



## Full wwPDB EM Validation Report ⓘ

Nov 7, 2023 – 08:43 am GMT

PDB ID : 7O80  
EMDB ID : EMD-12758  
Title : Rabbit 80S ribosome in complex with eRF1 and ABCE1 stalled at the STOP codon in the mutated SARS-CoV-2 slippery site  
Authors : Bhatt, P.R.; Scaiola, A.; Leibundgut, M.A.; Atkins, J.F.; Ban, N.  
Deposited on : 2021-04-14  
Resolution : 2.90 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](mailto: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>.

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

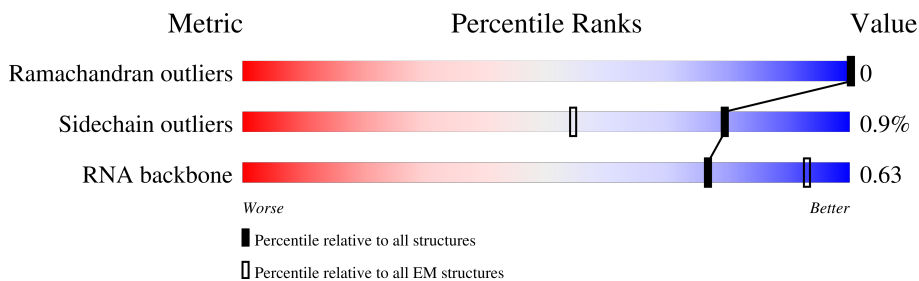
EMDB validation analysis : 0.0.1.dev70  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

# 1 Overall quality at a glance

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

The reported resolution of this entry is 2.90 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.




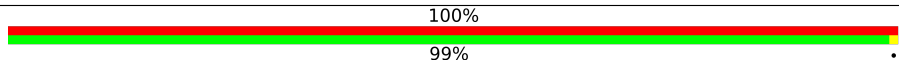

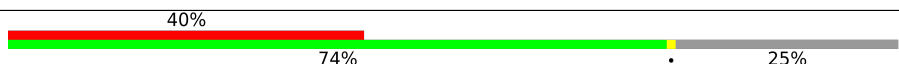
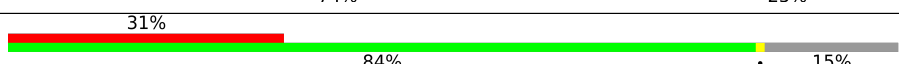
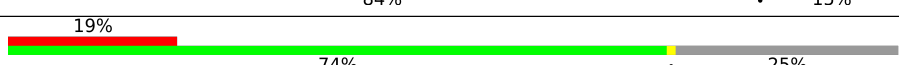

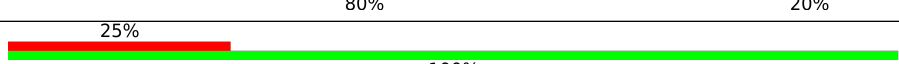
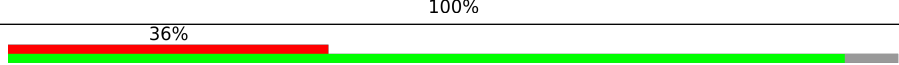
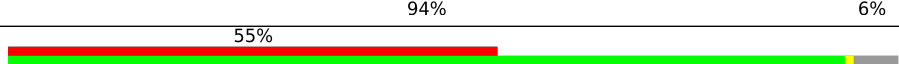

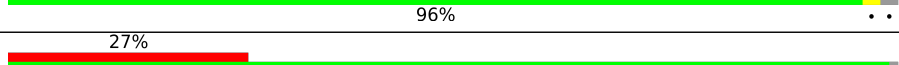
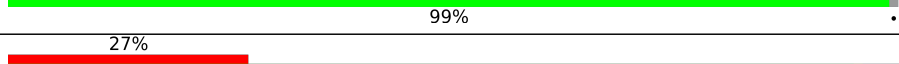
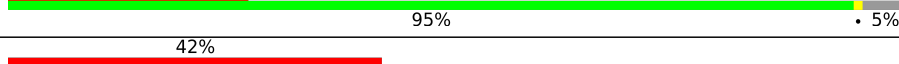
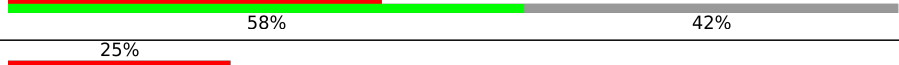
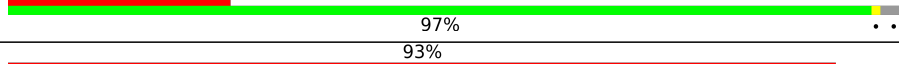

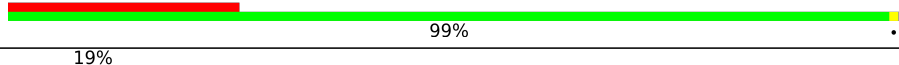
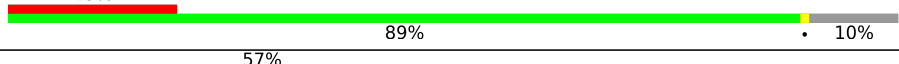
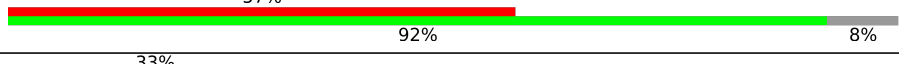
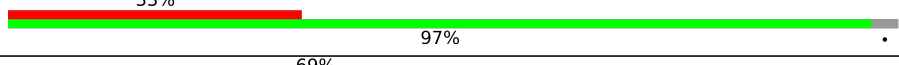
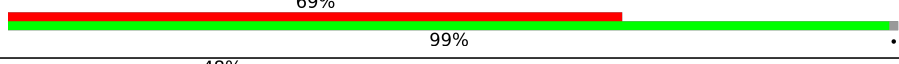
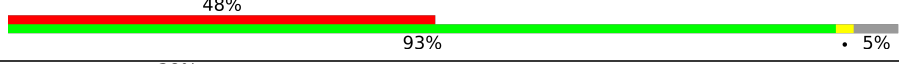
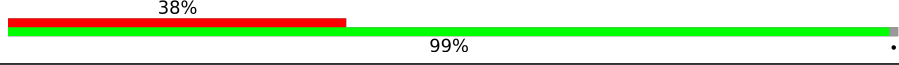

Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	A2	1870	
2	AA	84	
3	AB	69	
4	AC	156	
5	AD	133	
6	AE	115	
7	AF	317	
8	AG	56	

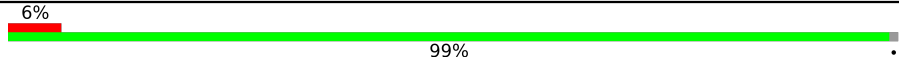
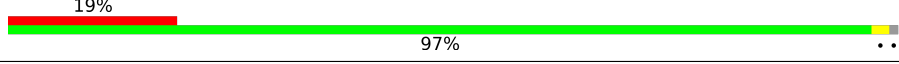
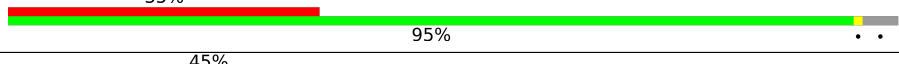

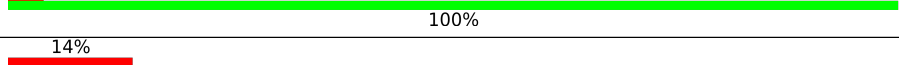
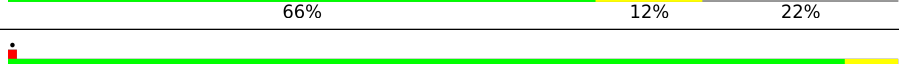
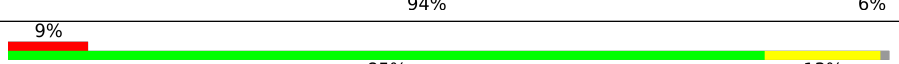
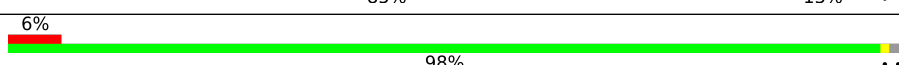
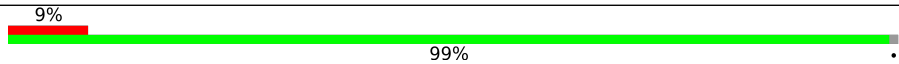

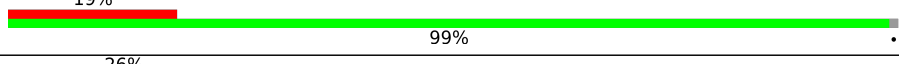
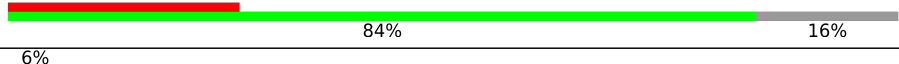
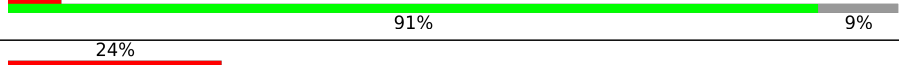

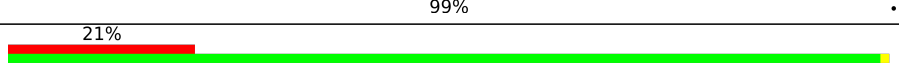
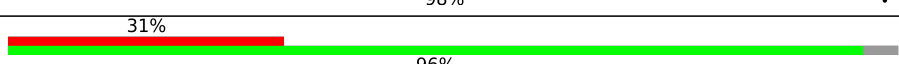
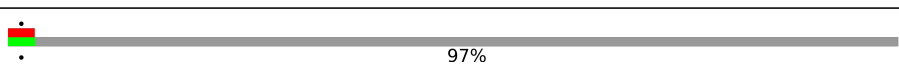
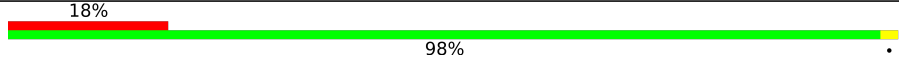

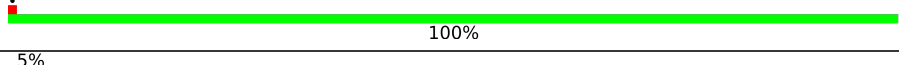
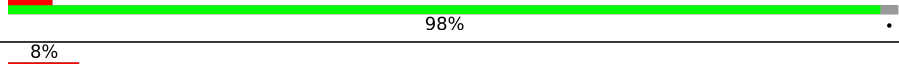

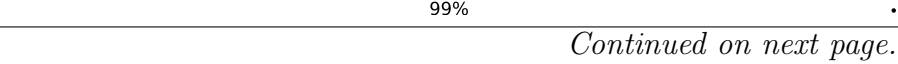


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Mol	Chain	Length	Quality of chain
9	AH	217	
10	AI	76	
11	AT	86	
12	AZ	295	
13	Aa	264	
14	Ab	293	
15	Ac	281	
16	Ad	263	
17	Ae	204	
18	Af	249	
19	Ag	194	
20	Ah	208	
21	Ai	194	
22	Aj	165	
23	Ak	158	
24	Al	132	
25	Am	151	
26	An	151	
27	Ao	145	
28	Ap	146	
29	Aq	135	
30	Ar	152	
31	As	145	
32	At	119	
33	Au	83	

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Mol	Chain	Length	Quality of chain
34	Av	130	
35	Aw	143	
36	Ax	130	
37	Ay	124	
38	Az	25	
39	B5	4808	
40	B7	119	
41	B8	158	
42	BA	257	
43	BB	403	
44	BC	413	
45	BD	297	
46	BE	291	
47	BF	247	
48	BG	266	
49	BH	192	
50	BI	214	
51	BJ	178	
52	BK	1071	
53	BL	211	
54	BM	218	
55	BN	204	
56	BO	203	
57	BP	184	
58	BQ	188	

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Mol	Chain	Length	Quality of chain
59	BR	196	18% 92% 8%
60	BS	176	7% 100%
61	BT	160	16% 99%
62	BU	128	38% 77% 23%
63	BV	140	15% 98%
64	BW	157	41% 76% 23%
65	BX	156	14% 76% 24%
66	BY	145	10% 91% 8%
67	BZ	136	16% 99%
68	Ba	148	7% 99%
69	Bb	245	21% 44% 56%
70	Bc	115	23% 94% 6%
71	Bd	125	13% 86% 14%
72	Be	135	7% 96%
73	Bf	110	7% 100%
74	Bg	117	14% 97%
75	Bh	123	13% 99%
76	Bi	105	20% 96%
77	Bj	97	87% 11%
78	Bk	70	46% 99%
79	Bl	51	14% 96%
80	Bm	128	7% 41% 59%
81	Bo	106	22% 98%
82	Bp	92	12% 99%
83	Br	137	9% 91% 8%

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Mol	Chain	Length	Quality of chain
84	Bs	318	
85	Bt	165	
86	Bv	217	
87	By	437	
88	Bz	599	

## 2 Entry composition

There are 95 unique types of molecules in this entry. The entry contains 235677 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	A2	1770	37833	16911	6781	12371	1770	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A2	1249	B8N	C	conflict	GB GBCT01000564.1
A2	1338	4AC	C	conflict	GB GBCT01000564.1
A2	1843	4AC	C	conflict	GB GBCT01000564.1

- Molecule 2 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	AA	83	651	408	121	115	7	0	0

- Molecule 3 is a protein called Ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	AB	63	495	302	98	93	2	0	0

- Molecule 4 is a protein called Ribosomal protein S27a.

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

- Molecule 5 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	AD	57	457	282	101	73	1	0	0

- Molecule 6 is a protein called Ribosomal protein eS26.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	AE	101	814	507	170	132	5	0	0

- Molecule 7 is a protein called RACK1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	AF	313	2436	1535	424	465	12	0	0

- Molecule 8 is a protein called uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	AG	55	459	286	94	74	5	0	0

- Molecule 9 is a RNA chain called mRNA containing SARS-CoV-2 sequence.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
9	AH	24	508	227	84	173	24	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AH	3466	U	A	conflict	GB NC_045512.2
AH	3468	A	C	conflict	GB NC_045512.2

- Molecule 10 is a RNA chain called E-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
10	AI	76	939	393	11	459	76	0	0

- Molecule 11 is a RNA chain called P-site Leu-tRNA(Leu).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
11	AT	86	1840	820	330	604	86	0	0

- Molecule 12 is a protein called 40S ribosomal protein SA.



Mol	Chain	Residues	Atoms					AltConf	Trace
12	AZ	221	Total	C	N	O	S	0	0
			1743	1107	305	323	8		

- Molecule 13 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	Aa	224	Total	C	N	O	S	0	0
			1815	1152	328	321	14		

- Molecule 14 is a protein called Ribosomal protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	Ab	220	Total	C	N	O	S	0	0
			1706	1105	292	300	9		

- Molecule 15 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	Ac	225	Total	C	N	O	S	0	0
			1751	1116	315	313	7		

- Molecule 16 is a protein called Ribosomal protein eS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Ad	262	Total	C	N	O	S	0	0
			2076	1324	386	358	8		

- Molecule 17 is a protein called Ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Ae	191	Total	C	N	O	S	0	0
			1509	943	286	273	7		

- Molecule 18 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Af	237	Total	C	N	O	S	0	0
			1923	1200	387	329	7		

- Molecule 19 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Ag	190	Total	C	N	O	S	0	0
			1529	975	281	272	1		

- Molecule 20 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	Ah	206	Total	C	N	O	S	0	0
			1686	1058	332	291	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Ah	47	ARG	GLY	conflict	UNP G1TJW1

- Molecule 21 is a protein called Ribosomal protein S9 (Predicted).

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Ai	185	Total	C	N	O	S	0	0
			1525	969	306	248	2		

- Molecule 22 is a protein called Ribosomal protein eS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Aj	96	Total	C	N	O	S	0	0
			810	530	143	131	6		

- Molecule 23 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Ak	154	Total	C	N	O	S	0	0
			1262	804	236	216	6		

- Molecule 24 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Al	124	Total	C	N	O	S	0	0
			958	600	170	179	9		

- Molecule 25 is a protein called uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	Am	150	1208	773	229	205	1	0	0

- Molecule 26 is a protein called 40S ribosomal protein uS11.

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

- Molecule 27 is a protein called 40S ribosomal protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	Ao	133	1091	694	205	185	7	0	0

- Molecule 28 is a protein called Ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	Ap	141	1124	715	212	194	3	0	0

- Molecule 29 is a protein called 40S ribosomal protein eS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	Aq	134	1080	678	201	197	4	0	0

- Molecule 30 is a protein called 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	Ar	145	1200	753	242	204	1	0	0

- Molecule 31 is a protein called Ribosomal protein eS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	As	143	1113	698	214	198	3	0	0

- Molecule 32 is a protein called 40S ribosomal protein uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	At	104	821	514	155	148	4	0	0

- Molecule 33 is a protein called Ribosomal protein eS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	Au	83	640	394	117	124	5	0	0

- Molecule 34 is a protein called Ribosomal protein S15a.

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

- Molecule 35 is a protein called 40S ribosomal protein S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	Aw	141	1099	693	219	184	3	0	0

- Molecule 36 is a protein called 40S ribosomal protein S24.

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

- Molecule 37 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	Ay	85	683	439	128	115	1	0	0

- Molecule 38 is a protein called 60s ribosomal protein l41.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
38	Az	25	239	145	64	27	3	0	0

- Molecule 39 is a RNA chain called 28S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
39	B5	3764	80772	36003	14762	26243	3764	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B5	3550	UY1	U	conflict	GB GBCN01009604.1

- Molecule 40 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
40	B7	119	2538	1131	451	837	119	0	0

- Molecule 41 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
41	B8	156	3319	1481	585	1097	156	0	0

- Molecule 42 is a protein called Ribosomal protein uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	BA	253	1940	1214	396	324	6	0	0

- Molecule 43 is a protein called Ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	BB	398	3206	2042	605	546	13	0	0

- Molecule 44 is a protein called 60S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
44	BC	362	2886	1814	577	481	14	0	0

- Molecule 45 is a protein called Ribosomal\_L18\_c domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
45	BD	294	2398	1516	439	429	14	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BD	2	AAC	GLY	conflict	UNP G1SYJ6

- Molecule 46 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
46	BE	243	1960	1258	378	321	3	0	0

- Molecule 47 is a protein called Ribosomal Protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
47	BF	226	1886	1211	362	304	9	0	0

- Molecule 48 is a protein called Ribosomal protein eL8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
48	BG	233	1877	1197	361	315	4	0	0

- Molecule 49 is a protein called 60S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
49	BH	190	1516	954	284	272	6	0	0

- Molecule 50 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
50	BI	213	1717	1086	332	285	14	0	0

- Molecule 51 is a protein called Ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	BJ	170	Total	C	N	O	S	0	0
			1362	861	254	241	6		

- Molecule 52 is a protein called Replicase polyprotein 1ab.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	BK	36	Total	C	N	O	S	0	0
			273	169	46	52	6		

- Molecule 53 is a protein called Ribosomal protein eL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	BL	210	Total	C	N	O	S	0	0
			1702	1065	354	279	4		

- Molecule 54 is a protein called Ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	BM	138	Total	C	N	O	S	0	0
			1137	727	221	182	7		

- Molecule 55 is a protein called Ribosomal protein L15.

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

- Molecule 56 is a protein called Ribosomal protein L13a.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	BO	199	Total	C	N	O	S	0	0
			1630	1051	319	255	5		

- Molecule 57 is a protein called uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	BP	159	Total	C	N	O	S	0	0
			1289	809	249	222	9		

- Molecule 58 is a protein called Ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	BQ	187	Total	C	N	O	S	0	0
			1515	946	315	250	4		

- Molecule 59 is a protein called 60S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	BR	180	Total	C	N	O	S	0	0
			1508	933	328	238	9		

- Molecule 60 is a protein called Ribosomal protein L18a.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	BS	176	Total	C	N	O	S	0	0
			1457	924	288	234	11		

- Molecule 61 is a protein called eL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	BT	159	Total	C	N	O	S	0	0
			1298	823	252	217	6		

- Molecule 62 is a protein called Ribosomal protein eL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	BU	99	Total	C	N	O	S	0	0
			806	516	141	147	2		

- Molecule 63 is a protein called Ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	BV	139	Total	C	N	O	S	0	0
			1034	648	199	182	5		

- Molecule 64 is a protein called eL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	BW	121	Total	C	N	O	S	0	0
			991	619	202	166	4		

- Molecule 65 is a protein called uL23.



Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
65	BX	118	967	618	181	167	1	0	0

- Molecule 66 is a protein called Ribosomal protein L26.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
66	BY	134	1115	700	226	186	3	0	0

- Molecule 67 is a protein called 60S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
67	BZ	135	1107	714	208	182	3	0	0

- Molecule 68 is a protein called 60S ribosomal protein L27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
68	Ba	147	1163	734	239	186	4	0	0

- Molecule 69 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
69	Bb	108	881	548	196	134	3	0	0

- Molecule 70 is a protein called eL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
70	Bc	108	836	530	148	151	7	0	0

- Molecule 71 is a protein called eL31.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
71	Bd	107	888	560	171	155	2	0	0

- Molecule 72 is a protein called eL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
72	Be	130	1070	676	221	168	5	0	0

- Molecule 73 is a protein called eL33.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
73	Bf	110	884	560	175	144	5	0	0

- Molecule 74 is a protein called 60S ribosomal protein L34.

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

- Molecule 75 is a protein called uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
75	Bh	122	1013	640	204	168	1	0	0

- Molecule 76 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
76	Bi	102	830	520	176	129	5	0	0

- Molecule 77 is a protein called Ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
77	Bj	86	705	434	155	111	5	0	0

- Molecule 78 is a protein called eL38.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Bk	24	LYS	ASN	conflict	UNP G1U001

- Molecule 79 is a protein called eL39.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
79	Bl	50	447	286	96	64	1	0	0

- Molecule 80 is a protein called 60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
80	Bm	52	432	269	90	67	6	0	0

- Molecule 81 is a protein called eL42.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
81	Bo	105	863	543	175	139	6	0	0

- Molecule 82 is a protein called eL43.

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

- Molecule 83 is a protein called Ribosomal protein eL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
83	Br	126	1014	629	209	170	6	0	0

- Molecule 84 is a protein called 60S acidic ribosomal protein P0.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
84	Bs	196	1507	959	263	276	9	0	0

- Molecule 85 is a protein called Ribosomal protein L12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
85	Bt	156	1178	733	221	220	4	0	0

- Molecule 86 is a protein called Ribosomal protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
86	Bv	212	1707	1092	308	299	8	0	0

- Molecule 87 is a protein called Eukaryotic peptide chain release factor subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
87	By	416	3280	2087	559	623	11	0	0

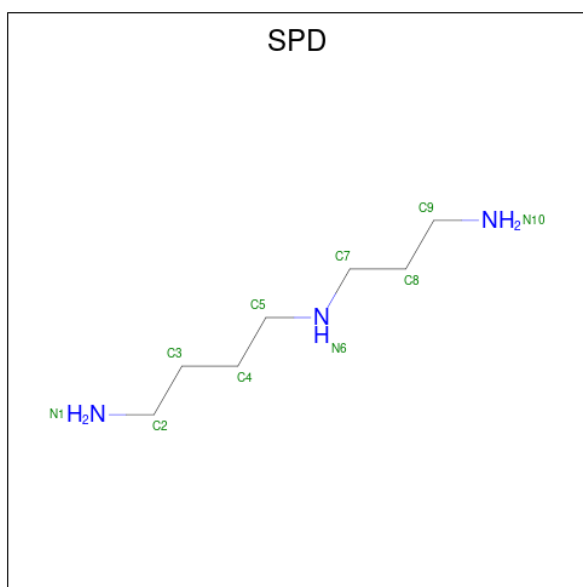
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
By	183	ALA	GLY	engineered mutation	UNP P62497
By	184	ALA	GLY	engineered mutation	UNP P62497

- Molecule 88 is a protein called ATP binding cassette subfamily E member 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
88	Bz	595	4668	2982	801	854	31	0	0

- Molecule 89 is SPERMIDINE (three-letter code: SPD) (formula: C<sub>7</sub>H<sub>19</sub>N<sub>3</sub>).



Mol	Chain	Residues	Atoms			AltConf
89	A2	1	Total	C	N	0
			10	7	3	

- Molecule 90 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
90	A2	102	Total	Mg	0
			102	102	
90	AH	1	Total	Mg	0
			1	1	
90	AT	2	Total	Mg	0
			2	2	
90	B5	235	Total	Mg	0
			235	235	
90	B7	4	Total	Mg	0
			4	4	
90	B8	6	Total	Mg	0
			6	6	
90	BI	1	Total	Mg	0
			1	1	
90	BP	1	Total	Mg	0
			1	1	
90	BR	1	Total	Mg	0
			1	1	
90	BV	1	Total	Mg	0
			1	1	
90	Ba	1	Total	Mg	0
			1	1	

- Molecule 91 is UNKNOWN ATOM OR ION (three-letter code: UNX) (formula: X).

Mol	Chain	Residues	Atoms		AltConf
91	A2	76	Total 76	X 76	0
91	AT	4	Total 4	X 4	0
91	Ab	1	Total 1	X 1	0
91	Ak	1	Total 1	X 1	0
91	Ar	1	Total 1	X 1	0
91	B5	244	Total 244	X 244	0
91	B7	10	Total 10	X 10	0
91	B8	16	Total 16	X 16	0
91	BA	2	Total 2	X 2	0
91	BB	3	Total 3	X 3	0
91	BC	1	Total 1	X 1	0
91	BH	1	Total 1	X 1	0
91	BI	1	Total 1	X 1	0
91	BL	1	Total 1	X 1	0
91	BN	2	Total 2	X 2	0
91	BP	1	Total 1	X 1	0
91	BQ	2	Total 2	X 2	0
91	BT	1	Total 1	X 1	0
91	Bb	1	Total 1	X 1	0
91	Be	2	Total 2	X 2	0
91	Bf	1	Total 1	X 1	0

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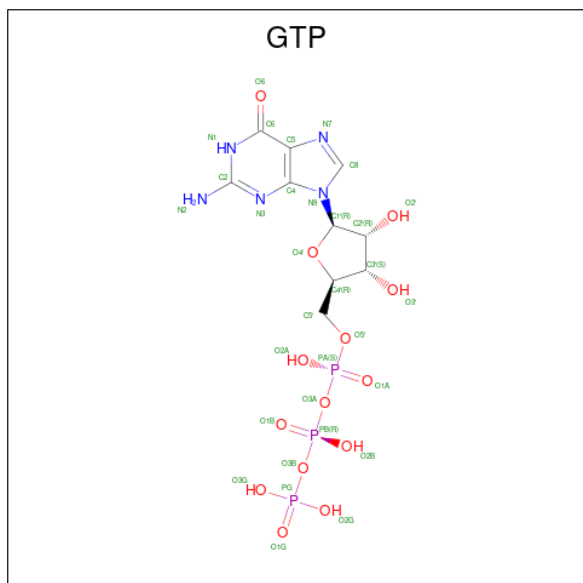
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Mol	Chain	Residues	Atoms	AltConf
91	Bg	1	Total X 1 1	0
91	Bo	1	Total X 1 1	0

- Molecule 92 is ZINC ION (three-letter code: ZN) (formula: Zn).

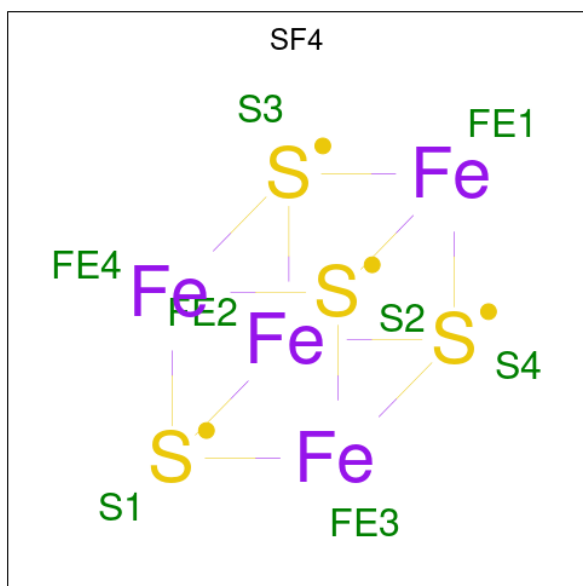
Mol	Chain	Residues	Atoms	AltConf
92	AC	1	Total Zn 1 1	0
92	AE	1	Total Zn 1 1	0
92	AG	1	Total Zn 1 1	0
92	Bg	1	Total Zn 1 1	0
92	Bj	1	Total Zn 1 1	0
92	Bm	1	Total Zn 1 1	0
92	Bo	1	Total Zn 1 1	0
92	Bp	1	Total Zn 1 1	0

- Molecule 93 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>14</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
93	B7	1	32	10	5	14	3	0

- Molecule 94 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
94	Bz	1	8	4	4	0
94	Bz	1	8	4	4	0

- Molecule 95 is water.

Mol	Chain	Residues	Atoms		AltConf
			Total	O	
95	A2	473	473	473	0
95	AH	10	10	10	0
95	AT	12	12	12	0
95	Aa	2	2	2	0
95	Ab	1	1	1	0
95	Ad	1	1	1	0
95	Af	2	2	2	0

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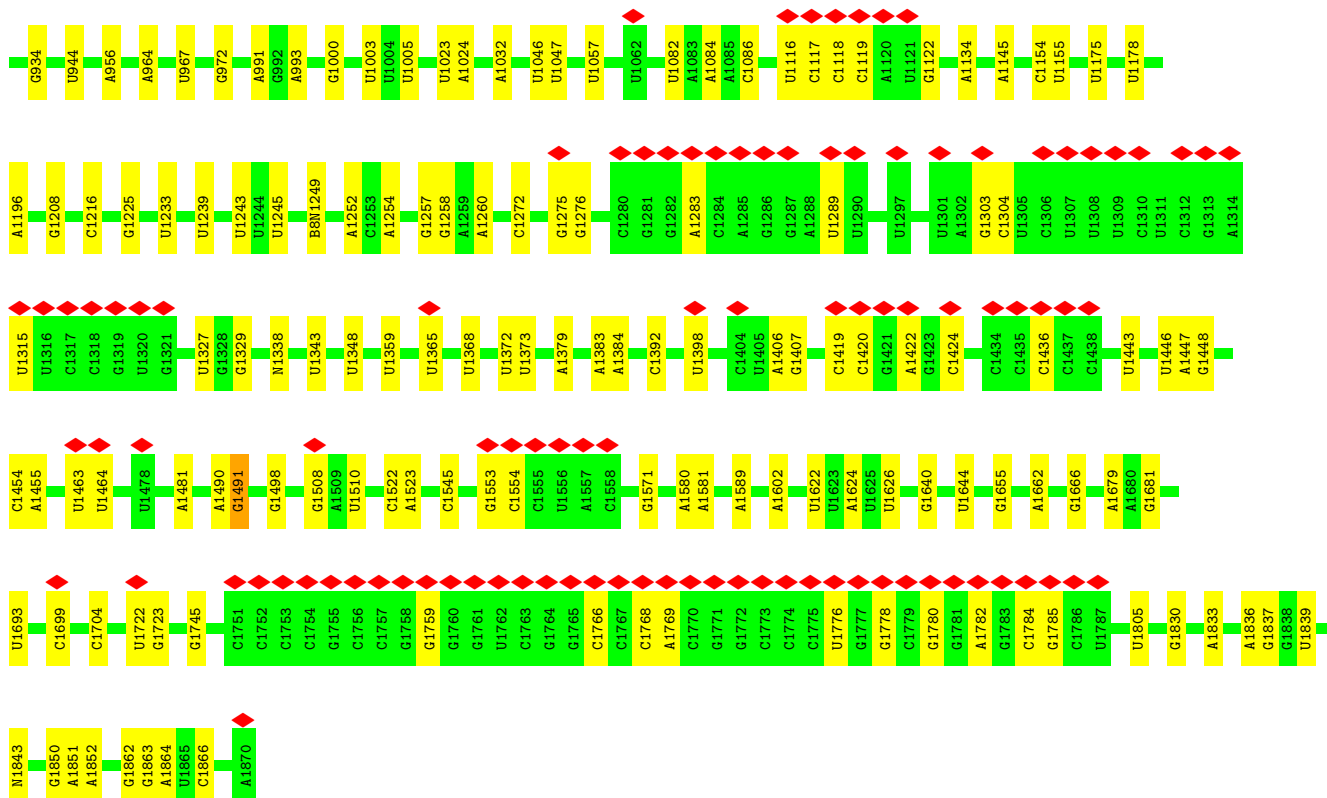
Mol	Chain	Residues	Atoms		AltConf
95	Ak	1	Total 1	O 1	0
95	Am	1	Total 1	O 1	0
95	An	2	Total 2	O 2	0
95	Ap	4	Total 4	O 4	0
95	Ar	1	Total 1	O 1	0
95	As	4	Total 4	O 4	0
95	Aw	4	Total 4	O 4	0
95	B5	1117	Total 1117	O 1117	0
95	B7	17	Total 17	O 17	0
95	B8	31	Total 31	O 31	0
95	BA	5	Total 5	O 5	0
95	BB	7	Total 7	O 7	0
95	BC	3	Total 3	O 3	0
95	BD	1	Total 1	O 1	0
95	BF	1	Total 1	O 1	0
95	BH	1	Total 1	O 1	0
95	BI	1	Total 1	O 1	0
95	BL	1	Total 1	O 1	0
95	BN	2	Total 2	O 2	0
95	BO	3	Total 3	O 3	0
95	BP	3	Total 3	O 3	0

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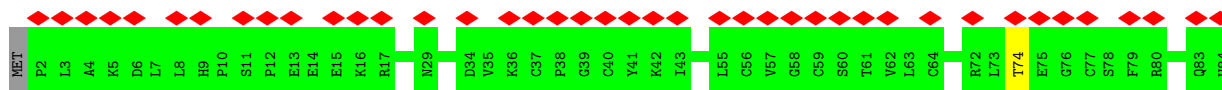
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Mol	Chain	Residues	Atoms		AltConf
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95	BV	4	Total 4	O 4	0
95	BX	1	Total 1	O 1	0
95	BY	1	Total 1	O 1	0
95	Ba	7	Total 7	O 7	0
95	Bb	1	Total 1	O 1	0
95	Bd	1	Total 1	O 1	0
95	Be	4	Total 4	O 4	0
95	Bf	1	Total 1	O 1	0
95	By	1	Total 1	O 1	0

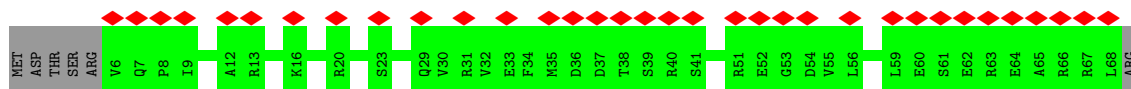
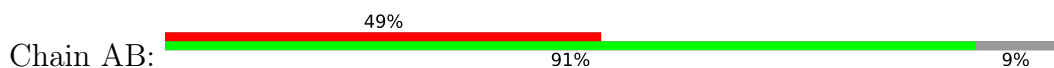




