



Full wwPDB EM Validation Report ⓘ

Dec 17, 2024 – 01:36 AM EST

PDB ID : 8EUB
EMDB ID : EMD-28610
Title : Hypopseudouridylated yeast 80S bound with Taura syndrome virus (TSV) internal ribosome entry site (IRES), eEF2 and GDP, Structure I
Authors : Zhao, Y.; Rai, J.; Li, H.
Deposited on : 2022-10-18
Resolution : 2.52 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

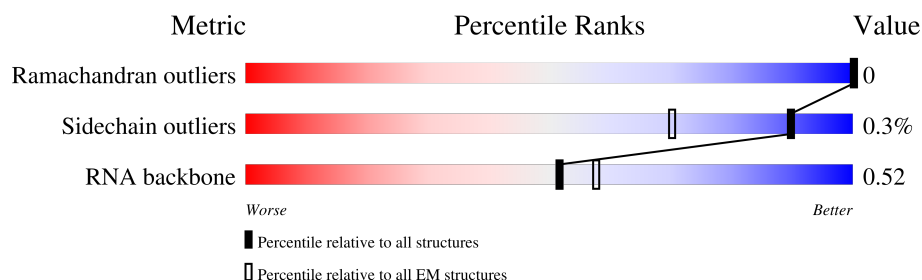
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.52 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.



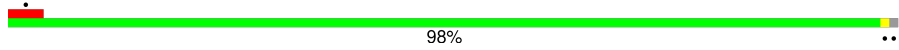
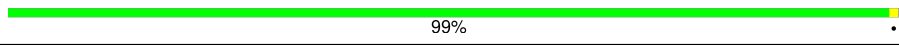
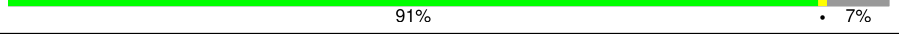
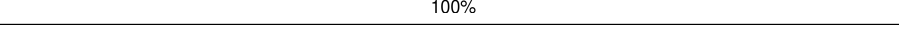
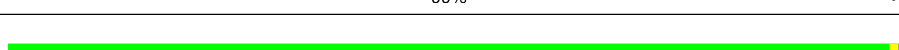
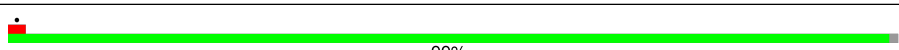

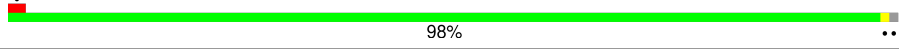
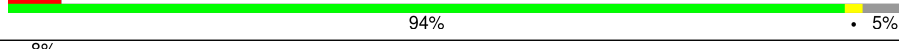
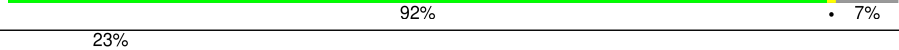
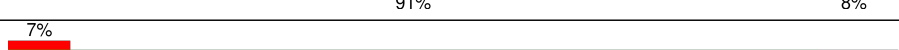
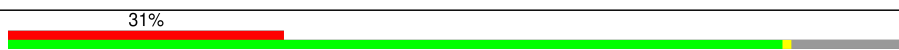
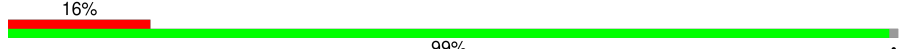

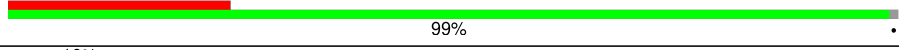
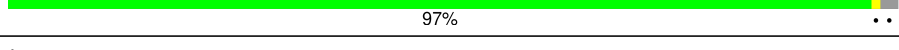
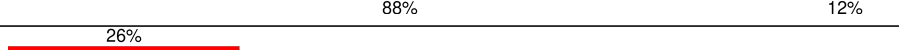

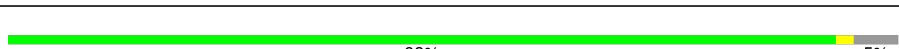
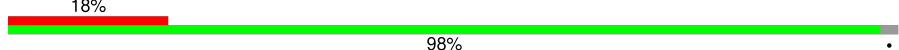

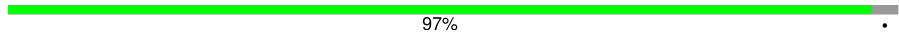



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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	

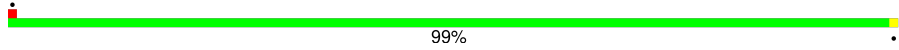
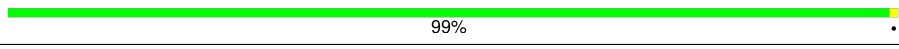

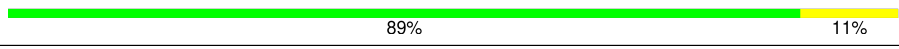

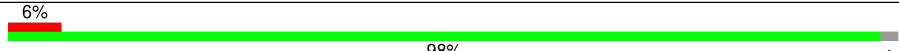
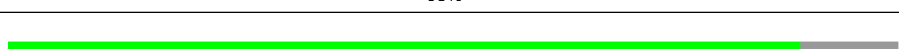
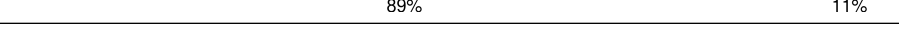
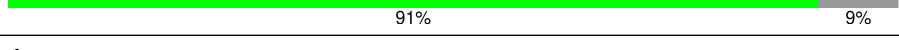

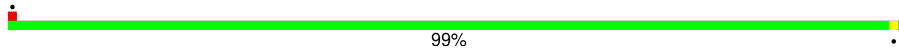
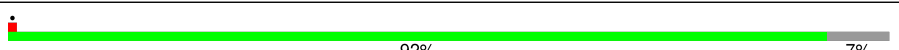
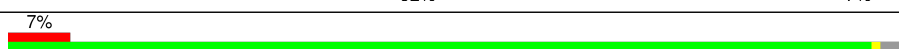
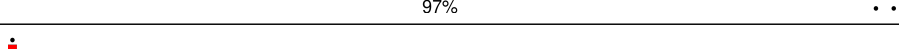
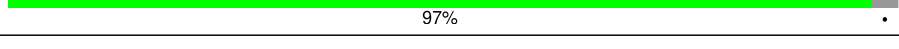
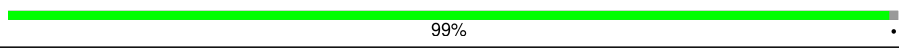

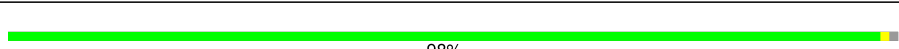
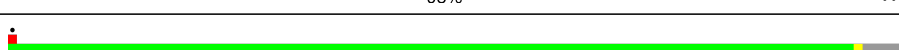
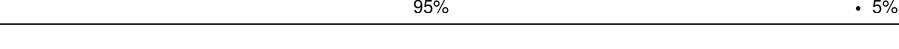
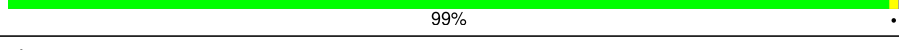
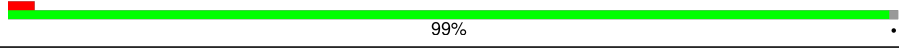
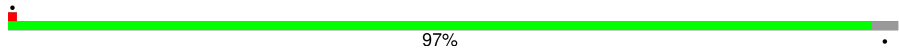
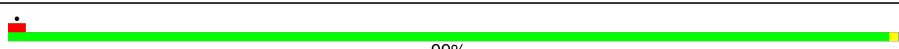
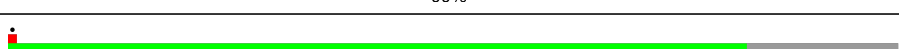
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Mol	Chain	Length	Quality of chain
9	BL	156	
10	BN	151	
11	BO	137	
12	BV	87	
13	BW	130	
14	BX	145	
15	BY	135	
16	Ba	119	
17	Bb	82	
18	Be	63	
19	BD	240	
20	BF	225	
21	BK	105	
22	BP	142	
23	BQ	143	
24	BR	136	
25	BS	146	
26	BT	144	
27	BU	121	
28	BZ	108	
29	Bc	67	
30	Bd	56	
31	Bg	319	
32	B5	1798	
33	AA	254	

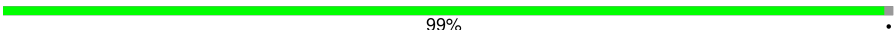
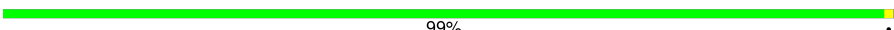
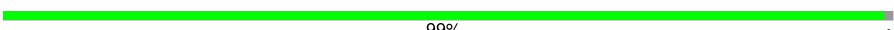
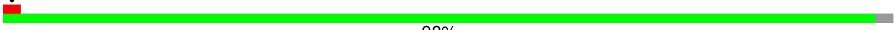








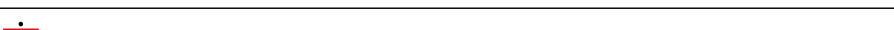
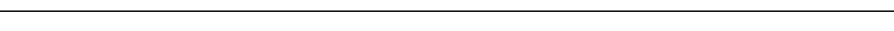
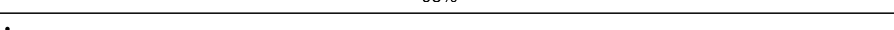

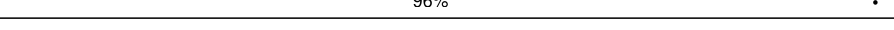
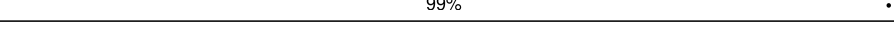
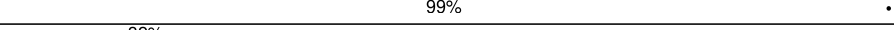
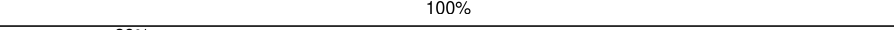

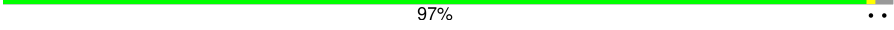


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Mol	Chain	Length	Quality of chain
34	AB	387	
35	AC	362	
36	A1	3360	
37	A3	121	
38	A4	158	
39	AD	297	
40	AE	176	
41	AF	244	
42	AG	256	
43	AH	191	
44	AI	221	
45	AJ	174	
46	AL	199	
47	AM	138	
48	AN	204	
49	AO	199	
50	AP	184	
51	AQ	186	
52	AR	189	
53	AS	178	
54	AT	160	
55	AU	121	
56	AV	137	
57	AW	155	
58	AX	142	

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Mol	Chain	Length	Quality of chain
59	AY	127	 99% .
60	AZ	136	 99% ..
61	Aa	149	 99% .
62	Ab	59	 98% .
63	Ac	105	 92% 8% .
64	Ad	113	 96% .
65	Ae	130	 98% .
66	Af	107	 99% .
67	Ag	121	 93% 7% .
68	Ah	120	 99% .
69	Ai	100	 99% .
70	Aj	88	 99% .
71	Ak	78	 99% .
72	Al	51	 98% .
73	Am	128	 41% 59% .
74	An	25	 96% .
75	Ao	106	 99% .
76	Ap	92	 99% .
77	E	217	 32% 100% .
78	EC	201	 29% 41% 55% .
79	DC	842	 7% 97% ..
80	Bf	152	 30% 49% 51% .
81	BM	143	 49% 87% 13% .
82	VA	312	 11% 61% 39% .

2 Entry composition

There are 85 unique types of molecules in this entry. The entry contains 214074 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

- Molecule 2 is a protein called RPS1A isoform 1.

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

- Molecule 3 is a protein called RPS2 isoform 1.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 13 is a protein called RPS22A isoform 1.

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

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

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

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

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

- Molecule 16 is a protein called RPS26B isoform 1.

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

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

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

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

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

- Molecule 19 is a protein called RPS3 isoform 1.

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

- Molecule 20 is a protein called Rps5p.

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

- 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	125	Total	C	N	O	S	0	0
			1000	625	188	185	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	69	Total	C	N	O	0	0
			558	357	103	98		

- 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 RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	B5	1782	Total	C	N	O	P	1	0
			38004	17005	6718	12499	1782		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B5	1280	4AC	C	conflict	GB 1329886537
B5	1773	4AC	C	conflict	GB 1329886537

- Molecule 33 is a protein called 60S ribosomal protein L2-A.

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

- Molecule 34 is a protein called 60S ribosomal protein L3.

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

- Molecule 35 is a protein called RPL4A isoform 1.

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

- Molecule 36 is a RNA chain called 28S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	A1	3198	Total	C	N	O	P	0	0
			68445	30596	12331	22320	3198		

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

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

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

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

- Molecule 39 is a protein called RPL5 isoform 1.

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

- Molecule 40 is a protein called 60S ribosomal protein L6-A.

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

- Molecule 41 is a protein called 60S ribosomal protein L7-A.

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

- Molecule 42 is a protein called 60S ribosomal protein L8-A.

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

- Molecule 43 is a protein called 60S ribosomal protein L9-A.

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

- Molecule 44 is a protein called RPL10 isoform 1.

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

- Molecule 45 is a protein called RPL11A isoform 1.

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

- Molecule 46 is a protein called 60S ribosomal protein L13-A.

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

- Molecule 47 is a protein called 60S ribosomal protein L14-A.

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

- Molecule 48 is a protein called 60S ribosomal protein L15-A.

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

- Molecule 49 is a protein called 60S ribosomal protein L16-A.

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

- Molecule 50 is a protein called 60S ribosomal protein L17-A.

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

- Molecule 51 is a protein called 60S ribosomal protein L18-A.

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

- Molecule 52 is a protein called 60S ribosomal protein L19-A.

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

- Molecule 53 is a protein called 60S ribosomal protein L20.

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

- Molecule 54 is a protein called 60S ribosomal protein L21-A.

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

- Molecule 55 is a protein called 60S ribosomal protein L22-A.

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

- Molecule 56 is a protein called 60S ribosomal protein L23-A.

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

- Molecule 57 is a protein called RPL24A isoform 1.

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

- Molecule 58 is a protein called 60S ribosomal protein L25.

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

- Molecule 59 is a protein called 60S ribosomal protein L26-A.

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

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

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

- Molecule 61 is a protein called 60S ribosomal protein L28.

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

- Molecule 62 is a protein called RPL29 isoform 1.

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

- Molecule 63 is a protein called 60S ribosomal protein L30.

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

- Molecule 64 is a protein called 60S ribosomal protein L31-A.

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

- Molecule 65 is a protein called RPL32 isoform 1.

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

- Molecule 66 is a protein called 60S ribosomal protein L33-A.

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

- Molecule 67 is a protein called 60S ribosomal protein L34-A.

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

- Molecule 68 is a protein called 60S ribosomal protein L35-A.

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

- Molecule 69 is a protein called 60S ribosomal protein L36-A.

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

- Molecule 70 is a protein called 60S ribosomal protein L37-A.

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

- Molecule 71 is a protein called RPL38 isoform 1.

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

- Molecule 72 is a protein called 60S ribosomal protein L39.

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

- Molecule 73 is a protein called Ubiquitin-60S ribosomal protein L40.

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

- Molecule 74 is a protein called 60S ribosomal protein L41-A.

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

- Molecule 75 is a protein called 60S ribosomal protein L42-A.

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

- Molecule 76 is a protein called 60S ribosomal protein L43-A.

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

- Molecule 77 is a protein called RPL1A isoform 1.

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

- Molecule 78 is a RNA chain called Taura syndrome virus (TSV) internal ribosome entry site (IRES) RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	EC	195	Total	C	N	O	P	0	0
			4128	1843	731	1359	195		

- Molecule 79 is a protein called Elongation factor 2.

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

- Molecule 80 is a protein called Ubiquitin-40S ribosomal protein S31.

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

- Molecule 81 is a protein called 40S ribosomal protein S12.

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

- Molecule 82 is a protein called 60S acidic ribosomal protein P0.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	VA	189	Total	C	N	O	S	0	0
			1473	942	257	270	4		

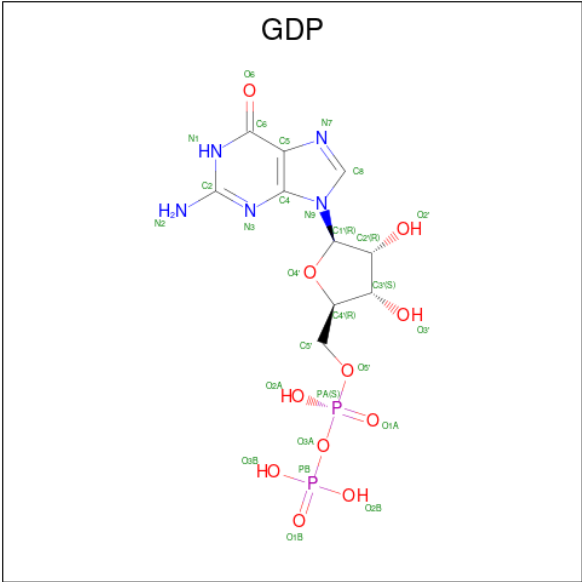
- Molecule 83 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
83	B5	51	Total 51	Mg 51	0
83	AB	1	Total 1	Mg 1	0
83	A1	187	Total 187	Mg 187	0
83	A3	2	Total 2	Mg 2	0
83	A4	5	Total 5	Mg 5	0
83	AG	1	Total 1	Mg 1	0
83	AN	3	Total 3	Mg 3	0
83	AO	2	Total 2	Mg 2	0
83	AP	1	Total 1	Mg 1	0
83	Af	1	Total 1	Mg 1	0
83	Aj	1	Total 1	Mg 1	0

- Molecule 84 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
84	Ao	1	Total 1	Zn 1	0

- Molecule 85 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂) (labeled as "Ligand of Interest" by depositor).




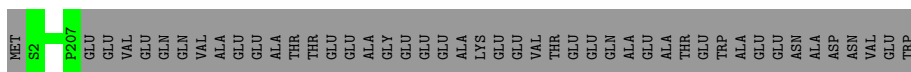
Mol	Chain	Residues	Atoms					AltConf
85	DC	1	Total	C	N	O	P	0
			28	10	5	11	2	

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.

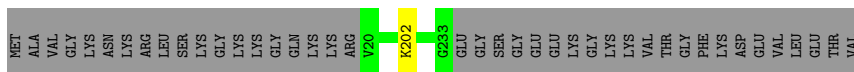
- Molecule 1: 40S ribosomal protein S0-A

Chain BA:  82% 18%




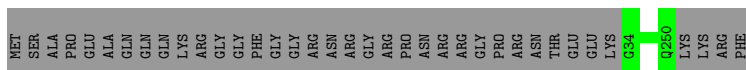
- Molecule 2: RPS1A isoform 1

Chain BB:  84% 16%



- Molecule 3: RPS2 isoform 1

Chain BC:  85% 15%



- Molecule 4: 40S ribosomal protein S4-A

Chain BE:  100%



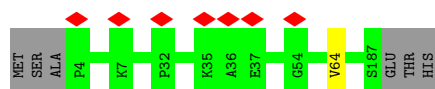
- Molecule 5: 40S ribosomal protein S6-A

Chain BG:  96%



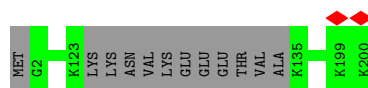
- Molecule 6: 40S ribosomal protein S7-A

Chain BH:  96%



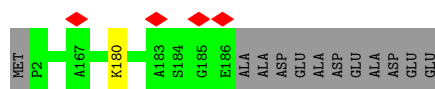
- Molecule 7: 40S ribosomal protein S8-A

Chain BI:  94%



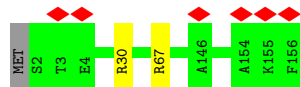
- Molecule 8: 40S ribosomal protein S9-A

Chain BJ:  93%



- Molecule 9: 40S ribosomal protein S11-A

Chain BL:  98%



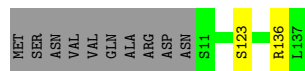
- Molecule 10: 40S ribosomal protein S13

Chain BN:  99%



- Molecule 11: 40S ribosomal protein S14-A

Chain BO:  91%



- Molecule 12: 40S ribosomal protein S21-A

Chain BV:  100%

There are no outlier residues recorded for this chain.

- Molecule 13: RPS22A isoform 1

Chain BW:  99%



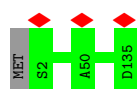
- Molecule 14: 40S ribosomal protein S23-A

Chain BX:  99%




- Molecule 15: 40S ribosomal protein S24-A

Chain BY:  99%



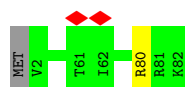
- Molecule 16: RPS26B isoform 1

Chain Ba:  81% 18%



- Molecule 17: 40S ribosomal protein S27-A

Chain Bb:  98%



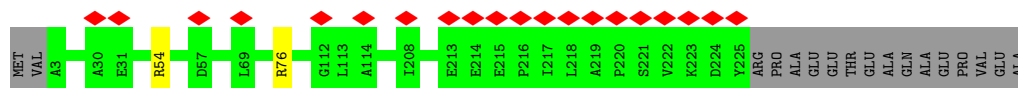
- Molecule 18: 40S ribosomal protein S30-A

Chain Be:  6% 94% 5%

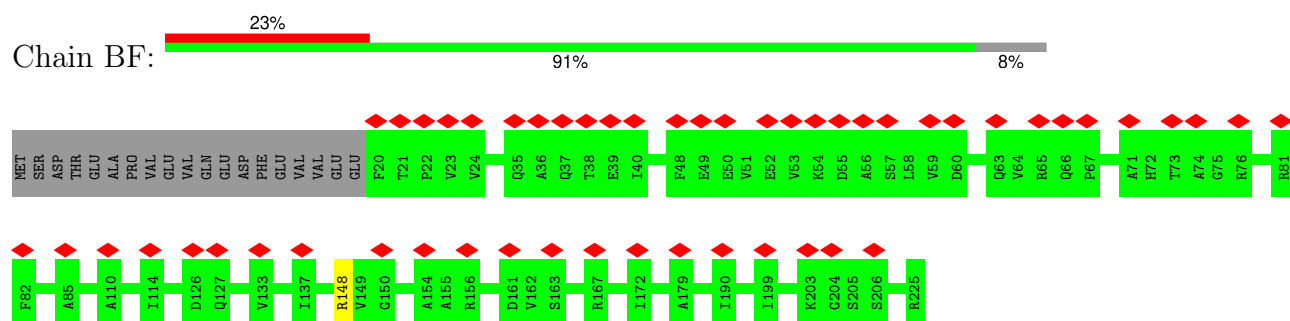


- Molecule 19: RPS3 isoform 1

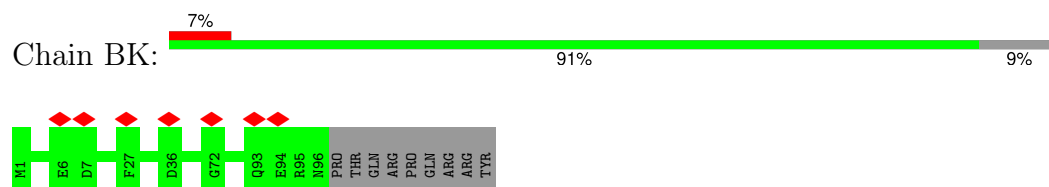
Chain BD:  8% 92% 7%



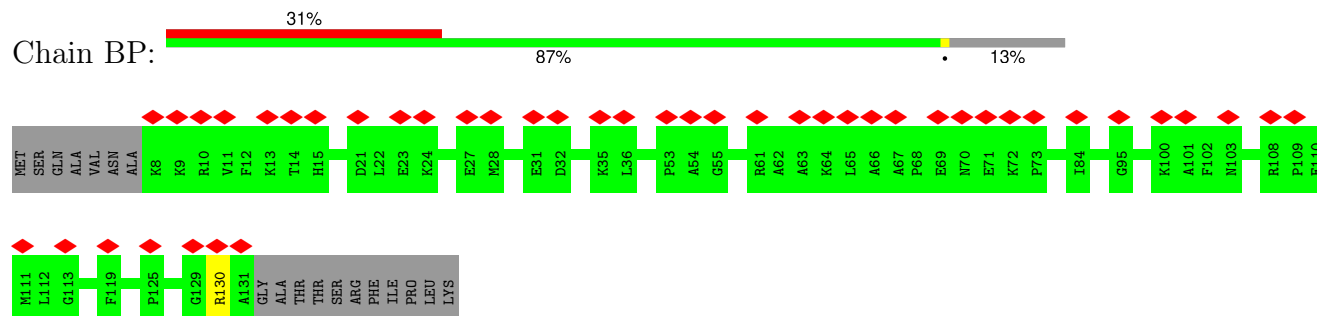
- Molecule 20: Rps5p



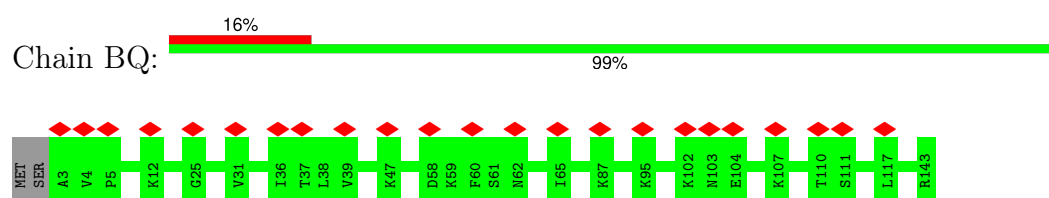
- Molecule 21: 40S ribosomal protein S10-A



