



Full wwPDB EM Validation Report ⓘ

Oct 12, 2024 – 11:35 AM EDT

PDB ID : 6OLZ
EMDB ID : EMD-0598
Title : Human ribosome nascent chain complex (PCSK9-RNC) stalled by a drug-like molecule with PP tRNA
Authors : Li, W.; Cate, J.H.D.
Deposited on : 2019-04-17
Resolution : 3.90 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) : 2.39

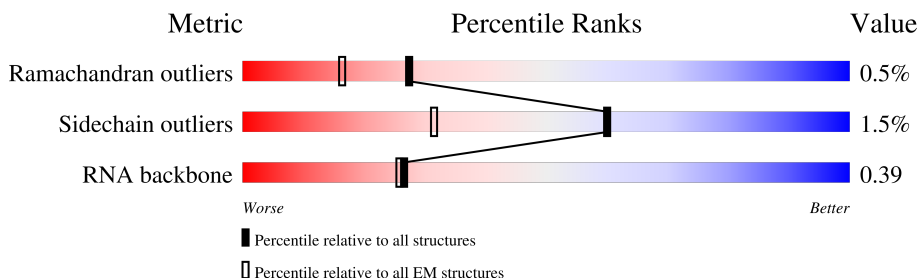
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.90 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	AA	248	
2	BA	215	
3	AB	394	
4	BB	212	
5	AC	363	
6	BC	222	
7	A3	157	
8	A4	119	

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Mol	Chain	Length	Quality of chain
9	AD	294	19% 97% .
10	AE	247	21% 88% 9%
11	AF	234	9% 97% .
12	AG	234	26% 99% .
13	AH	191	19% 99% .
14	AI	211	17% 95% ..
15	AJ	169	30% 99% .
16	AL	205	19% 95% .
17	AM	139	12% 99% .
18	AN	203	5% 98% .
19	AO	195	9% 97% .
20	AP	153	5% 100% .
21	AQ	187	13% 99% .
22	AR	181	17% 98% .
23	AS	175	8% 99% .
24	AT	157	13% 99% .
25	AU	99	34% 99% .
26	AV	129	11% 99% .
27	AW	121	55% 98% .
28	AX	117	10% 100% .
29	AY	127	7% 98% .
30	AZ	134	15% 99% .
31	Aa	147	10% 99% .
32	Ab	118	27% 76% 5% 18%
33	Ac	103	20% 98% .

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Mol	Chain	Length	Quality of chain
34	Ad	106	
35	Ae	129	
36	Af	109	
37	Ag	114	
38	Ah	122	
39	Ai	97	
40	Aj	84	
41	Ak	69	
42	Al	50	
43	Am	50	
44	An	25	
45	Ao	105	
46	Ap	91	
47	At	122	
48	A2	3643	
49	B1	1708	
50	BD	220	
51	BE	257	
52	BF	190	
53	BG	232	
54	BH	183	
55	BI	207	
56	BJ	179	
57	BK	98	
58	BL	153	

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Mol	Chain	Length	Quality of chain
59	BM	120	99% 98% .
60	BN	149	37% 99% .
61	BO	136	31% 99% .
62	BP	120	67% 97% .
63	BQ	139	68% 100% .
64	BR	125	68% 98% .
65	BS	139	65% 96% .
66	BT	143	69% 97% .
67	BU	97	70% 100% .
68	BV	81	41% 98% ..
69	BW	129	26% 98% .
70	BX	139	30% 99% .
71	BY	125	46% 98% .
72	BZ	86	72% 95% 5%
73	Ba	97	32% 99% .
74	Bb	80	41% 99% .
75	Bc	62	73% 97% .
76	Bd	51	59% 98% .
77	Be	55	47% 93% 7%
78	Bf	73	93% 99% .
79	Bg	314	92% 99% .
80	Bv	76	91% 58% 39% .
81	Bx	16	88% 44% 56% .
82	A	26	92% 81% 19% .

2 Entry composition

There are 85 unique types of molecules in this entry. The entry contains 214215 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 60S ribosomal protein L8.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	AA	248	Total	C	N	O	S	0	0
			1898	1189	389	314	6		

- Molecule 2 is a protein called 40S ribosomal protein SA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	BA	215	Total	C	N	O	S	0	0
			1704	1083	298	315	8		

- Molecule 3 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	AB	394	Total	C	N	O	S	0	0
			3178	2024	596	544	14		

- Molecule 4 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	BB	212	Total	C	N	O	S	0	0
			1722	1093	308	307	14		

- Molecule 5 is a protein called 60S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	AC	363	Total	C	N	O	S	0	0
			2888	1817	577	480	14		

- Molecule 6 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	BC	222	Total	C	N	O	S	0	0
			1724	1114	296	304	10		

- Molecule 7 is a RNA chain called 5.8S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	A3	157	Total	C	N	O	P	0	0
			3337	1489	587	1104	157		

- Molecule 8 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	A4	119	Total	C	N	O	P	0	0
			2541	1132	454	836	119		

- Molecule 9 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	AD	294	Total	C	N	O	S	0	0
			2392	1510	436	432	14		

- Molecule 10 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	AE	226	Total	C	N	O	S	0	0
			1838	1180	350	304	4		

- Molecule 11 is a protein called 60S ribosomal protein L7.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	AF	234	Total	C	N	O	S	0	0
			1950	1252	376	313	9		

- Molecule 12 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	AG	234	Total	C	N	O	S	0	0
			1880	1197	362	317	4		

- Molecule 13 is a protein called 60S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	AH	191	Total	C	N	O	S	0	0
			1526	960	285	275	6		

- Molecule 14 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	AI	208	Total	C	N	O	S	0	0
			1692	1074	327	278	13		

- Molecule 15 is a protein called 60S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	AJ	169	Total	C	N	O	S	0	0
			1353	855	252	240	6		

- Molecule 16 is a protein called 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	AL	205	Total	C	N	O	S	0	0
			1657	1036	344	273	4		

- Molecule 17 is a protein called 60S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	AM	139	Total	C	N	O	S	0	0
			1138	730	218	183	7		

- Molecule 18 is a protein called 60S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	AN	203	Total	C	N	O	S	0	0
			1701	1072	359	266	4		

- Molecule 19 is a protein called 60S ribosomal protein L13a.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	AO	195	Total	C	N	O	S	0	0
			1606	1034	315	252	5		

- Molecule 20 is a protein called 60S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	AP	153	Total	C	N	O	S	0	0
			1242	776	241	216	9		

- Molecule 21 is a protein called 60S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	AQ	187	Total	C	N	O	S	0	0
			1513	944	314	250	5		

- Molecule 22 is a protein called 60S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	AR	181	Total	C	N	O	S	0	0
			1517	938	329	241	9		

- Molecule 23 is a protein called 60S ribosomal protein L18a.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	AS	175	Total	C	N	O	S	0	0
			1449	921	283	234	11		

- Molecule 24 is a protein called 60S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	AT	157	Total	C	N	O	S	0	0
			1284	815	250	214	5		

- Molecule 25 is a protein called 60S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	AU	99	Total	C	N	O	S	0	0
			808	518	141	147	2		

- Molecule 26 is a protein called 60S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	AV	129	Total	C	N	O	S	0	0
			969	613	182	169	5		

- Molecule 27 is a protein called 60S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	AW	121	Total	C	N	O	S	0	0
			989	617	202	167	3		

- Molecule 28 is a protein called 60S ribosomal protein L23a.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	AX	117	Total	C	N	O	S	0	0
			958	612	180	165	1		

- Molecule 29 is a protein called 60S ribosomal protein L26.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	AY	127	Total	C	N	O	S	0	0
			1064	668	216	177	3		

- Molecule 30 is a protein called 60S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	AZ	134	Total	C	N	O	S	0	0
			1103	712	207	181	3		

- Molecule 31 is a protein called 60S ribosomal protein L27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Aa	147	Total	C	N	O	S	0	0
			1162	736	237	186	3		

- Molecule 32 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Ab	97	Total	C	N	O	S	0	0
			792	492	175	122	3		

- Molecule 33 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Ac	103	Total	C	N	O	S	0	0
			801	508	141	145	7		

- Molecule 34 is a protein called 60S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	Ad	106	Total	C	N	O	S	0	0
			879	555	170	152	2		

- Molecule 35 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	Ae	129	Total	C	N	O	S	0	0
			1064	673	220	166	5		

- Molecule 36 is a protein called 60S ribosomal protein L35a.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	Af	109	Total	C	N	O	S	0	0
			876	555	174	144	3		

- Molecule 37 is a protein called 60S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	Ag	114	Total	C	N	O	S	0	0
			906	566	187	147	6		

- Molecule 38 is a protein called 60S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	Ah	122	Total	C	N	O	S	0	0
			1015	641	205	168	1		

- Molecule 39 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	Ai	97	Total	C	N	O	S	0	0
			794	497	168	124	5		

- Molecule 40 is a protein called 60S ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	Aj	84	Total	C	N	O	S	0	0
			689	423	152	109	5		

- Molecule 41 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	Ak	69	Total	C	N	O	S	0	0
			569	366	103	99	1		

- Molecule 42 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	Al	50	Total	C	N	O	S	0	0
			444	281	98	64	1		

- Molecule 43 is a protein called 60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	Am	50	Total	C	N	O	S	0	0
			411	254	87	64	6		

- Molecule 44 is a protein called 60S ribosomal protein L41.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	An	25	Total	C	N	O	S	0	0
			240	145	64	28	3		

- Molecule 45 is a protein called 60S ribosomal protein L36a.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	Ao	105	Total	C	N	O	S	0	0
			863	542	175	140	6		

- Molecule 46 is a protein called 60S ribosomal protein L37a.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	Ap	91	Total	C	N	O	S	0	0
			708	445	136	120	7		

- Molecule 47 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	At	122	Total	C	N	O	S	0	0
			980	607	204	165	4		

- Molecule 48 is a RNA chain called 28S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	A2	3643	Total	C	N	O	P	0	0
			78102	34781	14290	25388	3643		

- Molecule 49 is a RNA chain called 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	B1	1708	Total	C	N	O	P	0	0
			36456	16274	6546	11928	1708		

- Molecule 50 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	BD	220	Total	C	N	O	S	0	0
			1709	1090	308	304	7		

- Molecule 51 is a protein called 40S ribosomal protein S4, Y isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	BE	257	Total	C	N	O	S	0	0
			2031	1298	381	344	8		

- Molecule 52 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	BF	190	Total	C	N	O	S	0	0
			1502	939	285	271	7		

- Molecule 53 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	BG	232	Total	C	N	O	S	0	0
			1884	1176	379	322	7		

- Molecule 54 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	BH	183	Total	C	N	O	S	0	0
			1479	941	272	265	1		

- Molecule 55 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	BI	207	Total	C	N	O	S	0	0
			1696	1064	334	293	5		

- Molecule 56 is a protein called 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	BJ	179	Total	C	N	O	S	0	0
			1495	953	299	241	2		

- Molecule 57 is a protein called 40S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	BK	98	Total	C	N	O	S	0	0
			827	539	148	134	6		

- Molecule 58 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	BL	153	Total	C	N	O	S	0	0
			1258	804	235	213	6		

- Molecule 59 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	BM	120	Total	C	N	O	S	0	0
			931	584	164	174	9		

- Molecule 60 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	BN	149	Total	C	N	O	S	0	0
			1202	770	228	203	1		

- Molecule 61 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	BO	136	Total	C	N	O	S	0	0
			1016	621	199	190	6		

- Molecule 62 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	BP	120	Total	C	N	O	S	0	0
			999	636	188	168	7		

- Molecule 63 is a protein called 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	BQ	139	Total	C	N	O	S	0	0
			1109	704	210	192	3		

- Molecule 64 is a protein called 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	BR	125	Total	C	N	O	S	0	0
			1011	634	187	186	4		

- Molecule 65 is a protein called 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	BS	139	Total	C	N	O	S	0	0
			1154	725	233	195	1		

- Molecule 66 is a protein called 40S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	BT	143	Total	C	N	O	S	0	0
			1112	697	214	198	3		

- Molecule 67 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	BU	97	Total	C	N	O	S	0	0
			769	483	144	138	4		

- Molecule 68 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	BV	81	Total	C	N	O	S	0	0
			617	380	114	118	5		

- Molecule 69 is a protein called 40S ribosomal protein S15a.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	BW	129	Total	C	N	O	S	0	0
			1034	659	193	176	6		

- Molecule 70 is a protein called 40S ribosomal protein S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	BX	139	Total	C	N	O	S	0	0
			1080	682	214	181	3		

- Molecule 71 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	BY	125	Total	C	N	O	S	0	0
			1015	642	199	169	5		

- Molecule 72 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	BZ	86	Total	C	N	O	S	0	0
			688	442	129	116	1		

- Molecule 73 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	Ba	97	Total	C	N	O	S	0	0
			774	481	160	128	5		

- Molecule 74 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	Bb	80	Total	C	N	O	S	0	0
			625	391	116	111	7		

- Molecule 75 is a protein called 40S ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	Bc	62	Total	C	N	O	S	0	0
			488	297	97	92	2		

- Molecule 76 is a protein called 40S ribosomal protein S29.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	Bd	51	Total	C	N	O	S	0	0
			427	269	87	66	5		

- Molecule 77 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	Be	55	Total	C	N	O	S	0	0
			437	272	96	68	1		

- Molecule 78 is a protein called Ubiquitin-40S ribosomal protein S27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	Bf	73	Total	C	N	O	S	0	0
			601	379	115	100	7		

- Molecule 79 is a protein called Receptor of activated protein C kinase 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	Bg	314	Total	C	N	O	S	0	0
			2440	1537	425	466	12		

- Molecule 80 is a RNA chain called tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	Bv	76	Total	C	N	O	P	0	0
			1623	723	290	534	76		

- Molecule 81 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	Bx	16	Total	C	N	O	P	0	0
			320	144	32	128	16		

- Molecule 82 is a protein called Proprotein convertase subtilisin/kexin type 9.

Mol	Chain	Residues	Atoms				AltConf	Trace
82	A	26	Total	C	N	O	0	0
			128	76	26	26		

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

Mol	Chain	Residues	Atoms		AltConf
83	AA	1	Total	Mg	0
			1	1	
83	AB	2	Total	Mg	0
			2	2	
83	BC	1	Total	Mg	0
			1	1	

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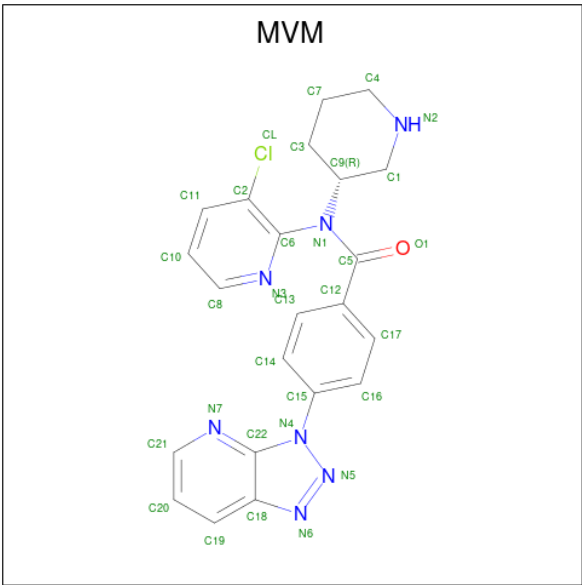
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Mol	Chain	Residues	Atoms		AltConf
83	A3	8	Total 8	Mg 8	0
83	A4	9	Total 9	Mg 9	0
83	AN	1	Total 1	Mg 1	0
83	AP	2	Total 2	Mg 2	0
83	Aa	2	Total 2	Mg 2	0
83	Ae	1	Total 1	Mg 1	0
83	Aj	1	Total 1	Mg 1	0
83	Al	1	Total 1	Mg 1	0
83	An	1	Total 1	Mg 1	0
83	A2	220	Total 220	Mg 220	0
83	B1	73	Total 73	Mg 73	0
83	BI	1	Total 1	Mg 1	0
83	Bv	2	Total 2	Mg 2	0

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

Mol	Chain	Residues	Atoms		AltConf
84	Aj	1	Total 1	Zn 1	0
84	Ao	1	Total 1	Zn 1	0
84	Ap	1	Total 1	Zn 1	0
84	Ba	1	Total 1	Zn 1	0
84	Bd	1	Total 1	Zn 1	0

- Molecule 85 is N-(3-chloropyridin-2-yl)-N-[(3R)-piperidin-3-yl]-4-(3H-[1,2,3]triazolo[4,5-b]pyridin-3-yl)benzamide (three-letter code: MVM) (formula: C₂₂H₂₀ClN₇O).

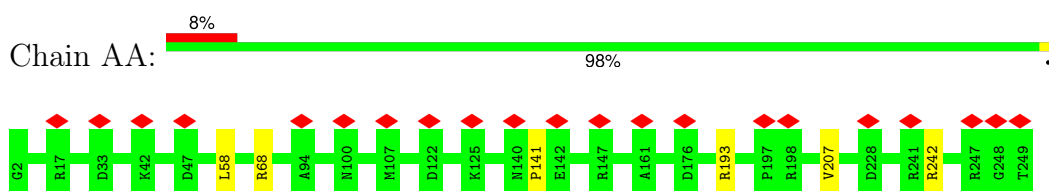


Mol	Chain	Residues	Atoms					AltConf
			Total	C	Cl	N	O	
85	A	1	31	22	1	7	1	0

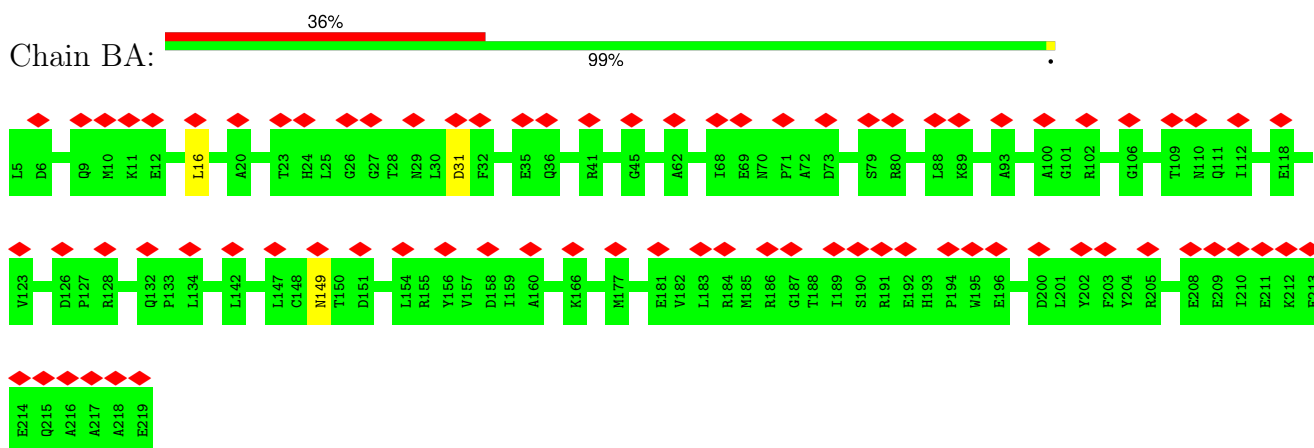
3 Residue-property plots [i](#)

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

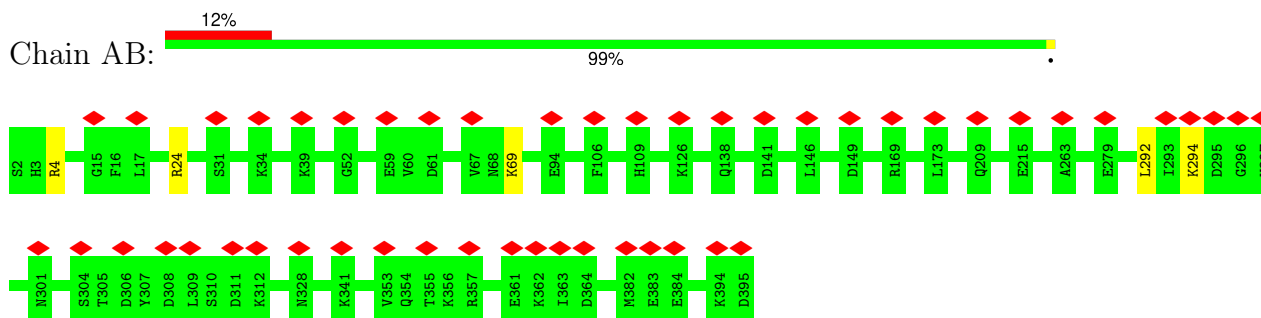
- Molecule 1: 60S ribosomal protein L8



- Molecule 2: 40S ribosomal protein SA

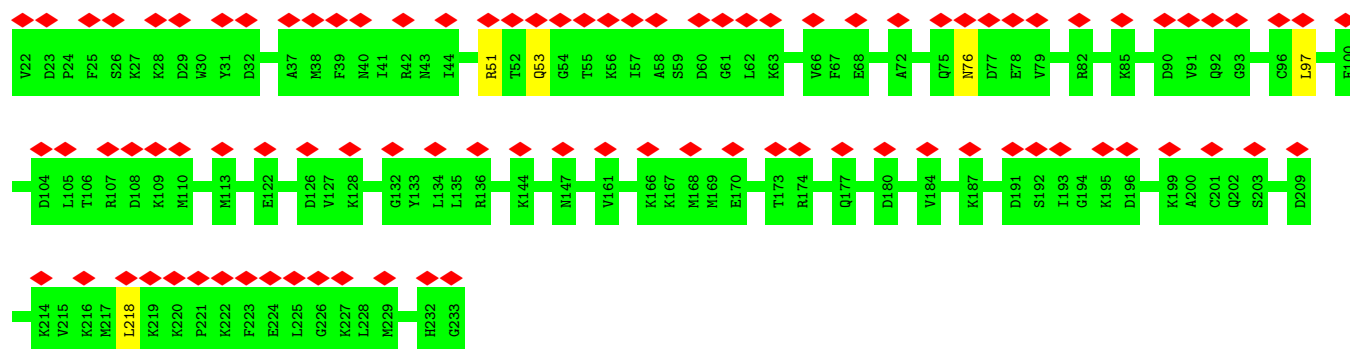


- Molecule 3: 60S ribosomal protein L3

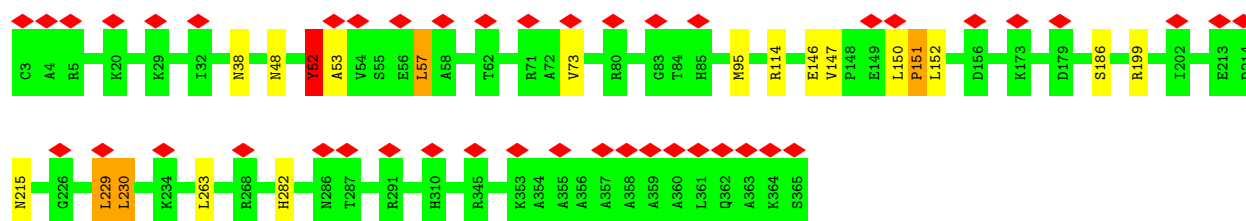


- Molecule 4: 40S ribosomal protein S3a

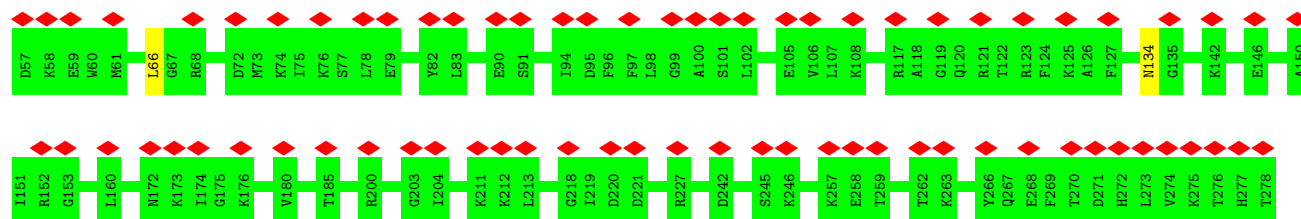




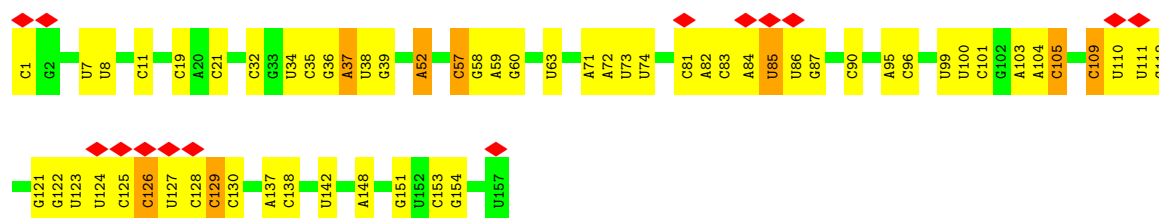
• Molecule 5: 60S ribosomal protein L4



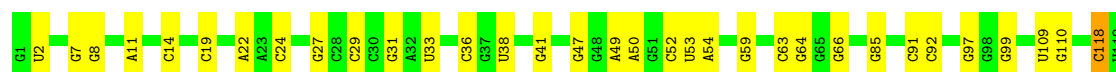
• Molecule 6: 40S ribosomal protein S2



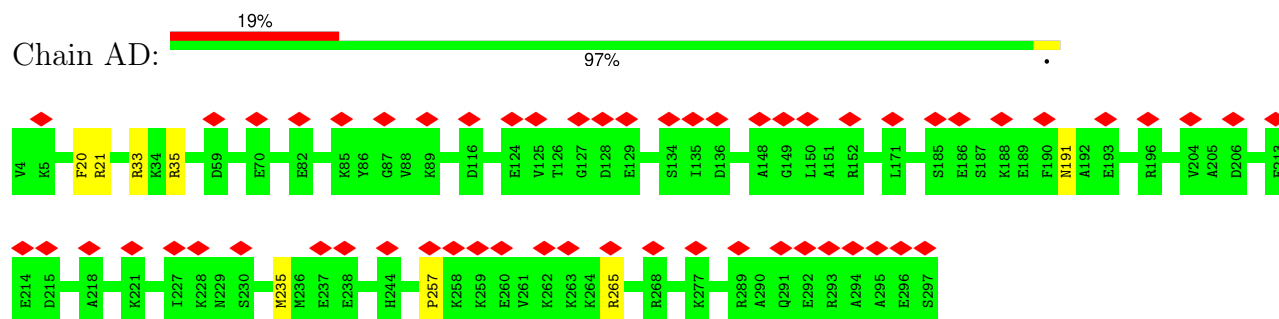
• Molecule 7: 5.8S ribosomal RNA



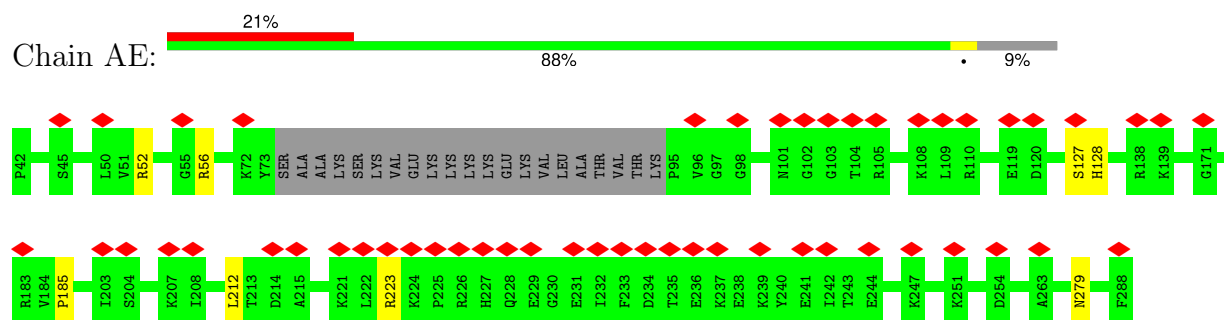
• Molecule 8: 5S ribosomal RNA



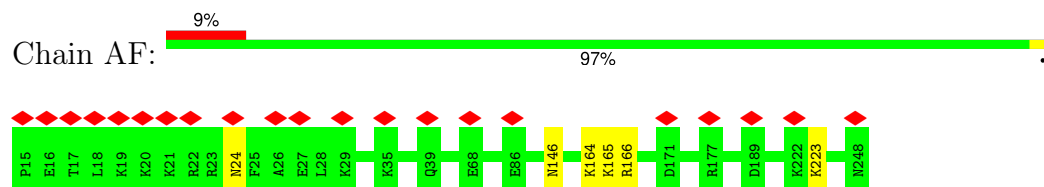
- Molecule 9: 60S ribosomal protein L5



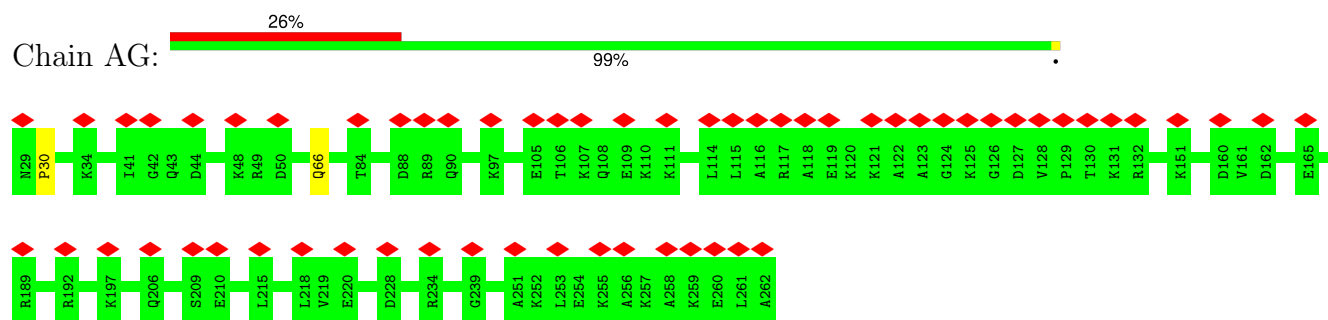
- Molecule 10: 60S ribosomal protein L6



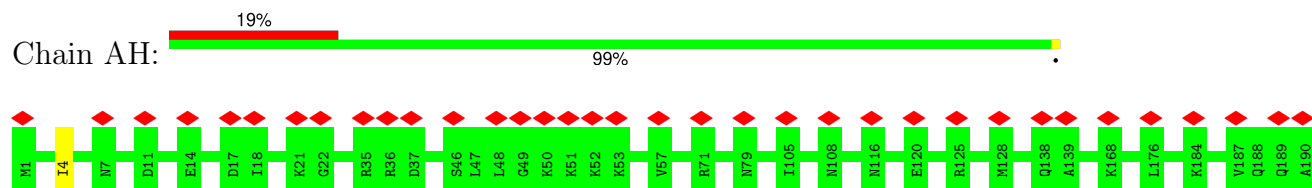
- Molecule 11: 60S ribosomal protein L7



- Molecule 12: 60S ribosomal protein L7a

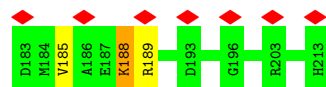
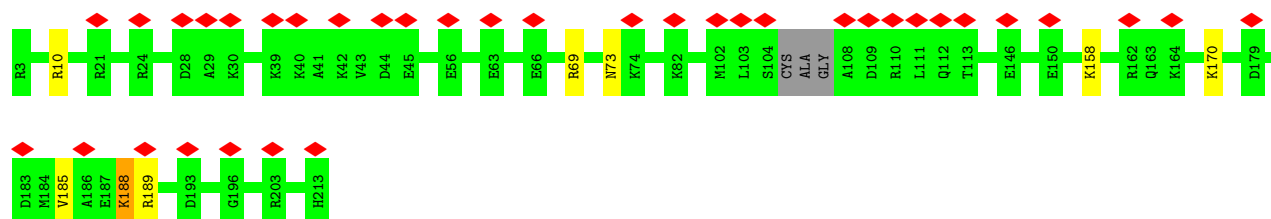


- Molecule 13: 60S ribosomal protein L9

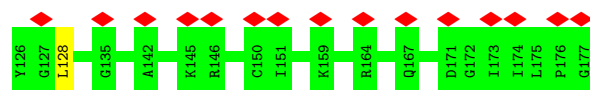
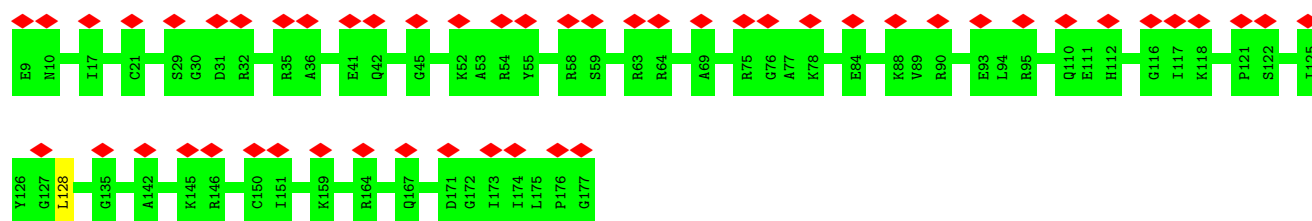




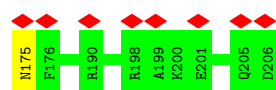
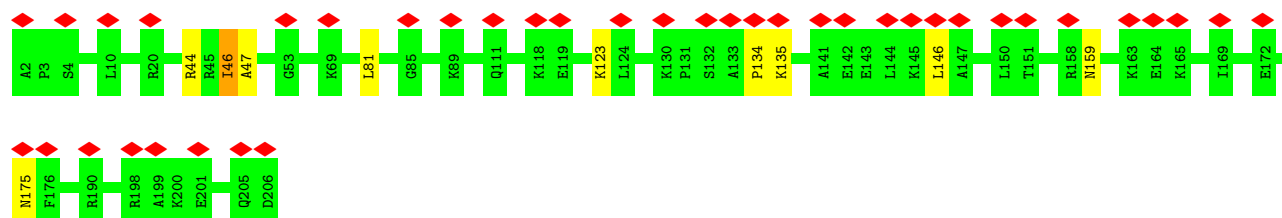
- Molecule 14: 60S ribosomal protein L10



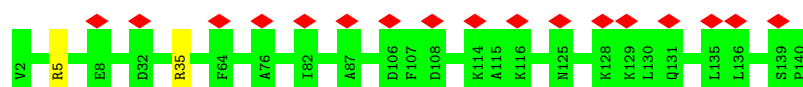
- Molecule 15: 60S ribosomal protein L11



- Molecule 16: 60S ribosomal protein L13

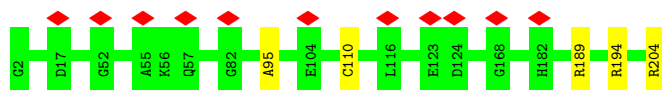


- Molecule 17: 60S ribosomal protein L14

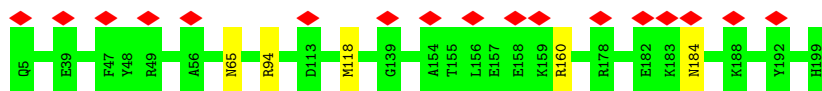


- Molecule 18: 60S ribosomal protein L15

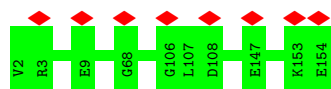




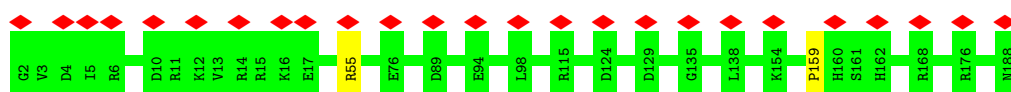
- Molecule 19: 60S ribosomal protein L13a



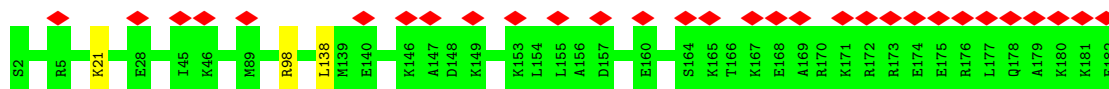
- Molecule 20: 60S ribosomal protein L17



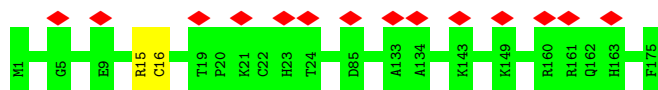
- Molecule 21: 60S ribosomal protein L18



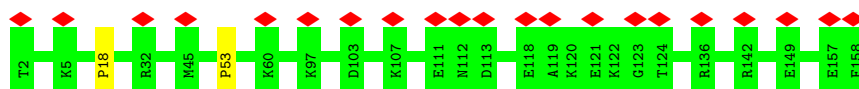
- Molecule 22: 60S ribosomal protein L19



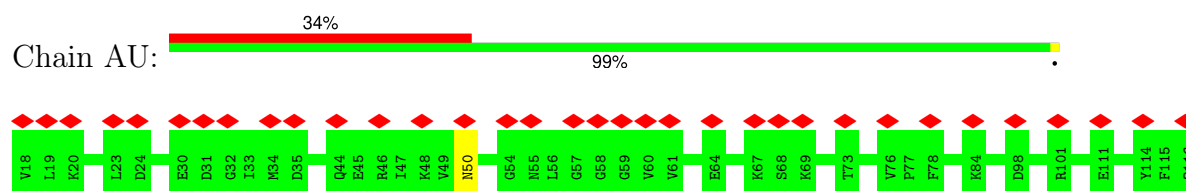
- Molecule 23: 60S ribosomal protein L18a



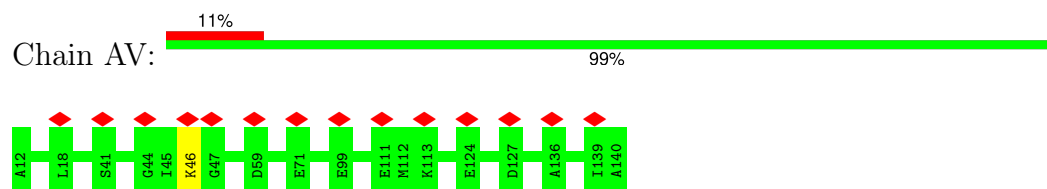
- Molecule 24: 60S ribosomal protein L21