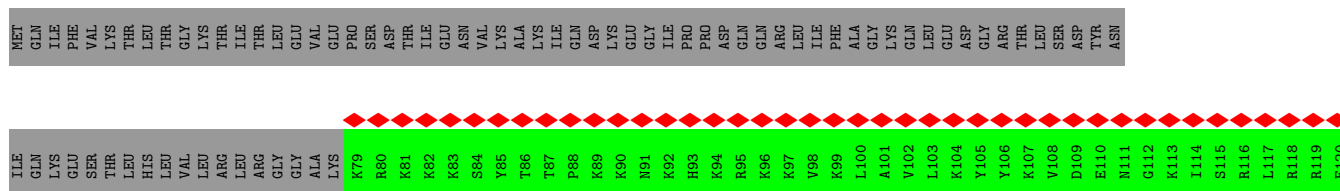
• Molecule 2: 40S ribosomal protein S27

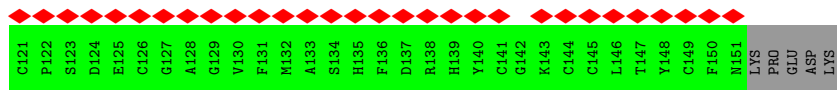


• Molecule 3: Ribosomal protein S28

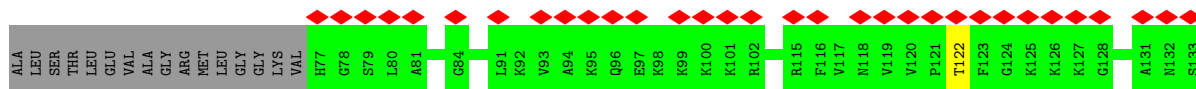
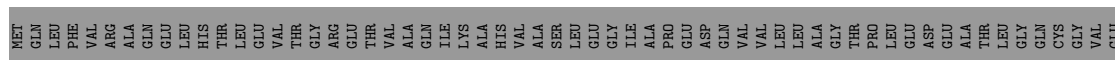
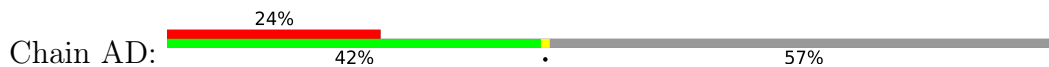


• Molecule 4: Ribosomal protein S27a

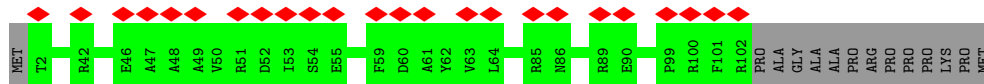
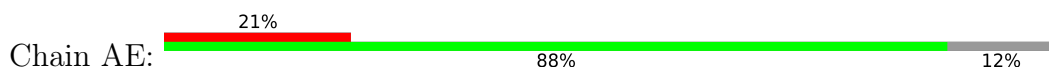




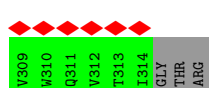
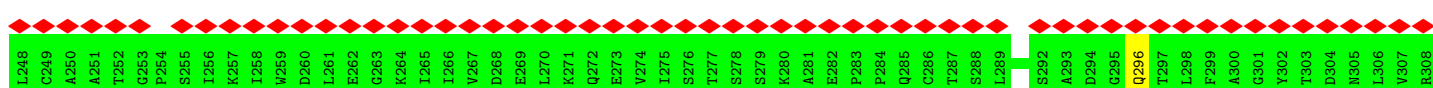
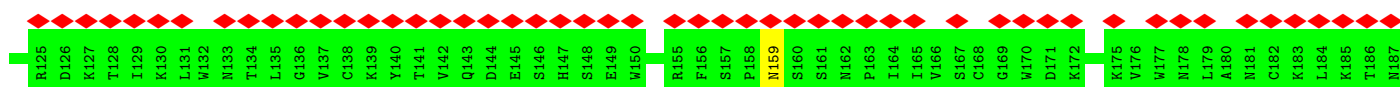
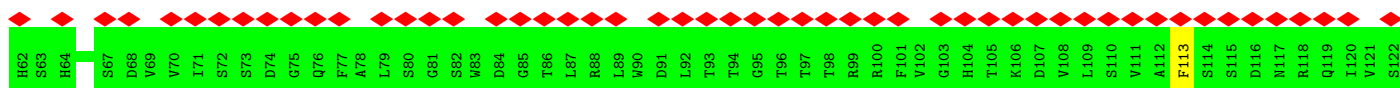
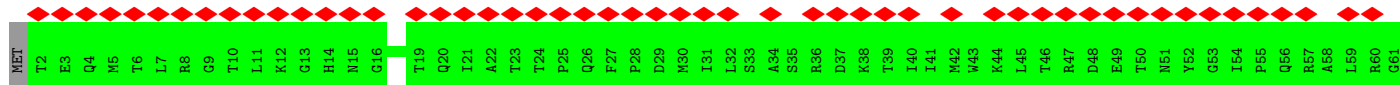
• Molecule 5: 40S ribosomal protein S30



• Molecule 6: Ribosomal protein eS26



• Molecule 7: RACK1



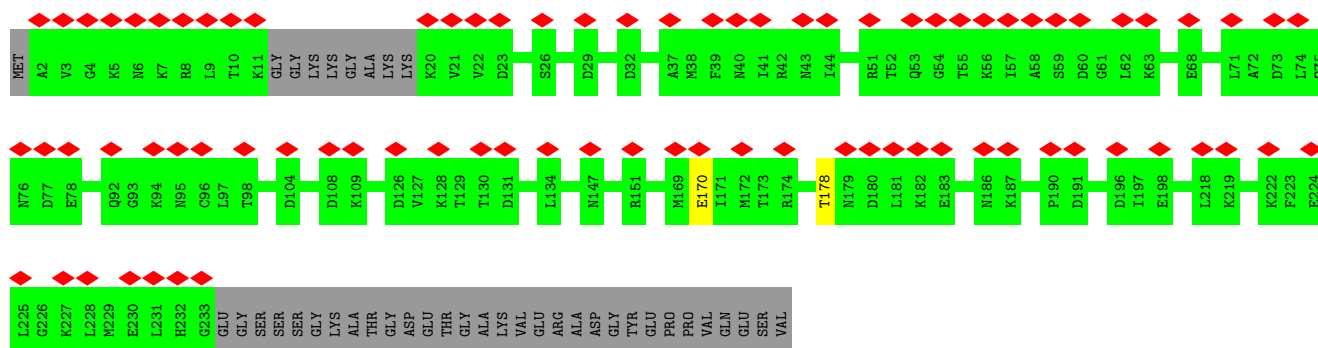
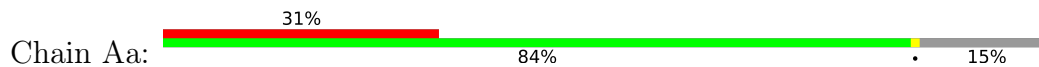
• Molecule 8: uS14



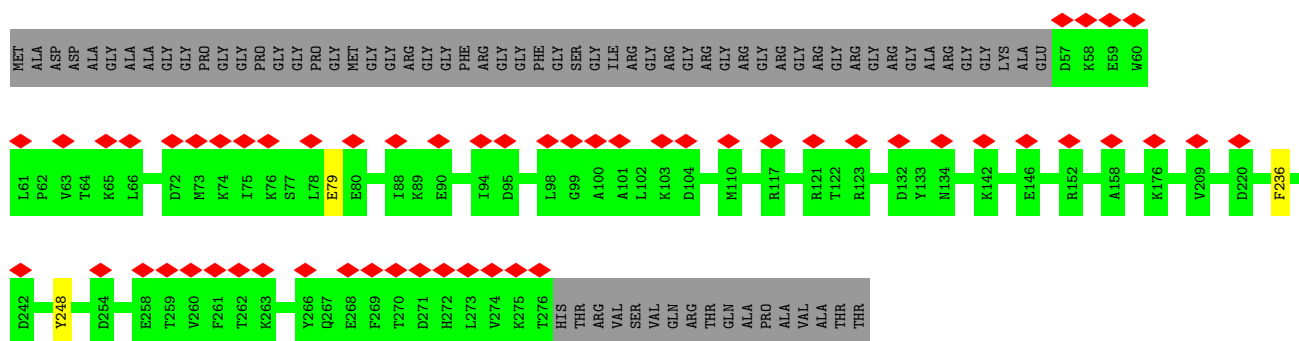
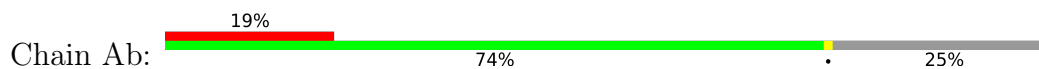


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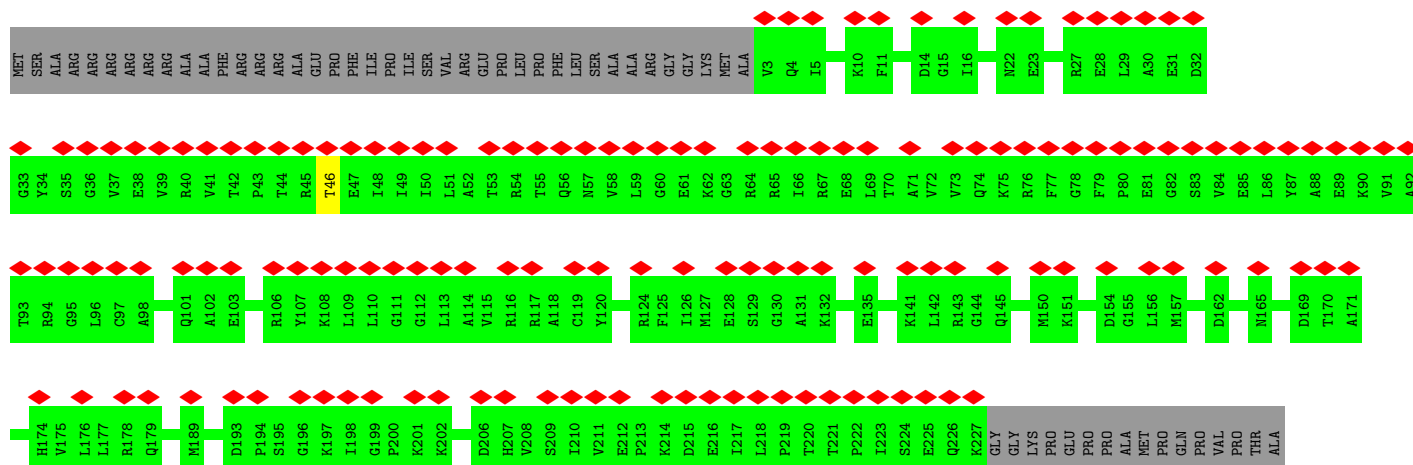
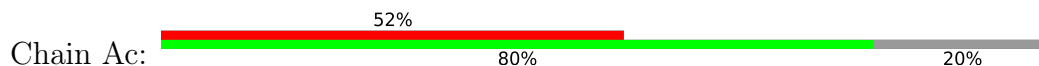
● Molecule 13: 40S ribosomal protein S3a



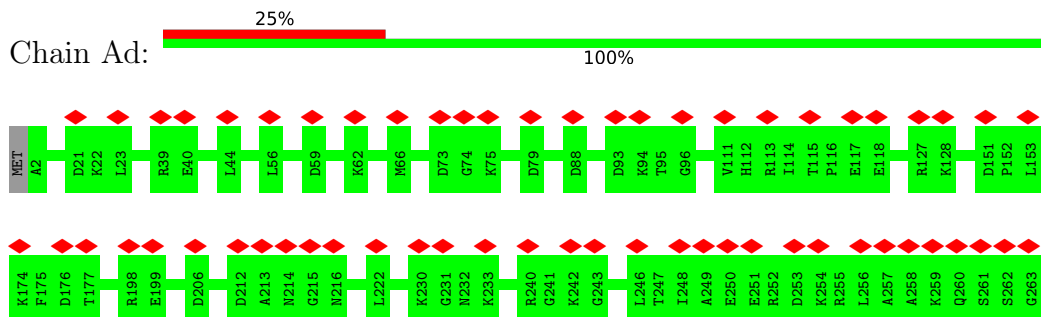
● Molecule 14: Ribosomal protein uS5



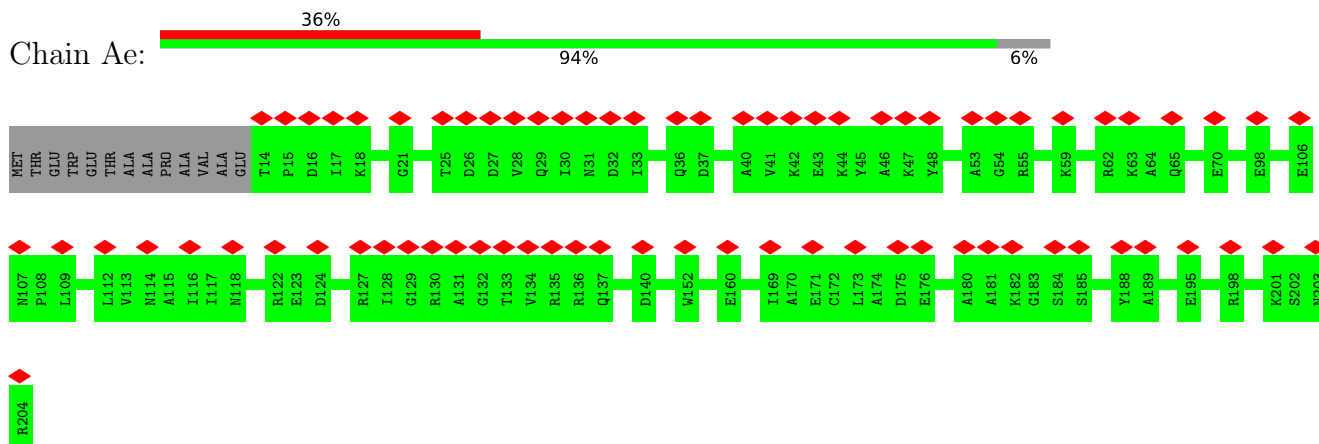
● Molecule 15: 40S ribosomal protein S3



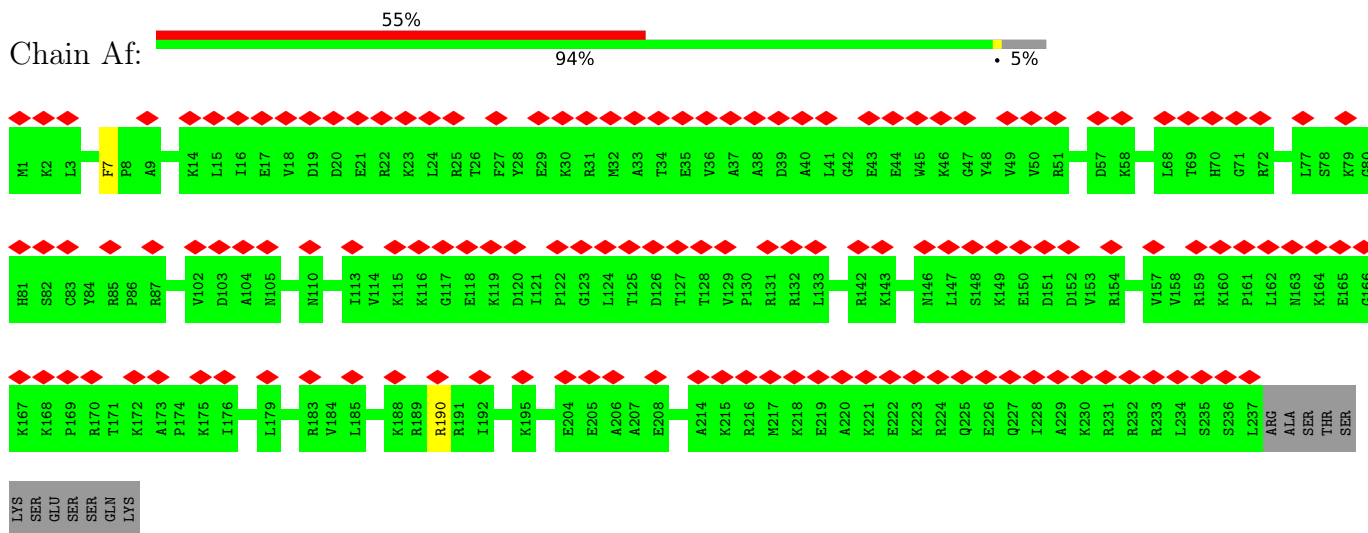
• Molecule 16: Ribosomal protein eS4



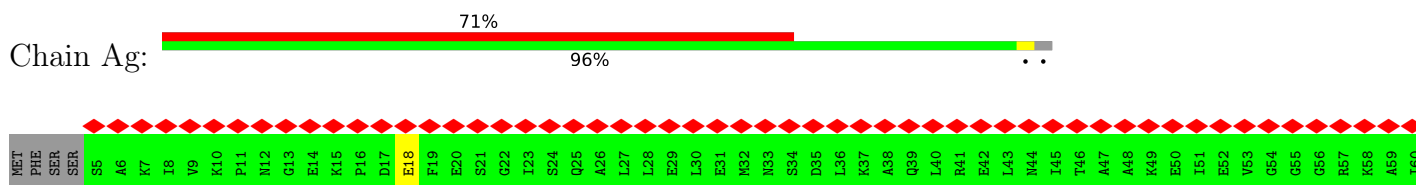
• Molecule 17: Ribosomal protein S5



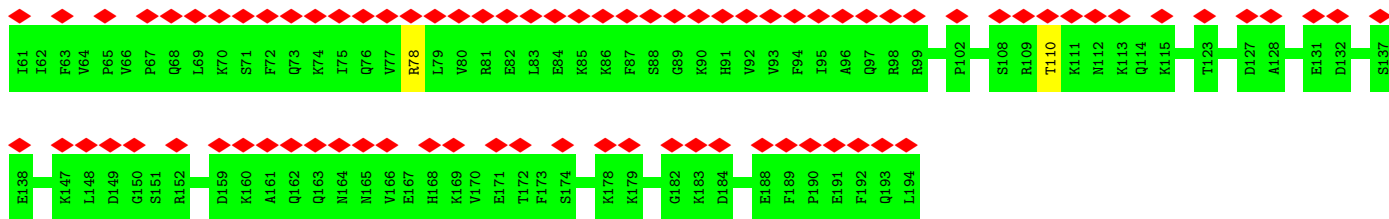
• Molecule 18: 40S ribosomal protein S6



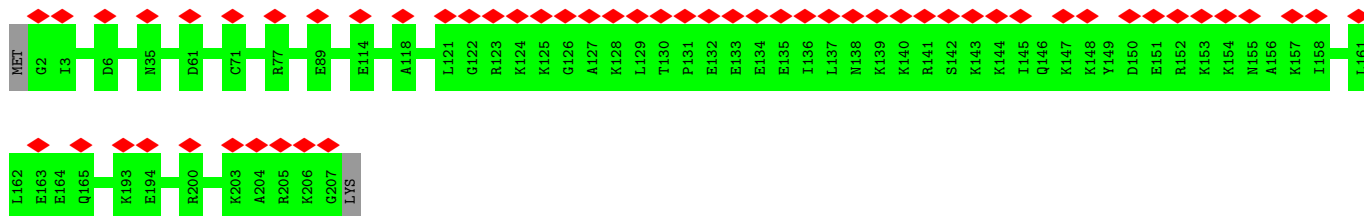
• Molecule 19: 40S ribosomal protein S7



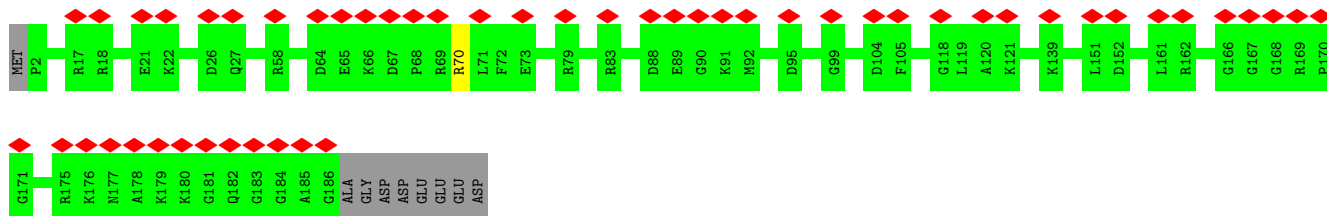




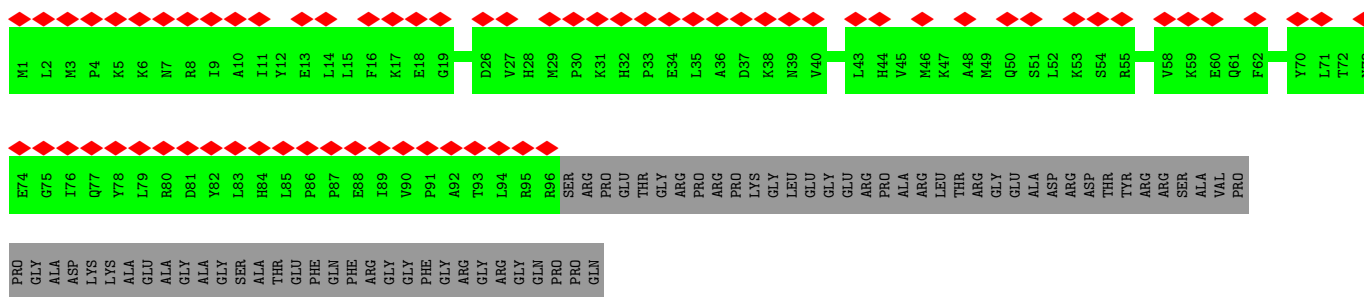
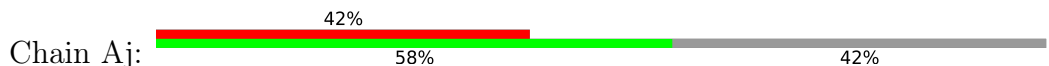
• Molecule 20: 40S ribosomal protein S8



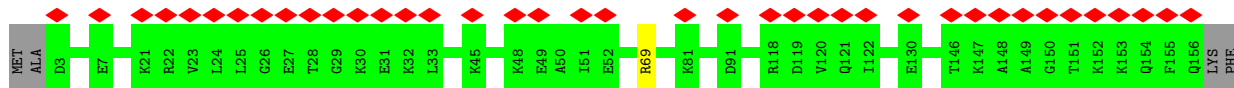
• Molecule 21: Ribosomal protein S9 (Predicted)



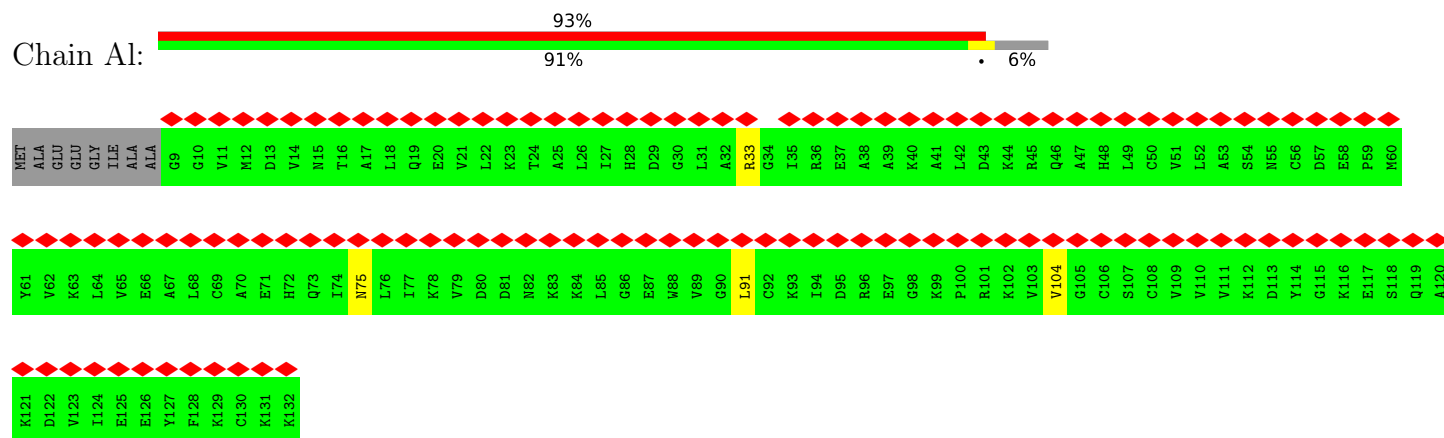
• Molecule 22: Ribosomal protein eS10



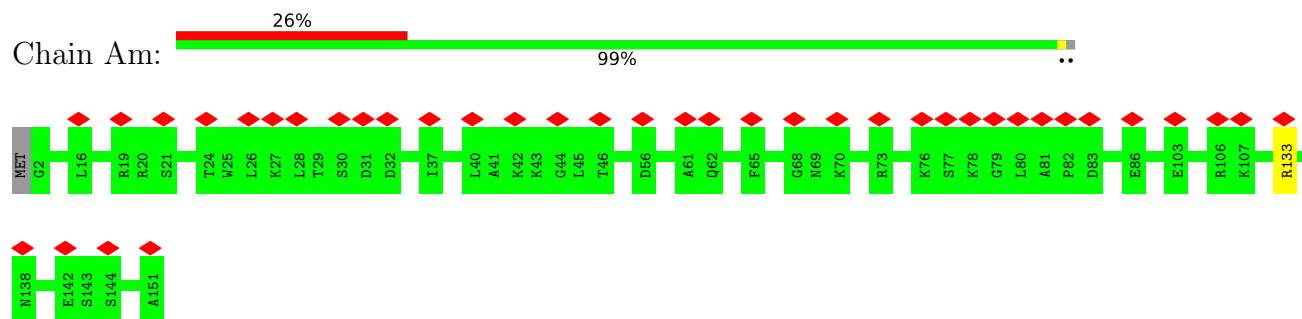
• Molecule 23: 40S ribosomal protein S11



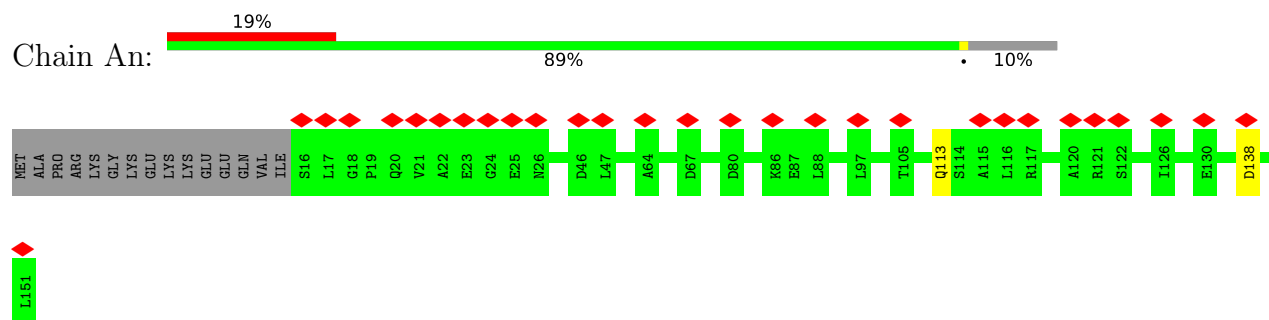
• Molecule 24: 40S ribosomal protein S12



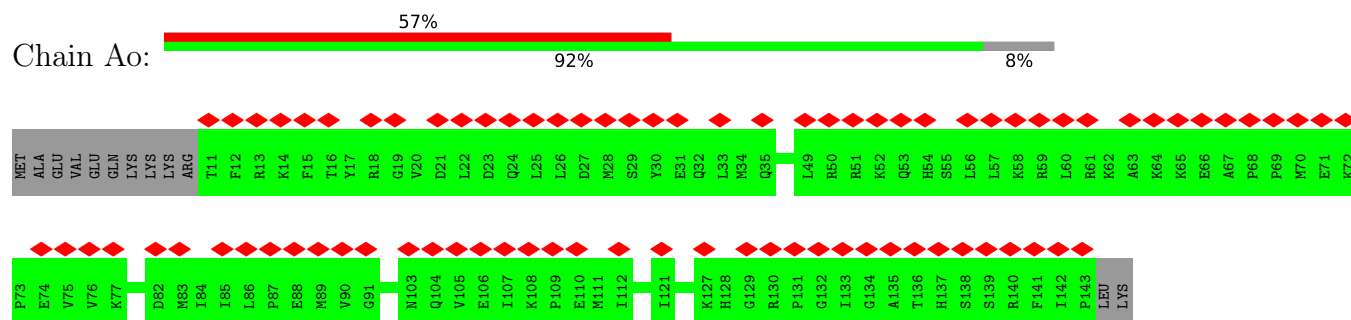
• Molecule 25: uS15



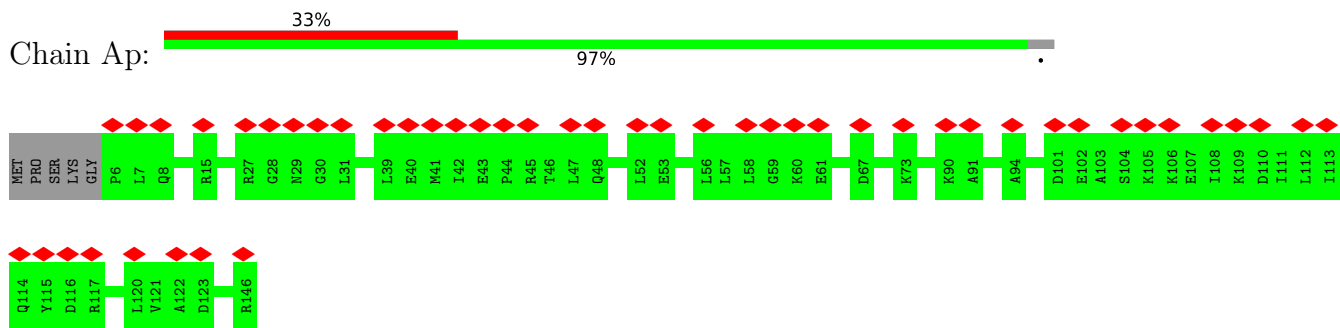
• Molecule 26: 40S ribosomal protein uS11



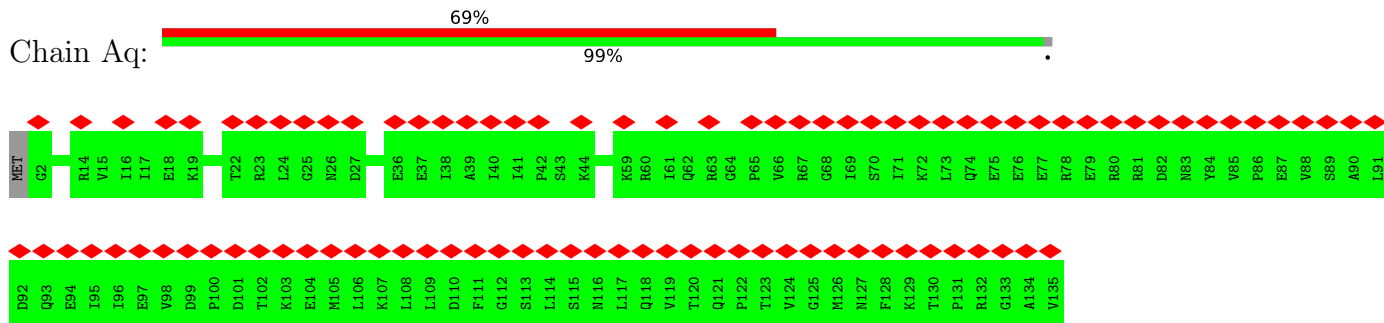
• Molecule 27: 40S ribosomal protein uS19



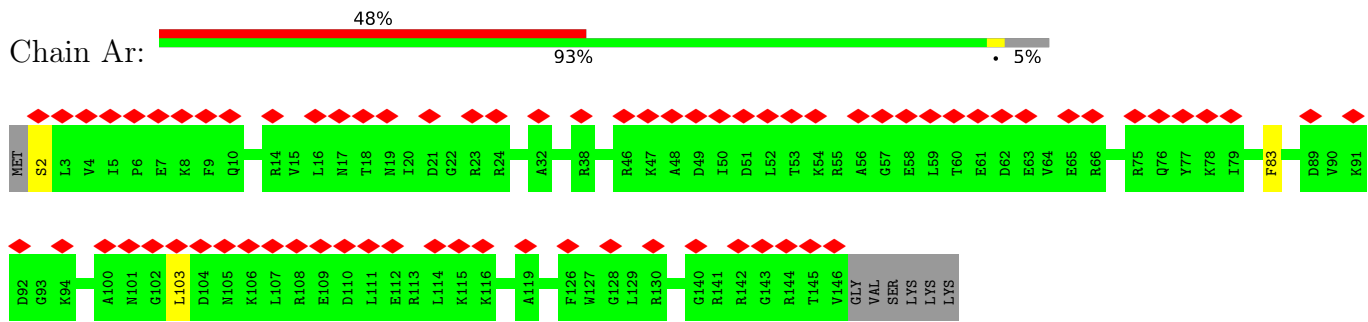
• Molecule 28: Ribosomal protein S16



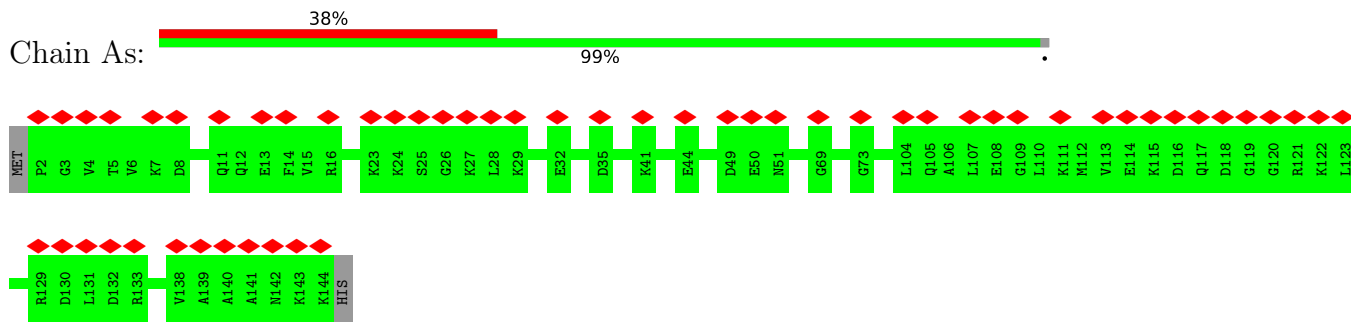
• Molecule 29: 40S ribosomal protein eS17