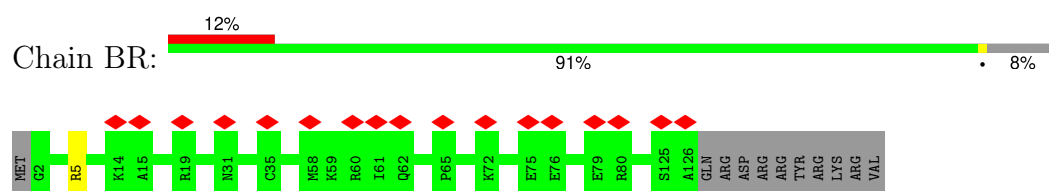
- Molecule 22: RPS15 isoform 1



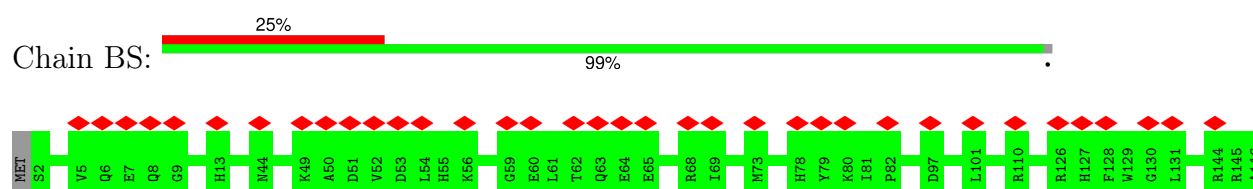
- Molecule 23: 40S ribosomal protein S16-A



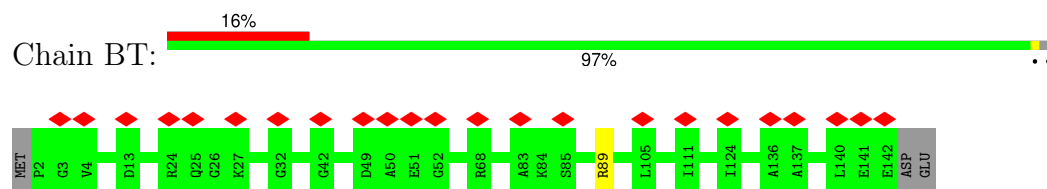
- Molecule 24: 40S ribosomal protein S17-A



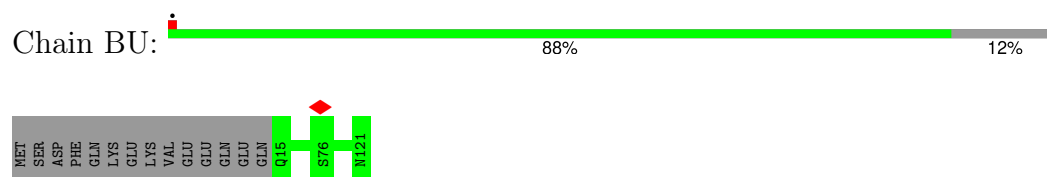
- Molecule 25: 40S ribosomal protein S18-A



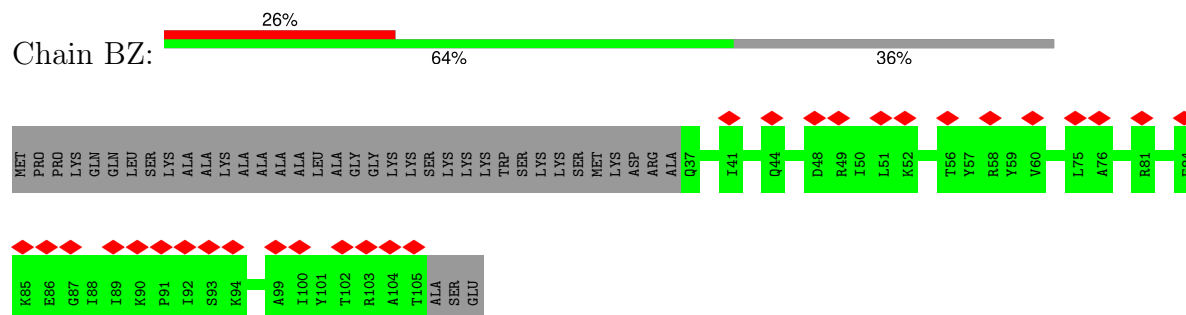
- Molecule 26: 40S ribosomal protein S19-A



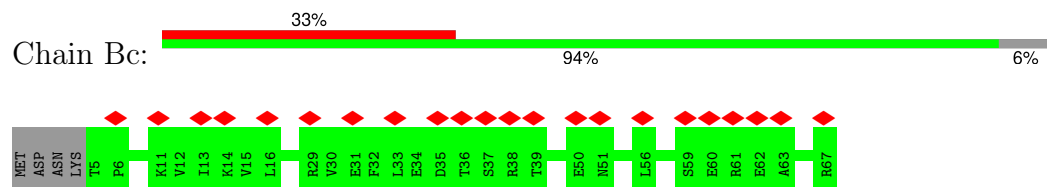
- Molecule 27: RPS20 isoform 1



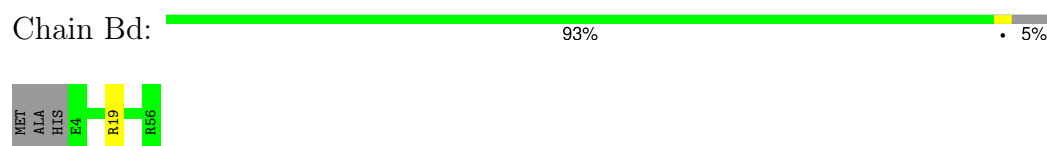
- Molecule 28: RPS25A isoform 1



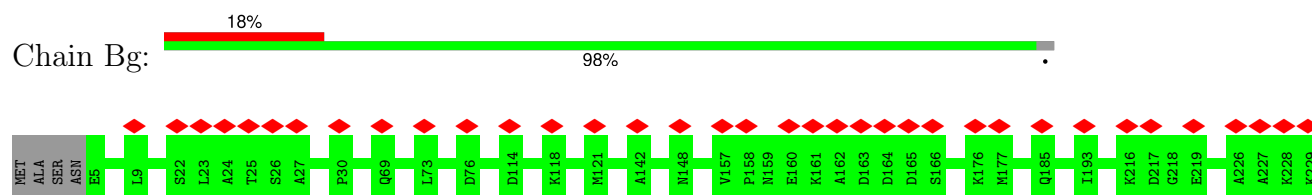
- Molecule 29: RPS28A isoform 1

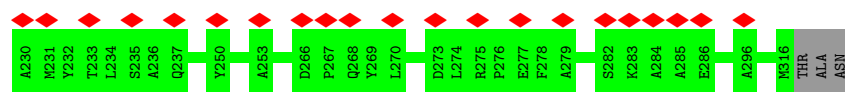


- Molecule 30: RPS29A isoform 1



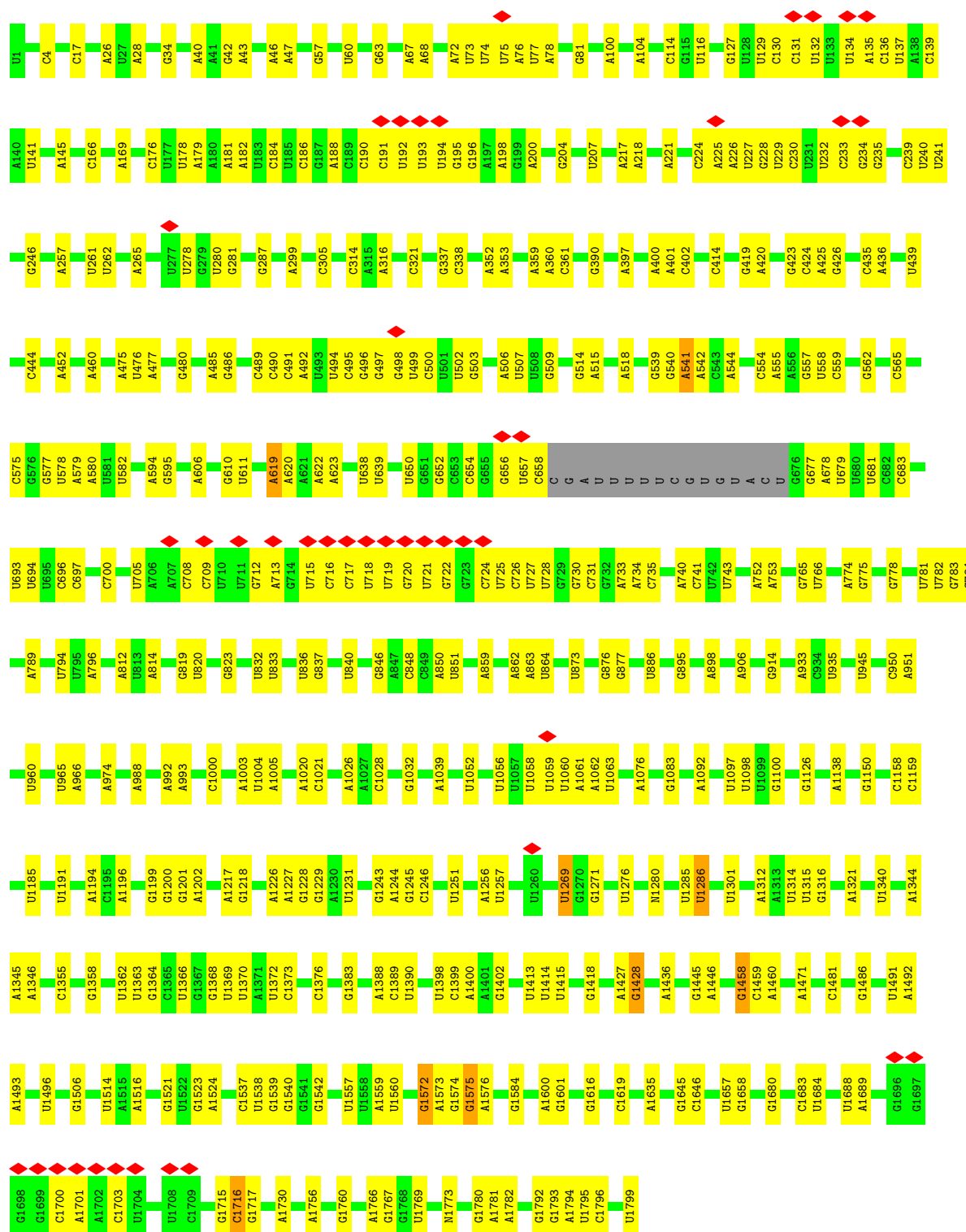
- Molecule 31: Guanine nucleotide-binding protein subunit beta-like protein





• Molecule 32: 18S rRNA

Chain B5: 75% 23%



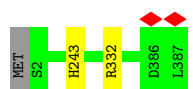
- Molecule 33: 60S ribosomal protein L2-A

Chain AA:  97%



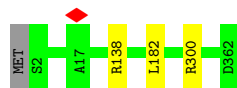
- Molecule 34: 60S ribosomal protein L3

Chain AB:  99%



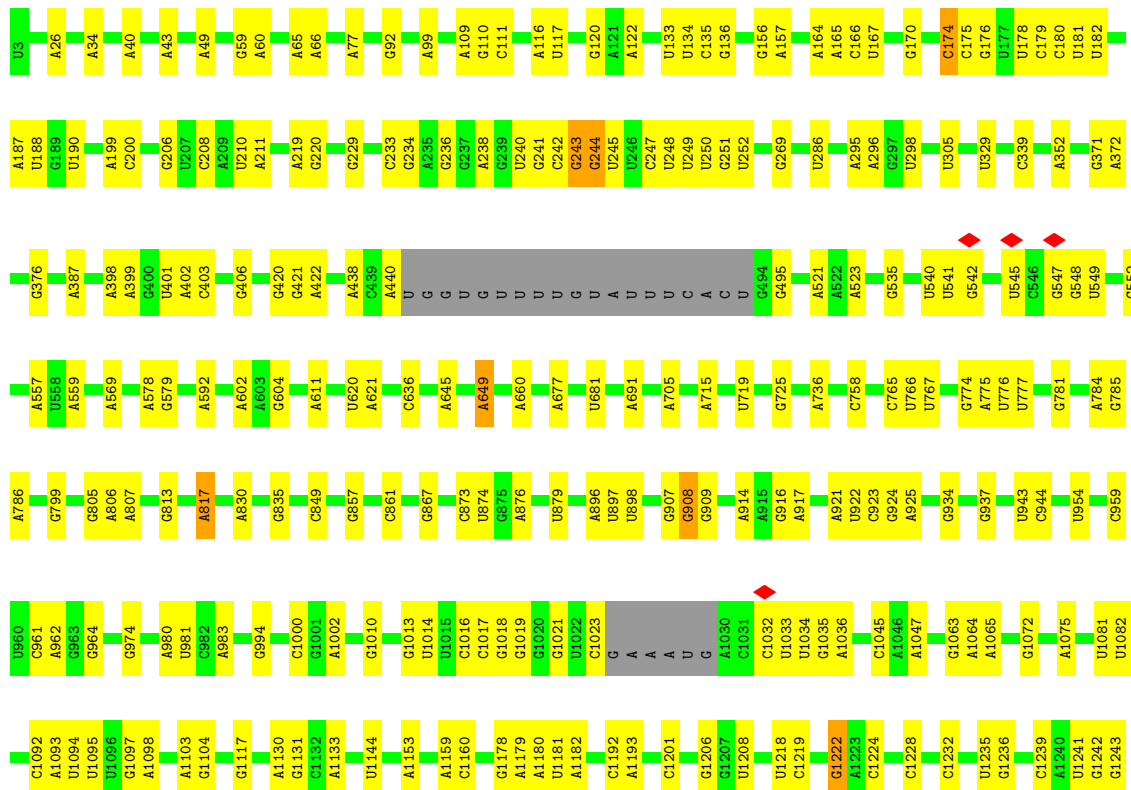
- Molecule 35: RPL4A isoform 1

Chain AC:  99%



- Molecule 36: 28S rRNA

Chain A1:  75% 19% 5%




G3276	U3121	G2874	G2690	U2537	G2452	G2288	A2131	U	G	C	A1589	C1849	G1431	A1244
U3281	A3122	C2876	A2691	U2538	U2453	G2307	U2140	G	C	C	A1593	A1850	G1434	A1245
G3289	A3130	A2887	A2694	C2539	U2455	C2308	U2141	U	U	U	G1604	C1866	U1252	G1246
A3294	U3131	U2888	A2704	U2541	A2458	U2310	A2142	A	A	C	A1605	G1878	C1437	U1253
G3303	A3142	C2889	A2705	U2542	A2459	A2313	A2143	A	C	C	G1608	U1860	C1254	C1254
U3304	C3143	G2898	U2712	U2544	U2460	U2314	A2144	C	U	U	A1449	U1886	G1255	G1256
A3305	U3153	U2921	G2713	G2549	A2461	G2315	A2145	G	G	G	U1628	A1886	G1262	G1262
U3313	U3304	G2922	G2714	C2552	A2462	U2318	C2146	C	U	U	U1629	U1887	G1263	G1263
A3314	U3156	U2923	U2719	U2553	G2463	U2318	A2158	C	A	A	U1630	U1888	G1264	G1264
A3316	U3157	U2935	U2724	U2554	G2467	U2334	G2169	U	C	C	A1642	A1893	U1265	U1265
U3319	A3165	A2936	U2728	A2554	A2468	G2335	A2188	G	U	U	A1643	A1896	A1468	A1468
U3341	A3170	A2941	U2729	A2561	C2470	C2337	C2197	U	C	C	A1683	G1899	A1476	A1476
A3342	C3171	C2942	G2737	A2562	U2471	U2340	G2201	G	U	U	U1724	G1906	A1481	G1282
G3345	A3172	A2946	U2750	U2569	C2472	U2347	G2206	U	G	G	A1729	G1906	A1502	C1283
U3351	G3173	G2947	C2572	U2571	C2473	A2347	A2206	C	U	C	G1734	A1932	C1496	A1286
G3352	A3174	C2948	G2573	C2572	G2474	C2366	A2207	U	U	U	U1739	U1950	A1503	A1287
U3353	U3175	G2948	G2754	G2573	G2475	A2373	U2209	C	G	G	G1735	A1936	C1508	U1293
G3356	G3176	G2977	G2755	G2585	C2476	C2374	A2220	U	U	U	U1736	C1943	U1523	G1295
U3359	U3179	C2983	G2777	G2586	C2478	G2376	A2225	G	C	C	U1737	G1953	U1526	G1307
C3378	C3181	G2990	G2778	C2593	C2479	G2376	U2225	C	U	C	A1750	G1954	A1539	U1308
U3389	A3187	G2997	G2791	C2594	A2480	C2383	C2237	A	U	U	G1751	U1955	U1555	U1309
G3390	U3196	A3011	G2792	G2606	A2485	U2388	U2241	C	C	C	C1762	G	A1557	A1330
U3396	G3197	A3012	G2796	G2607	A2486	U2487	A2242	G	U	U	U1763	G	A1558	U1331
C3207	U3198	G3022	G2799	G2614	A2488	C2391	G2249	U	U	U	U1764	G	C1562	U1348
A3217	U3207	A3032	A2801	G2619	C2489	G2393	G2250	C	C	C	G1765	G	U1563	G1349
G3219	C3217	A3033	A2802	U2634	A2491	A2397	G2251	U	U	U	G1766	G	U1564	A1350
G3224	A3218	G3034	A2803	U2634	A2492	A2402	A2255	C	C	C	G1775	G	G1565	U1351
U3224	G3219	U3037	C2810	G2648	A2494	A2404	A2256	U	U	U	G1778	G	A1566	A1352
A3234	U3057	U3056	G2814	G2651	A2496	U2411	A2259	C	C	C	G1796	G	U1567	U1353
A3243	U3058	G3059	G2815	U2652	C2496	G2412	U2260	U	U	U	A1797	G	U1568	G1354
G3246	G3059	U3078	G2816	A2656	C2497	U2417	C2267	C	C	C	A1813	G	U1569	A1355
G3247	U3079	U3079	A2817	G2672	U2501	G2418	U2268	U	U	U	A1814	G	U1572	U1356
G3256	A3086	A3087	A2845	A2673	A2502	U2421	A2271	A	U	U	U1815	C	U1573	A1357
U3259	U3087	C3092	A2851	A2674	U2505	A2439	A2272	C	C	C	U1816	G	C1574	A1386
G3263	G3092	U2860	A2851	G2677	U2506	G2442	G2272	U	U	U	G1817	G	A1575	C1391
U3270	U3109	G2870	A2871	A2678	C2507	G2442	C2278	G	C	C	U1820	C	G1576	A1393
C3271	C3272	A2872	U2688	A2679	A2511	A2445	A2279	U	U	U	U1821	C	A1579	A1399
A3273	U2873	U2873	U2689	U2681	U2514	U2446	A2281	C	C	C	A1842	C	A1583	G1400
					A2523	G2450	C2284	U	U	U	C1846	C	A1587	U1419
					A2524	G2451		G	G	G			A1588	
					C2531									

• Molecule 37: 5S rRNA

Chain A3:  89% 11%



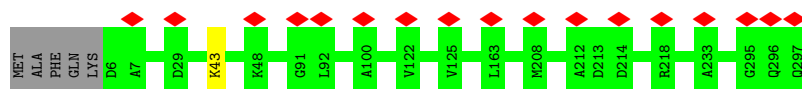
- Molecule 38: 5.8S rRNA

Chain A4:  80% 20%



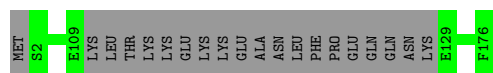
- Molecule 39: RPL5 isoform 1

Chain AD:  6% 98%



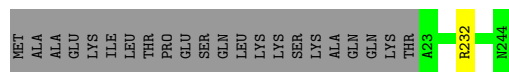
- Molecule 40: 60S ribosomal protein L6-A

Chain AE:  89% 11%



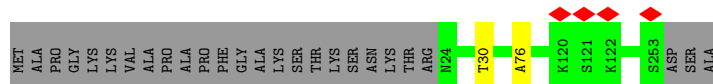
- Molecule 41: 60S ribosomal protein L7-A

Chain AF:  91% 9%



- Molecule 42: 60S ribosomal protein L8-A

Chain AG:  89% 10%



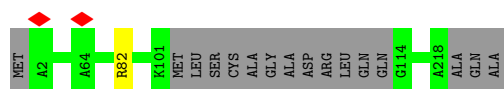
- Molecule 43: 60S ribosomal protein L9-A

Chain AH:  99%



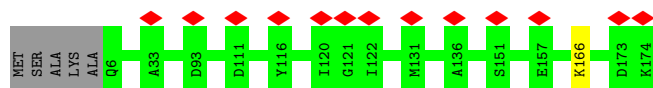
- Molecule 44: RPL10 isoform 1

Chain AI:  92% 7%



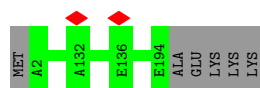
- Molecule 45: RPL11A isoform 1

Chain AJ:  7% 97%



- Molecule 46: 60S ribosomal protein L13-A

Chain AL:  97%



- Molecule 47: 60S ribosomal protein L14-A

Chain AM:  99%



- Molecule 48: 60S ribosomal protein L15-A

Chain AN:  100%



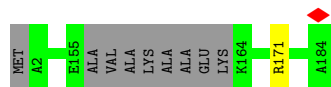
- Molecule 49: 60S ribosomal protein L16-A

Chain AO:  98%



- Molecule 50: 60S ribosomal protein L17-A

Chain AP:  95% 5%



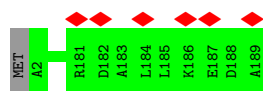
- Molecule 51: 60S ribosomal protein L18-A

Chain AQ:  99%



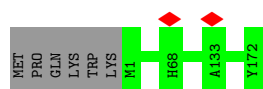
- Molecule 52: 60S ribosomal protein L19-A

Chain AR:  99%



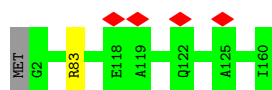
- Molecule 53: 60S ribosomal protein L20

Chain AS:  97%




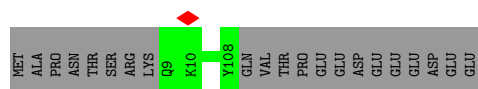
- Molecule 54: 60S ribosomal protein L21-A

Chain AT:  99%



- Molecule 55: 60S ribosomal protein L22-A

Chain AU:  83% 17%



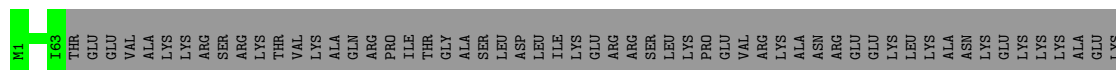
- Molecule 56: 60S ribosomal protein L23-A

Chain AV:  99%




- Molecule 57: RPL24A isoform 1

Chain AW:  41% 59%



ALA
ALA
ARG
LYS
LYS
GLU
LYS
LYS
ALA
SER
ALA
GLY
THR
GLN
SER
SER
LYS
PHE
SER
LYS
GLN
GLN
ALA
LYS
GLY
ALA
PHE
GLN
LYS
VAL
ALA
ALA
THR
SER
ARG

- Molecule 58: 60S ribosomal protein L25

Chain AX:  85% 15%

MET
ALA
PRO
SER
LYS
LYS
ALA
THR
ALA
ALA
LYS
LYS
VAL
VAL
GLY
THR
ASN
GLY
LYS
K22
T142

- Molecule 59: 60S ribosomal protein L26-A

Chain AY:  99% .