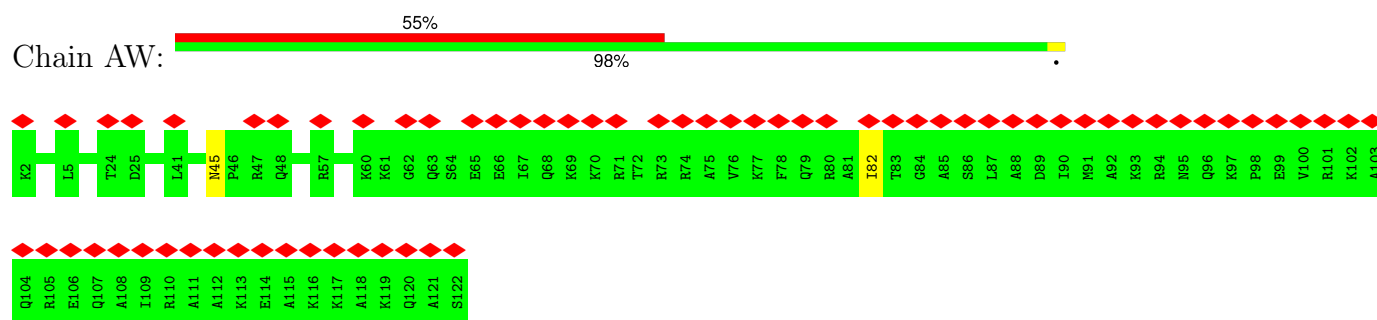
- Molecule 25: 60S ribosomal protein L22



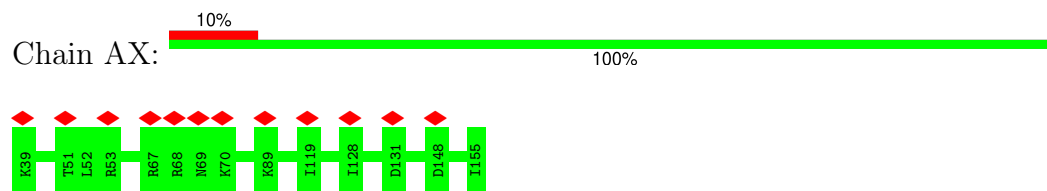
- Molecule 26: 60S ribosomal protein L23



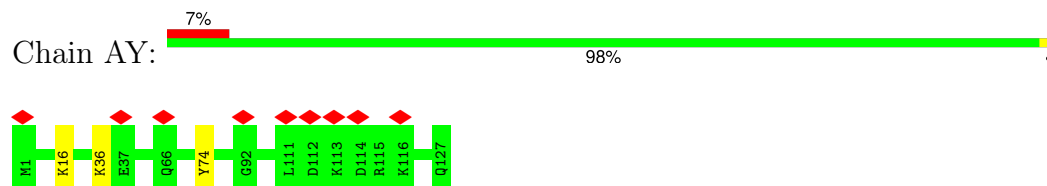
- Molecule 27: 60S ribosomal protein L24



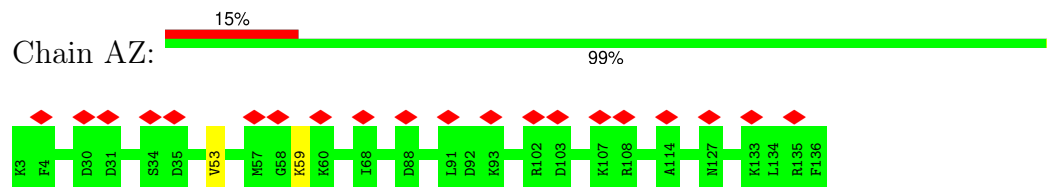
- Molecule 28: 60S ribosomal protein L23a



- Molecule 29: 60S ribosomal protein L26

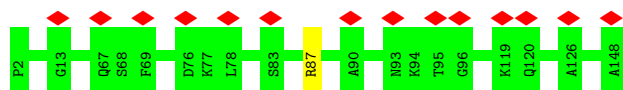


- Molecule 30: 60S ribosomal protein L27

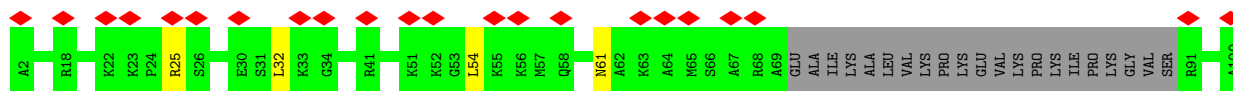
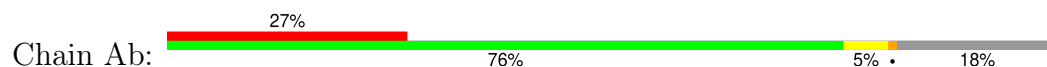


- Molecule 31: 60S ribosomal protein L27a

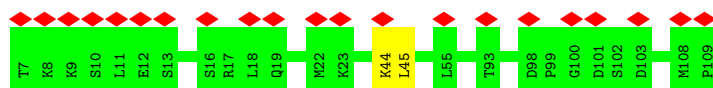




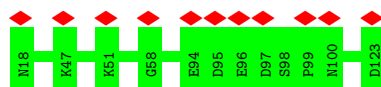
- Molecule 32: 60S ribosomal protein L29



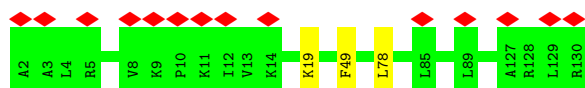
- Molecule 33: 60S ribosomal protein L30



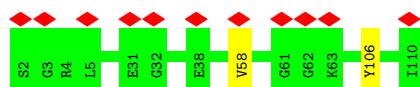
- Molecule 34: 60S ribosomal protein L31



- Molecule 35: 60S ribosomal protein L32

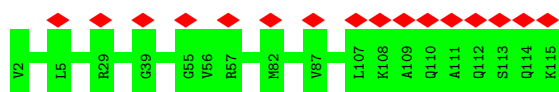


- Molecule 36: 60S ribosomal protein L35a

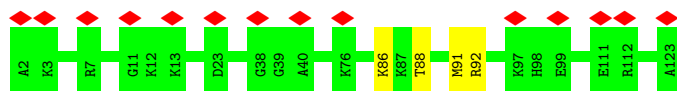


- Molecule 37: 60S ribosomal protein L34

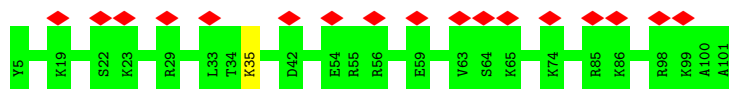




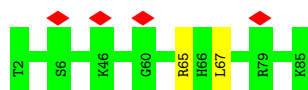
- Molecule 38: 60S ribosomal protein L35



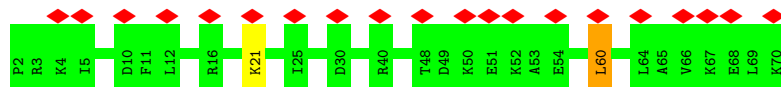
- Molecule 39: 60S ribosomal protein L36



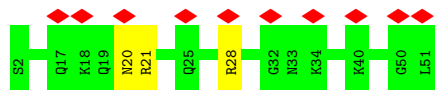
- Molecule 40: 60S ribosomal protein L37



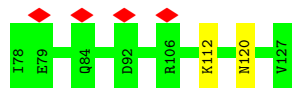
- Molecule 41: 60S ribosomal protein L38



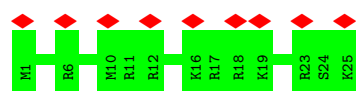
- Molecule 42: 60S ribosomal protein L39



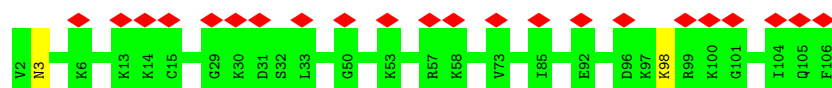
- Molecule 43: 60S ribosomal protein L40



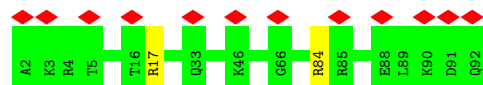
- Molecule 44: 60S ribosomal protein L41



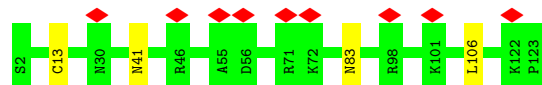
- Molecule 45: 60S ribosomal protein L36a



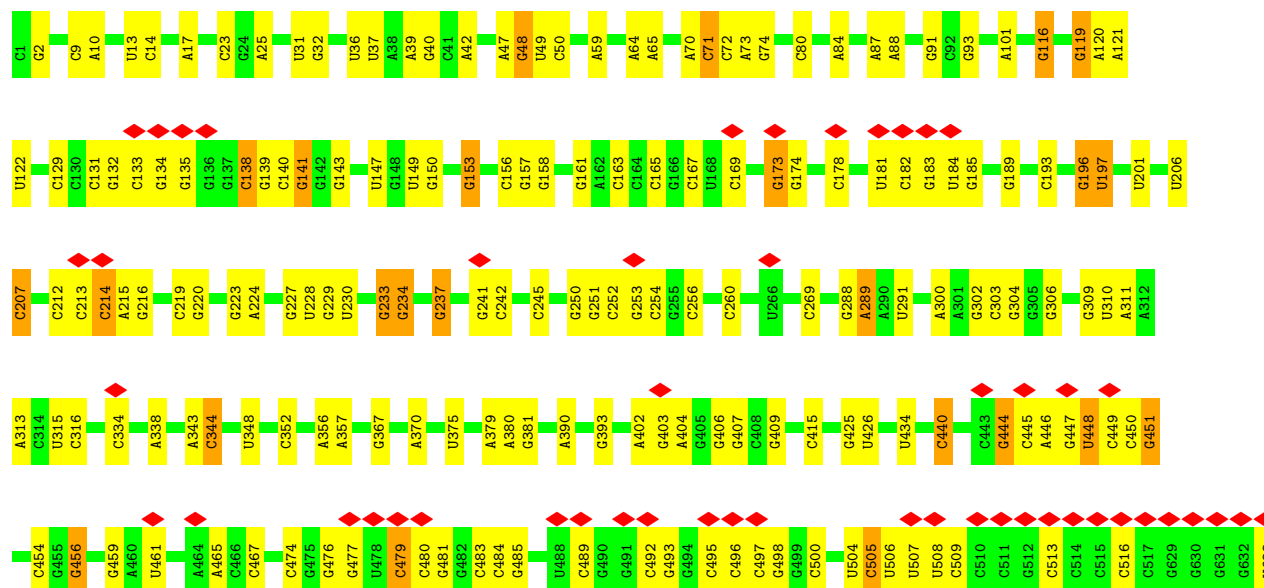
- Molecule 46: 60S ribosomal protein L37a

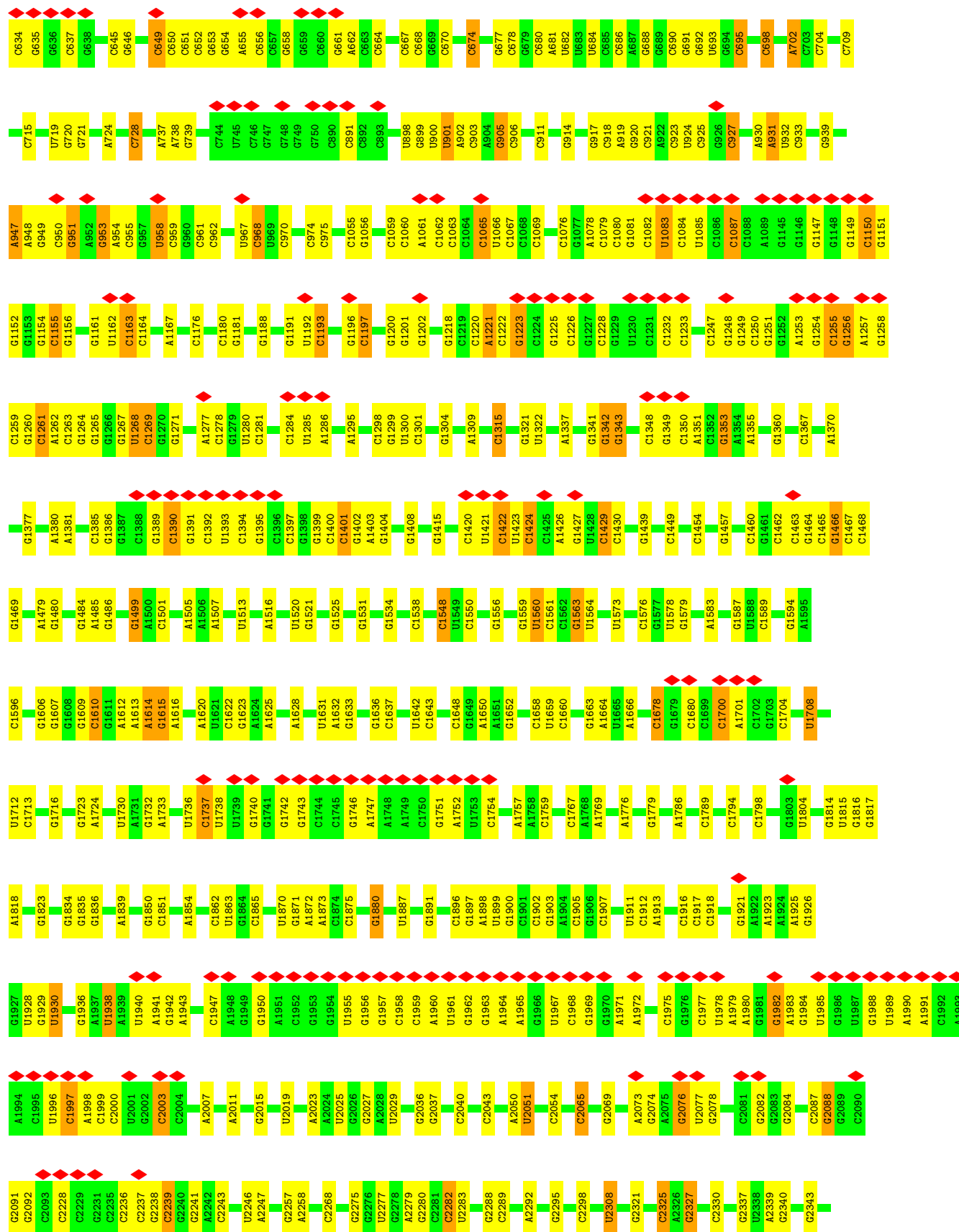


- Molecule 47: 60S ribosomal protein L28

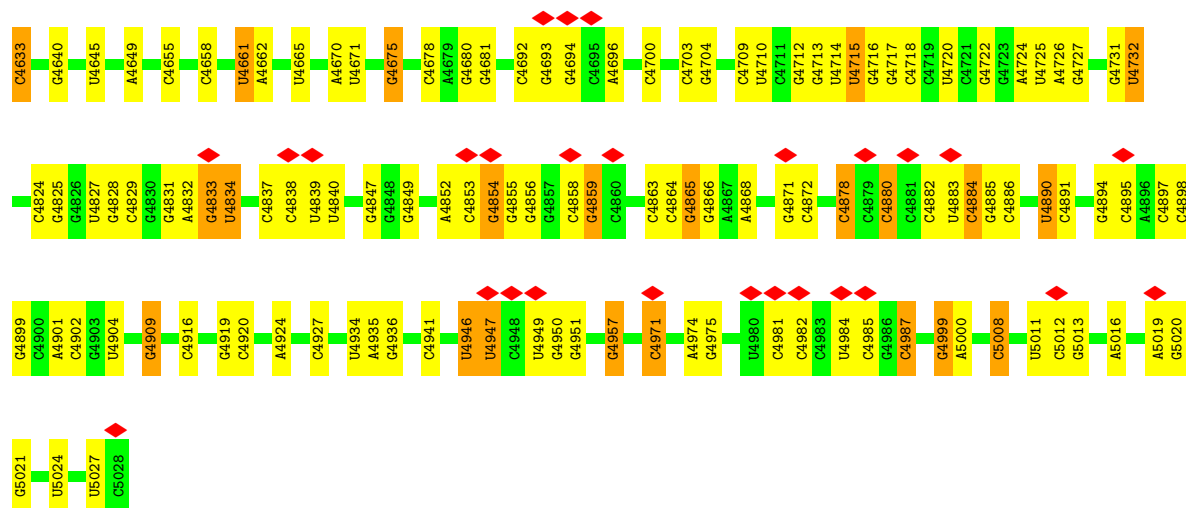


- Molecule 48: 28S ribosomal RNA

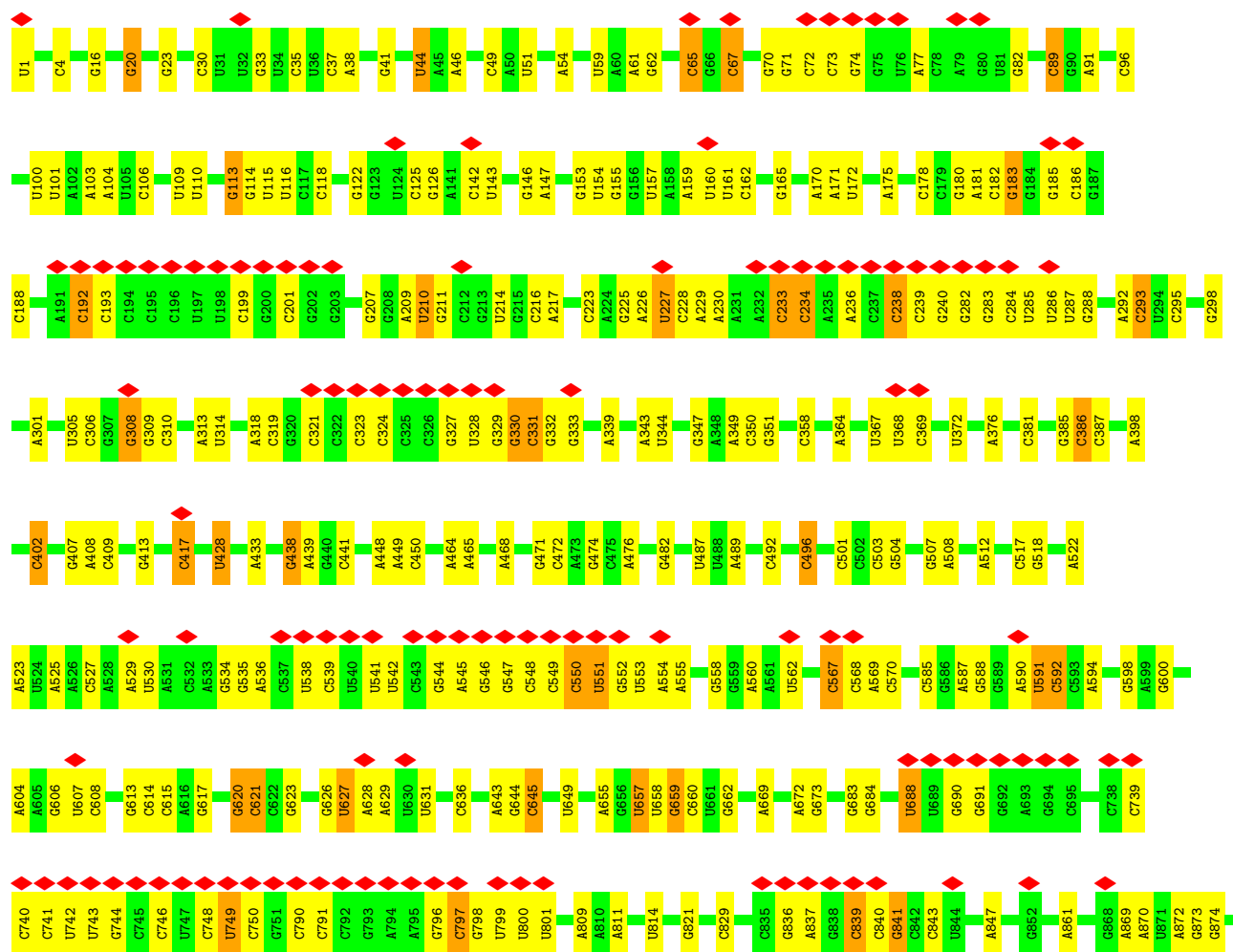


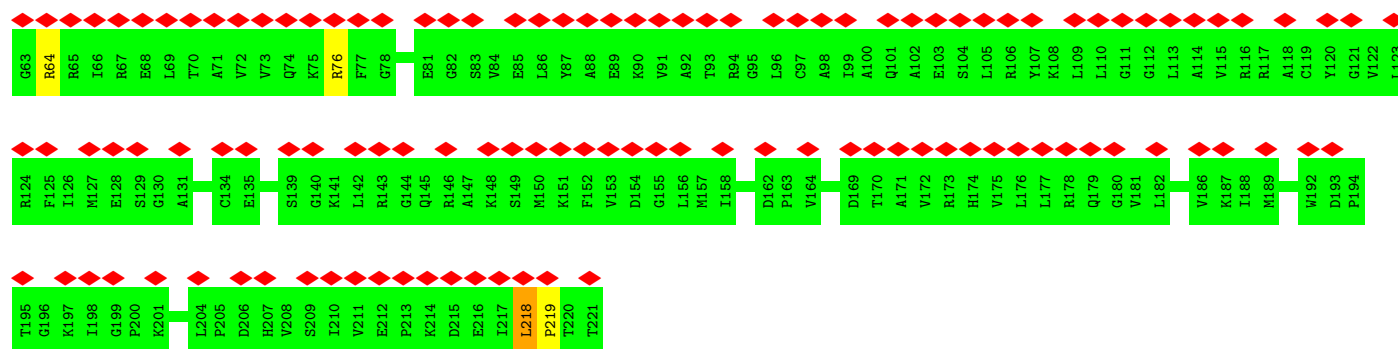


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A4475	G4333	G4216	U4087	G4012	C3867	C3621	A2824	G2690	C2567	
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A4510	A4340	A4231	U3761	A4018	G2834	C3644	G2834	C2706	U2469	
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	A4195	C4070	C3944	C4071	G3851	C3737	U3612	A2544	A2544	U2446
	C4205	A4072	G3945	C4072	C3852	U3741	A3613	G2545	G2545	U2447
	A4206	G4073	C3946	G4073	C3853	U3744	A3614	G2546	G2546	C2448
		A4074	C3947	A4074	G3856	U3747	U3615	G2547	G2547	C2449
		G4075	C3948	G4075	G3860	G3747	U3616	G2548	G2548	A2452
		G4076	G4004	G4076				G2555	G2555	G2453
		G4077	G4005	G4077				A2561	A2561	G2454
		G4078	G4006	G4078						
		G4079	G4007	G4079						
		U4080	C4008	U4080						
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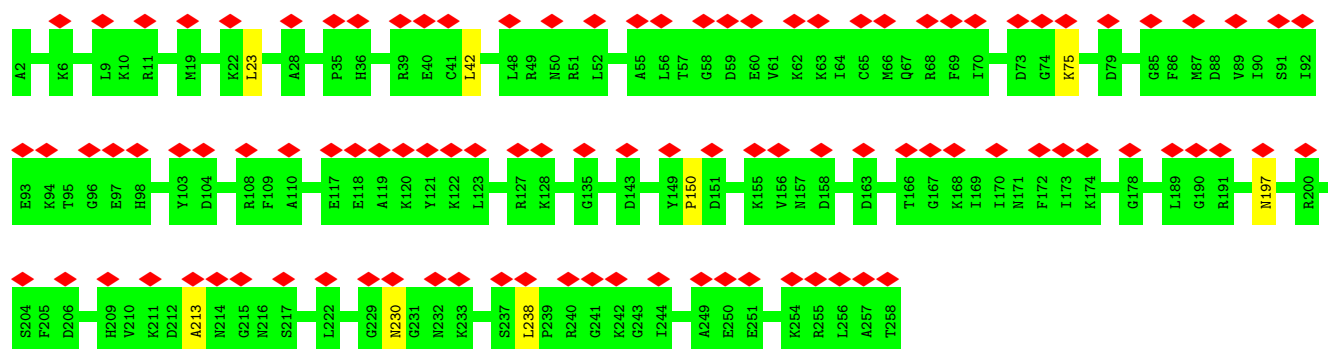
• Molecule 49: 18S ribosomal RNA





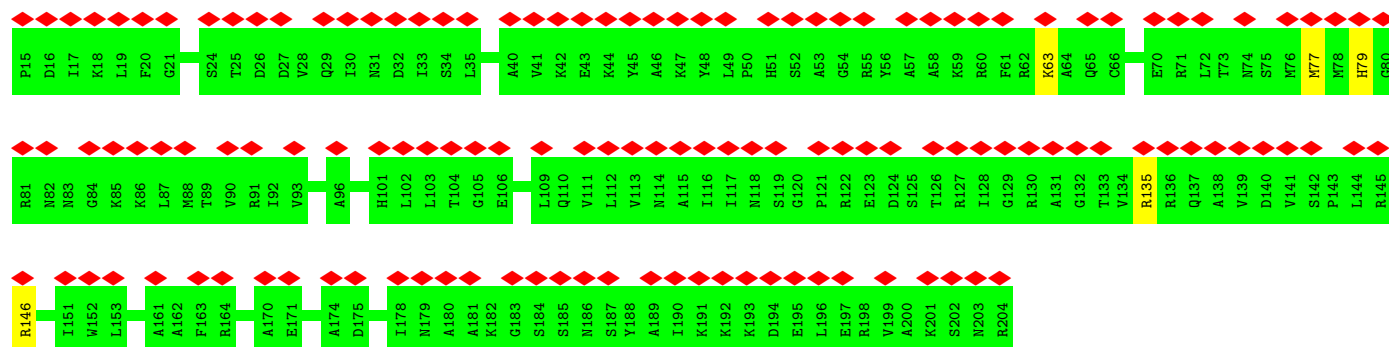
- Molecule 51: 40S ribosomal protein S4, Y isoform 1

Chain BE: 39% 97%



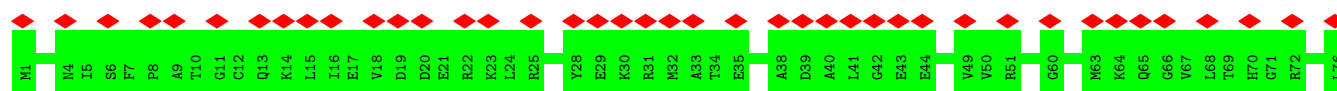
- Molecule 52: 40S ribosomal protein S5

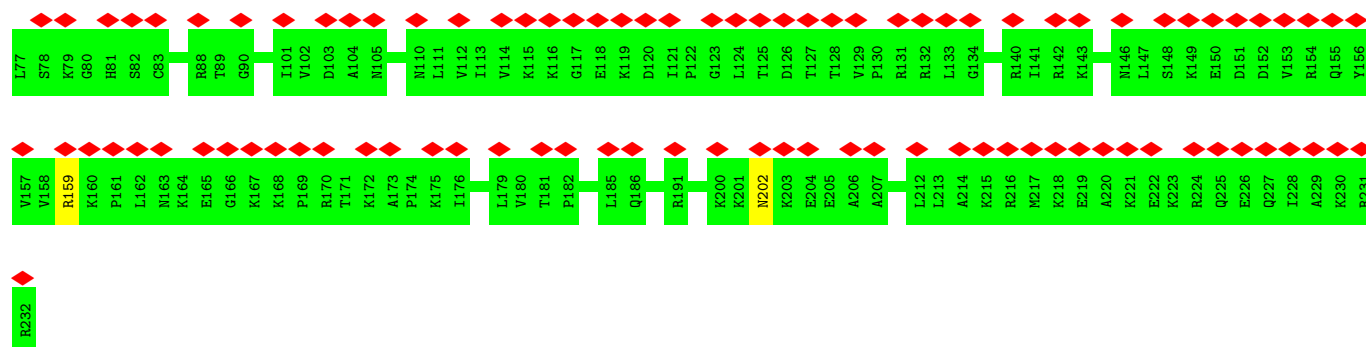
Chain BF: 70% 97%



- Molecule 53: 40S ribosomal protein S6

Chain BG: 57% 99%

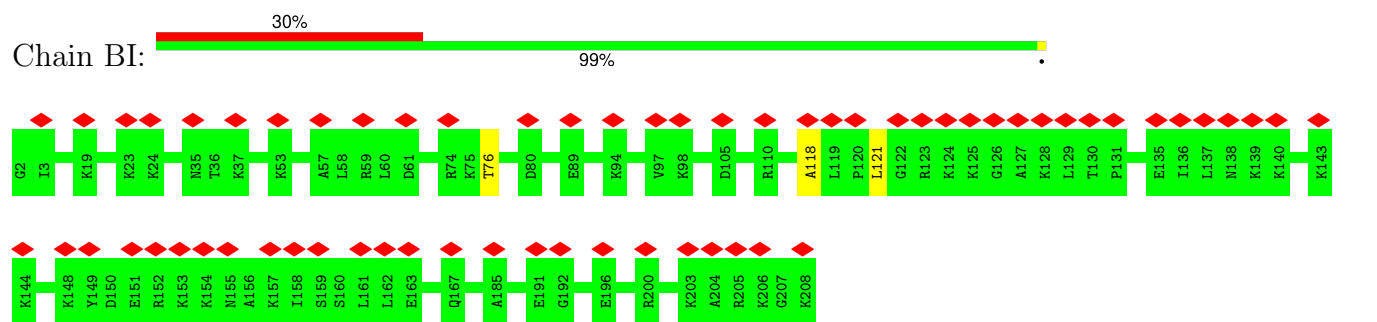




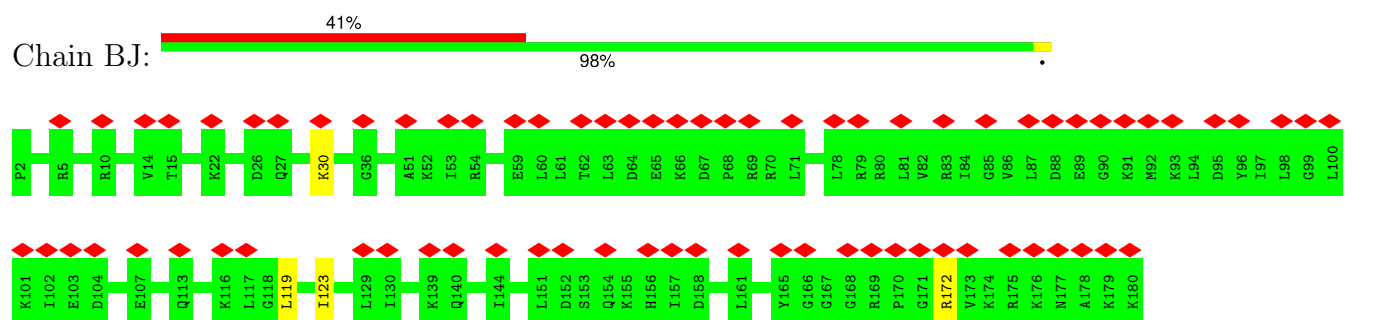
- Molecule 54: 40S ribosomal protein S7



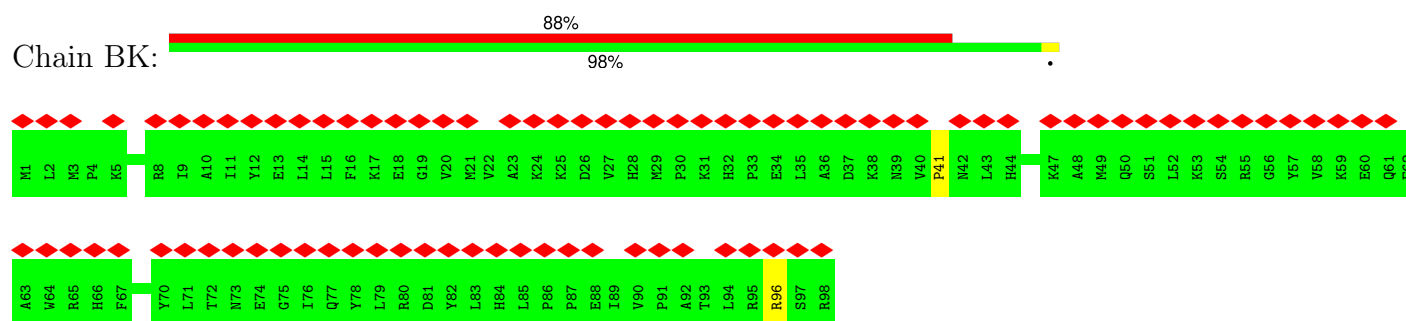
- Molecule 55: 40S ribosomal protein S8



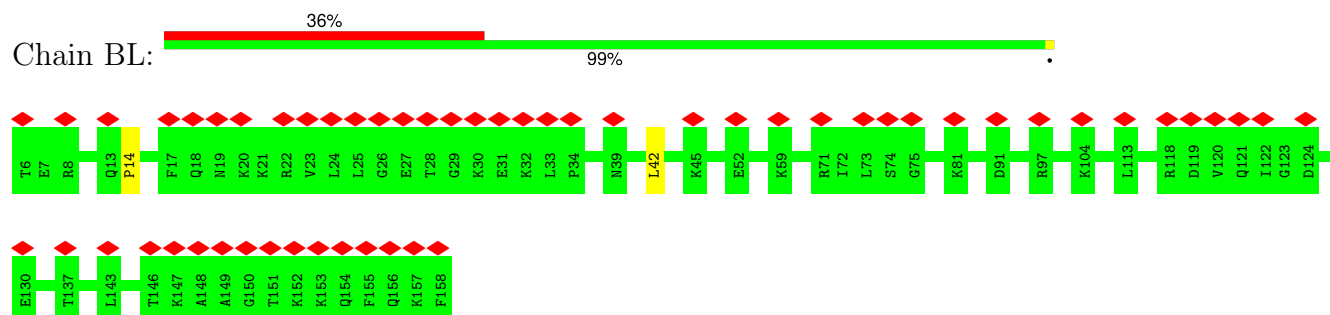
- Molecule 56: 40S ribosomal protein S9



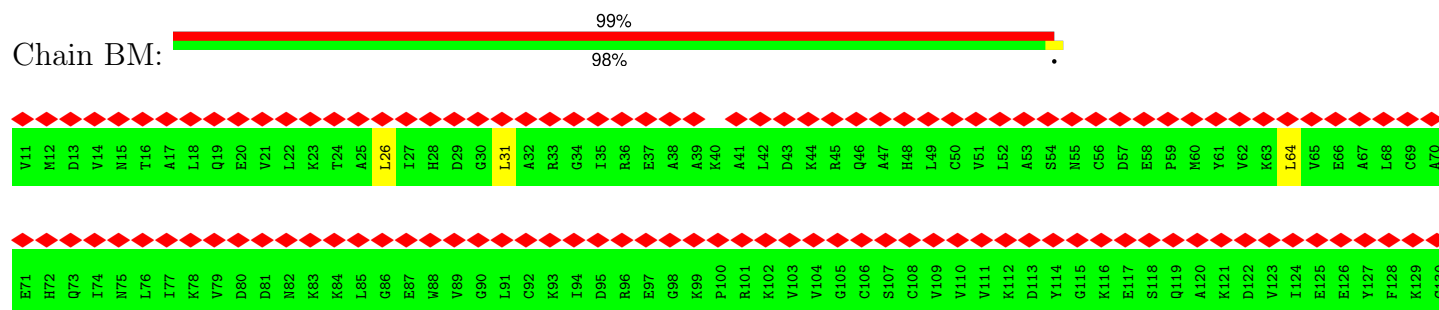
- Molecule 57: 40S ribosomal protein S10



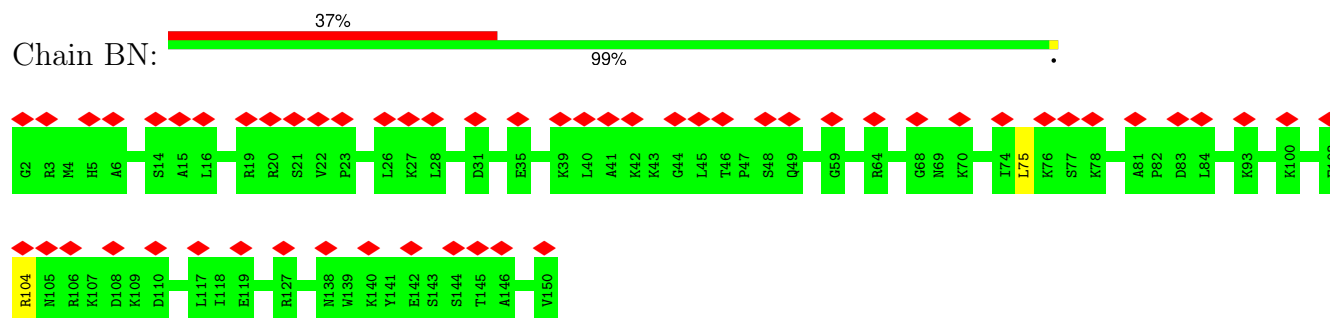
- Molecule 58: 40S ribosomal protein S11



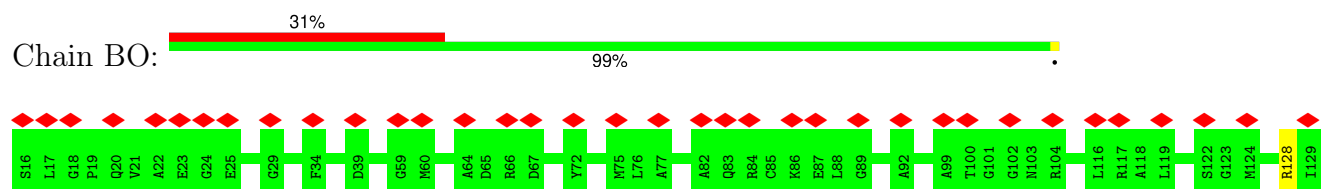
- Molecule 59: 40S ribosomal protein S12