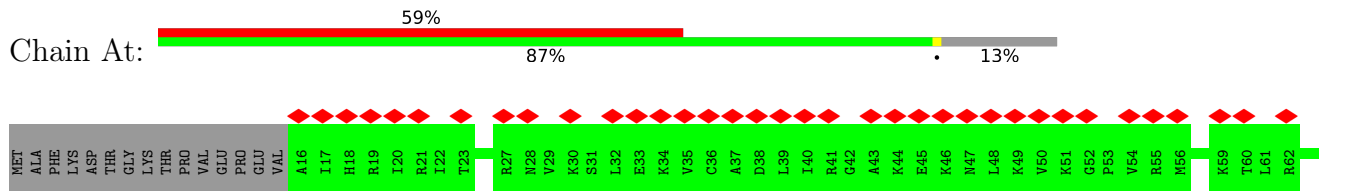
• Molecule 30: 40S ribosomal protein S18

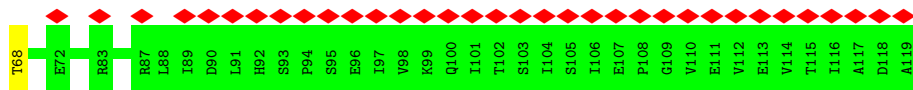


• Molecule 31: Ribosomal protein eS19

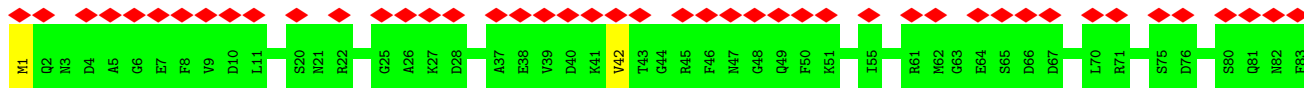


• Molecule 32: 40S ribosomal protein uS10

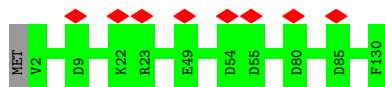




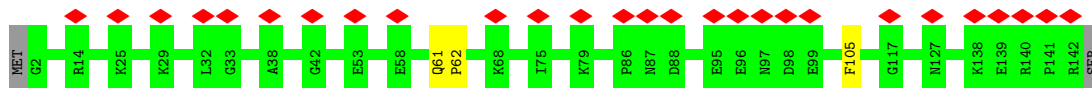
• Molecule 33: Ribosomal protein eS21



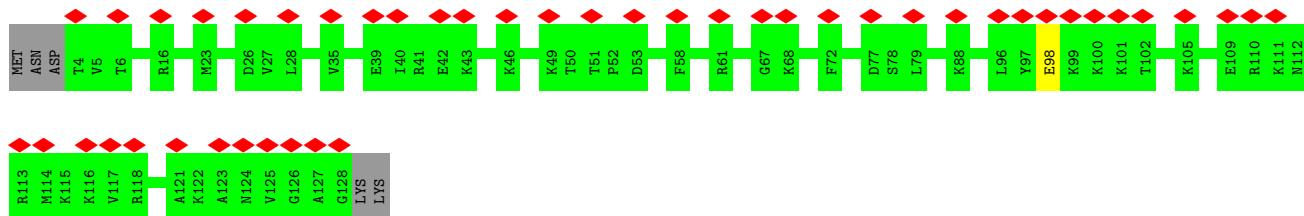
• Molecule 34: Ribosomal protein S15a



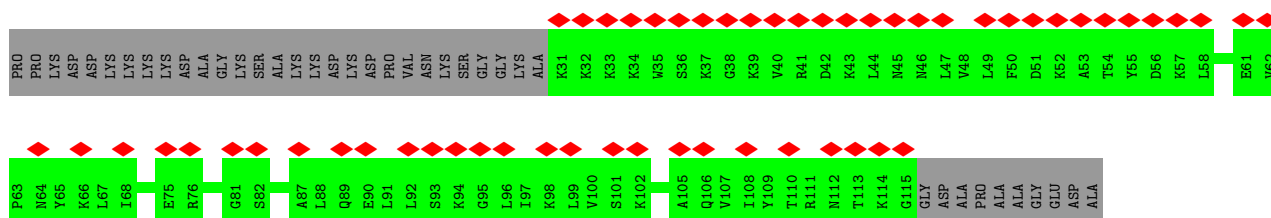
• Molecule 35: 40S ribosomal protein S23



• Molecule 36: 40S ribosomal protein S24



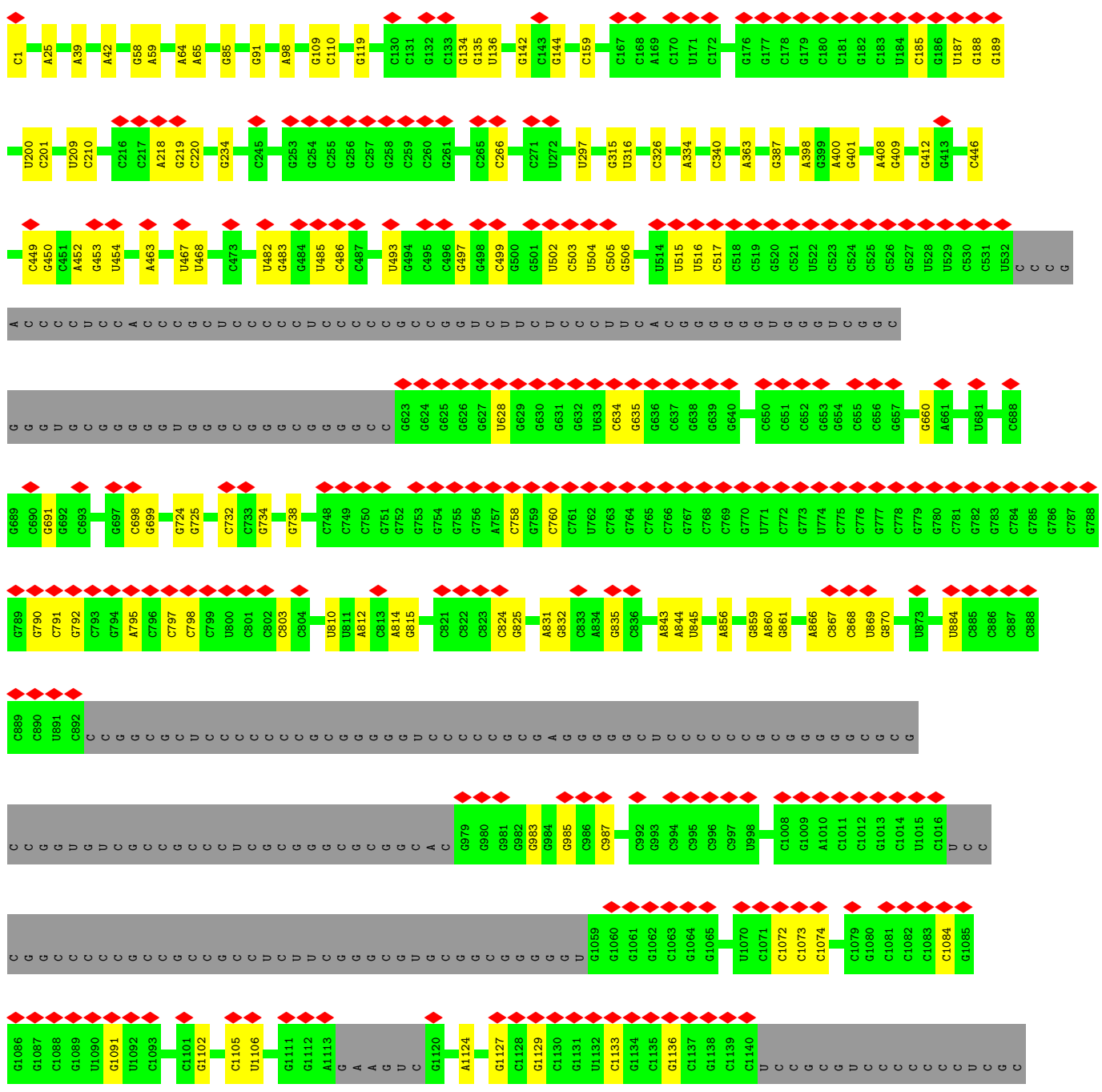
• Molecule 37: 40S ribosomal protein S25



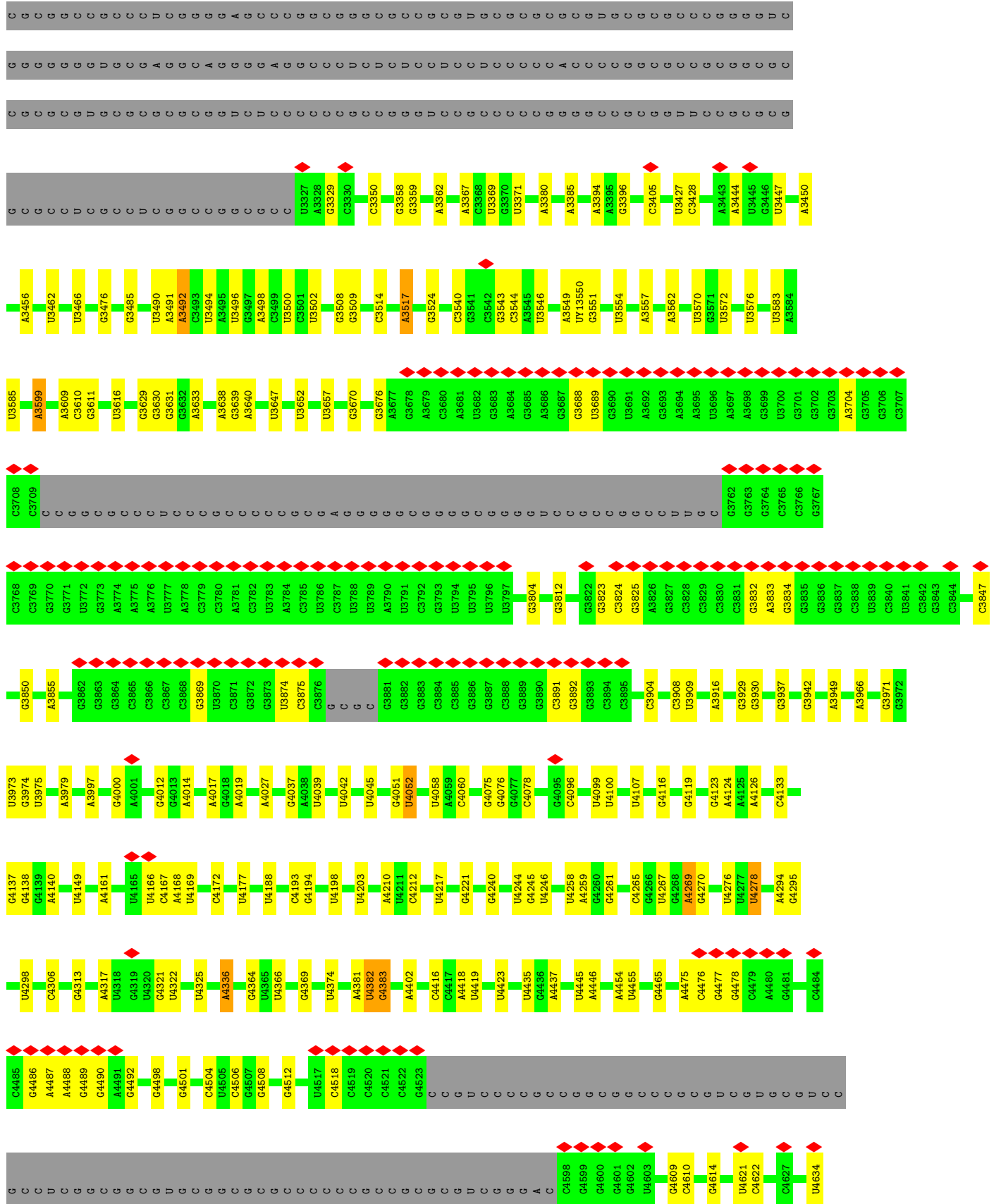
• Molecule 38: 60s ribosomal protein l41

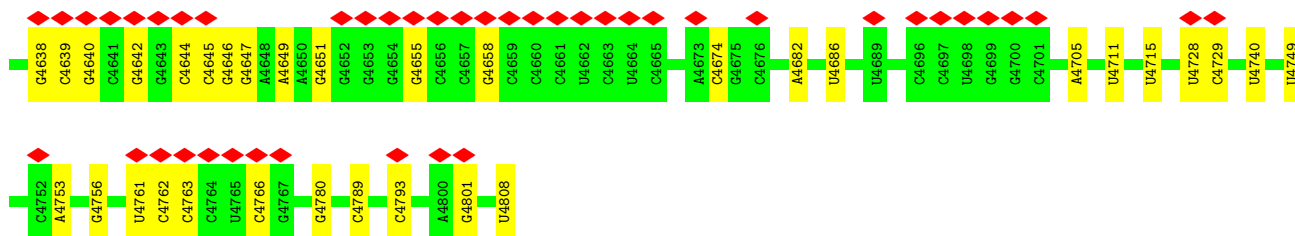


• Molecule 39: 28S rRNA

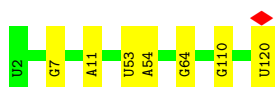




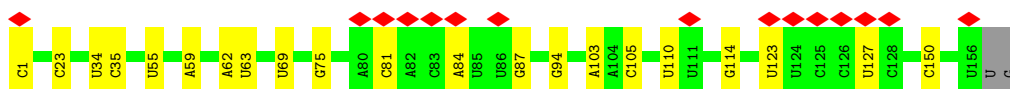
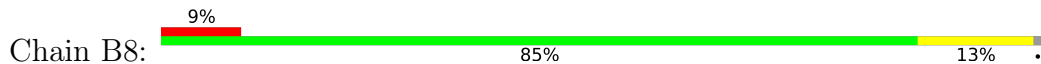




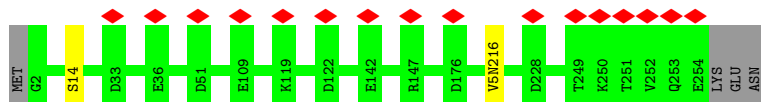
• Molecule 40: 5S rRNA



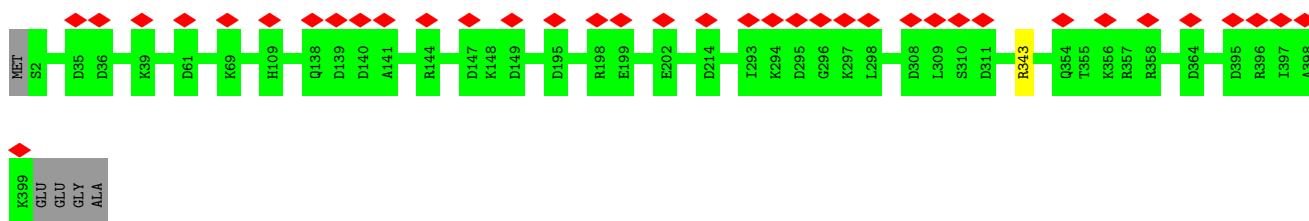
• Molecule 41: 5.8S rRNA



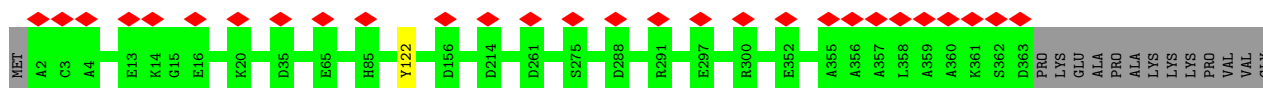
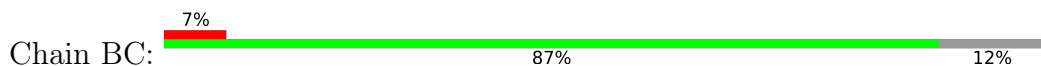
• Molecule 42: Ribosomal protein uL2



• Molecule 43: Ribosomal protein L3



• Molecule 44: 60S ribosomal protein L4

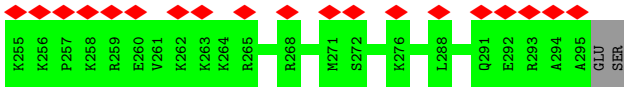
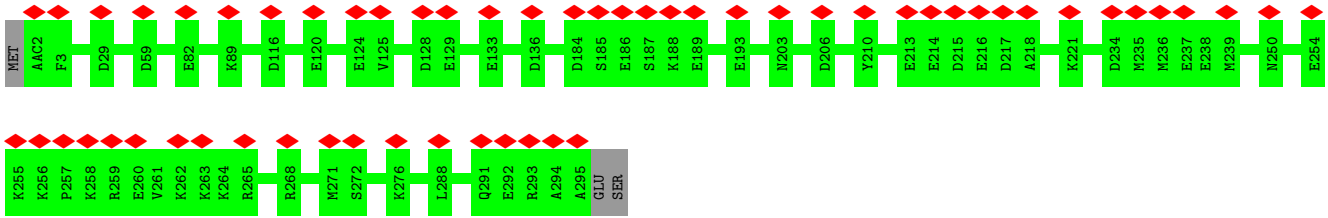




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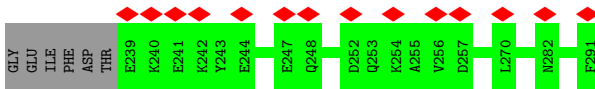
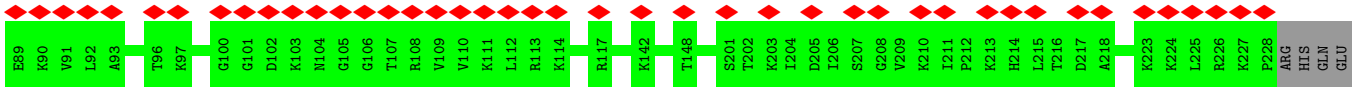
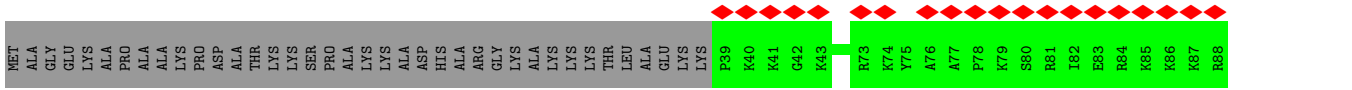
• Molecule 45: Ribosomal\_L18\_c domain-containing protein

Chain BD: 19% 99%



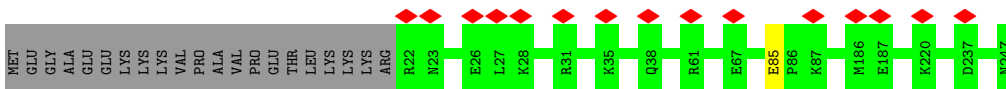
• Molecule 46: 60S ribosomal protein L6

Chain BE: 26% 84% 16%



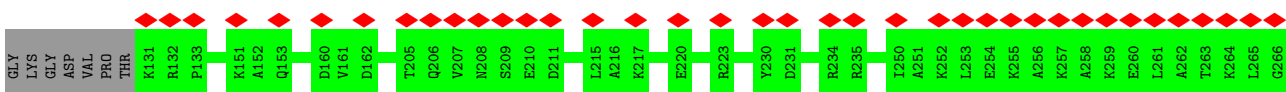
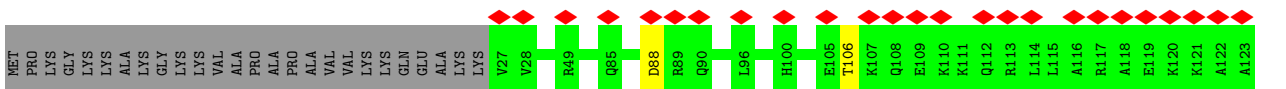
• Molecule 47: Ribosomal Protein uL30

Chain BF: 6% 91% 9%



• Molecule 48: Ribosomal protein eL8

Chain BG: 24% 87% 12%

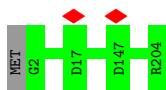


• Molecule 49: 60S ribosomal protein L9

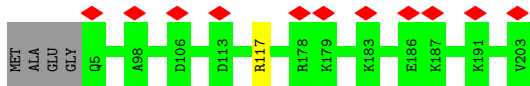
Chain BH: 19% 99%



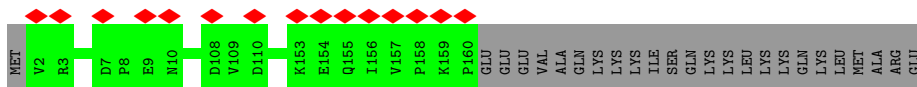
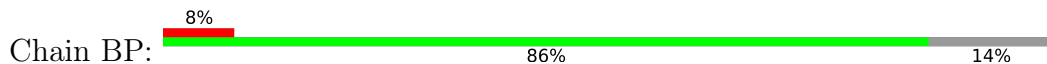




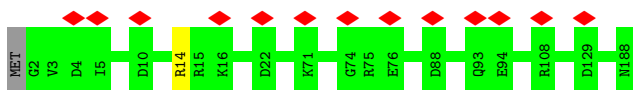
- Molecule 56: Ribosomal protein L13a



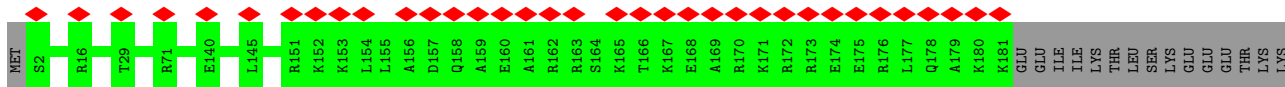
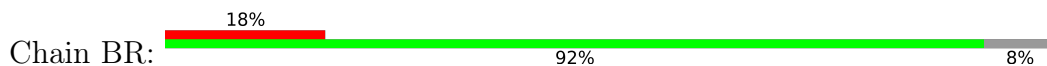
- Molecule 57: uL22



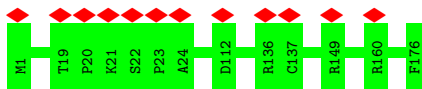
- Molecule 58: Ribosomal protein L18



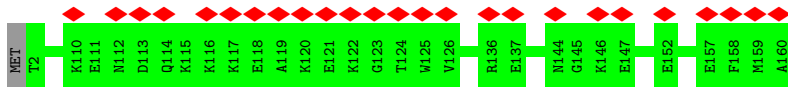
- Molecule 59: 60S ribosomal protein L19



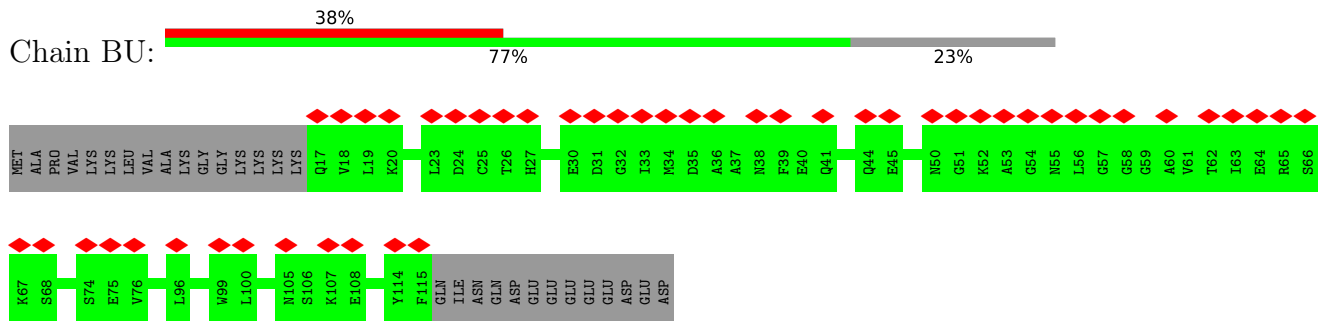
- Molecule 60: Ribosomal protein L18a



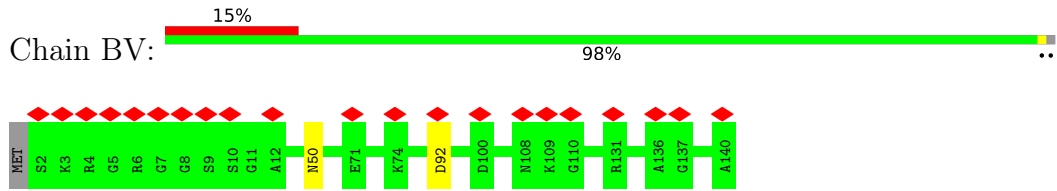
- Molecule 61: eL21



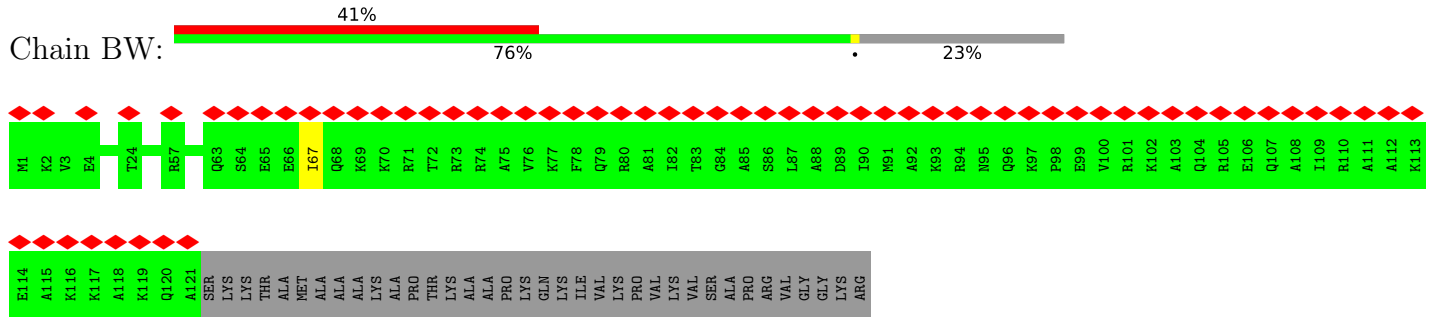
- Molecule 62: Ribosomal protein eL22



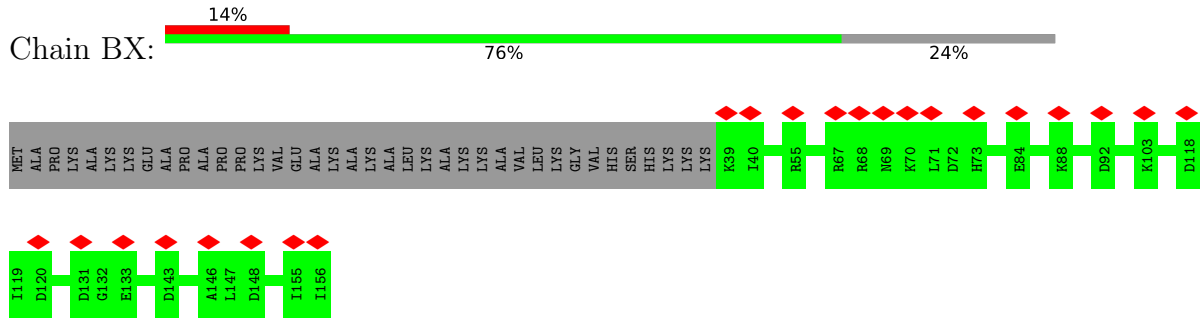
- Molecule 63: Ribosomal protein L23



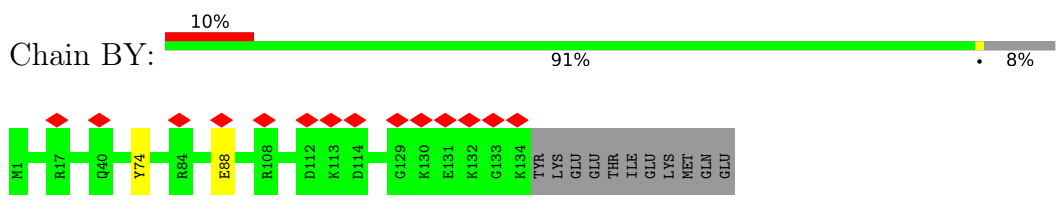
- Molecule 64: eL24



- Molecule 65: uL23



- Molecule 66: Ribosomal protein L26

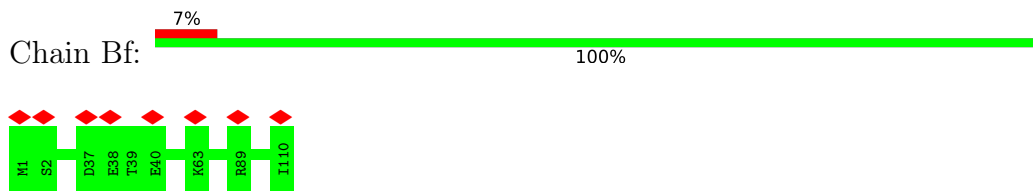


- Molecule 67: 60S ribosomal protein L27

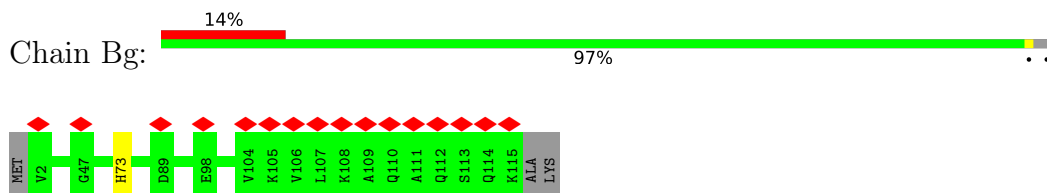




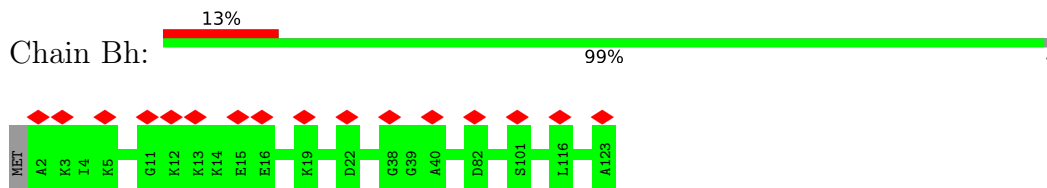
• Molecule 73: eL33



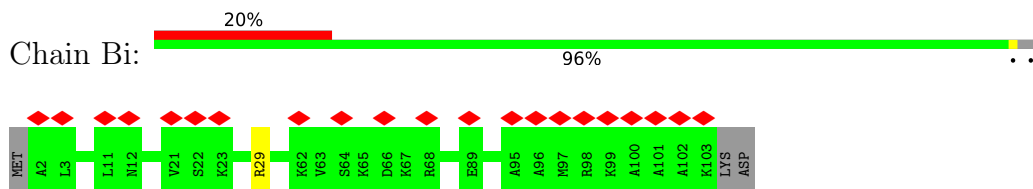
• Molecule 74: 60S ribosomal protein L34



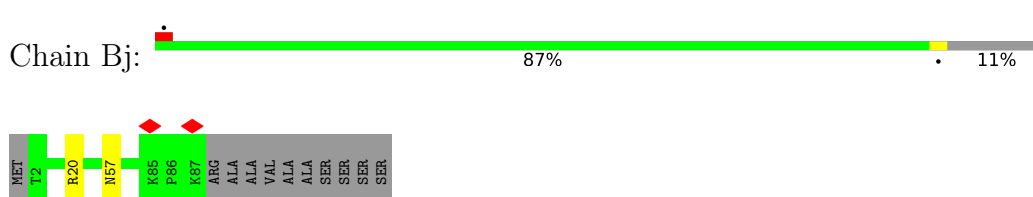
• Molecule 75: uL29



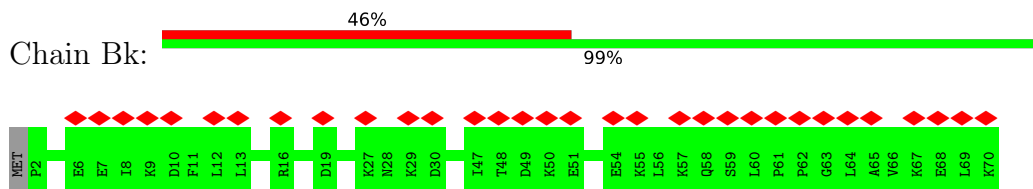
• Molecule 76: 60S ribosomal protein L36



• Molecule 77: Ribosomal protein L37



• Molecule 78: eL38

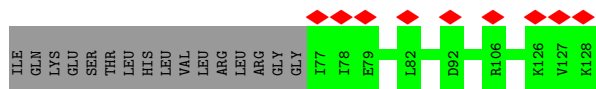
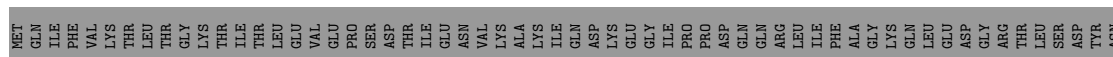
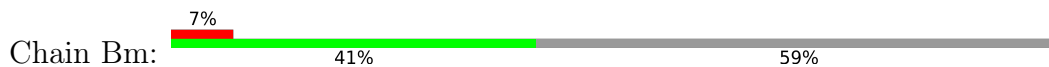