MET
A2
E127

- Molecule 60: 60S ribosomal protein L27-A

Chain AZ:  99% ..

MET
A2
K34
E138

- Molecule 61: 60S ribosomal protein L28

Chain Aa:  99% .

MET
P2
A149

- Molecule 62: RPL29 isoform 1

Chain Ab:  98% .

MET
A2
A57
K58
K59

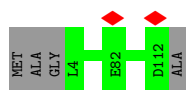
- Molecule 63: 60S ribosomal protein L30

Chain Ac:  92% 8%

MET
ALA
PRO
VAL
LYS
SER
GLN
GLU
S9
A105

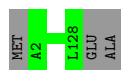
- Molecule 64: 60S ribosomal protein L31-A

Chain Ad:  96% .



- Molecule 65: RPL32 isoform 1

Chain Ae: 98%



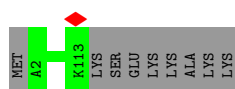
- Molecule 66: 60S ribosomal protein L33-A

Chain Af: 99%



- Molecule 67: 60S ribosomal protein L34-A

Chain Ag: 93% 7%



- Molecule 68: 60S ribosomal protein L35-A

Chain Ah: 99%



- Molecule 69: 60S ribosomal protein L36-A

Chain Ai: 99%



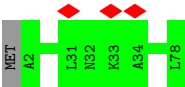
- Molecule 70: 60S ribosomal protein L37-A

Chain Aj: 99%



- Molecule 71: RPL38 isoform 1

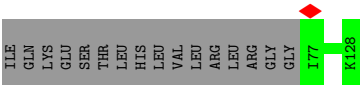
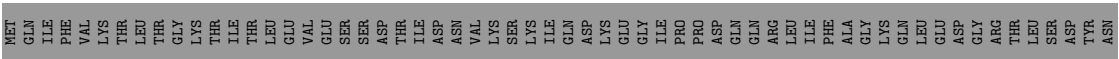
Chain Ak: 99%



• Molecule 72: 60S ribosomal protein L39



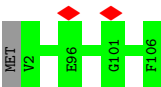
• Molecule 73: Ubiquitin-60S ribosomal protein L40



• Molecule 74: 60S ribosomal protein L41-A



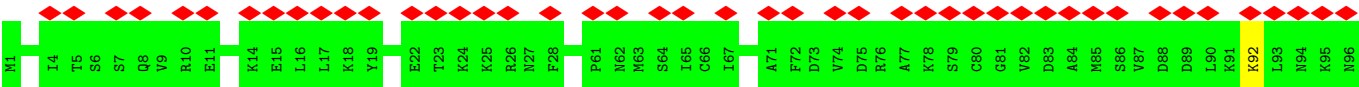
• Molecule 75: 60S ribosomal protein L42-A

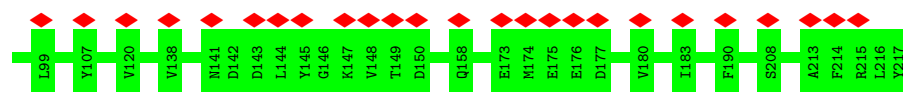


• Molecule 76: 60S ribosomal protein L43-A



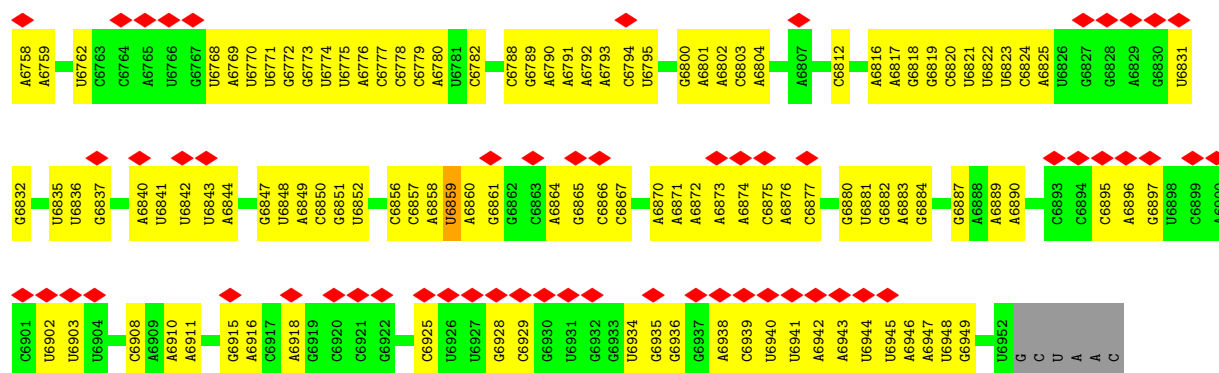
• Molecule 77: RPL1A isoform 1





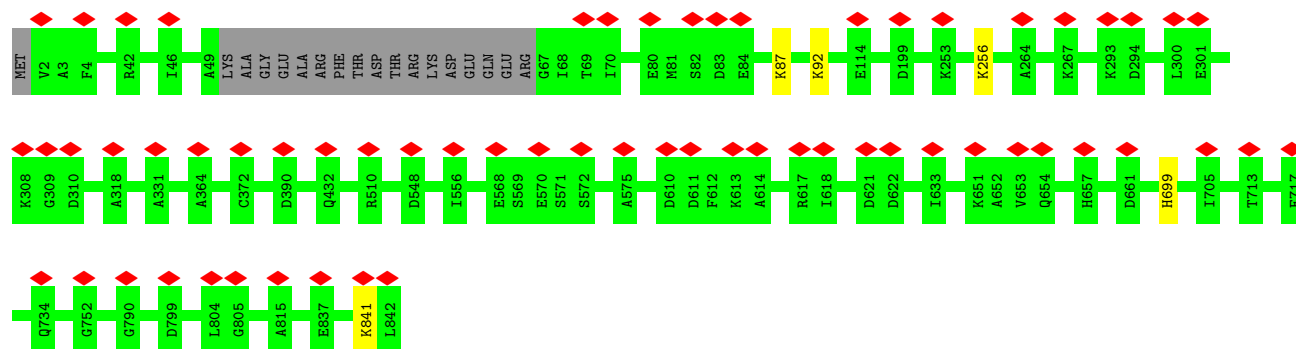
- Molecule 78: Taura syndrome virus (TSV) internal ribosome entry site (IRES) RNA

Chain EC: 29% 41% 55%



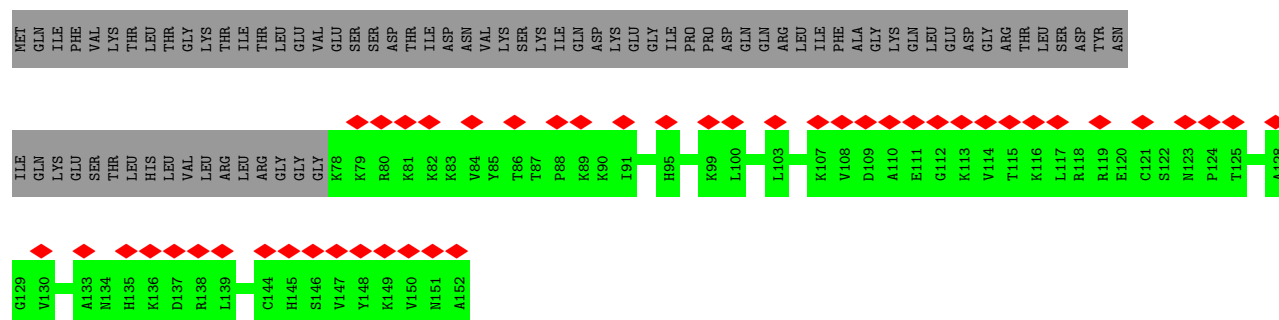
- Molecule 79: Elongation factor 2

Chain DC: 7% 97%



- Molecule 80: Ubiquitin-40S ribosomal protein S31

Chain Bf: 30% 49% 51%



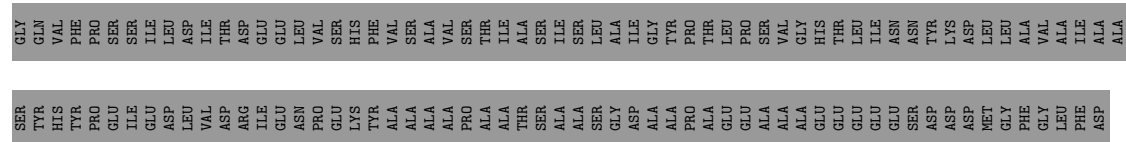
- Molecule 81: 40S ribosomal protein S12

Country	Percentage
U.S.	49%
China	87%
Russia	13%



- Molecule 82: 60S acidic ribosomal protein P0

Response	Percentage
Used a mobile app to book a flight	11%
Have not used a mobile app to book a flight	61%
Don't know	39%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	96683	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	4.770	Depositor
Minimum map value	-1.793	Depositor
Average map value	0.035	Depositor
Map value standard deviation	0.202	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 ⓘ

5.1 Standard geometry ⓘ

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

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	0.27	0/1653	0.55	0/2261
2	BB	0.26	0/1735	0.55	0/2335
3	BC	0.26	0/1665	0.48	0/2263
4	BE	0.26	0/2109	0.54	0/2839
5	BG	0.25	0/1844	0.56	0/2464
6	BH	0.25	0/1506	0.53	0/2028
7	BI	0.26	0/1514	0.58	0/2021
8	BJ	0.25	0/1519	0.54	0/2035
9	BL	0.27	0/1272	0.52	0/1712
10	BN	0.25	0/1215	0.51	0/1638
11	BO	0.28	0/952	0.66	0/1279
12	BV	0.28	0/693	0.55	0/935
13	BW	0.26	0/1038	0.52	0/1395
14	BX	0.26	0/1139	0.54	0/1518
15	BY	0.26	0/1087	0.55	0/1449
16	Ba	0.27	0/782	0.64	1/1047 (0.1%)
17	Bb	0.24	0/620	0.55	0/838
18	Be	0.23	0/483	0.54	0/643
19	BD	0.25	0/1759	0.53	0/2368
20	BF	0.25	0/1629	0.52	0/2202
21	BK	0.25	0/837	0.50	0/1131
22	BP	0.26	0/1012	0.59	0/1356
23	BQ	0.26	0/1125	0.51	0/1510
24	BR	0.26	0/1010	0.58	0/1355
25	BS	0.24	0/1211	0.54	0/1628
26	BT	0.26	0/1113	0.52	0/1494
27	BU	0.25	0/865	0.53	0/1169
28	BZ	0.24	0/566	0.56	0/761
29	Bc	0.25	0/499	0.67	0/670
30	Bd	0.26	0/452	0.59	0/600
31	Bg	0.24	0/2454	0.52	0/3340
32	B5	0.28	0/41880	0.80	10/65248 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	AA	0.30	0/1912	0.59	0/2569
34	AB	0.29	0/3139	0.55	0/4219
35	AC	0.28	0/2800	0.54	1/3790 (0.0%)
36	A1	0.41	0/75561	0.81	25/117806 (0.0%)
37	A3	0.35	0/2883	0.79	0/4491
38	A4	0.43	0/3746	0.78	0/5832
39	AD	0.28	0/2390	0.51	0/3225
40	AE	0.28	0/1260	0.52	0/1694
41	AF	0.29	0/1821	0.49	0/2451
42	AG	0.27	0/1830	0.49	0/2469
43	AH	0.28	0/1531	0.52	0/2062
44	AI	0.28	0/1708	0.52	0/2290
45	AJ	0.26	0/1374	0.56	0/1842
46	AL	0.27	0/1568	0.56	0/2106
47	AM	0.27	0/1068	0.52	0/1438
48	AN	0.30	0/1757	0.58	0/2354
49	AO	0.29	0/1585	0.52	0/2128
50	AP	0.28	0/1410	0.54	0/1893
51	AQ	0.28	0/1465	0.56	0/1965
52	AR	0.27	0/1538	0.57	0/2050
53	AS	0.29	0/1481	0.54	0/1990
54	AT	0.29	0/1300	0.53	0/1743
55	AU	0.29	0/812	0.54	0/1099
56	AV	0.29	0/1018	0.54	0/1369
57	AW	0.29	0/533	0.54	0/707
58	AX	0.30	0/983	0.48	0/1325
59	AY	0.29	0/1004	0.54	0/1341
60	AZ	0.29	0/1118	0.50	0/1497
61	Aa	0.30	0/1204	0.53	0/1612
62	Ab	0.25	0/473	0.46	0/629
63	Ac	0.29	0/751	0.50	0/1008
64	Ad	0.28	0/904	0.53	0/1213
65	Ae	0.28	0/1041	0.53	0/1394
66	Af	0.31	0/868	0.57	0/1168
67	Ag	0.29	0/890	0.57	0/1189
68	Ah	0.28	0/978	0.51	0/1301
69	Ai	0.26	0/778	0.56	0/1034
70	Aj	0.29	0/696	0.58	0/923
71	Ak	0.28	0/618	0.53	0/826
72	Al	0.25	0/443	0.58	0/588
73	Am	0.27	0/423	0.55	0/562
74	An	0.32	0/234	1.07	3/300 (1.0%)
75	Ao	0.29	0/860	0.54	0/1136

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
76	Ap	0.29	0/701	0.59	0/934
77	E	0.25	0/1745	0.53	0/2342
78	EC	0.28	1/4613 (0.0%)	0.83	1/7182 (0.0%)
79	DC	0.25	0/6521	0.52	0/8830
80	Bf	0.25	0/616	0.51	0/817
81	BM	0.24	0/943	0.53	0/1274
82	VA	0.27	0/1498	0.55	0/2025
All	All	0.33	1/227631 (0.0%)	0.71	41/333564 (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
11	BO	0	1
14	BX	0	1
39	AD	0	1
41	AF	0	1
42	AG	0	2
All	All	0	7

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
78	EC	6758	A	OP3-P	-10.63	1.48	1.61

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
74	An	15	ARG	CB-CG-CD	-7.98	90.86	111.60
36	A1	406	G	O4'-C1'-N9	7.80	114.44	108.20
32	B5	848	C	N3-C2-O2	-7.35	116.75	121.90
16	Ba	64	LEU	CA-CB-CG	7.09	131.61	115.30
36	A1	2237	C	N3-C2-O2	-6.67	117.23	121.90
32	B5	1716	C	C2-N1-C1'	6.63	126.09	118.80
32	B5	1716	C	N1-C2-O2	6.49	122.80	118.90
36	A1	835	G	O4'-C1'-N9	6.42	113.33	108.20
36	A1	922	U	C2-N1-C1'	6.33	125.29	117.70
78	EC	6859	U	O4'-C1'-N1	-6.17	103.27	108.20
36	A1	174	C	C2-N1-C1'	6.15	125.57	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	B5	1389	C	C2-N1-C1'	6.11	125.52	118.80
32	B5	965	U	C2-N1-C1'	6.09	125.01	117.70
35	AC	182	LEU	CA-CB-CG	6.07	129.26	115.30
36	A1	3034	C	C2-N1-C1'	6.01	125.41	118.80
36	A1	2237	C	N1-C2-O2	5.95	122.47	118.90
74	An	15	ARG	CG-CD-NE	5.95	124.30	111.80
74	An	15	ARG	CA-CB-CG	5.85	126.26	113.40
36	A1	1255	C	N3-C2-O2	-5.84	117.81	121.90
36	A1	174	C	N1-C2-O2	5.79	122.37	118.90
36	A1	1496	C	C2-N1-C1'	5.72	125.10	118.80
32	B5	848	C	N1-C2-O2	5.72	122.33	118.90
36	A1	1222	G	O4'-C1'-N9	5.56	112.65	108.20
32	B5	1458	G	N3-C4-C5	-5.50	125.85	128.60
36	A1	2506	U	C2-N1-C1'	5.50	124.30	117.70
36	A1	3058	U	C2-N1-C1'	5.33	124.10	117.70
36	A1	2225	U	N3-C2-O2	-5.30	118.49	122.20
36	A1	244	G	N3-C4-N9	-5.26	122.84	126.00
32	B5	1286	U	C2-N1-C1'	5.25	124.00	117.70
36	A1	1283	C	N3-C2-O2	-5.23	118.24	121.90
36	A1	1283	C	N1-C2-O2	5.18	122.01	118.90
36	A1	3057	U	N3-C2-O2	-5.18	118.57	122.20
36	A1	1283	C	C6-N1-C2	-5.16	118.24	120.30
36	A1	922	U	N1-C2-O2	5.16	126.41	122.80
32	B5	1560	U	C2-N1-C1'	5.13	123.85	117.70
36	A1	1604	G	C4-N9-C1'	5.12	133.15	126.50
36	A1	3037	U	C2-N1-C1'	5.08	123.80	117.70
36	A1	954	U	N3-C2-O2	-5.08	118.64	122.20
36	A1	243	G	N3-C4-N9	5.06	129.03	126.00
32	B5	1000	C	C2-N1-C1'	5.03	124.33	118.80
36	A1	3037	U	N3-C2-O2	-5.00	118.70	122.20

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
39	AD	43	LYS	Peptide
41	AF	232	ARG	Peptide
42	AG	30	THR	Peptide
42	AG	76	ALA	Peptide
6	BH	64	VAL	Peptide
11	BO	123	SER	Peptide
14	BX	88	PRO	Peptide

5.2 Too-close contacts

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

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	BA	204/252 (81%)	177 (87%)	27 (13%)	0	100	100
2	BB	212/255 (83%)	178 (84%)	34 (16%)	0	100	100
3	BC	215/254 (85%)	206 (96%)	9 (4%)	0	100	100
4	BE	258/261 (99%)	243 (94%)	15 (6%)	0	100	100
5	BG	224/236 (95%)	212 (95%)	12 (5%)	0	100	100
6	BH	182/190 (96%)	168 (92%)	14 (8%)	0	100	100
7	BI	184/200 (92%)	163 (89%)	21 (11%)	0	100	100
8	BJ	183/197 (93%)	172 (94%)	11 (6%)	0	100	100
9	BL	153/156 (98%)	142 (93%)	11 (7%)	0	100	100
10	BN	148/151 (98%)	139 (94%)	9 (6%)	0	100	100
11	BO	125/137 (91%)	114 (91%)	11 (9%)	0	100	100
12	BV	85/87 (98%)	75 (88%)	10 (12%)	0	100	100
13	BW	127/130 (98%)	117 (92%)	10 (8%)	0	100	100
14	BX	142/145 (98%)	123 (87%)	19 (13%)	0	100	100
15	BY	132/135 (98%)	122 (92%)	10 (8%)	0	100	100
16	Ba	95/119 (80%)	78 (82%)	17 (18%)	0	100	100
17	Bb	79/82 (96%)	69 (87%)	10 (13%)	0	100	100
18	Be	58/63 (92%)	50 (86%)	8 (14%)	0	100	100
19	BD	221/240 (92%)	204 (92%)	17 (8%)	0	100	100
20	BF	204/225 (91%)	192 (94%)	12 (6%)	0	100	100
21	BK	94/105 (90%)	85 (90%)	9 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
22	BP	122/142 (86%)	111 (91%)	11 (9%)	0	100	100
23	BQ	139/143 (97%)	133 (96%)	6 (4%)	0	100	100
24	BR	123/136 (90%)	116 (94%)	7 (6%)	0	100	100
25	BS	143/146 (98%)	125 (87%)	18 (13%)	0	100	100
26	BT	139/144 (96%)	129 (93%)	10 (7%)	0	100	100
27	BU	105/121 (87%)	98 (93%)	7 (7%)	0	100	100
28	BZ	67/108 (62%)	62 (92%)	5 (8%)	0	100	100
29	Bc	61/67 (91%)	55 (90%)	6 (10%)	0	100	100
30	Bd	51/56 (91%)	48 (94%)	3 (6%)	0	100	100
31	Bg	310/319 (97%)	277 (89%)	33 (11%)	0	100	100
33	AA	245/254 (96%)	231 (94%)	14 (6%)	0	100	100
34	AB	383/387 (99%)	365 (95%)	18 (5%)	0	100	100
35	AC	359/362 (99%)	332 (92%)	27 (8%)	0	100	100
39	AD	290/297 (98%)	271 (93%)	19 (7%)	0	100	100
40	AE	152/176 (86%)	139 (91%)	13 (9%)	0	100	100
41	AF	220/244 (90%)	212 (96%)	8 (4%)	0	100	100
42	AG	228/256 (89%)	209 (92%)	19 (8%)	0	100	100
43	AH	188/191 (98%)	174 (93%)	14 (7%)	0	100	100
44	AI	201/221 (91%)	188 (94%)	13 (6%)	0	100	100
45	AJ	167/174 (96%)	150 (90%)	17 (10%)	0	100	100
46	AL	191/199 (96%)	181 (95%)	10 (5%)	0	100	100
47	AM	134/138 (97%)	129 (96%)	5 (4%)	0	100	100
48	AN	201/204 (98%)	190 (94%)	11 (6%)	0	100	100
49	AO	195/199 (98%)	192 (98%)	3 (2%)	0	100	100
50	AP	171/184 (93%)	165 (96%)	6 (4%)	0	100	100
51	AQ	183/186 (98%)	177 (97%)	6 (3%)	0	100	100
52	AR	186/189 (98%)	179 (96%)	7 (4%)	0	100	100
53	AS	170/178 (96%)	162 (95%)	8 (5%)	0	100	100
54	AT	157/160 (98%)	147 (94%)	10 (6%)	0	100	100
55	AU	98/121 (81%)	89 (91%)	9 (9%)	0	100	100
56	AV	134/137 (98%)	131 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
57	AW	61/155 (39%)	61 (100%)	0	0	100	100
58	AX	119/142 (84%)	116 (98%)	3 (2%)	0	100	100
59	AY	124/127 (98%)	121 (98%)	3 (2%)	0	100	100
60	AZ	133/136 (98%)	129 (97%)	4 (3%)	0	100	100
61	Aa	146/149 (98%)	134 (92%)	12 (8%)	0	100	100
62	Ab	56/59 (95%)	50 (89%)	6 (11%)	0	100	100
63	Ac	95/105 (90%)	95 (100%)	0	0	100	100
64	Ad	107/113 (95%)	102 (95%)	5 (5%)	0	100	100
65	Ae	125/130 (96%)	122 (98%)	3 (2%)	0	100	100
66	Af	104/107 (97%)	101 (97%)	3 (3%)	0	100	100
67	Ag	110/121 (91%)	106 (96%)	4 (4%)	0	100	100
68	Ah	117/120 (98%)	113 (97%)	4 (3%)	0	100	100
69	Ai	97/100 (97%)	92 (95%)	5 (5%)	0	100	100
70	Aj	85/88 (97%)	81 (95%)	4 (5%)	0	100	100
71	Ak	75/78 (96%)	71 (95%)	4 (5%)	0	100	100
72	Al	48/51 (94%)	47 (98%)	1 (2%)	0	100	100
73	Am	50/128 (39%)	48 (96%)	2 (4%)	0	100	100
74	An	23/25 (92%)	23 (100%)	0	0	100	100
75	Ao	103/106 (97%)	92 (89%)	11 (11%)	0	100	100
76	Ap	89/92 (97%)	85 (96%)	4 (4%)	0	100	100
77	E	215/217 (99%)	197 (92%)	18 (8%)	0	100	100
79	DC	819/842 (97%)	754 (92%)	65 (8%)	0	100	100
80	Bf	73/152 (48%)	67 (92%)	6 (8%)	0	100	100
81	BM	122/143 (85%)	110 (90%)	12 (10%)	0	100	100
82	VA	187/312 (60%)	169 (90%)	18 (10%)	0	100	100
All	All	12121/13257 (91%)	11282 (93%)	839 (7%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	BA	173/210 (82%)	173 (100%)	0	100	100
2	BB	191/224 (85%)	190 (100%)	1 (0%)	86	94
3	BC	176/205 (86%)	176 (100%)	0	100	100
4	BE	221/222 (100%)	221 (100%)	0	100	100
5	BG	193/201 (96%)	193 (100%)	0	100	100
6	BH	165/170 (97%)	165 (100%)	0	100	100
7	BI	150/161 (93%)	150 (100%)	0	100	100
8	BJ	158/166 (95%)	157 (99%)	1 (1%)	84	93
9	BL	136/137 (99%)	134 (98%)	2 (2%)	60	80
10	BN	127/128 (99%)	126 (99%)	1 (1%)	79	91
11	BO	96/105 (91%)	95 (99%)	1 (1%)	73	87
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%)	69 (99%)	1 (1%)	62	82
18	Be	51/54 (94%)	50 (98%)	1 (2%)	50	74
19	BD	182/195 (93%)	180 (99%)	2 (1%)	70	86
20	BF	173/191 (91%)	172 (99%)	1 (1%)	84	93
21	BK	89/98 (91%)	89 (100%)	0	100	100
22	BP	104/118 (88%)	103 (99%)	1 (1%)	73	87
23	BQ	117/119 (98%)	117 (100%)	0	100	100
24	BR	113/124 (91%)	112 (99%)	1 (1%)	75	89
25	BS	128/129 (99%)	128 (100%)	0	100	100
26	BT	113/116 (97%)	112 (99%)	1 (1%)	75	89
27	BU	100/114 (88%)	100 (100%)	0	100	100
28	BZ	61/89 (68%)	61 (100%)	0	100	100
29	Bc	56/60 (93%)	56 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
30	Bd	47/49 (96%)	46 (98%)	1 (2%)	48	72
31	Bg	256/262 (98%)	256 (100%)	0	100	100
33	AA	189/196 (96%)	189 (100%)	0	100	100
34	AB	321/322 (100%)	320 (100%)	1 (0%)	91	96
35	AC	288/289 (100%)	286 (99%)	2 (1%)	81	92
39	AD	241/245 (98%)	241 (100%)	0	100	100
40	AE	134/153 (88%)	134 (100%)	0	100	100
41	AF	186/205 (91%)	186 (100%)	0	100	100
42	AG	189/208 (91%)	189 (100%)	0	100	100
43	AH	170/171 (99%)	169 (99%)	1 (1%)	84	93
44	AI	176/187 (94%)	175 (99%)	1 (1%)	84	93
45	AJ	147/150 (98%)	146 (99%)	1 (1%)	81	92
46	AL	154/159 (97%)	154 (100%)	0	100	100
47	AM	107/109 (98%)	107 (100%)	0	100	100
48	AN	175/176 (99%)	175 (100%)	0	100	100
49	AO	160/162 (99%)	159 (99%)	1 (1%)	84	93
50	AP	141/146 (97%)	140 (99%)	1 (1%)	81	92
51	AQ	150/151 (99%)	149 (99%)	1 (1%)	81	92
52	AR	153/154 (99%)	153 (100%)	0	100	100
53	AS	156/162 (96%)	156 (100%)	0	100	100
54	AT	136/137 (99%)	135 (99%)	1 (1%)	81	92
55	AU	87/107 (81%)	87 (100%)	0	100	100
56	AV	104/105 (99%)	104 (100%)	0	100	100
57	AW	55/129 (43%)	55 (100%)	0	100	100
58	AX	105/118 (89%)	105 (100%)	0	100	100
59	AY	109/110 (99%)	109 (100%)	0	100	100
60	AZ	115/116 (99%)	114 (99%)	1 (1%)	75	89
61	Aa	118/119 (99%)	118 (100%)	0	100	100
62	Ab	46/47 (98%)	46 (100%)	0	100	100
63	Ac	81/88 (92%)	81 (100%)	0	100	100
64	Ad	96/97 (99%)	96 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
65	Ae	109/111 (98%)	109 (100%)	0	100	100
66	Af	90/91 (99%)	90 (100%)	0	100	100
67	Ag	95/103 (92%)	95 (100%)	0	100	100
68	Ah	104/105 (99%)	104 (100%)	0	100	100
69	Ai	81/82 (99%)	81 (100%)	0	100	100
70	Aj	70/71 (99%)	70 (100%)	0	100	100
71	Ak	68/69 (99%)	68 (100%)	0	100	100
72	Al	45/46 (98%)	45 (100%)	0	100	100
73	Am	47/116 (40%)	47 (100%)	0	100	100
74	An	23/23 (100%)	23 (100%)	0	100	100
75	Ao	90/91 (99%)	90 (100%)	0	100	100
76	Ap	71/72 (99%)	71 (100%)	0	100	100
77	E	198/198 (100%)	197 (100%)	1 (0%)	86	94
79	DC	699/714 (98%)	695 (99%)	4 (1%)	84	93
80	Bf	66/135 (49%)	66 (100%)	0	100	100
81	BM	100/119 (84%)	100 (100%)	0	100	100
82	VA	160/254 (63%)	160 (100%)	0	100	100
All	All	10349/11154 (93%)	10318 (100%)	31 (0%)	90	96