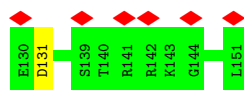


- Molecule 60: 40S ribosomal protein S13



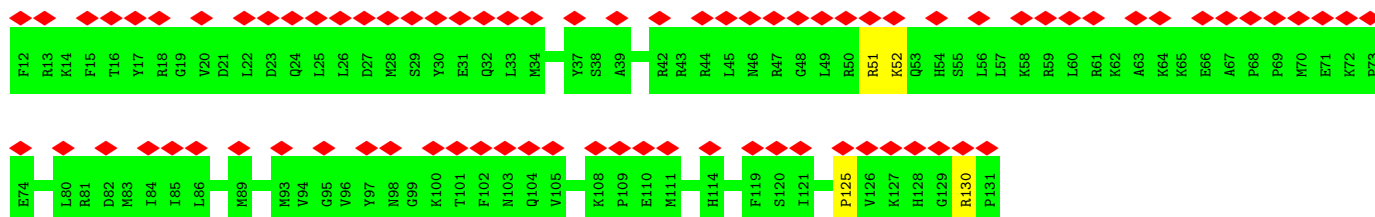
- Molecule 61: 40S ribosomal protein S14





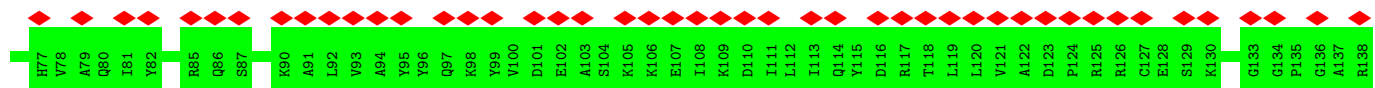
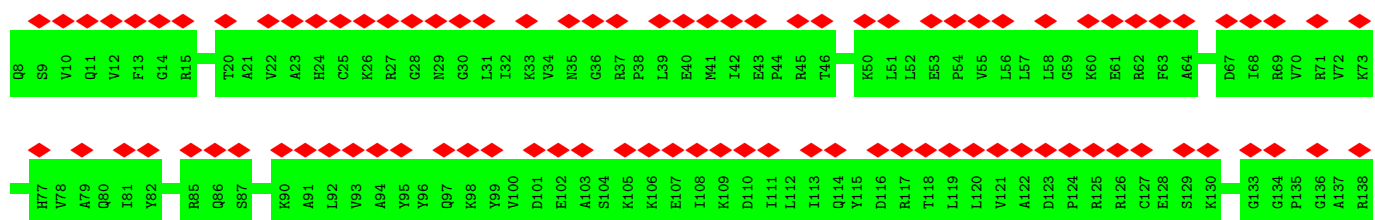
- Molecule 62: 40S ribosomal protein S15

Chain BP: 67% 97%



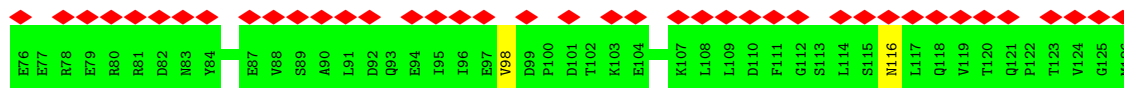
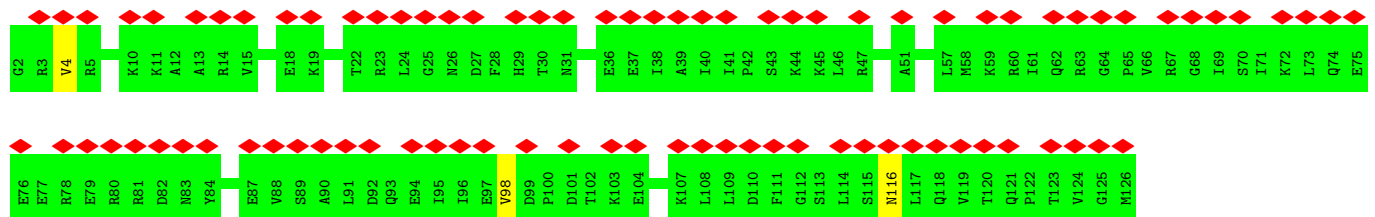
- Molecule 63: 40S ribosomal protein S16

Chain BQ: 68% 100%



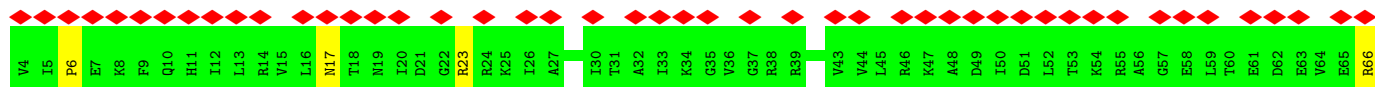
- Molecule 64: 40S ribosomal protein S17

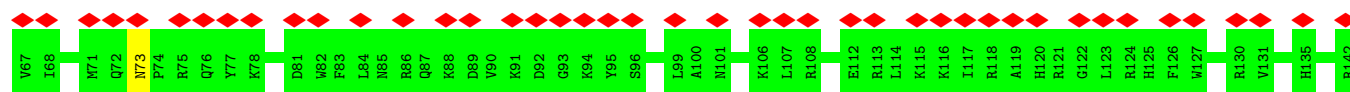
Chain BR: 68% 98%



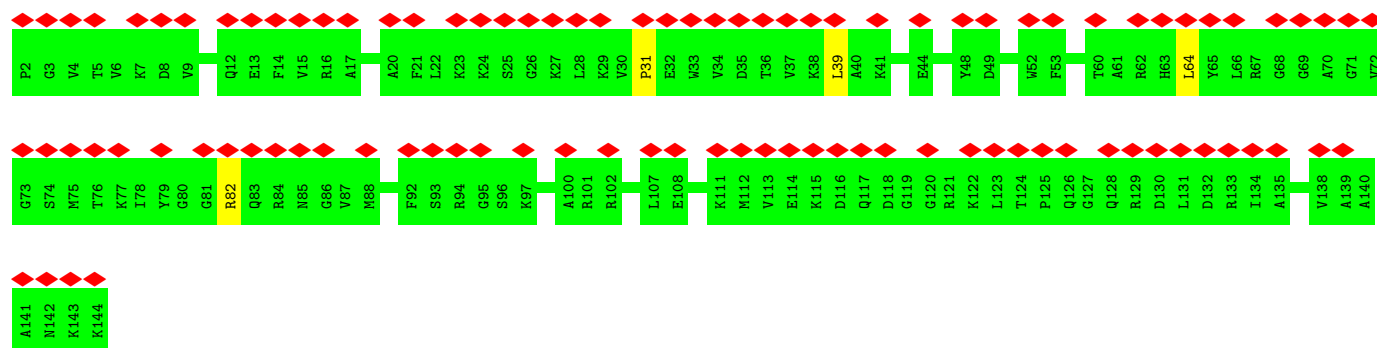
- Molecule 65: 40S ribosomal protein S18

Chain BS: 65% 96%

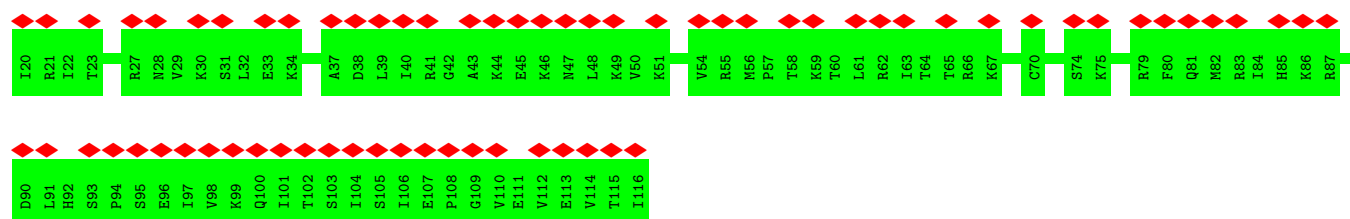
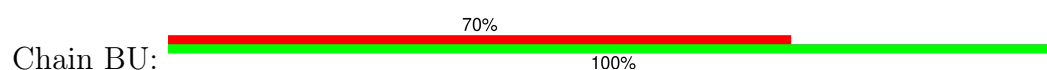




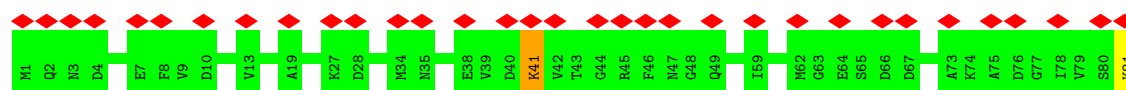
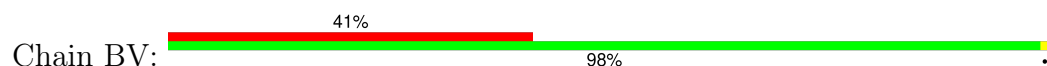
- Molecule 66: 40S ribosomal protein S19



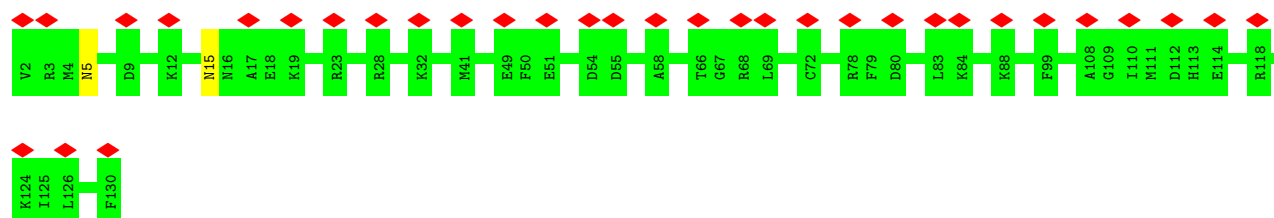
- Molecule 67: 40S ribosomal protein S20



- Molecule 68: 40S ribosomal protein S21

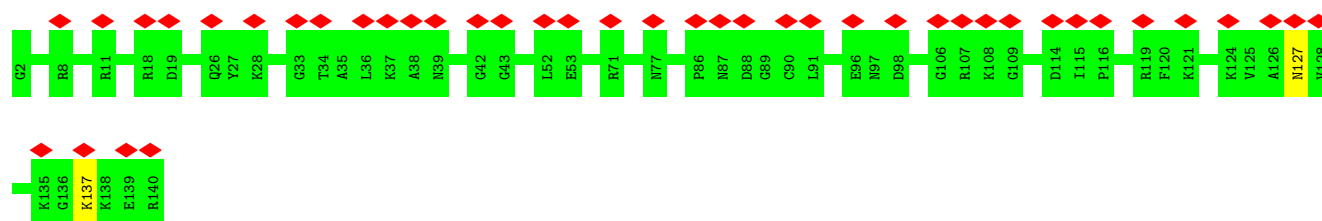


- Molecule 69: 40S ribosomal protein S15a



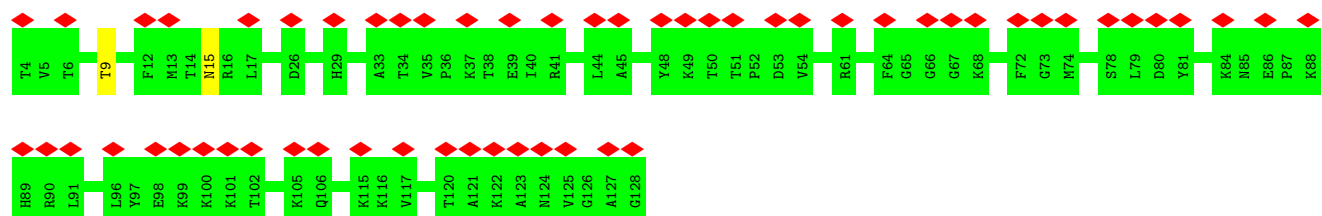
- Molecule 70: 40S ribosomal protein S23

Chain BX: 

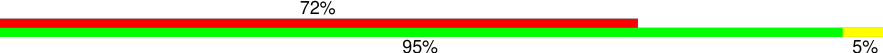


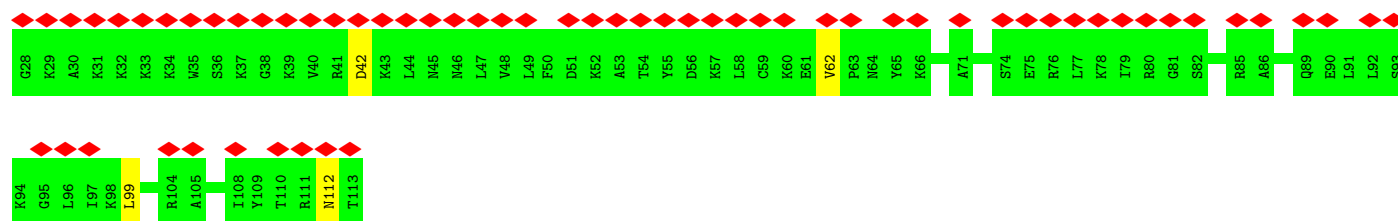
- Molecule 71: 40S ribosomal protein S24

Chain BY: 



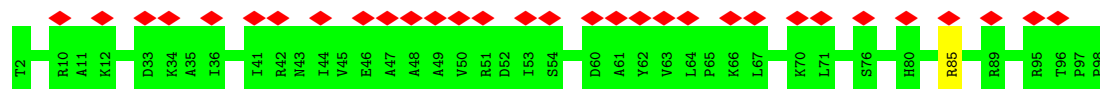
- Molecule 72: 40S ribosomal protein S25

Chain BZ: 

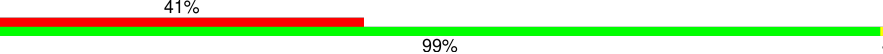


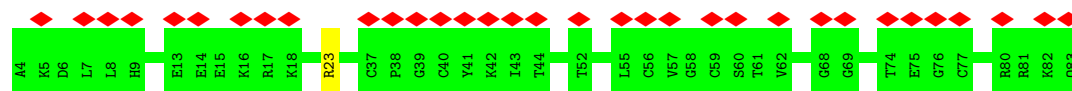
- Molecule 73: 40S ribosomal protein S26

Chain Ba: 

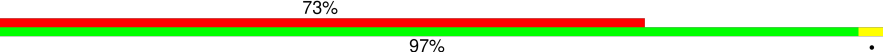


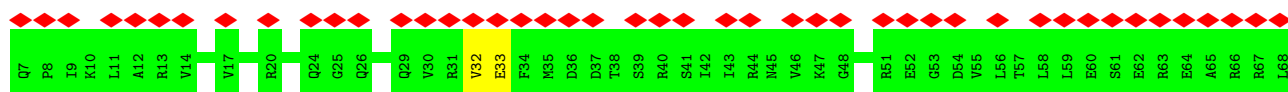
- Molecule 74: 40S ribosomal protein S27

Chain Bb: 

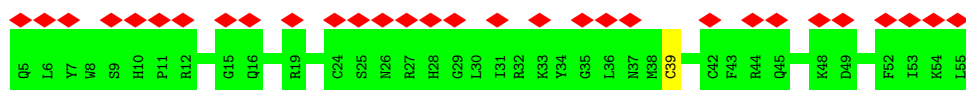


- Molecule 75: 40S ribosomal protein S28

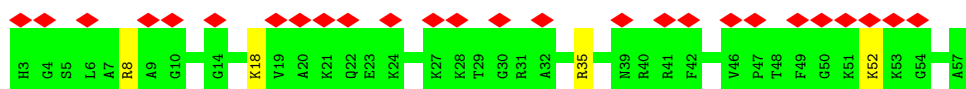
Chain Bc: 



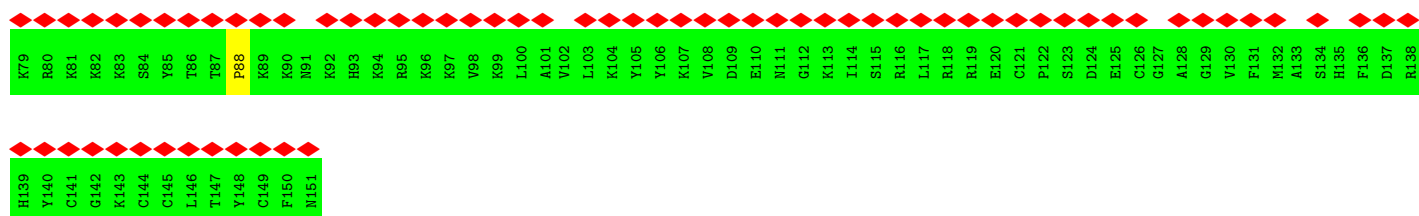
- Molecule 76: 40S ribosomal protein S29



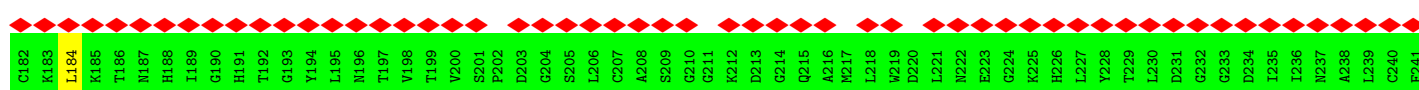
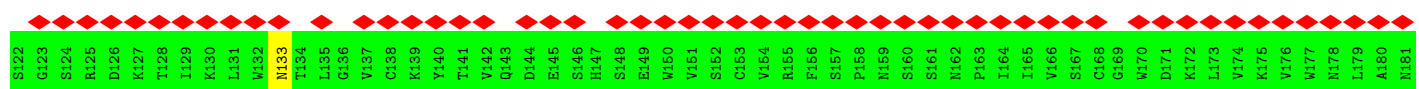
- Molecule 77: 40S ribosomal protein S30

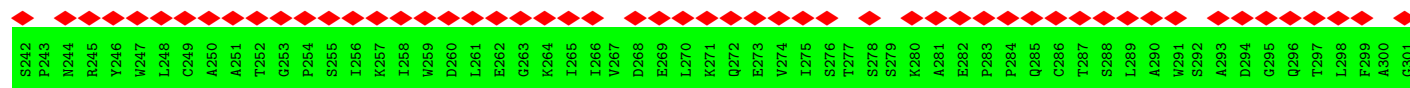


- Molecule 78: Ubiquitin-40S ribosomal protein S27a

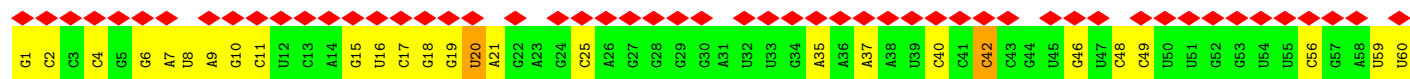


- Molecule 79: Receptor of activated protein C kinase 1

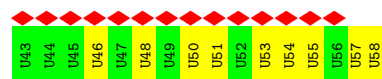




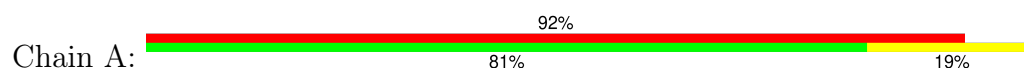
• Molecule 80: tRNA



• Molecule 81: mRNA



• Molecule 82: Proprotein convertase subtilisin/kexin type 9



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	7214	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.104	Depositor
Minimum map value	-0.058	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.022	Depositor
Map size (\AA)	488.0, 488.0, 488.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.22, 1.22, 1.22	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MVM, ZN, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	AA	0.55	0/1936	0.67	0/2596
2	BA	0.44	0/1741	0.71	1/2366 (0.0%)
3	AB	0.54	0/3246	0.71	1/4345 (0.0%)
4	BB	0.41	0/1749	0.71	1/2340 (0.0%)
5	AC	0.58	1/2942 (0.0%)	0.82	7/3951 (0.2%)
6	BC	0.46	0/1761	0.66	0/2379
7	A3	0.98	1/3726 (0.0%)	1.29	46/5804 (0.8%)
8	A4	0.91	0/2839	1.14	7/4425 (0.2%)
9	AD	0.46	0/2437	0.66	0/3262
10	AE	0.45	0/1876	0.75	1/2514 (0.0%)
11	AF	0.57	0/1986	0.72	2/2644 (0.1%)
12	AG	0.45	0/1913	0.68	0/2576
13	AH	0.46	0/1545	0.71	1/2077 (0.0%)
14	AI	0.50	0/1730	0.68	0/2311
15	AJ	0.44	0/1376	0.69	1/1841 (0.1%)
16	AL	0.53	0/1688	0.76	2/2260 (0.1%)
17	AM	0.47	0/1161	0.65	0/1554
18	AN	0.61	1/1746 (0.1%)	0.70	0/2338
19	AO	0.51	0/1638	0.70	0/2191
20	AP	0.50	0/1268	0.61	0/1701
21	AQ	0.58	0/1537	0.79	0/2052
22	AR	0.43	0/1533	0.68	1/2025 (0.0%)
23	AS	0.53	1/1488 (0.1%)	0.68	0/1997
24	AT	0.55	0/1312	0.69	0/1753
25	AU	0.43	0/822	0.65	0/1103
26	AV	0.48	0/983	0.68	0/1319
27	AW	0.46	0/1004	0.68	1/1332 (0.1%)
28	AX	0.45	0/975	0.67	0/1312
29	AY	0.48	0/1081	0.67	0/1439
30	AZ	0.52	0/1126	0.71	0/1502
31	Aa	0.55	0/1191	0.68	0/1591
32	Ab	2.58	2/804 (0.2%)	0.78	2/1060 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	Ac	0.48	0/812	0.64	0/1089
34	Ad	0.51	0/894	0.68	0/1204
35	Ae	0.55	0/1082	0.70	2/1443 (0.1%)
36	Af	0.56	0/895	0.73	0/1198
37	Ag	0.51	0/916	0.76	0/1220
38	Ah	0.55	1/1023 (0.1%)	0.73	0/1351
39	Ai	0.45	0/805	0.69	0/1065
40	Aj	0.55	0/703	0.76	1/929 (0.1%)
41	Ak	0.44	0/575	0.70	1/761 (0.1%)
42	Al	0.45	0/454	0.68	0/599
43	Am	0.45	0/417	0.67	0/553
44	An	0.49	0/241	0.85	0/305
45	Ao	0.51	0/877	0.69	0/1156
46	Ap	0.54	0/718	0.71	0/953
47	At	0.51	0/995	0.77	2/1334 (0.1%)
48	A2	1.27	17/87365 (0.0%)	1.27	737/136272 (0.5%)
49	B1	0.76	1/40767 (0.0%)	1.24	314/63536 (0.5%)
50	BD	0.40	0/1736	0.68	1/2338 (0.0%)
51	BE	0.41	0/2072	0.71	3/2793 (0.1%)
52	BF	0.39	0/1524	0.70	1/2048 (0.0%)
53	BG	0.38	0/1907	0.71	0/2538
54	BH	0.39	0/1501	0.70	1/2009 (0.0%)
55	BI	0.44	0/1725	0.70	0/2298
56	BJ	0.41	0/1520	0.70	1/2030 (0.0%)
57	BK	0.40	0/851	0.71	0/1147
58	BL	0.46	0/1281	0.74	1/1710 (0.1%)
59	BM	0.37	0/941	0.71	2/1264 (0.2%)
60	BN	0.40	0/1226	0.69	1/1649 (0.1%)
61	BO	0.45	1/1029 (0.1%)	0.70	0/1380
62	BP	0.41	0/1019	0.80	0/1361
63	BQ	0.37	0/1126	0.70	0/1506
64	BR	0.36	0/1023	0.68	0/1373
65	BS	0.39	0/1172	0.69	0/1570
66	BT	0.40	0/1131	0.70	1/1515 (0.1%)
67	BU	0.35	0/778	0.68	0/1045
68	BV	0.38	0/623	0.68	0/833
69	BW	0.44	0/1051	0.71	0/1406
70	BX	0.46	0/1097	0.69	0/1464
71	BY	0.37	0/1032	0.65	0/1371
72	BZ	0.36	0/696	0.77	1/929 (0.1%)
73	Ba	0.44	0/786	0.66	0/1053
74	Bb	0.46	0/637	0.72	0/854
75	Bc	0.32	0/490	0.70	0/656

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
76	Bd	0.43	0/437	0.79	1/580 (0.2%)
77	Be	0.38	0/443	0.71	0/583
78	Bf	0.35	0/613	0.66	0/811
79	Bg	0.35	0/2497	0.68	1/3399 (0.0%)
80	Bv	0.56	1/1813 (0.1%)	1.16	7/2823 (0.2%)
81	Bx	0.40	0/351	1.05	0/540
82	A	0.19	0/127	0.56	0/175
All	All	0.92	27/229954 (0.0%)	1.09	1153/337979 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
22	AR	0	1
52	BF	0	1
All	All	0	2

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	A2	1254	G	N3-C4	132.95	2.28	1.35
48	A2	1254	G	C2-N3	109.51	2.20	1.32
48	A2	1254	G	C6-N1	99.11	2.08	1.39
48	A2	1254	G	N1-C2	89.30	2.09	1.37
48	A2	1254	G	C5-C4	82.35	1.96	1.38
48	A2	1254	G	C5-C6	72.90	2.15	1.42
32	Ab	112	ILE	N-CA	71.70	2.89	1.46
80	Bv	1	G	OP3-P	-10.66	1.48	1.61
49	B1	1	U	OP3-P	-10.63	1.48	1.61
48	A2	1254	G	C6-O6	-10.24	1.15	1.24
7	A3	37	A	N9-C4	-9.07	1.32	1.37
32	Ab	112	ILE	CA-CB	8.71	1.74	1.54
5	AC	186	SER	CA-CB	-8.63	1.40	1.52
48	A2	4717	G	N9-C4	-6.71	1.32	1.38
38	Ah	86	LYS	CD-CE	6.47	1.67	1.51
48	A2	3624	A	N9-C4	-5.92	1.34	1.37
48	A2	3780	G	N9-C4	-5.63	1.33	1.38
18	AN	110	CYS	CA-CB	-5.60	1.41	1.53
48	A2	1839	A	N9-C4	-5.58	1.34	1.37
48	A2	1221	A	N9-C4	-5.57	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	A2	216	G	N3-C4	-5.46	1.31	1.35
23	AS	16	CYS	C-N	-5.46	1.21	1.34
48	A2	1484	G	N9-C4	-5.30	1.33	1.38
48	A2	1664	A	N9-C4	-5.21	1.34	1.37
61	BO	131	ASP	CA-CB	-5.08	1.42	1.53
48	A2	930	A	N9-C4	-5.07	1.34	1.37
48	A2	2766	A	N7-C5	-5.06	1.36	1.39