• Molecule 79: eL39

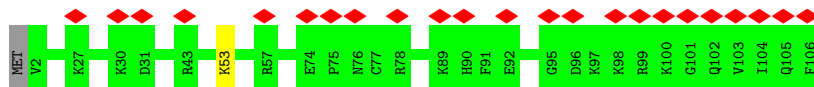




• Molecule 80: 60S ribosomal protein L40



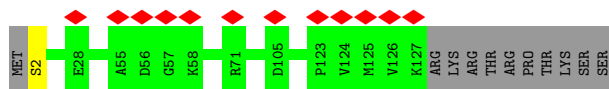
• Molecule 81: eL42



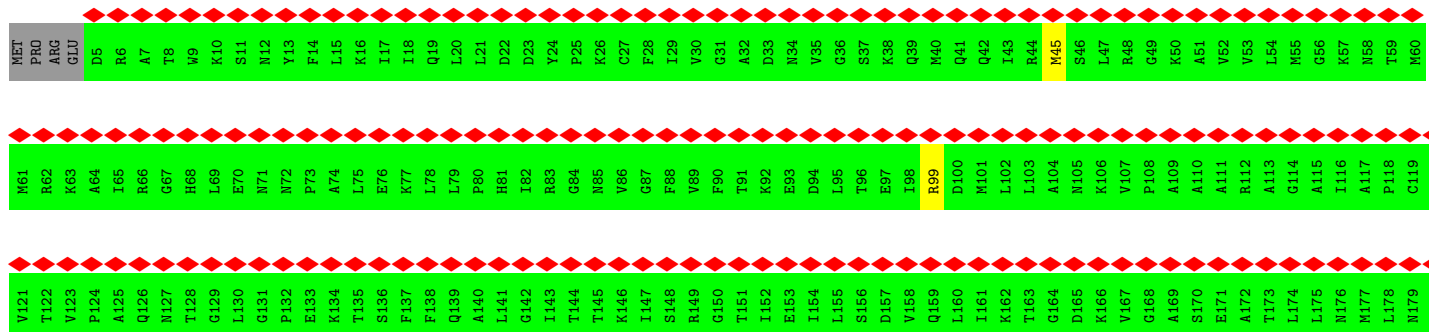
• Molecule 82: eL43



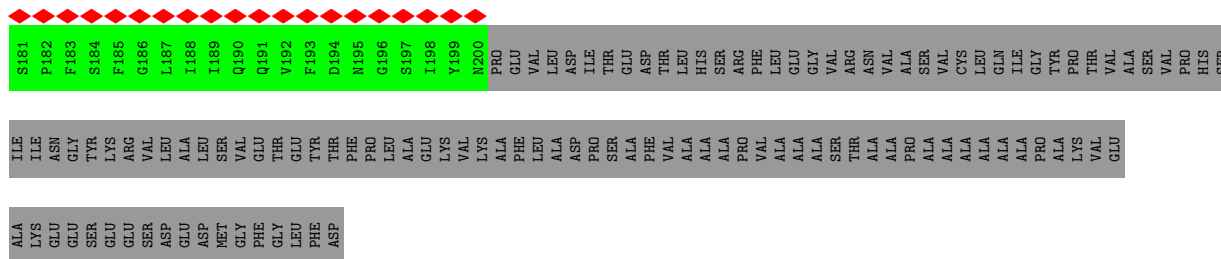
• Molecule 83: Ribosomal protein eL28



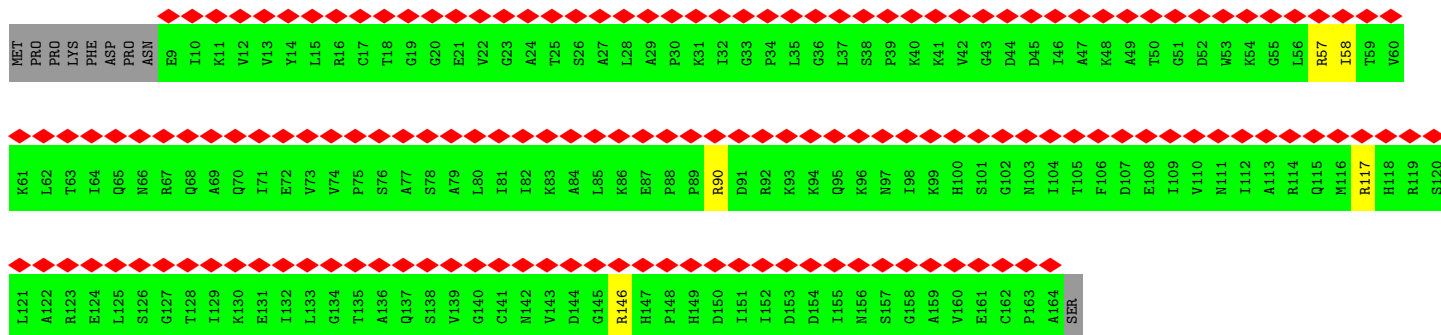
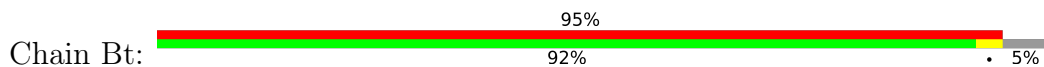
• Molecule 84: 60S acidic ribosomal protein P0



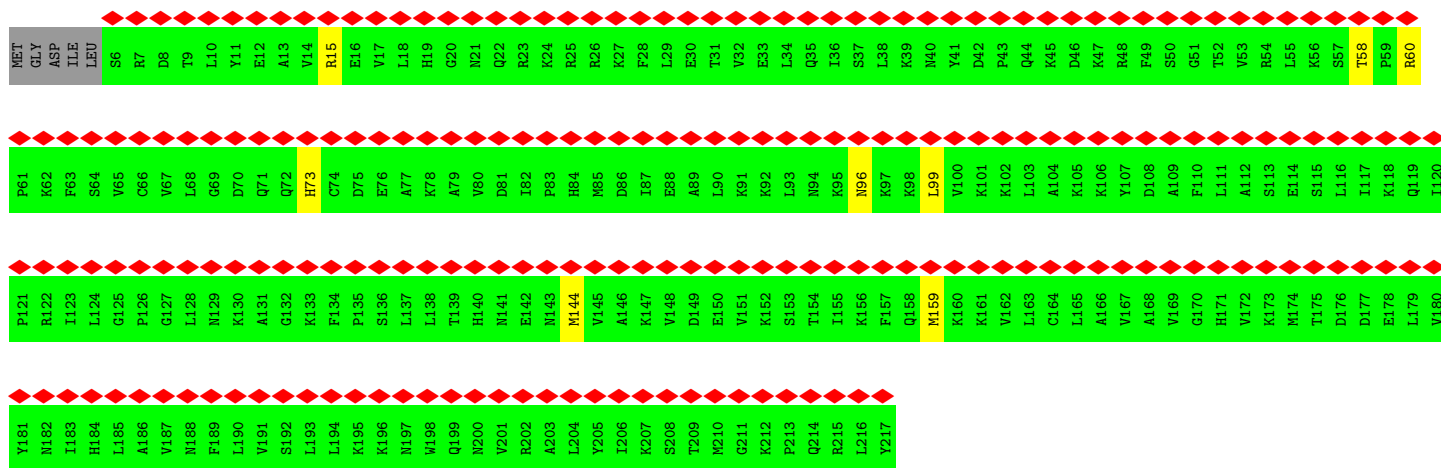




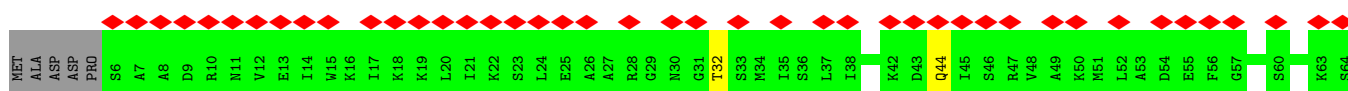
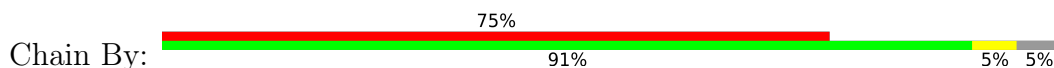
• Molecule 85: Ribosomal protein L12

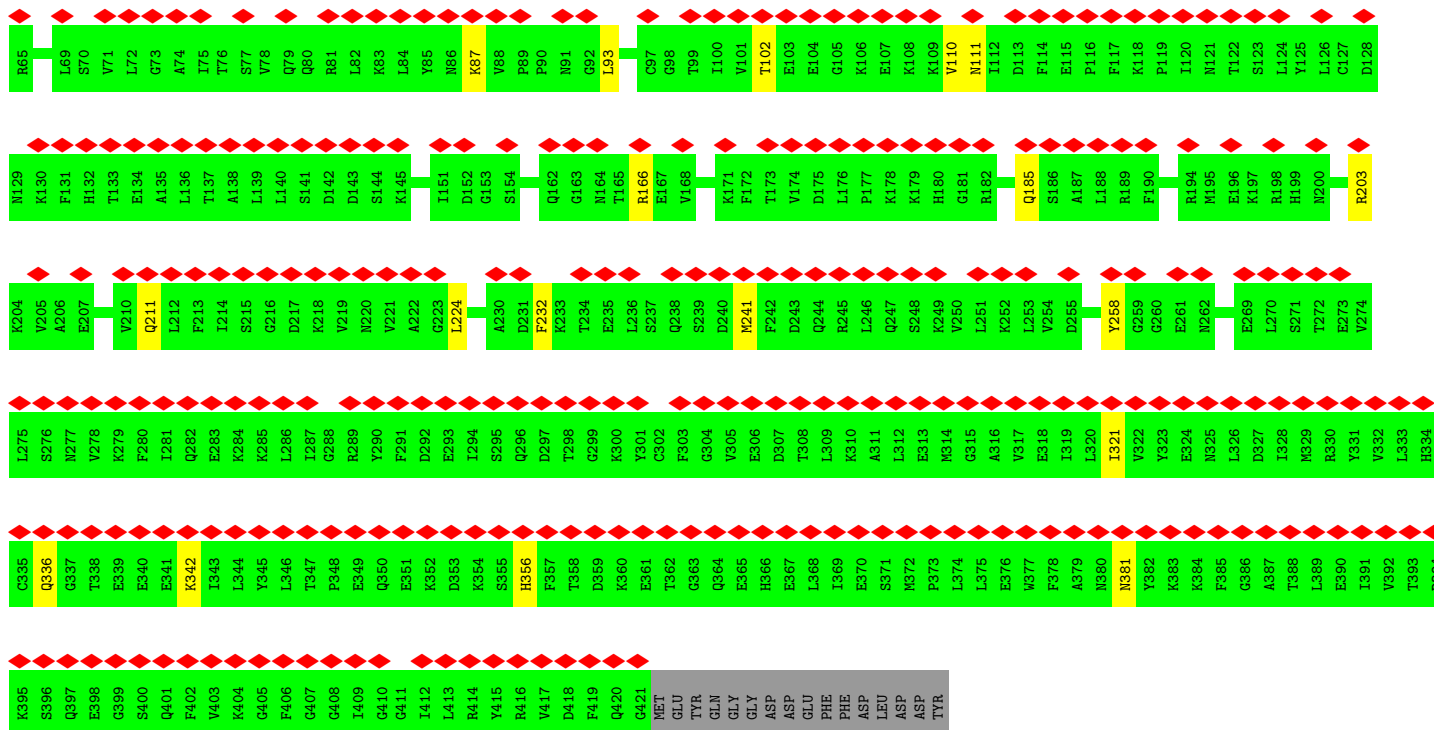


• Molecule 86: Ribosomal protein

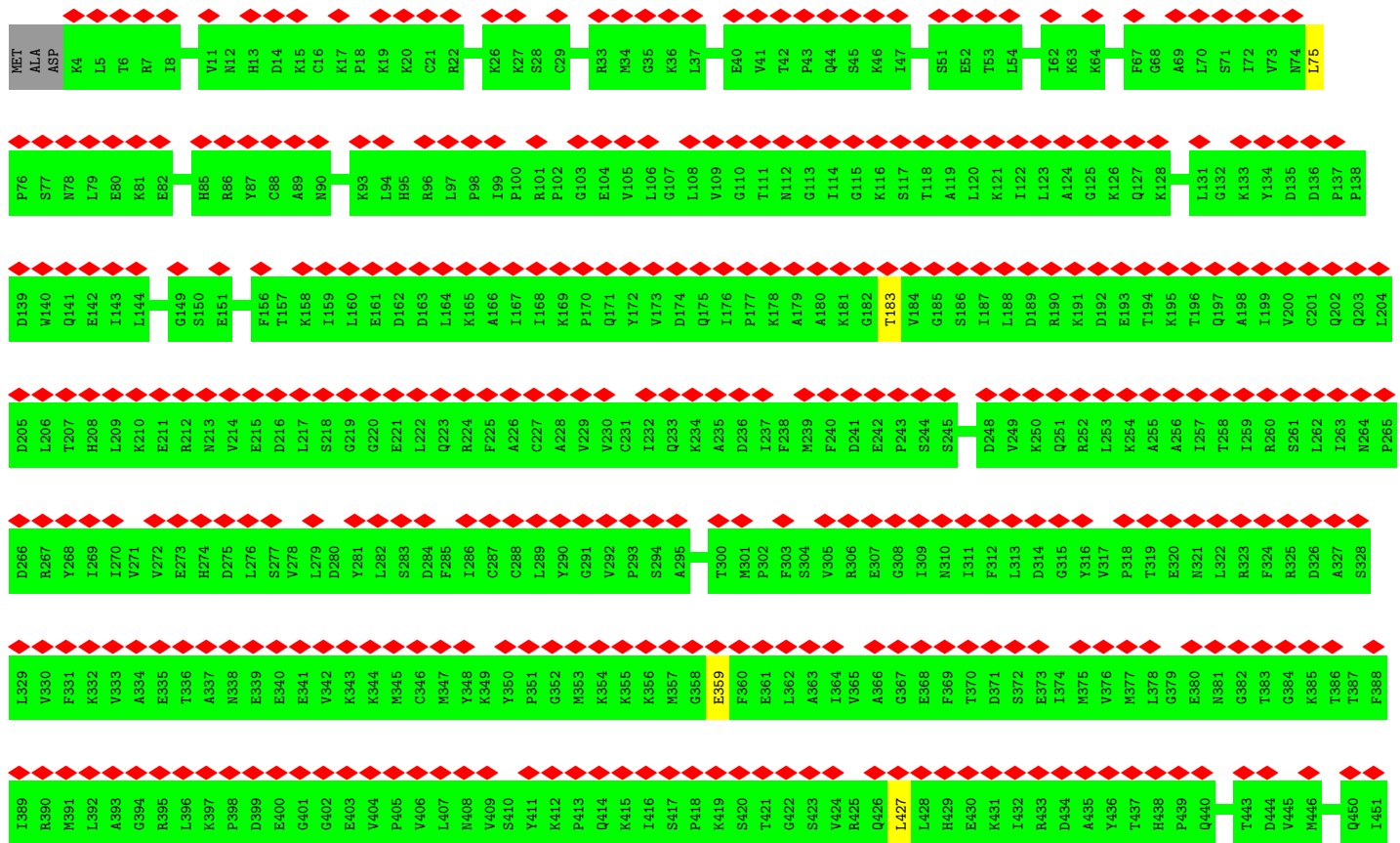
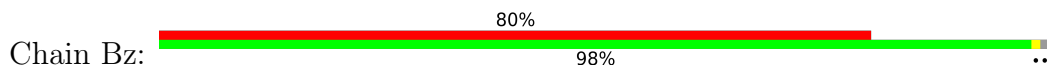


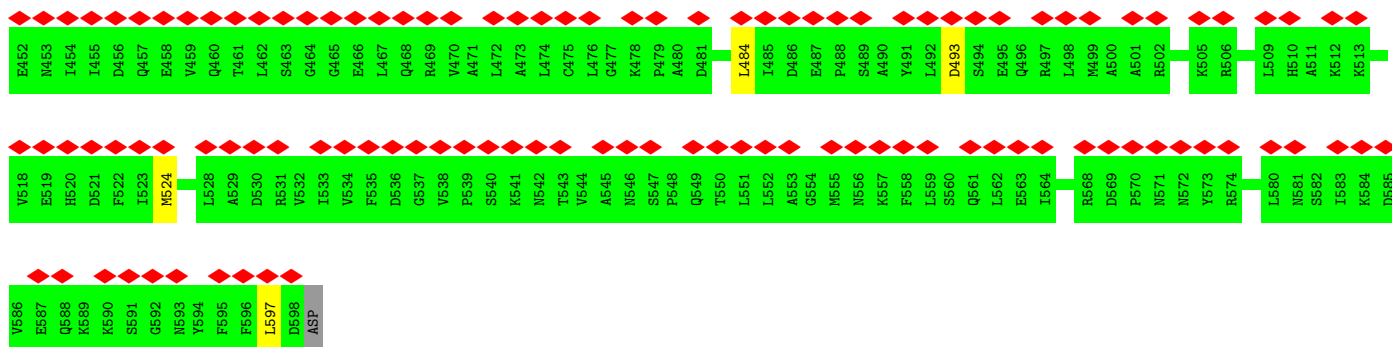
• Molecule 87: Eukaryotic peptide chain release factor subunit 1





● Molecule 88: ATP binding cassette subfamily E member 1





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	55057	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	60	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	56604	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	4.379	Depositor
Minimum map value	-1.818	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.131	Depositor
Recommended contour level	0.7	Depositor
Map size (Å)	593.6, 593.6, 593.6	wwPDB
Map dimensions	560, 560, 560	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

## 5 Model quality i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: AYA, AAC, GTP, HY3, SF4, PSU, 1MA, M3L, OMU, 5MU, AME, OMC, V5N, UNX, OMG, 6MZ, UY1, MA6, HIC, A2M, NMM, SPD, UR3, MLZ, 4AC, MG, SAC, 5MC, ZN, B8N, G7M

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A2	0.18	1/40342 (0.0%)	0.68	10/62877 (0.0%)
2	AA	0.24	0/665	0.46	0/891
3	AB	0.24	0/497	0.57	0/666
4	AC	0.24	0/613	0.50	0/811
5	AD	0.24	0/462	0.53	0/607
6	AE	0.24	0/828	0.53	0/1109
7	AF	0.23	0/2493	0.46	0/3394
8	AG	0.24	0/470	0.51	0/623
9	AH	0.13	0/566	0.66	0/879
10	AI	0.18	0/68	0.68	0/103
11	AT	0.28	1/2011 (0.0%)	0.68	0/3133
12	AZ	0.23	0/1771	0.46	0/2406
13	Aa	0.23	0/1841	0.46	0/2459
14	Ab	0.24	0/1742	0.45	0/2354
15	Ac	0.24	0/1779	0.48	0/2395
16	Ad	0.24	0/2118	0.50	0/2849
17	Ae	0.23	0/1531	0.48	0/2059
18	Af	0.24	0/1946	0.52	0/2590
19	Ag	0.24	0/1552	0.46	0/2079
20	Ah	0.24	0/1715	0.51	0/2287
21	Ai	0.23	0/1550	0.52	0/2069
22	Aj	0.24	0/834	0.42	0/1125
23	Ak	0.25	0/1284	0.51	0/1717
24	Al	0.23	0/968	0.41	0/1296
25	Am	0.23	0/1232	0.47	0/1656
26	An	0.24	0/1029	0.53	0/1380
27	Ao	0.25	0/1114	0.48	0/1490
28	Ap	0.24	0/1142	0.50	0/1528
29	Aq	0.23	0/1094	0.48	0/1469
30	Ar	0.23	0/1209	0.52	0/1620
31	As	0.23	0/1119	0.46	0/1498

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
32	At	0.23	0/831	0.52	0/1115
33	Au	0.24	0/636	0.48	0/852
34	Av	0.24	0/1051	0.48	0/1406
35	Aw	0.24	0/1107	0.50	0/1475
36	Ax	0.24	0/1032	0.50	0/1371
37	Ay	0.23	0/691	0.46	0/922
38	Az	0.22	0/240	0.66	0/305
39	B5	0.21	3/87403 (0.0%)	0.68	16/136359 (0.0%)
40	B7	0.18	0/2835	0.67	0/4418
41	B8	0.26	1/3635 (0.0%)	0.68	0/5661
42	BA	0.25	0/1965	0.54	0/2633
43	BB	0.25	0/3261	0.50	0/4364
44	BC	0.24	0/2932	0.50	0/3939
45	BD	0.25	0/2437	0.47	0/3264
46	BE	0.24	0/1998	0.50	0/2673
47	BF	0.25	0/1922	0.49	0/2563
48	BG	0.23	0/1908	0.48	0/2566
49	BH	0.24	0/1535	0.49	0/2063
50	BI	0.25	0/1756	0.50	0/2346
51	BJ	0.24	0/1385	0.51	0/1852
52	BK	0.25	0/277	0.46	0/372
53	BL	0.24	0/1733	0.53	0/2316
54	BM	0.24	0/1158	0.49	0/1547
55	BN	0.24	0/1746	0.54	0/2338
56	BO	0.24	0/1662	0.49	0/2222
57	BP	0.24	0/1317	0.48	0/1768
58	BQ	0.25	0/1539	0.56	0/2054
59	BR	0.23	0/1524	0.53	0/2013
60	BS	0.25	0/1497	0.53	0/2008
61	BT	0.25	0/1326	0.49	0/1770
62	BU	0.24	0/820	0.47	0/1100
63	BV	0.26	0/1048	0.51	0/1402
64	BW	0.24	0/1006	0.50	0/1334
65	BX	0.24	0/984	0.49	0/1323
66	BY	0.24	0/1132	0.52	0/1504
67	BZ	0.25	0/1130	0.49	0/1507
68	Ba	0.24	0/1179	0.50	0/1572
69	Bb	0.23	0/884	0.50	0/1169
70	Bc	0.24	0/847	0.43	0/1134
71	Bd	0.24	0/903	0.52	0/1216
72	Be	0.24	0/1088	0.52	0/1451
73	Bf	0.26	0/903	0.53	0/1208
74	Bg	0.24	0/916	0.54	0/1220

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
75	Bh	0.23	0/1021	0.50	0/1348
76	Bi	0.23	0/841	0.52	0/1112
77	Bj	0.25	0/720	0.57	0/952
78	Bk	0.24	0/575	0.45	0/761
79	Bl	0.23	0/459	0.51	0/608
80	Bm	0.23	0/426	0.50	0/564
81	Bo	0.25	0/866	0.51	0/1141
82	Bp	0.24	0/718	0.49	0/953
83	Br	0.23	0/1020	0.53	0/1366
84	Bs	0.24	0/1530	0.46	0/2064
85	Bt	0.23	0/1193	0.47	0/1609
86	Bv	0.23	0/1735	0.44	0/2328
87	By	0.24	0/3333	0.44	0/4483
88	Bz	0.24	0/4755	0.45	0/6421
All	All	0.22	6/243956 (0.0%)	0.61	26/356824 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
81	Bo	0	1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	B5	4761	U	C4-O4	12.82	1.33	1.23
11	AT	1	A	OP3-P	-10.68	1.48	1.61
41	B8	1	C	OP3-P	-10.62	1.48	1.61
1	A2	1	U	OP3-P	-10.59	1.48	1.61
39	B5	1	C	OP3-P	-10.52	1.48	1.61
39	B5	4761	U	N3-C4	-5.17	1.33	1.38

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	B5	4761	U	N3-C4-C5	12.16	121.89	114.60
39	B5	4761	U	C2-N3-C4	-11.63	120.02	127.00
39	B5	4761	U	C5-C4-O4	-9.76	120.04	125.90
1	A2	1454	C	C2-N1-C1'	7.92	127.52	118.80
1	A2	1454	C	N1-C2-O2	7.83	123.60	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	B5	2312	C	C2-N1-C1'	7.53	127.08	118.80
39	B5	2312	C	N1-C2-O2	7.41	123.35	118.90
39	B5	4761	U	N1-C2-N3	7.21	119.22	114.90
39	B5	2252	U	C2-N1-C1'	6.55	125.57	117.70
39	B5	1594	U	C2-N1-C1'	6.27	125.23	117.70
1	A2	1454	C	N3-C2-O2	-6.27	117.51	121.90
1	A2	1315	U	C2-N1-C1'	6.20	125.14	117.70
39	B5	2312	C	N3-C2-O2	-5.93	117.75	121.90
39	B5	2252	U	N1-C2-O2	5.83	126.88	122.80
1	A2	1023	U	C2-N1-C1'	5.78	124.64	117.70
1	A2	294	C	N1-C2-O2	5.71	122.32	118.90
39	B5	1594	U	N1-C2-O2	5.60	126.72	122.80
1	A2	294	C	C2-N1-C1'	5.47	124.82	118.80
1	A2	1454	C	C6-N1-C1'	-5.46	114.24	120.80
39	B5	2252	U	N3-C2-O2	-5.30	118.49	122.20
39	B5	1594	U	N3-C2-O2	-5.24	118.53	122.20
39	B5	4761	U	N1-C2-O2	-5.21	119.15	122.80
1	A2	1315	U	N1-C2-O2	5.21	126.45	122.80
1	A2	1454	C	C6-N1-C2	-5.20	118.22	120.30
39	B5	2312	C	C6-N1-C2	-5.17	118.23	120.30
39	B5	2312	C	C6-N1-C1'	-5.12	114.65	120.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
81	Bo	53	MLZ	Mainchain

## 5.2 Too-close contacts [i](#)

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

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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



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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AA	81/84 (96%)	79 (98%)	2 (2%)	0	100	100
3	AB	61/69 (88%)	61 (100%)	0	0	100	100
4	AC	71/156 (46%)	69 (97%)	2 (3%)	0	100	100
5	AD	55/133 (41%)	55 (100%)	0	0	100	100
6	AE	99/115 (86%)	99 (100%)	0	0	100	100
7	AF	311/317 (98%)	300 (96%)	11 (4%)	0	100	100
8	AG	53/56 (95%)	53 (100%)	0	0	100	100
12	AZ	219/295 (74%)	215 (98%)	4 (2%)	0	100	100
13	Aa	220/264 (83%)	218 (99%)	2 (1%)	0	100	100
14	Ab	218/293 (74%)	218 (100%)	0	0	100	100
15	Ac	223/281 (79%)	222 (100%)	1 (0%)	0	100	100
16	Ad	260/263 (99%)	256 (98%)	4 (2%)	0	100	100
17	Ae	189/204 (93%)	184 (97%)	5 (3%)	0	100	100
18	Af	235/249 (94%)	235 (100%)	0	0	100	100
19	Ag	188/194 (97%)	184 (98%)	4 (2%)	0	100	100
20	Ah	204/208 (98%)	203 (100%)	1 (0%)	0	100	100
21	Ai	183/194 (94%)	181 (99%)	2 (1%)	0	100	100
22	Aj	94/165 (57%)	93 (99%)	1 (1%)	0	100	100
23	Ak	152/158 (96%)	149 (98%)	3 (2%)	0	100	100
24	Al	122/132 (92%)	119 (98%)	3 (2%)	0	100	100
25	Am	148/151 (98%)	147 (99%)	1 (1%)	0	100	100
26	An	134/151 (89%)	133 (99%)	1 (1%)	0	100	100
27	Ao	131/145 (90%)	130 (99%)	1 (1%)	0	100	100
28	Ap	139/146 (95%)	133 (96%)	6 (4%)	0	100	100
29	Aq	132/135 (98%)	132 (100%)	0	0	100	100
30	Ar	143/152 (94%)	141 (99%)	2 (1%)	0	100	100
31	As	140/145 (97%)	139 (99%)	1 (1%)	0	100	100
32	At	102/119 (86%)	101 (99%)	1 (1%)	0	100	100
33	Au	81/83 (98%)	81 (100%)	0	0	100	100
34	Av	127/130 (98%)	126 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
35	Aw	138/143 (96%)	137 (99%)	1 (1%)	0	100	100
36	Ax	123/130 (95%)	121 (98%)	2 (2%)	0	100	100
37	Ay	83/124 (67%)	83 (100%)	0	0	100	100
38	Az	23/25 (92%)	23 (100%)	0	0	100	100
42	BA	250/257 (97%)	244 (98%)	6 (2%)	0	100	100
43	BB	395/403 (98%)	392 (99%)	3 (1%)	0	100	100
44	BC	360/413 (87%)	357 (99%)	3 (1%)	0	100	100
45	BD	291/297 (98%)	289 (99%)	2 (1%)	0	100	100
46	BE	239/291 (82%)	235 (98%)	4 (2%)	0	100	100
47	BF	224/247 (91%)	219 (98%)	5 (2%)	0	100	100
48	BG	229/266 (86%)	228 (100%)	1 (0%)	0	100	100
49	BH	188/192 (98%)	188 (100%)	0	0	100	100
50	BI	211/214 (99%)	208 (99%)	3 (1%)	0	100	100
51	BJ	168/178 (94%)	167 (99%)	1 (1%)	0	100	100
52	BK	34/1071 (3%)	34 (100%)	0	0	100	100
53	BL	208/211 (99%)	204 (98%)	4 (2%)	0	100	100
54	BM	136/218 (62%)	133 (98%)	3 (2%)	0	100	100
55	BN	201/204 (98%)	196 (98%)	5 (2%)	0	100	100
56	BO	197/203 (97%)	197 (100%)	0	0	100	100
57	BP	157/184 (85%)	156 (99%)	1 (1%)	0	100	100
58	BQ	185/188 (98%)	182 (98%)	3 (2%)	0	100	100
59	BR	178/196 (91%)	178 (100%)	0	0	100	100
60	BS	174/176 (99%)	174 (100%)	0	0	100	100
61	BT	157/160 (98%)	154 (98%)	3 (2%)	0	100	100
62	BU	97/128 (76%)	95 (98%)	2 (2%)	0	100	100
63	BV	137/140 (98%)	137 (100%)	0	0	100	100
64	BW	119/157 (76%)	119 (100%)	0	0	100	100
65	BX	116/156 (74%)	114 (98%)	2 (2%)	0	100	100
66	BY	132/145 (91%)	131 (99%)	1 (1%)	0	100	100
67	BZ	133/136 (98%)	133 (100%)	0	0	100	100
68	Ba	144/148 (97%)	139 (96%)	5 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
69	Bb	103/245 (42%)	97 (94%)	6 (6%)	0	100	100
70	Bc	106/115 (92%)	106 (100%)	0	0	100	100
71	Bd	105/125 (84%)	105 (100%)	0	0	100	100
72	Be	128/135 (95%)	128 (100%)	0	0	100	100
73	Bf	108/110 (98%)	108 (100%)	0	0	100	100
74	Bg	112/117 (96%)	111 (99%)	1 (1%)	0	100	100
75	Bh	120/123 (98%)	120 (100%)	0	0	100	100
76	Bi	100/105 (95%)	99 (99%)	1 (1%)	0	100	100
77	Bj	84/97 (87%)	84 (100%)	0	0	100	100
78	Bk	67/70 (96%)	67 (100%)	0	0	100	100
79	Bl	48/51 (94%)	48 (100%)	0	0	100	100
80	Bm	49/128 (38%)	49 (100%)	0	0	100	100
81	Bo	102/106 (96%)	100 (98%)	2 (2%)	0	100	100
82	Bp	89/92 (97%)	88 (99%)	1 (1%)	0	100	100
83	Br	124/137 (90%)	122 (98%)	2 (2%)	0	100	100
84	Bs	194/318 (61%)	190 (98%)	4 (2%)	0	100	100
85	Bt	154/165 (93%)	153 (99%)	1 (1%)	0	100	100
86	Bv	210/217 (97%)	203 (97%)	7 (3%)	0	100	100
87	By	414/437 (95%)	406 (98%)	8 (2%)	0	100	100
88	Bz	593/599 (99%)	582 (98%)	11 (2%)	0	100	100
All	All	12952/15680 (83%)	12789 (99%)	163 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AA	75/76 (99%)	74 (99%)	1 (1%)	69	90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	AB	56/62 (90%)	56 (100%)	0	100	100
4	AC	66/140 (47%)	66 (100%)	0	100	100
5	AD	47/106 (44%)	46 (98%)	1 (2%)	53	81
6	AE	88/98 (90%)	88 (100%)	0	100	100
7	AF	272/275 (99%)	269 (99%)	3 (1%)	73	92
8	AG	48/49 (98%)	48 (100%)	0	100	100
12	AZ	182/243 (75%)	180 (99%)	2 (1%)	73	92
13	Aa	203/231 (88%)	201 (99%)	2 (1%)	76	92
14	Ab	185/223 (83%)	182 (98%)	3 (2%)	62	86
15	Ac	189/232 (82%)	188 (100%)	1 (0%)	88	96
16	Ad	224/225 (100%)	224 (100%)	0	100	100
17	Ae	161/170 (95%)	161 (100%)	0	100	100
18	Af	207/218 (95%)	205 (99%)	2 (1%)	76	92
19	Ag	170/174 (98%)	167 (98%)	3 (2%)	59	85
20	Ah	178/180 (99%)	178 (100%)	0	100	100
21	Ai	161/168 (96%)	160 (99%)	1 (1%)	86	96
22	Aj	87/136 (64%)	87 (100%)	0	100	100
23	Ak	139/142 (98%)	138 (99%)	1 (1%)	84	95
24	Al	104/108 (96%)	100 (96%)	4 (4%)	33	67
25	Am	130/131 (99%)	129 (99%)	1 (1%)	81	94
26	An	106/119 (89%)	104 (98%)	2 (2%)	57	84
27	Ao	119/130 (92%)	119 (100%)	0	100	100
28	Ap	117/121 (97%)	117 (100%)	0	100	100
29	Aq	120/121 (99%)	120 (100%)	0	100	100
30	Ar	125/131 (95%)	123 (98%)	2 (2%)	62	86
31	As	112/114 (98%)	112 (100%)	0	100	100
32	At	94/107 (88%)	93 (99%)	1 (1%)	73	92
33	Au	67/67 (100%)	66 (98%)	1 (2%)	65	87
34	Av	112/113 (99%)	112 (100%)	0	100	100
35	Aw	112/114 (98%)	110 (98%)	2 (2%)	59	85
36	Ax	107/112 (96%)	106 (99%)	1 (1%)	78	93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
37	Ay	75/102 (74%)	75 (100%)	0	100	100
38	Az	24/24 (100%)	24 (100%)	0	100	100
42	BA	194/198 (98%)	193 (100%)	1 (0%)	88	96
43	BB	344/347 (99%)	343 (100%)	1 (0%)	92	98
44	BC	302/337 (90%)	301 (100%)	1 (0%)	92	98
45	BD	247/250 (99%)	247 (100%)	0	100	100
46	BE	216/251 (86%)	216 (100%)	0	100	100
47	BF	197/215 (92%)	196 (100%)	1 (0%)	88	96
48	BG	199/223 (89%)	197 (99%)	2 (1%)	76	92
49	BH	169/171 (99%)	169 (100%)	0	100	100
50	BI	180/181 (99%)	177 (98%)	3 (2%)	60	86
51	BJ	143/149 (96%)	143 (100%)	0	100	100
52	BK	31/936 (3%)	30 (97%)	1 (3%)	39	73
53	BL	175/176 (99%)	171 (98%)	4 (2%)	50	80
54	BM	117/161 (73%)	116 (99%)	1 (1%)	78	93
55	BN	171/172 (99%)	171 (100%)	0	100	100
56	BO	171/173 (99%)	170 (99%)	1 (1%)	86	96
57	BP	140/163 (86%)	140 (100%)	0	100	100
58	BQ	164/165 (99%)	163 (99%)	1 (1%)	86	96
59	BR	159/175 (91%)	159 (100%)	0	100	100
60	BS	154/154 (100%)	154 (100%)	0	100	100
61	BT	139/140 (99%)	139 (100%)	0	100	100
62	BU	88/113 (78%)	88 (100%)	0	100	100
63	BV	106/107 (99%)	104 (98%)	2 (2%)	57	84
64	BW	100/126 (79%)	99 (99%)	1 (1%)	76	92
65	BX	106/134 (79%)	106 (100%)	0	100	100
66	BY	124/135 (92%)	122 (98%)	2 (2%)	62	86
67	BZ	117/118 (99%)	117 (100%)	0	100	100
68	Ba	118/119 (99%)	118 (100%)	0	100	100
69	Bb	87/183 (48%)	87 (100%)	0	100	100
70	Bc	92/98 (94%)	92 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
71	Bd	98/110 (89%)	98 (100%)	0	100	100
72	Be	116/121 (96%)	116 (100%)	0	100	100
73	Bf	89/89 (100%)	89 (100%)	0	100	100
74	Bg	98/100 (98%)	97 (99%)	1 (1%)	76	92
75	Bh	109/110 (99%)	109 (100%)	0	100	100
76	Bi	86/89 (97%)	85 (99%)	1 (1%)	71	91
77	Bj	73/80 (91%)	71 (97%)	2 (3%)	44	77
78	Bk	64/65 (98%)	64 (100%)	0	100	100
79	Bl	47/48 (98%)	46 (98%)	1 (2%)	53	81
80	Bm	47/115 (41%)	47 (100%)	0	100	100
81	Bo	92/93 (99%)	92 (100%)	0	100	100
82	Bp	74/75 (99%)	74 (100%)	0	100	100
83	Br	109/120 (91%)	109 (100%)	0	100	100
84	Bs	164/258 (64%)	162 (99%)	2 (1%)	71	91
85	Bt	128/137 (93%)	123 (96%)	5 (4%)	32	66
86	Bv	191/195 (98%)	183 (96%)	8 (4%)	30	63
87	By	358/376 (95%)	338 (94%)	20 (6%)	21	52
88	Bz	516/526 (98%)	508 (98%)	8 (2%)	62	86
All	All	11271/13339 (84%)	11167 (99%)	104 (1%)	79	93