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	BB	202	LYS
8	BJ	180	LYS
9	BL	30	ARG
9	BL	67	ARG
10	BN	114	ARG
11	BO	136	ARG
17	Bb	80	ARG
18	Be	26	LYS
19	BD	54	ARG
19	BD	76	ARG
20	BF	148	ARG
22	BP	130	ARG
24	BR	5	ARG
26	BT	89	ARG

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Mol	Chain	Res	Type
30	Bd	19	ARG
34	AB	332	ARG
35	AC	138	ARG
35	AC	300	ARG
43	AH	23	ARG
44	AI	82	ARG
45	AJ	166	LYS
49	AO	117[A]	ARG
50	AP	171	ARG
51	AQ	92	ARG
54	AT	83	ARG
60	AZ	34	LYS
77	E	92	LYS
79	DC	87	LYS
79	DC	92	LYS
79	DC	256	LYS
79	DC	841	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (114) such sidechains are listed below:

Mol	Chain	Res	Type
1	BA	21	ASN
1	BA	30	GLN
1	BA	131	GLN
1	BA	140	ASN
2	BB	49	ASN
2	BB	92	GLN
3	BC	94	GLN
3	BC	108	ASN
3	BC	199	GLN
3	BC	209	ASN
4	BE	67	GLN
4	BE	130	GLN
4	BE	157	ASN
4	BE	231	GLN
5	BG	80	ASN
5	BG	197	ASN
5	BG	199	GLN
6	BH	5	GLN
6	BH	110	GLN
6	BH	180	GLN
7	BI	103	GLN

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Mol	Chain	Res	Type
9	BL	81	HIS
10	BN	151	ASN
11	BO	12	GLN
12	BV	74	GLN
14	BX	22	ASN
14	BX	65	ASN
14	BX	75	GLN
14	BX	99	ASN
15	BY	22	GLN
15	BY	77	ASN
16	Ba	43	ASN
18	Be	17	GLN
19	BD	101	GLN
19	BD	165	ASN
20	BF	63	GLN
20	BF	103	ASN
21	BK	9	ASN
21	BK	81	ASN
23	BQ	21	HIS
23	BQ	100	GLN
24	BR	31	ASN
25	BS	75	ASN
28	BZ	98	GLN
31	Bg	17	ASN
31	Bg	101	GLN
31	Bg	147	HIS
31	Bg	148	ASN
31	Bg	153	GLN
33	AA	24	GLN
33	AA	215	ASN
34	AB	377	HIS
35	AC	48	GLN
35	AC	260	GLN
35	AC	291	ASN
39	AD	151	GLN
39	AD	264	GLN
41	AF	93	ASN
41	AF	104	GLN
41	AF	199	ASN
41	AF	200	ASN
42	AG	59	GLN
42	AG	232	HIS

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Mol	Chain	Res	Type
42	AG	243	GLN
43	AH	9	GLN
43	AH	37	ASN
43	AH	157	ASN
44	AI	209	ASN
45	AJ	39	GLN
45	AJ	95	ASN
46	AL	103	ASN
47	AM	41	GLN
47	AM	119	GLN
48	AN	86	ASN
48	AN	182	ASN
49	AO	50[A]	ASN
51	AQ	45	ASN
51	AQ	126	GLN
51	AQ	145	ASN
52	AR	7	GLN
52	AR	39	ASN
52	AR	47	ASN
53	AS	62	ASN
53	AS	88	HIS
54	AT	112	ASN
54	AT	134	GLN
55	AU	87	ASN
55	AU	101	ASN
56	AV	98	ASN
58	AX	111	ASN
59	AY	42	GLN
59	AY	81	GLN
60	AZ	103	GLN
60	AZ	128	GLN
61	Aa	120	ASN
65	Ae	13	HIS
65	Ae	71	HIS
66	Af	17	GLN
66	Af	87	ASN
68	Ah	76	GLN
68	Ah	104	GLN
69	Ai	91	ASN
70	Aj	13	ASN
71	Ak	57	ASN
72	Al	43	ASN

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Mol	Chain	Res	Type
73	Am	120	GLN
77	E	96	ASN
77	E	200	ASN
79	DC	18	ASN
79	DC	216	HIS
79	DC	290	ASN
79	DC	603	ASN
79	DC	607	ASN
79	DC	654	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
32	B5	1775/1798 (98%)	398 (22%)	11 (0%)
36	A1	3194/3360 (95%)	614 (19%)	26 (0%)
37	A3	120/121 (99%)	12 (10%)	1 (0%)
38	A4	157/158 (99%)	31 (19%)	0
78	EC	192/201 (95%)	109 (56%)	8 (4%)
All	All	5438/5638 (96%)	1164 (21%)	46 (0%)

All (1164) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
32	B5	4	C
32	B5	17	C
32	B5	26	A
32	B5	34	G
32	B5	40	A
32	B5	42	G
32	B5	43	A
32	B5	46	A
32	B5	47	A
32	B5	57	G
32	B5	60	U
32	B5	63	G
32	B5	67	A
32	B5	68	A
32	B5	72	A
32	B5	73	U
32	B5	74	U
32	B5	75	U

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Mol	Chain	Res	Type
32	B5	76	A
32	B5	77	U
32	B5	78	A
32	B5	81	G
32	B5	104	A
32	B5	114	C
32	B5	116	U
32	B5	127	G
32	B5	129	U
32	B5	130	C
32	B5	131	C
32	B5	132	U
32	B5	134	U
32	B5	135	A
32	B5	136	C
32	B5	137	U
32	B5	139	C
32	B5	141	U
32	B5	145	A
32	B5	166	C
32	B5	169	A
32	B5	176	C
32	B5	178	U
32	B5	179	A
32	B5	181	A
32	B5	182	A
32	B5	184	C
32	B5	186	C
32	B5	188	A
32	B5	190	C
32	B5	191	C
32	B5	192	U
32	B5	193	U
32	B5	194	U
32	B5	195	G
32	B5	196	G
32	B5	198	A
32	B5	200	A
32	B5	204	G
32	B5	207	U
32	B5	217	A
32	B5	218	A

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Mol	Chain	Res	Type
32	B5	221	A
32	B5	224	C
32	B5	225	A
32	B5	226	A
32	B5	227	U
32	B5	228	G
32	B5	229	U
32	B5	230	C
32	B5	232	U
32	B5	233	C
32	B5	234	G
32	B5	235	G
32	B5	239	C
32	B5	240	U
32	B5	241	U
32	B5	246	G
32	B5	257	A
32	B5	261	U
32	B5	262	U
32	B5	265	A
32	B5	278	U
32	B5	280	U
32	B5	281	G
32	B5	287	G
32	B5	299	A
32	B5	305	C
32	B5	314	C
32	B5	316	A
32	B5	321	C
32	B5	337	G
32	B5	338	C
32	B5	352	A
32	B5	353	A
32	B5	359	A
32	B5	360	A
32	B5	361	C
32	B5	390	G
32	B5	397	A
32	B5	400	A
32	B5	401	A
32	B5	402	C
32	B5	419	G

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Mol	Chain	Res	Type
32	B5	423	G
32	B5	424	C
32	B5	425	A
32	B5	426	G
32	B5	435	C
32	B5	439	U
32	B5	444	C
32	B5	452	A
32	B5	460	A
32	B5	475	A
32	B5	476	U
32	B5	477	A
32	B5	480	G
32	B5	485	A
32	B5	486	G
32	B5	489	C
32	B5	490	C
32	B5	491	C
32	B5	492	A
32	B5	494	U
32	B5	495	C
32	B5	496	G
32	B5	497	G
32	B5	498	G
32	B5	499	U
32	B5	500	C
32	B5	502	U
32	B5	503	G
32	B5	506	A
32	B5	507	U
32	B5	509	G
32	B5	514	G
32	B5	515	A
32	B5	518	A
32	B5	539	G
32	B5	540	G
32	B5	541	A2M
32	B5	542	A
32	B5	544	A
32	B5	554	C
32	B5	555	A
32	B5	557	G

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Mol	Chain	Res	Type
32	B5	558	U
32	B5	559	C
32	B5	565	C
32	B5	575	C
32	B5	577	G
32	B5	579	A
32	B5	580	A
32	B5	582	U
32	B5	594	A
32	B5	595	G
32	B5	606	A
32	B5	610	G
32	B5	611	U
32	B5	619	A2M
32	B5	620	A
32	B5	622	A
32	B5	623	A
32	B5	638	U
32	B5	639	U
32	B5	650	U
32	B5	652	G
32	B5	654	C
32	B5	656	G
32	B5	657	U
32	B5	658	C
32	B5	677	G
32	B5	678	A
32	B5	679	U
32	B5	681	U
32	B5	683	C
32	B5	693	U
32	B5	694	U
32	B5	696	C
32	B5	697	C
32	B5	700	C
32	B5	705	U
32	B5	708	C
32	B5	709	C
32	B5	712	G
32	B5	713	A
32	B5	715	U
32	B5	716	C

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Mol	Chain	Res	Type
32	B5	717	C
32	B5	718	U
32	B5	719	U
32	B5	720	G
32	B5	721	U
32	B5	722	G
32	B5	724	C
32	B5	725	U
32	B5	726	C
32	B5	727	U
32	B5	728	U
32	B5	730	G
32	B5	731	C
32	B5	733	A
32	B5	734	A
32	B5	735	C
32	B5	740	A
32	B5	741	C
32	B5	743	U
32	B5	753	A
32	B5	765	G
32	B5	766	U
32	B5	774	A
32	B5	775	G
32	B5	778	G
32	B5	781	U
32	B5	782	U
32	B5	783	G
32	B5	784	C
32	B5	789	A
32	B5	794	U
32	B5	812	A
32	B5	814	A
32	B5	819	G
32	B5	820	U
32	B5	823	G
32	B5	832	U
32	B5	833	U
32	B5	836	U
32	B5	837	G
32	B5	840	U
32	B5	846	G

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Mol	Chain	Res	Type
32	B5	850	A
32	B5	851	U
32	B5	859	A
32	B5	863	A
32	B5	864	U
32	B5	873	U
32	B5	876	G
32	B5	877	G
32	B5	886	U
32	B5	895	G
32	B5	898	A
32	B5	906	A
32	B5	914	G
32	B5	933	A
32	B5	935	U
32	B5	945	U
32	B5	951	A
32	B5	960	U
32	B5	966	A
32	B5	988	A
32	B5	992	A
32	B5	993	A
32	B5	1003	A
32	B5	1004	U
32	B5	1005	A
32	B5	1020	A
32	B5	1021	C
32	B5	1026	A
32	B5	1028	C
32	B5	1032	G
32	B5	1039	A
32	B5	1052	U
32	B5	1056	U
32	B5	1058	U
32	B5	1059	U
32	B5	1060	U
32	B5	1061	A
32	B5	1062	A
32	B5	1063	U
32	B5	1076	A
32	B5	1083	G
32	B5	1092	A

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Mol	Chain	Res	Type
32	B5	1097	U
32	B5	1098	U
32	B5	1100	G
32	B5	1138	A
32	B5	1150	G
32	B5	1158	C
32	B5	1159	C
32	B5	1185	U
32	B5	1194	A
32	B5	1196	A
32	B5	1199	G
32	B5	1200	G
32	B5	1201	G
32	B5	1202	A
32	B5	1217	A
32	B5	1218	G
32	B5	1226	A
32	B5	1227	A
32	B5	1228	G
32	B5	1229	G
32	B5	1231	U
32	B5	1243	G
32	B5	1244	A
32	B5	1245	G
32	B5	1246	C
32	B5	1251	U
32	B5	1256	A
32	B5	1257	U
32	B5	1269	OMU
32	B5	1276	U
32	B5	1286	U
32	B5	1301	U
32	B5	1312	A
32	B5	1314	U
32	B5	1315	U
32	B5	1316	G
32	B5	1321	A
32	B5	1340	U
32	B5	1345	A
32	B5	1346	A
32	B5	1355	C
32	B5	1358	G

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Mol	Chain	Res	Type
32	B5	1362	U
32	B5	1363	U
32	B5	1364	G
32	B5	1366	U
32	B5	1368	G
32	B5	1370	U
32	B5	1372	U
32	B5	1373	C
32	B5	1376	C
32	B5	1383	G
32	B5	1388	A
32	B5	1390	U
32	B5	1398	U
32	B5	1399	C
32	B5	1400	A
32	B5	1402	G
32	B5	1413	U
32	B5	1414	U
32	B5	1415	U
32	B5	1418	G
32	B5	1427	A
32	B5	1428	OMG
32	B5	1436	A
32	B5	1445	G
32	B5	1446	A
32	B5	1459	C
32	B5	1460	A
32	B5	1471	A
32	B5	1481	C
32	B5	1486	G
32	B5	1491	U
32	B5	1492	A
32	B5	1493	A
32	B5	1496	U
32	B5	1506	G
32	B5	1514	U
32	B5	1516	A
32	B5	1521	G
32	B5	1523	G
32	B5	1524	A
32	B5	1537	C
32	B5	1538	U

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Mol	Chain	Res	Type
32	B5	1539	G
32	B5	1540	G
32	B5	1542	G
32	B5	1557	U
32	B5	1559	A
32	B5	1572	OMG
32	B5	1573	A
32	B5	1574	G
32	B5	1575	G7M
32	B5	1576	A
32	B5	1584	G
32	B5	1600	A
32	B5	1601	G
32	B5	1616	G
32	B5	1619	C
32	B5	1635	A
32	B5	1645	G
32	B5	1646	C
32	B5	1657	U
32	B5	1658	G
32	B5	1680	G
32	B5	1683	C
32	B5	1684	U
32	B5	1688	U
32	B5	1689	A
32	B5	1700	C
32	B5	1701	A
32	B5	1703	C
32	B5	1715	G
32	B5	1716	C
32	B5	1717	G
32	B5	1730	A
32	B5	1756[A]	A
32	B5	1760	G
32	B5	1766	A
32	B5	1767	G
32	B5	1769	U
32	B5	1780	G
32	B5	1792	G
32	B5	1793	G
32	B5	1794	A
32	B5	1795	U

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Mol	Chain	Res	Type
32	B5	1796	C
32	B5	1799	U
36	A1	26	A
36	A1	34	A
36	A1	40	A
36	A1	43	A
36	A1	49	A
36	A1	59	G
36	A1	60	A
36	A1	65	A
36	A1	66	A
36	A1	77	A
36	A1	92	G
36	A1	99	A
36	A1	109	A
36	A1	110	G
36	A1	111	C
36	A1	116	A
36	A1	117	U
36	A1	120	G
36	A1	122	A
36	A1	133	U
36	A1	134	U
36	A1	135	C
36	A1	136	G
36	A1	156	G
36	A1	157	A
36	A1	164	A
36	A1	165	A
36	A1	166	C
36	A1	167	U
36	A1	170	G
36	A1	174	C
36	A1	175	C
36	A1	176	G
36	A1	178	U
36	A1	179	C
36	A1	180	C
36	A1	181	U
36	A1	182	U
36	A1	187	A
36	A1	188	U

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Mol	Chain	Res	Type
36	A1	190	U
36	A1	199	A
36	A1	200	C
36	A1	206	G
36	A1	208	C
36	A1	210	U
36	A1	211	A
36	A1	219	A
36	A1	220	G
36	A1	229	G
36	A1	233	C
36	A1	234	G
36	A1	236	G
36	A1	238	A
36	A1	240	U
36	A1	241	G
36	A1	242	C
36	A1	243	G
36	A1	244	G
36	A1	245	U
36	A1	247	C
36	A1	248	U
36	A1	249	U
36	A1	250	U
36	A1	251	G
36	A1	252	U
36	A1	269	G
36	A1	286	U
36	A1	295	A
36	A1	296	A
36	A1	298	U
36	A1	305	U
36	A1	329	U
36	A1	339	C
36	A1	352	A
36	A1	371	G
36	A1	372	A
36	A1	376	G
36	A1	387	A
36	A1	398	A
36	A1	399	A
36	A1	401	U

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Mol	Chain	Res	Type
36	A1	402	A
36	A1	403	C
36	A1	420	G
36	A1	421	G
36	A1	422	A
36	A1	438	A
36	A1	440	A
36	A1	495	G
36	A1	521	A
36	A1	523	A
36	A1	535	G
36	A1	540	U
36	A1	541	U
36	A1	542	G
36	A1	545	U
36	A1	547	G
36	A1	548	G
36	A1	549	U
36	A1	552	G
36	A1	557	A
36	A1	559	A
36	A1	569	A
36	A1	578	A
36	A1	579	G
36	A1	592	A
36	A1	602	A
36	A1	604	G
36	A1	611	A
36	A1	620	U
36	A1	621	A
36	A1	636	C
36	A1	649	A2M
36	A1	660	A
36	A1	677	A
36	A1	681	U
36	A1	691	A
36	A1	705	A
36	A1	715	A
36	A1	719	U
36	A1	725	G
36	A1	736	A
36	A1	758	C

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Mol	Chain	Res	Type
36	A1	765	C
36	A1	766	U
36	A1	767	U
36	A1	774	G
36	A1	775	A
36	A1	776	U
36	A1	777	U
36	A1	781	G
36	A1	784	A
36	A1	785	G
36	A1	786	A
36	A1	799	G
36	A1	806	A
36	A1	813	G
36	A1	817	A2M
36	A1	830	A
36	A1	849	C
36	A1	857	G
36	A1	861	C
36	A1	874	U
36	A1	879	U
36	A1	896	A
36	A1	897	U
36	A1	907	G
36	A1	908	OMG
36	A1	909	G
36	A1	914	A
36	A1	916	G
36	A1	917	A
36	A1	921	A
36	A1	923	C
36	A1	924	G
36	A1	925	A
36	A1	934	G
36	A1	937	G
36	A1	943	U
36	A1	944	C
36	A1	959	C
36	A1	961	C
36	A1	962	A
36	A1	964	G
36	A1	974	G

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Mol	Chain	Res	Type
36	A1	980	A
36	A1	981	U
36	A1	983	A
36	A1	994	G
36	A1	1000	C
36	A1	1002	A
36	A1	1010	G
36	A1	1013	G
36	A1	1014	U
36	A1	1016	C
36	A1	1017	C
36	A1	1018	G
36	A1	1019	G
36	A1	1021	G
36	A1	1023	C
36	A1	1032	C
36	A1	1033	U
36	A1	1034	U
36	A1	1035	G
36	A1	1036	A
36	A1	1045	C
36	A1	1047	A
36	A1	1063	G
36	A1	1064	A
36	A1	1065	A
36	A1	1072	G
36	A1	1075	A
36	A1	1081	U
36	A1	1082	U
36	A1	1093	A
36	A1	1094	U
36	A1	1095	U
36	A1	1097	G
36	A1	1098	A
36	A1	1103	A
36	A1	1104	G
36	A1	1117	G
36	A1	1130	A
36	A1	1131	G
36	A1	1144	U
36	A1	1153	A
36	A1	1159	A

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Mol	Chain	Res	Type
36	A1	1160	C
36	A1	1178	G
36	A1	1179	A
36	A1	1180	A
36	A1	1181	U
36	A1	1182	A
36	A1	1192	C
36	A1	1193	A
36	A1	1201	C
36	A1	1206	G
36	A1	1208	U
36	A1	1219	C
36	A1	1222	G
36	A1	1224	C
36	A1	1228	C
36	A1	1232	C
36	A1	1235	U
36	A1	1236	G
36	A1	1239	C
36	A1	1241	U
36	A1	1243	G
36	A1	1245	A
36	A1	1246	G
36	A1	1252	A
36	A1	1253	U
36	A1	1256	G
36	A1	1262	G
36	A1	1263	A
36	A1	1265	U
36	A1	1279	C
36	A1	1281	G
36	A1	1282	G
36	A1	1283	C
36	A1	1286	A
36	A1	1287	A
36	A1	1292	C
36	A1	1293	U
36	A1	1295	G
36	A1	1307	G
36	A1	1309	U
36	A1	1317	A
36	A1	1330	A

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Mol	Chain	Res	Type
36	A1	1331	U
36	A1	1348	U
36	A1	1350	A
36	A1	1351	U
36	A1	1352	A
36	A1	1353	U
36	A1	1354	G
36	A1	1355	A
36	A1	1356	U
36	A1	1357	G
36	A1	1386	A
36	A1	1391	C
36	A1	1393	A
36	A1	1399	A
36	A1	1400	G
36	A1	1419	A
36	A1	1431	G
36	A1	1434	G
36	A1	1437	OMC
36	A1	1446	A
36	A1	1455	U
36	A1	1468	A
36	A1	1475	A
36	A1	1476	G
36	A1	1481	A
36	A1	1502	C
36	A1	1503	A
36	A1	1508	C
36	A1	1523	U
36	A1	1526	U
36	A1	1539	A
36	A1	1555	U
36	A1	1556	C
36	A1	1558	A
36	A1	1562	C
36	A1	1564	U
36	A1	1565	G
36	A1	1566	A
36	A1	1567	U
36	A1	1568	U
36	A1	1569	U
36	A1	1572	U