All (1153) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	A2	1254	G	C2-N3-C4	39.26	131.53	111.90
48	A2	1254	G	C4-C5-N7	-37.76	95.70	110.80
48	A2	1254	G	N3-C4-C5	-34.88	111.16	128.60
48	A2	1254	G	N3-C4-N9	33.78	146.27	126.00
48	A2	1254	G	N1-C2-N3	-29.77	106.04	123.90
48	A2	1254	G	N7-C8-N9	26.10	126.15	113.10
48	A2	1254	G	C5-C6-N1	19.41	121.20	111.50
5	AC	150	LEU	C-N-CD	-18.47	79.97	120.60
48	A2	1254	G	C6-C5-N7	17.93	141.16	130.40
48	A2	1254	G	C5-C6-O6	-16.82	118.51	128.60
48	A2	1254	G	N3-C2-N2	16.79	131.65	119.90
48	A2	4085	C	N1-C2-O2	14.92	127.85	118.90
7	A3	38	U	C2-N3-C4	12.96	134.77	127.00
48	A2	1254	G	C5-N7-C8	12.75	110.68	104.30
7	A3	38	U	N1-C2-N3	-12.41	107.45	114.90
48	A2	4085	C	N3-C2-O2	-12.40	113.22	121.90
48	A2	2228	C	C2-N1-C1'	12.01	132.01	118.80
49	B1	1472	C	N1-C2-O2	11.51	125.81	118.90
48	A2	2236	C	N1-C2-O2	11.38	125.73	118.90
48	A2	649	C	N1-C2-O2	11.10	125.56	118.90
48	A2	2228	C	N1-C2-O2	11.07	125.54	118.90
48	A2	2236	C	C2-N1-C1'	11.04	130.94	118.80
49	B1	1309	C	N1-C2-O2	10.70	125.32	118.90
48	A2	4085	C	C2-N1-C1'	10.63	130.49	118.80
48	A2	4545	C	N1-C2-O2	10.59	125.25	118.90
48	A2	1982	G	C6-C5-N7	-10.50	124.10	130.40
49	B1	1472	C	C2-N1-C1'	10.41	130.25	118.80
49	B1	96	C	N3-C2-O2	-10.19	114.77	121.90
48	A2	918	C	N1-C2-O2	10.16	125.00	118.90
49	B1	1464	C	N3-C2-O2	-10.04	114.87	121.90
48	A2	4717	G	N3-C4-N9	-10.03	119.98	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	B1	118	C	N1-C2-O2	10.00	124.90	118.90
49	B1	67	C	N1-C2-O2	9.97	124.89	118.90
48	A2	4545	C	C2-N1-C1'	9.92	129.71	118.80
48	A2	4717	G	N3-C4-C5	9.92	133.56	128.60
49	B1	1555	U	C2-N1-C1'	9.88	129.55	117.70
48	A2	444	G	O4'-C1'-N9	9.86	116.09	108.20
49	B1	118	C	N3-C2-O2	-9.76	115.07	121.90
48	A2	216	G	N3-C2-N2	-9.74	113.08	119.90
49	B1	67	C	C2-N1-C1'	9.68	129.44	118.80
48	A2	484	C	C6-N1-C2	-9.63	116.45	120.30
49	B1	1464	C	N1-C2-O2	9.53	124.62	118.90
49	B1	1472	C	N3-C2-O2	-9.51	115.25	121.90
49	B1	89	C	C2-N1-C1'	9.40	129.14	118.80
49	B1	89	C	N1-C2-O2	9.40	124.54	118.90
49	B1	428	U	N1-C2-O2	9.40	129.38	122.80
48	A2	219	C	C2-N1-C1'	9.37	129.11	118.80
48	A2	1997	C	N1-C2-O2	9.36	124.51	118.90
48	A2	2478	C	N1-C2-O2	9.31	124.49	118.90
49	B1	96	C	C2-N1-C1'	9.28	129.01	118.80
49	B1	96	C	N1-C2-O2	9.21	124.43	118.90
48	A2	2389	C	N1-C2-O2	9.12	124.38	118.90
48	A2	1982	G	N7-C8-N9	9.06	117.63	113.10
48	A2	2065	C	N1-C2-O2	9.04	124.33	118.90
48	A2	918	C	C2-N1-C1'	8.92	128.61	118.80
49	B1	118	C	C2-N1-C1'	8.88	128.57	118.80
49	B1	428	U	C2-N1-C1'	8.83	128.29	117.70
48	A2	3919	C	C5-C6-N1	8.77	125.39	121.00
7	A3	126	C	N1-C2-O2	8.75	124.15	118.90
49	B1	1398	G	C4-N9-C1'	8.74	137.86	126.50
48	A2	1637	C	N1-C2-O2	8.73	124.14	118.90
48	A2	116	G	N3-C4-N9	-8.70	120.78	126.00
48	A2	2228	C	N3-C2-O2	-8.70	115.81	121.90
49	B1	89	C	N3-C2-O2	-8.69	115.82	121.90
49	B1	539	C	C6-N1-C2	-8.68	116.83	120.30
48	A2	2771	C	C6-N1-C2	-8.66	116.84	120.30
48	A2	1422	C	C5-C6-N1	8.60	125.30	121.00
48	A2	484	C	C5-C6-N1	8.60	125.30	121.00
48	A2	4545	C	C6-N1-C1'	-8.59	110.50	120.80
7	A3	126	C	C2-N1-C1'	8.58	128.24	118.80
49	B1	1586	U	N3-C2-O2	-8.56	116.21	122.20
49	B1	1442	U	C2-N1-C1'	8.48	127.88	117.70
49	B1	1586	U	N1-C2-O2	8.48	128.73	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	A2	1930	U	N3-C2-O2	-8.48	116.27	122.20
48	A2	1982	G	C8-N9-C4	-8.47	103.01	106.40
48	A2	2236	C	N3-C2-O2	-8.46	115.98	121.90
48	A2	918	C	N3-C2-O2	-8.43	116.00	121.90
48	A2	2228	C	C6-N1-C1'	-8.39	110.72	120.80
48	A2	4069	G	C4-N9-C1'	8.39	137.41	126.50
48	A2	2389	C	N3-C2-O2	-8.39	116.03	121.90
48	A2	4858	C	C6-N1-C2	-8.38	116.95	120.30
48	A2	2727	C	C2-N1-C1'	8.38	128.02	118.80
48	A2	1422	C	C6-N1-C2	-8.35	116.96	120.30
48	A2	1083	U	C2-N1-C1'	8.28	127.64	117.70
48	A2	1197	C	N1-C2-O2	8.23	123.84	118.90
49	B1	1117	C	N1-C2-O2	8.21	123.83	118.90
48	A2	214	C	N1-C2-O2	8.17	123.80	118.90
7	A3	57	C	C6-N1-C2	-8.10	117.06	120.30
49	B1	496	C	C2-N1-C1'	8.10	127.71	118.80
49	B1	1117	C	C2-N1-C1'	8.09	127.70	118.80
48	A2	649	C	N3-C2-O2	-8.08	116.24	121.90
49	B1	428	U	N3-C2-O2	-8.08	116.55	122.20
49	B1	233	C	N1-C2-O2	8.06	123.73	118.90
48	A2	2228	C	C6-N1-C2	-8.04	117.08	120.30
49	B1	1555	U	N1-C2-O2	8.04	128.43	122.80
49	B1	892	U	C5-C6-N1	8.02	126.71	122.70
48	A2	3919	C	C6-N1-C2	-8.02	117.09	120.30
48	A2	2236	C	C6-N1-C1'	-8.01	111.19	120.80
47	At	106	LEU	CA-CB-CG	8.00	133.71	115.30
49	B1	1237	C	N1-C2-O2	8.00	123.70	118.90
7	A3	129	C	N1-C2-O2	7.96	123.68	118.90
48	A2	1256	G	N3-C4-N9	7.94	130.76	126.00
48	A2	4085	C	C6-N1-C2	-7.93	117.13	120.30
49	B1	1309	C	C2-N1-C1'	7.92	127.51	118.80
49	B1	496	C	N1-C2-O2	7.91	123.64	118.90
49	B1	67	C	N3-C2-O2	-7.90	116.37	121.90
49	B1	1309	C	N3-C2-O2	-7.84	116.41	121.90
48	A2	4406	C	N1-C2-O2	7.83	123.60	118.90
48	A2	650	C	N1-C2-O2	7.80	123.58	118.90
49	B1	1156	U	C2-N1-C1'	7.79	127.05	117.70
49	B1	89	C	C6-N1-C2	-7.78	117.19	120.30
48	A2	2241	G	C4-N9-C1'	7.76	136.59	126.50
7	A3	126	C	N3-C2-O2	-7.74	116.48	121.90
49	B1	118	C	C6-N1-C2	-7.73	117.21	120.30
48	A2	4545	C	N3-C2-O2	-7.73	116.49	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	A2	288	G	N3-C4-N9	-7.72	121.37	126.00
48	A2	4946	U	OP1-P-O3'	7.71	122.17	105.20
49	B1	1156	U	N3-C2-O2	-7.71	116.81	122.20
48	A2	2282	C	C6-N1-C2	-7.69	117.23	120.30
48	A2	3569	C	N1-C2-O2	7.68	123.51	118.90
48	A2	189	G	C8-N9-C4	-7.66	103.33	106.40
5	AC	150	LEU	C-N-CA	7.65	154.13	122.00
48	A2	2499	C	C2-N1-C1'	7.65	127.22	118.80
48	A2	1079	C	C6-N1-C2	-7.64	117.24	120.30
48	A2	1083	U	C5-C6-N1	7.64	126.52	122.70
48	A2	1484	G	N3-C4-N9	-7.64	121.42	126.00
48	A2	2470	C	C5-C6-N1	7.64	124.82	121.00
49	B1	688	U	N1-C2-O2	7.63	128.14	122.80
49	B1	843	C	C6-N1-C2	-7.63	117.25	120.30
48	A2	695	C	C6-N1-C2	-7.62	117.25	120.30
48	A2	1982	G	N1-C6-O6	7.61	124.46	119.90
49	B1	627	U	N3-C2-O2	-7.58	116.89	122.20
48	A2	962	C	C6-N1-C2	-7.58	117.27	120.30
48	A2	2467	C	C6-N1-C2	-7.57	117.27	120.30
48	A2	3616	U	N3-C2-O2	-7.57	116.90	122.20
49	B1	1490	G	O5'-P-OP2	-7.56	98.89	105.70
48	A2	153	G	N3-C2-N2	-7.56	114.61	119.90
48	A2	219	C	N1-C2-O2	7.55	123.43	118.90
49	B1	1398	G	C8-N9-C4	-7.51	103.40	106.40
48	A2	1499	G	C4-N9-C1'	7.47	136.21	126.50
48	A2	1422	C	C2-N1-C1'	7.47	127.01	118.80
49	B1	688	U	C2-N1-C1'	7.46	126.66	117.70
48	A2	1576	C	N3-C2-O2	-7.46	116.68	121.90
49	B1	1555	U	N3-C2-O2	-7.44	116.99	122.20
48	A2	1155	C	C6-N1-C2	-7.43	117.33	120.30
48	A2	220	G	C4-N9-C1'	7.43	136.16	126.50
48	A2	715	C	N3-C2-O2	-7.41	116.71	121.90
48	A2	4583	C	C6-N1-C2	-7.41	117.34	120.30
49	B1	1287	A	C2-N3-C4	7.41	114.30	110.60
48	A2	670	C	N1-C2-O2	7.41	123.34	118.90
48	A2	4633	C	N1-C2-O2	7.41	123.34	118.90
49	B1	1120	U	N1-C2-O2	7.41	127.98	122.80
7	A3	83	C	C6-N1-C2	-7.40	117.34	120.30
48	A2	670	C	N3-C2-O2	-7.40	116.72	121.90
48	A2	1232	C	C5-C6-N1	7.38	124.69	121.00
49	B1	592	C	N1-C2-O2	7.38	123.33	118.90
48	A2	4946	U	P-O3'-C3'	7.38	128.56	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	B1	1688	C	N1-C2-O2	7.38	123.33	118.90
48	A2	1564	U	C2-N1-C1'	7.37	126.55	117.70
48	A2	2499	C	N3-C2-O2	-7.37	116.74	121.90
48	A2	649	C	C2-N1-C1'	7.37	126.90	118.80
48	A2	456	G	N3-C4-N9	7.36	130.42	126.00
49	B1	1111	U	C2-N1-C1'	7.36	126.53	117.70
49	B1	1271	C	C6-N1-C2	-7.35	117.36	120.30
48	A2	2241	G	N3-C4-C5	-7.34	124.93	128.60
49	B1	989	C	N1-C2-O2	7.34	123.31	118.90
49	B1	797	C	P-O3'-C3'	7.33	128.49	119.70
48	A2	667	C	N3-C2-O2	-7.32	116.77	121.90
48	A2	3946	C	C5-C6-N1	7.32	124.66	121.00
48	A2	3616	U	N1-C2-O2	7.30	127.91	122.80
7	A3	105	C	C5-C4-N4	-7.29	115.09	120.20
48	A2	958	U	C2-N1-C1'	7.28	126.44	117.70
49	B1	96	C	C6-N1-C2	-7.27	117.39	120.30
48	A2	1254	G	C4-N9-C1'	7.26	135.94	126.50
48	A2	1254	G	N9-C4-C5	-7.25	102.50	105.40
7	A3	11	C	C6-N1-C2	-7.24	117.40	120.30
48	A2	1163	C	C6-N1-C2	-7.21	117.42	120.30
49	B1	1120	U	N3-C2-O2	-7.21	117.16	122.20
48	A2	4971	C	C6-N1-C2	-7.21	117.42	120.30
49	B1	1472	C	C6-N1-C1'	-7.20	112.16	120.80
48	A2	1254	G	C4-C5-C6	7.18	123.11	118.80
48	A2	2499	C	N1-C2-O2	7.18	123.21	118.90
49	B1	233	C	C2-N1-C1'	7.17	126.69	118.80
48	A2	1982	G	C5-C6-O6	-7.16	124.31	128.60
48	A2	1678	C	C6-N1-C2	-7.15	117.44	120.30
48	A2	3849	C	N1-C2-O2	7.14	123.18	118.90
48	A2	2283	U	N1-C2-O2	7.13	127.79	122.80
48	A2	4727	G	N3-C2-N2	-7.13	114.91	119.90
48	A2	901	U	P-O3'-C3'	7.12	128.24	119.70
48	A2	1430	C	C6-N1-C2	-7.12	117.45	120.30
49	B1	1442	U	C5-C6-N1	7.11	126.25	122.70
48	A2	3783	C	N1-C2-O2	7.09	123.16	118.90
48	A2	220	G	C8-N9-C1'	-7.08	117.79	127.00
51	BE	23	LEU	CA-CB-CG	7.08	131.59	115.30
48	A2	2766	A	N7-C8-N9	7.08	117.34	113.80
49	B1	887	U	C2-N1-C1'	7.08	126.19	117.70
49	B1	1053	C	C6-N1-C2	-7.08	117.47	120.30
48	A2	2373	G	C4-N9-C1'	7.07	135.69	126.50
48	A2	2241	G	N3-C4-N9	7.07	130.24	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	B1	645	C	C5-C6-N1	7.07	124.53	121.00
48	A2	4085	C	C6-N1-C1'	-7.05	112.33	120.80
48	A2	2373	G	C6-C5-N7	-7.04	126.17	130.40
48	A2	116	G	N3-C4-C5	7.04	132.12	128.60
48	A2	891	C	C5-C6-N1	7.02	124.51	121.00
58	BL	42	LEU	CA-CB-CG	7.02	131.45	115.30
7	A3	129	C	N3-C2-O2	-7.02	116.98	121.90
49	B1	797	C	OP2-P-O3'	7.02	120.64	105.20
48	A2	2478	C	N3-C2-O2	-7.01	116.99	121.90
48	A2	2228	C	C5-C6-N1	7.01	124.51	121.00
49	B1	621	C	C2-N1-C1'	7.00	126.50	118.80
49	B1	1111	U	N1-C2-O2	7.00	127.70	122.80
56	BJ	119	LEU	CA-CB-CG	6.99	131.38	115.30
48	A2	1637	C	N3-C2-O2	-6.99	117.01	121.90
48	A2	4717	G	N3-C2-N2	-6.98	115.01	119.90
48	A2	269	C	N1-C2-O2	6.98	123.09	118.90
49	B1	227	U	P-O3'-C3'	6.97	128.07	119.70
48	A2	4878	C	C6-N1-C2	-6.96	117.51	120.30
49	B1	1464	C	C6-N1-C2	-6.95	117.52	120.30
48	A2	197	U	N3-C2-O2	-6.94	117.34	122.20
49	B1	843	C	N3-C2-O2	-6.92	117.06	121.90
48	A2	1322	U	C2-N1-C1'	6.92	126.00	117.70
48	A2	119	G	N3-C4-C5	-6.91	125.14	128.60
48	A2	1466	G	C4-N9-C1'	6.91	135.48	126.50
48	A2	1401	C	N1-C2-O2	6.90	123.04	118.90
49	B1	1442	U	N1-C2-O2	6.89	127.62	122.80
49	B1	1557	C	N1-C2-O2	6.89	123.03	118.90
48	A2	4916	C	C5-C6-N1	6.88	124.44	121.00
48	A2	2778	G	C6-C5-N7	-6.88	126.27	130.40
48	A2	2846	C	N1-C2-O2	6.86	123.02	118.90
49	B1	186	C	C6-N1-C2	-6.85	117.56	120.30
48	A2	119	G	N3-C4-N9	6.83	130.10	126.00
49	B1	201	C	C6-N1-C2	-6.83	117.57	120.30
48	A2	219	C	N3-C2-O2	-6.81	117.13	121.90
49	B1	1261	C	C2-N1-C1'	6.81	126.29	118.80
49	B1	1557	C	C2-N1-C1'	6.80	126.28	118.80
7	A3	153	C	N1-C2-O2	6.79	122.98	118.90
49	B1	1586	U	C2-N1-C1'	6.79	125.85	117.70
48	A2	4717	G	C4-N9-C1'	-6.79	117.68	126.50
48	A2	2337	G	C5-C6-O6	-6.78	124.53	128.60
48	A2	4299	C	N1-C2-O2	6.78	122.97	118.90
48	A2	219	C	C6-N1-C2	-6.77	117.59	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	A2	2076	G	C4-N9-C1'	6.77	135.31	126.50
48	A2	1789	C	C6-N1-C2	-6.77	117.59	120.30
48	A2	4069	G	C8-N9-C1'	-6.77	118.20	127.00
48	A2	2000	C	N1-C2-O2	6.77	122.96	118.90
48	A2	2727	C	N1-C2-O2	6.76	122.96	118.90
7	A3	126	C	C6-N1-C2	-6.76	117.60	120.30
49	B1	1472	C	C6-N1-C2	-6.76	117.60	120.30
48	A2	1982	G	C4-C5-N7	6.76	113.50	110.80
48	A2	4880	C	N1-C2-O2	6.75	122.95	118.90
49	B1	539	C	C5-C6-N1	6.75	124.38	121.00
49	B1	959	G	C8-N9-C4	-6.75	103.70	106.40
48	A2	691	G	N3-C2-N2	-6.75	115.18	119.90
48	A2	456	G	C6-C5-N7	-6.74	126.36	130.40
48	A2	4947	U	C2-N1-C1'	6.73	125.78	117.70
48	A2	138	C	N1-C2-O2	6.73	122.94	118.90
49	B1	1426	U	N3-C2-O2	-6.73	117.49	122.20
48	A2	1163	C	C2-N1-C1'	6.72	126.19	118.80
11	AF	164	LYS	N-CA-C	-6.71	92.87	111.00
49	B1	1708	C	C6-N1-C2	-6.71	117.61	120.30
48	A2	448	U	O5'-P-OP1	-6.71	99.66	105.70
48	A2	197	U	C2-N1-C1'	6.71	125.75	117.70
48	A2	2373	G	C4-C5-N7	6.71	113.48	110.80
49	B1	496	C	C6-N1-C1'	-6.71	112.75	120.80
7	A3	100	U	N3-C2-O2	-6.70	117.51	122.20
48	A2	2738	G	O4'-C1'-N9	6.70	113.56	108.20
48	A2	1385	C	N1-C2-O2	6.69	122.91	118.90
48	A2	245	C	C6-N1-C2	-6.68	117.63	120.30
48	A2	1466	G	N3-C4-N9	6.68	130.01	126.00
49	B1	749	U	N1-C2-O2	6.68	127.48	122.80
48	A2	4951	G	N3-C4-N9	-6.68	121.99	126.00
49	B1	814	U	N1-C2-O2	6.68	127.47	122.80
48	A2	197	U	N1-C2-O2	6.67	127.47	122.80
48	A2	2688	C	C6-N1-C2	-6.67	117.63	120.30
48	A2	2065	C	N3-C2-O2	-6.67	117.23	121.90
49	B1	67	C	C6-N1-C1'	-6.65	112.82	120.80
48	A2	1576	C	N1-C2-O2	6.65	122.89	118.90
48	A2	4947	U	N1-C2-O2	6.64	127.45	122.80
48	A2	4205	C	N1-C2-O2	6.63	122.88	118.90
48	A2	4916	C	C6-N1-C2	-6.63	117.65	120.30
48	A2	5008	C	C6-N1-C2	-6.63	117.65	120.30
48	A2	2241	G	C8-N9-C1'	-6.63	118.39	127.00
80	Bv	25	C	C6-N1-C2	-6.62	117.65	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A3	37	A	N3-C4-C5	6.61	131.43	126.80
32	Ab	112	ILE	N-CA-C	6.61	128.85	111.00
48	A2	196	G	N3-C4-N9	-6.61	122.04	126.00
48	A2	1342	G	OP2-P-O3'	6.61	119.73	105.20
7	A3	38	U	N1-C2-O2	6.60	127.42	122.80
48	A2	4878	C	C5-C6-N1	6.60	124.30	121.00
48	A2	4633	C	C2-N1-C1'	6.60	126.06	118.80
48	A2	1594	G	C4-N9-C1'	6.59	135.07	126.50
48	A2	1997	C	C2-N3-C4	6.59	123.20	119.90
48	A2	1880	G	C4-N9-C1'	6.59	135.07	126.50
48	A2	698	C	N1-C2-O2	6.59	122.85	118.90
48	A2	4858	C	C5-C6-N1	6.58	124.29	121.00
48	A2	4678	C	C6-N1-C2	-6.58	117.67	120.30
48	A2	2556	C	C6-N1-C2	-6.57	117.67	120.30
48	A2	1176	C	N1-C2-O2	6.56	122.84	118.90
49	B1	1847	G	C4-C5-N7	6.55	113.42	110.80
48	A2	2003	C	N1-C2-O2	6.55	122.83	118.90
48	A2	2236	C	C5-C6-N1	6.55	124.28	121.00
48	A2	1082	C	C6-N1-C2	-6.55	117.68	120.30
48	A2	219	C	O4'-C1'-N1	6.54	113.43	108.20
48	A2	1256	G	C4-N9-C1'	6.54	135.01	126.50
48	A2	918	C	C6-N1-C1'	-6.53	112.96	120.80
48	A2	4715	U	N3-C2-O2	-6.53	117.63	122.20
49	B1	989	C	N3-C2-O2	-6.53	117.33	121.90
41	Ak	60	LEU	CA-CB-CG	6.52	130.30	115.30
48	A2	48	G	C4-N9-C1'	-6.52	118.02	126.50
48	A2	1594	G	C4-C5-N7	6.52	113.41	110.80
49	B1	1156	U	N1-C2-O2	6.52	127.36	122.80
80	Bv	42	C	C2-N1-C1'	6.52	125.97	118.80
48	A2	1737	C	C6-N1-C2	-6.51	117.69	120.30
48	A2	4951	G	N3-C2-N2	-6.51	115.34	119.90
48	A2	1268	U	C5-C6-N1	-6.51	119.44	122.70
48	A2	2728	C	C6-N1-C2	-6.51	117.70	120.30
49	B1	106	C	C5-C6-N1	6.50	124.25	121.00
48	A2	504	U	C5-C6-N1	6.50	125.95	122.70
48	A2	2325	C	N3-C2-O2	-6.50	117.35	121.90
48	A2	958	U	N1-C2-O2	6.49	127.34	122.80
48	A2	1087	C	N1-C2-O2	6.49	122.80	118.90
49	B1	1555	U	C6-N1-C1'	-6.49	112.11	121.20
48	A2	1254	G	N1-C2-N2	6.49	122.04	116.20
49	B1	621	C	C6-N1-C2	-6.48	117.71	120.30
48	A2	4645	U	N3-C2-O2	-6.48	117.67	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	A2	2650	C	C6-N1-C2	-6.47	117.71	120.30
49	B1	959	G	C6-C5-N7	-6.47	126.52	130.40
48	A2	1390	C	N1-C2-O2	6.47	122.78	118.90
48	A2	1875	C	C6-N1-C2	-6.47	117.71	120.30
49	B1	1553	C	C6-N1-C2	-6.46	117.72	120.30
54	BH	115	LYS	C-N-CA	6.46	137.85	121.70
49	B1	201	C	C5-C6-N1	6.46	124.23	121.00
48	A2	2574	C	C6-N1-C2	-6.46	117.72	120.30
49	B1	620	G	N3-C4-C5	-6.46	125.37	128.60
7	A3	1	C	C6-N1-C2	-6.45	117.72	120.30
49	B1	35	C	C6-N1-C2	-6.45	117.72	120.30
49	B1	843	C	N1-C2-O2	6.45	122.77	118.90
48	A2	1907	C	C6-N1-C2	-6.45	117.72	120.30
49	B1	67	C	C6-N1-C2	-6.44	117.72	120.30
49	B1	1398	G	C8-N9-C1'	-6.44	118.63	127.00
49	B1	1203	G	C4-C5-N7	6.43	113.37	110.80
48	A2	1385	C	C6-N1-C2	-6.43	117.73	120.30
49	B1	814	U	N3-C2-O2	-6.43	117.70	122.20
48	A2	36	U	C5-C6-N1	6.42	125.91	122.70
48	A2	1163	C	C5-C6-N1	6.41	124.21	121.00
49	B1	238	C	C6-N1-C2	-6.41	117.73	120.30
49	B1	959	G	N7-C8-N9	6.41	116.31	113.10
48	A2	1484	G	N3-C4-C5	6.40	131.80	128.60
49	B1	183	G	N3-C4-C5	-6.40	125.40	128.60
48	A2	1982	G	N3-C4-N9	6.40	129.84	126.00
48	A2	2727	C	C6-N1-C1'	-6.39	113.13	120.80
48	A2	3749	U	N1-C2-O2	6.39	127.27	122.80
48	A2	2398	C	C2-N1-C1'	6.38	125.82	118.80
8	A4	118	C	N1-C2-O2	6.38	122.73	118.90
49	B1	387	C	C5-C6-N1	6.37	124.19	121.00
48	A2	3590	G	C4-C5-N7	6.37	113.35	110.80
49	B1	1837	G	N3-C4-N9	-6.37	122.18	126.00
7	A3	129	C	C2-N1-C1'	6.36	125.80	118.80
48	A2	219	C	C6-N1-C1'	-6.36	113.17	120.80
48	A2	4713	G	N3-C4-C5	6.36	131.78	128.60
7	A3	57	C	C5-C6-N1	6.35	124.18	121.00
48	A2	2480	C	C6-N1-C2	-6.35	117.76	120.30
48	A2	4880	C	C2-N1-C1'	6.35	125.79	118.80
49	B1	1230	C	N1-C2-O2	6.35	122.71	118.90
49	B1	1664	A	O4'-C1'-N9	6.35	113.28	108.20
48	A2	667	C	N1-C2-O2	6.35	122.71	118.90
49	B1	1441	U	N3-C2-O2	-6.35	117.76	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	B1	1495	G	C8-N9-C4	-6.34	103.86	106.40
49	B1	1600	G	N3-C4-N9	6.34	129.81	126.00
48	A2	1499	G	C8-N9-C1'	-6.34	118.76	127.00
49	B1	1398	G	N7-C8-N9	6.34	116.27	113.10
48	A2	74	G	C5-C6-O6	-6.34	124.80	128.60
48	A2	958	U	N3-C2-O2	-6.32	117.77	122.20
48	A2	1563	G	C4-N9-C1'	6.32	134.72	126.50
48	A2	1648	C	C6-N1-C2	-6.32	117.77	120.30
48	A2	1501	C	C6-N1-C2	-6.32	117.77	120.30
49	B1	627	U	N1-C2-O2	6.32	127.22	122.80
48	A2	237	G	C2-N3-C4	-6.31	108.74	111.90
48	A2	2389	C	C6-N1-C2	-6.31	117.78	120.30
48	A2	119	G	C4-N9-C1'	6.31	134.70	126.50
48	A2	4008	C	C5-C6-N1	6.31	124.15	121.00
48	A2	4406	C	N3-C2-O2	-6.31	117.49	121.90
48	A2	1256	G	C8-N9-C1'	-6.30	118.81	127.00
48	A2	233	G	N3-C2-N2	-6.30	115.49	119.90
49	B1	1286	G	OP1-P-O3'	6.29	119.05	105.20
7	A3	57	C	N1-C2-O2	6.29	122.67	118.90
48	A2	4717	G	C8-N9-C1'	6.28	135.17	127.00
48	A2	476	G	N3-C4-N9	-6.28	122.23	126.00
48	A2	2282	C	C5-C6-N1	6.28	124.14	121.00
48	A2	3947	C	C6-N1-C2	-6.28	117.79	120.30
48	A2	2778	G	C4-C5-N7	6.27	113.31	110.80
48	A2	2065	C	C2-N1-C1'	6.27	125.69	118.80
49	B1	1203	G	C6-C5-N7	-6.26	126.64	130.40
48	A2	634	C	N1-C2-O2	6.26	122.65	118.90
48	A2	207	C	N1-C2-O2	6.25	122.65	118.90
48	A2	709	C	N3-C2-O2	-6.25	117.52	121.90
48	A2	2325	C	N1-C2-O2	6.25	122.65	118.90
49	B1	38	A	O5'-P-OP1	-6.25	100.08	105.70
49	B1	1683	C	N1-C2-O2	6.25	122.65	118.90
48	A2	4583	C	C5-C6-N1	6.24	124.12	121.00
48	A2	1401	C	C5-C6-N1	6.24	124.12	121.00
59	BM	26	LEU	CA-CB-CG	6.24	129.64	115.30
48	A2	450	C	C6-N1-C2	-6.23	117.81	120.30
48	A2	2051	U	C2-N1-C1'	6.22	125.17	117.70
48	A2	4971	C	C5-C6-N1	6.22	124.11	121.00
48	A2	2846	C	N3-C2-O2	-6.22	117.55	121.90
48	A2	698	C	C2-N1-C1'	6.22	125.64	118.80
7	A3	100	U	N1-C2-O2	6.21	127.15	122.80
48	A2	2283	U	N3-C2-O2	-6.21	117.85	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	A2	947	A	P-O3'-C3'	6.21	127.15	119.70
49	B1	330	G	C2-N3-C4	6.21	115.00	111.90
49	B1	331	C	C6-N1-C2	-6.21	117.82	120.30
49	B1	496	C	N3-C2-O2	-6.21	117.56	121.90
48	A2	474	C	C6-N1-C2	-6.20	117.82	120.30
48	A2	3818	C	C6-N1-C2	-6.20	117.82	120.30
49	B1	113	G	OP2-P-O3'	6.20	118.85	105.20
48	A2	702	A	N1-C6-N6	-6.20	114.88	118.60
48	A2	465	A	C8-N9-C4	-6.20	103.32	105.80
48	A2	1548	C	N1-C2-O2	6.20	122.62	118.90
49	B1	106	C	C6-N1-C2	-6.19	117.82	120.30
49	B1	1117	C	O4'-C1'-N1	6.19	113.15	108.20
48	A2	1083	U	N1-C2-O2	6.18	127.13	122.80
48	A2	3946	C	C6-N1-C2	-6.18	117.83	120.30
48	A2	4837	C	C6-N1-C2	-6.17	117.83	120.30
48	A2	715	C	N1-C2-O2	6.17	122.60	118.90
48	A2	961	C	C6-N1-C2	-6.17	117.83	120.30
48	A2	1422	C	N1-C2-O2	6.17	122.60	118.90
48	A2	2533	U	N3-C2-O2	-6.17	117.88	122.20
48	A2	2051	U	N1-C2-O2	6.17	127.12	122.80
48	A2	288	G	N3-C4-C5	6.16	131.68	128.60
49	B1	951	C	C6-N1-C2	-6.16	117.83	120.30
7	A3	57	C	N3-C2-O2	-6.16	117.59	121.90
49	B1	1837	G	C4-N9-C1'	-6.16	118.49	126.50
48	A2	974	C	C6-N1-C2	-6.16	117.84	120.30
48	A2	2236	C	C6-N1-C2	-6.16	117.83	120.30
48	A2	4947	U	C5-C6-N1	6.16	125.78	122.70
49	B1	1847	G	C6-C5-N7	-6.16	126.70	130.40
15	AJ	128	LEU	CA-CB-CG	6.16	129.46	115.30
49	B1	1542	C	C6-N1-C2	-6.16	117.84	120.30
48	A2	2441	C	C5-C6-N1	6.15	124.08	121.00
48	A2	1367	C	C6-N1-C2	-6.15	117.84	120.30
48	A2	3659	U	C5-C6-N1	6.15	125.78	122.70
49	B1	234	C	C6-N1-C2	-6.15	117.84	120.30
48	A2	1834	G	C8-N9-C4	-6.14	103.94	106.40
48	A2	2690	G	N3-C4-C5	6.13	131.67	128.60
49	B1	1117	C	N3-C2-O2	-6.13	117.61	121.90
48	A2	1254	G	C8-N9-C1'	-6.13	119.03	127.00
48	A2	4670	A	C2-N3-C4	6.13	113.66	110.60
76	Bd	39	CYS	C-N-CA	6.12	137.00	121.70
80	Bv	20	U	N1-C2-O2	6.12	127.08	122.80
10	AE	212	LEU	CA-CB-CG	6.12	129.37	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	B1	1600	G	N3-C4-C5	-6.12	125.54	128.60
49	B1	1111	U	C5-C6-N1	6.11	125.75	122.70
49	B1	688	U	C5-C6-N1	6.09	125.75	122.70
48	A2	2373	G	N7-C8-N9	6.09	116.15	113.10
49	B1	940	U	N3-C2-O2	-6.09	117.94	122.20
49	B1	984	C	C6-N1-C2	-6.09	117.86	120.30
49	B1	1546	G	N7-C8-N9	6.08	116.14	113.10
72	BZ	99	LEU	CA-CB-CG	6.08	129.28	115.30
48	A2	653	G	C4-N9-C1'	-6.08	118.60	126.50
48	A2	2758	C	C5-C6-N1	6.08	124.04	121.00
7	A3	153	C	N3-C2-O2	-6.07	117.65	121.90
48	A2	2676	A	N1-C6-N6	-6.07	114.96	118.60
48	A2	3749	U	C2-N1-C1'	6.06	124.98	117.70
49	B1	20	G	N3-C4-N9	6.06	129.64	126.00
48	A2	3749	U	N3-C2-O2	-6.06	117.96	122.20
48	A2	1815	U	N1-C2-O2	6.06	127.04	122.80
48	A2	1151	G	C6-C5-N7	-6.05	126.77	130.40
48	A2	2727	C	N3-C2-O2	-6.05	117.66	121.90
48	A2	4854	G	N3-C4-C5	6.05	131.63	128.60
49	B1	1742	C	N1-C2-O2	6.05	122.53	118.90
2	BA	31	ASP	CB-CG-OD1	6.05	123.74	118.30
48	A2	288	G	C8-N9-C1'	6.04	134.86	127.00
49	B1	1085	C	N1-C2-O2	6.04	122.53	118.90
49	B1	1557	C	N3-C2-O2	-6.04	117.67	121.90
48	A2	1385	C	C5-C6-N1	6.04	124.02	121.00
48	A2	1322	U	N1-C2-O2	6.04	127.03	122.80
48	A2	2667	G	C4-N9-C1'	6.04	134.35	126.50
49	B1	1237	C	N3-C2-O2	-6.04	117.67	121.90
5	AC	229	LEU	CA-CB-CG	6.03	129.18	115.30
48	A2	1576	C	C2-N1-C1'	6.03	125.44	118.80
48	A2	899	G	N3-C4-N9	6.03	129.62	126.00
48	A2	3888	A	C8-N9-C4	-6.03	103.39	105.80
49	B1	1593	C	C6-N1-C2	-6.03	117.89	120.30
48	A2	224	A	N1-C6-N6	6.02	122.21	118.60
48	A2	698	C	N3-C2-O2	-6.02	117.69	121.90
48	A2	237	G	N3-C4-N9	-6.02	122.39	126.00
48	A2	1865	C	C5-C6-N1	6.02	124.01	121.00
49	B1	1442	U	N3-C2-O2	-6.02	117.99	122.20
49	B1	96	C	C6-N1-C1'	-6.00	113.59	120.80
48	A2	1193	C	N1-C2-O2	6.00	122.50	118.90
49	B1	1747	C	N1-C2-O2	6.00	122.50	118.90
49	B1	1261	C	C6-N1-C2	-6.00	117.90	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	A2	3749	U	C5-C6-N1	6.00	125.70	122.70
48	A2	1298	C	N1-C2-O2	5.99	122.50	118.90
48	A2	4270	C	C6-N1-C2	-5.99	117.91	120.30
48	A2	1982	G	C4-C5-C6	5.98	122.39	118.80
49	B1	37	C	C6-N1-C2	-5.98	117.91	120.30
48	A2	1466	G	C8-N9-C1'	-5.98	119.23	127.00
49	B1	428	U	C6-N1-C1'	-5.98	112.83	121.20
48	A2	970	C	C5-C6-N1	5.97	123.99	121.00
3	AB	292	LEU	CA-CB-CG	5.97	129.04	115.30
48	A2	4909	G	C4-N9-C1'	5.97	134.26	126.50
11	AF	165	LYS	CA-CB-CG	5.97	126.53	113.40
49	B1	1460	C	C6-N1-C2	-5.97	117.91	120.30
48	A2	454	C	C6-N1-C2	-5.97	117.91	120.30
48	A2	927	C	N3-C2-O2	-5.96	117.72	121.90
48	A2	4069	G	N3-C4-C5	-5.96	125.62	128.60
48	A2	2766	A	C4-N9-C1'	5.96	137.02	126.30
48	A2	3659	U	N3-C2-O2	-5.96	118.03	122.20
48	A2	3621	C	C6-N1-C2	-5.95	117.92	120.30
48	A2	1424	C	C2-N1-C1'	5.95	125.35	118.80
48	A2	2690	G	N3-C4-N9	-5.95	122.43	126.00
48	A2	2766	A	C8-N9-C4	-5.95	103.42	105.80
49	B1	1677	U	C5-C6-N1	5.95	125.67	122.70
7	A3	85	U	N3-C2-O2	-5.94	118.04	122.20
48	A2	667	C	C6-N1-C2	-5.94	117.92	120.30
49	B1	89	C	C6-N1-C1'	-5.94	113.67	120.80
49	B1	1717	C	C6-N1-C2	-5.94	117.92	120.30
48	A2	1197	C	N3-C2-O2	-5.94	117.74	121.90
48	A2	3659	U	C6-N1-C2	-5.94	117.44	121.00
49	B1	1546	G	C8-N9-C4	-5.94	104.02	106.40
48	A2	2829	A	C2-N3-C4	5.93	113.57	110.60
48	A2	4884	C	C6-N1-C2	-5.93	117.93	120.30
8	A4	52	C	C6-N1-C2	-5.93	117.93	120.30
48	A2	634	C	C6-N1-C2	-5.93	117.93	120.30
48	A2	3932	G	C4-C5-N7	5.93	113.17	110.80
48	A2	3837	C	C6-N1-C2	-5.92	117.93	120.30
48	A2	1564	U	C6-N1-C1'	-5.92	112.91	121.20
48	A2	196	G	C4-N9-C1'	-5.92	118.81	126.50
48	A2	2000	C	N3-C2-O2	-5.91	117.76	121.90
48	A2	1056	G	N3-C2-N2	-5.91	115.76	119.90
49	B1	1753	C	C6-N1-C2	-5.90	117.94	120.30
48	A2	1151	G	N3-C4-N9	5.90	129.54	126.00
48	A2	4715	U	N1-C2-O2	5.90	126.93	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	A2	4658	C	N1-C2-O2	5.90	122.44	118.90
48	A2	220	G	N3-C4-N9	5.90	129.54	126.00
49	B1	238	C	C5-C6-N1	5.89	123.95	121.00
49	B1	741	C	N1-C2-O2	5.89	122.43	118.90
48	A2	653	G	N3-C4-N9	-5.89	122.47	126.00
48	A2	316	C	N1-C2-O2	5.89	122.43	118.90
48	A2	4859	G	N3-C4-N9	5.89	129.53	126.00
48	A2	1880	G	C8-N9-C1'	-5.88	119.35	127.00
49	B1	234	C	C5-C6-N1	5.88	123.94	121.00
48	A2	71	C	P-O3'-C3'	5.88	126.76	119.70
48	A2	1708	U	N3-C2-O2	-5.88	118.08	122.20
48	A2	4717	G	N1-C2-N2	5.88	121.49	116.20
49	B1	1444	U	N1-C2-O2	5.88	126.92	122.80
48	A2	1982	G	C5-N7-C8	-5.88	101.36	104.30
48	A2	2441	C	C6-N1-C2	-5.88	117.95	120.30
48	A2	3656	C	C5-C6-N1	5.88	123.94	121.00
49	B1	1696	C	C5-C6-N1	5.87	123.94	121.00
48	A2	1353	G	O5'-P-OP1	-5.87	100.42	105.70
48	A2	898	U	C5-C6-N1	5.87	125.63	122.70
48	A2	2076	G	N3-C4-C5	-5.86	125.67	128.60
48	A2	1067	C	N1-C2-O2	5.86	122.42	118.90
48	A2	2461	C	C6-N1-C2	-5.86	117.96	120.30
49	B1	1317	C	N1-C2-O2	5.85	122.41	118.90
7	A3	109	C	P-O3'-C3'	5.85	126.72	119.70
48	A2	931	A	N7-C8-N9	5.85	116.72	113.80
48	A2	1484	G	C8-N9-C1'	5.85	134.60	127.00
48	A2	1460	C	C5-C6-N1	5.84	123.92	121.00
48	A2	4050	C	N1-C2-O2	5.84	122.41	118.90
48	A2	650	C	N3-C2-O2	-5.84	117.81	121.90
48	A2	4080	U	N3-C2-O2	-5.84	118.11	122.20
49	B1	659	G	N3-C4-C5	-5.84	125.68	128.60
48	A2	1982	G	N3-C4-C5	-5.84	125.68	128.60
48	A2	3621	C	N1-C2-O2	5.84	122.40	118.90
49	B1	1600	G	C4-N9-C1'	5.83	134.09	126.50
48	A2	2373	G	N3-C4-N9	5.83	129.50	126.00
7	A3	129	C	C6-N1-C2	-5.83	117.97	120.30
48	A2	4295	C	C6-N1-C2	-5.83	117.97	120.30
8	A4	36	C	C6-N1-C2	-5.82	117.97	120.30
48	A2	1737	C	N3-C2-O2	-5.82	117.83	121.90
48	A2	2691	G	C4-N9-C1'	5.82	134.06	126.50
48	A2	119	G	C2-N3-C4	5.81	114.81	111.90
48	A2	2327	G	N3-C4-N9	-5.81	122.52	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A3	57	C	C2-N1-C1'	5.81	125.19	118.80