All (104) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	AA	74	THR
5	AD	122	THR
7	AF	113	PHE
7	AF	159	ASN
7	AF	296	GLN
12	AZ	121	LEU
12	AZ	206	ASP
13	Aa	170	GLU
13	Aa	178	THR
14	Ab	79	GLU
14	Ab	236	PHE
14	Ab	248	TYR
15	Ac	46	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
18	Af	7	PHE
18	Af	190	ARG
19	Ag	18	GLU
19	Ag	78	ARG
19	Ag	110	THR
21	Ai	70	ARG
23	Ak	69	ARG
24	Al	33	ARG
24	Al	75	ASN
24	Al	91	LEU
24	Al	104	VAL
25	Am	133	ARG
26	An	113	GLN
26	An	138	ASP
30	Ar	83	PHE
30	Ar	103	LEU
32	At	68	THR
33	Au	42	VAL
35	Aw	61	GLN
35	Aw	105	PHE
36	Ax	98	GLU
42	BA	14	SER
43	BB	343	ARG
44	BC	122	TYR
47	BF	85	GLU
48	BG	88	ASP
48	BG	106	THR
50	BI	102	MET
50	BI	110	ARG
50	BI	163	GLN
52	BK	4400	LEU
53	BL	63	THR
53	BL	67	HIS
53	BL	115	GLN
53	BL	129	ARG
54	BM	126	GLU
56	BO	117	ARG
58	BQ	14	ARG
63	BV	50	ASN
63	BV	92	ASP
64	BW	67	ILE
66	BY	74	TYR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
66	BY	88	GLU
74	Bg	73	HIS
76	Bi	29	ARG
77	Bj	20	ARG
77	Bj	57	ASN
79	Bl	28	TRP
84	Bs	45	MET
84	Bs	99	ARG
85	Bt	57	ARG
85	Bt	58	ILE
85	Bt	90	ARG
85	Bt	117	ARG
85	Bt	146	ARG
86	Bv	15	ARG
86	Bv	58	THR
86	Bv	60	ARG
86	Bv	73	HIS
86	Bv	96	ASN
86	Bv	99	LEU
86	Bv	144	MET
86	Bv	159	MET
87	By	32	THR
87	By	44	GLN
87	By	87	LYS
87	By	93	LEU
87	By	102	THR
87	By	110	VAL
87	By	111	ASN
87	By	166	ARG
87	By	185	GLN
87	By	203	ARG
87	By	211	GLN
87	By	224	LEU
87	By	232	PHE
87	By	241	MET
87	By	258	TYR
87	By	321	ILE
87	By	336	GLN
87	By	342	LYS
87	By	356	HIS
87	By	381	ASN
88	Bz	75	LEU

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Mol	Chain	Res	Type
88	Bz	183	THR
88	Bz	359	GLU
88	Bz	427	LEU
88	Bz	484	LEU
88	Bz	493	ASP
88	Bz	524	MET
88	Bz	597	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (110) such sidechains are listed below:

Mol	Chain	Res	Type
2	AA	29	ASN
2	AA	51	GLN
5	AD	89	GLN
6	AE	72	HIS
7	AF	62	HIS
7	AF	159	ASN
7	AF	296	GLN
8	AG	16	GLN
8	AG	37	ASN
12	AZ	141	ASN
12	AZ	193	HIS
13	Aa	186	ASN
15	Ac	145	GLN
15	Ac	174	HIS
16	Ad	142	HIS
16	Ad	157	ASN
17	Ae	65	GLN
17	Ae	83	ASN
20	Ah	7	ASN
20	Ah	146	GLN
20	Ah	167	GLN
22	Aj	32	HIS
22	Aj	77	GLN
24	Al	28	HIS
27	Ao	103	ASN
27	Ao	104	GLN
28	Ap	24	HIS
28	Ap	80	GLN
28	Ap	86	GLN
28	Ap	97	GLN
28	Ap	114	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
30	Ar	72	GLN
31	As	12	GLN
33	Au	2	GLN
34	Av	90	GLN
42	BA	50	HIS
42	BA	140	ASN
42	BA	205	ASN
43	BB	175	GLN
43	BB	184	GLN
43	BB	289	GLN
43	BB	354	GLN
44	BC	50	GLN
44	BC	310	HIS
45	BD	122	GLN
45	BD	202	GLN
45	BD	222	GLN
45	BD	225	GLN
46	BE	131	HIS
47	BF	57	HIS
47	BF	118	ASN
48	BG	64	GLN
48	BG	81	ASN
49	BH	42	ASN
49	BH	102	ASN
50	BI	59	GLN
50	BI	163	GLN
53	BL	188	ASN
54	BM	33	GLN
56	BO	180	GLN
58	BQ	160	HIS
59	BR	40	GLN
59	BR	75	HIS
59	BR	143	HIS
60	BS	125	GLN
61	BT	131	GLN
61	BT	144	ASN
62	BU	17	GLN
64	BW	79	GLN
64	BW	96	GLN
64	BW	120	GLN
66	BY	14	ASN
66	BY	56	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
67	BZ	78	ASN
68	Ba	66	ASN
69	Bb	17	HIS
72	Be	23	HIS
74	Bg	114	GLN
76	Bi	36	HIS
78	Bk	58	GLN
79	Bl	4	HIS
80	Bm	117	HIS
83	Br	4	HIS
83	Br	6	GLN
84	Bs	39	GLN
84	Bs	190	GLN
84	Bs	191	GLN
85	Bt	97	ASN
86	Bv	96	ASN
87	By	44	GLN
87	By	67	ASN
87	By	79	GLN
87	By	80	GLN
87	By	111	ASN
87	By	162	GLN
87	By	185	GLN
87	By	211	GLN
87	By	238	GLN
87	By	350	GLN
87	By	381	ASN
87	By	401	GLN
87	By	420	GLN
88	Bz	85	HIS
88	Bz	127	GLN
88	Bz	153	GLN
88	Bz	251	GLN
88	Bz	321	ASN
88	Bz	440	GLN
88	Bz	460	GLN
88	Bz	549	GLN

### 5.3.3 RNA

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A2	1758/1870 (94%)	231 (13%)	1 (0%)
10	AI	2/76 (2%)	1 (50%)	0
11	AT	85/86 (98%)	15 (17%)	0
39	B5	3750/4808 (77%)	469 (12%)	1 (0%)
40	B7	118/119 (99%)	7 (5%)	0
41	B8	155/158 (98%)	17 (10%)	0
9	AH	23/217 (10%)	8 (34%)	0
All	All	5891/7334 (80%)	748 (12%)	2 (0%)

All (748) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A2	3	C
1	A2	17	C
1	A2	26	U
1	A2	33	G
1	A2	41	G
1	A2	44	U
1	A2	46	A
1	A2	56	G
1	A2	58	C
1	A2	67	C
1	A2	68	A
1	A2	73	C
1	A2	74	G
1	A2	77	A
1	A2	79	A
1	A2	103	A
1	A2	113	G
1	A2	114	G
1	A2	115	U
1	A2	126	G
1	A2	130	G
1	A2	142	C
1	A2	143	U
1	A2	155	G
1	A2	162	C
1	A2	163	U
1	A2	168	C
1	A2	170	A
1	A2	178	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A2	180	G
1	A2	184	G
1	A2	188	C
1	A2	192	C
1	A2	226	A
1	A2	228	C
1	A2	282	C
1	A2	298	A
1	A2	303	A
1	A2	306	U
1	A2	308	G
1	A2	310	G
1	A2	313	G
1	A2	320	C
1	A2	325	U
1	A2	327	C
1	A2	328	G
1	A2	329	U
1	A2	330	G
1	A2	348	G
1	A2	365	A
1	A2	369	U
1	A2	370	C
1	A2	386	G
1	A2	387	C
1	A2	401	C
1	A2	410	C
1	A2	439	G
1	A2	449	A
1	A2	450	A
1	A2	451	C
1	A2	465	A
1	A2	466	A
1	A2	467	G
1	A2	472	G
1	A2	473	C
1	A2	474	A
1	A2	475	G
1	A2	483	G
1	A2	488	U
1	A2	493	C
1	A2	509	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A2	513	A2M
1	A2	526	A
1	A2	542	U
1	A2	543	U
1	A2	544	C
1	A2	550	C
1	A2	556	A
1	A2	557	U
1	A2	565	A
1	A2	569	C
1	A2	584	A
1	A2	590	G
1	A2	592	U
1	A2	605	A
1	A2	607	G
1	A2	609	C
1	A2	615	C
1	A2	629	A
1	A2	632	U
1	A2	644	A
1	A2	645	OMG
1	A2	656	A
1	A2	661	C
1	A2	669	A2M
1	A2	670	A
1	A2	672	A
1	A2	673	A
1	A2	698	G
1	A2	734	C
1	A2	747	C
1	A2	748	U
1	A2	749	C
1	A2	753	G
1	A2	755	G
1	A2	795	A
1	A2	796	A
1	A2	800	U
1	A2	812	A
1	A2	822	G
1	A2	823	PSU
1	A2	831	A
1	A2	832	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A2	837	G
1	A2	838	A
1	A2	839	G
1	A2	840	C
1	A2	841	C
1	A2	842	G
1	A2	848	A
1	A2	870	A
1	A2	871	A
1	A2	872	U
1	A2	873	A
1	A2	892	G
1	A2	914	A
1	A2	915	U
1	A2	921	A
1	A2	923	A
1	A2	931	C
1	A2	934	G
1	A2	944	U
1	A2	956	A
1	A2	964	A
1	A2	972	G
1	A2	991	A
1	A2	993	A
1	A2	1000	G
1	A2	1003	U
1	A2	1024	A
1	A2	1084	A
1	A2	1086	C
1	A2	1116	U
1	A2	1117	C
1	A2	1118	C
1	A2	1119	C
1	A2	1122	G
1	A2	1134	A
1	A2	1145	A
1	A2	1154	C
1	A2	1155	U
1	A2	1196	A
1	A2	1208	G
1	A2	1216	C
1	A2	1225	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A2	1243	U
1	A2	1252	A
1	A2	1254	A
1	A2	1257	G
1	A2	1258	G
1	A2	1260	A
1	A2	1272	C
1	A2	1275	G
1	A2	1276	G
1	A2	1283	A
1	A2	1303	G
1	A2	1304	C
1	A2	1343	U
1	A2	1359	U
1	A2	1365	U
1	A2	1372	U
1	A2	1373	U
1	A2	1379	A
1	A2	1383	A
1	A2	1398	U
1	A2	1406	A
1	A2	1407	G
1	A2	1419	C
1	A2	1420	C
1	A2	1422	A
1	A2	1424	C
1	A2	1436	C
1	A2	1447	A
1	A2	1455	A
1	A2	1463	U
1	A2	1464	U
1	A2	1481	A
1	A2	1490	A
1	A2	1491	OMG
1	A2	1498	G
1	A2	1508	G
1	A2	1510	U
1	A2	1522	C
1	A2	1523	A
1	A2	1545	C
1	A2	1553	G
1	A2	1554	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A2	1571	G
1	A2	1580	A
1	A2	1581	A
1	A2	1589	A
1	A2	1602	A
1	A2	1622	U
1	A2	1624	A
1	A2	1655	G
1	A2	1662	A
1	A2	1666	G
1	A2	1681	G
1	A2	1699	C
1	A2	1722	U
1	A2	1723	G
1	A2	1745	G
1	A2	1759	G
1	A2	1766	C
1	A2	1768	C
1	A2	1769	A
1	A2	1776	U
1	A2	1778	G
1	A2	1780	G
1	A2	1782	A
1	A2	1784	C
1	A2	1785	G
1	A2	1830	G
1	A2	1836	A
1	A2	1837	G
1	A2	1839	U
1	A2	1850	G
1	A2	1862	G
1	A2	1863	G
1	A2	1864	A
1	A2	1866	C
9	AH	3457	U
9	AH	3458	C
9	AH	3459	G
9	AH	3466	U
9	AH	3470	G
9	AH	3473	U
9	AH	3474	U
9	AH	3477	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
10	AI	76	A
11	AT	9	G
11	AT	10	G
11	AT	14	A
11	AT	16	U
11	AT	18	G
11	AT	19	U
11	AT	20	U
11	AT	21	A
11	AT	22	A
11	AT	45	G
11	AT	46	G
11	AT	50	A
11	AT	52	U
11	AT	59	G
11	AT	69	A
39	B5	25	A
39	B5	39	A
39	B5	42	A
39	B5	58	G
39	B5	59	A
39	B5	64	A
39	B5	65	A
39	B5	85	G
39	B5	91	G
39	B5	98	A
39	B5	109	G
39	B5	110	C
39	B5	119	G
39	B5	134	G
39	B5	135	G
39	B5	136	U
39	B5	142	G
39	B5	144	G
39	B5	159	C
39	B5	185	C
39	B5	187	U
39	B5	188	G
39	B5	189	G
39	B5	200	U
39	B5	201	C
39	B5	209	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
39	B5	210	C
39	B5	218	A
39	B5	219	G
39	B5	220	C
39	B5	234	G
39	B5	266	C
39	B5	297	U
39	B5	315	G
39	B5	316	U
39	B5	326	C
39	B5	334	A
39	B5	340	C
39	B5	363	A
39	B5	387	G
39	B5	401	G
39	B5	408	A
39	B5	409	G
39	B5	412	G
39	B5	446	C
39	B5	449	C
39	B5	450	G
39	B5	452	A
39	B5	453	G
39	B5	454	U
39	B5	463	A
39	B5	467	U
39	B5	468	U
39	B5	482	U
39	B5	483	G
39	B5	485	U
39	B5	486	C
39	B5	493	U
39	B5	497	G
39	B5	499	C
39	B5	502	U
39	B5	503	C
39	B5	504	U
39	B5	505	C
39	B5	506	G
39	B5	515	U
39	B5	516	U
39	B5	517	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
39	B5	628	U
39	B5	634	C
39	B5	635	G
39	B5	660	G
39	B5	691	G
39	B5	698	C
39	B5	699	G
39	B5	724	G
39	B5	725	G
39	B5	732	C
39	B5	734	G
39	B5	738	G
39	B5	758	C
39	B5	760	C
39	B5	790	G
39	B5	791	C
39	B5	792	G
39	B5	795	A
39	B5	797	C
39	B5	798	C
39	B5	803	C
39	B5	810	U
39	B5	812	A
39	B5	814	A
39	B5	815	G
39	B5	824	C
39	B5	825	G
39	B5	831	A
39	B5	832	G
39	B5	835	G
39	B5	843	A
39	B5	844	A
39	B5	845	U
39	B5	856	A
39	B5	859	G
39	B5	860	A
39	B5	861	G
39	B5	866	A
39	B5	867	C
39	B5	868	C
39	B5	869	U
39	B5	870	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
39	B5	884	U
39	B5	983	G
39	B5	985	G
39	B5	987	C
39	B5	1072	C
39	B5	1073	C
39	B5	1074	C
39	B5	1084	C
39	B5	1091	G
39	B5	1102	G
39	B5	1105	C
39	B5	1106	U
39	B5	1124	A
39	B5	1127	G
39	B5	1129	G
39	B5	1133	C
39	B5	1136	G
39	B5	1202	C
39	B5	1214	A
39	B5	1215	G
39	B5	1216	C
39	B5	1217	G
39	B5	1221	G
39	B5	1228	G
39	B5	1231	G
39	B5	1239	U
39	B5	1240	G
39	B5	1247	A
39	B5	1270	A2M
39	B5	1298	A
39	B5	1299	G
39	B5	1303	G
39	B5	1308	U
39	B5	1309	C
39	B5	1310	G
39	B5	1312	A
39	B5	1323	C
39	B5	1331	A
39	B5	1341	A
39	B5	1367	G
39	B5	1375	A
39	B5	1391	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
39	B5	1393	C
39	B5	1401	C
39	B5	1452	A
39	B5	1453	G
39	B5	1457	G
39	B5	1480	A
39	B5	1489	A2M
39	B5	1490	C
39	B5	1502	A
39	B5	1521	C
39	B5	1533	U
39	B5	1546	U
39	B5	1551	U
39	B5	1579	G
39	B5	1580	OMG
39	B5	1586	A
39	B5	1588	G
39	B5	1589	A
39	B5	1593	A
39	B5	1596	G
39	B5	1609	G
39	B5	1616	C
39	B5	1631	C
39	B5	1632	PSU
39	B5	1633	C
39	B5	1646	G
39	B5	1653	C
39	B5	1657	C
39	B5	1658	C
39	B5	1673	G
39	B5	1694	C
39	B5	1704	A
39	B5	1705	A
39	B5	1726	A
39	B5	1743	A
39	B5	1745	G
39	B5	1754	G
39	B5	1767	C
39	B5	1774	G
39	B5	1775	G
39	B5	1776	A
39	B5	1781	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
39	B5	1794	G
39	B5	1808	G
39	B5	1830	A
39	B5	1832	C
39	B5	1836	A
39	B5	1857	U
39	B5	1859	C
39	B5	1860	C
39	B5	1861	G
39	B5	1870	C
39	B5	1871	A
39	B5	1879	G
39	B5	1887	G
39	B5	1890	G
39	B5	1898	U
39	B5	1900	G
39	B5	1913	U
39	B5	1914	G
39	B5	1915	G
39	B5	1917	C
39	B5	1923	A
39	B5	1937	A
39	B5	1940	G
39	B5	1942	G
39	B5	1963	G
39	B5	1965	A
39	B5	1983	U
39	B5	1985	G
39	B5	1987	U
39	B5	1994	G
39	B5	1995	G
39	B5	2008	A
39	B5	2023	U
39	B5	2032	G
39	B5	2037	G
39	B5	2041	G
39	B5	2043	A
39	B5	2044	A
39	B5	2045	G
39	B5	2046	A
39	B5	2050	U
39	B5	2143	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
39	B5	2144	G
39	B5	2149	G
39	B5	2156	A
39	B5	2157	G
39	B5	2174	G
39	B5	2191	G
39	B5	2194	OMC
39	B5	2207	OMG
39	B5	2238	A
39	B5	2260	A
39	B5	2264	G
39	B5	2268	U
39	B5	2322	G
39	B5	2332	C
39	B5	2333	U
39	B5	2349	G
39	B5	2356	A
39	B5	2372	A
39	B5	2380	A
39	B5	2386	A
39	B5	2387	G
39	B5	2388	U
39	B5	2390	G
39	B5	2397	U
39	B5	2409	G
39	B5	2429	G
39	B5	2430	A
39	B5	2432	C
39	B5	2444	A
39	B5	2496	C
39	B5	2503	A
39	B5	2504	U
39	B5	2512	C
39	B5	2530	U
39	B5	2537	G
39	B5	2538	A
39	B5	2539	A
39	B5	2551	U
39	B5	2552	C
39	B5	2553	C
39	B5	2554	G
39	B5	2564	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
39	B5	2586	A
39	B5	2606	U
39	B5	2612	U
39	B5	2631	U
39	B5	2633	U
39	B5	2641	A
39	B5	2657	C
39	B5	2658	A2M
39	B5	2669	U
39	B5	2670	G
39	B5	2672	U
39	B5	2698	G
39	B5	2745	G
39	B5	3329	G
39	B5	3350	C
39	B5	3358	G
39	B5	3362	A
39	B5	3367	A
39	B5	3380	A
39	B5	3385	A
39	B5	3394	A
39	B5	3396	G
39	B5	3405	C
39	B5	3428	C
39	B5	3444	A
39	B5	3485	G
39	B5	3491	A
39	B5	3492	A2M
39	B5	3498	A
39	B5	3508	G
39	B5	3509	G
39	B5	3517	A2M
39	B5	3543	G
39	B5	3544	C
39	B5	3546	U
39	B5	3549	A
39	B5	3551	G
39	B5	3570	U
39	B5	3572	U
39	B5	3599	A2M
39	B5	3609	A
39	B5	3610	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
39	B5	3611	G
39	B5	3629	G
39	B5	3630	G
39	B5	3633	A
39	B5	3638	A
39	B5	3639	G
39	B5	3640	A
39	B5	3647	U
39	B5	3670	G
39	B5	3688	G
39	B5	3689	U
39	B5	3704	A
39	B5	3804	G
39	B5	3812	G
39	B5	3823	G
39	B5	3824	C
39	B5	3825	G
39	B5	3832	G
39	B5	3833	A
39	B5	3834	G
39	B5	3847	C
39	B5	3850	G
39	B5	3855	A
39	B5	3869	G
39	B5	3874	U
39	B5	3875	C
39	B5	3891	C
39	B5	3892	G
39	B5	3904	C
39	B5	3908	C
39	B5	3909	U
39	B5	3916	A
39	B5	3929	G
39	B5	3930	G
39	B5	3937	G
39	B5	3949	A
39	B5	3971	G
39	B5	3975	U
39	B5	3979	A
39	B5	3997	A
39	B5	4000	G
39	B5	4012	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
39	B5	4014	A
39	B5	4017	A
39	B5	4019	A
39	B5	4027	A
39	B5	4037	G
39	B5	4051	G
39	B5	4052	OMU
39	B5	4060	C
39	B5	4075	G
39	B5	4076	G
39	B5	4078	C
39	B5	4096	C
39	B5	4100	U
39	B5	4119	G
39	B5	4123	G
39	B5	4124	A
39	B5	4126	A
39	B5	4133	C
39	B5	4137	G
39	B5	4140	A
39	B5	4161	A
39	B5	4167	C
39	B5	4168	A
39	B5	4172	C
39	B5	4194	G
39	B5	4198	U
39	B5	4210	A
39	B5	4212	C
39	B5	4221	G
39	B5	4258	U
39	B5	4259	A
39	B5	4261	G
39	B5	4265	C
39	B5	4269	A2M
39	B5	4270	G
39	B5	4278	PSU
39	B5	4294	A
39	B5	4295	G
39	B5	4306	C
39	B5	4313	G
39	B5	4321	G
39	B5	4336	A2M

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
39	B5	4381	A
39	B5	4382	PSU
39	B5	4383	OMG
39	B5	4402	A
39	B5	4416	C
39	B5	4418	A
39	B5	4423	U
39	B5	4437	A
39	B5	4445	U
39	B5	4446	A
39	B5	4454	A
39	B5	4455	U
39	B5	4465	G
39	B5	4475	A
39	B5	4476	C
39	B5	4477	G
39	B5	4478	G
39	B5	4486	G
39	B5	4487	A
39	B5	4488	A
39	B5	4489	G
39	B5	4490	G
39	B5	4492	G
39	B5	4498	G
39	B5	4501	G
39	B5	4504	C
39	B5	4506	C
39	B5	4508	G
39	B5	4512	G
39	B5	4518	C
39	B5	4609	G
39	B5	4610	C
39	B5	4614	G
39	B5	4621	U
39	B5	4622	C
39	B5	4634	U
39	B5	4638	G
39	B5	4639	C
39	B5	4640	G
39	B5	4642	G
39	B5	4644	C
39	B5	4645	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
39	B5	4646	G
39	B5	4647	G
39	B5	4649	A
39	B5	4651	G
39	B5	4655	G
39	B5	4658	G
39	B5	4674	C
39	B5	4682	A
39	B5	4686	U
39	B5	4705	A
39	B5	4715	U
39	B5	4728	U
39	B5	4729	C
39	B5	4753	A
39	B5	4756	G
39	B5	4762	C
39	B5	4763	C
39	B5	4766	C
39	B5	4780	G
39	B5	4789	C
39	B5	4793	C
39	B5	4801	G
39	B5	4808	U
40	B7	7	G
40	B7	11	A
40	B7	53	U
40	B7	54	A
40	B7	64	G
40	B7	110	G
40	B7	120	U
41	B8	23	C
41	B8	34	U
41	B8	35	C
41	B8	59	A
41	B8	62	A
41	B8	63	U
41	B8	81	C
41	B8	84	A
41	B8	87	G
41	B8	94	G
41	B8	103	A
41	B8	105	C

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Mol	Chain	Res	Type
41	B8	110	U
41	B8	114	G
41	B8	123	U
41	B8	127	U
41	B8	150	C