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Mol	Chain	Res	Type
36	A1	1574	C
36	A1	1575	A
36	A1	1576	G
36	A1	1579	C
36	A1	1583	A
36	A1	1587	A
36	A1	1589	A
36	A1	1593	A
36	A1	1605	A
36	A1	1608	C
36	A1	1628	C
36	A1	1629	U
36	A1	1630	U
36	A1	1642	A
36	A1	1643	A
36	A1	1683	A
36	A1	1724	U
36	A1	1729	A
36	A1	1734	G
36	A1	1736	G
36	A1	1738	C
36	A1	1739	U
36	A1	1741	A
36	A1	1750	A
36	A1	1751	G
36	A1	1762	C
36	A1	1763	U
36	A1	1764	U
36	A1	1765	U
36	A1	1766	G
36	A1	1775	G
36	A1	1778	G
36	A1	1796	G
36	A1	1797	A
36	A1	1813	A
36	A1	1815	U
36	A1	1816	A
36	A1	1817	G
36	A1	1820	U
36	A1	1821	U
36	A1	1842	A
36	A1	1846	C

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Mol	Chain	Res	Type
36	A1	1849	C
36	A1	1850	A
36	A1	1866	C
36	A1	1878	G
36	A1	1880	U
36	A1	1886	A
36	A1	1893	A
36	A1	1896	A
36	A1	1899	G
36	A1	1906	G
36	A1	1932	A
36	A1	1936	A
36	A1	1943	C
36	A1	1950	U
36	A1	1951	C
36	A1	1953	G
36	A1	1954	G
36	A1	1955	U
36	A1	2094	C
36	A1	2110	G
36	A1	2111	G
36	A1	2112	U
36	A1	2114	C
36	A1	2122	G
36	A1	2131	A
36	A1	2140	U
36	A1	2144	A
36	A1	2146	C
36	A1	2158	A
36	A1	2169	G
36	A1	2188	A
36	A1	2197	OMC
36	A1	2201	G
36	A1	2206	G
36	A1	2207	A
36	A1	2209	U
36	A1	2242	A
36	A1	2249	G
36	A1	2251	G
36	A1	2255	A
36	A1	2256	A2M
36	A1	2259	A

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Mol	Chain	Res	Type
36	A1	2260	U
36	A1	2267	C
36	A1	2269	U
36	A1	2270	A
36	A1	2272	G
36	A1	2273	G
36	A1	2280	A2M
36	A1	2281	A2M
36	A1	2284	C
36	A1	2307	G
36	A1	2308	C
36	A1	2310	U
36	A1	2313	A
36	A1	2314	U
36	A1	2315	G
36	A1	2318	U
36	A1	2334	U
36	A1	2336	U
36	A1	2340	U
36	A1	2366	C
36	A1	2373	A
36	A1	2374	C
36	A1	2375	G
36	A1	2376	G
36	A1	2383	C
36	A1	2388	U
36	A1	2391	G
36	A1	2393	G
36	A1	2397	A
36	A1	2402	A
36	A1	2403	G
36	A1	2404	A
36	A1	2411	U
36	A1	2412	G
36	A1	2418	G
36	A1	2438	A
36	A1	2442	G
36	A1	2445	A
36	A1	2446	U
36	A1	2450	G
36	A1	2451	G
36	A1	2452	G

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Mol	Chain	Res	Type
36	A1	2453	U
36	A1	2454	G
36	A1	2455	U
36	A1	2458	A
36	A1	2459	A
36	A1	2460	U
36	A1	2461	A
36	A1	2462	A
36	A1	2463	G
36	A1	2467	G
36	A1	2468	A
36	A1	2469	G
36	A1	2470	C
36	A1	2473	C
36	A1	2474	G
36	A1	2475	G
36	A1	2477	G
36	A1	2479	C
36	A1	2480	A
36	A1	2485	A
36	A1	2486	A
36	A1	2487	U
36	A1	2488	A
36	A1	2489	C
36	A1	2490	C
36	A1	2492	C
36	A1	2493	U
36	A1	2494	A
36	A1	2495	C
36	A1	2496	C
36	A1	2497	U
36	A1	2498	U
36	A1	2500	A
36	A1	2502	A
36	A1	2503	G
36	A1	2504	U
36	A1	2505	U
36	A1	2506	U
36	A1	2507	C
36	A1	2511	A
36	A1	2514	U
36	A1	2523	A

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Mol	Chain	Res	Type
36	A1	2524	A
36	A1	2531	C
36	A1	2538	U
36	A1	2539	C
36	A1	2540	A
36	A1	2541	U
36	A1	2542	U
36	A1	2544	U
36	A1	2549	G
36	A1	2552	C
36	A1	2554	A
36	A1	2561	A
36	A1	2562	A
36	A1	2569	A
36	A1	2571	U
36	A1	2573	G
36	A1	2585	G
36	A1	2586	G
36	A1	2593	A
36	A1	2594	C
36	A1	2606	G
36	A1	2607	G
36	A1	2614	G
36	A1	2648	G
36	A1	2651	G
36	A1	2652	U
36	A1	2656	A
36	A1	2672	G
36	A1	2674	A
36	A1	2677	G
36	A1	2678	A
36	A1	2680	A
36	A1	2681	U
36	A1	2688	U
36	A1	2689	A
36	A1	2690	G
36	A1	2691	A
36	A1	2694	A
36	A1	2704	A
36	A1	2705	A
36	A1	2712	U
36	A1	2714	G

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Mol	Chain	Res	Type
36	A1	2719	U
36	A1	2728	G
36	A1	2729	OMU
36	A1	2737	C
36	A1	2752	U
36	A1	2753	G
36	A1	2755	C
36	A1	2777	G
36	A1	2778	G
36	A1	2796	G
36	A1	2799	A
36	A1	2800	G
36	A1	2801	A
36	A1	2803	A
36	A1	2810	C
36	A1	2814	G
36	A1	2817	A
36	A1	2842	U
36	A1	2845	A
36	A1	2851	A
36	A1	2860	U
36	A1	2871	G
36	A1	2872	A
36	A1	2873	U
36	A1	2875	U
36	A1	2876	C
36	A1	2887	A
36	A1	2889	C
36	A1	2898	G
36	A1	2923	U
36	A1	2935	U
36	A1	2936	A
36	A1	2941	A
36	A1	2942	C
36	A1	2947	G
36	A1	2977	G
36	A1	2983	C
36	A1	2990	G
36	A1	2997	G
36	A1	3011	A
36	A1	3012	A
36	A1	3022	G

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Mol	Chain	Res	Type
36	A1	3032	A
36	A1	3056	U
36	A1	3059	G
36	A1	3078	U
36	A1	3079	U
36	A1	3086	A
36	A1	3087	A
36	A1	3092	C
36	A1	3109	G
36	A1	3113	A
36	A1	3122	A
36	A1	3130	A
36	A1	3131	U
36	A1	3142	A
36	A1	3143	C
36	A1	3153	U
36	A1	3154	C
36	A1	3155	U
36	A1	3156	U
36	A1	3157	U
36	A1	3165	A
36	A1	3170	A
36	A1	3172	A
36	A1	3173	G
36	A1	3174	A
36	A1	3176	G
36	A1	3179	U
36	A1	3181	C
36	A1	3187	A
36	A1	3196	U
36	A1	3198	U
36	A1	3207	U
36	A1	3217	C
36	A1	3218	A
36	A1	3219	G
36	A1	3224	G
36	A1	3234	A
36	A1	3243	A
36	A1	3246	G
36	A1	3247	G
36	A1	3256	G
36	A1	3259	U

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Mol	Chain	Res	Type
36	A1	3263	G
36	A1	3270	U
36	A1	3271	G
36	A1	3273	A
36	A1	3276	G
36	A1	3281	U
36	A1	3289	G
36	A1	3294	A
36	A1	3303	G
36	A1	3304	U
36	A1	3305	A
36	A1	3313	U
36	A1	3314	A
36	A1	3316	A
36	A1	3319	U
36	A1	3341	U
36	A1	3342	A
36	A1	3345	G
36	A1	3351	U
36	A1	3352	U
36	A1	3353	G
36	A1	3354	U
36	A1	3355	U
36	A1	3356	G
36	A1	3369	G
36	A1	3378	C
36	A1	3389	U
36	A1	3390	G
37	A3	48	U
37	A3	53	U
37	A3	54	U
37	A3	55	A
37	A3	64	A
37	A3	65	G
37	A3	74	C
37	A3	76	A
37	A3	78	U
37	A3	102	A
37	A3	112	G
37	A3	121	U
38	A4	23	U
38	A4	34	U

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Mol	Chain	Res	Type
38	A4	35	C
38	A4	46	G
38	A4	51	G
38	A4	52	A
38	A4	53	A
38	A4	58	G
38	A4	59	A
38	A4	60	U
38	A4	62	C
38	A4	63	G
38	A4	75	G
38	A4	76	C
38	A4	81	U
38	A4	83	C
38	A4	86	U
38	A4	87	G
38	A4	88	A
38	A4	90	U
38	A4	95	G
38	A4	104	A
38	A4	106	C
38	A4	107	G
38	A4	111	A
38	A4	112	U
38	A4	113	U
38	A4	116	G
38	A4	125	U
38	A4	152	G
38	A4	158	U
78	EC	6759	A
78	EC	6762	U
78	EC	6768	U
78	EC	6769	A
78	EC	6770	U
78	EC	6771	U
78	EC	6772	G
78	EC	6773	G
78	EC	6774	U
78	EC	6775	U
78	EC	6776	A
78	EC	6777	C
78	EC	6778	C

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Mol	Chain	Res	Type
78	EC	6779	C
78	EC	6780	A
78	EC	6782	C
78	EC	6788	C
78	EC	6789	G
78	EC	6790	A
78	EC	6791	A
78	EC	6792	A
78	EC	6793	A
78	EC	6794	C
78	EC	6795	U
78	EC	6800	G
78	EC	6801	A
78	EC	6802	A
78	EC	6803	C
78	EC	6804	A
78	EC	6812	C
78	EC	6816	A
78	EC	6817	A
78	EC	6818	G
78	EC	6819	G
78	EC	6820	C
78	EC	6821	U
78	EC	6822	U
78	EC	6823	U
78	EC	6824	C
78	EC	6825	A
78	EC	6831	U
78	EC	6832	G
78	EC	6835	U
78	EC	6836	U
78	EC	6837	G
78	EC	6840	A
78	EC	6841	U
78	EC	6842	U
78	EC	6843	U
78	EC	6844	A
78	EC	6847	G
78	EC	6848	U
78	EC	6849	A
78	EC	6850	C
78	EC	6852	U

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Mol	Chain	Res	Type
78	EC	6856	C
78	EC	6857	C
78	EC	6858	A
78	EC	6859	U
78	EC	6860	A
78	EC	6861	G
78	EC	6864	A
78	EC	6865	G
78	EC	6866	C
78	EC	6867	C
78	EC	6870	A
78	EC	6871	A
78	EC	6872	A
78	EC	6873	A
78	EC	6874	A
78	EC	6875	C
78	EC	6877	C
78	EC	6880	G
78	EC	6881	U
78	EC	6882	G
78	EC	6883	A
78	EC	6884	G
78	EC	6887	G
78	EC	6889	A
78	EC	6890	A
78	EC	6895	C
78	EC	6896	A
78	EC	6897	G
78	EC	6902	U
78	EC	6903	U
78	EC	6908	C
78	EC	6910	A
78	EC	6911	A
78	EC	6915	G
78	EC	6916	A
78	EC	6918	A
78	EC	6925	C
78	EC	6928	G
78	EC	6929	C
78	EC	6934	U
78	EC	6935	G
78	EC	6936	G

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Mol	Chain	Res	Type
78	EC	6938	A
78	EC	6939	C
78	EC	6940	U
78	EC	6941	U
78	EC	6942	A
78	EC	6943	A
78	EC	6944	U
78	EC	6945	U
78	EC	6946	A
78	EC	6947	A
78	EC	6948	U
78	EC	6949	G

All (46) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
32	B5	240	U
32	B5	752	A
32	B5	819	G
32	B5	862	A
32	B5	950	C
32	B5	1285	U
32	B5	1344	A
32	B5	1369	U
32	B5	1458	G
32	B5	1572	OMG
32	B5	1645	G
36	A1	116	A
36	A1	122	A
36	A1	165	A
36	A1	178	U
36	A1	210	U
36	A1	241	G
36	A1	249	U
36	A1	873	C
36	A1	916	G
36	A1	1092	C
36	A1	1218	U
36	A1	1242	G
36	A1	1278	A
36	A1	1292	C
36	A1	1349	G

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Mol	Chain	Res	Type
36	A1	1354	G
36	A1	1565	G
36	A1	1629	U
36	A1	2241	U
36	A1	2469	G
36	A1	2493	U
36	A1	2494	A
36	A1	2506	U
36	A1	2801	A
36	A1	2875	U
36	A1	3121	U
37	A3	52	G
78	EC	6789	G
78	EC	6817	A
78	EC	6831	U
78	EC	6851	G
78	EC	6876	A
78	EC	6889	A
78	EC	6939	C
78	EC	6943	A

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

68 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$
32	A2M	B5	420	32	18,25,26	0.90	1 (5%)	20,36,39	1.22	2 (10%)
32	A2M	B5	796	32	18,25,26	0.90	1 (5%)	20,36,39	1.41	3 (15%)
36	OMG	A1	805	36	19,26,27	0.89	1 (5%)	21,38,41	1.15	2 (9%)
36	A2M	A1	2281	36	18,25,26	0.76	0	20,36,39	2.03	5 (25%)
36	OMC	A1	2959	36	19,22,23	0.78	0	25,31,34	0.82	0
79	DDE	DC	699	79	15,20,21	0.98	1 (6%)	11,28,30	0.98	1 (9%)
36	A2M	A1	2220	36	18,25,26	0.85	1 (5%)	20,36,39	1.25	2 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	OMC	B5	1639	32	19,22,23	0.76	0	25,31,34	0.71	0
36	OMU	A1	2417	36	19,22,23	1.23	3 (15%)	25,31,34	1.82	5 (20%)
36	OMG	A1	867	36,83	19,26,27	0.90	1 (5%)	21,38,41	1.04	2 (9%)
36	OMC	A1	1437	36,83	19,22,23	0.82	0	25,31,34	1.02	2 (8%)
36	A2M	A1	2946	36,83	18,25,26	0.85	1 (5%)	20,36,39	1.47	4 (20%)
32	OMG	B5	1126	32	19,26,27	0.89	1 (5%)	21,38,41	1.19	2 (9%)
36	5MC	A1	2278	36,83	19,22,23	1.54	3 (15%)	26,32,35	1.21	3 (11%)
36	A2M	A1	2280	36	18,25,26	0.84	0	20,36,39	1.27	2 (10%)
36	OMU	A1	2421	36	19,22,23	1.26	3 (15%)	25,31,34	1.85	5 (20%)
36	A2M	A1	2640	36	18,25,26	0.86	0	20,36,39	1.15	2 (10%)
32	OMG	B5	1428	32,83	19,26,27	0.89	1 (5%)	21,38,41	1.04	2 (9%)
36	OMC	A1	2197	36	19,22,23	0.79	0	25,31,34	0.88	0
36	1MA	A1	645	36,83	17,25,26	1.45	2 (11%)	17,37,40	1.16	2 (11%)
36	OMG	A1	2922	36	19,26,27	0.87	1 (5%)	21,38,41	1.02	1 (4%)
32	G7M	B5	1575	32	20,26,27	2.73	5 (25%)	16,39,42	1.77	4 (25%)
32	OMU	B5	1269	32	19,22,23	1.25	4 (21%)	25,31,34	1.85	5 (20%)
32	MA6	B5	1781	32	19,26,27	1.00	1 (5%)	18,38,41	1.89	4 (22%)
36	OMU	A1	1888	36	19,22,23	1.28	3 (15%)	25,31,34	1.87	5 (20%)
36	1MA	A1	2142	36,83	17,25,26	1.50	2 (11%)	17,37,40	1.20	2 (11%)
32	OMC	B5	414	32	19,22,23	0.79	0	25,31,34	0.80	1 (4%)
36	OMG	A1	2791	36	19,26,27	0.88	1 (5%)	21,38,41	1.02	2 (9%)
36	OMU	A1	2729	36	19,22,23	1.24	3 (15%)	25,31,34	1.79	4 (16%)
36	OMG	A1	2815	36	19,26,27	0.88	1 (5%)	21,38,41	1.01	2 (9%)
36	OMG	A1	2288	36	19,26,27	0.88	1 (5%)	21,38,41	1.01	1 (4%)
36	A2M	A1	817	36,83	18,25,26	0.86	0	20,36,39	1.23	2 (10%)
36	A2M	A1	1449	36,83	18,25,26	0.86	0	20,36,39	1.19	2 (10%)
32	A2M	B5	28	32	18,25,26	0.89	1 (5%)	20,36,39	1.15	2 (10%)
36	OMU	A1	2724	36	19,22,23	1.24	3 (15%)	25,31,34	1.83	6 (24%)
36	A2M	A1	1133	36	18,25,26	0.83	1 (5%)	20,36,39	1.40	3 (15%)
32	OMG	B5	562	32	19,26,27	0.90	1 (5%)	21,38,41	1.02	2 (9%)
32	A2M	B5	974	32	18,25,26	0.85	0	20,36,39	1.15	2 (10%)
36	OMC	A1	650	36,83	19,22,23	0.79	0	25,31,34	0.86	0
32	A2M	B5	541	32	18,25,26	0.86	0	20,36,39	1.21	2 (10%)
36	A2M	A1	876	36	18,25,26	0.82	0	20,36,39	1.16	2 (10%)
36	OMU	A1	2921	36	19,22,23	1.26	3 (15%)	25,31,34	1.83	4 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
36	OMC	A1	2337	36	19,22,23	0.77	0	25,31,34	0.85	1 (4%)
32	A2M	B5	100	32,83	18,25,26	0.87	1 (5%)	20,36,39	1.23	2 (10%)
32	4AC	B5	1773	32	21,24,25	1.05	2 (9%)	28,34,37	2.58	7 (25%)
36	OMU	A1	2347	36	19,22,23	1.29	3 (15%)	25,31,34	1.82	5 (20%)
32	A2M	B5	619	32,83	18,25,26	0.80	0	20,36,39	1.23	2 (10%)
32	OMC	B5	1007	32	19,22,23	0.78	0	25,31,34	0.81	0
36	OMU	A1	898	36	19,22,23	1.25	3 (15%)	25,31,34	1.81	4 (16%)
36	OMG	A1	1450	36	19,26,27	0.88	1 (5%)	21,38,41	1.01	1 (4%)
32	OMG	B5	1572	32	19,26,27	0.88	1 (5%)	21,38,41	1.42	3 (14%)
32	XSX	B5	1191	32	24,28,29	1.00	1 (4%)	30,40,43	3.70	5 (16%)
32	4AC	B5	1280	32	21,24,25	1.06	1 (4%)	28,34,37	1.07	2 (7%)
36	OMG	A1	908	36	19,26,27	0.97	1 (5%)	21,38,41	1.17	2 (9%)
36	A2M	A1	807	36	18,25,26	0.80	0	20,36,39	1.36	4 (20%)
36	OMC	A1	2948	36	19,22,23	0.78	0	25,31,34	0.89	1 (4%)
32	OMG	B5	1271	32	19,26,27	0.88	1 (5%)	21,38,41	1.04	2 (9%)
34	HIC	AB	243	34	8,11,12	1.62	2 (25%)	5,14,16	0.95	0
36	OMC	A1	663	36	19,22,23	0.81	0	25,31,34	0.74	0
32	MA6	B5	1782	32	19,26,27	1.00	1 (5%)	18,38,41	1.91	3 (16%)
36	A2M	A1	2256	36	18,25,26	0.85	0	20,36,39	1.29	2 (10%)
36	OMG	A1	2619	36	19,26,27	0.89	1 (5%)	21,38,41	1.01	2 (9%)
36	5MC	A1	2870	36	19,22,23	1.61	3 (15%)	26,32,35	1.23	3 (11%)
36	OMG	A1	2793	36	19,26,27	0.89	1 (5%)	21,38,41	1.09	2 (9%)
32	A2M	B5	436	32	18,25,26	0.86	0	20,36,39	1.27	2 (10%)
36	UR3	A1	2634	36	19,22,23	0.96	0	26,32,35	1.77	2 (7%)
32	OMU	B5	578	32	19,22,23	1.19	3 (15%)	25,31,34	1.81	5 (20%)
36	A2M	A1	649	36	18,25,26	0.79	0	20,36,39	1.18	2 (10%)

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
32	A2M	B5	420	32	-	1/5/27/28	0/3/3/3
32	A2M	B5	796	32	-	0/5/27/28	0/3/3/3
36	OMG	A1	805	36	-	0/5/27/28	0/3/3/3
36	A2M	A1	2281	36	-	2/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	OMC	A1	2959	36	-	0/9/27/28	0/2/2/2
79	DDE	DC	699	79	-	8/20/21/23	0/1/1/1
36	A2M	A1	2220	36	-	1/5/27/28	0/3/3/3
32	OMC	B5	1639	32	-	0/9/27/28	0/2/2/2
36	OMU	A1	2417	36	-	1/9/27/28	0/2/2/2
36	OMG	A1	867	36,83	-	0/5/27/28	0/3/3/3
36	OMC	A1	1437	36,83	-	4/9/27/28	0/2/2/2
36	A2M	A1	2946	36,83	-	0/5/27/28	0/3/3/3
32	OMG	B5	1126	32	-	1/5/27/28	0/3/3/3
36	5MC	A1	2278	36,83	-	1/7/25/26	0/2/2/2
36	A2M	A1	2280	36	-	2/5/27/28	0/3/3/3
36	OMU	A1	2421	36	-	1/9/27/28	0/2/2/2
36	A2M	A1	2640	36	-	0/5/27/28	0/3/3/3
32	OMG	B5	1428	32,83	-	2/5/27/28	0/3/3/3
36	OMC	A1	2197	36	-	6/9/27/28	0/2/2/2
36	1MA	A1	645	36,83	-	0/3/25/26	0/3/3/3
36	OMG	A1	2922	36	-	1/5/27/28	0/3/3/3
32	G7M	B5	1575	32	-	0/3/25/26	0/3/3/3
32	OMU	B5	1269	32	-	4/9/27/28	0/2/2/2
32	MA6	B5	1781	32	-	0/7/29/30	0/3/3/3
36	OMU	A1	1888	36	-	1/9/27/28	0/2/2/2
36	1MA	A1	2142	36,83	-	0/3/25/26	0/3/3/3
32	OMC	B5	414	32	-	1/9/27/28	0/2/2/2
36	OMG	A1	2791	36	-	1/5/27/28	0/3/3/3
36	OMU	A1	2729	36	-	3/9/27/28	0/2/2/2
36	OMG	A1	2815	36	-	0/5/27/28	0/3/3/3
36	OMG	A1	2288	36	-	0/5/27/28	0/3/3/3
36	A2M	A1	817	36,83	-	1/5/27/28	0/3/3/3
36	A2M	A1	1449	36,83	-	0/5/27/28	0/3/3/3
32	A2M	B5	28	32	-	0/5/27/28	0/3/3/3
36	OMU	A1	2724	36	-	1/9/27/28	0/2/2/2
36	A2M	A1	1133	36	-	0/5/27/28	0/3/3/3
32	OMG	B5	562	32	-	1/5/27/28	0/3/3/3
32	A2M	B5	974	32	-	0/5/27/28	0/3/3/3
36	OMC	A1	650	36,83	-	0/9/27/28	0/2/2/2
32	A2M	B5	541	32	-	3/5/27/28	0/3/3/3
36	A2M	A1	876	36	-	0/5/27/28	0/3/3/3
36	OMU	A1	2921	36	-	0/9/27/28	0/2/2/2
36	OMC	A1	2337	36	-	1/9/27/28	0/2/2/2
32	A2M	B5	100	32,83	-	0/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	4AC	B5	1773	32	-	4/11/29/30	0/2/2/2
36	OMU	A1	2347	36	-	0/9/27/28	0/2/2/2
32	A2M	B5	619	32,83	-	2/5/27/28	0/3/3/3
32	OMC	B5	1007	32	-	0/9/27/28	0/2/2/2
36	OMU	A1	898	36	-	0/9/27/28	0/2/2/2
36	OMG	A1	1450	36	-	1/5/27/28	0/3/3/3
32	OMG	B5	1572	32	-	2/5/27/28	0/3/3/3
32	XSX	B5	1191	32	-	6/16/34/35	0/2/2/2
32	4AC	B5	1280	32	-	4/11/29/30	0/2/2/2
36	OMG	A1	908	36	-	0/5/27/28	0/3/3/3
36	A2M	A1	807	36	-	0/5/27/28	0/3/3/3
36	OMC	A1	2948	36	-	0/9/27/28	0/2/2/2
32	OMG	B5	1271	32	-	1/5/27/28	0/3/3/3
34	HIC	AB	243	34	-	2/5/6/8	0/1/1/1
36	OMC	A1	663	36	-	1/9/27/28	0/2/2/2
32	MA6	B5	1782	32	-	2/7/29/30	0/3/3/3
36	A2M	A1	2256	36	-	3/5/27/28	0/3/3/3
36	OMG	A1	2619	36	-	1/5/27/28	0/3/3/3
36	5MC	A1	2870	36	-	4/7/25/26	0/2/2/2
36	OMG	A1	2793	36	-	1/5/27/28	0/3/3/3
32	A2M	B5	436	32	-	0/5/27/28	0/3/3/3
36	UR3	A1	2634	36	-	0/7/25/26	0/2/2/2
32	OMU	B5	578	32	-	0/9/27/28	0/2/2/2
36	A2M	A1	649	36	-	0/5/27/28	0/3/3/3