48	A2	1484	G	C4-N9-C1'	-5.81	118.95	126.50
48	A2	2676	A	C4-C5-C6	-5.81	114.10	117.00
48	A2	2766	A	C5-N7-C8	-5.81	101.00	103.90
80	Bv	4	C	N1-C2-O2	5.81	122.39	118.90
49	B1	1163	C	C2-N1-C1'	5.80	125.18	118.80
48	A2	1429	C	C6-N1-C2	-5.80	117.98	120.30
48	A2	4299	C	N3-C2-O2	-5.80	117.84	121.90
49	B1	1752	C	C6-N1-C2	-5.80	117.98	120.30
48	A2	1281	C	N1-C2-O2	5.80	122.38	118.90
48	A2	3837	C	C5-C6-N1	5.80	123.90	121.00
48	A2	1225	G	N3-C4-C5	-5.79	125.70	128.60
49	B1	659	G	C4-N9-C1'	5.79	134.03	126.50
48	A2	2054	C	C6-N1-C2	-5.79	117.98	120.30
49	B1	1794	C	C6-N1-C2	-5.79	117.98	120.30
48	A2	1466	G	N3-C4-C5	-5.78	125.71	128.60
7	A3	38	U	C4-C5-C6	-5.78	116.23	119.70
48	A2	2699	C	C6-N1-C2	-5.78	117.99	120.30
49	B1	621	C	N3-C2-O2	-5.78	117.86	121.90
48	A2	1079	C	C5-C6-N1	5.78	123.89	121.00
35	Ae	19	LYS	CA-CB-CG	5.77	126.10	113.40
48	A2	269	C	N3-C2-O2	-5.77	117.86	121.90
48	A2	4858	C	N1-C2-O2	5.77	122.36	118.90
48	A2	1499	G	N3-C4-N9	5.77	129.46	126.00
48	A2	1930	U	N1-C2-O2	5.77	126.84	122.80
48	A2	4909	G	C6-C5-N7	-5.76	126.94	130.40
48	A2	653	G	C8-N9-C1'	5.76	134.49	127.00
48	A2	1907	C	C5-C6-N1	5.76	123.88	121.00
48	A2	3853	C	N1-C2-O2	5.76	122.36	118.90
48	A2	1737	C	N1-C2-O2	5.76	122.36	118.90
49	B1	1271	C	C5-C6-N1	5.76	123.88	121.00
49	B1	1117	C	C6-N1-C1'	-5.76	113.89	120.80
48	A2	1594	G	C8-N9-C1'	-5.75	119.52	127.00
48	A2	1550	C	C6-N1-C2	-5.75	118.00	120.30
48	A2	2325	C	C2-N1-C1'	5.75	125.13	118.80
49	B1	1163	C	N1-C2-O2	5.75	122.35	118.90
7	A3	86	U	C5-C6-N1	5.74	125.57	122.70
48	A2	4920	C	C5-C6-N1	5.74	123.87	121.00
48	A2	485	G	C2-N3-C4	5.74	114.77	111.90
7	A3	126	C	C6-N1-C1'	-5.73	113.92	120.80
48	A2	1401	C	C6-N1-C2	-5.73	118.01	120.30
49	B1	1111	U	N3-C2-O2	-5.73	118.19	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	B1	20	G	C4-N9-C1'	5.73	133.95	126.50
49	B1	989	C	C2-N1-C1'	5.72	125.09	118.80
49	B1	438	G	N3-C2-N2	-5.72	115.90	119.90
48	A2	1056	G	N3-C4-N9	-5.71	122.57	126.00
48	A2	1322	U	C5-C6-N1	5.71	125.56	122.70
48	A2	1614	A	C2-N3-C4	5.71	113.46	110.60
49	B1	233	C	N3-C2-O2	-5.71	117.90	121.90
48	A2	2706	C	C6-N1-C2	-5.71	118.02	120.30
48	A2	1151	G	C4-N9-C1'	5.71	133.92	126.50
48	A2	4397	U	N3-C2-O2	-5.71	118.20	122.20
48	A2	214	C	N3-C2-O2	-5.70	117.91	121.90
48	A2	289	A	C4-N9-C1'	5.70	136.57	126.30
48	A2	1079	C	N1-C2-O2	5.70	122.32	118.90
48	A2	4837	C	C5-C6-N1	5.70	123.85	121.00
48	A2	951	G	N3-C4-N9	5.70	129.42	126.00
48	A2	3737	A	O4'-C1'-N9	5.69	112.75	108.20
48	A2	4941	C	C6-N1-C2	-5.69	118.02	120.30
49	B1	193	C	N1-C2-O2	5.69	122.31	118.90
49	B1	1683	C	C6-N1-C2	-5.69	118.03	120.30
7	A3	86	U	N3-C2-O2	-5.69	118.22	122.20
48	A2	1871	G	C4-C5-N7	5.68	113.07	110.80
48	A2	2478	C	C2-N1-C1'	5.68	125.05	118.80
48	A2	1594	G	C6-C5-N7	-5.68	126.99	130.40
48	A2	2533	U	N1-C2-O2	5.68	126.78	122.80
48	A2	3780	G	N3-C4-C5	5.68	131.44	128.60
48	A2	1424	C	N1-C2-O2	5.68	122.31	118.90
49	B1	1593	C	N1-C2-O2	5.67	122.30	118.90
49	B1	165	G	N3-C4-N9	-5.67	122.60	126.00
48	A2	2388	U	C2-N1-C1'	5.67	124.50	117.70
52	BF	77	MET	CA-CB-CG	5.67	122.93	113.30
7	A3	138	C	C6-N1-C2	-5.66	118.03	120.30
48	A2	709	C	N1-C2-O2	5.66	122.30	118.90
48	A2	2076	G	N3-C4-N9	5.66	129.40	126.00
49	B1	626	G	C4-C5-N7	5.66	113.06	110.80
49	B1	887	U	N1-C2-O2	5.66	126.76	122.80
48	A2	74	G	N1-C6-O6	5.66	123.29	119.90
48	A2	4834	U	C2-N3-C4	5.66	130.39	127.00
48	A2	4008	C	C6-N1-C2	-5.66	118.04	120.30
49	B1	330	G	N3-C4-C5	-5.66	125.77	128.60
49	B1	1555	U	C5-C6-N1	5.66	125.53	122.70
7	A3	100	U	C2-N1-C1'	5.65	124.48	117.70
48	A2	970	C	C6-N1-C2	-5.65	118.04	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	B1	749	U	N3-C2-O2	-5.65	118.24	122.20
48	A2	1269	C	C6-N1-C2	-5.65	118.04	120.30
48	A2	4563	U	C2-N1-C1'	5.65	124.48	117.70
49	B1	65	C	C6-N1-C2	-5.65	118.04	120.30
48	A2	2480	C	C5-C6-N1	5.65	123.82	121.00
7	A3	7	U	N3-C2-O2	-5.65	118.25	122.20
48	A2	4624	C	C6-N1-C2	-5.65	118.04	120.30
48	A2	1740	G	N3-C4-C5	-5.64	125.78	128.60
49	B1	402	C	C5-C6-N1	5.64	123.82	121.00
16	AL	81	LEU	CA-CB-CG	5.64	128.27	115.30
49	B1	796	G	N3-C4-C5	-5.64	125.78	128.60
49	B1	1683	C	N3-C2-O2	-5.64	117.95	121.90
48	A2	2604	U	N3-C2-O2	-5.63	118.26	122.20
48	A2	344	C	N3-C2-O2	-5.63	117.96	121.90
48	A2	2793	C	C2-N1-C1'	5.62	124.99	118.80
48	A2	2604	U	N1-C2-O2	5.62	126.74	122.80
49	B1	1254	C	N1-C2-O2	5.62	122.28	118.90
48	A2	4069	G	N7-C8-N9	5.62	115.91	113.10
49	B1	1006	C	C6-N1-C2	-5.62	118.05	120.30
48	A2	2758	C	C6-N1-C2	-5.62	118.05	120.30
49	B1	67	C	C5-C6-N1	5.62	123.81	121.00
49	B1	1593	C	C5-C6-N1	5.61	123.81	121.00
48	A2	216	G	C8-N9-C4	-5.61	104.16	106.40
48	A2	1678	C	C5-C6-N1	5.61	123.81	121.00
48	A2	116	G	C8-N9-C1'	5.61	134.29	127.00
48	A2	4021	C	C6-N1-C2	-5.60	118.06	120.30
48	A2	4371	C	C6-N1-C2	-5.60	118.06	120.30
48	A2	1221	A	N3-C4-C5	5.60	130.72	126.80
49	B1	1309	C	C6-N1-C2	-5.60	118.06	120.30
48	A2	4069	G	N3-C4-N9	5.60	129.36	126.00
48	A2	3606	A	N1-C6-N6	5.60	121.96	118.60
48	A2	1424	C	C6-N1-C2	-5.59	118.06	120.30
48	A2	3670	C	C6-N1-C2	-5.59	118.06	120.30
8	A4	92	C	C6-N1-C2	-5.59	118.06	120.30
48	A2	4101	C	C5-C6-N1	5.59	123.79	121.00
49	B1	192	C	N1-C2-O2	5.59	122.25	118.90
48	A2	3762	C	N1-C2-O2	5.59	122.25	118.90
48	A2	1256	G	N3-C4-C5	-5.59	125.81	128.60
48	A2	1637	C	C2-N1-C1'	5.59	124.94	118.80
48	A2	3621	C	N3-C2-O2	-5.58	117.99	121.90
5	AC	52	TYR	CA-CB-CG	5.58	124.00	113.40
49	B1	1053	C	C5-C6-N1	5.58	123.79	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	A2	1958	C	C6-N1-C2	-5.58	118.07	120.30
48	A2	927	C	N1-C2-O2	5.57	122.24	118.90
48	A2	2088	G	C8-N9-C4	-5.57	104.17	106.40
48	A2	1065	C	C6-N1-C2	-5.57	118.07	120.30
49	B1	1120	U	C2-N1-C1'	5.57	124.38	117.70
48	A2	3853	C	C6-N1-C2	-5.57	118.07	120.30
49	B1	1837	G	C8-N9-C1'	5.57	134.24	127.00
49	B1	1473	G	O4'-C1'-N9	5.57	112.65	108.20
48	A2	4397	U	N1-C2-O2	5.56	126.69	122.80
48	A2	2863	G	C4-N9-C1'	5.56	133.73	126.50
48	A2	4713	G	N3-C4-N9	-5.56	122.67	126.00
48	A2	196	G	C8-N9-C1'	5.55	134.22	127.00
49	B1	1112	U	C5-C6-N1	5.55	125.47	122.70
49	B1	688	U	C2-N3-C4	5.55	130.33	127.00
49	B1	1268	C	C6-N1-C2	-5.55	118.08	120.30
49	B1	1237	C	C2-N1-C1'	5.54	124.90	118.80
48	A2	649	C	C6-N1-C2	-5.54	118.08	120.30
49	B1	891	G	N3-C4-N9	5.54	129.33	126.00
48	A2	4489	G	N3-C4-C5	-5.54	125.83	128.60
49	B1	165	G	N3-C4-C5	5.54	131.37	128.60
48	A2	4304	C	N3-C2-O2	-5.53	118.03	121.90
48	A2	483	C	N1-C2-O2	5.53	122.22	118.90
48	A2	2480	C	N1-C2-O2	5.53	122.22	118.90
49	B1	308	G	C4-N9-C1'	5.53	133.69	126.50
48	A2	3853	C	N3-C2-O2	-5.53	118.03	121.90
48	A2	1223	G	N3-C4-C5	-5.53	125.83	128.60
48	A2	1460	C	C6-N1-C2	-5.53	118.09	120.30
49	B1	1837	G	N3-C4-C5	5.52	131.36	128.60
48	A2	2076	G	C8-N9-C1'	-5.52	119.82	127.00
48	A2	3849	C	N3-C2-O2	-5.52	118.03	121.90
49	B1	1398	G	N3-C4-C5	-5.52	125.84	128.60
48	A2	899	G	C6-C5-N7	-5.52	127.09	130.40
48	A2	227	G	C6-C5-N7	-5.51	127.09	130.40
48	A2	1610	C	C6-N1-C2	-5.51	118.09	120.30
48	A2	2706	C	C5-C6-N1	5.51	123.76	121.00
48	A2	2770	C	C6-N1-C2	-5.51	118.10	120.30
48	A2	2373	G	C8-N9-C4	-5.51	104.20	106.40
49	B1	1705	C	C6-N1-C2	-5.51	118.10	120.30
49	B1	657	U	N1-C2-O2	5.51	126.66	122.80
48	A2	2289	C	C6-N1-C2	-5.50	118.10	120.30
49	B1	165	G	N3-C2-N2	-5.50	116.05	119.90
7	A3	86	U	N1-C2-O2	5.50	126.65	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	Ae	78	LEU	CA-CB-CG	5.50	127.95	115.30
48	A2	440	C	N1-C2-O2	5.50	122.20	118.90
48	A2	1538	C	C6-N1-C2	-5.50	118.10	120.30
48	A2	4205	C	N3-C2-O2	-5.50	118.05	121.90
7	A3	37	A	O4'-C1'-N9	-5.49	103.81	108.20
48	A2	48	G	C8-N9-C1'	5.49	134.14	127.00
48	A2	2389	C	C2-N1-C1'	5.49	124.84	118.80
5	AC	230	LEU	CA-CB-CG	5.49	127.93	115.30
48	A2	899	G	N1-C2-N2	-5.48	111.27	116.20
49	B1	1752	C	C5-C6-N1	5.48	123.74	121.00
48	A2	650	C	C2-N1-C1'	5.48	124.83	118.80
48	A2	1704	C	C5-C6-N1	5.48	123.74	121.00
48	A2	3569	C	C6-N1-C2	-5.48	118.11	120.30
49	B1	118	C	C6-N1-C1'	-5.48	114.22	120.80
48	A2	3681	G	C4-N9-C1'	5.48	133.62	126.50
48	A2	74	G	N9-C4-C5	-5.47	103.21	105.40
48	A2	1633	G	C6-C5-N7	-5.47	127.11	130.40
48	A2	3881	C	C6-N1-C2	-5.47	118.11	120.30
48	A2	951	G	N3-C4-C5	-5.47	125.86	128.60
48	A2	3731	A	C2-N3-C4	5.47	113.33	110.60
79	Bg	184	LEU	CA-CB-CG	5.47	127.88	115.30
49	B1	1279	C	C6-N1-C2	-5.46	118.11	120.30
48	A2	500	C	C6-N1-C2	-5.46	118.11	120.30
48	A2	1232	C	C6-N1-C2	-5.46	118.11	120.30
7	A3	105	C	N3-C4-N4	5.46	121.82	118.00
48	A2	649	C	C5-C6-N1	5.46	123.73	121.00
48	A2	653	G	N3-C4-C5	5.46	131.33	128.60
48	A2	974	C	C2-N1-C1'	5.45	124.80	118.80
48	A2	2637	G	C4-C5-N7	5.45	112.98	110.80
48	A2	2706	C	N1-C2-O2	5.45	122.17	118.90
49	B1	1472	C	C5-C6-N1	5.45	123.73	121.00
48	A2	1150	C	C6-N1-C2	-5.45	118.12	120.30
48	A2	3659	U	N1-C2-O2	5.45	126.62	122.80
48	A2	704	C	N3-C2-O2	-5.45	118.09	121.90
49	B1	433	A	C8-N9-C4	5.45	107.98	105.80
48	A2	71	C	N3-C4-C5	5.45	124.08	121.90
48	A2	3569	C	N3-C2-O2	-5.45	118.09	121.90
48	A2	4957	G	C5-C6-O6	-5.45	125.33	128.60
48	A2	2606	C	C6-N1-C2	-5.44	118.12	120.30
48	A2	4333	G	P-O3'-C3'	5.44	126.23	119.70
48	A2	4624	C	N3-C2-O2	-5.44	118.09	121.90
49	B1	1688	C	N3-C2-O2	-5.44	118.09	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	B1	1708	C	C5-C6-N1	5.44	123.72	121.00
48	A2	1997	C	N3-C2-O2	-5.43	118.09	121.90
48	A2	227	G	N7-C8-N9	5.43	115.81	113.10
49	B1	1203	G	C4-N9-C1'	5.43	133.56	126.50
48	A2	1466	G	C6-C5-N7	-5.43	127.14	130.40
48	A2	686	C	N1-C2-O2	5.42	122.15	118.90
48	A2	2646	C	N3-C2-O2	-5.42	118.10	121.90
48	A2	4833	G	C8-N9-C1'	-5.42	119.95	127.00
49	B1	1292	C	C6-N1-C2	-5.42	118.13	120.30
49	B1	1292	C	N1-C2-O2	5.42	122.15	118.90
49	B1	1292	C	N3-C2-O2	-5.42	118.11	121.90
48	A2	302	G	C4-C5-N7	5.42	112.97	110.80
48	A2	2778	G	C4-N9-C1'	5.42	133.54	126.50
48	A2	1067	C	N3-C2-O2	-5.42	118.11	121.90
49	B1	1309	C	C6-N1-C1'	-5.41	114.30	120.80
48	A2	1759	C	N1-C2-O2	5.41	122.15	118.90
49	B1	293	C	C2-N1-C1'	5.41	124.75	118.80
49	B1	994	C	C6-N1-C2	-5.41	118.14	120.30
49	B1	1065	G	C8-N9-C4	5.41	108.56	106.40
49	B1	1444	U	N3-C2-O2	-5.41	118.42	122.20
48	A2	1151	G	C8-N9-C1'	-5.40	119.97	127.00
7	A3	83	C	N3-C2-O2	-5.40	118.12	121.90
48	A2	974	C	N1-C2-O2	5.40	122.14	118.90
48	A2	4126	C	C6-N1-C2	-5.40	118.14	120.30
48	A2	4833	G	C4-N9-C1'	5.40	133.52	126.50
48	A2	905	G	N1-C2-N3	5.40	127.14	123.90
48	A2	1315	C	C5-C6-N1	5.40	123.70	121.00
48	A2	1564	U	O4'-C1'-N1	5.40	112.52	108.20
49	B1	688	U	N3-C2-O2	-5.40	118.42	122.20
48	A2	129	C	C2-N1-C1'	-5.40	112.86	118.80
48	A2	1069	C	C6-N1-C2	-5.40	118.14	120.30
49	B1	550	C	N1-C2-O2	5.39	122.14	118.90
16	AL	146	LEU	CA-CB-CG	5.39	127.69	115.30
66	BT	64	LEU	CA-CB-CG	5.39	127.69	115.30
49	B1	636	C	N1-C2-O2	5.39	122.13	118.90
49	B1	790	C	C6-N1-C2	-5.39	118.15	120.30
8	A4	118	C	N3-C2-O2	-5.38	118.13	121.90
49	B1	30	C	C6-N1-C2	-5.38	118.15	120.30
5	AC	57	LEU	CA-CB-CG	5.38	127.67	115.30
48	A2	80	C	C6-N1-C2	-5.38	118.15	120.30
48	A2	1176	C	C6-N1-C2	-5.38	118.15	120.30
48	A2	4829	C	N3-C4-N4	-5.37	114.24	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	A2	4891	C	C6-N1-C2	-5.37	118.15	120.30
48	A2	4406	C	C2-N1-C1'	5.37	124.71	118.80
49	B1	1237	C	C6-N1-C2	-5.37	118.15	120.30
48	A2	163	C	N1-C2-O2	5.37	122.12	118.90
48	A2	3780	G	N3-C4-N9	-5.37	122.78	126.00
49	B1	1755	C	C6-N1-C2	-5.37	118.15	120.30
48	A2	1385	C	N3-C2-O2	-5.36	118.15	121.90
49	B1	970	G	C4-N9-C1'	-5.36	119.53	126.50
48	A2	1063	C	C6-N1-C2	-5.36	118.16	120.30
48	A2	1637	C	C5-C6-N1	5.36	123.68	121.00
48	A2	5021	G	C4-N9-C1'	5.36	133.47	126.50
48	A2	4385	U	C5-C6-N1	5.36	125.38	122.70
7	A3	19	C	C6-N1-C2	-5.35	118.16	120.30
48	A2	2467	C	C5-C6-N1	5.35	123.67	121.00
48	A2	1754	C	C6-N1-C2	-5.35	118.16	120.30
48	A2	4865	G	P-O3'-C3'	5.35	126.12	119.70
48	A2	961	C	C5-C6-N1	5.35	123.67	121.00
48	A2	1079	C	N3-C2-O2	-5.34	118.16	121.90
48	A2	2373	G	C8-N9-C1'	-5.34	120.05	127.00
48	A2	3797	C	C6-N1-C2	-5.34	118.16	120.30
49	B1	193	C	C5-C6-N1	5.34	123.67	121.00
49	B1	1091	C	C6-N1-C2	-5.34	118.16	120.30
48	A2	256	C	N1-C2-O2	5.34	122.10	118.90
48	A2	1563	G	C8-N9-C1'	-5.34	120.06	127.00
48	A2	1880	G	N3-C4-N9	5.34	129.20	126.00
49	B1	402	C	C6-N1-C2	-5.33	118.17	120.30
48	A2	1930	U	C6-N1-C2	-5.33	117.80	121.00
49	B1	551	U	N3-C2-O2	-5.33	118.47	122.20
49	B1	1252	C	C6-N1-C2	-5.33	118.17	120.30
49	B1	293	C	C5-C4-N4	-5.33	116.47	120.20
7	A3	126	C	O4'-C1'-N1	5.33	112.46	108.20
48	A2	1218	G	N3-C4-N9	-5.33	122.80	126.00
48	A2	4633	C	N3-C2-O2	-5.33	118.17	121.90
49	B1	621	C	N1-C2-O2	5.33	122.10	118.90
48	A2	1648	C	C5-C6-N1	5.33	123.66	121.00
48	A2	4971	C	N1-C2-O2	5.33	122.09	118.90
51	BE	213	ALA	C-N-CA	5.33	135.01	121.70
48	A2	1083	U	C6-N1-C1'	-5.32	113.75	121.20
49	B1	89	C	C5-C6-N1	5.32	123.66	121.00
49	B1	1117	C	C5-C6-N1	5.32	123.66	121.00
48	A2	4894	G	OP1-P-O3'	5.32	116.91	105.20
48	A2	4101	C	C6-N1-C2	-5.31	118.17	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	B1	1310	U	C5-C6-N1	5.31	125.36	122.70
48	A2	3759	C	N1-C2-O2	5.31	122.09	118.90
49	B1	295	C	N3-C2-O2	-5.31	118.18	121.90
49	B1	295	C	N1-C2-O2	5.31	122.09	118.90
48	A2	4661	U	OP1-P-O3'	5.31	116.88	105.20
49	B1	567	C	C6-N1-C2	-5.31	118.18	120.30
48	A2	905	G	C4-N9-C1'	5.30	133.40	126.50
49	B1	1060	A	C4-N9-C1'	5.30	135.85	126.30
48	A2	1390	C	N3-C2-O2	-5.30	118.19	121.90
48	A2	2327	G	C8-N9-C1'	5.30	133.89	127.00
49	B1	387	C	C6-N1-C2	-5.30	118.18	120.30
49	B1	1572	C	C6-N1-C2	-5.30	118.18	120.30
48	A2	4880	C	C6-N1-C1'	-5.30	114.44	120.80
48	A2	224	A	C4-C5-N7	5.29	113.35	110.70
48	A2	1737	C	C2-N1-C1'	5.29	124.62	118.80
49	B1	1117	C	C6-N1-C2	-5.29	118.18	120.30
48	A2	2327	G	C4-N9-C1'	-5.29	119.62	126.50
49	B1	186	C	C5-C6-N1	5.28	123.64	121.00
48	A2	1300	U	C5-C4-O4	5.28	129.07	125.90
49	B1	918	U	N3-C2-O2	-5.28	118.51	122.20
49	B1	940	U	N1-C2-O2	5.28	126.49	122.80
48	A2	1977	C	C6-N1-C2	-5.27	118.19	120.30
49	B1	182	C	C5-C6-N1	5.27	123.64	121.00
48	A2	207	C	N3-C2-O2	-5.27	118.21	121.90
49	B1	1185	C	C5-C6-N1	5.27	123.64	121.00
48	A2	1268	U	C6-N1-C2	5.27	124.16	121.00
4	BB	97	LEU	CA-CB-CG	5.27	127.42	115.30
49	B1	1391	C	C6-N1-C2	-5.27	118.19	120.30
48	A2	1255	C	C6-N1-C2	-5.27	118.19	120.30
48	A2	2613	C	N1-C2-O2	5.27	122.06	118.90
5	AC	263	LEU	CA-CB-CG	5.26	127.41	115.30
48	A2	116	G	C4-N9-C1'	-5.26	119.66	126.50
48	A2	728	C	C2-N1-C1'	-5.26	113.01	118.80
49	B1	1747	C	N3-C2-O2	-5.26	118.22	121.90
22	AR	138	LEU	CA-CB-CG	5.26	127.40	115.30
48	A2	974	C	N3-C2-O2	-5.26	118.22	121.90
48	A2	1056	G	C4-N9-C1'	-5.26	119.66	126.50
49	B1	233	C	C6-N1-C1'	-5.26	114.48	120.80
48	A2	302	G	C6-C5-N7	-5.26	127.24	130.40
49	B1	1482	C	C5-C6-N1	5.26	123.63	121.00
80	Bv	20	U	N3-C2-O2	-5.26	118.52	122.20
48	A2	2688	C	C5-C6-N1	5.26	123.63	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	A2	3932	G	C6-C5-N7	-5.26	127.24	130.40
49	B1	210	U	N3-C2-O2	-5.26	118.52	122.20
48	A2	1700	C	N1-C2-O2	5.26	122.06	118.90
48	A2	1248	G	N3-C4-C5	-5.26	125.97	128.60
48	A2	2386	G	N3-C4-C5	-5.26	125.97	128.60
49	B1	417	C	C6-N1-C2	-5.25	118.20	120.30
48	A2	288	G	C8-N9-C4	-5.25	104.30	106.40
48	A2	2308	U	C5-C6-N1	5.25	125.33	122.70
7	A3	52	A	C2-N3-C4	5.25	113.22	110.60
48	A2	3783	C	N3-C2-O2	-5.25	118.22	121.90
48	A2	4661	U	P-O3'-C3'	5.25	126.00	119.70
49	B1	841	G	N1-C6-O6	-5.25	116.75	119.90
48	A2	141	G	N7-C8-N9	5.25	115.72	113.10
49	B1	1675	A	O4'-C1'-N9	5.25	112.40	108.20
48	A2	233	G	N1-C2-N2	5.25	120.92	116.20
48	A2	674	C	C6-N1-C2	-5.25	118.20	120.30
48	A2	1367	C	C5-C6-N1	5.25	123.62	121.00
48	A2	1865	C	C6-N1-C2	-5.25	118.20	120.30
49	B1	1426	U	N1-C2-O2	5.25	126.47	122.80
49	B1	1442	U	C6-N1-C2	-5.25	117.85	121.00
48	A2	214	C	C2-N1-C1'	5.24	124.57	118.80
48	A2	1424	C	N3-C2-O2	-5.24	118.23	121.90
48	A2	2667	G	C8-N9-C1'	-5.24	120.18	127.00
48	A2	3762	C	C2-N1-C1'	5.24	124.57	118.80
48	A2	1081	G	C5-C6-O6	-5.24	125.46	128.60
7	A3	38	U	C5-C6-N1	5.24	125.32	122.70
49	B1	912	C	N3-C4-C5	5.23	123.99	121.90
48	A2	4139	C	C6-N1-C2	-5.23	118.21	120.30
49	B1	539	C	C2-N1-C1'	5.23	124.55	118.80
80	Bv	68	C	N1-C2-O2	5.23	122.04	118.90
48	A2	1871	G	N1-C6-O6	5.23	123.04	119.90
49	B1	1705	C	N3-C2-O2	-5.23	118.24	121.90
48	A2	2676	A	N1-C2-N3	-5.23	126.69	129.30
49	B1	970	G	C8-N9-C1'	5.23	133.79	127.00
48	A2	4085	C	C5-C6-N1	5.22	123.61	121.00
49	B1	1622	U	N1-C2-O2	5.22	126.46	122.80
48	A2	2239	C	C2-N1-C1'	5.22	124.54	118.80
48	A2	3731	A	N3-C4-N9	5.22	131.57	127.40
48	A2	656	C	N1-C2-O2	5.21	122.03	118.90
48	A2	1938	U	N1-C2-O2	5.21	126.45	122.80
48	A2	2499	C	C6-N1-C2	-5.21	118.21	120.30
48	A2	1559	G	C4-N9-C1'	5.21	133.28	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	A2	219	C	C5-C6-N1	5.21	123.61	121.00
48	A2	4400	U	N1-C2-O2	5.21	126.45	122.80
48	A2	415	C	C6-N1-C2	-5.21	118.22	120.30
48	A2	4101	C	N1-C2-O2	5.21	122.03	118.90
48	A2	968	C	C5-C6-N1	5.21	123.60	121.00
48	A2	4040	U	C2-N1-C1'	5.21	123.95	117.70
50	BD	218	LEU	C-N-CD	-5.21	109.15	120.60
48	A2	1633	G	C4-N9-C1'	5.21	133.27	126.50
48	A2	2499	C	C6-N1-C1'	-5.20	114.56	120.80
49	B1	1287	A	N1-C6-N6	-5.20	115.48	118.60
48	A2	2582	C	C6-N1-C2	-5.20	118.22	120.30
49	B1	657	U	N3-C2-O2	-5.20	118.56	122.20
48	A2	344	C	N1-C2-O2	5.20	122.02	118.90
48	A2	3853	C	C2-N1-C1'	5.20	124.52	118.80
60	BN	75	LEU	CA-CB-CG	5.20	127.25	115.30
48	A2	237	G	N3-C4-C5	5.19	131.20	128.60
48	A2	634	C	N3-C2-O2	-5.19	118.27	121.90
40	Aj	67	LEU	CA-CB-CG	5.19	127.23	115.30
48	A2	1615	G	P-O3'-C3'	5.19	125.93	119.70
49	B1	282	G	C4-N9-C1'	5.18	133.24	126.50
49	B1	1132	C	C5-C6-N1	5.18	123.59	121.00
13	AH	4	ILE	CG1-CB-CG2	-5.18	100.00	111.40
48	A2	968	C	C6-N1-C2	-5.18	118.23	120.30
49	B1	20	G	C8-N9-C1'	-5.18	120.27	127.00
48	A2	2040	C	C6-N1-C2	-5.18	118.23	120.30
48	A2	2424	C	N3-C2-O2	-5.18	118.28	121.90
48	A2	3870	G	C4-C5-N7	5.18	112.87	110.80
49	B1	1126	G	N3-C4-N9	5.18	129.11	126.00
8	A4	118	C	C6-N1-C2	-5.17	118.23	120.30
49	B1	192	C	N3-C2-O2	-5.17	118.28	121.90
49	B1	1482	C	C6-N1-C2	-5.17	118.23	120.30
49	B1	1794	C	C5-C6-N1	5.17	123.58	121.00
49	B1	386	C	N1-C2-O2	5.17	122.00	118.90
49	B1	688	U	O4'-C1'-N1	5.17	112.33	108.20
49	B1	887	U	C6-N1-C1'	-5.17	113.96	121.20
32	Ab	112	ILE	CB-CA-C	-5.17	101.27	111.60
48	A2	1982	G	C4-N9-C1'	5.17	133.22	126.50
48	A2	2386	G	N3-C4-N9	5.17	129.10	126.00
48	A2	4717	G	C2-N3-C4	-5.17	109.32	111.90
48	A2	4732	U	C5-C6-N1	5.16	125.28	122.70
49	B1	891	G	C8-N9-C1'	-5.16	120.29	127.00
48	A2	3621	C	C2-N1-C1'	5.16	124.48	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	B1	323	C	C6-N1-C2	-5.16	118.23	120.30
48	A2	516	C	C6-N1-C2	-5.16	118.24	120.30
48	A2	1343	G	O5'-P-OP2	-5.16	101.06	105.70
48	A2	4859	G	C4-N9-C1'	5.16	133.21	126.50
48	A2	2646	C	N1-C2-O2	5.16	122.00	118.90
48	A2	4825	G	C2-N3-C4	5.16	114.48	111.90
48	A2	119	G	C8-N9-C1'	-5.16	120.30	127.00
48	A2	4006	G	N7-C8-N9	5.15	115.68	113.10
49	B1	962	A	C4-N9-C1'	5.15	135.58	126.30
48	A2	1267	G	C8-N9-C4	-5.15	104.34	106.40
49	B1	239	C	C5-C6-N1	5.15	123.58	121.00
48	A2	165	C	C6-N1-C2	-5.15	118.24	120.30
48	A2	505	C	N1-C2-O2	5.15	121.99	118.90
48	A2	4633	C	C6-N1-C1'	-5.15	114.62	120.80
48	A2	1397	C	N1-C2-O2	5.15	121.99	118.90
49	B1	1600	G	C8-N9-C1'	-5.15	120.31	127.00
48	A2	4069	G	C8-N9-C4	-5.14	104.34	106.40
49	B1	185	G	O4'-C1'-N9	5.14	112.32	108.20
49	B1	659	G	N3-C4-N9	5.14	129.09	126.00
48	A2	4872	C	C6-N1-C2	-5.14	118.24	120.30
48	A2	4645	U	N1-C2-O2	5.14	126.40	122.80
48	A2	2528	G	C4-N9-C1'	5.14	133.18	126.50
48	A2	477	G	N3-C4-N9	-5.14	122.92	126.00
48	A2	4419	U	N3-C2-O2	-5.14	118.61	122.20
48	A2	3643	G	C2-N3-C4	-5.13	109.33	111.90
7	A3	85	U	N1-C2-O2	5.13	126.39	122.80
48	A2	4858	C	N3-C2-O2	-5.13	118.31	121.90
48	A2	1499	G	C4-C5-N7	5.13	112.85	110.80
48	A2	2867	G	C4-N9-C1'	5.13	133.17	126.50
48	A2	899	G	N9-C4-C5	-5.13	103.35	105.40
48	A2	2484	C	C6-N1-C2	-5.13	118.25	120.30
48	A2	2667	G	N3-C4-N9	5.13	129.08	126.00
48	A2	1268	U	C2-N1-C1'	-5.13	111.55	117.70
48	A2	4891	C	C5-C6-N1	5.13	123.56	121.00
49	B1	839	C	C6-N1-C2	-5.13	118.25	120.30
48	A2	234	G	N3-C2-N2	-5.12	116.31	119.90
48	A2	1083	U	C2-N3-C4	5.12	130.07	127.00
48	A2	2420	C	C6-N1-C2	-5.12	118.25	120.30
48	A2	951	G	C4-N9-C1'	5.12	133.16	126.50
49	B1	1412	C	C5-C6-N1	5.12	123.56	121.00
49	B1	1542	C	C5-C6-N1	5.12	123.56	121.00
48	A2	224	A	C5-N7-C8	-5.11	101.34	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	A2	316	C	C6-N1-C2	-5.11	118.25	120.30
49	B1	1078	C	N3-C2-O2	-5.11	118.32	121.90
49	B1	1495	G	N7-C8-N9	5.11	115.66	113.10
48	A2	901	U	OP1-P-O3'	5.11	116.44	105.20
48	A2	891	C	C6-N1-C2	-5.11	118.26	120.30
48	A2	1315	C	C6-N1-C2	-5.11	118.26	120.30
48	A2	4999	G	N3-C4-C5	5.11	131.16	128.60
48	A2	516	C	C5-C6-N1	5.11	123.55	121.00
48	A2	2478	C	C6-N1-C2	-5.11	118.26	120.30
48	A2	898	U	C2-N1-C1'	5.11	123.83	117.70
48	A2	1150	C	O4'-C1'-N1	5.10	112.28	108.20
48	A2	4270	C	C5-C6-N1	5.10	123.55	121.00
48	A2	4890	U	N3-C2-O2	-5.10	118.63	122.20
49	B1	44	U	C2-N1-C1'	5.10	123.82	117.70
49	B1	891	G	C4-N9-C1'	5.10	133.13	126.50
47	At	13	CYS	CA-CB-SG	5.10	123.18	114.00
48	A2	4400	U	C5-C6-N1	5.10	125.25	122.70
49	B1	1674	G	N9-C4-C5	-5.10	103.36	105.40
48	A2	2650	C	C5-C6-N1	5.10	123.55	121.00
48	A2	3569	C	C2-N1-C1'	5.10	124.41	118.80
48	A2	316	C	N3-C2-O2	-5.09	118.33	121.90
48	A2	637	C	N1-C2-O2	5.09	121.96	118.90
48	A2	4517	U	O4'-C1'-N1	5.09	112.28	108.20
48	A2	4941	C	C5-C6-N1	5.09	123.55	121.00
49	B1	298	G	C4-N9-C1'	5.09	133.12	126.50
48	A2	456	G	N9-C4-C5	-5.09	103.36	105.40
48	A2	1564	U	N1-C2-O2	5.09	126.36	122.80
48	A2	4675	G	C4-N9-C1'	5.09	133.12	126.50
49	B1	321	C	C5-C6-N1	5.09	123.55	121.00
48	A2	1449	C	C6-N1-C2	-5.09	118.26	120.30
48	A2	2778	G	N3-C4-N9	5.09	129.05	126.00
48	A2	173	G	C4-C5-N7	5.09	112.83	110.80
48	A2	1223	G	N3-C4-N9	5.09	129.05	126.00
48	A2	1560	U	C5-C6-N1	5.08	125.24	122.70
48	A2	1561	C	C6-N1-C2	-5.08	118.27	120.30
48	A2	456	G	C4-C5-N7	5.08	112.83	110.80
48	A2	1628	A	C8-N9-C4	-5.08	103.77	105.80
48	A2	2470	C	C4-C5-C6	-5.08	114.86	117.40
48	A2	476	G	C8-N9-C1'	5.08	133.60	127.00
49	B1	549	C	N1-C2-O2	5.08	121.95	118.90
49	B1	620	G	N3-C4-N9	5.08	129.05	126.00
49	B1	626	G	C5-N7-C8	-5.08	101.76	104.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	A2	914	G	N3-C4-C5	5.08	131.14	128.60
48	A2	1905	C	C6-N1-C2	-5.08	118.27	120.30
48	A2	178	C	N1-C2-O2	5.08	121.95	118.90
48	A2	1261	C	C6-N1-C2	-5.08	118.27	120.30
48	A2	1871	G	C6-C5-N7	-5.08	127.36	130.40
48	A2	1880	G	N3-C4-C5	-5.08	126.06	128.60
80	Bv	4	C	C6-N1-C2	-5.08	118.27	120.30
48	A2	1738	U	N1-C2-O2	5.07	126.35	122.80
48	A2	1147	G	N3-C4-N9	5.07	129.04	126.00
49	B1	1862	G	OP1-P-O3'	5.07	116.36	105.20
48	A2	4205	C	C2-N1-C1'	5.07	124.38	118.80
48	A2	1176	C	N3-C2-O2	-5.07	118.35	121.90
48	A2	4304	C	N1-C2-O2	5.07	121.94	118.90
49	B1	350	C	C6-N1-C2	-5.07	118.27	120.30
48	A2	4315	U	C2-N1-C1'	5.06	123.78	117.70
48	A2	1614	A	C4-N9-C1'	5.06	135.41	126.30
48	A2	4987	C	C6-N1-C2	-5.06	118.28	120.30
48	A2	2681	C	C6-N1-C2	-5.06	118.28	120.30
48	A2	4624	C	N1-C2-O2	5.06	121.94	118.90
49	B1	428	U	C5-C6-N1	5.06	125.23	122.70
27	AW	82	ILE	CG1-CB-CG2	-5.06	100.27	111.40
49	B1	591	U	N3-C2-O2	-5.06	118.66	122.20
49	B1	1593	C	N3-C2-O2	-5.06	118.36	121.90
48	A2	1087	C	N3-C2-O2	-5.06	118.36	121.90
49	B1	223	C	C6-N1-C2	-5.06	118.28	120.30
7	A3	153	C	C6-N1-C2	-5.05	118.28	120.30
48	A2	3570	A	N1-C6-N6	5.05	121.63	118.60
49	B1	841	G	C5-C6-O6	5.05	131.63	128.60
48	A2	1499	G	N3-C4-C5	-5.05	126.08	128.60
48	A2	3590	G	N9-C4-C5	-5.05	103.38	105.40
48	A2	2051	U	C5-C6-N1	5.05	125.22	122.70
48	A2	2863	G	C8-N9-C1'	-5.05	120.44	127.00
48	A2	1060	C	C2-N1-C1'	5.04	124.34	118.80
49	B1	1121	G	C4-N9-C1'	5.04	133.05	126.50
48	A2	4658	C	N3-C2-O2	-5.04	118.37	121.90
48	A2	479	C	OP1-P-O3'	5.04	116.28	105.20
48	A2	953	G	OP2-P-O3'	5.04	116.28	105.20
48	A2	1300	U	N3-C4-O4	-5.04	115.88	119.40
48	A2	1256	G	C4-C5-N7	5.03	112.81	110.80
48	A2	1401	C	N3-C2-O2	-5.03	118.38	121.90
48	A2	3756	A	C5-C6-N6	-5.03	119.67	123.70
48	A2	3870	G	C6-C5-N7	-5.03	127.38	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	B1	37	C	N1-C2-O2	5.03	121.92	118.90
7	A3	126	C	C5-C6-N1	5.03	123.52	121.00
48	A2	456	G	C4-N9-C1'	5.03	133.03	126.50
48	A2	1063	C	C5-C6-N1	5.03	123.51	121.00
48	A2	4582	U	N3-C2-O2	-5.03	118.68	122.20
48	A2	451	G	N3-C2-N2	-5.03	116.38	119.90
48	A2	4999	G	N3-C4-N9	-5.03	122.98	126.00
48	A2	1056	G	C8-N9-C1'	5.02	133.53	127.00
48	A2	1633	G	C8-N9-C1'	-5.02	120.47	127.00
48	A2	4854	G	C4-N9-C1'	-5.02	119.97	126.50
48	A2	4974	A	N7-C8-N9	5.02	116.31	113.80
49	B1	538	U	N1-C2-O2	5.02	126.31	122.80
49	B1	1442	U	C6-N1-C1'	-5.02	114.17	121.20
8	A4	47	G	O4'-C1'-N9	5.02	112.21	108.20
59	BM	64	LEU	CB-CG-CD1	-5.02	102.47	111.00
48	A2	1065	C	C5-C6-N1	5.01	123.51	121.00
48	A2	4220	C	C5-C6-N1	5.01	123.51	121.00
51	BE	42	LEU	CA-CB-CG	5.01	126.83	115.30
48	A2	1067	C	C6-N1-C2	-5.01	118.30	120.30
48	A2	3890	C	C5-C6-N1	5.01	123.51	121.00
48	A2	4854	G	N3-C4-N9	-5.01	122.99	126.00
48	A2	899	G	N3-C2-N2	5.01	123.41	119.90
48	A2	456	G	C8-N9-C1'	-5.01	120.49	127.00
7	A3	21	C	C6-N1-C2	-5.00	118.30	120.30
48	A2	681	A	N7-C8-N9	5.00	116.30	113.80
48	A2	2402	A	C5-N7-C8	-5.00	101.40	103.90
48	A2	4256	C	N1-C2-O2	5.00	121.90	118.90
48	A2	254	C	C6-N1-C2	-5.00	118.30	120.30
48	A2	1080	C	C5-C6-N1	5.00	123.50	121.00
48	A2	4853	C	C6-N1-C2	-5.00	118.30	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
22	AR	21	LYS	Peptide
52	BF	79	HIS	Peptide