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A2	549	C
39	B5	4445	U

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
39	PSU	B5	3616	39	18,21,22	1.38	2 (11%)	22,30,33	1.93	3 (13%)
39	PSU	B5	1720	39	18,21,22	1.36	2 (11%)	22,30,33	1.88	3 (13%)
1	PSU	A2	1446	1	18,21,22	1.34	2 (11%)	22,30,33	1.91	4 (18%)
39	PSU	B5	4188	39	18,21,22	1.35	2 (11%)	22,30,33	1.92	3 (13%)
39	PSU	B5	4325	39	18,21,22	1.35	2 (11%)	22,30,33	1.89	3 (13%)
39	A2M	B5	1810	90,39	18,25,26	1.01	1 (5%)	18,36,39	1.24	2 (11%)
39	PSU	B5	4166	39	18,21,22	1.37	2 (11%)	22,30,33	1.81	3 (13%)
39	PSU	B5	3490	39	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)
39	A2M	B5	4269	90,39	18,25,26	1.01	1 (5%)	18,36,39	1.25	2 (11%)
1	PSU	A2	864	1	18,21,22	1.36	2 (11%)	22,30,33	1.86	3 (13%)
81	MLZ	B <sub>o</sub>	53	81	8,9,10	0.48	0	4,9,11	0.09	0
39	PSU	B5	4374	39	18,21,22	1.35	2 (11%)	22,30,33	1.92	3 (13%)
39	OMU	B5	4244	39	19,22,23	1.21	2 (10%)	26,31,34	1.74	5 (19%)
39	OMG	B5	3942	11,39	18,26,27	0.92	1 (5%)	19,38,41	1.09	3 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
39	A2M	B5	3562	39	18,25,26	1.01	1 (5%)	18,36,39	1.24	2 (11%)
1	OMG	A2	1448	1	18,26,27	0.92	1 (5%)	19,38,41	1.08	2 (10%)
39	PSU	B5	4039	39	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
1	OMC	A2	463	1	19,22,23	0.81	0	26,31,34	0.82	0
1	A2M	A2	1679	1	18,25,26	1.02	1 (5%)	18,36,39	1.24	2 (11%)
1	PSU	A2	967	1	18,21,22	1.35	2 (11%)	22,30,33	1.89	3 (13%)
1	A2M	A2	1032	1	18,25,26	1.01	1 (5%)	18,36,39	1.26	2 (11%)
1	PSU	A2	687	1	18,21,22	1.33	2 (11%)	22,30,33	1.89	3 (13%)
1	PSU	A2	816	1	18,21,22	1.34	2 (11%)	22,30,33	1.89	3 (13%)
1	PSU	A2	36	1	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)
1	MA6	A2	1852	1	19,26,27	0.95	1 (5%)	18,38,41	1.46	3 (16%)
1	A2M	A2	591	1	18,25,26	1.05	1 (5%)	18,36,39	1.21	2 (11%)
39	A2M	B5	2244	90,39	18,25,26	1.01	1 (5%)	18,36,39	1.22	2 (11%)
1	PSU	A2	867	1	18,21,22	1.35	2 (11%)	22,30,33	1.89	3 (13%)
1	MA6	A2	1851	1	19,26,27	0.95	1 (5%)	18,38,41	1.61	3 (16%)
39	OMC	B5	4202	39	19,22,23	0.82	0	26,31,34	0.80	0
1	B8N	A2	1249	1	24,29,30	1.28	3 (12%)	29,42,45	1.30	3 (10%)
39	1MA	B5	1266	90,39	16,25,26	1.54	2 (12%)	18,37,40	1.06	3 (16%)
39	PSU	B5	3500	39	18,21,22	1.36	2 (11%)	22,30,33	1.86	3 (13%)
39	PSU	B5	4042	39	18,21,22	1.33	2 (11%)	22,30,33	1.92	3 (13%)
39	PSU	B5	4278	39	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
1	OMU	A2	172	1	19,22,23	1.19	2 (10%)	26,31,34	1.71	4 (15%)
1	PSU	A2	1626	1	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)
68	V5N	Ba	39	68	4,11,12	0.77	0	5,14,16	1.54	1 (20%)
41	PSU	B8	69	41	18,21,22	1.36	2 (11%)	22,30,33	1.92	3 (13%)
39	PSU	B5	3652	90,39	18,21,22	1.36	2 (11%)	22,30,33	1.88	3 (13%)
39	OMG	B5	3359	39	18,26,27	0.93	1 (5%)	19,38,41	1.13	2 (10%)
39	OMC	B5	3433	39	19,22,23	0.80	0	26,31,34	0.80	0
1	PSU	A2	802	1	18,21,22	1.34	2 (11%)	22,30,33	1.89	3 (13%)
39	OMU	B5	4052	39	19,22,23	1.24	3 (15%)	26,31,34	1.69	5 (19%)
39	PSU	B5	1721	39	18,21,22	1.35	2 (11%)	22,30,33	1.90	4 (18%)
39	OMG	B5	2267	39	18,26,27	0.92	1 (5%)	19,38,41	1.06	2 (10%)
39	PSU	B5	3496	39	18,21,22	1.34	2 (11%)	22,30,33	1.92	4 (18%)
1	PSU	A2	93	1	18,21,22	1.36	2 (11%)	22,30,33	1.87	3 (13%)
1	A2M	A2	669	90,1	18,25,26	0.97	1 (5%)	18,36,39	1.32	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
39	PSU	B5	1632	39	18,21,22	1.35	2 (11%)	22,30,33	1.89	4 (18%)
39	PSU	B5	4099	39	18,21,22	1.34	2 (11%)	22,30,33	1.91	3 (13%)
39	PSU	B5	4169	39	18,21,22	1.34	2 (11%)	22,30,33	1.86	3 (13%)
1	OMU	A2	355	1	19,22,23	1.22	2 (10%)	26,31,34	1.73	4 (15%)
39	PSU	B5	3466	39	18,21,22	1.33	2 (11%)	22,30,33	1.89	4 (18%)
39	OMU	B5	3973	39	19,22,23	1.24	3 (15%)	26,31,34	1.69	4 (15%)
1	G7M	A2	1640	11,1	20,26,27	2.62	4 (20%)	17,39,42	0.93	1 (5%)
1	PSU	A2	34	1	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
39	PSU	B5	3502	39	18,21,22	1.34	2 (11%)	22,30,33	1.89	3 (13%)
39	PSU	B5	4740	39	18,21,22	1.36	2 (11%)	22,30,33	1.89	3 (13%)
39	PSU	B5	1537	39	18,21,22	1.36	2 (11%)	22,30,33	1.88	3 (13%)
39	OMC	B5	3573	39	19,22,23	0.80	0	26,31,34	0.82	0
1	A2M	A2	99	90,1	18,25,26	1.04	1 (5%)	18,36,39	1.25	2 (11%)
1	A2M	A2	1384	1	18,25,26	1.02	1 (5%)	18,36,39	1.20	2 (11%)
39	OMG	B5	1477	39	18,26,27	0.94	1 (5%)	19,38,41	1.09	2 (10%)
39	OMC	B5	3601	39	19,22,23	0.82	0	26,31,34	0.76	0
1	A2M	A2	166	1	18,25,26	1.05	1 (5%)	18,36,39	1.28	2 (11%)
11	PSU	AT	65	11	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
39	OMC	B5	2647	39	19,22,23	0.81	0	26,31,34	0.81	0
1	OMU	A2	628	1	19,22,23	1.18	2 (10%)	26,31,34	1.71	5 (19%)
39	A2M	B5	2630	90,39	18,25,26	0.96	1 (5%)	18,36,39	1.34	2 (11%)
39	PSU	B5	1683	39	18,21,22	1.33	2 (11%)	22,30,33	1.90	3 (13%)
1	PSU	A2	407	1	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
39	OMU	B5	4366	39	19,22,23	1.24	4 (21%)	26,31,34	1.75	4 (15%)
1	A2M	A2	159	1	18,25,26	1.02	1 (5%)	18,36,39	1.39	2 (11%)
1	OMU	A2	1327	90,1	19,22,23	1.20	2 (10%)	26,31,34	1.71	5 (19%)
39	PSU	B5	1801	39	18,21,22	1.34	2 (11%)	22,30,33	1.92	4 (18%)
1	PSU	A2	650	1	18,21,22	1.34	2 (11%)	22,30,33	1.90	4 (18%)
39	PSU	B5	1731	39	18,21,22	1.35	2 (11%)	22,30,33	1.89	3 (13%)
39	PSU	B5	3447	39	18,21,22	1.36	2 (11%)	22,30,33	1.91	3 (13%)
1	PSU	A2	1175	1	18,21,22	1.36	2 (11%)	22,30,33	1.93	3 (13%)
1	PSU	A2	815	1	18,21,22	1.33	2 (11%)	22,30,33	1.87	3 (13%)
1	A2M	A2	27	90,1	18,25,26	1.02	1 (5%)	18,36,39	1.23	2 (11%)
31	NMM	As	67	31	9,11,12	0.59	0	6,12,14	0.39	0
39	OMU	B5	2680	39	19,22,23	1.23	2 (10%)	26,31,34	1.75	5 (19%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	PSU	A2	1245	1	18,21,22	1.33	2 (11%)	22,30,33	1.90	3 (13%)
39	PSU	B5	4246	39	18,21,22	1.34	2 (11%)	22,30,33	1.92	3 (13%)
1	OMC	A2	174	90,1	19,22,23	0.82	0	26,31,34	0.80	0
11	5MU	AT	64	11	19,22,23	1.42	5 (26%)	28,32,35	2.02	5 (17%)
39	PSU	B5	3576	39	18,21,22	1.36	2 (11%)	22,30,33	1.88	3 (13%)
1	PSU	A2	218	1	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)
39	A2M	B5	1270	39	18,25,26	0.95	1 (5%)	18,36,39	1.26	2 (11%)
39	OMG	B5	4240	39	18,26,27	0.94	1 (5%)	19,38,41	1.08	2 (10%)
1	OMG	A2	1329	1	18,26,27	0.94	1 (5%)	19,38,41	1.10	2 (10%)
39	A2M	B5	3599	39	18,25,26	0.99	1 (5%)	18,36,39	1.22	2 (11%)
39	A2M	B5	3450	39	18,25,26	1.02	1 (5%)	18,36,39	1.21	2 (11%)
1	PSU	A2	682	1	18,21,22	1.36	2 (11%)	22,30,33	1.89	3 (13%)
33	AME	Au	1	33	9,10,11	0.48	0	9,11,13	0.85	1 (11%)
39	PSU	B5	4107	39	18,21,22	1.37	2 (11%)	22,30,33	1.88	3 (13%)
39	A2M	B5	4317	39	18,25,26	1.01	1 (5%)	18,36,39	1.27	2 (11%)
1	PSU	A2	1057	1	18,21,22	1.34	2 (11%)	22,30,33	1.89	3 (13%)
39	PSU	B5	4267	90,39	18,21,22	1.35	2 (11%)	22,30,33	1.94	4 (18%)
39	A2M	B5	3517	39	18,25,26	0.92	1 (5%)	18,36,39	1.38	2 (11%)
1	OMG	A2	437	1	18,26,27	0.92	1 (5%)	19,38,41	1.09	2 (10%)
1	4AC	A2	1843	1	21,24,25	1.11	2 (9%)	29,34,37	1.21	3 (10%)
39	PSU	B5	2351	39	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
1	PSU	A2	573	1	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
1	PSU	A2	1046	1	18,21,22	1.35	2 (11%)	22,30,33	1.90	3 (13%)
39	OMU	B5	3657	39	19,22,23	1.23	2 (10%)	26,31,34	1.74	5 (19%)
1	PSU	A2	1693	1	18,21,22	1.37	2 (11%)	22,30,33	1.88	3 (13%)
39	UY1	B5	3550	39	19,22,23	1.36	3 (15%)	22,31,34	1.96	5 (22%)
39	PSU	B5	3585	90,39	18,21,22	1.36	2 (11%)	22,30,33	1.86	3 (13%)
43	HIC	BB	245	43	8,11,12	0.88	0	6,14,16	0.84	0
1	OMU	A2	1289	1	19,22,23	1.22	3 (15%)	26,31,34	1.66	4 (15%)
39	OMG	B5	1260	39	18,26,27	0.93	1 (5%)	19,38,41	1.17	2 (10%)
39	A2M	B5	4336	39	18,25,26	1.02	1 (5%)	18,36,39	1.20	2 (11%)
39	OMU	B5	2258	39	19,22,23	1.21	3 (15%)	26,31,34	1.68	4 (15%)
35	HY3	Aw	62	35	6,8,9	2.13	1 (16%)	5,10,12	1.12	1 (20%)
12	SAC	AZ	2	12	7,8,9	0.53	0	8,9,11	0.86	1 (12%)
1	OMC	A2	518	1	19,22,23	0.81	0	26,31,34	0.81	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
39	PSU	B5	3583	39	18,21,22	1.35	2 (11%)	22,30,33	1.91	3 (13%)
39	PSU	B5	4217	39	18,21,22	1.36	2 (11%)	22,30,33	1.86	3 (13%)
39	OMC	B5	3619	39	19,22,23	0.81	0	26,31,34	0.78	0
39	PSU	B5	4419	39	18,21,22	1.35	2 (11%)	22,30,33	1.90	3 (13%)
39	A2M	B5	3492	39	18,25,26	1.03	1 (5%)	18,36,39	1.33	2 (11%)
1	PSU	A2	105	1	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
1	OMG	A2	684	1	18,26,27	0.92	1 (5%)	19,38,41	1.12	2 (10%)
39	OMG	B5	4116	39	18,26,27	0.94	1 (5%)	19,38,41	1.07	2 (10%)
39	A2M	B5	3456	39	18,25,26	1.03	1 (5%)	18,36,39	1.22	2 (11%)
39	6MZ	B5	3966	39	18,25,26	0.86	1 (5%)	16,36,39	2.19	4 (25%)
1	OMU	A2	116	1	19,22,23	1.19	2 (10%)	26,31,34	1.69	5 (19%)
39	PSU	B5	3369	39	18,21,22	1.35	2 (11%)	22,30,33	1.90	4 (18%)
39	OMG	B5	3974	39	18,26,27	0.89	1 (5%)	19,38,41	1.12	2 (10%)
39	PSU	B5	4045	39	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)
1	PSU	A2	210	1	18,21,22	1.34	2 (11%)	22,30,33	1.85	3 (13%)
1	A2M	A2	469	1	18,25,26	1.02	1 (5%)	18,36,39	1.24	2 (11%)
1	A2M	A2	513	1	18,25,26	1.01	1 (5%)	18,36,39	1.19	2 (11%)
39	OMG	B5	3631	39	18,26,27	0.94	1 (5%)	19,38,41	1.09	2 (10%)
39	OMG	B5	3524	39	18,26,27	0.93	1 (5%)	19,38,41	1.07	2 (10%)
39	PSU	B5	4749	39	18,21,22	1.34	2 (11%)	22,30,33	1.91	3 (13%)
1	PSU	A2	823	1	18,21,22	1.36	2 (11%)	22,30,33	1.91	4 (18%)
39	A2M	B5	3557	39	18,25,26	1.01	1 (5%)	18,36,39	1.20	2 (11%)
1	A2M	A2	577	1	18,25,26	1.01	1 (5%)	18,36,39	1.22	2 (11%)
39	PSU	B5	2475	39	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
1	OMG	A2	602	1	18,26,27	0.93	1 (5%)	19,38,41	1.07	2 (10%)
39	PSU	B5	3554	39	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
1	OMG	A2	1491	90,1	18,26,27	0.92	1 (5%)	19,38,41	1.08	2 (10%)
39	OMG	B5	3476	39	18,26,27	0.93	1 (5%)	19,38,41	1.09	2 (10%)
39	A2M	B5	398	39	18,25,26	1.01	1 (5%)	18,36,39	1.25	2 (11%)
39	PSU	B5	4177	39	18,21,22	1.35	2 (11%)	22,30,33	1.89	3 (13%)
41	OMG	B8	75	41	18,26,27	0.94	1 (5%)	19,38,41	1.08	2 (10%)
42	V5N	BA	216	42	4,11,12	0.77	0	5,14,16	1.54	1 (20%)
1	6MZ	A2	1833	90,1	18,25,26	0.92	1 (5%)	16,36,39	1.77	4 (25%)
39	A2M	B5	2658	39	18,25,26	1.01	1 (5%)	18,36,39	1.23	2 (11%)
39	OMC	B5	2667	39	19,22,23	0.81	0	26,31,34	0.84	1 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
39	OMG	B5	4138	39	18,26,27	0.92	1 (5%)	19,38,41	1.10	2 (10%)
1	PSU	A2	1368	1	18,21,22	1.34	2 (11%)	22,30,33	1.90	3 (13%)
1	OMG	A2	510	90,1	18,26,27	0.94	1 (5%)	19,38,41	1.08	2 (10%)
39	PSU	B5	1718	39	18,21,22	1.33	2 (11%)	22,30,33	1.88	3 (13%)
1	PSU	A2	652	1	18,21,22	1.35	2 (11%)	22,30,33	1.92	4 (18%)
1	PSU	A2	1644	90,1	18,21,22	1.34	2 (11%)	22,30,33	1.86	3 (13%)
1	4AC	A2	1338	1	21,24,25	1.06	1 (4%)	29,34,37	1.27	3 (10%)
1	PSU	A2	1082	1	18,21,22	1.36	2 (11%)	22,30,33	1.86	3 (13%)
39	5MC	B5	3514	90,39	18,22,23	0.96	2 (11%)	26,32,35	1.20	3 (11%)
39	OMC	B5	2704	39	19,22,23	0.81	0	26,31,34	0.77	0
39	OMG	B5	4245	39	18,26,27	0.93	1 (5%)	19,38,41	1.05	2 (10%)
39	PSU	B5	4435	39	18,21,22	1.36	2 (11%)	22,30,33	1.94	3 (13%)
39	OMG	B5	1580	39	18,26,27	0.94	1 (5%)	19,38,41	1.08	2 (10%)
1	OMG	A2	868	1	18,26,27	0.95	1 (5%)	19,38,41	1.08	2 (10%)
1	OMG	A2	645	1	18,26,27	0.93	1 (5%)	19,38,41	1.10	2 (10%)
1	PSU	A2	1348	1	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
39	OMC	B5	1820	90,39	19,22,23	0.80	0	26,31,34	0.83	0
39	PSU	B5	4058	39	18,21,22	1.36	2 (11%)	22,30,33	1.91	3 (13%)
1	OMC	A2	1704	1	19,22,23	0.81	0	26,31,34	0.84	1 (3%)
1	PSU	A2	1239	1	18,21,22	1.36	2 (11%)	22,30,33	1.89	3 (13%)
39	PSU	B5	1799	39	18,21,22	1.36	2 (11%)	22,30,33	1.93	3 (13%)
39	OMC	B5	4282	39	19,22,23	0.82	0	26,31,34	0.82	0
39	OMG	B5	2207	39	18,26,27	0.93	1 (5%)	19,38,41	1.08	2 (10%)
39	OMG	B5	4364	39	18,26,27	0.93	1 (5%)	19,38,41	1.10	2 (10%)
39	PSU	B5	4711	39	18,21,22	1.34	2 (11%)	22,30,33	1.89	4 (18%)
80	M3L	Bm	98	80	10,11,12	0.82	0	9,14,16	0.47	0
1	PSU	A2	119	1	18,21,22	1.35	2 (11%)	22,30,33	1.86	3 (13%)
1	PSU	A2	1178	1	18,21,22	1.35	2 (11%)	22,30,33	1.90	3 (13%)
39	UR3	B5	4276	39	19,22,23	0.99	0	26,32,35	1.43	1 (3%)
39	A2M	B5	1479	39	18,25,26	1.02	1 (5%)	18,36,39	1.26	2 (11%)
39	PSU	B5	1491	39	18,21,22	1.35	2 (11%)	22,30,33	1.89	3 (13%)
1	OMU	A2	1805	1	19,22,23	1.23	3 (15%)	26,31,34	1.71	4 (15%)
39	PSU	B5	4203	39	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)
39	OMG	B5	3676	39	18,26,27	0.92	1 (5%)	19,38,41	1.11	2 (10%)
39	PSU	B5	4322	39	18,21,22	1.35	2 (11%)	22,30,33	1.89	3 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
39	A2M	B5	400	39	18,25,26	1.00	1 (5%)	18,36,39	1.22	2 (11%)
39	PSU	B5	3427	39	18,21,22	1.37	2 (11%)	22,30,33	1.89	3 (13%)
1	A2M	A2	485	1	18,25,26	1.02	1 (5%)	18,36,39	1.22	2 (11%)
39	PSU	B5	4149	39	18,21,22	1.36	2 (11%)	22,30,33	1.94	4 (18%)
1	OMU	A2	429	1	19,22,23	1.19	2 (10%)	26,31,34	1.70	5 (19%)
39	OMC	B5	2208	90,39	19,22,23	0.82	0	26,31,34	0.79	0
39	OMC	B5	2265	90,39	19,22,23	0.82	0	26,31,34	0.88	1 (3%)
39	OMG	B5	4383	39	18,26,27	0.94	1 (5%)	19,38,41	1.08	2 (10%)
1	OMU	A2	121	1	19,22,23	1.23	3 (15%)	26,31,34	1.70	4 (15%)
1	OMU	A2	1443	90,1	19,22,23	1.23	2 (10%)	26,31,34	1.70	4 (15%)
30	SAC	Ar	2	30	7,8,9	0.54	0	8,9,11	0.92	1 (12%)
39	PSU	B5	4382	39	18,21,22	1.33	2 (11%)	22,30,33	1.88	3 (13%)
39	5MC	B5	4193	39	18,22,23	0.98	2 (11%)	26,32,35	1.19	2 (7%)
39	PSU	B5	1638	39	18,21,22	1.36	2 (11%)	22,30,33	1.94	3 (13%)
39	A2M	B5	2206	90,39	18,25,26	1.00	1 (5%)	18,36,39	1.22	2 (11%)
39	PSU	B5	3462	39	18,21,22	1.34	2 (11%)	22,30,33	1.91	3 (13%)
39	PSU	B5	3494	39	18,21,22	1.38	2 (11%)	22,30,33	1.89	3 (13%)
39	OMC	B5	2194	90,39	19,22,23	0.82	0	26,31,34	0.92	2 (7%)
39	OMG	B5	4369	39	18,26,27	0.94	1 (5%)	19,38,41	1.12	2 (10%)
41	PSU	B8	55	41	18,21,22	1.34	2 (11%)	22,30,33	1.91	4 (18%)
39	OMG	B5	2719	39	18,26,27	0.92	1 (5%)	19,38,41	1.07	2 (10%)
39	PSU	B5	4298	39	18,21,22	1.34	2 (11%)	22,30,33	1.92	3 (13%)
83	SAC	Br	2	83	7,8,9	0.53	0	8,9,11	0.82	1 (12%)
39	A2M	B5	1489	90,39	18,25,26	1.00	1 (5%)	18,36,39	1.33	2 (11%)
39	PSU	B5	3371	39	18,21,22	1.37	2 (11%)	22,30,33	1.89	3 (13%)
39	OMC	B5	1284	39	19,22,23	0.83	0	26,31,34	0.80	0
69	MLZ	Bb	5	69	8,9,10	0.49	0	4,9,11	0.24	0
44	AYA	BC	2	44	6,7,8	0.76	0	5,8,10	0.28	0
1	PSU	A2	1047	1	18,21,22	1.36	2 (11%)	22,30,33	1.89	3 (13%)
39	OMC	B5	3540	39	19,22,23	0.82	0	26,31,34	0.84	1 (3%)
1	PSU	A2	109	1	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
1	OMC	A2	1392	1	19,22,23	0.82	0	26,31,34	0.88	1 (3%)
1	PSU	A2	1005	1	18,21,22	1.33	2 (11%)	22,30,33	1.87	3 (13%)
1	PSU	A2	1233	1	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)

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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	PSU	B5	3616	39	-	0/7/25/26	0/2/2/2
39	PSU	B5	1720	39	-	0/7/25/26	0/2/2/2
1	PSU	A2	1446	1	-	0/7/25/26	0/2/2/2
39	PSU	B5	4188	39	-	0/7/25/26	0/2/2/2
39	PSU	B5	4325	39	-	0/7/25/26	0/2/2/2
39	A2M	B5	1810	90,39	-	2/5/27/28	0/3/3/3
39	PSU	B5	4166	39	-	1/7/25/26	0/2/2/2
39	PSU	B5	3490	39	-	0/7/25/26	0/2/2/2
39	A2M	B5	4269	90,39	-	2/5/27/28	0/3/3/3
1	PSU	A2	864	1	-	0/7/25/26	0/2/2/2
81	MLZ	Bo	53	81	-	0/7/8/10	-
39	PSU	B5	4374	39	-	0/7/25/26	0/2/2/2
39	OMU	B5	4244	39	-	0/9/27/28	0/2/2/2
39	OMG	B5	3942	11,39	-	0/5/27/28	0/3/3/3
39	A2M	B5	3562	39	-	0/5/27/28	0/3/3/3
1	OMG	A2	1448	1	-	3/5/27/28	0/3/3/3
39	PSU	B5	4039	39	-	0/7/25/26	0/2/2/2
1	OMC	A2	463	1	-	0/9/27/28	0/2/2/2
1	A2M	A2	1679	1	-	0/5/27/28	0/3/3/3
1	PSU	A2	967	1	-	0/7/25/26	0/2/2/2
1	A2M	A2	1032	1	-	0/5/27/28	0/3/3/3
1	PSU	A2	687	1	-	0/7/25/26	0/2/2/2
1	PSU	A2	816	1	-	0/7/25/26	0/2/2/2
1	PSU	A2	36	1	-	0/7/25/26	0/2/2/2
1	MA6	A2	1852	1	-	1/7/29/30	0/3/3/3
1	A2M	A2	591	1	-	0/5/27/28	0/3/3/3
39	A2M	B5	2244	90,39	-	0/5/27/28	0/3/3/3
1	PSU	A2	867	1	-	0/7/25/26	0/2/2/2
1	MA6	A2	1851	1	-	0/7/29/30	0/3/3/3
39	OMC	B5	4202	39	-	0/9/27/28	0/2/2/2
1	B8N	A2	1249	1	-	4/16/34/35	0/2/2/2
39	1MA	B5	1266	90,39	-	0/3/25/26	0/3/3/3
39	PSU	B5	3500	39	-	0/7/25/26	0/2/2/2
39	PSU	B5	4042	39	-	0/7/25/26	0/2/2/2
39	PSU	B5	4278	39	-	2/7/25/26	0/2/2/2
1	OMU	A2	172	1	-	0/9/27/28	0/2/2/2
1	PSU	A2	1626	1	-	0/7/25/26	0/2/2/2
68	V5N	Ba	39	68	-	0/5/10/12	0/1/1/1
41	PSU	B8	69	41	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	PSU	B5	3652	90,39	-	0/7/25/26	0/2/2/2
39	OMG	B5	3359	39	-	0/5/27/28	0/3/3/3
39	OMC	B5	3433	39	-	4/9/27/28	0/2/2/2
1	PSU	A2	802	1	-	0/7/25/26	0/2/2/2
39	OMU	B5	4052	39	-	0/9/27/28	0/2/2/2
39	PSU	B5	1721	39	-	0/7/25/26	0/2/2/2
39	OMG	B5	2267	39	-	0/5/27/28	0/3/3/3
39	PSU	B5	3496	39	-	0/7/25/26	0/2/2/2
1	PSU	A2	93	1	-	0/7/25/26	0/2/2/2
1	A2M	A2	669	90,1	-	2/5/27/28	0/3/3/3
39	PSU	B5	1632	39	-	3/7/25/26	0/2/2/2
39	PSU	B5	4099	39	-	0/7/25/26	0/2/2/2
39	PSU	B5	4169	39	-	0/7/25/26	0/2/2/2
1	OMU	A2	355	1	-	0/9/27/28	0/2/2/2
39	PSU	B5	3466	39	-	0/7/25/26	0/2/2/2
39	OMU	B5	3973	39	-	1/9/27/28	0/2/2/2
1	G7M	A2	1640	11,1	-	0/3/25/26	0/3/3/3
1	PSU	A2	34	1	-	0/7/25/26	0/2/2/2
39	PSU	B5	3502	39	-	0/7/25/26	0/2/2/2
39	PSU	B5	4740	39	-	0/7/25/26	0/2/2/2
39	PSU	B5	1537	39	-	0/7/25/26	0/2/2/2
39	OMC	B5	3573	39	-	0/9/27/28	0/2/2/2
1	A2M	A2	99	90,1	-	2/5/27/28	0/3/3/3
1	A2M	A2	1384	1	-	0/5/27/28	0/3/3/3
39	OMG	B5	1477	39	-	0/5/27/28	0/3/3/3
39	OMC	B5	3601	39	-	0/9/27/28	0/2/2/2
1	A2M	A2	166	1	-	0/5/27/28	0/3/3/3
11	PSU	AT	65	11	-	0/7/25/26	0/2/2/2
39	OMC	B5	2647	39	-	0/9/27/28	0/2/2/2
1	OMU	A2	628	1	-	3/9/27/28	0/2/2/2
39	A2M	B5	2630	90,39	-	0/5/27/28	0/3/3/3
39	PSU	B5	1683	39	-	0/7/25/26	0/2/2/2
1	PSU	A2	407	1	-	0/7/25/26	0/2/2/2
39	OMU	B5	4366	39	-	0/9/27/28	0/2/2/2
1	A2M	A2	159	1	-	1/5/27/28	0/3/3/3
1	OMU	A2	1327	90,1	-	0/9/27/28	0/2/2/2
39	PSU	B5	1801	39	-	0/7/25/26	0/2/2/2
1	PSU	A2	650	1	-	0/7/25/26	0/2/2/2
39	PSU	B5	1731	39	-	0/7/25/26	0/2/2/2
39	PSU	B5	3447	39	-	0/7/25/26	0/2/2/2
1	PSU	A2	1175	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	A2	815	1	-	0/7/25/26	0/2/2/2
1	A2M	A2	27	90,1	-	0/5/27/28	0/3/3/3
31	NMM	As	67	31	-	0/9/11/13	-
39	OMU	B5	2680	39	-	1/9/27/28	0/2/2/2
1	PSU	A2	1245	1	-	0/7/25/26	0/2/2/2
39	PSU	B5	4246	39	-	1/7/25/26	0/2/2/2
1	OMC	A2	174	90,1	-	0/9/27/28	0/2/2/2
11	5MU	AT	64	11	-	0/7/25/26	0/2/2/2
39	PSU	B5	3576	39	-	1/7/25/26	0/2/2/2
1	PSU	A2	218	1	-	0/7/25/26	0/2/2/2
39	A2M	B5	1270	39	-	0/5/27/28	0/3/3/3
39	OMG	B5	4240	39	-	0/5/27/28	0/3/3/3
1	OMG	A2	1329	1	-	0/5/27/28	0/3/3/3
39	A2M	B5	3599	39	-	2/5/27/28	0/3/3/3
39	A2M	B5	3450	39	-	1/5/27/28	0/3/3/3
1	PSU	A2	682	1	-	0/7/25/26	0/2/2/2
33	AME	Au	1	33	-	2/9/10/12	-
39	PSU	B5	4107	39	-	0/7/25/26	0/2/2/2
39	A2M	B5	4317	39	-	0/5/27/28	0/3/3/3
1	PSU	A2	1057	1	-	0/7/25/26	0/2/2/2
39	PSU	B5	4267	90,39	-	0/7/25/26	0/2/2/2
39	A2M	B5	3517	39	-	1/5/27/28	0/3/3/3
1	OMG	A2	437	1	-	0/5/27/28	0/3/3/3
1	4AC	A2	1843	1	-	2/11/29/30	0/2/2/2
39	PSU	B5	2351	39	-	0/7/25/26	0/2/2/2
1	PSU	A2	573	1	-	0/7/25/26	0/2/2/2
1	PSU	A2	1046	1	-	0/7/25/26	0/2/2/2
39	OMU	B5	3657	39	-	0/9/27/28	0/2/2/2
1	PSU	A2	1693	1	-	0/7/25/26	0/2/2/2
39	UY1	B5	3550	39	-	1/9/27/28	0/2/2/2
39	PSU	B5	3585	90,39	-	0/7/25/26	0/2/2/2
43	HIC	BB	245	43	-	1/5/6/8	0/1/1/1
1	OMU	A2	1289	1	-	2/9/27/28	0/2/2/2
39	OMG	B5	1260	39	-	1/5/27/28	0/3/3/3
39	A2M	B5	4336	39	-	1/5/27/28	0/3/3/3
39	OMU	B5	2258	39	-	0/9/27/28	0/2/2/2
35	HY3	Aw	62	35	-	1/1/12/14	0/1/1/1
12	SAC	AZ	2	12	-	1/7/8/10	-
1	OMC	A2	518	1	-	0/9/27/28	0/2/2/2
39	PSU	B5	3583	39	-	0/7/25/26	0/2/2/2
39	PSU	B5	4217	39	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	OMC	B5	3619	39	-	2/9/27/28	0/2/2/2
39	PSU	B5	4419	39	-	0/7/25/26	0/2/2/2
39	A2M	B5	3492	39	-	0/5/27/28	0/3/3/3
1	PSU	A2	105	1	-	0/7/25/26	0/2/2/2
1	OMG	A2	684	1	-	3/5/27/28	0/3/3/3
39	OMG	B5	4116	39	-	0/5/27/28	0/3/3/3
39	A2M	B5	3456	39	-	0/5/27/28	0/3/3/3
39	6MZ	B5	3966	39	-	0/5/27/28	0/3/3/3
1	OMU	A2	116	1	-	1/9/27/28	0/2/2/2
39	PSU	B5	3369	39	-	0/7/25/26	0/2/2/2
39	OMG	B5	3974	39	-	0/5/27/28	0/3/3/3
39	PSU	B5	4045	39	-	0/7/25/26	0/2/2/2
1	PSU	A2	210	1	-	0/7/25/26	0/2/2/2
1	A2M	A2	469	1	-	1/5/27/28	0/3/3/3
1	A2M	A2	513	1	-	2/5/27/28	0/3/3/3
39	OMG	B5	3631	39	-	1/5/27/28	0/3/3/3
39	OMG	B5	3524	39	-	0/5/27/28	0/3/3/3
39	PSU	B5	4749	39	-	0/7/25/26	0/2/2/2
1	PSU	A2	823	1	-	0/7/25/26	0/2/2/2
39	A2M	B5	3557	39	-	1/5/27/28	0/3/3/3
1	A2M	A2	577	1	-	2/5/27/28	0/3/3/3
39	PSU	B5	2475	39	-	0/7/25/26	0/2/2/2
1	OMG	A2	602	1	-	0/5/27/28	0/3/3/3
39	PSU	B5	3554	39	-	0/7/25/26	0/2/2/2
1	OMG	A2	1491	90,1	-	1/5/27/28	0/3/3/3
39	OMG	B5	3476	39	-	1/5/27/28	0/3/3/3
39	A2M	B5	398	39	-	2/5/27/28	0/3/3/3
39	PSU	B5	4177	39	-	0/7/25/26	0/2/2/2
41	OMG	B8	75	41	-	1/5/27/28	0/3/3/3
42	V5N	BA	216	42	-	1/5/10/12	0/1/1/1
1	6MZ	A2	1833	90,1	-	1/5/27/28	0/3/3/3
39	A2M	B5	2658	39	-	2/5/27/28	0/3/3/3
39	OMC	B5	2667	39	-	1/9/27/28	0/2/2/2
39	OMG	B5	4138	39	-	0/5/27/28	0/3/3/3
1	PSU	A2	1368	1	-	0/7/25/26	0/2/2/2
1	OMG	A2	510	90,1	-	1/5/27/28	0/3/3/3
39	PSU	B5	1718	39	-	0/7/25/26	0/2/2/2
1	PSU	A2	652	1	-	0/7/25/26	0/2/2/2
1	PSU	A2	1644	90,1	-	0/7/25/26	0/2/2/2
1	4AC	A2	1338	1	-	4/11/29/30	0/2/2/2
1	PSU	A2	1082	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	5MC	B5	3514	90,39	-	0/7/25/26	0/2/2/2
39	OMC	B5	2704	39	-	0/9/27/28	0/2/2/2
39	OMG	B5	4245	39	-	0/5/27/28	0/3/3/3
39	PSU	B5	4435	39	-	0/7/25/26	0/2/2/2
39	OMG	B5	1580	39	-	0/5/27/28	0/3/3/3
1	OMG	A2	868	1	-	0/5/27/28	0/3/3/3
1	OMG	A2	645	1	-	3/5/27/28	0/3/3/3
1	PSU	A2	1348	1	-	0/7/25/26	0/2/2/2
39	OMC	B5	1820	90,39	-	1/9/27/28	0/2/2/2
39	PSU	B5	4058	39	-	0/7/25/26	0/2/2/2
1	OMC	A2	1704	1	-	2/9/27/28	0/2/2/2
1	PSU	A2	1239	1	-	0/7/25/26	0/2/2/2
39	PSU	B5	1799	39	-	0/7/25/26	0/2/2/2
39	OMC	B5	4282	39	-	0/9/27/28	0/2/2/2
39	OMG	B5	2207	39	-	2/5/27/28	0/3/3/3
39	OMG	B5	4364	39	-	0/5/27/28	0/3/3/3
39	PSU	B5	4711	39	-	0/7/25/26	0/2/2/2
80	M3L	Bm	98	80	-	0/9/10/12	-
1	PSU	A2	119	1	-	0/7/25/26	0/2/2/2
1	PSU	A2	1178	1	-	0/7/25/26	0/2/2/2
39	UR3	B5	4276	39	-	0/7/25/26	0/2/2/2
39	A2M	B5	1479	39	-	0/5/27/28	0/3/3/3
39	PSU	B5	1491	39	-	0/7/25/26	0/2/2/2
1	OMU	A2	1805	1	-	0/9/27/28	0/2/2/2
39	PSU	B5	4203	39	-	0/7/25/26	0/2/2/2
39	OMG	B5	3676	39	-	0/5/27/28	0/3/3/3
39	PSU	B5	4322	39	-	0/7/25/26	0/2/2/2
39	A2M	B5	400	39	-	0/5/27/28	0/3/3/3
39	PSU	B5	3427	39	-	0/7/25/26	0/2/2/2
1	A2M	A2	485	1	-	0/5/27/28	0/3/3/3
39	PSU	B5	4149	39	-	0/7/25/26	0/2/2/2
1	OMU	A2	429	1	-	6/9/27/28	0/2/2/2
39	OMC	B5	2208	90,39	-	0/9/27/28	0/2/2/2
39	OMC	B5	2265	90,39	-	1/9/27/28	0/2/2/2
39	OMG	B5	4383	39	-	1/5/27/28	0/3/3/3
1	OMU	A2	121	1	-	0/9/27/28	0/2/2/2
1	OMU	A2	1443	90,1	-	2/9/27/28	0/2/2/2
30	SAC	Ar	2	30	-	0/7/8/10	-
39	PSU	B5	4382	39	-	4/7/25/26	0/2/2/2
39	5MC	B5	4193	39	-	4/7/25/26	0/2/2/2
39	PSU	B5	1638	39	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	A2M	B5	2206	90,39	-	0/5/27/28	0/3/3/3
39	PSU	B5	3462	39	-	0/7/25/26	0/2/2/2
39	PSU	B5	3494	39	-	2/7/25/26	0/2/2/2
39	OMC	B5	2194	90,39	-	2/9/27/28	0/2/2/2
39	OMG	B5	4369	39	-	1/5/27/28	0/3/3/3
41	PSU	B8	55	41	-	0/7/25/26	0/2/2/2
39	OMG	B5	2719	39	-	0/5/27/28	0/3/3/3
39	PSU	B5	4298	39	-	0/7/25/26	0/2/2/2
83	SAC	Br	2	83	-	0/7/8/10	-
39	A2M	B5	1489	90,39	-	1/5/27/28	0/3/3/3
39	PSU	B5	3371	39	-	0/7/25/26	0/2/2/2
39	OMC	B5	1284	39	-	2/9/27/28	0/2/2/2
69	MLZ	Bb	5	69	-	2/7/8/10	-
44	AYA	BC	2	44	-	3/4/6/8	-
1	PSU	A2	1047	1	-	0/7/25/26	0/2/2/2
39	OMC	B5	3540	39	-	1/9/27/28	0/2/2/2
1	PSU	A2	109	1	-	0/7/25/26	0/2/2/2
1	OMC	A2	1392	1	-	0/9/27/28	0/2/2/2
1	PSU	A2	1005	1	-	0/7/25/26	0/2/2/2
1	PSU	A2	1233	1	-	0/7/25/26	0/2/2/2