All (77) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	B5	1575	G7M	C8-N9	7.41	1.46	1.33
32	B5	1575	G7M	C8-N7	7.12	1.46	1.33
36	A1	2870	5MC	C5-C4	5.60	1.48	1.44
36	A1	2278	5MC	C5-C4	5.39	1.48	1.44
36	A1	2142	1MA	C2-N3	4.85	1.34	1.28
36	A1	645	1MA	C2-N3	4.50	1.34	1.28
32	B5	1575	G7M	C5-C4	4.21	1.47	1.39
34	AB	243	HIC	CD2-CG	3.39	1.41	1.36
36	A1	645	1MA	C6-N6	3.06	1.35	1.27
32	B5	1280	4AC	C4-N4	-2.97	1.35	1.39
36	A1	1888	OMU	C4-N3	-2.95	1.33	1.38
36	A1	2870	5MC	C6-C5	2.91	1.39	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	A1	2347	OMU	C4-N3	-2.88	1.33	1.38
36	A1	2921	OMU	C4-N3	-2.87	1.33	1.38
36	A1	2417	OMU	C4-N3	-2.85	1.33	1.38
36	A1	898	OMU	C4-N3	-2.84	1.33	1.38
36	A1	2421	OMU	C4-N3	-2.83	1.33	1.38
36	A1	2142	1MA	C6-N6	2.82	1.34	1.27
36	A1	2724	OMU	C4-N3	-2.79	1.33	1.38
36	A1	2729	OMU	C4-N3	-2.78	1.33	1.38
32	B5	1782	MA6	C6-C5	2.78	1.49	1.44
36	A1	2278	5MC	C6-C5	2.76	1.39	1.34
32	B5	1269	OMU	C4-N3	-2.70	1.34	1.38
36	A1	867	OMG	C6-N1	-2.65	1.33	1.37
36	A1	2815	OMG	C6-N1	-2.64	1.33	1.37
32	B5	1781	MA6	C6-C5	2.60	1.48	1.44
36	A1	908	OMG	C6-N1	-2.59	1.33	1.37
36	A1	1450	OMG	C6-N1	-2.59	1.33	1.37
36	A1	2619	OMG	C6-N1	-2.59	1.33	1.37
36	A1	2288	OMG	C6-N1	-2.57	1.33	1.37
32	B5	578	OMU	C4-N3	-2.52	1.34	1.38
36	A1	2791	OMG	C6-N1	-2.49	1.34	1.37
36	A1	805	OMG	C6-N1	-2.49	1.34	1.37
36	A1	2793	OMG	C6-N1	-2.47	1.34	1.37
36	A1	2347	OMU	C2-N3	-2.47	1.33	1.38
36	A1	2421	OMU	C2-N3	-2.46	1.33	1.38
32	B5	1575	G7M	C2'-C3'	-2.45	1.46	1.53
36	A1	2921	OMU	C2-N3	-2.44	1.33	1.38
36	A1	2922	OMG	C6-N1	-2.44	1.34	1.37
32	B5	562	OMG	C6-N1	-2.42	1.34	1.37
32	B5	1428	OMG	C6-N1	-2.41	1.34	1.37
36	A1	1888	OMU	C2-N3	-2.40	1.33	1.38
36	A1	2729	OMU	C2-N3	-2.38	1.33	1.38
36	A1	898	OMU	C2-N3	-2.38	1.33	1.38
36	A1	2724	OMU	C2-N3	-2.37	1.33	1.38
36	A1	2417	OMU	C2-N3	-2.37	1.33	1.38
32	B5	1271	OMG	C6-N1	-2.37	1.34	1.37
32	B5	1126	OMG	C6-N1	-2.28	1.34	1.37
32	B5	1773	4AC	C4-N4	-2.28	1.36	1.39
36	A1	2729	OMU	C5-C4	-2.27	1.38	1.43
32	B5	1773	4AC	C6-N1	-2.25	1.32	1.38
36	A1	2724	OMU	C5-C4	-2.25	1.38	1.43
32	B5	1572	OMG	C6-N1	-2.25	1.34	1.37
32	B5	1575	G7M	C6-N1	-2.24	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	A1	2870	5MC	C6-N1	-2.24	1.34	1.38
36	A1	2278	5MC	C6-N1	-2.24	1.34	1.38
32	B5	1269	OMU	C2-N3	-2.22	1.34	1.38
32	B5	1269	OMU	C2-N1	2.22	1.41	1.38
36	A1	2347	OMU	C5-C4	-2.22	1.38	1.43
36	A1	2417	OMU	C5-C4	-2.20	1.38	1.43
36	A1	2946	A2M	O4'-C1'	2.17	1.43	1.40
36	A1	2220	A2M	O4'-C1'	2.15	1.43	1.40
32	B5	578	OMU	C2-N3	-2.14	1.34	1.38
32	B5	420	A2M	O4'-C1'	2.13	1.43	1.40
36	A1	2421	OMU	C5-C4	-2.13	1.39	1.43
79	DC	699	DDE	CD2-NE2	2.12	1.39	1.36
32	B5	796	A2M	O4'-C1'	2.11	1.43	1.40
36	A1	898	OMU	C5-C4	-2.10	1.39	1.43
34	AB	243	HIC	CZ-NE2	-2.09	1.42	1.48
36	A1	2921	OMU	C5-C4	-2.09	1.39	1.43
32	B5	28	A2M	O4'-C1'	2.08	1.43	1.40
32	B5	1191	XSX	C2-N1	2.04	1.41	1.38
32	B5	1269	OMU	C5-C4	-2.04	1.39	1.43
32	B5	100	A2M	O4'-C1'	2.04	1.43	1.40
36	A1	1133	A2M	O4'-C1'	2.01	1.43	1.40
36	A1	1888	OMU	C5-C4	-2.01	1.39	1.43
32	B5	578	OMU	C5-C4	-2.01	1.39	1.43

All (168) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	B5	1191	XSX	C3-C1-N3	18.82	145.05	112.16
32	B5	1773	4AC	N4-C4-N3	9.43	129.18	113.87
36	A1	2634	UR3	C4-N3-C2	-7.12	118.85	124.58
32	B5	1773	4AC	C5-C4-N4	-6.04	112.76	122.94
32	B5	1781	MA6	C2-N1-C6	5.70	122.43	116.84
32	B5	1782	MA6	C2-N1-C6	5.56	122.29	116.84
36	A1	2421	OMU	C4-N3-C2	-5.01	120.39	126.61
36	A1	2281	A2M	O4'-C1'-N9	5.01	115.38	108.75
36	A1	1888	OMU	C4-N3-C2	-5.00	120.40	126.61
32	B5	1191	XSX	C4-N3-C2	-4.91	118.89	124.66
36	A1	2921	OMU	C4-N3-C2	-4.90	120.52	126.61
32	B5	578	OMU	C4-N3-C2	-4.89	120.54	126.61
36	A1	898	OMU	C4-N3-C2	-4.89	120.55	126.61
36	A1	2417	OMU	C4-N3-C2	-4.85	120.60	126.61
36	A1	2724	OMU	C4-N3-C2	-4.78	120.68	126.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A1	2347	OMU	C4-N3-C2	-4.71	120.76	126.61
36	A1	2729	OMU	C4-N3-C2	-4.71	120.77	126.61
32	B5	1269	OMU	C4-N3-C2	-4.64	120.86	126.61
32	B5	1773	4AC	C6-C5-C4	4.57	122.51	117.00
36	A1	1888	OMU	N3-C2-N1	4.52	120.78	114.89
36	A1	2421	OMU	N3-C2-N1	4.31	120.50	114.89
36	A1	2921	OMU	N3-C2-N1	4.29	120.48	114.89
36	A1	2417	OMU	N3-C2-N1	4.27	120.45	114.89
36	A1	2729	OMU	N3-C2-N1	4.27	120.45	114.89
36	A1	898	OMU	N3-C2-N1	4.26	120.44	114.89
32	B5	1269	OMU	N3-C2-N1	4.24	120.42	114.89
36	A1	2281	A2M	C4'-O4'-C1'	-4.23	106.05	109.92
32	B5	578	OMU	N3-C2-N1	4.14	120.29	114.89
36	A1	2724	OMU	N3-C2-N1	4.11	120.24	114.89
36	A1	2347	OMU	N3-C2-N1	4.08	120.21	114.89
36	A1	2421	OMU	C5-C4-N3	4.06	120.49	114.80
36	A1	2347	OMU	C5-C4-N3	4.01	120.42	114.80
36	A1	2921	OMU	C5-C4-N3	4.00	120.40	114.80
36	A1	898	OMU	C5-C4-N3	3.96	120.34	114.80
36	A1	2220	A2M	N3-C2-N1	-3.95	123.31	128.67
36	A1	2870	5MC	C5-C6-N1	-3.95	119.03	123.31
36	A1	2724	OMU	C5-C4-N3	3.94	120.32	114.80
36	A1	2417	OMU	C5-C4-N3	3.94	120.32	114.80
36	A1	2729	OMU	C5-C4-N3	3.89	120.25	114.80
32	B5	1782	MA6	N3-C2-N1	-3.86	123.43	128.67
36	A1	1888	OMU	C5-C4-N3	3.86	120.20	114.80
36	A1	1133	A2M	N3-C2-N1	-3.85	123.45	128.67
32	B5	578	OMU	C5-C4-N3	3.83	120.17	114.80
32	B5	1575	G7M	O2'-C2'-C3'	3.83	124.08	111.82
32	B5	1269	OMU	C5-C4-N3	3.79	120.11	114.80
36	A1	649	A2M	N3-C2-N1	-3.78	123.55	128.67
36	A1	2946	A2M	N3-C2-N1	-3.75	123.58	128.67
36	A1	2281	A2M	N3-C2-N1	-3.74	123.59	128.67
36	A1	876	A2M	N3-C2-N1	-3.74	123.60	128.67
32	B5	796	A2M	N3-C2-N1	-3.70	123.66	128.67
36	A1	2640	A2M	N3-C2-N1	-3.69	123.66	128.67
36	A1	2256	A2M	N3-C2-N1	-3.69	123.66	128.67
32	B5	436	A2M	N3-C2-N1	-3.68	123.68	128.67
36	A1	1449	A2M	N3-C2-N1	-3.68	123.68	128.67
32	B5	1781	MA6	N3-C2-N1	-3.66	123.70	128.67
32	B5	100	A2M	N3-C2-N1	-3.66	123.71	128.67
36	A1	817	A2M	N3-C2-N1	-3.66	123.71	128.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	B5	420	A2M	N3-C2-N1	-3.64	123.73	128.67
32	B5	1575	G7M	O3'-C3'-C4'	3.64	121.53	111.08
32	B5	974	A2M	N3-C2-N1	-3.63	123.75	128.67
32	B5	619	A2M	N3-C2-N1	-3.61	123.77	128.67
36	A1	2280	A2M	N3-C2-N1	-3.61	123.77	128.67
32	B5	541	A2M	N3-C2-N1	-3.60	123.78	128.67
32	B5	28	A2M	N3-C2-N1	-3.58	123.81	128.67
32	B5	1280	4AC	N4-C4-N3	3.57	119.66	113.87
32	B5	1126	OMG	C8-N7-C5	3.49	108.48	102.55
32	B5	1782	MA6	C4-C5-N7	-3.40	105.74	109.34
36	A1	807	A2M	N3-C2-N1	-3.39	124.07	128.67
36	A1	2634	UR3	C5-C4-N3	3.25	119.32	115.04
36	A1	2724	OMU	O4-C4-C5	-3.25	119.56	125.16
36	A1	2417	OMU	O4-C4-C5	-3.14	119.75	125.16
32	B5	1781	MA6	C4-C5-N7	-3.10	106.06	109.34
36	A1	2421	OMU	O4-C4-C5	-3.09	119.83	125.16
32	B5	578	OMU	O4-C4-C5	-3.09	119.83	125.16
36	A1	2729	OMU	O4-C4-C5	-3.08	119.85	125.16
32	B5	1773	4AC	CM7-C7-N4	3.08	120.23	115.27
36	A1	2347	OMU	O4-C4-C5	-3.07	119.87	125.16
36	A1	2278	5MC	O2-C2-N3	-3.03	117.55	122.33
32	B5	1269	OMU	O4-C4-C5	-3.03	119.94	125.16
36	A1	898	OMU	O4-C4-C5	-2.97	120.04	125.16
32	B5	1572	OMG	CM2-O2'-C2'	-2.97	106.86	114.47
36	A1	2921	OMU	O4-C4-C5	-2.96	120.06	125.16
32	B5	1572	OMG	C8-N7-C5	2.96	107.59	102.55
36	A1	867	OMG	C8-N7-C5	2.95	107.58	102.55
36	A1	2278	5MC	C5-C6-N1	-2.93	120.13	123.31
32	B5	1773	4AC	C5-C4-N3	-2.90	118.06	122.60
36	A1	2793	OMG	C8-N7-C5	2.89	107.46	102.55
32	B5	562	OMG	C8-N7-C5	2.85	107.40	102.55
36	A1	645	1MA	C8-N7-C5	2.84	107.38	102.55
36	A1	2791	OMG	C8-N7-C5	2.83	107.38	102.55
36	A1	2278	5MC	C5-C4-N3	-2.83	118.85	121.75
32	B5	1271	OMG	C8-N7-C5	2.83	107.36	102.55
36	A1	805	OMG	C8-N7-C5	2.81	107.33	102.55
36	A1	2922	OMG	C8-N7-C5	2.81	107.33	102.55
32	B5	1773	4AC	C1'-N1-C2	2.80	124.63	118.44
36	A1	1437	OMC	O2-C2-N3	-2.80	117.92	122.33
36	A1	2619	OMG	C8-N7-C5	2.80	107.31	102.55
32	B5	796	A2M	C4-C5-N7	-2.79	106.39	109.34
32	B5	1428	OMG	C8-N7-C5	2.78	107.28	102.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A1	1888	OMU	O4-C4-C5	-2.78	120.37	125.16
32	B5	1191	XSX	C5-C4-N3	2.77	119.47	115.64
36	A1	1450	OMG	C8-N7-C5	2.76	107.25	102.55
36	A1	807	A2M	C4-C5-N7	-2.76	106.42	109.34
36	A1	2288	OMG	C8-N7-C5	2.71	107.16	102.55
32	B5	1269	OMU	C1'-N1-C2	2.71	122.46	117.59
36	A1	2815	OMG	C8-N7-C5	2.71	107.16	102.55
32	B5	619	A2M	C4-C5-N7	-2.71	106.48	109.34
36	A1	2946	A2M	O4'-C1'-N9	2.70	112.33	108.75
32	B5	436	A2M	C4-C5-N7	-2.68	106.50	109.34
36	A1	817	A2M	C4-C5-N7	-2.67	106.52	109.34
36	A1	2280	A2M	C4-C5-N7	-2.66	106.53	109.34
36	A1	1133	A2M	C4-C5-N7	-2.62	106.57	109.34
36	A1	2870	5MC	C5-C4-N3	-2.61	119.08	121.75
32	B5	420	A2M	C4-C5-N7	-2.60	106.59	109.34
36	A1	2946	A2M	C4-C5-N7	-2.59	106.60	109.34
36	A1	2256	A2M	C4-C5-N7	-2.57	106.62	109.34
32	B5	1575	G7M	CN7-N7-C8	-2.57	113.05	125.43
32	B5	100	A2M	C4-C5-N7	-2.57	106.62	109.34
36	A1	2347	OMU	C1'-N1-C2	2.57	122.20	117.59
36	A1	908	OMG	C8-N7-C5	2.55	106.89	102.55
36	A1	2142	1MA	C5-C6-N1	2.55	117.61	113.95
32	B5	974	A2M	C4-C5-N7	-2.55	106.64	109.34
36	A1	649	A2M	C4-C5-N7	-2.53	106.66	109.34
32	B5	28	A2M	C4-C5-N7	-2.51	106.69	109.34
36	A1	2142	1MA	C8-N7-C5	2.51	106.82	102.55
36	A1	2640	A2M	C4-C5-N7	-2.48	106.72	109.34
32	B5	578	OMU	O2-C2-N1	-2.47	119.58	122.80
32	B5	796	A2M	C2'-C1'-N9	-2.42	107.19	112.56
36	A1	2281	A2M	C2'-C1'-N9	-2.41	107.20	112.56
32	B5	541	A2M	C4-C5-N7	-2.41	106.79	109.34
36	A1	645	1MA	C5-C6-N1	2.40	117.40	113.95
36	A1	2220	A2M	C4-C5-N7	-2.40	106.80	109.34
36	A1	876	A2M	C4-C5-N7	-2.40	106.80	109.34
36	A1	1449	A2M	C4-C5-N7	-2.40	106.81	109.34
36	A1	2417	OMU	O2-C2-N1	-2.39	119.68	122.80
36	A1	2946	A2M	C2'-C1'-N9	-2.35	107.33	112.56
32	B5	1575	G7M	O4'-C1'-N9	2.32	111.83	108.75
32	B5	1280	4AC	C6-C5-C4	2.32	119.80	117.00
36	A1	2281	A2M	C4-C5-N7	-2.31	106.90	109.34
36	A1	2948	OMC	O2-C2-N3	-2.28	118.73	122.33
32	B5	1191	XSX	C1-N3-C4	2.19	121.34	117.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	B5	1773	4AC	C1'-N1-C6	-2.19	116.10	120.78
36	A1	2870	5MC	O2-C2-N3	-2.19	118.89	122.33
32	B5	1126	OMG	C5-C6-N1	2.17	118.20	114.07
36	A1	805	OMG	C5-C6-N1	2.17	118.20	114.07
36	A1	2337	OMC	O2-C2-N3	-2.17	118.92	122.33
36	A1	2421	OMU	O2-C2-N1	-2.14	120.01	122.80
36	A1	2724	OMU	O2-C2-N1	-2.14	120.01	122.80
32	B5	1572	OMG	C5-C6-N1	2.13	118.13	114.07
36	A1	2791	OMG	C5-C6-N1	2.11	118.09	114.07
36	A1	2815	OMG	C5-C6-N1	2.10	118.08	114.07
36	A1	2793	OMG	C5-C6-N1	2.09	118.06	114.07
36	A1	1888	OMU	O2-C2-N1	-2.09	120.08	122.80
32	B5	1781	MA6	N1-C6-N6	2.07	119.22	116.83
36	A1	2724	OMU	C1'-N1-C2	2.07	121.31	117.59
32	B5	1191	XSX	C6-N1-C2	-2.06	120.12	121.80
36	A1	2619	OMG	C5-C6-N1	2.06	118.00	114.07
79	DC	699	DDE	CAU-CBW-CBI	-2.04	107.22	111.22
36	A1	807	A2M	O4'-C1'-N9	2.04	111.45	108.75
32	B5	1271	OMG	C5-C6-N1	2.04	117.96	114.07
36	A1	807	A2M	C4'-O4'-C1'	-2.04	108.06	109.92
32	B5	1428	OMG	C5-C6-N1	2.03	117.95	114.07
36	A1	867	OMG	C5-C6-N1	2.03	117.94	114.07
32	B5	414	OMC	O2-C2-N3	-2.03	119.13	122.33
32	B5	562	OMG	C5-C6-N1	2.02	117.93	114.07
36	A1	908	OMG	C5-C6-N1	2.02	117.93	114.07
36	A1	1133	A2M	C2'-C1'-N9	-2.02	108.08	112.56
36	A1	1437	OMC	C1'-N1-C2	2.01	122.87	118.44

There are no chirality outliers.

All (82) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	B5	414	OMC	C1'-C2'-O2'-CM2
32	B5	420	A2M	C1'-C2'-O2'-CM'
32	B5	562	OMG	C1'-C2'-O2'-CM2
32	B5	1191	XSX	C3-C1-N3-C2
32	B5	1191	XSX	C3-C1-N3-C4
32	B5	1191	XSX	N4-C7-C9-O11
32	B5	1269	OMU	O4'-C1'-N1-C2
32	B5	1269	OMU	O4'-C1'-N1-C6
32	B5	1271	OMG	C1'-C2'-O2'-CM2
34	AB	243	HIC	CA-CB-CG-ND1

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Mol	Chain	Res	Type	Atoms
79	DC	699	DDE	O-C-CA-CB
79	DC	699	DDE	CAU-CAT-CE1-NE2
79	DC	699	DDE	CBI-CBW-NCB-CAB
79	DC	699	DDE	CBI-CBW-NCB-CAC
79	DC	699	DDE	CBI-CBW-NCB-CAA
79	DC	699	DDE	CAU-CBW-NCB-CAB
79	DC	699	DDE	CAU-CBW-NCB-CAC
79	DC	699	DDE	CAU-CBW-NCB-CAA
32	B5	1280	4AC	N3-C4-N4-C7
32	B5	1280	4AC	C5-C4-N4-C7
32	B5	1280	4AC	O7-C7-N4-C4
32	B5	1280	4AC	CM7-C7-N4-C4
32	B5	1773	4AC	N3-C4-N4-C7
36	A1	663	OMC	C1'-C2'-O2'-CM2
36	A1	1437	OMC	C1'-C2'-O2'-CM2
36	A1	2197	OMC	C2'-C1'-N1-C2
36	A1	2197	OMC	C2'-C1'-N1-C6
36	A1	2220	A2M	C1'-C2'-O2'-CM'
36	A1	2337	OMC	C1'-C2'-O2'-CM2
36	A1	2421	OMU	C1'-C2'-O2'-CM2
36	A1	2619	OMG	C1'-C2'-O2'-CM2
36	A1	2724	OMU	C1'-C2'-O2'-CM2
36	A1	2729	OMU	O4'-C4'-C5'-O5'
36	A1	2791	OMG	C1'-C2'-O2'-CM2
32	B5	1572	OMG	C3'-C4'-C5'-O5'
32	B5	1782	MA6	O4'-C4'-C5'-O5'
36	A1	2197	OMC	O4'-C4'-C5'-O5'
36	A1	2280	A2M	C3'-C4'-C5'-O5'
36	A1	2729	OMU	C3'-C4'-C5'-O5'
32	B5	1191	XSX	N4-C7-C9-O10
32	B5	541	A2M	O4'-C4'-C5'-O5'
32	B5	1572	OMG	O4'-C4'-C5'-O5'
36	A1	1437	OMC	C3'-C4'-C5'-O5'
36	A1	1437	OMC	O4'-C4'-C5'-O5'
36	A1	2197	OMC	C3'-C4'-C5'-O5'
36	A1	2280	A2M	O4'-C4'-C5'-O5'
32	B5	541	A2M	C3'-C4'-C5'-O5'
32	B5	619	A2M	C3'-C4'-C5'-O5'
32	B5	619	A2M	O4'-C4'-C5'-O5'
32	B5	1782	MA6	C3'-C4'-C5'-O5'
36	A1	2870	5MC	C2'-C1'-N1-C6
32	B5	1428	OMG	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
36	A1	2281	A2M	O4'-C4'-C5'-O5'
32	B5	541	A2M	C4'-C5'-O5'-P
36	A1	2256	A2M	O4'-C4'-C5'-O5'
36	A1	2256	A2M	C3'-C4'-C5'-O5'
36	A1	2281	A2M	C3'-C4'-C5'-O5'
32	B5	1773	4AC	O7-C7-N4-C4
32	B5	1773	4AC	CM7-C7-N4-C4
36	A1	2729	OMU	C1'-C2'-O2'-CM2
36	A1	817	A2M	C4'-C5'-O5'-P
36	A1	2870	5MC	O4'-C1'-N1-C6
34	AB	243	HIC	CA-CB-CG-CD2
32	B5	1191	XSX	C3-C7-C9-O11
36	A1	2870	5MC	O4'-C1'-N1-C2
36	A1	2922	OMG	C3'-C2'-O2'-CM2
36	A1	2197	OMC	O4'-C1'-N1-C6
36	A1	2870	5MC	C2'-C1'-N1-C2
36	A1	2793	OMG	C3'-C2'-O2'-CM2
32	B5	1428	OMG	C4'-C5'-O5'-P
36	A1	2256	A2M	C4'-C5'-O5'-P
36	A1	1888	OMU	C3'-C2'-O2'-CM2
36	A1	2197	OMC	O4'-C1'-N1-C2
32	B5	1269	OMU	O4'-C4'-C5'-O5'
36	A1	2417	OMU	O4'-C4'-C5'-O5'
32	B5	1773	4AC	C5-C4-N4-C7
32	B5	1191	XSX	C3-C7-C9-O10
36	A1	2278	5MC	O4'-C4'-C5'-O5'
36	A1	1450	OMG	C4'-C5'-O5'-P
32	B5	1126	OMG	C4'-C5'-O5'-P
32	B5	1269	OMU	C4'-C5'-O5'-P
36	A1	1437	OMC	C2'-C1'-N1-C2

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 257 ligands modelled in this entry, 256 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
85	GDP	DC	901	-	25,30,30	0.94	1 (4%)	30,47,47	1.08	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	GDP	DC	901	-	-	2/12/32/32	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
85	DC	901	GDP	C6-N1	-2.28	1.34	1.37

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
85	DC	901	GDP	C8-N7-C5	2.92	107.52	102.55
85	DC	901	GDP	C5-C6-N1	2.01	117.89	114.07

There are no chirality outliers.