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles ⓘ

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	AA	246/248 (99%)	216 (88%)	29 (12%)	1 (0%)	30	65
2	BA	213/215 (99%)	193 (91%)	20 (9%)	0	100	100
3	AB	392/394 (100%)	352 (90%)	39 (10%)	1 (0%)	37	70
4	BB	210/212 (99%)	175 (83%)	34 (16%)	1 (0%)	25	60
5	AC	361/363 (99%)	323 (90%)	32 (9%)	6 (2%)	7	36
6	BC	220/222 (99%)	196 (89%)	24 (11%)	0	100	100
9	AD	292/294 (99%)	261 (89%)	30 (10%)	1 (0%)	37	70
10	AE	222/247 (90%)	184 (83%)	35 (16%)	3 (1%)	9	39
11	AF	232/234 (99%)	201 (87%)	30 (13%)	1 (0%)	30	65
12	AG	232/234 (99%)	208 (90%)	23 (10%)	1 (0%)	30	65
13	AH	189/191 (99%)	172 (91%)	17 (9%)	0	100	100
14	AI	204/211 (97%)	181 (89%)	21 (10%)	2 (1%)	13	46
15	AJ	167/169 (99%)	146 (87%)	21 (13%)	0	100	100
16	AL	203/205 (99%)	174 (86%)	26 (13%)	3 (2%)	8	39
17	AM	137/139 (99%)	119 (87%)	18 (13%)	0	100	100
18	AN	201/203 (99%)	172 (86%)	28 (14%)	1 (0%)	25	60
19	AO	193/195 (99%)	183 (95%)	10 (5%)	0	100	100
20	AP	151/153 (99%)	142 (94%)	9 (6%)	0	100	100
21	AQ	185/187 (99%)	165 (89%)	19 (10%)	1 (0%)	25	60
22	AR	179/181 (99%)	170 (95%)	9 (5%)	0	100	100
23	AS	173/175 (99%)	153 (88%)	20 (12%)	0	100	100
24	AT	155/157 (99%)	131 (84%)	22 (14%)	2 (1%)	10	41
25	AU	97/99 (98%)	94 (97%)	3 (3%)	0	100	100
26	AV	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
27	AW	119/121 (98%)	103 (87%)	16 (13%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	AX	115/117 (98%)	104 (90%)	11 (10%)	0	100	100
29	AY	125/127 (98%)	116 (93%)	9 (7%)	0	100	100
30	AZ	132/134 (98%)	116 (88%)	16 (12%)	0	100	100
31	Aa	145/147 (99%)	124 (86%)	21 (14%)	0	100	100
32	Ab	93/118 (79%)	81 (87%)	9 (10%)	3 (3%)	3	26
33	Ac	101/103 (98%)	94 (93%)	7 (7%)	0	100	100
34	Ad	104/106 (98%)	91 (88%)	13 (12%)	0	100	100
35	Ae	127/129 (98%)	107 (84%)	20 (16%)	0	100	100
36	Af	107/109 (98%)	96 (90%)	11 (10%)	0	100	100
37	Ag	112/114 (98%)	97 (87%)	15 (13%)	0	100	100
38	Ah	120/122 (98%)	112 (93%)	8 (7%)	0	100	100
39	Ai	95/97 (98%)	81 (85%)	13 (14%)	1 (1%)	12	45
40	Aj	82/84 (98%)	75 (92%)	7 (8%)	0	100	100
41	Ak	67/69 (97%)	62 (92%)	5 (8%)	0	100	100
42	Al	48/50 (96%)	43 (90%)	5 (10%)	0	100	100
43	Am	48/50 (96%)	43 (90%)	5 (10%)	0	100	100
44	An	23/25 (92%)	22 (96%)	1 (4%)	0	100	100
45	Ao	103/105 (98%)	92 (89%)	11 (11%)	0	100	100
46	Ap	89/91 (98%)	78 (88%)	11 (12%)	0	100	100
47	At	120/122 (98%)	106 (88%)	14 (12%)	0	100	100
50	BD	218/220 (99%)	193 (88%)	23 (11%)	2 (1%)	14	48
51	BE	255/257 (99%)	231 (91%)	23 (9%)	1 (0%)	30	65
52	BF	188/190 (99%)	163 (87%)	25 (13%)	0	100	100
53	BG	230/232 (99%)	197 (86%)	33 (14%)	0	100	100
54	BH	181/183 (99%)	158 (87%)	22 (12%)	1 (1%)	22	57
55	BI	205/207 (99%)	170 (83%)	34 (17%)	1 (0%)	25	60
56	BJ	177/179 (99%)	157 (89%)	19 (11%)	1 (1%)	22	57
57	BK	96/98 (98%)	77 (80%)	18 (19%)	1 (1%)	13	46
58	BL	151/153 (99%)	131 (87%)	19 (13%)	1 (1%)	19	54
59	BM	118/120 (98%)	110 (93%)	8 (7%)	0	100	100
60	BN	147/149 (99%)	129 (88%)	18 (12%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
61	BO	134/136 (98%)	116 (87%)	18 (13%)	0	100	100
62	BP	118/120 (98%)	100 (85%)	16 (14%)	2 (2%)	7	36
63	BQ	137/139 (99%)	121 (88%)	16 (12%)	0	100	100
64	BR	123/125 (98%)	107 (87%)	15 (12%)	1 (1%)	16	51
65	BS	137/139 (99%)	117 (85%)	19 (14%)	1 (1%)	19	54
66	BT	141/143 (99%)	126 (89%)	14 (10%)	1 (1%)	19	54
67	BU	95/97 (98%)	87 (92%)	8 (8%)	0	100	100
68	BV	79/81 (98%)	72 (91%)	6 (8%)	1 (1%)	10	41
69	BW	127/129 (98%)	117 (92%)	10 (8%)	0	100	100
70	BX	137/139 (99%)	124 (90%)	13 (10%)	0	100	100
71	BY	123/125 (98%)	113 (92%)	10 (8%)	0	100	100
72	BZ	84/86 (98%)	71 (84%)	12 (14%)	1 (1%)	11	43
73	Ba	95/97 (98%)	84 (88%)	10 (10%)	1 (1%)	12	45
74	Bb	78/80 (98%)	68 (87%)	10 (13%)	0	100	100
75	Bc	60/62 (97%)	52 (87%)	6 (10%)	2 (3%)	3	25
76	Bd	49/51 (96%)	38 (78%)	11 (22%)	0	100	100
77	Be	53/55 (96%)	45 (85%)	8 (15%)	0	100	100
78	Bf	71/73 (97%)	61 (86%)	9 (13%)	1 (1%)	9	39
79	Bg	312/314 (99%)	273 (88%)	39 (12%)	0	100	100
82	A	24/26 (92%)	16 (67%)	3 (12%)	5 (21%)	0	1
All	All	11199/11402 (98%)	9901 (88%)	1246 (11%)	52 (0%)	27	60

All (52) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	AB	4	ARG
5	AC	53	ALA
5	AC	151	PRO
14	AI	189	ARG
16	AL	46	ILE
16	AL	47	ALA
32	Ab	25	ARG
50	BD	219	PRO
62	BP	51	ARG
82	A	5	PRO

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Mol	Chain	Res	Type
82	A	10	LEU
82	A	20	ARG
5	AC	152	LEU
10	AE	128	HIS
18	AN	95	ALA
32	Ab	112	ILE
39	Ai	35	LYS
57	BK	41	PRO
58	BL	14	PRO
72	BZ	42	ASP
82	A	9	LEU
5	AC	57	LEU
14	AI	188	LYS
24	AT	53	PRO
32	Ab	113	ALA
56	BJ	123	ILE
66	BT	31	PRO
5	AC	52	TYR
5	AC	73	VAL
11	AF	223	LYS
24	AT	18	PRO
51	BE	150	PRO
54	BH	115	LYS
55	BI	118	ALA
68	BV	41	LYS
73	Ba	85	ARG
82	A	16	PRO
4	BB	53	GLN
9	AD	257	PRO
10	AE	127	SER
16	AL	134	PRO
21	AQ	159	PRO
62	BP	125	PRO
75	Bc	33	GLU
10	AE	185	PRO
50	BD	218	LEU
64	BR	4	VAL
75	Bc	32	VAL
1	AA	141	PRO
78	Bf	88	PRO
65	BS	6	PRO
12	AG	30	PRO

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	AA	190/190 (100%)	185 (97%)	5 (3%)	41	61
2	BA	180/180 (100%)	178 (99%)	2 (1%)	70	79
3	AB	343/343 (100%)	340 (99%)	3 (1%)	75	83
4	BB	193/193 (100%)	190 (98%)	3 (2%)	58	73
5	AC	302/302 (100%)	289 (96%)	13 (4%)	25	49
6	BC	188/188 (100%)	186 (99%)	2 (1%)	70	79
9	AD	248/248 (100%)	241 (97%)	7 (3%)	38	59
10	AE	202/220 (92%)	198 (98%)	4 (2%)	50	68
11	AF	203/203 (100%)	200 (98%)	3 (2%)	60	74
12	AG	199/199 (100%)	198 (100%)	1 (0%)	86	90
13	AH	170/170 (100%)	170 (100%)	0	100	100
14	AI	178/179 (99%)	171 (96%)	7 (4%)	27	51
15	AJ	142/142 (100%)	142 (100%)	0	100	100
16	AL	171/171 (100%)	165 (96%)	6 (4%)	31	54
17	AM	118/118 (100%)	116 (98%)	2 (2%)	56	72
18	AN	171/171 (100%)	168 (98%)	3 (2%)	54	71
19	AO	168/168 (100%)	163 (97%)	5 (3%)	36	58
20	AP	134/134 (100%)	134 (100%)	0	100	100
21	AQ	164/164 (100%)	163 (99%)	1 (1%)	84	88
22	AR	160/160 (100%)	159 (99%)	1 (1%)	84	88
23	AS	156/156 (100%)	155 (99%)	1 (1%)	84	88
24	AT	138/138 (100%)	138 (100%)	0	100	100
25	AU	89/89 (100%)	88 (99%)	1 (1%)	70	79
26	AV	100/100 (100%)	99 (99%)	1 (1%)	73	81
27	AW	100/100 (100%)	99 (99%)	1 (1%)	73	81
28	AX	105/105 (100%)	105 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
29	AY	119/119 (100%)	116 (98%)	3 (2%)	42	62
30	AZ	117/117 (100%)	115 (98%)	2 (2%)	56	72
31	Aa	120/120 (100%)	119 (99%)	1 (1%)	79	84
32	Ab	79/98 (81%)	75 (95%)	4 (5%)	20	45
33	Ac	88/88 (100%)	86 (98%)	2 (2%)	45	64
34	Ad	97/97 (100%)	97 (100%)	0	100	100
35	Ae	115/115 (100%)	114 (99%)	1 (1%)	75	83
36	Af	88/88 (100%)	86 (98%)	2 (2%)	45	64
37	Ag	98/98 (100%)	98 (100%)	0	100	100
38	Ah	109/109 (100%)	106 (97%)	3 (3%)	38	59
39	Ai	83/83 (100%)	83 (100%)	0	100	100
40	Aj	71/71 (100%)	70 (99%)	1 (1%)	62	75
41	Ak	64/64 (100%)	62 (97%)	2 (3%)	35	56
42	Al	47/47 (100%)	44 (94%)	3 (6%)	14	39
43	Am	46/46 (100%)	44 (96%)	2 (4%)	25	49
44	An	24/24 (100%)	24 (100%)	0	100	100
45	Ao	93/93 (100%)	91 (98%)	2 (2%)	47	65
46	Ap	74/74 (100%)	72 (97%)	2 (3%)	40	60
47	At	106/106 (100%)	104 (98%)	2 (2%)	52	70
50	BD	183/183 (100%)	181 (99%)	2 (1%)	70	79
51	BE	220/220 (100%)	216 (98%)	4 (2%)	54	71
52	BF	160/160 (100%)	157 (98%)	3 (2%)	52	70
53	BG	202/202 (100%)	200 (99%)	2 (1%)	73	81
54	BH	164/164 (100%)	162 (99%)	2 (1%)	67	78
55	BI	179/179 (100%)	177 (99%)	2 (1%)	70	79
56	BJ	160/160 (100%)	158 (99%)	2 (1%)	65	76
57	BK	89/89 (100%)	88 (99%)	1 (1%)	70	79
58	BL	138/138 (100%)	138 (100%)	0	100	100
59	BM	102/102 (100%)	101 (99%)	1 (1%)	73	81
60	BN	130/130 (100%)	129 (99%)	1 (1%)	79	84
61	BO	106/106 (100%)	105 (99%)	1 (1%)	75	83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
62	BP	109/109 (100%)	107 (98%)	2 (2%)	54	71
63	BQ	115/115 (100%)	115 (100%)	0	100	100
64	BR	113/113 (100%)	111 (98%)	2 (2%)	54	71
65	BS	121/121 (100%)	117 (97%)	4 (3%)	33	56
66	BT	113/113 (100%)	111 (98%)	2 (2%)	54	71
67	BU	90/90 (100%)	90 (100%)	0	100	100
68	BV	65/65 (100%)	63 (97%)	2 (3%)	35	56
69	BW	112/112 (100%)	110 (98%)	2 (2%)	54	71
70	BX	111/111 (100%)	109 (98%)	2 (2%)	54	71
71	BY	107/107 (100%)	105 (98%)	2 (2%)	52	70
72	BZ	75/75 (100%)	73 (97%)	2 (3%)	40	60
73	Ba	84/84 (100%)	84 (100%)	0	100	100
74	Bb	72/72 (100%)	71 (99%)	1 (1%)	62	75
75	Bc	55/55 (100%)	55 (100%)	0	100	100
76	Bd	45/45 (100%)	45 (100%)	0	100	100
77	Be	44/44 (100%)	40 (91%)	4 (9%)	7	28
78	Bf	66/66 (100%)	66 (100%)	0	100	100
79	Bg	272/272 (100%)	271 (100%)	1 (0%)	89	91
All	All	9752/9790 (100%)	9601 (98%)	151 (2%)	60	74

All (151) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AA	58	LEU
1	AA	68	ARG
1	AA	193	ARG
1	AA	207	VAL
1	AA	242	ARG
2	BA	16	LEU
2	BA	149	ASN
3	AB	24	ARG
3	AB	69	LYS
3	AB	294	LYS
4	BB	51	ARG
4	BB	76	ASN
4	BB	218	LEU

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Mol	Chain	Res	Type
5	AC	38	ASN
5	AC	48	ASN
5	AC	52	TYR
5	AC	95	MET
5	AC	114	ARG
5	AC	146	GLU
5	AC	147	VAL
5	AC	151	PRO
5	AC	199	ARG
5	AC	215	ASN
5	AC	229	LEU
5	AC	230	LEU
5	AC	282	HIS
6	BC	66	LEU
6	BC	134	ASN
9	AD	20	PHE
9	AD	21	ARG
9	AD	33	ARG
9	AD	35	ARG
9	AD	191	ASN
9	AD	235	MET
9	AD	265	ARG
10	AE	52	ARG
10	AE	56	ARG
10	AE	223	ARG
10	AE	279	ASN
11	AF	24	ASN
11	AF	146	ASN
11	AF	166	ARG
12	AG	66	GLN
14	AI	10	ARG
14	AI	69	ARG
14	AI	73	ASN
14	AI	158	LYS
14	AI	170	LYS
14	AI	185	VAL
14	AI	188	LYS
16	AL	44	ARG
16	AL	46	ILE
16	AL	123	LYS
16	AL	135	LYS
16	AL	159	ASN

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Mol	Chain	Res	Type
16	AL	175	ASN
17	AM	5	ARG
17	AM	35	ARG
18	AN	189	ARG
18	AN	194	ARG
18	AN	204	ARG
19	AO	65	ASN
19	AO	94	ARG
19	AO	118	MET
19	AO	160	ARG
19	AO	184	ASN
21	AQ	55	ARG
22	AR	98	ARG
23	AS	15	ARG
25	AU	50	ASN
26	AV	46	LYS
27	AW	45	ASN
29	AY	16	LYS
29	AY	36	LYS
29	AY	74	TYR
30	AZ	53	VAL
30	AZ	59	LYS
31	Aa	87	ARG
32	Ab	32	LEU
32	Ab	54	LEU
32	Ab	61	ASN
32	Ab	116	LEU
33	Ac	44	LYS
33	Ac	45	LEU
35	Ae	49	PHE
36	Af	58	VAL
36	Af	106	TYR
38	Ah	88	THR
38	Ah	91	MET
38	Ah	92	ARG
40	Aj	65	ARG
41	Ak	21	LYS
41	Ak	60	LEU
42	Al	20	ASN
42	Al	21	ARG
42	Al	28	ARG
43	Am	112	LYS

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Mol	Chain	Res	Type
43	Am	120	ASN
45	Ao	3	ASN
45	Ao	98	LYS
46	Ap	17	ARG
46	Ap	84	ARG
47	At	41	ASN
47	At	83	ASN
50	BD	64	ARG
50	BD	76	ARG
51	BE	75	LYS
51	BE	197	ASN
51	BE	230	ASN
51	BE	238	LEU
52	BF	63	LYS
52	BF	135	ARG
52	BF	146	ARG
53	BG	159	ARG
53	BG	202	ASN
54	BH	152	ARG
54	BH	156	VAL
55	BI	76	THR
55	BI	121	LEU
56	BJ	30	LYS
56	BJ	172	ARG
57	BK	96	ARG
59	BM	31	LEU
60	BN	104	ARG
61	BO	128	ARG
62	BP	52	LYS
62	BP	130	ARG
64	BR	98	VAL
64	BR	116	ASN
65	BS	17	ASN
65	BS	23	ARG
65	BS	66	ARG
65	BS	73	ASN
66	BT	39	LEU
66	BT	82	ARG
68	BV	41	LYS
68	BV	81	LYS
69	BW	5	ASN
69	BW	15	ASN

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Mol	Chain	Res	Type
70	BX	127	ASN
70	BX	137	LYS
71	BY	9	THR
71	BY	15	ASN
72	BZ	62	VAL
72	BZ	112	ASN
74	Bb	23	ARG
77	Be	8	ARG
77	Be	18	LYS
77	Be	35	ARG
77	Be	52	LYS
79	Bg	133	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (127) such sidechains are listed below:

Mol	Chain	Res	Type
1	AA	50	HIS
1	AA	132	ASN
1	AA	209	HIS
1	AA	216	HIS
1	AA	218	HIS
2	BA	149	ASN
2	BA	169	HIS
3	AB	25	HIS
3	AB	175	GLN
3	AB	204	GLN
3	AB	245	HIS
3	AB	380	GLN
4	BB	75	GLN
4	BB	76	ASN
4	BB	149	GLN
4	BB	208	HIS
5	AC	38	ASN
5	AC	50	GLN
5	AC	215	ASN
5	AC	299	GLN
6	BC	134	ASN
6	BC	235	ASN
9	AD	39	GLN
9	AD	111	ASN
9	AD	191	ASN
9	AD	198	HIS

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Mol	Chain	Res	Type
9	AD	244	HIS
9	AD	282	GLN
10	AE	136	HIS
10	AE	191	GLN
10	AE	279	ASN
11	AF	24	ASN
11	AF	131	ASN
11	AF	146	ASN
12	AG	43	GLN
13	AH	189	GLN
14	AI	14	ASN
14	AI	86	HIS
14	AI	144	ASN
14	AI	147	HIS
16	AL	149	GLN
16	AL	159	ASN
16	AL	175	ASN
17	AM	70	GLN
18	AN	8	GLN
18	AN	37	HIS
18	AN	87	HIS
18	AN	109	HIS
18	AN	145	ASN
18	AN	199	GLN
18	AN	201	HIS
19	AO	50	ASN
19	AO	65	ASN
19	AO	184	ASN
20	AP	40	HIS
20	AP	75	GLN
20	AP	80	GLN
21	AQ	44	ASN
22	AR	58	HIS
24	AT	3	ASN
24	AT	98	HIS
25	AU	50	ASN
25	AU	105	ASN
26	AV	135	ASN
27	AW	45	ASN
27	AW	50	ASN
28	AX	107	HIS
29	AY	96	HIS

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Mol	Chain	Res	Type
31	Aa	60	HIS
31	Aa	67	GLN
31	Aa	74	ASN
32	Ab	60	ASN
34	Ad	79	ASN
36	Af	99	HIS
37	Ag	73	HIS
40	Aj	13	ASN
40	Aj	57	ASN
42	Al	19	GLN
42	Al	43	HIS
43	Am	120	ASN
45	Ao	3	ASN
45	Ao	45	GLN
47	At	6	GLN
47	At	30	ASN
47	At	41	ASN
47	At	83	ASN
51	BE	197	ASN
51	BE	230	ASN
52	BF	79	HIS
52	BF	82	ASN
52	BF	114	ASN
52	BF	179	ASN
53	BG	56	ASN
53	BG	81	HIS
53	BG	202	ASN
56	BJ	134	HIS
57	BK	7	ASN
58	BL	11	GLN
58	BL	18	GLN
58	BL	19	ASN
58	BL	83	GLN
59	BM	46	GLN
59	BM	82	ASN
60	BN	105	ASN
61	BO	43	HIS
62	BP	79	HIS
63	BQ	142	GLN
64	BR	31	ASN
65	BS	17	ASN
65	BS	19	ASN

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Mol	Chain	Res	Type
69	BW	5	ASN
69	BW	16	ASN
69	BW	44	HIS
70	BX	61	GLN
70	BX	127	ASN
71	BY	15	ASN
71	BY	22	GLN
71	BY	29	HIS
72	BZ	89	GLN
72	BZ	106	GLN
72	BZ	112	ASN
73	Ba	7	ASN
75	Bc	24	GLN
76	Bd	41	GLN
79	Bg	133	ASN
79	Bg	143	GLN
79	Bg	272	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
48	A2	3626/3643 (99%)	1021 (28%)	12 (0%)
49	B1	1701/1708 (99%)	533 (31%)	6 (0%)
7	A3	156/157 (99%)	49 (31%)	1 (0%)
8	A4	118/119 (99%)	29 (24%)	0
80	Bv	75/76 (98%)	28 (37%)	0
81	Bx	15/16 (93%)	9 (60%)	0
All	All	5691/5719 (99%)	1669 (29%)	19 (0%)

All (1669) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
7	A3	8	U
7	A3	32	C
7	A3	34	U
7	A3	35	C
7	A3	36	G
7	A3	37	A
7	A3	39	G
7	A3	52	A
7	A3	57	C

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Mol	Chain	Res	Type
7	A3	58	G
7	A3	59	A
7	A3	60	G
7	A3	63	U
7	A3	71	A
7	A3	72	A
7	A3	73	U
7	A3	74	U
7	A3	81	C
7	A3	82	A
7	A3	84	A
7	A3	85	U
7	A3	87	G
7	A3	90	C
7	A3	95	A
7	A3	96	C
7	A3	99	U
7	A3	101	C
7	A3	103	A
7	A3	104	A
7	A3	105	C
7	A3	109	C
7	A3	110	U
7	A3	111	U
7	A3	112	G
7	A3	121	G
7	A3	122	G
7	A3	123	U
7	A3	124	U
7	A3	125	C
7	A3	126	C
7	A3	127	U
7	A3	128	C
7	A3	129	C
7	A3	130	C
7	A3	137	A
7	A3	142	U
7	A3	148	A
7	A3	151	G
7	A3	154	G
8	A4	2	U
8	A4	7	G

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Mol	Chain	Res	Type
8	A4	8	G
8	A4	11	A
8	A4	14	C
8	A4	19	C
8	A4	22	A
8	A4	24	C
8	A4	27	G
8	A4	29	C
8	A4	31	G
8	A4	33	U
8	A4	38	U
8	A4	41	G
8	A4	49	A
8	A4	50	A
8	A4	53	U
8	A4	54	A
8	A4	59	G
8	A4	63	C
8	A4	64	G
8	A4	66	G
8	A4	85	G
8	A4	91	C
8	A4	97	G
8	A4	99	G
8	A4	109	U
8	A4	110	G
8	A4	118	C
48	A2	2	G
48	A2	9	C
48	A2	10	A
48	A2	13	U
48	A2	14	C
48	A2	17	A
48	A2	23	C
48	A2	25	A
48	A2	32	G
48	A2	37	U
48	A2	39	A
48	A2	40	G
48	A2	42	A
48	A2	47	A
48	A2	48	G

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Mol	Chain	Res	Type
48	A2	49	U
48	A2	50	C
48	A2	59	A
48	A2	64	A
48	A2	65	A
48	A2	70	A
48	A2	71	C
48	A2	72	C
48	A2	73	A
48	A2	84	A
48	A2	87	A
48	A2	88	A
48	A2	91	G
48	A2	93	G
48	A2	101	A
48	A2	116	G
48	A2	119	G
48	A2	120	A
48	A2	121	A
48	A2	122	U
48	A2	131	C
48	A2	132	G
48	A2	133	C
48	A2	134	G
48	A2	135	G
48	A2	138	C
48	A2	139	G
48	A2	140	C
48	A2	141	G
48	A2	143	G
48	A2	147	U
48	A2	149	U
48	A2	150	G
48	A2	153	G
48	A2	156	C
48	A2	157	G
48	A2	158	G
48	A2	161	G
48	A2	167	C
48	A2	169	C
48	A2	173	G
48	A2	174	G

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Mol	Chain	Res	Type
48	A2	181	U
48	A2	182	C
48	A2	183	G
48	A2	184	U
48	A2	185	G
48	A2	193	C
48	A2	196	G
48	A2	197	U
48	A2	201	U
48	A2	206	U
48	A2	207	C
48	A2	212	C
48	A2	213	C
48	A2	214	C
48	A2	215	A
48	A2	223	G
48	A2	228	U
48	A2	229	G
48	A2	230	U
48	A2	233	G
48	A2	234	G
48	A2	237	G
48	A2	241	G
48	A2	242	C
48	A2	250	G
48	A2	251	G
48	A2	252	C
48	A2	253	G
48	A2	260	C
48	A2	289	A
48	A2	291	U
48	A2	300	A
48	A2	303	C
48	A2	304	G
48	A2	306	G
48	A2	309	G
48	A2	310	U
48	A2	311	A
48	A2	313	A
48	A2	315	U
48	A2	334	C
48	A2	338	A

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Mol	Chain	Res	Type
48	A2	343	A
48	A2	344	C
48	A2	348	U
48	A2	352	C
48	A2	356	A
48	A2	357	A
48	A2	367	G
48	A2	370	A
48	A2	375	U
48	A2	379	A
48	A2	380	A
48	A2	381	G
48	A2	390	A
48	A2	393	G
48	A2	402	A
48	A2	403	G
48	A2	404	A
48	A2	406	G
48	A2	407	G
48	A2	409	G
48	A2	425	G
48	A2	426	U
48	A2	434	U
48	A2	440	C
48	A2	444	G
48	A2	445	C
48	A2	446	A
48	A2	447	G
48	A2	448	U
48	A2	449	C
48	A2	451	G
48	A2	456	G
48	A2	459	G
48	A2	461	U
48	A2	467	C
48	A2	479	C
48	A2	480	C
48	A2	481	G
48	A2	489	C
48	A2	492	C
48	A2	493	G
48	A2	495	C

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Mol	Chain	Res	Type
48	A2	496	C
48	A2	497	C
48	A2	498	G
48	A2	505	C
48	A2	506	U
48	A2	507	U
48	A2	508	U
48	A2	509	C
48	A2	513	C
48	A2	633	U
48	A2	635	G
48	A2	645	C
48	A2	646	G
48	A2	649	C
48	A2	651	C
48	A2	652	C
48	A2	654	G
48	A2	655	A
48	A2	658	G
48	A2	661	G
48	A2	662	A
48	A2	664	C
48	A2	668	C
48	A2	674	C
48	A2	677	G
48	A2	678	C
48	A2	680	C
48	A2	682	U
48	A2	684	U
48	A2	688	G
48	A2	690	C
48	A2	692	G
48	A2	693	U
48	A2	695	C
48	A2	698	C
48	A2	702	A
48	A2	719	U
48	A2	720	G
48	A2	721	G
48	A2	724	A
48	A2	728	C
48	A2	737	A

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Mol	Chain	Res	Type
48	A2	738	A
48	A2	739	G
48	A2	900	U
48	A2	901	U
48	A2	902	A
48	A2	903	C
48	A2	905	G
48	A2	906	C
48	A2	911	C
48	A2	917	G
48	A2	919	A
48	A2	920	G
48	A2	921	C
48	A2	923	C
48	A2	924	U
48	A2	925	C
48	A2	927	C
48	A2	931	A
48	A2	932	U
48	A2	933	C
48	A2	939	G
48	A2	947	A
48	A2	948	A
48	A2	949	G
48	A2	950	C
48	A2	951	G
48	A2	953	G
48	A2	954	A
48	A2	955	C
48	A2	958	U
48	A2	959	C
48	A2	967	U
48	A2	968	C
48	A2	975	C
48	A2	1055	C
48	A2	1059	C
48	A2	1061	A
48	A2	1062	C
48	A2	1065	C
48	A2	1066	U
48	A2	1076	C
48	A2	1078	A

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Mol	Chain	Res	Type
48	A2	1083	U
48	A2	1084	C
48	A2	1085	U
48	A2	1087	C
48	A2	1149	G
48	A2	1150	C
48	A2	1152	G
48	A2	1154	G
48	A2	1155	C
48	A2	1156	G
48	A2	1161	G
48	A2	1162	U
48	A2	1163	C
48	A2	1164	C
48	A2	1167	A
48	A2	1180	C
48	A2	1181	G
48	A2	1188	G
48	A2	1191	G
48	A2	1192	U
48	A2	1193	C
48	A2	1196	G
48	A2	1197	C
48	A2	1200	G
48	A2	1201	G
48	A2	1202	G
48	A2	1220	C
48	A2	1221	A
48	A2	1222	C
48	A2	1223	G
48	A2	1226	C
48	A2	1228	C
48	A2	1233	C
48	A2	1247	C
48	A2	1249	G
48	A2	1250	C
48	A2	1251	G
48	A2	1253	A
48	A2	1255	C
48	A2	1256	G
48	A2	1257	A
48	A2	1258	G

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Mol	Chain	Res	Type
48	A2	1259	C
48	A2	1260	G
48	A2	1261	C
48	A2	1262	A
48	A2	1263	C
48	A2	1264	G
48	A2	1265	G
48	A2	1268	U
48	A2	1269	C
48	A2	1271	G
48	A2	1277	A
48	A2	1278	C
48	A2	1280	U
48	A2	1284	C
48	A2	1285	U
48	A2	1286	A
48	A2	1295	A
48	A2	1299	G
48	A2	1301	C
48	A2	1304	G
48	A2	1309	A
48	A2	1315	C
48	A2	1321	G
48	A2	1337	A
48	A2	1341	G
48	A2	1342	G
48	A2	1343	G
48	A2	1348	C
48	A2	1349	G
48	A2	1350	C
48	A2	1351	A
48	A2	1353	G
48	A2	1355	A
48	A2	1360	G
48	A2	1370	A
48	A2	1377	G
48	A2	1380	A
48	A2	1381	A
48	A2	1386	G
48	A2	1389	G
48	A2	1390	C
48	A2	1391	G

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Mol	Chain	Res	Type
48	A2	1392	C
48	A2	1393	U
48	A2	1394	C
48	A2	1395	G
48	A2	1399	G
48	A2	1400	C
48	A2	1401	C
48	A2	1402	G
48	A2	1403	A
48	A2	1404	G
48	A2	1408	G
48	A2	1415	G
48	A2	1420	C
48	A2	1421	U
48	A2	1422	C
48	A2	1423	U
48	A2	1424	C
48	A2	1426	A
48	A2	1427	G
48	A2	1429	C
48	A2	1439	G
48	A2	1454	C
48	A2	1457	G
48	A2	1462	C
48	A2	1463	C
48	A2	1464	G
48	A2	1465	C
48	A2	1466	G
48	A2	1467	C
48	A2	1468	C
48	A2	1469	G
48	A2	1479	A
48	A2	1480	G
48	A2	1485	A
48	A2	1486	G
48	A2	1499	G
48	A2	1505	A
48	A2	1507	A
48	A2	1513	U
48	A2	1516	A
48	A2	1520	U
48	A2	1521	G

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Mol	Chain	Res	Type
48	A2	1525	G
48	A2	1531	G
48	A2	1534	G
48	A2	1548	C
48	A2	1556	G
48	A2	1560	U
48	A2	1563	G
48	A2	1573	U
48	A2	1578	U
48	A2	1579	G
48	A2	1583	A
48	A2	1587	G
48	A2	1589	C
48	A2	1596	C
48	A2	1606	G
48	A2	1607	G
48	A2	1609	G
48	A2	1610	C
48	A2	1612	A
48	A2	1613	A
48	A2	1614	A
48	A2	1615	G
48	A2	1616	A
48	A2	1620	A
48	A2	1622	C
48	A2	1623	G
48	A2	1625	A
48	A2	1631	U
48	A2	1632	A
48	A2	1636	G
48	A2	1642	U
48	A2	1643	C
48	A2	1650	A
48	A2	1652	G
48	A2	1658	C
48	A2	1659	U
48	A2	1660	C
48	A2	1663	G
48	A2	1666	A
48	A2	1678	C
48	A2	1680	C
48	A2	1700	C

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Mol	Chain	Res	Type
48	A2	1701	A
48	A2	1708	U
48	A2	1712	U
48	A2	1713	C
48	A2	1716	G
48	A2	1723	G
48	A2	1724	A
48	A2	1730	U
48	A2	1732	G
48	A2	1733	A
48	A2	1736	U
48	A2	1737	C
48	A2	1742	G
48	A2	1743	G
48	A2	1746	G
48	A2	1747	A
48	A2	1751	G
48	A2	1752	A
48	A2	1757	A
48	A2	1767	C
48	A2	1769	A
48	A2	1776	A
48	A2	1779	G
48	A2	1786	A
48	A2	1794	C
48	A2	1798	C
48	A2	1804	U
48	A2	1814	G
48	A2	1816	G
48	A2	1817	G
48	A2	1818	A
48	A2	1823	G
48	A2	1835	G
48	A2	1836	G
48	A2	1850	G
48	A2	1851	C
48	A2	1854	A
48	A2	1862	C
48	A2	1863	U
48	A2	1870	U
48	A2	1872	A
48	A2	1873	A

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Mol	Chain	Res	Type
48	A2	1880	G
48	A2	1887	U
48	A2	1891	G
48	A2	1896	C
48	A2	1897	G
48	A2	1898	A
48	A2	1899	U
48	A2	1900	G
48	A2	1902	C
48	A2	1903	G
48	A2	1911	U
48	A2	1912	C
48	A2	1913	A
48	A2	1916	C
48	A2	1917	C
48	A2	1918	C
48	A2	1921	G
48	A2	1923	A
48	A2	1925	A
48	A2	1926	G
48	A2	1928	U
48	A2	1929	G
48	A2	1930	U
48	A2	1936	G
48	A2	1938	U
48	A2	1940	U
48	A2	1941	A
48	A2	1942	G
48	A2	1943	A
48	A2	1947	C
48	A2	1950	G
48	A2	1955	U
48	A2	1956	G
48	A2	1957	G
48	A2	1959	C
48	A2	1960	A
48	A2	1961	U
48	A2	1962	G
48	A2	1963	G
48	A2	1964	A
48	A2	1965	A
48	A2	1967	U

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Mol	Chain	Res	Type
48	A2	1968	C
48	A2	1969	G
48	A2	1971	A
48	A2	1972	A
48	A2	1975	C
48	A2	1978	U
48	A2	1979	A
48	A2	1980	A
48	A2	1982	G
48	A2	1983	A
48	A2	1984	G
48	A2	1985	U
48	A2	1988	G
48	A2	1989	U
48	A2	1990	A
48	A2	1991	A
48	A2	1996	U
48	A2	1997	C
48	A2	1998	A
48	A2	1999	C
48	A2	2003	C
48	A2	2007	A
48	A2	2011	A
48	A2	2015	G
48	A2	2019	U
48	A2	2023	A
48	A2	2025	U
48	A2	2027	G
48	A2	2029	U
48	A2	2036	G
48	A2	2037	G
48	A2	2043	C
48	A2	2050	A
48	A2	2051	U
48	A2	2065	C
48	A2	2069	G
48	A2	2073	A
48	A2	2074	G
48	A2	2076	G
48	A2	2077	U
48	A2	2078	G
48	A2	2082	G

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Mol	Chain	Res	Type
48	A2	2084	G
48	A2	2087	C
48	A2	2088	G
48	A2	2091	G
48	A2	2092	G
48	A2	2237	C
48	A2	2238	G
48	A2	2239	C
48	A2	2243	C
48	A2	2246	U
48	A2	2247	A
48	A2	2257	G
48	A2	2258	A
48	A2	2268	C
48	A2	2275	G
48	A2	2277	U
48	A2	2279	A
48	A2	2280	G
48	A2	2282	C
48	A2	2288	G
48	A2	2292	A
48	A2	2295	G
48	A2	2298	C
48	A2	2308	U
48	A2	2321	G
48	A2	2325	C
48	A2	2327	G
48	A2	2330	C
48	A2	2339	A
48	A2	2340	G
48	A2	2343	G
48	A2	2348	U
48	A2	2352	C
48	A2	2358	A
48	A2	2363	U
48	A2	2366	G
48	A2	2370	G
48	A2	2375	A
48	A2	2376	G
48	A2	2400	G
48	A2	2401	C
48	A2	2405	U

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Mol	Chain	Res	Type
48	A2	2416	C
48	A2	2417	A
48	A2	2420	C
48	A2	2426	U
48	A2	2429	G
48	A2	2432	A
48	A2	2439	A
48	A2	2442	G
48	A2	2446	U
48	A2	2447	U
48	A2	2449	C
48	A2	2452	A
48	A2	2453	G
48	A2	2454	G
48	A2	2467	C
48	A2	2468	C
48	A2	2469	U
48	A2	2473	U
48	A2	2478	C
48	A2	2480	C
48	A2	2482	G
48	A2	2483	C
48	A2	2484	C
48	A2	2485	G
48	A2	2486	A
48	A2	2490	A
48	A2	2492	A
48	A2	2499	C
48	A2	2509	U
48	A2	2523	G
48	A2	2524	U
48	A2	2525	G
48	A2	2527	C
48	A2	2532	A
48	A2	2533	U
48	A2	2545	G
48	A2	2555	G
48	A2	2560	A
48	A2	2561	A
48	A2	2565	G
48	A2	2566	A
48	A2	2567	C