All (326) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A2	1640	G7M	C8-N9	7.41	1.46	1.33
1	A2	1640	G7M	C8-N7	7.15	1.46	1.33
35	Aw	62	HY3	C3-CA	-4.91	1.50	1.55
39	B5	1266	1MA	C2-N3	4.72	1.34	1.29
1	A2	1640	G7M	C5-C4	4.29	1.47	1.39
39	B5	3550	UY1	C6-C5	3.59	1.39	1.35
1	A2	1175	PSU	C6-C5	3.27	1.39	1.35
1	A2	210	PSU	C6-C5	3.22	1.39	1.35
39	B5	1266	1MA	C6-N6	3.22	1.35	1.27
39	B5	3447	PSU	C6-C5	3.21	1.39	1.35
11	AT	65	PSU	C6-C5	3.20	1.39	1.35
39	B5	4166	PSU	C6-C5	3.19	1.39	1.35
39	B5	3500	PSU	C6-C5	3.16	1.39	1.35
1	A2	1239	PSU	C6-C5	3.16	1.39	1.35
1	A2	407	PSU	C6-C5	3.16	1.39	1.35
1	A2	573	PSU	C6-C5	3.15	1.39	1.35
39	B5	3494	PSU	C6-C5	3.15	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	B5	3462	PSU	C6-C5	3.14	1.39	1.35
1	A2	802	PSU	C6-C5	3.14	1.39	1.35
1	A2	967	PSU	C6-C5	3.13	1.39	1.35
39	B5	4107	PSU	C6-C5	3.13	1.39	1.35
39	B5	4740	PSU	C6-C5	3.13	1.39	1.35
1	A2	1178	PSU	C6-C5	3.13	1.39	1.35
39	B5	1799	PSU	C6-C5	3.12	1.39	1.35
1	A2	1047	PSU	C6-C5	3.12	1.39	1.35
1	A2	652	PSU	C6-C5	3.12	1.39	1.35
1	A2	109	PSU	C6-C5	3.12	1.39	1.35
39	B5	3496	PSU	C6-C5	3.11	1.38	1.35
1	A2	1046	PSU	C6-C5	3.11	1.38	1.35
1	A2	93	PSU	C6-C5	3.10	1.38	1.35
1	A2	823	PSU	C6-C5	3.10	1.38	1.35
1	A2	1005	PSU	C6-C5	3.10	1.38	1.35
39	B5	1731	PSU	C6-C5	3.10	1.38	1.35
39	B5	1721	PSU	C6-C5	3.10	1.38	1.35
39	B5	4322	PSU	C6-C5	3.10	1.38	1.35
39	B5	3502	PSU	C6-C5	3.10	1.38	1.35
39	B5	4278	PSU	C6-C5	3.09	1.38	1.35
1	A2	119	PSU	C6-C5	3.09	1.38	1.35
1	A2	1693	PSU	C6-C5	3.09	1.38	1.35
39	B5	2475	PSU	C6-C5	3.09	1.38	1.35
1	A2	1249	B8N	C4-N3	-3.09	1.34	1.40
39	B5	4711	PSU	C6-C5	3.09	1.38	1.35
39	B5	4169	PSU	C6-C5	3.09	1.38	1.35
1	A2	815	PSU	C6-C5	3.09	1.38	1.35
39	B5	4217	PSU	C6-C5	3.09	1.38	1.35
1	A2	105	PSU	C6-C5	3.08	1.38	1.35
1	A2	1446	PSU	C6-C5	3.08	1.38	1.35
1	A2	218	PSU	C6-C5	3.08	1.38	1.35
1	A2	36	PSU	C6-C5	3.08	1.38	1.35
1	A2	867	PSU	C6-C5	3.08	1.38	1.35
1	A2	34	PSU	C6-C5	3.07	1.38	1.35
1	A2	650	PSU	C6-C5	3.07	1.38	1.35
1	A2	816	PSU	C6-C5	3.07	1.38	1.35
1	A2	864	PSU	C6-C5	3.07	1.38	1.35
39	B5	3427	PSU	C6-C5	3.07	1.38	1.35
1	A2	1368	PSU	C6-C5	3.06	1.38	1.35
39	B5	1718	PSU	C6-C5	3.06	1.38	1.35
39	B5	4749	PSU	C6-C5	3.06	1.38	1.35
1	A2	1626	PSU	C6-C5	3.06	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	B5	1683	PSU	C6-C5	3.06	1.38	1.35
41	B8	69	PSU	C6-C5	3.06	1.38	1.35
41	B8	55	PSU	C6-C5	3.06	1.38	1.35
1	A2	682	PSU	C6-C5	3.05	1.38	1.35
39	B5	4099	PSU	C6-C5	3.05	1.38	1.35
39	B5	4325	PSU	C6-C5	3.05	1.38	1.35
39	B5	4435	PSU	C6-C5	3.05	1.38	1.35
1	A2	1233	PSU	C6-C5	3.05	1.38	1.35
1	A2	1644	PSU	C6-C5	3.05	1.38	1.35
1	A2	1348	PSU	C6-C5	3.05	1.38	1.35
39	B5	4419	PSU	C6-C5	3.04	1.38	1.35
39	B5	4045	PSU	C6-C5	3.04	1.38	1.35
39	B5	4039	PSU	C6-C5	3.04	1.38	1.35
39	B5	3466	PSU	C6-C5	3.04	1.38	1.35
39	B5	4382	PSU	C6-C5	3.04	1.38	1.35
39	B5	1720	PSU	C6-C5	3.04	1.38	1.35
1	A2	1082	PSU	C6-C5	3.03	1.38	1.35
39	B5	3576	PSU	C6-C5	3.03	1.38	1.35
39	B5	4246	PSU	C6-C5	3.03	1.38	1.35
39	B5	4267	PSU	C6-C5	3.03	1.38	1.35
39	B5	1638	PSU	C6-C5	3.03	1.38	1.35
1	A2	1057	PSU	C6-C5	3.03	1.38	1.35
39	B5	3490	PSU	C6-C5	3.03	1.38	1.35
39	B5	1632	PSU	C6-C5	3.03	1.38	1.35
1	A2	687	PSU	C6-C5	3.02	1.38	1.35
39	B5	3616	PSU	C6-C5	3.02	1.38	1.35
39	B5	3554	PSU	C6-C5	3.02	1.38	1.35
39	B5	1537	PSU	C6-C5	3.02	1.38	1.35
39	B5	3371	PSU	C6-C5	3.01	1.38	1.35
1	A2	1245	PSU	C6-C5	3.01	1.38	1.35
39	B5	4058	PSU	C6-C5	3.01	1.38	1.35
39	B5	4042	PSU	C6-C5	3.00	1.38	1.35
39	B5	4188	PSU	C6-C5	3.00	1.38	1.35
39	B5	4203	PSU	C6-C5	3.00	1.38	1.35
39	B5	2351	PSU	C6-C5	2.99	1.38	1.35
39	B5	1491	PSU	C6-C5	2.98	1.38	1.35
39	B5	1801	PSU	C6-C5	2.98	1.38	1.35
39	B5	3369	PSU	C6-C5	2.98	1.38	1.35
39	B5	4177	PSU	C6-C5	2.98	1.38	1.35
39	B5	4298	PSU	C6-C5	2.98	1.38	1.35
39	B5	3583	PSU	C6-C5	2.98	1.38	1.35
39	B5	4374	PSU	C6-C5	2.98	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A2	1249	B8N	C6-C5	2.97	1.39	1.34
39	B5	3585	PSU	C6-C5	2.97	1.38	1.35
39	B5	3652	PSU	C6-C5	2.95	1.38	1.35
1	A2	1843	4AC	C4-N4	-2.95	1.35	1.39
39	B5	4149	PSU	C6-C5	2.92	1.38	1.35
1	A2	1338	4AC	C4-N4	-2.85	1.35	1.39
39	B5	3652	PSU	C4-N3	-2.84	1.33	1.38
39	B5	3616	PSU	C4-N3	-2.82	1.33	1.38
39	B5	3369	PSU	C4-N3	-2.81	1.33	1.38
39	B5	3371	PSU	C4-N3	-2.81	1.33	1.38
39	B5	4149	PSU	C4-N3	-2.80	1.33	1.38
39	B5	3427	PSU	C4-N3	-2.78	1.33	1.38
39	B5	1491	PSU	C4-N3	-2.78	1.33	1.38
41	B8	69	PSU	C4-N3	-2.77	1.33	1.38
39	B5	1801	PSU	C4-N3	-2.77	1.33	1.38
39	B5	4267	PSU	C4-N3	-2.77	1.33	1.38
39	B5	3576	PSU	C4-N3	-2.77	1.33	1.38
39	B5	4203	PSU	C4-N3	-2.77	1.33	1.38
1	A2	1082	PSU	C4-N3	-2.76	1.33	1.38
39	B5	3585	PSU	C4-N3	-2.76	1.33	1.38
39	B5	4039	PSU	C4-N3	-2.76	1.33	1.38
39	B5	4435	PSU	C4-N3	-2.75	1.33	1.38
39	B5	4177	PSU	C4-N3	-2.75	1.33	1.38
39	B5	2351	PSU	C4-N3	-2.75	1.33	1.38
39	B5	4298	PSU	C4-N3	-2.75	1.33	1.38
1	A2	867	PSU	C4-N3	-2.74	1.33	1.38
39	B5	4188	PSU	C4-N3	-2.74	1.33	1.38
1	A2	105	PSU	C4-N3	-2.74	1.33	1.38
39	B5	1721	PSU	C4-N3	-2.74	1.33	1.38
1	A2	1693	PSU	C4-N3	-2.74	1.33	1.38
39	B5	4107	PSU	C4-N3	-2.74	1.33	1.38
39	B5	1638	PSU	C4-N3	-2.73	1.33	1.38
1	A2	1046	PSU	C4-N3	-2.73	1.33	1.38
39	B5	3500	PSU	C4-N3	-2.73	1.33	1.38
39	B5	4058	PSU	C4-N3	-2.73	1.33	1.38
1	A2	652	PSU	C4-N3	-2.72	1.33	1.38
11	AT	64	5MU	C6-C5	2.72	1.39	1.34
39	B5	1720	PSU	C4-N3	-2.72	1.33	1.38
39	B5	1731	PSU	C4-N3	-2.72	1.33	1.38
1	A2	407	PSU	C4-N3	-2.72	1.33	1.38
39	B5	4193	5MC	C6-C5	2.72	1.39	1.34
39	B5	4740	PSU	C4-N3	-2.72	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	B5	1799	PSU	C4-N3	-2.72	1.33	1.38
1	A2	682	PSU	C4-N3	-2.72	1.33	1.38
39	B5	4322	PSU	C4-N3	-2.72	1.33	1.38
39	B5	3496	PSU	C4-N3	-2.71	1.33	1.38
1	A2	93	PSU	C4-N3	-2.71	1.33	1.38
39	B5	2475	PSU	C4-N3	-2.71	1.33	1.38
39	B5	4382	PSU	C4-N3	-2.71	1.33	1.38
41	B8	55	PSU	C4-N3	-2.71	1.33	1.38
1	A2	1368	PSU	C4-N3	-2.71	1.33	1.38
1	A2	218	PSU	C4-N3	-2.70	1.33	1.38
1	A2	864	PSU	C4-N3	-2.70	1.33	1.38
39	B5	3583	PSU	C4-N3	-2.70	1.33	1.38
39	B5	4419	PSU	C4-N3	-2.70	1.33	1.38
39	B5	4099	PSU	C4-N3	-2.70	1.33	1.38
1	A2	1245	PSU	C4-N3	-2.70	1.33	1.38
39	B5	3466	PSU	C4-N3	-2.70	1.33	1.38
39	B5	1537	PSU	C4-N3	-2.70	1.33	1.38
1	A2	1047	PSU	C4-N3	-2.70	1.33	1.38
1	A2	650	PSU	C4-N3	-2.70	1.33	1.38
1	A2	1233	PSU	C4-N3	-2.70	1.33	1.38
39	B5	4217	PSU	C4-N3	-2.70	1.33	1.38
39	B5	3554	PSU	C4-N3	-2.69	1.33	1.38
1	A2	1446	PSU	C4-N3	-2.69	1.33	1.38
39	B5	4711	PSU	C4-N3	-2.69	1.33	1.38
39	B5	4374	PSU	C4-N3	-2.69	1.33	1.38
39	B5	4042	PSU	C4-N3	-2.69	1.33	1.38
39	B5	4325	PSU	C4-N3	-2.69	1.33	1.38
1	A2	34	PSU	C4-N3	-2.68	1.33	1.38
1	A2	815	PSU	C4-N3	-2.68	1.33	1.38
1	A2	1057	PSU	C4-N3	-2.68	1.33	1.38
11	AT	65	PSU	C4-N3	-2.68	1.33	1.38
1	A2	1644	PSU	C4-N3	-2.68	1.33	1.38
1	A2	816	PSU	C4-N3	-2.68	1.33	1.38
1	A2	1005	PSU	C4-N3	-2.68	1.33	1.38
39	B5	3462	PSU	C4-N3	-2.68	1.33	1.38
39	B5	4246	PSU	C4-N3	-2.68	1.33	1.38
39	B5	3657	OMU	C4-N3	-2.68	1.33	1.38
1	A2	1178	PSU	C4-N3	-2.68	1.33	1.38
39	B5	3490	PSU	C4-N3	-2.68	1.33	1.38
39	B5	3447	PSU	C4-N3	-2.67	1.33	1.38
1	A2	687	PSU	C4-N3	-2.67	1.33	1.38
1	A2	1239	PSU	C4-N3	-2.67	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A2	119	PSU	C4-N3	-2.67	1.33	1.38
1	A2	1348	PSU	C4-N3	-2.67	1.33	1.38
39	B5	1718	PSU	C4-N3	-2.67	1.33	1.38
1	A2	1626	PSU	C4-N3	-2.67	1.33	1.38
1	A2	1175	PSU	C4-N3	-2.66	1.33	1.38
39	B5	3550	UY1	C2-N1	2.66	1.40	1.36
1	A2	109	PSU	C4-N3	-2.66	1.33	1.38
1	A2	967	PSU	C4-N3	-2.66	1.33	1.38
39	B5	4169	PSU	C4-N3	-2.65	1.33	1.38
39	B5	4045	PSU	C4-N3	-2.65	1.33	1.38
39	B5	4278	PSU	C4-N3	-2.65	1.33	1.38
1	A2	573	PSU	C4-N3	-2.64	1.33	1.38
39	B5	3502	PSU	C4-N3	-2.64	1.33	1.38
39	B5	4749	PSU	C4-N3	-2.64	1.33	1.38
1	A2	823	PSU	C4-N3	-2.64	1.33	1.38
39	B5	4052	OMU	C4-N3	-2.64	1.33	1.38
39	B5	1683	PSU	C4-N3	-2.64	1.33	1.38
39	B5	4366	OMU	C4-N3	-2.64	1.33	1.38
39	B5	3494	PSU	C4-N3	-2.63	1.33	1.38
39	B5	1632	PSU	C4-N3	-2.63	1.34	1.38
1	A2	36	PSU	C4-N3	-2.61	1.34	1.38
39	B5	3514	5MC	C6-C5	2.61	1.38	1.34
1	A2	802	PSU	C4-N3	-2.60	1.34	1.38
11	AT	64	5MU	C4-N3	-2.60	1.34	1.38
39	B5	3973	OMU	C4-N3	-2.59	1.33	1.38
1	A2	210	PSU	C4-N3	-2.59	1.34	1.38
39	B5	3524	OMG	C6-N1	-2.58	1.34	1.37
39	B5	4244	OMU	C4-N3	-2.58	1.33	1.38
1	A2	355	OMU	C4-N3	-2.57	1.33	1.38
1	A2	121	OMU	C4-N3	-2.57	1.34	1.38
39	B5	4116	OMG	C6-N1	-2.57	1.34	1.37
39	B5	2207	OMG	C6-N1	-2.57	1.34	1.37
1	A2	1443	OMU	C4-N3	-2.57	1.34	1.38
39	B5	4166	PSU	C4-N3	-2.56	1.34	1.38
39	B5	2680	OMU	C4-N3	-2.56	1.34	1.38
39	B5	1260	OMG	C6-N1	-2.55	1.34	1.37
39	B5	4138	OMG	C6-N1	-2.55	1.34	1.37
39	B5	1477	OMG	C6-N1	-2.55	1.34	1.37
1	A2	591	A2M	C5-C4	2.55	1.47	1.40
39	B5	2267	OMG	C6-N1	-2.54	1.34	1.37
39	B5	3631	OMG	C6-N1	-2.54	1.34	1.37
39	B5	2258	OMU	C4-N3	-2.54	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	B5	4240	OMG	C6-N1	-2.53	1.34	1.37
1	A2	1327	OMU	C4-N3	-2.53	1.34	1.38
1	A2	510	OMG	C6-N1	-2.53	1.34	1.37
39	B5	1580	OMG	C6-N1	-2.51	1.34	1.37
39	B5	3942	OMG	C6-N1	-2.51	1.34	1.37
1	A2	1805	OMU	C4-N3	-2.51	1.34	1.38
39	B5	4245	OMG	C6-N1	-2.50	1.34	1.37
39	B5	4383	OMG	C6-N1	-2.50	1.34	1.37
1	A2	166	A2M	C5-C4	2.50	1.47	1.40
41	B8	75	OMG	C6-N1	-2.50	1.34	1.37
39	B5	3492	A2M	C5-C4	2.49	1.47	1.40
1	A2	1491	OMG	C6-N1	-2.49	1.34	1.37
39	B5	4364	OMG	C6-N1	-2.49	1.34	1.37
1	A2	602	OMG	C6-N1	-2.48	1.34	1.37
1	A2	116	OMU	C4-N3	-2.48	1.34	1.38
1	A2	429	OMU	C4-N3	-2.48	1.34	1.38
39	B5	4369	OMG	C6-N1	-2.47	1.34	1.37
1	A2	159	A2M	C5-C4	2.47	1.47	1.40
1	A2	469	A2M	C5-C4	2.47	1.47	1.40
39	B5	1479	A2M	C5-C4	2.47	1.47	1.40
1	A2	577	A2M	C5-C4	2.46	1.47	1.40
1	A2	1249	B8N	C2-N3	-2.46	1.34	1.38
39	B5	3450	A2M	C5-C4	2.46	1.47	1.40
39	B5	3476	OMG	C6-N1	-2.46	1.34	1.37
1	A2	1851	MA6	C5-C4	2.46	1.47	1.40
39	B5	2719	OMG	C6-N1	-2.46	1.34	1.37
1	A2	645	OMG	C6-N1	-2.45	1.34	1.37
39	B5	3359	OMG	C6-N1	-2.45	1.34	1.37
1	A2	1852	MA6	C5-C4	2.45	1.47	1.40
1	A2	1329	OMG	C6-N1	-2.45	1.34	1.37
1	A2	485	A2M	C5-C4	2.45	1.47	1.40
1	A2	437	OMG	C6-N1	-2.45	1.34	1.37
1	A2	868	OMG	C6-N1	-2.45	1.34	1.37
1	A2	172	OMU	C4-N3	-2.45	1.34	1.38
1	A2	1289	OMU	C4-N3	-2.44	1.34	1.38
39	B5	3599	A2M	C5-C4	2.44	1.47	1.40
1	A2	1679	A2M	C5-C4	2.44	1.47	1.40
39	B5	398	A2M	C5-C4	2.44	1.47	1.40
39	B5	2206	A2M	C5-C4	2.43	1.47	1.40
39	B5	2630	A2M	C5-C4	2.43	1.47	1.40
39	B5	400	A2M	C5-C4	2.43	1.47	1.40
39	B5	2244	A2M	C5-C4	2.43	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A2	99	A2M	C5-C4	2.42	1.47	1.40
1	A2	628	OMU	C4-N3	-2.42	1.34	1.38
1	A2	513	A2M	C5-C4	2.42	1.47	1.40
1	A2	684	OMG	C6-N1	-2.42	1.34	1.37
39	B5	3514	5MC	C6-N1	-2.42	1.33	1.38
39	B5	3557	A2M	C5-C4	2.42	1.47	1.40
1	A2	27	A2M	C5-C4	2.42	1.47	1.40
39	B5	4336	A2M	C5-C4	2.41	1.47	1.40
39	B5	3456	A2M	C5-C4	2.41	1.47	1.40
39	B5	3966	6MZ	C5-C4	2.41	1.47	1.40
1	A2	1384	A2M	C5-C4	2.41	1.47	1.40
1	A2	1448	OMG	C6-N1	-2.40	1.34	1.37
1	A2	1032	A2M	C5-C4	2.40	1.47	1.40
39	B5	2658	A2M	C5-C4	2.40	1.47	1.40
39	B5	4317	A2M	C5-C4	2.40	1.47	1.40
1	A2	669	A2M	C5-C4	2.39	1.47	1.40
39	B5	3974	OMG	C6-N1	-2.39	1.34	1.37
39	B5	1489	A2M	C5-C4	2.37	1.47	1.40
39	B5	4269	A2M	C5-C4	2.37	1.47	1.40
39	B5	1810	A2M	C5-C4	2.36	1.47	1.40
39	B5	3562	A2M	C5-C4	2.35	1.47	1.40
39	B5	3676	OMG	C6-N1	-2.35	1.34	1.37
11	AT	64	5MU	C2-N1	2.33	1.42	1.38
11	AT	64	5MU	C4-C5	2.32	1.48	1.44
1	A2	1833	6MZ	C5-C4	2.31	1.47	1.40
39	B5	1270	A2M	C5-C4	2.31	1.47	1.40
39	B5	4193	5MC	C6-N1	-2.31	1.34	1.38
1	A2	1640	G7M	C6-N1	-2.29	1.34	1.37
39	B5	3657	OMU	C2-N3	-2.27	1.33	1.38
39	B5	3973	OMU	C2-N3	-2.27	1.33	1.38
11	AT	64	5MU	C6-N1	-2.26	1.34	1.38
39	B5	3517	A2M	C5-C4	2.26	1.46	1.40
39	B5	2680	OMU	C2-N3	-2.25	1.34	1.38
39	B5	4366	OMU	C2-N3	-2.25	1.34	1.38
39	B5	3550	UY1	C6-N1	-2.24	1.32	1.36
1	A2	1443	OMU	C2-N3	-2.24	1.34	1.38
1	A2	1843	4AC	C7-N4	-2.24	1.33	1.37
1	A2	121	OMU	C2-N3	-2.23	1.34	1.38
1	A2	1805	OMU	C2-N3	-2.23	1.34	1.38
39	B5	4052	OMU	C2-N3	-2.21	1.34	1.38
1	A2	355	OMU	C2-N3	-2.19	1.34	1.38
39	B5	4244	OMU	C2-N3	-2.18	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	B5	2258	OMU	C2-N3	-2.17	1.34	1.38
1	A2	1327	OMU	C2-N3	-2.16	1.34	1.38
1	A2	429	OMU	C2-N3	-2.15	1.34	1.38
1	A2	172	OMU	C2-N3	-2.15	1.34	1.38
1	A2	628	OMU	C2-N3	-2.15	1.34	1.38
1	A2	1289	OMU	C2-N3	-2.14	1.34	1.38
1	A2	116	OMU	C2-N3	-2.11	1.34	1.38
1	A2	1289	OMU	C2-N1	2.10	1.41	1.38
39	B5	3973	OMU	C2-N1	2.08	1.41	1.38
1	A2	1805	OMU	C2-N1	2.07	1.41	1.38
39	B5	4052	OMU	C5-C4	-2.03	1.39	1.43
39	B5	4366	OMU	C5-C4	-2.02	1.39	1.43
1	A2	121	OMU	C5-C4	-2.02	1.39	1.43
39	B5	2258	OMU	C5-C4	-2.00	1.39	1.43
39	B5	4366	OMU	C2-N1	2.00	1.41	1.38