All (2) torsion outliers are listed below:

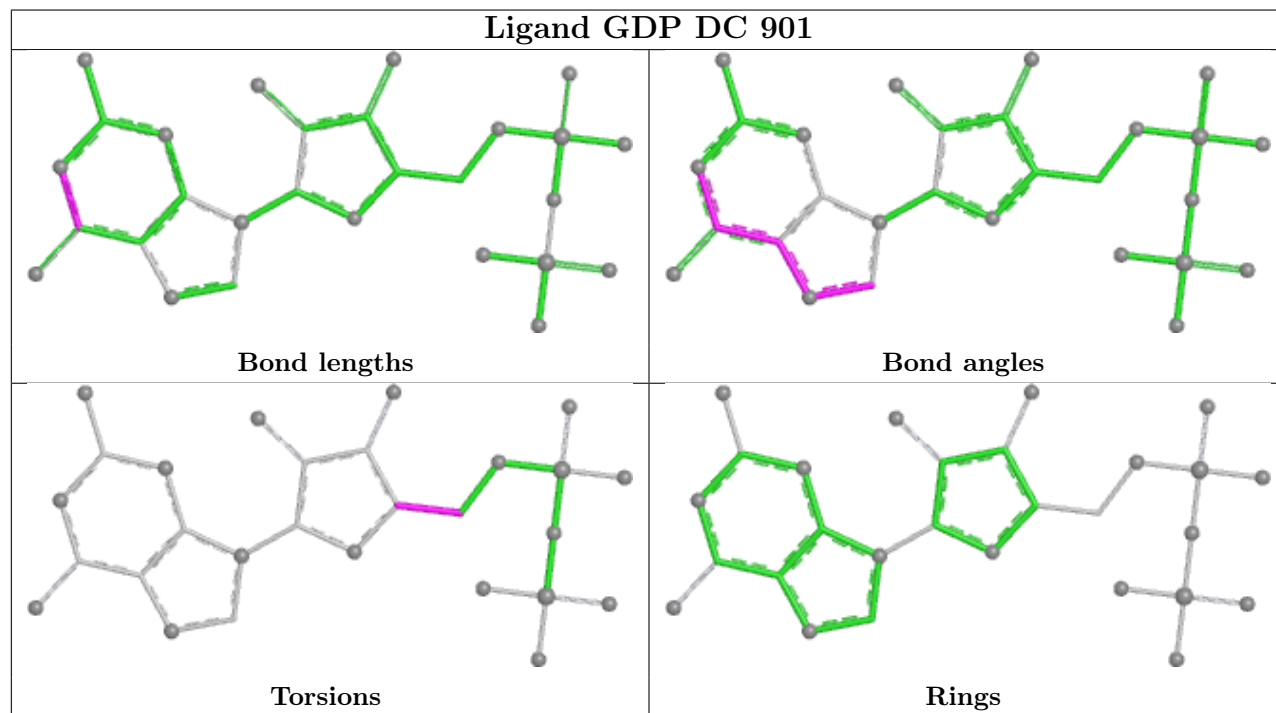
Mol	Chain	Res	Type	Atoms
85	DC	901	GDP	C3'-C4'-C5'-O5'
85	DC	901	GDP	O4'-C4'-C5'-O5'

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](#)

There are no chain breaks in this entry.

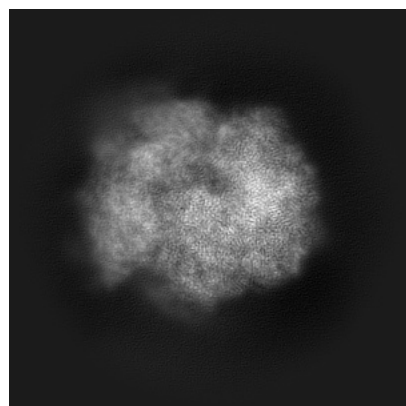
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-28610. These allow visual inspection of the internal detail of the map and identification of artifacts.

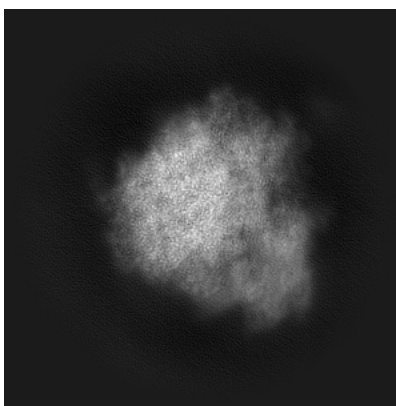
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

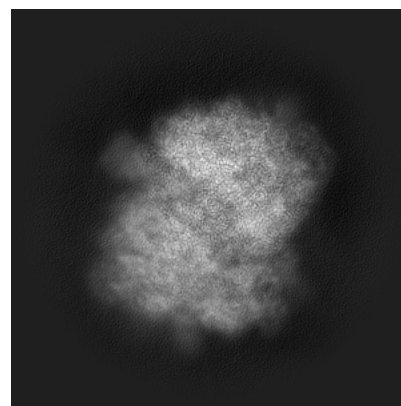
6.1.1 Primary map



X

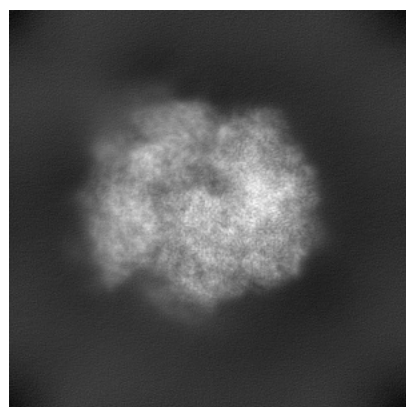


Y

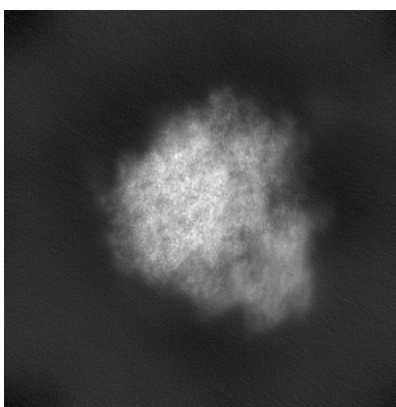


Z

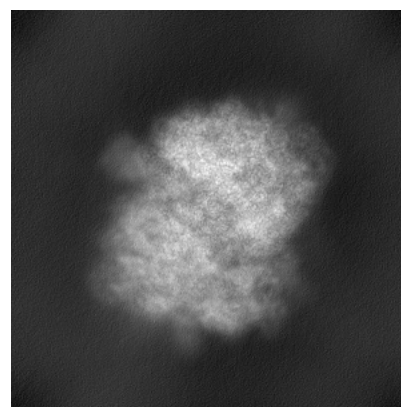
6.1.2 Raw map



X



Y

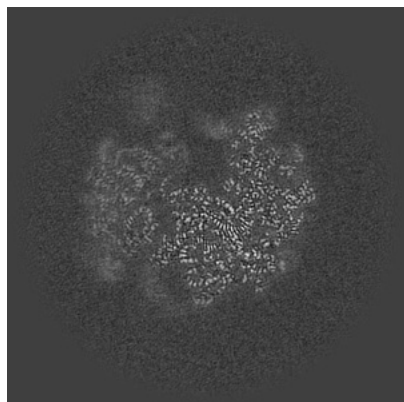


Z

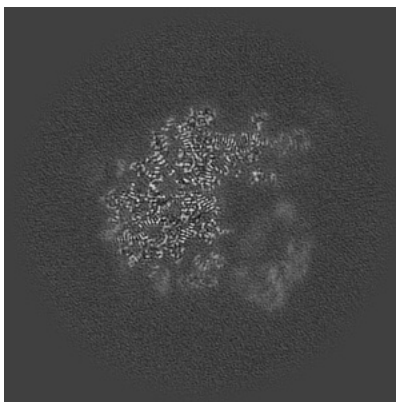
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

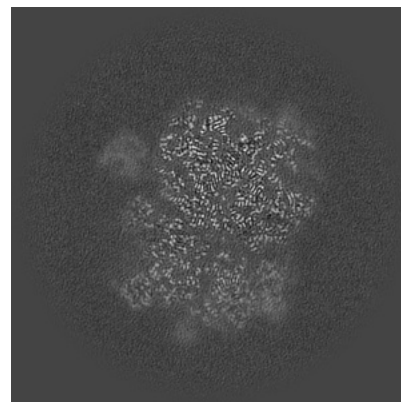
6.2.1 Primary map



X Index: 200

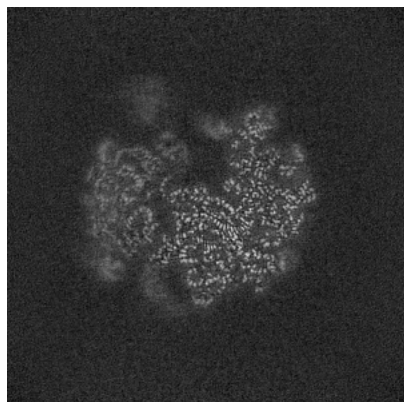


Y Index: 200

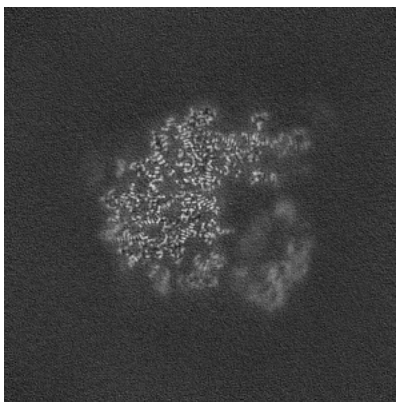


Z Index: 200

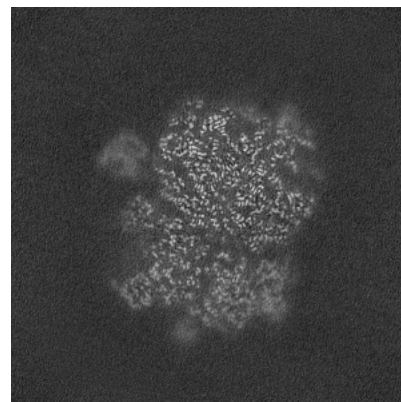
6.2.2 Raw map



X Index: 200



Y Index: 200

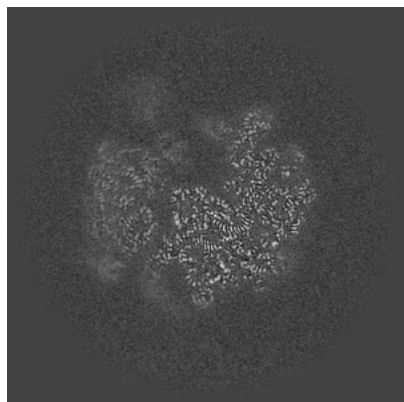


Z Index: 200

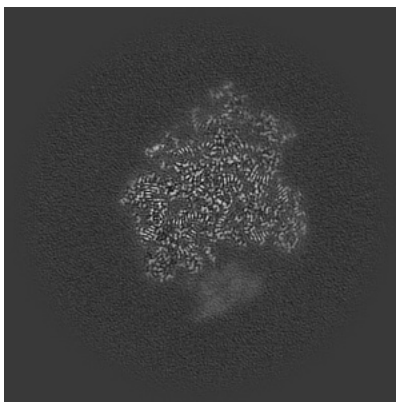
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

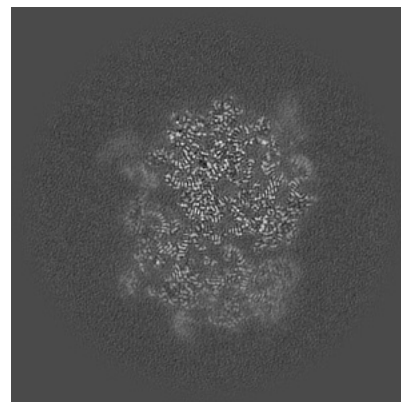
6.3.1 Primary map



X Index: 201

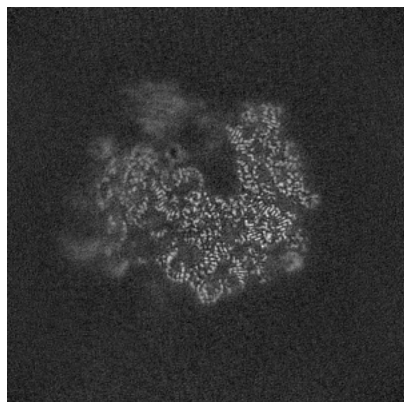


Y Index: 246

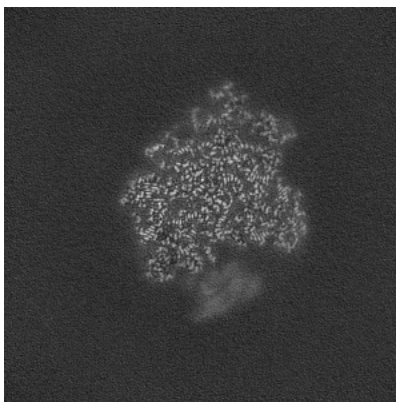


Z Index: 190

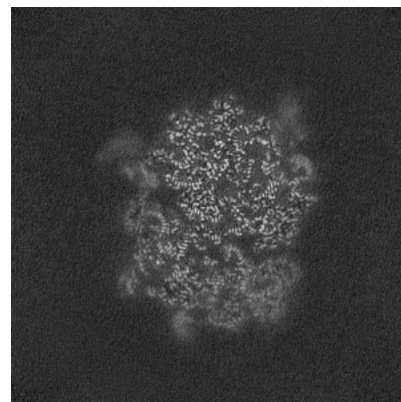
6.3.2 Raw map



X Index: 186



Y Index: 246

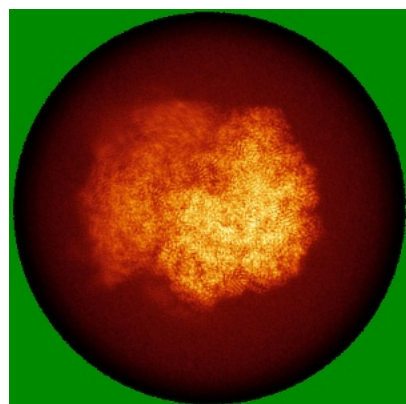


Z Index: 190

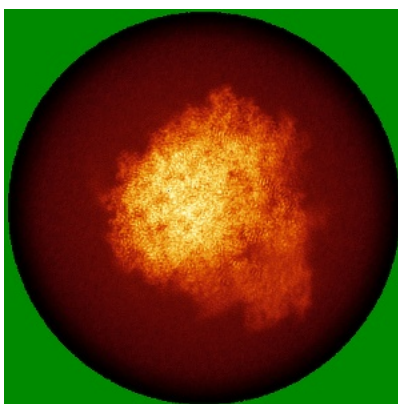
The images above show the largest variance slices of the map in three orthogonal directions.

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

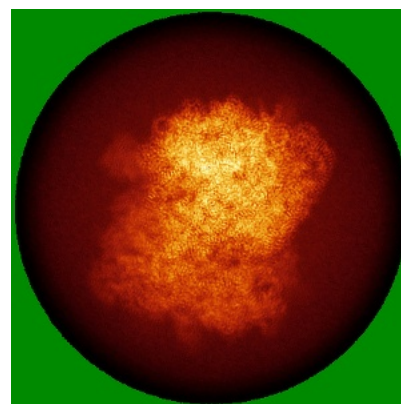
6.4.1 Primary map



X

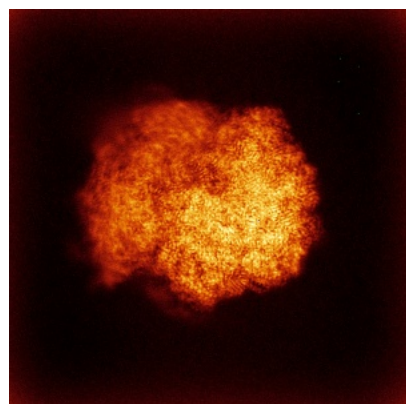


Y

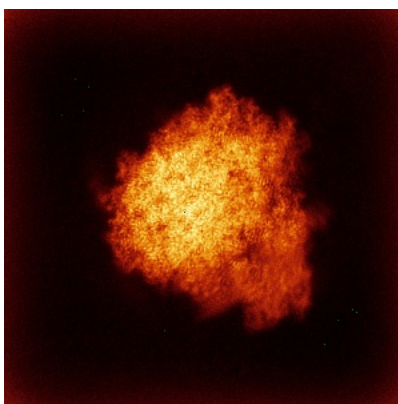


Z

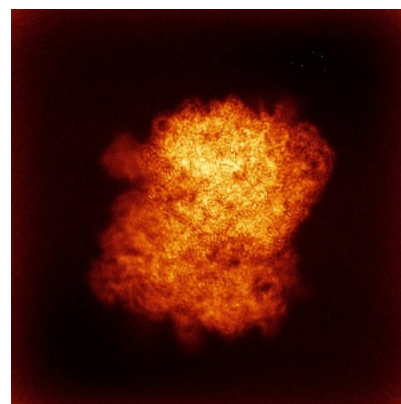
6.4.2 Raw map



X



Y

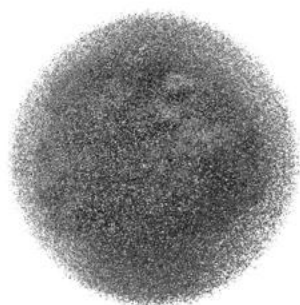


Z

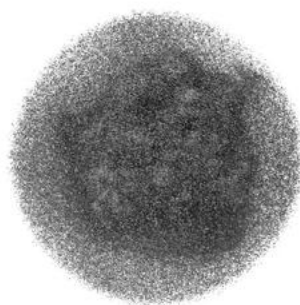
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

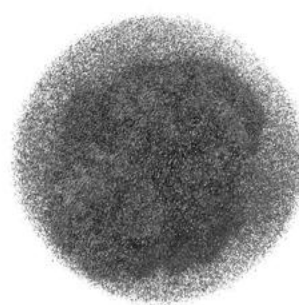
6.5.1 Primary map



X



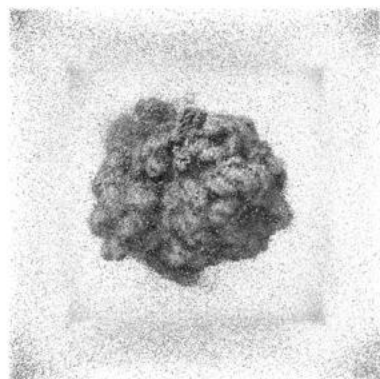
Y



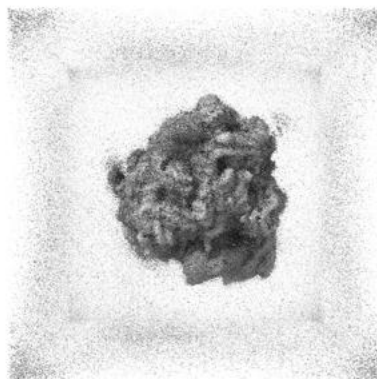
Z

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.

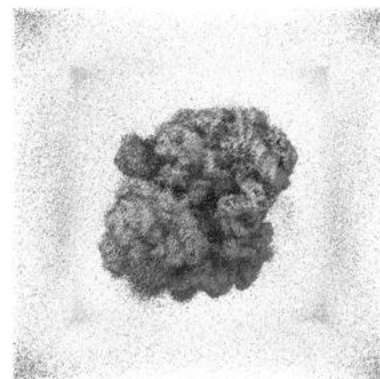
6.5.2 Raw map



X



Y



Z

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.