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Mol	Chain	Res	Type
48	A2	2568	C
48	A2	2569	G
48	A2	2580	A
48	A2	2584	G
48	A2	2585	G
48	A2	2601	G
48	A2	2606	C
48	A2	2617	G
48	A2	2619	G
48	A2	2632	C
48	A2	2640	U
48	A2	2642	G
48	A2	2646	C
48	A2	2648	C
48	A2	2652	G
48	A2	2653	A
48	A2	2665	G
48	A2	2666	U
48	A2	2673	G
48	A2	2674	A
48	A2	2675	A
48	A2	2676	A
48	A2	2682	G
48	A2	2684	G
48	A2	2686	U
48	A2	2687	U
48	A2	2689	C
48	A2	2690	G
48	A2	2691	G
48	A2	2699	C
48	A2	2700	G
48	A2	2704	A
48	A2	2705	G
48	A2	2719	U
48	A2	2720	U
48	A2	2722	A
48	A2	2723	A
48	A2	2734	A
48	A2	2737	G
48	A2	2740	U
48	A2	2741	G
48	A2	2742	U

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Mol	Chain	Res	Type
48	A2	2743	A
48	A2	2745	A
48	A2	2746	U
48	A2	2766	A
48	A2	2767	U
48	A2	2769	U
48	A2	2773	C
48	A2	2776	C
48	A2	2778	G
48	A2	2782	U
48	A2	2785	A
48	A2	2794	A
48	A2	2805	U
48	A2	2806	G
48	A2	2814	A
48	A2	2822	U
48	A2	2824	A
48	A2	2829	A
48	A2	2831	U
48	A2	2832	C
48	A2	2834	G
48	A2	2835	C
48	A2	2837	A
48	A2	2842	G
48	A2	2846	C
48	A2	2854	C
48	A2	2858	A
48	A2	2860	A
48	A2	2863	G
48	A2	2876	G
48	A2	2881	G
48	A2	3570	A
48	A2	3572	C
48	A2	3576	C
48	A2	3579	A
48	A2	3586	G
48	A2	3591	G
48	A2	3596	G
48	A2	3597	G
48	A2	3601	A
48	A2	3602	U
48	A2	3606	A

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Mol	Chain	Res	Type
48	A2	3612	U
48	A2	3613	A
48	A2	3614	A
48	A2	3615	U
48	A2	3619	A
48	A2	3627	A
48	A2	3633	A
48	A2	3643	G
48	A2	3644	C
48	A2	3646	G
48	A2	3649	G
48	A2	3651	U
48	A2	3656	C
48	A2	3659	U
48	A2	3663	A
48	A2	3665	U
48	A2	3683	A
48	A2	3686	U
48	A2	3688	A
48	A2	3700	U
48	A2	3704	A
48	A2	3707	A
48	A2	3721	G
48	A2	3724	G
48	A2	3731	A
48	A2	3732	C
48	A2	3733	U
48	A2	3738	C
48	A2	3741	U
48	A2	3744	U
48	A2	3747	G
48	A2	3748	G
48	A2	3751	G
48	A2	3754	A
48	A2	3755	A
48	A2	3756	A
48	A2	3761	U
48	A2	3774	A
48	A2	3781	C
48	A2	3782	G
48	A2	3783	C
48	A2	3784	A

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Mol	Chain	Res	Type
48	A2	3788	A
48	A2	3789	U
48	A2	3790	G
48	A2	3795	A
48	A2	3800	G
48	A2	3809	U
48	A2	3810	G
48	A2	3811	U
48	A2	3814	C
48	A2	3822	U
48	A2	3829	C
48	A2	3836	A
48	A2	3838	A
48	A2	3840	C
48	A2	3847	A
48	A2	3848	A
48	A2	3849	C
48	A2	3850	G
48	A2	3851	G
48	A2	3853	C
48	A2	3856	G
48	A2	3860	G
48	A2	3861	A
48	A2	3866	G
48	A2	3868	G
48	A2	3872	A
48	A2	3876	A
48	A2	3877	A
48	A2	3878	G
48	A2	3879	A
48	A2	3885	U
48	A2	3886	U
48	A2	3889	G
48	A2	3894	A
48	A2	3909	G
48	A2	3918	A
48	A2	3922	G
48	A2	3935	U
48	A2	3937	A
48	A2	3943	A
48	A2	3944	G
48	A2	4005	G

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Mol	Chain	Res	Type
48	A2	4009	G
48	A2	4011	C
48	A2	4012	G
48	A2	4013	G
48	A2	4014	U
48	A2	4016	A
48	A2	4018	A
48	A2	4019	U
48	A2	4027	C
48	A2	4029	C
48	A2	4033	U
48	A2	4034	C
48	A2	4035	G
48	A2	4037	U
48	A2	4038	U
48	A2	4040	U
48	A2	4041	U
48	A2	4046	G
48	A2	4047	A
48	A2	4058	C
48	A2	4065	G
48	A2	4067	G
48	A2	4068	A
48	A2	4069	G
48	A2	4070	C
48	A2	4071	C
48	A2	4072	C
48	A2	4074	A
48	A2	4076	G
48	A2	4083	C
48	A2	4084	G
48	A2	4086	U
48	A2	4088	C
48	A2	4090	G
48	A2	4091	G
48	A2	4093	G
48	A2	4097	A
48	A2	4104	G
48	A2	4106	C
48	A2	4109	G
48	A2	4110	C
48	A2	4112	G

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Mol	Chain	Res	Type
48	A2	4119	A
48	A2	4120	C
48	A2	4124	C
48	A2	4126	C
48	A2	4130	G
48	A2	4132	A
48	A2	4145	G
48	A2	4150	U
48	A2	4153	G
48	A2	4156	U
48	A2	4167	A
48	A2	4174	A
48	A2	4175	A
48	A2	4176	A
48	A2	4187	G
48	A2	4188	G
48	A2	4191	U
48	A2	4195	A
48	A2	4206	A
48	A2	4211	G
48	A2	4215	A
48	A2	4216	G
48	A2	4219	A
48	A2	4228	G
48	A2	4229	G
48	A2	4230	A
48	A2	4234	G
48	A2	4235	A
48	A2	4238	G
48	A2	4241	A
48	A2	4242	A
48	A2	4243	A
48	A2	4244	A
48	A2	4252	U
48	A2	4253	G
48	A2	4265	C
48	A2	4266	A
48	A2	4267	G
48	A2	4268	U
48	A2	4276	C
48	A2	4279	A
48	A2	4281	C

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Mol	Chain	Res	Type
48	A2	4291	G
48	A2	4292	G
48	A2	4294	C
48	A2	4299	C
48	A2	4301	A
48	A2	4310	A
48	A2	4311	C
48	A2	4316	U
48	A2	4319	G
48	A2	4327	C
48	A2	4330	G
48	A2	4333	G
48	A2	4334	U
48	A2	4337	C
48	A2	4339	G
48	A2	4340	A
48	A2	4341	A
48	A2	4342	A
48	A2	4349	C
48	A2	4353	G
48	A2	4355	G
48	A2	4356	A
48	A2	4360	C
48	A2	4372	G
48	A2	4382	U
48	A2	4384	A
48	A2	4395	G
48	A2	4406	C
48	A2	4410	G
48	A2	4414	U
48	A2	4415	C
48	A2	4426	A
48	A2	4428	C
48	A2	4437	G
48	A2	4441	A
48	A2	4443	U
48	A2	4453	G
48	A2	4455	U
48	A2	4466	C
48	A2	4474	U
48	A2	4475	A
48	A2	4477	G

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Mol	Chain	Res	Type
48	A2	4480	A
48	A2	4510	A
48	A2	4522	C
48	A2	4531	U
48	A2	4532	G
48	A2	4535	G
48	A2	4537	G
48	A2	4546	A
48	A2	4551	A
48	A2	4552	A
48	A2	4561	A
48	A2	4576	G
48	A2	4579	G
48	A2	4590	U
48	A2	4593	G
48	A2	4597	A
48	A2	4598	U
48	A2	4614	G
48	A2	4618	A
48	A2	4619	U
48	A2	4620	G
48	A2	4621	G
48	A2	4624	C
48	A2	4630	U
48	A2	4632	C
48	A2	4633	C
48	A2	4640	G
48	A2	4649	A
48	A2	4655	C
48	A2	4662	A
48	A2	4665	U
48	A2	4671	U
48	A2	4675	G
48	A2	4680	G
48	A2	4681	G
48	A2	4692	C
48	A2	4693	G
48	A2	4694	G
48	A2	4696	A
48	A2	4700	C
48	A2	4703	C
48	A2	4704	G

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Mol	Chain	Res	Type
48	A2	4709	C
48	A2	4710	U
48	A2	4712	G
48	A2	4714	U
48	A2	4715	U
48	A2	4716	G
48	A2	4718	C
48	A2	4720	U
48	A2	4722	G
48	A2	4724	A
48	A2	4725	U
48	A2	4726	A
48	A2	4731	G
48	A2	4732	U
48	A2	4824	C
48	A2	4827	U
48	A2	4828	G
48	A2	4831	G
48	A2	4832	A
48	A2	4833	G
48	A2	4834	U
48	A2	4838	C
48	A2	4839	U
48	A2	4840	U
48	A2	4847	G
48	A2	4849	G
48	A2	4852	A
48	A2	4854	G
48	A2	4855	G
48	A2	4856	G
48	A2	4859	G
48	A2	4863	C
48	A2	4864	C
48	A2	4865	G
48	A2	4866	G
48	A2	4868	A
48	A2	4871	G
48	A2	4878	C
48	A2	4880	C
48	A2	4882	C
48	A2	4883	U
48	A2	4884	C

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Mol	Chain	Res	Type
48	A2	4885	G
48	A2	4886	C
48	A2	4890	U
48	A2	4895	C
48	A2	4897	C
48	A2	4898	C
48	A2	4899	G
48	A2	4901	A
48	A2	4902	C
48	A2	4904	U
48	A2	4909	G
48	A2	4919	G
48	A2	4924	A
48	A2	4927	C
48	A2	4934	U
48	A2	4935	A
48	A2	4936	G
48	A2	4946	U
48	A2	4947	U
48	A2	4949	U
48	A2	4950	G
48	A2	4957	G
48	A2	4971	C
48	A2	4975	G
48	A2	4981	C
48	A2	4982	C
48	A2	4984	U
48	A2	4985	C
48	A2	4987	C
48	A2	4999	G
48	A2	5000	A
48	A2	5008	C
48	A2	5011	U
48	A2	5012	C
48	A2	5013	G
48	A2	5016	A
48	A2	5019	A
48	A2	5020	G
48	A2	5024	U
48	A2	5027	U
49	B1	4	C
49	B1	16	G

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Mol	Chain	Res	Type
49	B1	20	G
49	B1	23	G
49	B1	33	G
49	B1	41	G
49	B1	44	U
49	B1	46	A
49	B1	49	C
49	B1	51	U
49	B1	54	A
49	B1	59	U
49	B1	61	A
49	B1	62	G
49	B1	65	C
49	B1	67	C
49	B1	70	G
49	B1	71	G
49	B1	72	C
49	B1	73	C
49	B1	74	G
49	B1	77	A
49	B1	82	G
49	B1	89	C
49	B1	91	A
49	B1	100	U
49	B1	101	U
49	B1	103	A
49	B1	104	A
49	B1	109	U
49	B1	110	U
49	B1	113	G
49	B1	114	G
49	B1	115	U
49	B1	116	U
49	B1	122	G
49	B1	125	C
49	B1	126	G
49	B1	142	C
49	B1	143	U
49	B1	146	G
49	B1	147	A
49	B1	153	G
49	B1	154	U

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Mol	Chain	Res	Type
49	B1	155	G
49	B1	157	U
49	B1	159	A
49	B1	160	U
49	B1	161	U
49	B1	162	C
49	B1	170	A
49	B1	171	A
49	B1	172	U
49	B1	175	A
49	B1	178	C
49	B1	180	G
49	B1	181	A
49	B1	183	G
49	B1	188	C
49	B1	192	C
49	B1	199	C
49	B1	207	G
49	B1	209	A
49	B1	210	U
49	B1	211	G
49	B1	214	U
49	B1	217	A
49	B1	225	G
49	B1	226	A
49	B1	227	U
49	B1	228	C
49	B1	229	A
49	B1	230	A
49	B1	233	C
49	B1	234	C
49	B1	236	A
49	B1	238	C
49	B1	240	G
49	B1	283	G
49	B1	284	C
49	B1	285	U
49	B1	286	U
49	B1	287	U
49	B1	288	G
49	B1	292	A
49	B1	293	C

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Mol	Chain	Res	Type
49	B1	301	A
49	B1	305	U
49	B1	306	C
49	B1	308	G
49	B1	309	G
49	B1	310	C
49	B1	313	A
49	B1	314	U
49	B1	318	A
49	B1	319	C
49	B1	324	C
49	B1	327	G
49	B1	328	U
49	B1	329	G
49	B1	330	G
49	B1	331	C
49	B1	332	G
49	B1	333	G
49	B1	339	A
49	B1	343	A
49	B1	344	U
49	B1	347	G
49	B1	349	A
49	B1	351	G
49	B1	358	C
49	B1	364	A
49	B1	367	U
49	B1	368	U
49	B1	369	C
49	B1	372	U
49	B1	376	A
49	B1	381	C
49	B1	385	G
49	B1	386	C
49	B1	398	A
49	B1	402	C
49	B1	407	G
49	B1	408	A
49	B1	409	C
49	B1	413	G
49	B1	417	C
49	B1	428	U

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Mol	Chain	Res	Type
49	B1	438	G
49	B1	439	A
49	B1	441	C
49	B1	448	A
49	B1	449	A
49	B1	450	C
49	B1	464	A
49	B1	465	A
49	B1	468	A
49	B1	471	G
49	B1	472	C
49	B1	474	G
49	B1	476	A
49	B1	482	G
49	B1	487	U
49	B1	489	A
49	B1	492	C
49	B1	496	C
49	B1	501	C
49	B1	503	C
49	B1	504	G
49	B1	507	G
49	B1	508	A
49	B1	512	A
49	B1	517	C
49	B1	518	G
49	B1	522	A
49	B1	523	A
49	B1	525	A
49	B1	527	C
49	B1	529	A
49	B1	530	U
49	B1	534	G
49	B1	535	G
49	B1	536	A
49	B1	541	U
49	B1	542	U
49	B1	544	G
49	B1	545	A
49	B1	546	G
49	B1	547	G
49	B1	548	C

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Mol	Chain	Res	Type
49	B1	550	C
49	B1	551	U
49	B1	552	G
49	B1	553	U
49	B1	554	A
49	B1	555	A
49	B1	558	G
49	B1	560	A
49	B1	562	U
49	B1	567	C
49	B1	568	C
49	B1	569	A
49	B1	570	C
49	B1	585	C
49	B1	587	A
49	B1	588	G
49	B1	590	A
49	B1	591	U
49	B1	592	C
49	B1	594	A
49	B1	598	G
49	B1	600	G
49	B1	604	A
49	B1	606	G
49	B1	607	U
49	B1	608	C
49	B1	613	G
49	B1	614	C
49	B1	615	C
49	B1	617	G
49	B1	620	G
49	B1	621	C
49	B1	623	G
49	B1	627	U
49	B1	628	A
49	B1	629	A
49	B1	631	U
49	B1	643	A
49	B1	644	G
49	B1	645	C
49	B1	649	U
49	B1	655	A

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Mol	Chain	Res	Type
49	B1	657	U
49	B1	658	U
49	B1	659	G
49	B1	660	C
49	B1	662	G
49	B1	669	A
49	B1	672	A
49	B1	673	G
49	B1	683	G
49	B1	684	G
49	B1	688	U
49	B1	690	G
49	B1	691	G
49	B1	739	C
49	B1	740	C
49	B1	742	U
49	B1	743	U
49	B1	744	G
49	B1	746	C
49	B1	748	C
49	B1	749	U
49	B1	750	C
49	B1	791	C
49	B1	797	C
49	B1	798	G
49	B1	799	U
49	B1	800	U
49	B1	801	U
49	B1	809	A
49	B1	811	A
49	B1	821	G
49	B1	829	C
49	B1	836	G
49	B1	837	A
49	B1	839	C
49	B1	840	C
49	B1	841	G
49	B1	847	A
49	B1	861	A
49	B1	870	A
49	B1	872	A
49	B1	873	G

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Mol	Chain	Res	Type
49	B1	874	G
49	B1	881	G
49	B1	887	U
49	B1	888	U
49	B1	890	U
49	B1	893	U
49	B1	905	C
49	B1	909	G
49	B1	912	C
49	B1	913	A
49	B1	914	U
49	B1	917	U
49	B1	919	A
49	B1	920	A
49	B1	928	G
49	B1	929	G
49	B1	933	G
49	B1	943	U
49	B1	950	C
49	B1	955	A
49	B1	956	G
49	B1	958	G
49	B1	960	U
49	B1	962	A
49	B1	963	A
49	B1	969	U
49	B1	970	G
49	B1	971	G
49	B1	973	C
49	B1	975	G
49	B1	983	A
49	B1	988	C
49	B1	990	A
49	B1	992	A
49	B1	996	A
49	B1	997	A
49	B1	1001	A
49	B1	1002	U
49	B1	1008	A
49	B1	1017	U
49	B1	1022	U
49	B1	1023	A

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Mol	Chain	Res	Type
49	B1	1028	A
49	B1	1032	C
49	B1	1037	G
49	B1	1040	G
49	B1	1044	G
49	B1	1049	A
49	B1	1050	A
49	B1	1055	A
49	B1	1061	U
49	B1	1064	C
49	B1	1069	U
49	B1	1076	G
49	B1	1080	A
49	B1	1085	C
49	B1	1086	G
49	B1	1087	A
49	B1	1088	U
49	B1	1089	G
49	B1	1100	A
49	B1	1102	G
49	B1	1109	C
49	B1	1114	U
49	B1	1115	U
49	B1	1116	C
49	B1	1117	C
49	B1	1118	C
49	B1	1119	A
49	B1	1120	U
49	B1	1121	G
49	B1	1123	C
49	B1	1126	G
49	B1	1133	A
49	B1	1139	C
49	B1	1140	G
49	B1	1146	C
49	B1	1149	A
49	B1	1150	A
49	B1	1154	U
49	B1	1155	U
49	B1	1157	G
49	B1	1158	G
49	B1	1163	C

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Mol	Chain	Res	Type
49	B1	1166	G
49	B1	1170	A
49	B1	1175	G
49	B1	1176	G
49	B1	1195	A
49	B1	1196	A
49	B1	1197	G
49	B1	1199	A
49	B1	1203	G
49	B1	1207	G
49	B1	1210	G
49	B1	1211	G
49	B1	1215	C
49	B1	1216	C
49	B1	1221	G
49	B1	1224	G
49	B1	1237	C
49	B1	1240	A
49	B1	1242	U
49	B1	1250	A
49	B1	1251	A
49	B1	1256	G
49	B1	1257	G
49	B1	1258	A
49	B1	1259	A
49	B1	1260	A
49	B1	1261	C
49	B1	1262	C
49	B1	1264	C
49	B1	1275	G
49	B1	1276	A
49	B1	1278	A
49	B1	1281	G
49	B1	1283	C
49	B1	1285	G
49	B1	1287	A
49	B1	1288	U
49	B1	1289	U
49	B1	1290	G
49	B1	1297	U
49	B1	1301	A
49	B1	1302	G

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Mol	Chain	Res	Type
49	B1	1309	C
49	B1	1310	U
49	B1	1312	G
49	B1	1313	A
49	B1	1315	U
49	B1	1316	C
49	B1	1318	G
49	B1	1321	G
49	B1	1329	U
49	B1	1330	G
49	B1	1331	C
49	B1	1341	C
49	B1	1343	U
49	B1	1347	U
49	B1	1348	G
49	B1	1371	U
49	B1	1372	U
49	B1	1376	A
49	B1	1378	A
49	B1	1381	G
49	B1	1382	A
49	B1	1393	G
49	B1	1396	A
49	B1	1397	U
49	B1	1398	G
49	B1	1399	C
49	B1	1401	A
49	B1	1403	C
49	B1	1404	U
49	B1	1406	G
49	B1	1409	A
49	B1	1411	G
49	B1	1412	C
49	B1	1417	C
49	B1	1418	C
49	B1	1419	C
49	B1	1420	G
49	B1	1421	A
49	B1	1424	G
49	B1	1439	A
49	B1	1441	U
49	B1	1446	A

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Mol	Chain	Res	Type
49	B1	1450	G
49	B1	1452	A
49	B1	1454	A
49	B1	1455	A
49	B1	1458	G
49	B1	1462	U
49	B1	1463	U
49	B1	1464	C
49	B1	1469	A
49	B1	1477	U
49	B1	1478	U
49	B1	1484	A
49	B1	1487	A
49	B1	1489	A
49	B1	1494	U
49	B1	1495	G
49	B1	1497	G
49	B1	1498	A
49	B1	1502	C
49	B1	1505	U
49	B1	1509	U
49	B1	1512	C
49	B1	1519	U
49	B1	1520	G
49	B1	1521	C
49	B1	1522	A
49	B1	1533	A
49	B1	1534	C
49	B1	1535	U
49	B1	1536	G
49	B1	1540	G
49	B1	1544	C
49	B1	1547	C
49	B1	1551	U
49	B1	1552	G
49	B1	1553	C
49	B1	1554	C
49	B1	1555	U
49	B1	1557	C
49	B1	1558	C
49	B1	1567	G
49	B1	1578	U

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Mol	Chain	Res	Type
49	B1	1580	A
49	B1	1584	G
49	B1	1585	U
49	B1	1586	U
49	B1	1587	G
49	B1	1588	A
49	B1	1594	A
49	B1	1599	U
49	B1	1600	G
49	B1	1601	A
49	B1	1605	G
49	B1	1606	G
49	B1	1618	C
49	B1	1620	A
49	B1	1622	U
49	B1	1623	A
49	B1	1624	U
49	B1	1632	G
49	B1	1637	A
49	B1	1640	A
49	B1	1646	C
49	B1	1660	C
49	B1	1661	A
49	B1	1662	U
49	B1	1663	A
49	B1	1665	G
49	B1	1666	C
49	B1	1671	G
49	B1	1672	U
49	B1	1674	G
49	B1	1678	A
49	B1	1695	A
49	B1	1699	A
49	B1	1703	C
49	B1	1721	U
49	B1	1726	G
49	B1	1742	C
49	B1	1744	G
49	B1	1746	U
49	B1	1753	C
49	B1	1756	C
49	B1	1757	G

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Mol	Chain	Res	Type
49	B1	1777	G
49	B1	1783	C
49	B1	1784	G
49	B1	1799	G
49	B1	1801	A
49	B1	1803	U
49	B1	1811	C
49	B1	1822	A
49	B1	1826	G
49	B1	1829	G
49	B1	1830	U
49	B1	1832	A
49	B1	1834	A
49	B1	1835	A
49	B1	1838	U
49	B1	1839	U
49	B1	1840	U
49	B1	1845	A
49	B1	1849	G
49	B1	1851	A
49	B1	1852	C
49	B1	1855	G
49	B1	1861	G
49	B1	1863	A
49	B1	1865	C
49	B1	1866	A
49	B1	1869	A
80	Bv	2	C
80	Bv	6	G
80	Bv	7	A
80	Bv	8	U
80	Bv	9	A
80	Bv	10	G
80	Bv	11	C
80	Bv	15	G
80	Bv	16	U
80	Bv	17	C
80	Bv	18	G
80	Bv	19	G
80	Bv	20	U
80	Bv	21	A
80	Bv	35	A

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Mol	Chain	Res	Type
80	Bv	37	A
80	Bv	40	C
80	Bv	42	C
80	Bv	46	G
80	Bv	48	C
80	Bv	49	C
80	Bv	56	C
80	Bv	59	U
80	Bv	60	U
80	Bv	62	C
80	Bv	65	G
80	Bv	67	C
80	Bv	76	A
81	Bx	46	U
81	Bx	48	U
81	Bx	50	U
81	Bx	51	U
81	Bx	53	U
81	Bx	54	U
81	Bx	55	U
81	Bx	57	U
81	Bx	58	U

All (19) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
7	A3	109	C
48	A2	31	U
48	A2	71	C
48	A2	901	U
48	A2	947	A
48	A2	1161	G
48	A2	1222	C
48	A2	2407	A
48	A2	3755	A
48	A2	4333	G
48	A2	4661	U
48	A2	4865	G
48	A2	4946	U
49	B1	160	U
49	B1	216	C
49	B1	227	U

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Mol	Chain	Res	Type
49	B1	797	C
49	B1	869	A
49	B1	1398	G

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 332 ligands modelled in this entry, 331 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	MVM	A	101	-	32,35,35	1.78	7 (21%)	39,49,49	2.50	16 (41%)

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	MVM	A	101	-	-	2/20/28/28	0/5/5/5

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
85	A	101	MVM	C5-N1	5.72	1.45	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
85	A	101	MVM	N5-N4	-4.53	1.30	1.37
85	A	101	MVM	C6-N1	2.73	1.45	1.39
85	A	101	MVM	O1-C5	-2.18	1.18	1.22
85	A	101	MVM	C2-CL	2.09	1.78	1.73
85	A	101	MVM	C1-C9	2.07	1.54	1.52
85	A	101	MVM	C7-C3	-2.03	1.48	1.53

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
85	A	101	MVM	C15-N4-C22	-7.03	121.07	130.09
85	A	101	MVM	C15-N4-N5	4.81	127.66	119.95
85	A	101	MVM	C6-N1-C5	-4.76	117.24	122.94
85	A	101	MVM	N3-C6-N1	4.26	120.91	116.35
85	A	101	MVM	C21-N7-C22	4.05	121.65	116.81
85	A	101	MVM	C7-C3-C9	3.83	118.09	110.81
85	A	101	MVM	C19-C18-N6	3.44	135.79	130.19
85	A	101	MVM	C8-N3-C6	3.16	122.20	115.05
85	A	101	MVM	C20-C21-N7	-2.67	120.04	123.97
85	A	101	MVM	C12-C5-N1	2.49	121.66	118.36
85	A	101	MVM	C17-C12-C13	2.37	121.58	118.57
85	A	101	MVM	C6-N1-C9	2.34	121.88	118.40
85	A	101	MVM	C1-C9-N1	-2.34	110.29	116.16
85	A	101	MVM	O1-C5-C12	-2.19	115.94	120.29
85	A	101	MVM	N6-N5-N4	2.08	108.69	106.37
85	A	101	MVM	C6-C2-CL	-2.06	119.56	121.50

There are no chirality outliers.

All (2) torsion outliers are listed below:

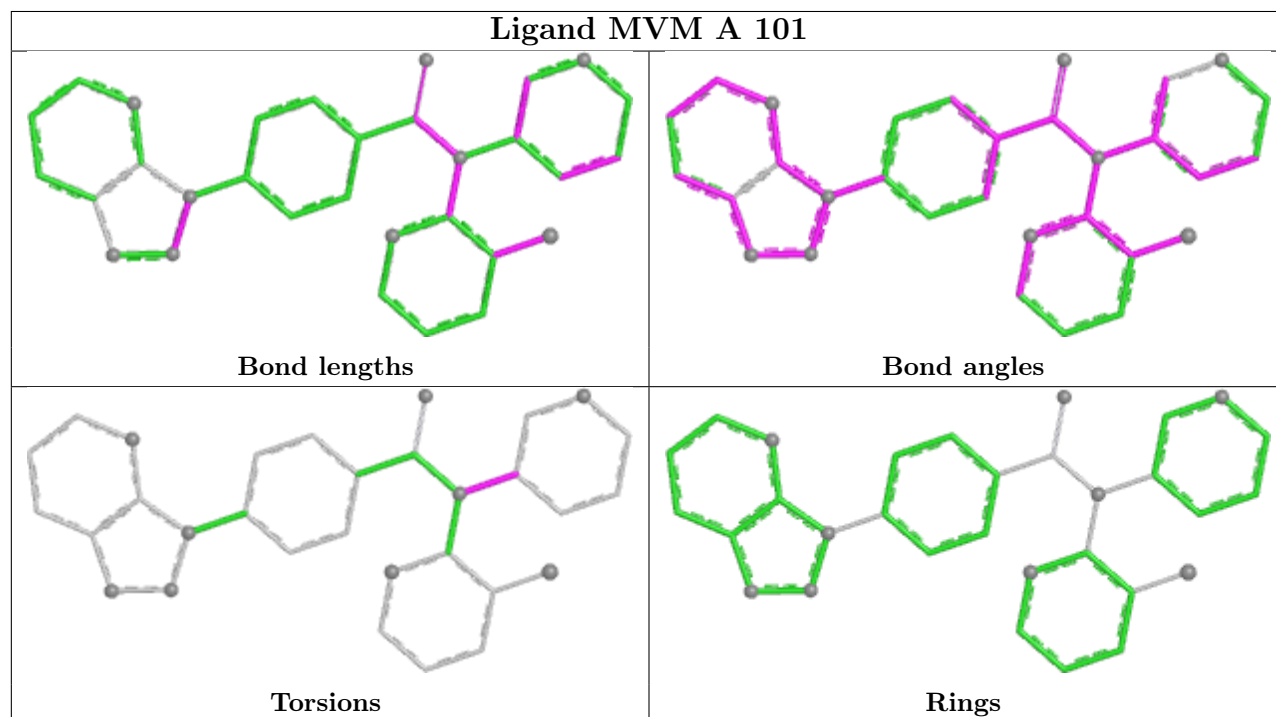
Mol	Chain	Res	Type	Atoms
85	A	101	MVM	C3-C9-N1-C5
85	A	101	MVM	C3-C9-N1-C6

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
48	A2	16
49	B1	6

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A2	3923:A	O3'	3930:U	P	31.28
1	B1	126:G	O3'	141:A	P	22.59

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A2	2231:G	O3'	2235:C	P	21.97
1	A2	3948:C	O3'	4004:G	P	18.85
1	B1	1426:U	O3'	1438:A	P	18.66
1	A2	1680:C	O3'	1699:C	P	18.34
1	A2	517:C	O3'	629:G	P	18.29
1	B1	751:G	O3'	790:C	P	17.33
1	A2	4734:C	O3'	4818:G	P	17.05
1	A2	2881:G	O3'	3569:C	P	16.41
1	A2	750:G	O3'	890:C	P	16.33
1	B1	696:G	O3'	737:G	P	15.56
1	A2	976:U	O3'	1047:G	P	15.44
1	B1	1757:G	O3'	1775:U	P	15.15
1	A2	1233:C	O3'	1243:G	P	14.69
1	A2	2093:C	O3'	2228:C	P	14.13
1	A2	1089:A	O3'	1145:G	P	14.10
1	B1	240:G	O3'	282:G	P	13.82
1	A2	955:C	O3'	957:G	P	8.96
1	A2	2229:C	O3'	2231:G	P	8.58
1	A2	1202:G	O3'	1216:G	P	8.51
1	A2	962:C	O3'	963:G	P	5.47

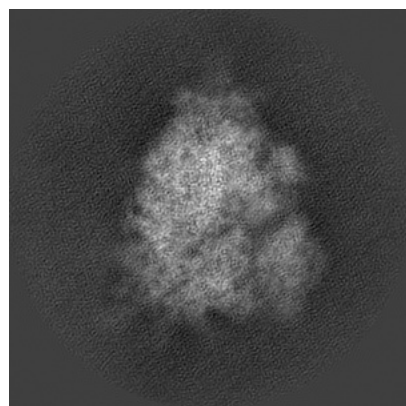
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0598. These allow visual inspection of the internal detail of the map and identification of artifacts.

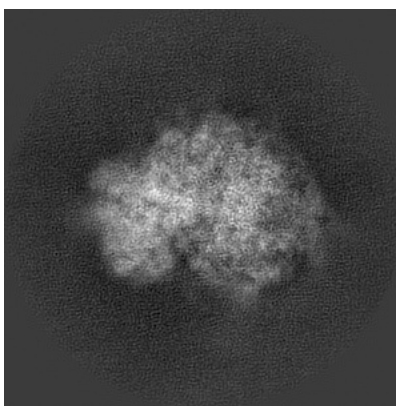
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

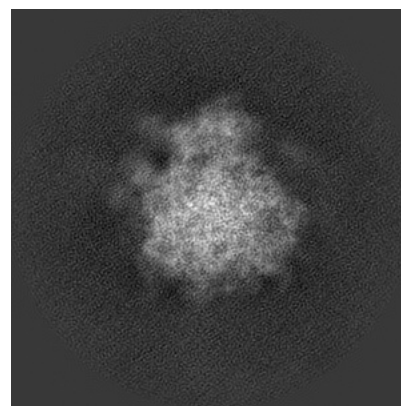
6.1.1 Primary map



X

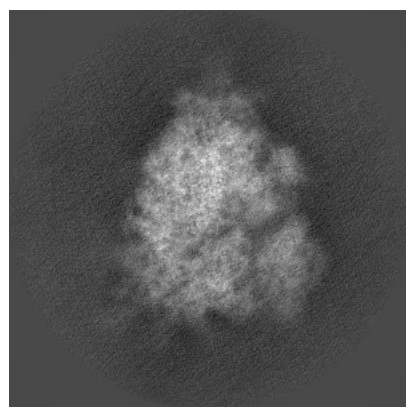


Y

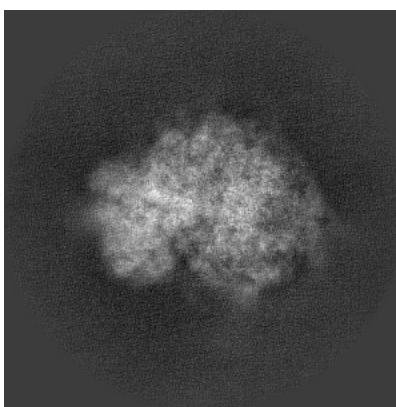


Z

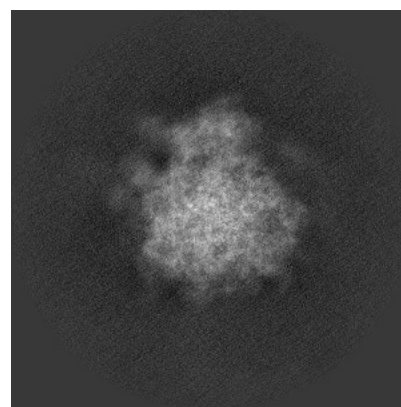
6.1.2 Raw map



X



Y

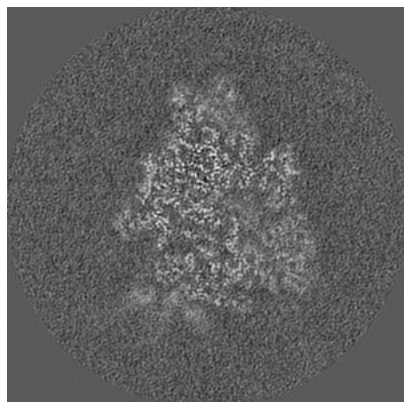


Z

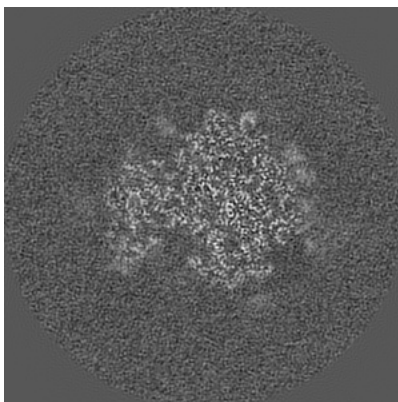
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

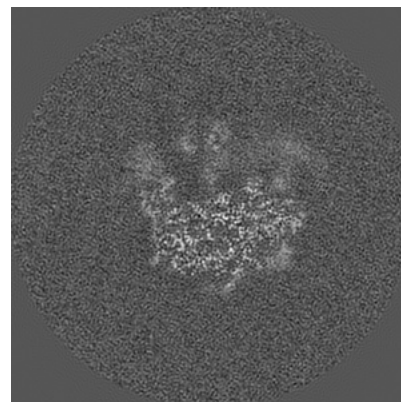
6.2.1 Primary map



X Index: 200

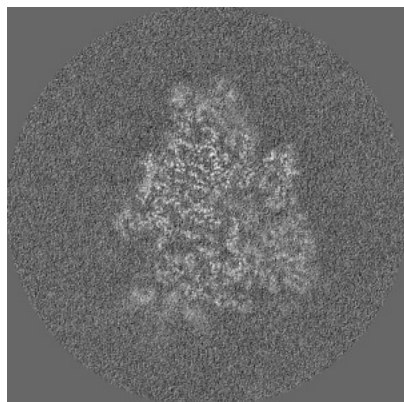


Y Index: 200

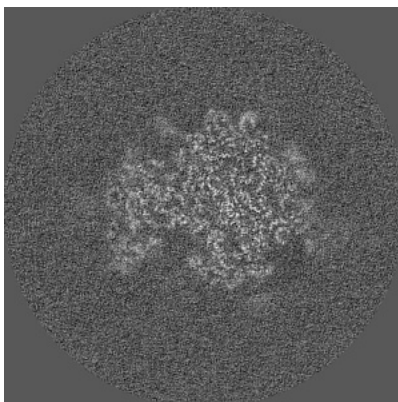


Z Index: 200

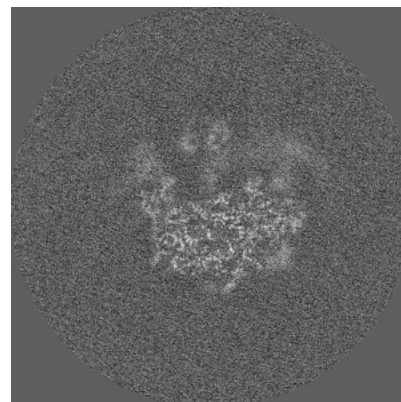
6.2.2 Raw map



X Index: 200



Y Index: 200

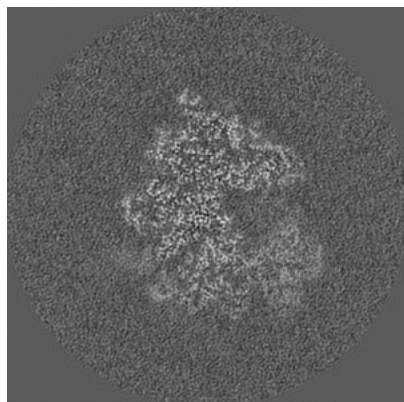


Z Index: 200

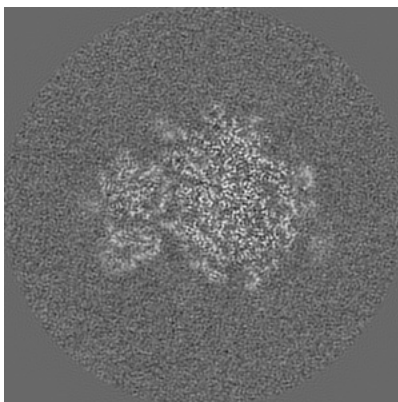
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

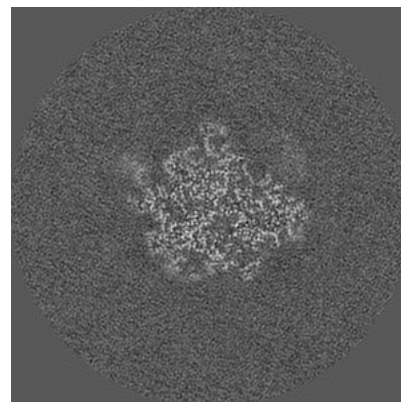
6.3.1 Primary map



X Index: 217

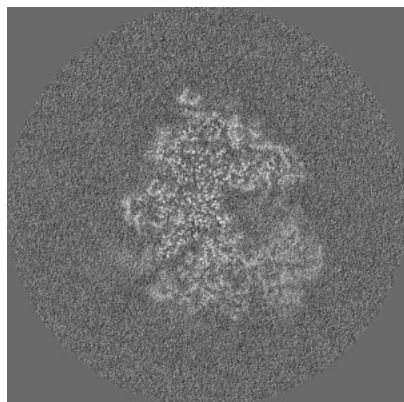


Y Index: 194

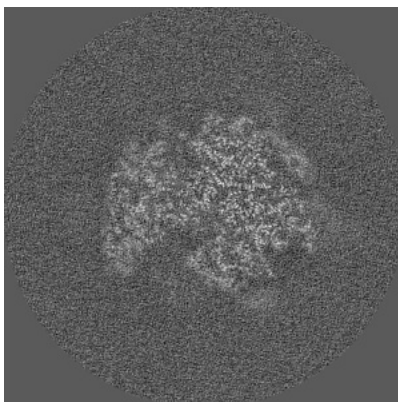


Z Index: 220

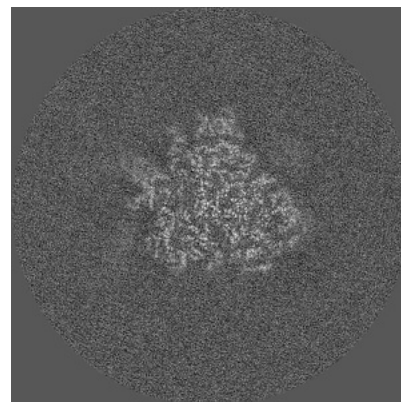
6.3.2 Raw map



X Index: 217



Y Index: 205

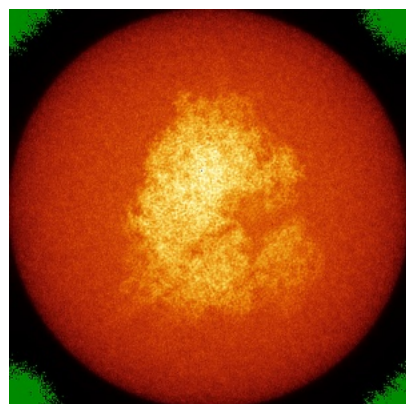


Z Index: 228

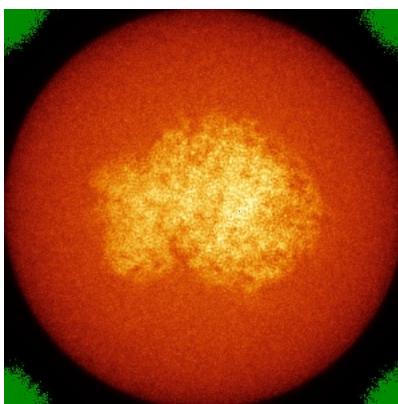
The images above show the largest variance slices of the map in three orthogonal directions.

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

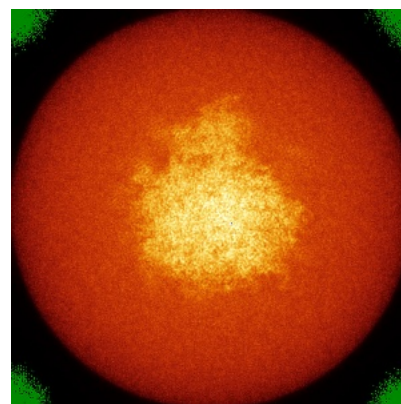
6.4.1 Primary map



X

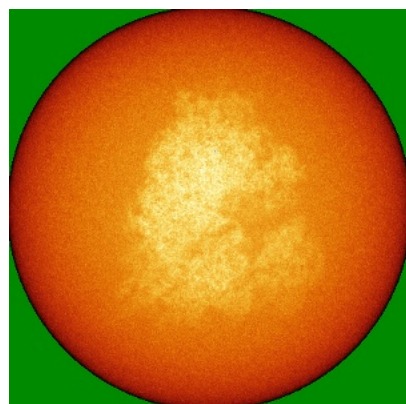


Y

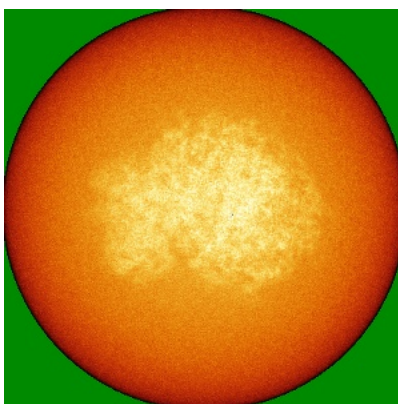


Z

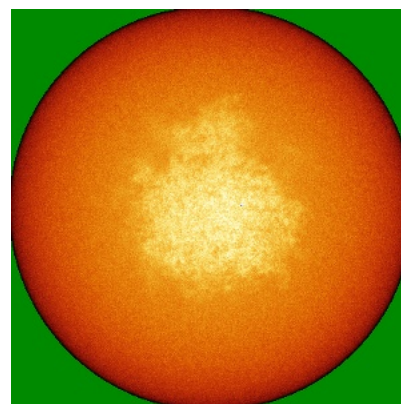
6.4.2 Raw map



X



Y

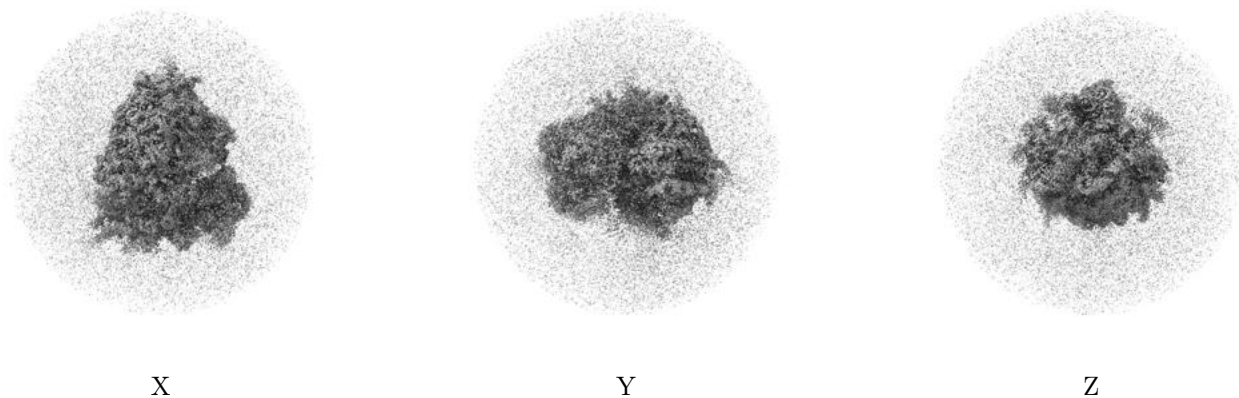


Z

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

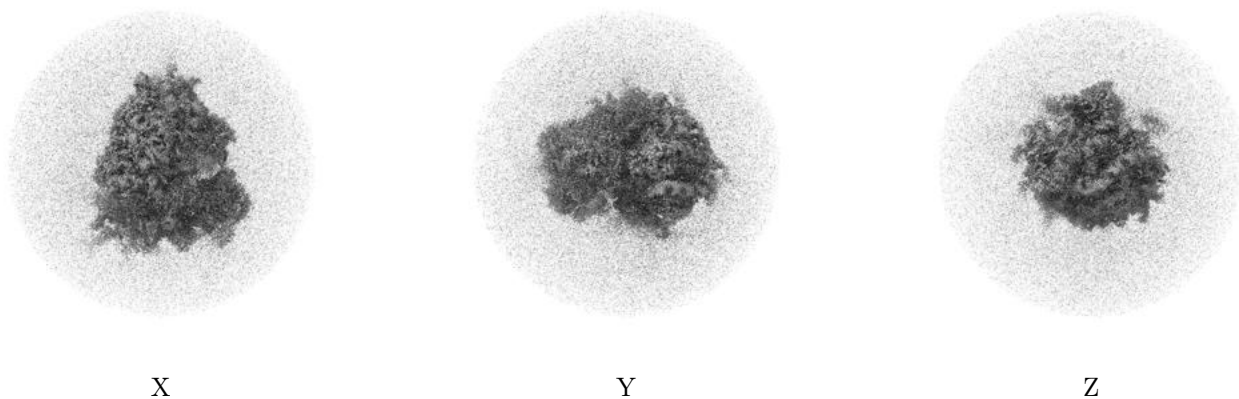
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.022. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

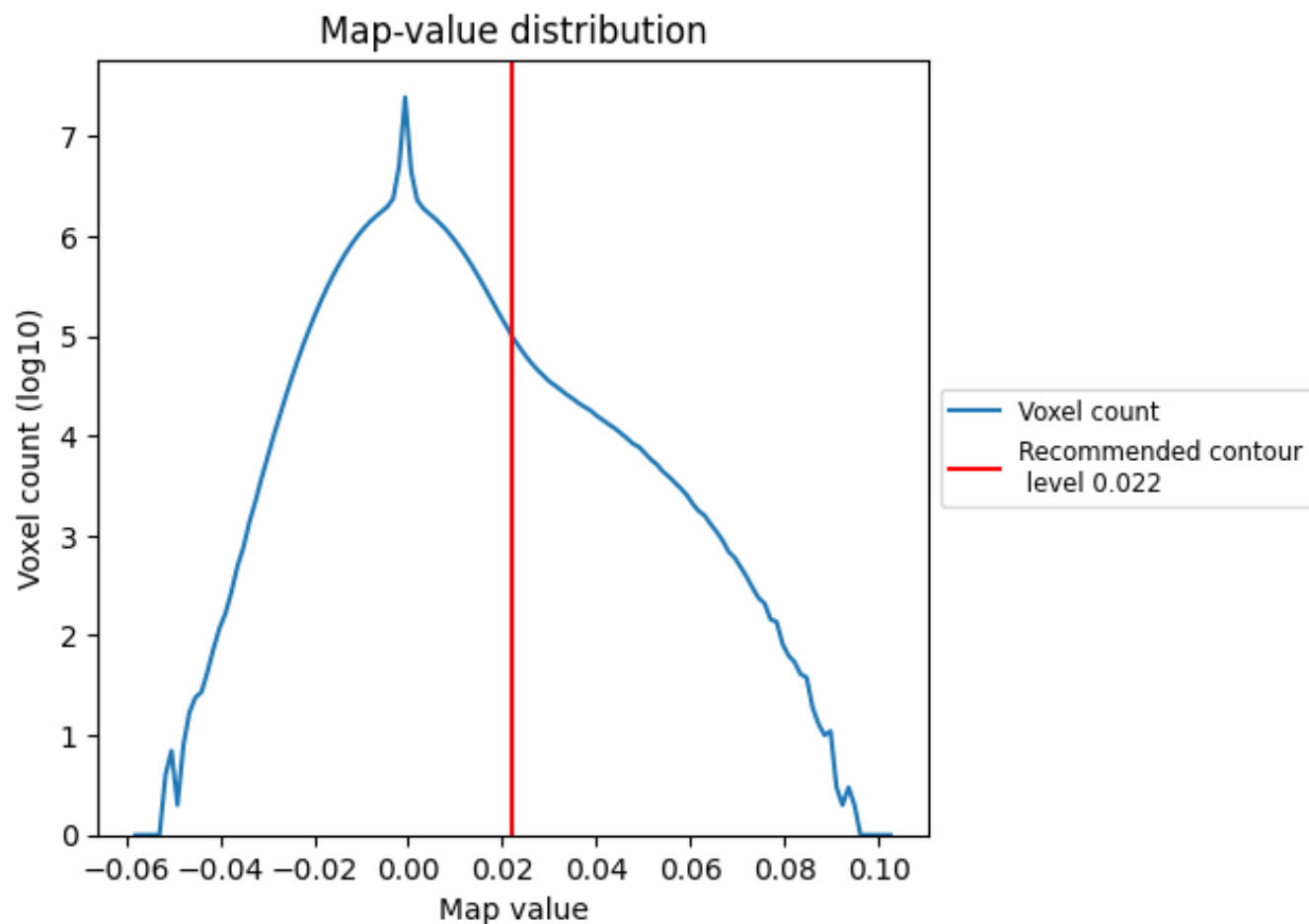
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

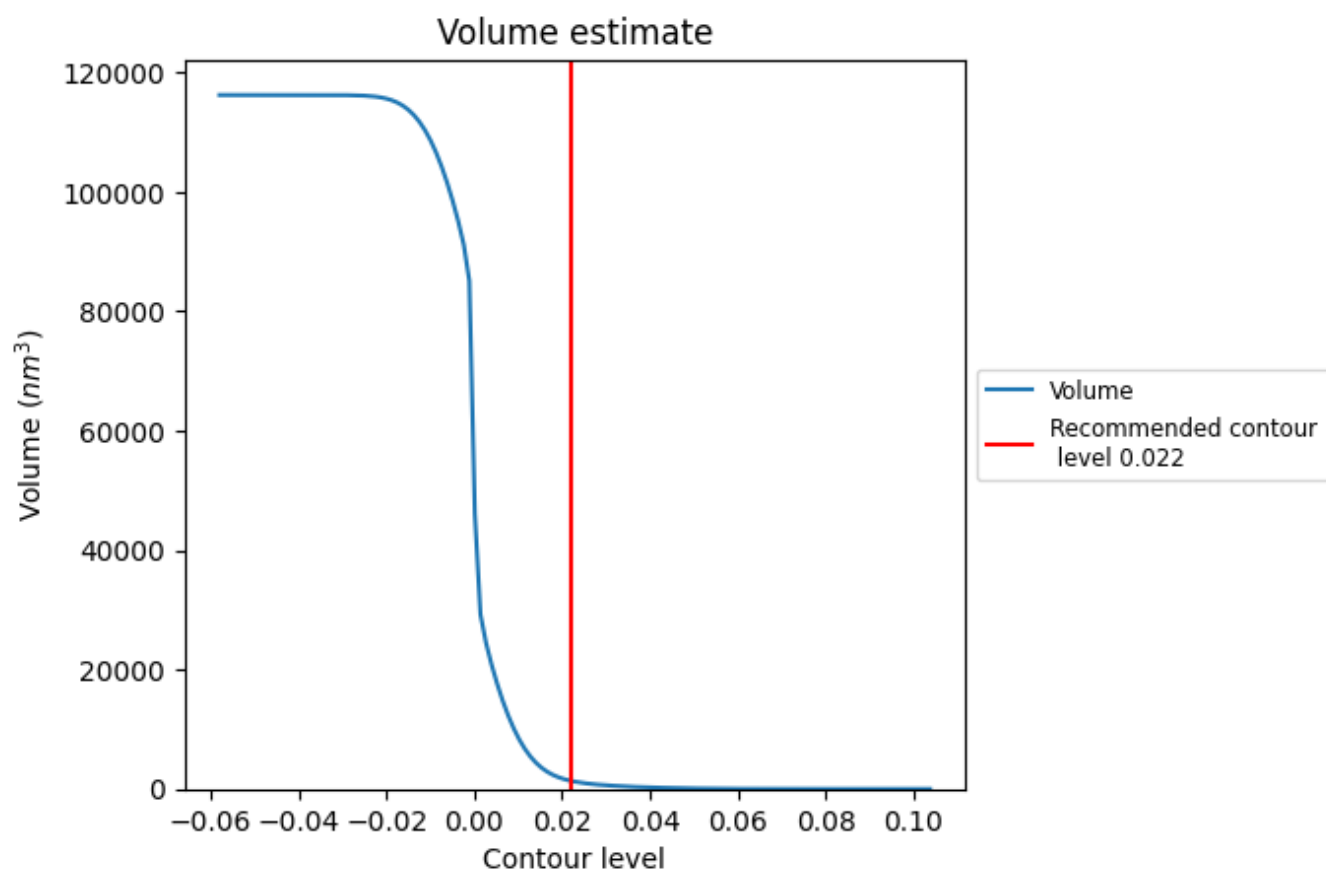
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

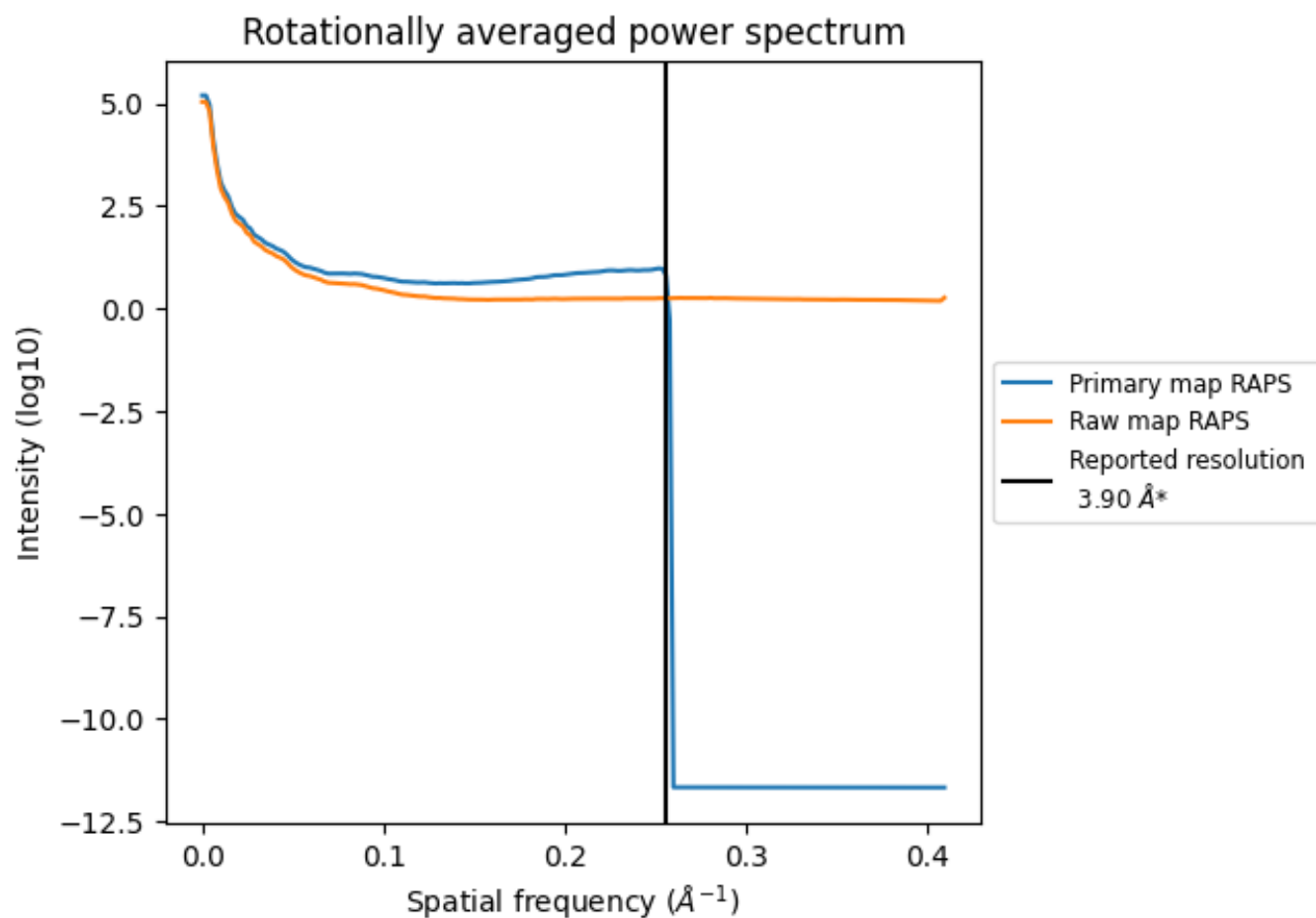
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1361 nm³; this corresponds to an approximate mass of 1230 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 ⓘ

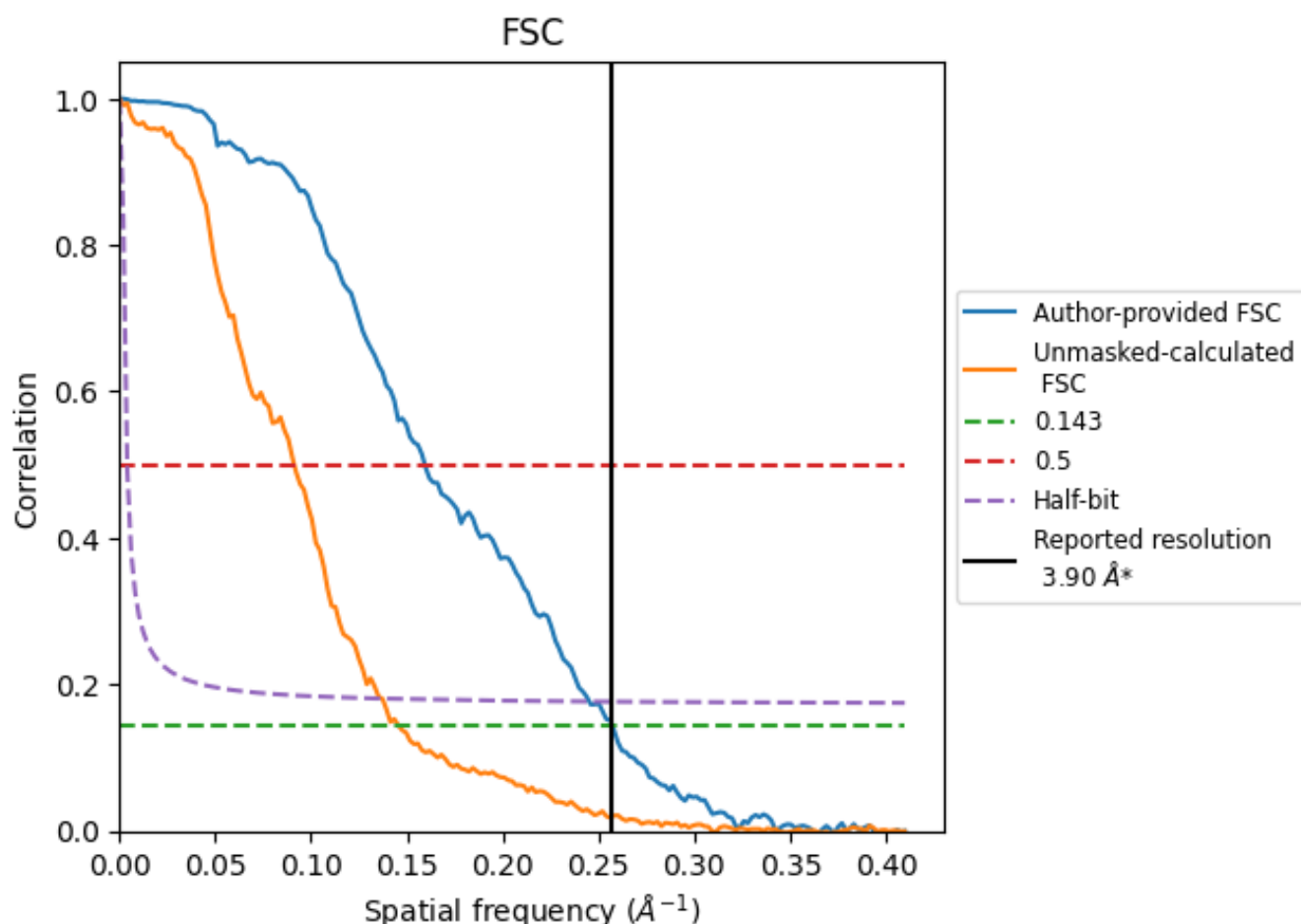


*Reported resolution corresponds to spatial frequency of 0.256 \AA^{-1}

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 0.256 Å⁻¹

8.2 Resolution estimates [i](#)

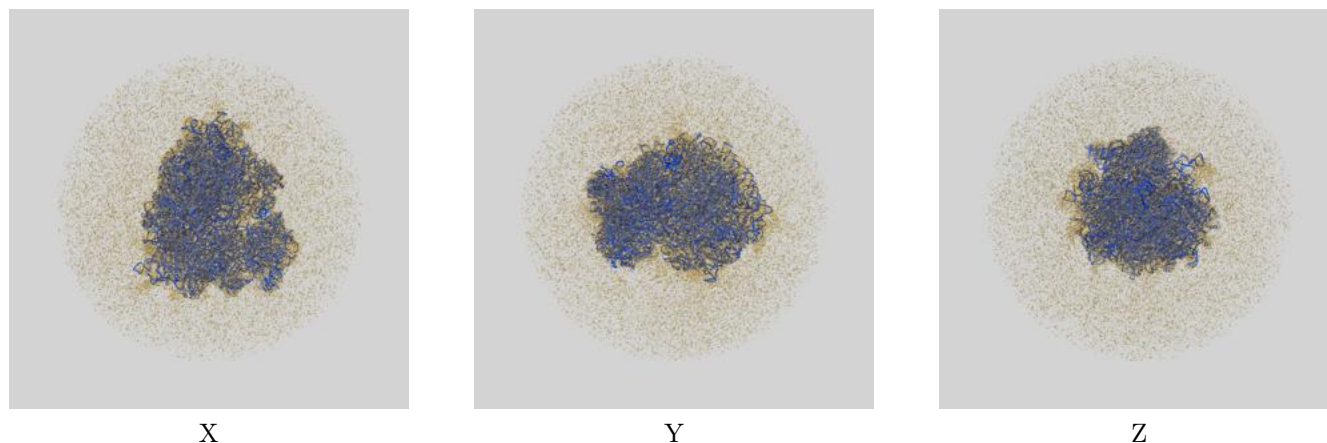
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.90	-	-
Author-provided FSC curve	3.89	6.27	4.08
Unmasked-calculated*	6.86	10.96	7.30

*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 6.86 differs from the reported value 3.9 by more than 10 %

9 Map-model fit [i](#)

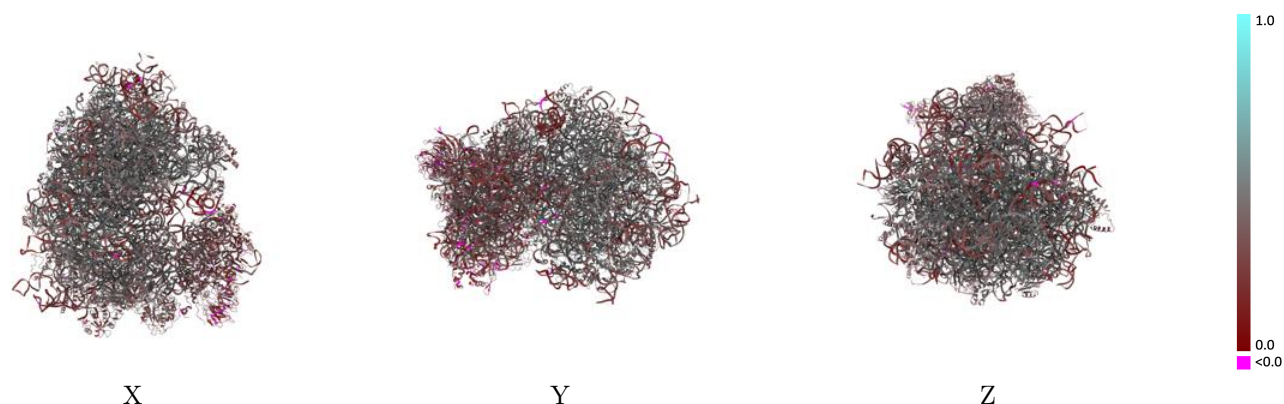
This section contains information regarding the fit between EMDB map EMD-0598 and PDB model 6OLZ. Per-residue inclusion information can be found in [section 3](#) on [page 20](#).

9.1 Map-model overlay [i](#)



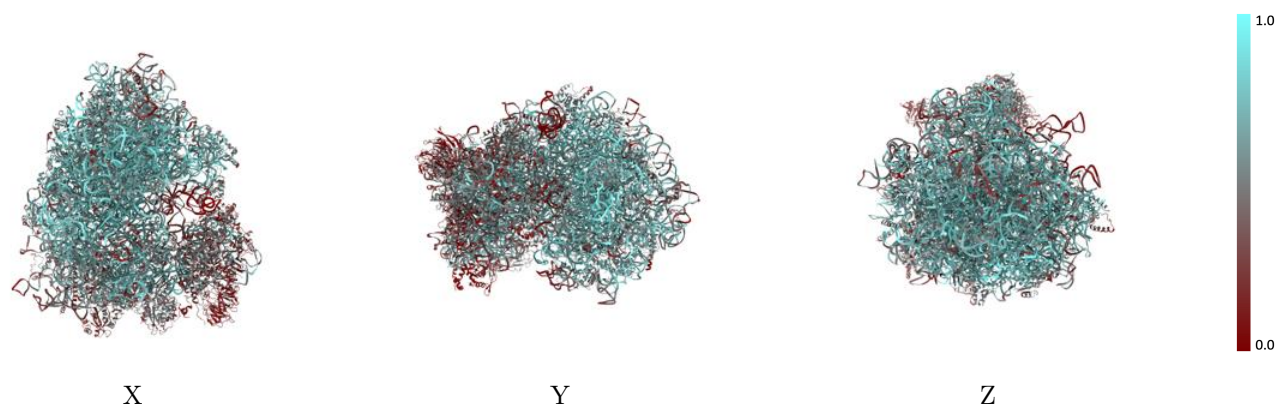
The images above show the 3D surface view of the map at the recommended contour level 0.022 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



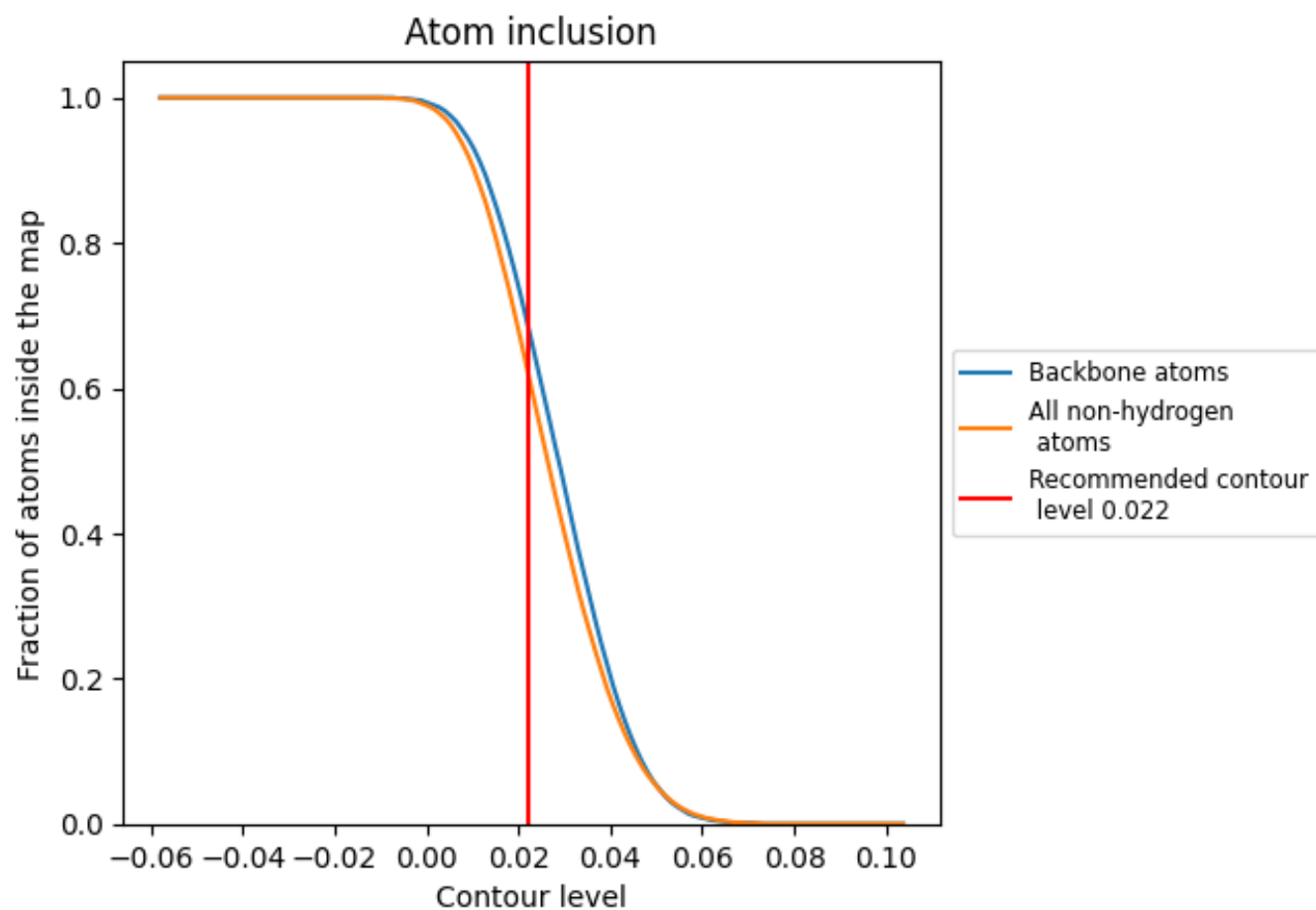
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.022).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 69% of all backbone atoms, 62% 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 (0.022) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6240	 0.3940
A	 0.2520	 0.3190
A2	 0.7480	 0.4090
A3	 0.7580	 0.4190
A4	 0.8400	 0.4390
AA	 0.6540	 0.4800
AB	 0.6310	 0.4530
AC	 0.6540	 0.4610
AD	 0.5620	 0.3920
AE	 0.5300	 0.3990
AF	 0.6220	 0.4410
AG	 0.5420	 0.4000
AH	 0.5620	 0.4300
AI	 0.5920	 0.4410
AJ	 0.5140	 0.3780
AL	 0.5930	 0.4140
AM	 0.6250	 0.4380
AN	 0.6920	 0.4760
AO	 0.6330	 0.4560
AP	 0.6660	 0.4730
AQ	 0.6440	 0.4640
AR	 0.5940	 0.4170
AS	 0.6480	 0.4620
AT	 0.6090	 0.4610
AU	 0.5110	 0.3850
AV	 0.6180	 0.4720
AW	 0.3680	 0.3430
AX	 0.6280	 0.4480
AY	 0.6480	 0.4620
AZ	 0.6010	 0.4220
Aa	 0.6750	 0.4650
Ab	 0.5330	 0.3850
Ac	 0.5540	 0.4100
Ad	 0.6220	 0.4460
Ae	 0.6570	 0.4720















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Chain	Atom inclusion	Q-score
Af	 0.6400	 0.4720
Ag	 0.6110	 0.4530
Ah	 0.6110	 0.4220
Ai	 0.6020	 0.4130
Aj	 0.7160	 0.4890
Ak	 0.5080	 0.3880
Al	 0.5850	 0.4380
Am	 0.6370	 0.4520
An	 0.5270	 0.4190
Ao	 0.6230	 0.4480
Ap	 0.6100	 0.4430
At	 0.6580	 0.4510
B1	 0.6440	 0.3640
BA	 0.4470	 0.3730
BB	 0.4620	 0.3870
BC	 0.4960	 0.3990
BD	 0.2440	 0.2790
BE	 0.4570	 0.3800
BF	 0.3020	 0.3080
BG	 0.3640	 0.3210
BH	 0.3390	 0.3290
BI	 0.5160	 0.4110
BJ	 0.4450	 0.3500
BK	 0.2030	 0.2460
BL	 0.4870	 0.4030
BM	 0.0440	 0.1750
BN	 0.4890	 0.3940
BO	 0.4960	 0.4110
BP	 0.2920	 0.2920
BQ	 0.3180	 0.2950
BR	 0.2880	 0.2990
BS	 0.3140	 0.2870
BT	 0.2930	 0.2630
BU	 0.2850	 0.2960
BV	 0.4330	 0.3670
BW	 0.5260	 0.4170
BX	 0.5180	 0.4040
BY	 0.4190	 0.3250
BZ	 0.2400	 0.2770
Ba	 0.5190	 0.4030
Bb	 0.4800	 0.4030
Bc	 0.2530	 0.3040

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Chain	Atom inclusion	Q-score
Bd	 0.3440	 0.3100
Be	 0.4240	 0.3860
Bf	 0.1100	 0.2150
Bg	 0.1370	 0.2190
Bv	 0.2000	 0.2750
Bx	 0.1250	 0.2270