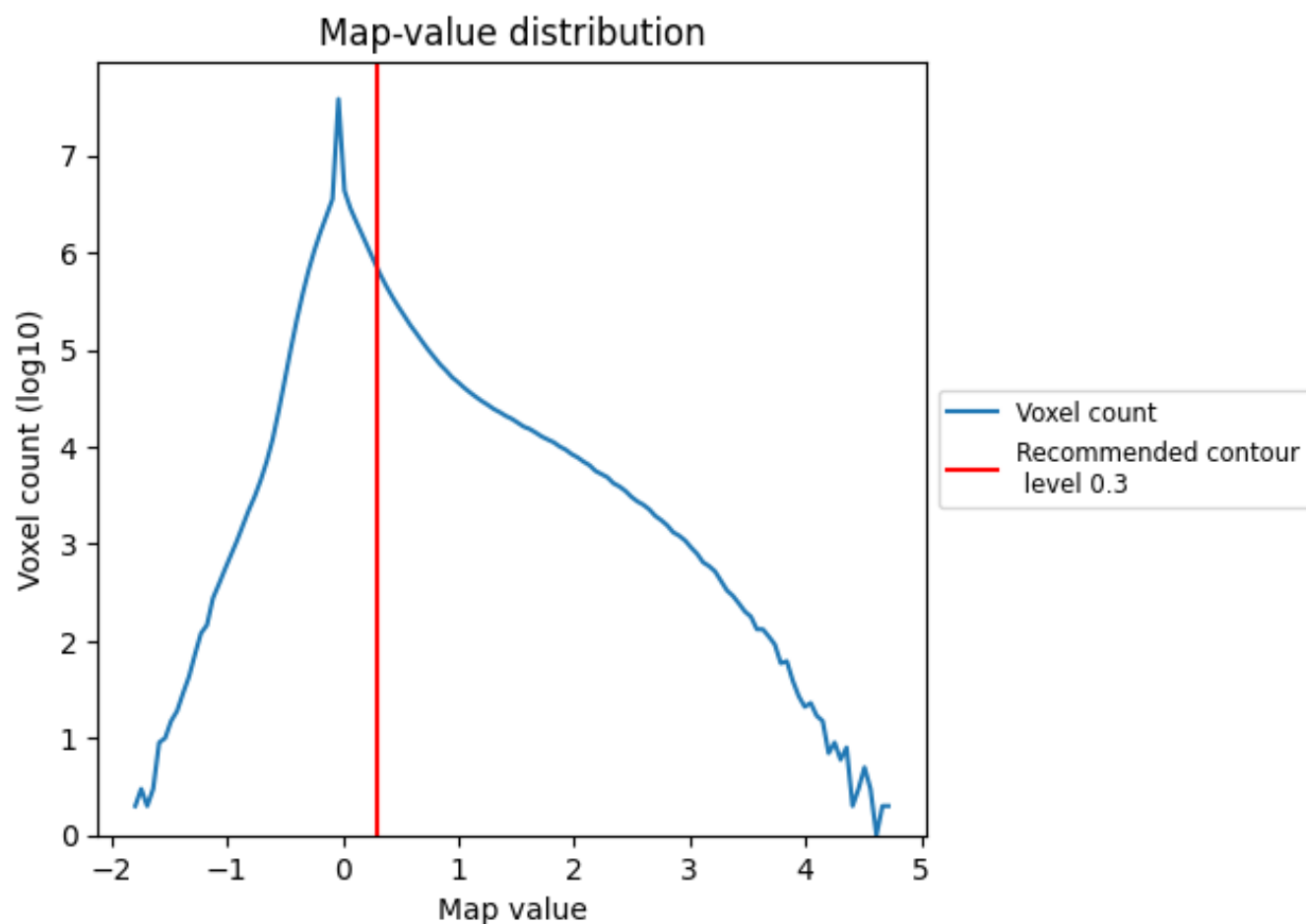
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

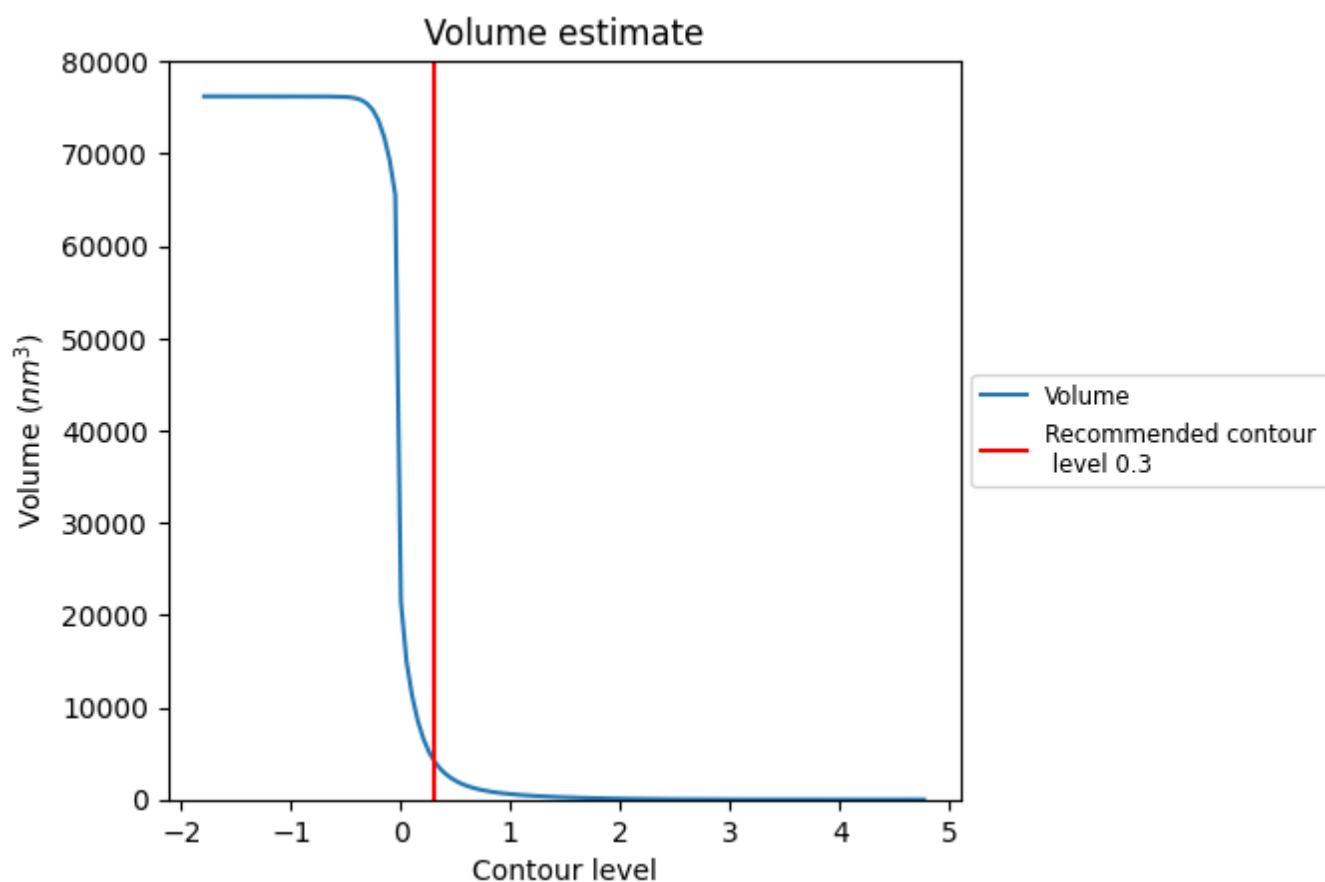
This section contains the results of statistical analysis of the map.

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.

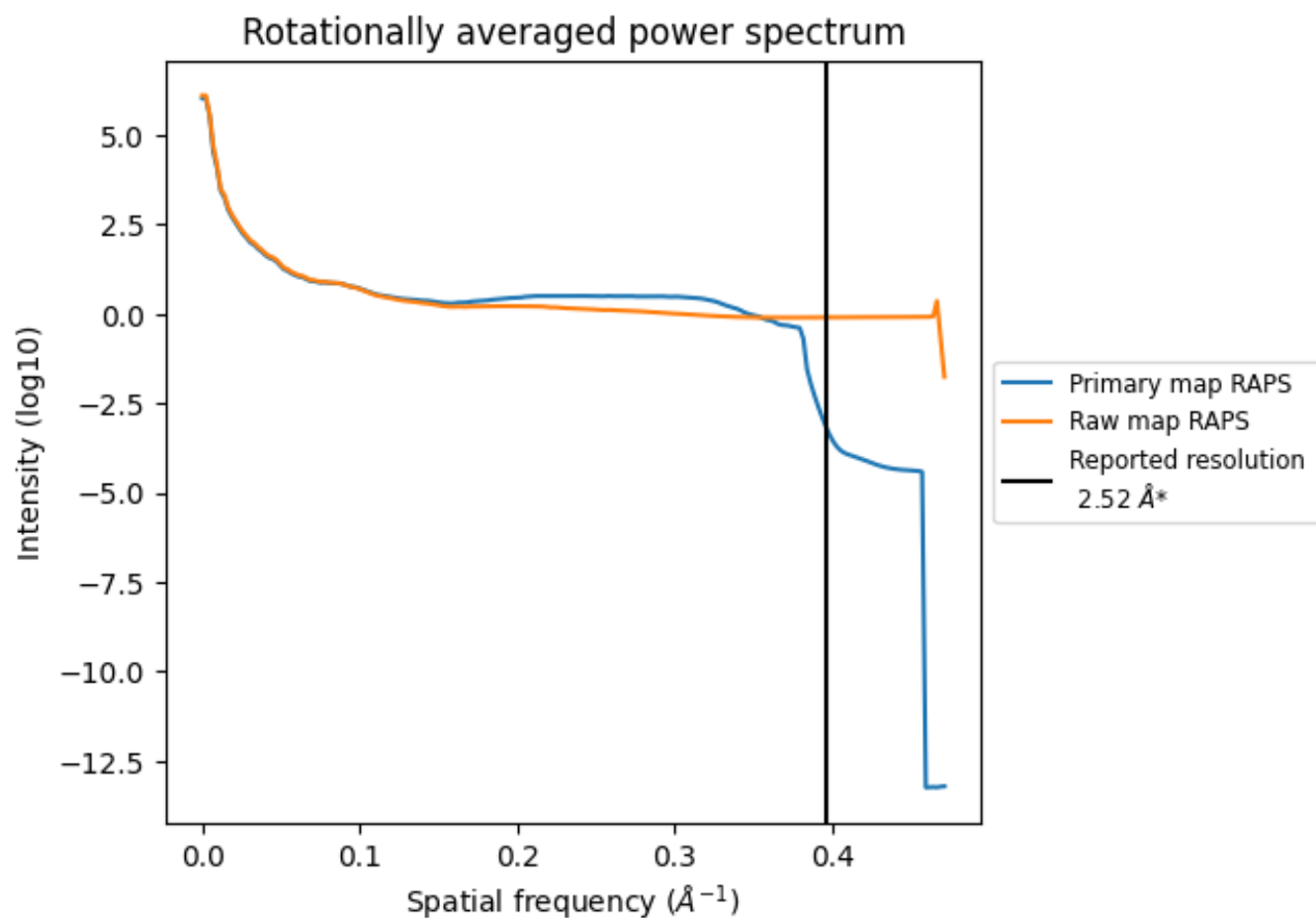
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 4289 nm^3 ; this corresponds to an approximate mass of 3874 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

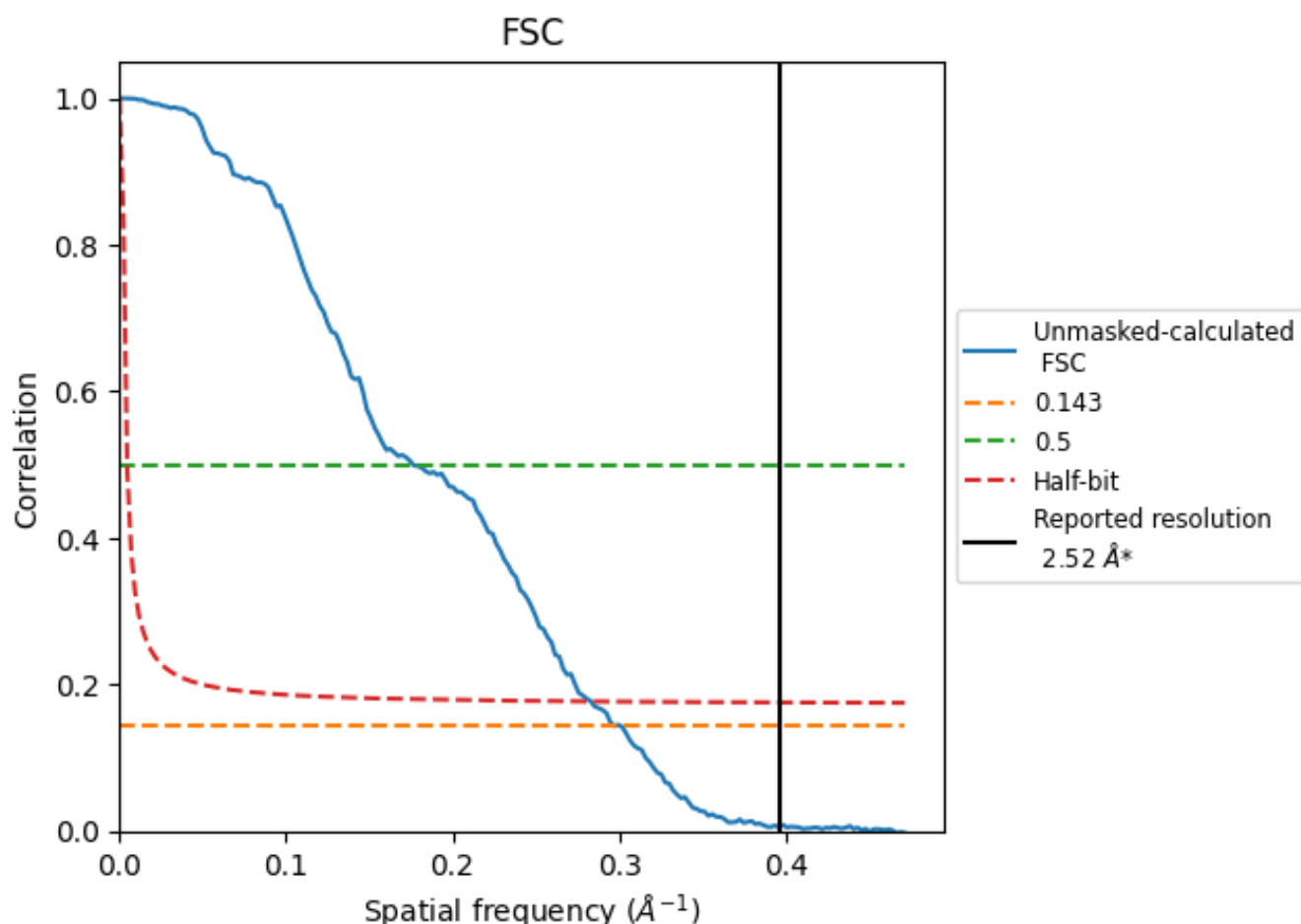


*Reported resolution corresponds to spatial frequency of 0.397 Å⁻¹

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 0.397 Å⁻¹

8.2 Resolution estimates [i](#)

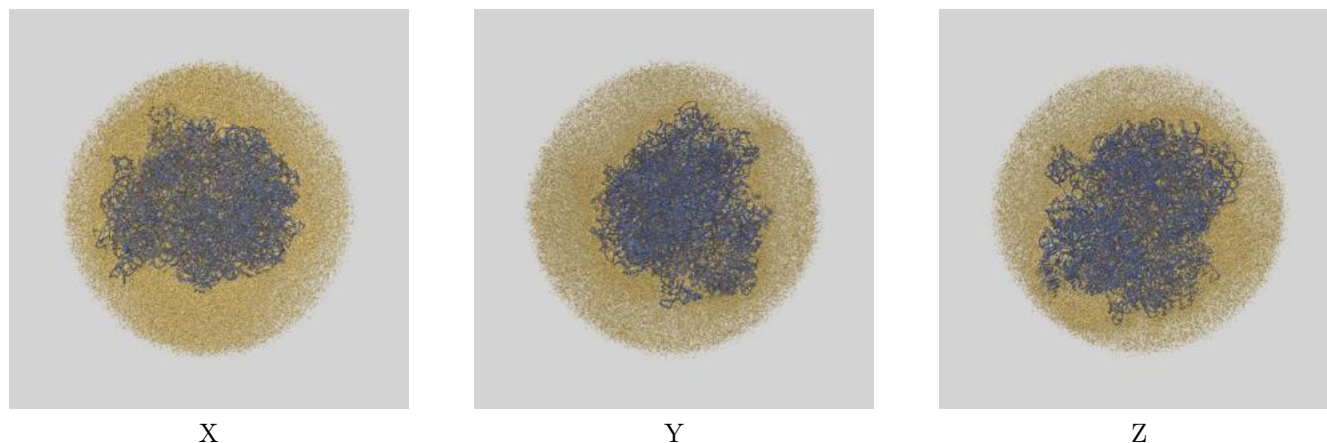
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.52	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.37	5.67	3.53

*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 3.37 differs from the reported value 2.52 by more than 10 %

9 Map-model fit [i](#)

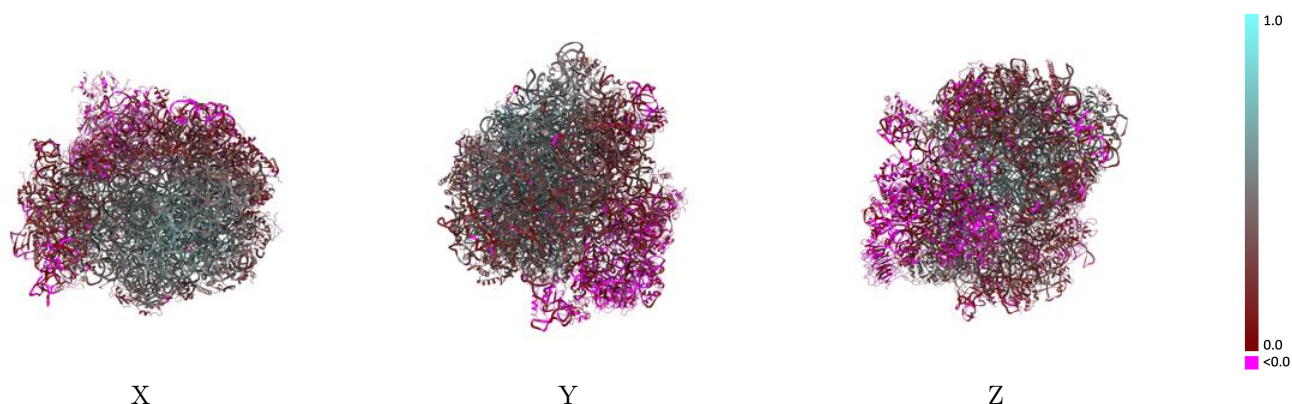
This section contains information regarding the fit between EMDB map EMD-28610 and PDB model 8EUB. Per-residue inclusion information can be found in section [3](#) on page [20](#).

9.1 Map-model overlay [i](#)



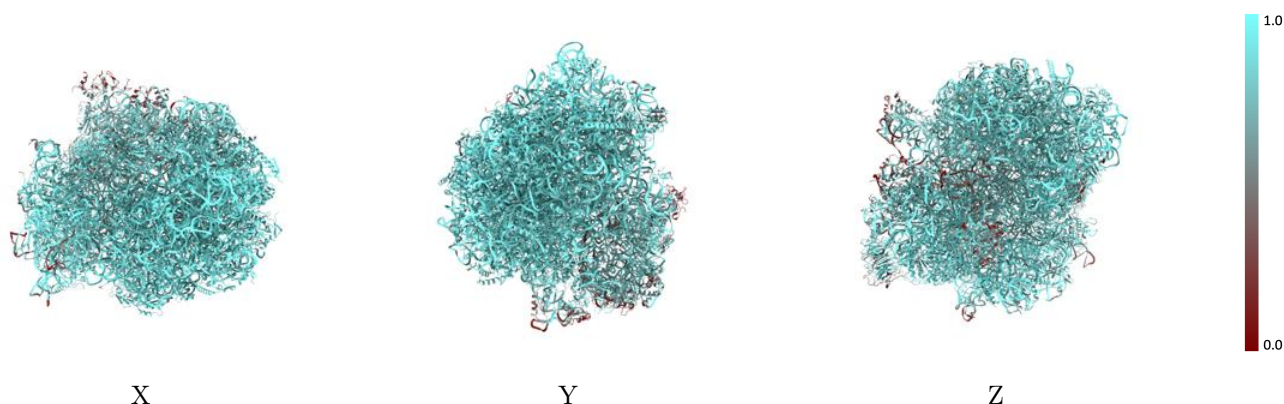
The images above show the 3D surface view of the map at the recommended contour level 0.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



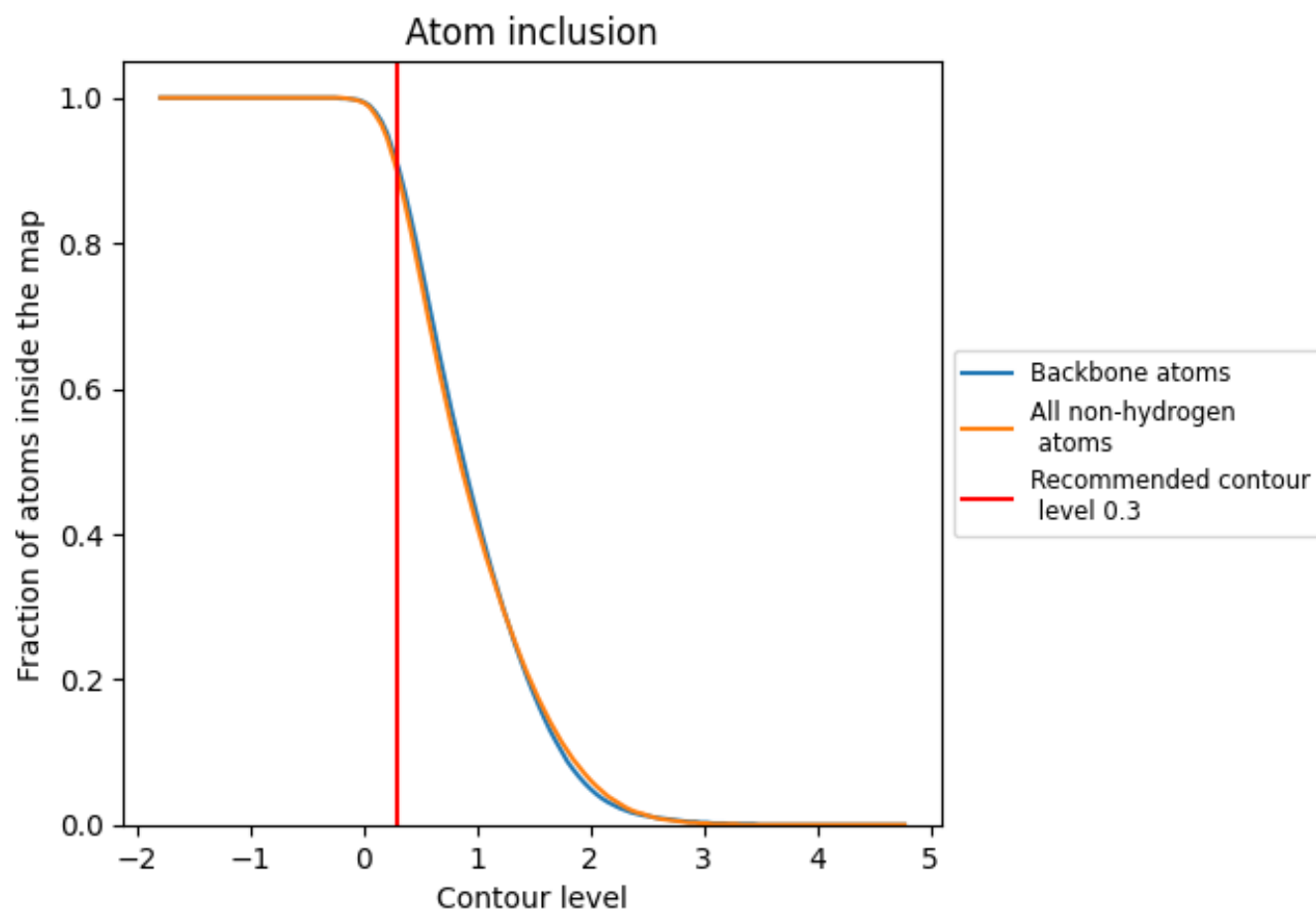
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 91% of all backbone atoms, 90% 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	 0.8960	 0.3190
A1	 0.9640	 0.4260
A3	 0.9010	 0.2260
A4	 0.9740	 0.4720
AA	 0.9870	 0.5900
AB	 0.9600	 0.4800
AC	 0.9080	 0.3380
AD	 0.7540	 0.0920
AE	 0.9300	 0.3710
AF	 0.8930	 0.2610
AG	 0.8840	 0.3370
AH	 0.8490	 0.2560
AI	 0.8640	 0.2530
AJ	 0.7480	 0.1020
AL	 0.8820	 0.2630
AM	 0.8750	 0.2830
AN	 0.9560	 0.4520
AO	 0.9580	 0.4650
AP	 0.9840	 0.5890
AQ	 0.8770	 0.2750
AR	 0.9110	 0.4220
AS	 0.8470	 0.2250
AT	 0.8610	 0.2410
AU	 0.8730	 0.2700
AV	 0.9350	 0.4410
AW	 0.9510	 0.4180
AX	 0.9190	 0.3810
AY	 0.9270	 0.3720
AZ	 0.9190	 0.3610
Aa	 0.8850	 0.3200
Ab	 0.8830	 0.2320
Ac	 0.9450	 0.4620
Ad	 0.9490	 0.4800
Ae	 0.9750	 0.4920
Af	 0.9790	 0.5020















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Chain	Atom inclusion	Q-score
Ag	 0.9580	 0.4780
Ah	 0.8940	 0.3110
Ai	 0.8910	 0.2990
Aj	 0.9800	 0.5260
Ak	 0.8360	 0.2890
Al	 0.9810	 0.5460
Am	 0.8960	 0.3090
An	 0.9670	 0.4900
Ao	 0.8960	 0.3540
Ap	 0.9760	 0.5740
B5	 0.9140	 0.2600
BA	 0.9550	 0.4160
BB	 0.9180	 0.4220
BC	 0.9390	 0.3920
BD	 0.7680	 0.0650
BE	 0.9050	 0.2300
BF	 0.6140	 -0.0070
BG	 0.8730	 0.1930
BH	 0.8650	 0.3080
BI	 0.9050	 0.3060
BJ	 0.8930	 0.2510
BK	 0.7550	 0.0320
BL	 0.8870	 0.3650
BM	 0.3970	 0.0290
BN	 0.9510	 0.4650
BO	 0.9510	 0.4430
BP	 0.5560	 -0.0090
BQ	 0.7070	 -0.0180
BR	 0.7360	 0.1220
BS	 0.5970	 -0.0140
BT	 0.7040	 -0.0060
BU	 0.8440	 0.0780
BV	 0.9410	 0.3980
BW	 0.9640	 0.4410
BX	 0.9300	 0.3930
BY	 0.8640	 0.1710
BZ	 0.5240	 -0.0250
Ba	 0.9490	 0.4860
Bb	 0.9180	 0.4140
Bc	 0.6060	 0.0420
Bd	 0.8940	 0.0820
Be	 0.8500	 0.2190

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Chain	Atom inclusion	Q-score
Bf	 0.3450	 0.0010
Bg	 0.7110	 -0.0050
DC	 0.7690	 0.1330
E	 0.5780	 0.0160
EC	 0.6050	 0.0380
VA	 0.6510	 0.1170