All (562) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	B5	1638	PSU	N1-C2-N3	6.15	122.10	115.13
41	B8	69	PSU	N1-C2-N3	6.15	122.10	115.13
39	B5	4149	PSU	N1-C2-N3	6.15	122.09	115.13
39	B5	3494	PSU	N1-C2-N3	6.14	122.08	115.13
39	B5	4246	PSU	N1-C2-N3	6.13	122.07	115.13
39	B5	4435	PSU	N1-C2-N3	6.13	122.07	115.13
1	A2	652	PSU	N1-C2-N3	6.12	122.06	115.13
39	B5	1632	PSU	N1-C2-N3	6.12	122.06	115.13
39	B5	4188	PSU	N1-C2-N3	6.11	122.06	115.13
39	B5	3583	PSU	N1-C2-N3	6.11	122.05	115.13
39	B5	4267	PSU	N1-C2-N3	6.11	122.05	115.13
39	B5	1799	PSU	N1-C2-N3	6.10	122.04	115.13
39	B5	3616	PSU	N1-C2-N3	6.09	122.03	115.13
39	B5	4099	PSU	N1-C2-N3	6.09	122.03	115.13
39	B5	4749	PSU	N1-C2-N3	6.08	122.02	115.13
39	B5	4374	PSU	N1-C2-N3	6.08	122.02	115.13
39	B5	4042	PSU	N1-C2-N3	6.08	122.02	115.13
39	B5	3447	PSU	N1-C2-N3	6.08	122.01	115.13
39	B5	3496	PSU	N1-C2-N3	6.07	122.01	115.13
1	A2	682	PSU	N1-C2-N3	6.07	122.00	115.13
39	B5	1801	PSU	N1-C2-N3	6.06	122.00	115.13
41	B8	55	PSU	N1-C2-N3	6.06	122.00	115.13
1	A2	1175	PSU	N1-C2-N3	6.05	121.99	115.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	B5	3462	PSU	N1-C2-N3	6.05	121.99	115.13
39	B5	4058	PSU	N1-C2-N3	6.05	121.99	115.13
1	A2	1446	PSU	N1-C2-N3	6.05	121.98	115.13
1	A2	823	PSU	N1-C2-N3	6.05	121.98	115.13
1	A2	802	PSU	N1-C2-N3	6.05	121.98	115.13
1	A2	967	PSU	N1-C2-N3	6.04	121.98	115.13
39	B5	3369	PSU	N1-C2-N3	6.04	121.97	115.13
39	B5	3966	6MZ	C2-N1-C6	6.04	121.77	116.59
39	B5	4298	PSU	N1-C2-N3	6.03	121.97	115.13
1	A2	1057	PSU	N1-C2-N3	6.03	121.96	115.13
39	B5	4322	PSU	N1-C2-N3	6.03	121.96	115.13
39	B5	4419	PSU	N1-C2-N3	6.03	121.96	115.13
1	A2	1693	PSU	N1-C2-N3	6.02	121.96	115.13
39	B5	3371	PSU	N1-C2-N3	6.02	121.95	115.13
1	A2	1245	PSU	N1-C2-N3	6.02	121.95	115.13
1	A2	687	PSU	N1-C2-N3	6.02	121.95	115.13
1	A2	1046	PSU	N1-C2-N3	6.02	121.95	115.13
39	B5	4325	PSU	N1-C2-N3	6.01	121.94	115.13
1	A2	34	PSU	N1-C2-N3	6.01	121.94	115.13
39	B5	1683	PSU	N1-C2-N3	6.01	121.94	115.13
39	B5	3576	PSU	N1-C2-N3	6.01	121.94	115.13
39	B5	4177	PSU	N1-C2-N3	6.01	121.94	115.13
1	A2	1239	PSU	N1-C2-N3	6.00	121.93	115.13
1	A2	1368	PSU	N1-C2-N3	6.00	121.93	115.13
1	A2	816	PSU	N1-C2-N3	6.00	121.93	115.13
39	B5	3554	PSU	N1-C2-N3	6.00	121.93	115.13
1	A2	1047	PSU	N1-C2-N3	6.00	121.92	115.13
39	B5	4740	PSU	N1-C2-N3	6.00	121.92	115.13
1	A2	1178	PSU	N1-C2-N3	5.99	121.92	115.13
39	B5	3652	PSU	N1-C2-N3	5.99	121.92	115.13
39	B5	4107	PSU	N1-C2-N3	5.99	121.92	115.13
39	B5	3427	PSU	N1-C2-N3	5.99	121.92	115.13
39	B5	1537	PSU	N1-C2-N3	5.99	121.92	115.13
1	A2	650	PSU	N1-C2-N3	5.99	121.91	115.13
39	B5	1721	PSU	N1-C2-N3	5.98	121.91	115.13
39	B5	1720	PSU	N1-C2-N3	5.98	121.91	115.13
1	A2	105	PSU	N1-C2-N3	5.98	121.90	115.13
39	B5	4217	PSU	N1-C2-N3	5.98	121.90	115.13
39	B5	2475	PSU	N1-C2-N3	5.98	121.90	115.13
39	B5	4382	PSU	N1-C2-N3	5.97	121.90	115.13
1	A2	36	PSU	N1-C2-N3	5.96	121.89	115.13
1	A2	867	PSU	N1-C2-N3	5.96	121.89	115.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	B5	1731	PSU	N1-C2-N3	5.96	121.89	115.13
39	B5	3466	PSU	N1-C2-N3	5.96	121.88	115.13
39	B5	3500	PSU	N1-C2-N3	5.96	121.88	115.13
39	B5	3502	PSU	N1-C2-N3	5.96	121.88	115.13
39	B5	4711	PSU	N1-C2-N3	5.96	121.88	115.13
1	A2	109	PSU	N1-C2-N3	5.96	121.88	115.13
39	B5	1491	PSU	N1-C2-N3	5.96	121.88	115.13
1	A2	864	PSU	N1-C2-N3	5.95	121.88	115.13
1	A2	93	PSU	N1-C2-N3	5.95	121.88	115.13
1	A2	573	PSU	N1-C2-N3	5.95	121.88	115.13
1	A2	407	PSU	N1-C2-N3	5.95	121.87	115.13
39	B5	4045	PSU	N1-C2-N3	5.95	121.87	115.13
39	B5	4278	PSU	N1-C2-N3	5.95	121.87	115.13
39	B5	4039	PSU	N1-C2-N3	5.95	121.87	115.13
39	B5	4203	PSU	N1-C2-N3	5.95	121.87	115.13
39	B5	1718	PSU	N1-C2-N3	5.94	121.86	115.13
39	B5	2351	PSU	N1-C2-N3	5.94	121.86	115.13
1	A2	1626	PSU	N1-C2-N3	5.94	121.86	115.13
1	A2	815	PSU	N1-C2-N3	5.93	121.85	115.13
1	A2	1348	PSU	N1-C2-N3	5.93	121.85	115.13
1	A2	1644	PSU	N1-C2-N3	5.93	121.85	115.13
11	AT	65	PSU	N1-C2-N3	5.93	121.85	115.13
1	A2	119	PSU	N1-C2-N3	5.92	121.84	115.13
39	B5	3490	PSU	N1-C2-N3	5.92	121.84	115.13
39	B5	4169	PSU	N1-C2-N3	5.92	121.84	115.13
1	A2	1005	PSU	N1-C2-N3	5.91	121.83	115.13
1	A2	1233	PSU	N1-C2-N3	5.91	121.83	115.13
1	A2	1082	PSU	N1-C2-N3	5.91	121.82	115.13
39	B5	3585	PSU	N1-C2-N3	5.90	121.82	115.13
1	A2	210	PSU	N1-C2-N3	5.90	121.82	115.13
39	B5	4276	UR3	C4-N3-C2	-5.90	119.00	124.56
1	A2	218	PSU	N1-C2-N3	5.89	121.81	115.13
39	B5	4166	PSU	N1-C2-N3	5.72	121.61	115.13
1	A2	1833	6MZ	C2-N1-C6	5.48	121.29	116.59
39	B5	3550	UY1	C4-N3-C2	-5.39	118.57	126.34
11	AT	64	5MU	C4-N3-C2	-4.93	120.97	127.35
11	AT	64	5MU	N3-C2-N1	4.76	121.21	114.89
1	A2	1338	4AC	N4-C4-N3	4.67	121.70	113.85
39	B5	4244	OMU	C4-N3-C2	-4.61	120.50	126.58
39	B5	3657	OMU	C4-N3-C2	-4.60	120.51	126.58
39	B5	2680	OMU	C4-N3-C2	-4.57	120.55	126.58
1	A2	1327	OMU	C4-N3-C2	-4.54	120.59	126.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A2	429	OMU	C4-N3-C2	-4.53	120.61	126.58
1	A2	628	OMU	C4-N3-C2	-4.52	120.62	126.58
39	B5	3966	6MZ	C9-N6-C6	-4.52	118.98	122.87
39	B5	4366	OMU	C4-N3-C2	-4.49	120.66	126.58
1	A2	1443	OMU	C4-N3-C2	-4.48	120.68	126.58
1	A2	355	OMU	C4-N3-C2	-4.47	120.68	126.58
39	B5	3973	OMU	C4-N3-C2	-4.46	120.70	126.58
39	B5	3550	UY1	N1-C2-N3	4.45	120.17	115.13
1	A2	172	OMU	C4-N3-C2	-4.45	120.71	126.58
1	A2	121	OMU	C4-N3-C2	-4.45	120.71	126.58
39	B5	2258	OMU	C4-N3-C2	-4.39	120.80	126.58
1	A2	116	OMU	C4-N3-C2	-4.38	120.80	126.58
1	A2	1851	MA6	N1-C6-N6	4.35	121.64	117.06
39	B5	4244	OMU	N3-C2-N1	4.32	120.62	114.89
1	A2	1805	OMU	C4-N3-C2	-4.30	120.91	126.58
39	B5	4052	OMU	C4-N3-C2	-4.28	120.94	126.58
11	AT	64	5MU	C5-C4-N3	4.28	118.96	115.31
1	A2	1289	OMU	C4-N3-C2	-4.26	120.96	126.58
1	A2	1843	4AC	N4-C4-N3	4.24	120.96	113.85
39	B5	4366	OMU	N3-C2-N1	4.23	120.50	114.89
39	B5	2680	OMU	N3-C2-N1	4.19	120.45	114.89
39	B5	3657	OMU	N3-C2-N1	4.18	120.44	114.89
1	A2	355	OMU	N3-C2-N1	4.16	120.42	114.89
1	A2	172	OMU	N3-C2-N1	4.15	120.40	114.89
39	B5	3973	OMU	N3-C2-N1	4.11	120.34	114.89
1	A2	628	OMU	N3-C2-N1	4.10	120.34	114.89
1	A2	429	OMU	N3-C2-N1	4.10	120.33	114.89
39	B5	4267	PSU	C4-N3-C2	-4.09	120.44	126.34
39	B5	1632	PSU	C4-N3-C2	-4.09	120.45	126.34
39	B5	4149	PSU	C4-N3-C2	-4.06	120.48	126.34
39	B5	3369	PSU	C4-N3-C2	-4.06	120.50	126.34
1	A2	1327	OMU	N3-C2-N1	4.05	120.27	114.89
39	B5	1801	PSU	C4-N3-C2	-4.05	120.50	126.34
1	A2	116	OMU	N3-C2-N1	4.04	120.25	114.89
39	B5	1638	PSU	C4-N3-C2	-4.04	120.52	126.34
39	B5	3496	PSU	C4-N3-C2	-4.03	120.53	126.34
39	B5	4298	PSU	C4-N3-C2	-4.03	120.53	126.34
39	B5	4052	OMU	N3-C2-N1	4.03	120.24	114.89
39	B5	4042	PSU	C4-N3-C2	-4.03	120.53	126.34
1	A2	1805	OMU	N3-C2-N1	4.02	120.22	114.89
1	A2	1175	PSU	C4-N3-C2	-4.01	120.56	126.34
41	B8	69	PSU	C4-N3-C2	-4.01	120.57	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	B5	3583	PSU	C4-N3-C2	-3.99	120.58	126.34
39	B5	1721	PSU	C4-N3-C2	-3.99	120.59	126.34
39	B5	3616	PSU	C4-N3-C2	-3.99	120.59	126.34
1	A2	650	PSU	C4-N3-C2	-3.99	120.59	126.34
1	A2	1446	PSU	C4-N3-C2	-3.99	120.59	126.34
39	B5	4749	PSU	C4-N3-C2	-3.99	120.59	126.34
41	B8	55	PSU	C4-N3-C2	-3.99	120.59	126.34
39	B5	4374	PSU	C4-N3-C2	-3.99	120.59	126.34
39	B5	4188	PSU	C4-N3-C2	-3.99	120.59	126.34
1	A2	1178	PSU	C4-N3-C2	-3.99	120.60	126.34
1	A2	652	PSU	C4-N3-C2	-3.98	120.60	126.34
1	A2	121	OMU	N3-C2-N1	3.98	120.17	114.89
39	B5	1491	PSU	C4-N3-C2	-3.98	120.61	126.34
1	A2	687	PSU	C4-N3-C2	-3.97	120.62	126.34
39	B5	1799	PSU	C4-N3-C2	-3.97	120.62	126.34
1	A2	867	PSU	C4-N3-C2	-3.97	120.62	126.34
39	B5	3462	PSU	C4-N3-C2	-3.97	120.62	126.34
39	B5	3502	PSU	C4-N3-C2	-3.97	120.62	126.34
1	A2	1245	PSU	C4-N3-C2	-3.97	120.62	126.34
1	A2	1368	PSU	C4-N3-C2	-3.97	120.62	126.34
39	B5	4711	PSU	C4-N3-C2	-3.96	120.63	126.34
39	B5	4058	PSU	C4-N3-C2	-3.96	120.63	126.34
39	B5	4246	PSU	C4-N3-C2	-3.96	120.63	126.34
39	B5	4435	PSU	C4-N3-C2	-3.96	120.63	126.34
39	B5	3466	PSU	C4-N3-C2	-3.96	120.64	126.34
1	A2	816	PSU	C4-N3-C2	-3.95	120.65	126.34
39	B5	4419	PSU	C4-N3-C2	-3.95	120.65	126.34
1	A2	1233	PSU	C4-N3-C2	-3.94	120.66	126.34
39	B5	4099	PSU	C4-N3-C2	-3.94	120.66	126.34
1	A2	1057	PSU	C4-N3-C2	-3.94	120.66	126.34
1	A2	1046	PSU	C4-N3-C2	-3.94	120.67	126.34
39	B5	4039	PSU	C4-N3-C2	-3.93	120.67	126.34
1	A2	1239	PSU	C4-N3-C2	-3.93	120.67	126.34
1	A2	1443	OMU	N3-C2-N1	3.93	120.11	114.89
39	B5	4740	PSU	C4-N3-C2	-3.93	120.68	126.34
39	B5	1731	PSU	C4-N3-C2	-3.93	120.68	126.34
39	B5	4045	PSU	C4-N3-C2	-3.92	120.69	126.34
1	A2	1289	OMU	N3-C2-N1	3.92	120.09	114.89
39	B5	3447	PSU	C4-N3-C2	-3.92	120.69	126.34
39	B5	4177	PSU	C4-N3-C2	-3.92	120.69	126.34
39	B5	1683	PSU	C4-N3-C2	-3.91	120.70	126.34
39	B5	3652	PSU	C4-N3-C2	-3.91	120.70	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A2	823	PSU	C4-N3-C2	-3.91	120.70	126.34
39	B5	2351	PSU	C4-N3-C2	-3.91	120.70	126.34
11	AT	64	5MU	O4-C4-C5	-3.91	120.37	124.90
1	A2	407	PSU	C4-N3-C2	-3.91	120.71	126.34
1	A2	573	PSU	C4-N3-C2	-3.91	120.71	126.34
39	B5	3554	PSU	C4-N3-C2	-3.91	120.71	126.34
39	B5	4107	PSU	C4-N3-C2	-3.90	120.71	126.34
11	AT	65	PSU	C4-N3-C2	-3.90	120.71	126.34
39	B5	4193	5MC	C5-C6-N1	-3.90	119.32	123.34
1	A2	109	PSU	C4-N3-C2	-3.90	120.72	126.34
1	A2	218	PSU	C4-N3-C2	-3.90	120.72	126.34
1	A2	1693	PSU	C4-N3-C2	-3.90	120.72	126.34
1	A2	802	PSU	C4-N3-C2	-3.90	120.72	126.34
1	A2	1348	PSU	C4-N3-C2	-3.90	120.72	126.34
1	A2	34	PSU	C4-N3-C2	-3.90	120.72	126.34
39	B5	3427	PSU	C4-N3-C2	-3.90	120.72	126.34
39	B5	4203	PSU	C4-N3-C2	-3.90	120.72	126.34
1	A2	1047	PSU	C4-N3-C2	-3.90	120.73	126.34
39	B5	3371	PSU	C4-N3-C2	-3.89	120.73	126.34
1	A2	682	PSU	C4-N3-C2	-3.89	120.73	126.34
1	A2	815	PSU	C4-N3-C2	-3.89	120.74	126.34
1	A2	1626	PSU	C4-N3-C2	-3.89	120.74	126.34
39	B5	4278	PSU	C4-N3-C2	-3.88	120.75	126.34
1	A2	1005	PSU	C4-N3-C2	-3.88	120.75	126.34
39	B5	1718	PSU	C4-N3-C2	-3.88	120.75	126.34
39	B5	3576	PSU	C4-N3-C2	-3.88	120.75	126.34
39	B5	1720	PSU	C4-N3-C2	-3.88	120.75	126.34
39	B5	2258	OMU	N3-C2-N1	3.87	120.03	114.89
39	B5	4322	PSU	C4-N3-C2	-3.87	120.76	126.34
39	B5	2475	PSU	C4-N3-C2	-3.87	120.76	126.34
1	A2	967	PSU	C4-N3-C2	-3.87	120.77	126.34
39	B5	4325	PSU	C4-N3-C2	-3.86	120.77	126.34
39	B5	1537	PSU	C4-N3-C2	-3.86	120.78	126.34
1	A2	105	PSU	C4-N3-C2	-3.85	120.78	126.34
39	B5	4169	PSU	C4-N3-C2	-3.85	120.80	126.34
39	B5	3490	PSU	C4-N3-C2	-3.85	120.80	126.34
1	A2	36	PSU	C4-N3-C2	-3.84	120.80	126.34
1	A2	93	PSU	C4-N3-C2	-3.84	120.81	126.34
1	A2	119	PSU	C4-N3-C2	-3.84	120.81	126.34
39	B5	3585	PSU	C4-N3-C2	-3.83	120.82	126.34
1	A2	1082	PSU	C4-N3-C2	-3.83	120.83	126.34
1	A2	864	PSU	C4-N3-C2	-3.82	120.83	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A2	210	PSU	C4-N3-C2	-3.81	120.84	126.34
39	B5	4382	PSU	C4-N3-C2	-3.81	120.85	126.34
39	B5	4217	PSU	C4-N3-C2	-3.81	120.85	126.34
39	B5	3500	PSU	C4-N3-C2	-3.80	120.86	126.34
1	A2	1644	PSU	C4-N3-C2	-3.80	120.86	126.34
39	B5	3494	PSU	C4-N3-C2	-3.78	120.90	126.34
1	A2	1443	OMU	C5-C4-N3	3.76	120.46	114.84
1	A2	1852	MA6	N1-C6-N6	3.76	121.01	117.06
39	B5	4435	PSU	O2-C2-N1	-3.71	118.70	122.79
39	B5	3657	OMU	C5-C4-N3	3.69	120.35	114.84
39	B5	2258	OMU	C5-C4-N3	3.67	120.33	114.84
1	A2	1175	PSU	O2-C2-N1	-3.66	118.76	122.79
39	B5	2680	OMU	C5-C4-N3	3.65	120.30	114.84
1	A2	121	OMU	C5-C4-N3	3.63	120.28	114.84
39	B5	3494	PSU	O2-C2-N1	-3.63	118.79	122.79
39	B5	1799	PSU	O2-C2-N1	-3.62	118.81	122.79
1	A2	1327	OMU	C5-C4-N3	3.61	120.24	114.84
1	A2	429	OMU	C5-C4-N3	3.61	120.23	114.84
1	A2	628	OMU	C5-C4-N3	3.60	120.23	114.84
39	B5	3973	OMU	C5-C4-N3	3.59	120.22	114.84
1	A2	1805	OMU	C5-C4-N3	3.59	120.20	114.84
39	B5	4366	OMU	C5-C4-N3	3.58	120.19	114.84
1	A2	355	OMU	C5-C4-N3	3.57	120.19	114.84
1	A2	116	OMU	C5-C4-N3	3.57	120.18	114.84
39	B5	4244	OMU	C5-C4-N3	3.57	120.18	114.84
39	B5	1638	PSU	O2-C2-N1	-3.57	118.86	122.79
39	B5	4325	PSU	O2-C2-N1	-3.56	118.87	122.79
39	B5	4166	PSU	C4-N3-C2	-3.56	121.22	126.34
1	A2	1289	OMU	C5-C4-N3	3.55	120.15	114.84
39	B5	3462	PSU	O2-C2-N1	-3.54	118.89	122.79
39	B5	4149	PSU	O2-C2-N1	-3.54	118.90	122.79
39	B5	1537	PSU	O2-C2-N1	-3.53	118.90	122.79
39	B5	3616	PSU	O2-C2-N1	-3.53	118.91	122.79
39	B5	3447	PSU	O2-C2-N1	-3.53	118.91	122.79
39	B5	4298	PSU	O2-C2-N1	-3.52	118.92	122.79
39	B5	3490	PSU	O2-C2-N1	-3.52	118.92	122.79
39	B5	4374	PSU	O2-C2-N1	-3.51	118.92	122.79
39	B5	4052	OMU	C5-C4-N3	3.50	120.08	114.84
1	A2	1368	PSU	O2-C2-N1	-3.49	118.94	122.79
39	B5	4058	PSU	O2-C2-N1	-3.49	118.95	122.79
1	A2	172	OMU	C5-C4-N3	3.48	120.05	114.84
39	B5	1683	PSU	O2-C2-N1	-3.47	118.97	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A2	823	PSU	O2-C2-N1	-3.47	118.97	122.79
39	B5	3514	5MC	C5-C6-N1	-3.47	119.77	123.34
1	A2	1046	PSU	O2-C2-N1	-3.46	118.98	122.79
39	B5	3554	PSU	O2-C2-N1	-3.46	118.99	122.79
41	B8	69	PSU	O2-C2-N1	-3.46	118.99	122.79
1	A2	1047	PSU	O2-C2-N1	-3.45	118.99	122.79
39	B5	4382	PSU	O2-C2-N1	-3.45	118.99	122.79
39	B5	1718	PSU	O2-C2-N1	-3.45	118.99	122.79
1	A2	802	PSU	O2-C2-N1	-3.45	119.00	122.79
39	B5	4322	PSU	O2-C2-N1	-3.45	119.00	122.79
39	B5	4246	PSU	O2-C2-N1	-3.44	119.00	122.79
1	A2	109	PSU	O2-C2-N1	-3.44	119.00	122.79
39	B5	1632	PSU	O2-C2-N1	-3.44	119.01	122.79
1	A2	652	PSU	O2-C2-N1	-3.43	119.01	122.79
39	B5	3371	PSU	O2-C2-N1	-3.43	119.01	122.79
39	B5	3502	PSU	O2-C2-N1	-3.43	119.02	122.79
39	B5	4278	PSU	O2-C2-N1	-3.43	119.02	122.79
1	A2	1245	PSU	O2-C2-N1	-3.42	119.02	122.79
41	B8	55	PSU	O2-C2-N1	-3.42	119.02	122.79
1	A2	36	PSU	O2-C2-N1	-3.42	119.03	122.79
39	B5	4419	PSU	O2-C2-N1	-3.42	119.03	122.79
1	A2	650	PSU	O2-C2-N1	-3.42	119.03	122.79
39	B5	1491	PSU	O2-C2-N1	-3.42	119.03	122.79
1	A2	573	PSU	O2-C2-N1	-3.41	119.03	122.79
1	A2	1005	PSU	O2-C2-N1	-3.41	119.03	122.79
39	B5	4188	PSU	O2-C2-N1	-3.41	119.04	122.79
1	A2	867	PSU	O2-C2-N1	-3.41	119.04	122.79
39	B5	1801	PSU	O2-C2-N1	-3.41	119.04	122.79
39	B5	4749	PSU	O2-C2-N1	-3.41	119.04	122.79
1	A2	1348	PSU	O2-C2-N1	-3.41	119.04	122.79
1	A2	93	PSU	O2-C2-N1	-3.40	119.04	122.79
1	A2	682	PSU	O2-C2-N1	-3.40	119.04	122.79
39	B5	4711	PSU	O2-C2-N1	-3.40	119.04	122.79
39	B5	1720	PSU	O2-C2-N1	-3.40	119.05	122.79
39	B5	3466	PSU	O2-C2-N1	-3.40	119.05	122.79
1	A2	1057	PSU	O2-C2-N1	-3.40	119.05	122.79
39	B5	4099	PSU	O2-C2-N1	-3.40	119.05	122.79
39	B5	3427	PSU	O2-C2-N1	-3.40	119.05	122.79
39	B5	4267	PSU	O2-C2-N1	-3.39	119.05	122.79
39	B5	4740	PSU	O2-C2-N1	-3.39	119.05	122.79
1	A2	816	PSU	O2-C2-N1	-3.39	119.06	122.79
11	AT	64	5MU	C5-C6-N1	-3.39	119.86	123.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A2	967	PSU	O2-C2-N1	-3.39	119.06	122.79
39	B5	3500	PSU	O2-C2-N1	-3.38	119.06	122.79
39	B5	3576	PSU	O2-C2-N1	-3.38	119.06	122.79
39	B5	3583	PSU	O2-C2-N1	-3.38	119.07	122.79
39	B5	4177	PSU	O2-C2-N1	-3.38	119.07	122.79
1	A2	687	PSU	O2-C2-N1	-3.37	119.08	122.79
1	A2	1178	PSU	O2-C2-N1	-3.37	119.08	122.79
1	A2	1249	B8N	C4-N3-C2	-3.37	121.20	125.46
1	A2	1626	PSU	O2-C2-N1	-3.37	119.08	122.79
39	B5	3585	PSU	O2-C2-N1	-3.37	119.08	122.79
39	B5	3496	PSU	O2-C2-N1	-3.36	119.09	122.79
1	A2	407	PSU	O2-C2-N1	-3.36	119.09	122.79
39	B5	4166	PSU	O2-C2-N1	-3.36	119.09	122.79
39	B5	3517	A2M	N3-C2-N1	-3.35	123.44	128.68
1	A2	1644	PSU	O2-C2-N1	-3.35	119.10	122.79
39	B5	2475	PSU	O2-C2-N1	-3.35	119.10	122.79
39	B5	1731	PSU	O2-C2-N1	-3.35	119.10	122.79
39	B5	4042	PSU	O2-C2-N1	-3.34	119.11	122.79
1	A2	119	PSU	O2-C2-N1	-3.33	119.12	122.79
1	A2	210	PSU	O2-C2-N1	-3.33	119.12	122.79
1	A2	864	PSU	O2-C2-N1	-3.33	119.12	122.79
1	A2	218	PSU	O2-C2-N1	-3.33	119.12	122.79
39	B5	4039	PSU	O2-C2-N1	-3.33	119.13	122.79
1	A2	1446	PSU	O2-C2-N1	-3.33	119.13	122.79
39	B5	1721	PSU	O2-C2-N1	-3.32	119.13	122.79
39	B5	4169	PSU	O2-C2-N1	-3.32	119.14	122.79
1	A2	1233	PSU	O2-C2-N1	-3.32	119.14	122.79
1	A2	1239	PSU	O2-C2-N1	-3.31	119.14	122.79
1	A2	34	PSU	O2-C2-N1	-3.31	119.14	122.79
1	A2	1693	PSU	O2-C2-N1	-3.31	119.14	122.79
1	A2	105	PSU	O2-C2-N1	-3.30	119.15	122.79
39	B5	4217	PSU	O2-C2-N1	-3.30	119.16	122.79
39	B5	4045	PSU	O2-C2-N1	-3.30	119.16	122.79
39	B5	1270	A2M	N3-C2-N1	-3.28	123.55	128.68
1	A2	1032	A2M	N3-C2-N1	-3.28	123.56	128.68
39	B5	3966	6MZ	N3-C2-N1	-3.27	123.57	128.68
39	B5	2351	PSU	O2-C2-N1	-3.26	119.20	122.79
39	B5	3652	PSU	O2-C2-N1	-3.26	119.20	122.79
1	A2	815	PSU	O2-C2-N1	-3.25	119.22	122.79
39	B5	4269	A2M	N3-C2-N1	-3.24	123.61	128.68
39	B5	1489	A2M	N3-C2-N1	-3.24	123.61	128.68
39	B5	4203	PSU	O2-C2-N1	-3.24	119.23	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	B5	4317	A2M	N3-C2-N1	-3.24	123.62	128.68
1	A2	27	A2M	N3-C2-N1	-3.23	123.62	128.68
1	A2	591	A2M	N3-C2-N1	-3.23	123.63	128.68
39	B5	2658	A2M	N3-C2-N1	-3.23	123.63	128.68
1	A2	99	A2M	N3-C2-N1	-3.23	123.64	128.68
11	AT	65	PSU	O2-C2-N1	-3.22	119.24	122.79
39	B5	3557	A2M	N3-C2-N1	-3.21	123.66	128.68
39	B5	4107	PSU	O2-C2-N1	-3.21	119.26	122.79
39	B5	3456	A2M	N3-C2-N1	-3.21	123.66	128.68
39	B5	3492	A2M	N3-C2-N1	-3.20	123.67	128.68
1	A2	1679	A2M	N3-C2-N1	-3.20	123.67	128.68
39	B5	398	A2M	N3-C2-N1	-3.20	123.68	128.68
1	A2	166	A2M	N3-C2-N1	-3.19	123.69	128.68
39	B5	4336	A2M	N3-C2-N1	-3.19	123.69	128.68
39	B5	2244	A2M	N3-C2-N1	-3.19	123.70	128.68
39	B5	2630	A2M	N3-C2-N1	-3.19	123.70	128.68
39	B5	3562	A2M	N3-C2-N1	-3.18	123.70	128.68
39	B5	1810	A2M	N3-C2-N1	-3.18	123.71	128.68
39	B5	3450	A2M	N3-C2-N1	-3.18	123.71	128.68
39	B5	1479	A2M	N3-C2-N1	-3.18	123.71	128.68
1	A2	669	A2M	N3-C2-N1	-3.17	123.72	128.68
39	B5	3369	PSU	O2-C2-N1	-3.17	119.30	122.79
1	A2	577	A2M	N3-C2-N1	-3.17	123.72	128.68
39	B5	2206	A2M	N3-C2-N1	-3.17	123.72	128.68
1	A2	1852	MA6	N3-C2-N1	-3.16	123.73	128.68
39	B5	3599	A2M	N3-C2-N1	-3.16	123.74	128.68
1	A2	159	A2M	N3-C2-N1	-3.16	123.74	128.68
1	A2	469	A2M	N3-C2-N1	-3.16	123.74	128.68
39	B5	400	A2M	N3-C2-N1	-3.16	123.74	128.68
1	A2	485	A2M	N3-C2-N1	-3.15	123.76	128.68
1	A2	1384	A2M	N3-C2-N1	-3.15	123.76	128.68
1	A2	1851	MA6	N3-C2-N1	-3.14	123.77	128.68
1	A2	1082	PSU	O2-C2-N1	-3.12	119.36	122.79
1	A2	1833	6MZ	N3-C2-N1	-3.12	123.81	128.68
1	A2	513	A2M	N3-C2-N1	-3.11	123.82	128.68
1	A2	1249	B8N	N3-C2-N1	3.11	121.14	116.76
1	A2	1851	MA6	C4-C5-N7	-3.09	106.18	109.40
39	B5	2258	OMU	O4-C4-C5	-3.08	119.75	125.16
1	A2	1805	OMU	O4-C4-C5	-3.07	119.77	125.16
1	A2	116	OMU	O4-C4-C5	-3.06	119.79	125.16
1	A2	429	OMU	O4-C4-C5	-3.05	119.79	125.16
1	A2	121	OMU	O4-C4-C5	-3.04	119.81	125.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	B5	2680	OMU	O4-C4-C5	-3.03	119.83	125.16
1	A2	1443	OMU	O4-C4-C5	-3.03	119.84	125.16
39	B5	3657	OMU	O4-C4-C5	-3.02	119.85	125.16
1	A2	1327	OMU	O4-C4-C5	-3.01	119.86	125.16
39	B5	4244	OMU	O4-C4-C5	-3.00	119.89	125.16
1	A2	628	OMU	O4-C4-C5	-2.99	119.89	125.16
1	A2	355	OMU	O4-C4-C5	-2.99	119.90	125.16
39	B5	4052	OMU	O4-C4-C5	-2.98	119.92	125.16
1	A2	172	OMU	O4-C4-C5	-2.97	119.94	125.16
39	B5	3550	UY1	C6-C5-C4	2.96	120.27	118.20
39	B5	4366	OMU	O4-C4-C5	-2.95	119.98	125.16
1	A2	1852	MA6	C4-C5-N7	-2.93	106.35	109.40
1	A2	1289	OMU	O4-C4-C5	-2.92	120.03	125.16
39	B5	3973	OMU	O4-C4-C5	-2.87	120.12	125.16
1	A2	166	A2M	C4-C5-N7	-2.82	106.46	109.40
39	B5	1489	A2M	C4-C5-N7	-2.79	106.50	109.40
1	A2	1032	A2M	C4-C5-N7	-2.78	106.50	109.40
39	B5	2244	A2M	C4-C5-N7	-2.76	106.52	109.40
1	A2	513	A2M	C4-C5-N7	-2.75	106.53	109.40
1	A2	469	A2M	C4-C5-N7	-2.74	106.55	109.40
39	B5	3492	A2M	C4-C5-N7	-2.74	106.55	109.40
1	A2	159	A2M	C4-C5-N7	-2.73	106.55	109.40
1	A2	27	A2M	C4-C5-N7	-2.73	106.56	109.40
39	B5	3456	A2M	C4-C5-N7	-2.72	106.56	109.40
39	B5	4317	A2M	C4-C5-N7	-2.69	106.59	109.40
39	B5	3966	6MZ	C4-C5-N7	-2.68	106.60	109.40
39	B5	2206	A2M	C4-C5-N7	-2.68	106.60	109.40
1	A2	577	A2M	C4-C5-N7	-2.68	106.61	109.40
1	A2	1640	G7M	CN7-N7-C8	-2.67	112.56	125.43
39	B5	3562	A2M	C4-C5-N7	-2.67	106.62	109.40
1	A2	485	A2M	C4-C5-N7	-2.66	106.62	109.40
39	B5	3599	A2M	C4-C5-N7	-2.66	106.62	109.40
39	B5	3450	A2M	C4-C5-N7	-2.66	106.63	109.40
39	B5	398	A2M	C4-C5-N7	-2.65	106.63	109.40
1	A2	669	A2M	C4-C5-N7	-2.65	106.64	109.40
39	B5	2658	A2M	C4-C5-N7	-2.64	106.64	109.40
39	B5	4269	A2M	C4-C5-N7	-2.64	106.65	109.40
1	A2	1679	A2M	C4-C5-N7	-2.64	106.65	109.40
1	A2	1384	A2M	C4-C5-N7	-2.63	106.66	109.40
39	B5	400	A2M	C4-C5-N7	-2.62	106.67	109.40
39	B5	1479	A2M	C4-C5-N7	-2.61	106.68	109.40
39	B5	1270	A2M	C4-C5-N7	-2.61	106.68	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	B5	3557	A2M	C4-C5-N7	-2.61	106.68	109.40
39	B5	3514	5MC	C5-C4-N3	-2.60	118.87	121.67
39	B5	1810	A2M	C4-C5-N7	-2.57	106.72	109.40
39	B5	4336	A2M	C4-C5-N7	-2.57	106.72	109.40
1	A2	99	A2M	C4-C5-N7	-2.56	106.74	109.40
39	B5	4193	5MC	C5-C4-N3	-2.54	118.93	121.67
39	B5	2630	A2M	C4-C5-N7	-2.53	106.76	109.40
1	A2	591	A2M	C4-C5-N7	-2.52	106.77	109.40
39	B5	3517	A2M	C4-C5-N7	-2.50	106.79	109.40
42	BA	216	V5N	O-C-CA	-2.47	118.30	124.78
1	A2	1338	4AC	C5-C4-N4	-2.47	118.64	122.92
39	B5	1477	OMG	C8-N7-C5	2.46	107.67	102.99
30	Ar	2	SAC	O-C-CA	-2.46	118.34	124.78
1	A2	1843	4AC	C6-C5-C4	2.45	119.96	116.96
68	Ba	39	V5N	O-C-CA	-2.45	118.36	124.78
33	Au	1	AME	O-C-CA	-2.45	118.36	124.78
39	B5	3550	UY1	O2-C2-N1	-2.43	120.12	122.79
39	B5	1260	OMG	C5-C6-N1	2.42	118.22	113.95
39	B5	3942	OMG	C5-C6-N1	2.42	118.22	113.95
1	A2	1491	OMG	C5-C6-N1	2.40	118.20	113.95
1	A2	684	OMG	C8-N7-C5	2.40	107.57	102.99
39	B5	4116	OMG	C5-C6-N1	2.39	118.17	113.95
39	B5	4138	OMG	C5-C6-N1	2.39	118.16	113.95
1	A2	1338	4AC	C6-C5-C4	2.38	119.88	116.96
39	B5	3476	OMG	C8-N7-C5	2.38	107.53	102.99
39	B5	3676	OMG	C8-N7-C5	2.36	107.48	102.99
39	B5	4369	OMG	C8-N7-C5	2.35	107.47	102.99
39	B5	4138	OMG	C8-N7-C5	2.35	107.46	102.99
39	B5	4116	OMG	C8-N7-C5	2.35	107.46	102.99
1	A2	437	OMG	C8-N7-C5	2.35	107.46	102.99
39	B5	1260	OMG	C8-N7-C5	2.34	107.46	102.99
39	B5	4383	OMG	C8-N7-C5	2.34	107.45	102.99
39	B5	3974	OMG	C8-N7-C5	2.34	107.45	102.99
39	B5	4245	OMG	C8-N7-C5	2.34	107.45	102.99
39	B5	2719	OMG	C5-C6-N1	2.34	118.08	113.95
41	B8	75	OMG	C8-N7-C5	2.34	107.44	102.99
39	B5	1477	OMG	C5-C6-N1	2.33	118.07	113.95
39	B5	2207	OMG	C8-N7-C5	2.33	107.44	102.99
39	B5	3359	OMG	C8-N7-C5	2.33	107.43	102.99
1	A2	684	OMG	C5-C6-N1	2.33	118.07	113.95
39	B5	3359	OMG	C5-C6-N1	2.33	118.07	113.95
1	A2	1329	OMG	C8-N7-C5	2.33	107.43	102.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	B5	4240	OMG	C8-N7-C5	2.33	107.42	102.99
1	A2	645	OMG	C8-N7-C5	2.33	107.42	102.99
1	A2	868	OMG	C8-N7-C5	2.32	107.42	102.99
39	B5	2267	OMG	C5-C6-N1	2.32	118.05	113.95
12	AZ	2	SAC	O-C-CA	-2.32	118.69	124.78
1	A2	437	OMG	C5-C6-N1	2.32	118.04	113.95
1	A2	645	OMG	C5-C6-N1	2.32	118.04	113.95
39	B5	1580	OMG	C8-N7-C5	2.32	107.40	102.99
1	A2	602	OMG	C8-N7-C5	2.31	107.40	102.99
39	B5	3631	OMG	C8-N7-C5	2.31	107.40	102.99
1	A2	1329	OMG	C5-C6-N1	2.31	118.04	113.95
41	B8	75	OMG	C5-C6-N1	2.31	118.03	113.95
39	B5	4383	OMG	C5-C6-N1	2.31	118.03	113.95
1	A2	868	OMG	C5-C6-N1	2.31	118.03	113.95
39	B5	4364	OMG	C5-C6-N1	2.31	118.02	113.95
39	B5	2719	OMG	C8-N7-C5	2.31	107.38	102.99
39	B5	4369	OMG	C5-C6-N1	2.30	118.02	113.95
39	B5	3676	OMG	C5-C6-N1	2.30	118.01	113.95
1	A2	602	OMG	C5-C6-N1	2.30	118.01	113.95
39	B5	3476	OMG	C5-C6-N1	2.30	118.01	113.95
39	B5	4364	OMG	C8-N7-C5	2.29	107.36	102.99
39	B5	1580	OMG	C5-C6-N1	2.29	118.00	113.95
1	A2	510	OMG	C8-N7-C5	2.29	107.35	102.99
39	B5	1266	1MA	C5-C6-N1	2.29	117.31	113.90
1	A2	1327	OMU	O2-C2-N1	-2.28	119.76	122.79
1	A2	429	OMU	O2-C2-N1	-2.28	119.76	122.79
1	A2	1448	OMG	C8-N7-C5	2.28	107.33	102.99
1	A2	510	OMG	C5-C6-N1	2.28	117.97	113.95
39	B5	4240	OMG	C5-C6-N1	2.28	117.97	113.95
39	B5	3524	OMG	C5-C6-N1	2.27	117.97	113.95
39	B5	1266	1MA	C8-N7-C5	2.27	107.32	102.99
1	A2	1448	OMG	C5-C6-N1	2.27	117.95	113.95
1	A2	1491	OMG	C8-N7-C5	2.27	107.31	102.99
39	B5	2265	OMC	O2-C2-N3	-2.26	118.65	122.33
39	B5	4245	OMG	C5-C6-N1	2.25	117.93	113.95
39	B5	2194	OMC	O2-C2-N3	-2.25	118.67	122.33
39	B5	3514	5MC	O2-C2-N3	-2.25	118.67	122.33
39	B5	3974	OMG	C5-C6-N1	2.25	117.92	113.95
39	B5	3631	OMG	C5-C6-N1	2.25	117.92	113.95
39	B5	2207	OMG	C5-C6-N1	2.24	117.92	113.95
39	B5	4244	OMU	O2-C2-N1	-2.24	119.81	122.79
39	B5	2267	OMG	C8-N7-C5	2.24	107.25	102.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	B5	3524	OMG	C8-N7-C5	2.23	107.23	102.99
35	Aw	62	HY3	O-C-CA	-2.22	118.63	124.83
39	B5	3942	OMG	C8-N7-C5	2.22	107.21	102.99
83	Br	2	SAC	O-C-CA	-2.19	119.03	124.78
39	B5	3550	UY1	CM2-O2'-C2'	-2.17	108.83	114.52
39	B5	2680	OMU	O2-C2-N1	-2.16	119.92	122.79
1	A2	1833	6MZ	C4-C5-N7	-2.15	107.16	109.40
39	B5	4267	PSU	C5-C6-N1	-2.15	118.89	122.11
1	A2	1704	OMC	O2-C2-N3	-2.14	118.84	122.33
1	A2	628	OMU	O2-C2-N1	-2.12	119.97	122.79
1	A2	1392	OMC	O2-C2-N3	-2.10	118.91	122.33
1	A2	1843	4AC	C5-C4-N4	-2.09	119.29	122.92
1	A2	1249	B8N	C5-C4-N3	2.09	120.04	116.17
1	A2	1833	6MZ	C9-N6-C6	-2.08	121.08	122.87
1	A2	823	PSU	O4'-C1'-C2'	2.07	108.06	105.14
39	B5	1632	PSU	C5-C6-N1	-2.07	119.01	122.11
39	B5	1266	1MA	N1-C2-N3	-2.06	123.62	126.02
39	B5	3369	PSU	C5-C6-N1	-2.05	119.03	122.11
39	B5	3657	OMU	O2-C2-N1	-2.05	120.06	122.79
39	B5	1801	PSU	C5-C6-N1	-2.04	119.04	122.11
1	A2	652	PSU	C5-C6-N1	-2.03	119.06	122.11
39	B5	1721	PSU	C5-C6-N1	-2.03	119.07	122.11
1	A2	1446	PSU	C5-C6-N1	-2.03	119.07	122.11
1	A2	116	OMU	O2-C2-N1	-2.03	120.09	122.79
1	A2	650	PSU	C5-C6-N1	-2.02	119.07	122.11
39	B5	3540	OMC	O2-C2-N3	-2.02	119.04	122.33
39	B5	4149	PSU	C5-C6-N1	-2.02	119.07	122.11
39	B5	4052	OMU	C1'-N1-C2	2.02	121.23	117.57
39	B5	2194	OMC	C1'-N1-C2	2.01	122.92	118.42
39	B5	4711	PSU	C5-C6-N1	-2.01	119.09	122.11
39	B5	3466	PSU	C5-C6-N1	-2.01	119.09	122.11
39	B5	3942	OMG	O6-C6-C5	-2.01	120.44	124.37
39	B5	2667	OMC	O2-C2-N3	-2.01	119.07	122.33
39	B5	3496	PSU	C5-C6-N1	-2.00	119.10	122.11
41	B8	55	PSU	C5-C6-N1	-2.00	119.11	122.11

There are no chirality outliers.

All (118) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A2	159	A2M	C1'-C2'-O2'-CM'
1	A2	429	OMU	C2'-C1'-N1-C2

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Mol	Chain	Res	Type	Atoms
1	A2	429	OMU	C2'-C1'-N1-C6
1	A2	513	A2M	O4'-C4'-C5'-O5'
1	A2	645	OMG	O4'-C4'-C5'-O5'
1	A2	645	OMG	C3'-C4'-C5'-O5'
39	B5	2207	OMG	O4'-C4'-C5'-O5'
39	B5	3433	OMC	C2'-C1'-N1-C2
39	B5	3433	OMC	C2'-C1'-N1-C6
39	B5	4166	PSU	C2'-C1'-C5-C4
39	B5	4382	PSU	O4'-C1'-C5-C4
39	B5	4382	PSU	O4'-C1'-C5-C6
39	B5	4382	PSU	C3'-C4'-C5'-O5'
43	BB	245	HIC	CA-CB-CG-ND1
1	A2	1249	B8N	N34-C33-C34-O35
1	A2	1338	4AC	N3-C4-N4-C7
1	A2	1338	4AC	C5-C4-N4-C7
1	A2	1338	4AC	O7-C7-N4-C4
1	A2	1338	4AC	CM7-C7-N4-C4
1	A2	1843	4AC	N3-C4-N4-C7
1	A2	1843	4AC	C5-C4-N4-C7
42	BA	216	V5N	O-C-CA-CB
39	B5	4336	A2M	C4'-C5'-O5'-P
1	A2	99	A2M	O4'-C4'-C5'-O5'
1	A2	669	A2M	O4'-C4'-C5'-O5'
1	A2	669	A2M	C3'-C4'-C5'-O5'
39	B5	2207	OMG	C3'-C4'-C5'-O5'
39	B5	2658	A2M	O4'-C4'-C5'-O5'
39	B5	2658	A2M	C3'-C4'-C5'-O5'
44	BC	2	AYA	CM-CT-N-CA
44	BC	2	AYA	OT-CT-N-CA
33	Au	1	AME	CT2-CT1-N-CA
33	Au	1	AME	OT-CT1-N-CA
1	A2	1249	B8N	N34-C33-C34-O36
1	A2	513	A2M	C3'-C4'-C5'-O5'
1	A2	684	OMG	O4'-C4'-C5'-O5'
1	A2	1448	OMG	C3'-C4'-C5'-O5'
39	B5	398	A2M	O4'-C4'-C5'-O5'
39	B5	4382	PSU	O4'-C4'-C5'-O5'
39	B5	4193	5MC	C2'-C1'-N1-C6
1	A2	577	A2M	C3'-C4'-C5'-O5'
39	B5	1632	PSU	C3'-C4'-C5'-O5'
39	B5	1632	PSU	O4'-C4'-C5'-O5'
39	B5	3599	A2M	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
1	A2	577	A2M	O4'-C4'-C5'-O5'
1	A2	1448	OMG	O4'-C4'-C5'-O5'
1	A2	1704	OMC	O4'-C4'-C5'-O5'
39	B5	398	A2M	C3'-C4'-C5'-O5'
39	B5	3494	PSU	C3'-C4'-C5'-O5'
1	A2	684	OMG	C3'-C4'-C5'-O5'
39	B5	4269	A2M	O4'-C4'-C5'-O5'
1	A2	99	A2M	C3'-C4'-C5'-O5'
1	A2	1443	OMU	C1'-C2'-O2'-CM2
1	A2	1852	MA6	C4'-C5'-O5'-P
44	BC	2	AYA	C-CA-N-CT
39	B5	3576	PSU	C4'-C5'-O5'-P
39	B5	4246	PSU	C4'-C5'-O5'-P
39	B5	3550	UY1	C4'-C5'-O5'-P
12	AZ	2	SAC	C-CA-N-C1A
39	B5	4193	5MC	C2'-C1'-N1-C2
39	B5	1260	OMG	C3'-C2'-O2'-CM2
39	B5	1820	OMC	C3'-C2'-O2'-CM2
39	B5	3540	OMC	C3'-C2'-O2'-CM2
39	B5	3631	OMG	C3'-C2'-O2'-CM2
39	B5	3973	OMU	C3'-C2'-O2'-CM2
39	B5	4193	5MC	O4'-C1'-N1-C6
69	Bb	5	MLZ	N-CA-CB-CG
1	A2	1249	B8N	C32-C33-C34-O36
69	Bb	5	MLZ	C-CA-CB-CG
1	A2	645	OMG	C4'-C5'-O5'-P
39	B5	4193	5MC	O4'-C1'-N1-C2
39	B5	3494	PSU	O4'-C4'-C5'-O5'
39	B5	3433	OMC	O4'-C1'-N1-C6
1	A2	1249	B8N	C32-C33-C34-O35
1	A2	628	OMU	C2'-C1'-N1-C6
1	A2	429	OMU	O4'-C4'-C5'-O5'
1	A2	684	OMG	C3'-C2'-O2'-CM2
1	A2	1448	OMG	C3'-C2'-O2'-CM2
1	A2	1491	OMG	C3'-C2'-O2'-CM2
39	B5	2680	OMU	C3'-C2'-O2'-CM2
39	B5	3619	OMC	C3'-C2'-O2'-CM2
39	B5	4369	OMG	C3'-C2'-O2'-CM2
1	A2	429	OMU	O4'-C1'-N1-C6
1	A2	116	OMU	C3'-C2'-O2'-CM2
1	A2	1289	OMU	C3'-C2'-O2'-CM2
1	A2	1443	OMU	C3'-C2'-O2'-CM2

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Mol	Chain	Res	Type	Atoms
39	B5	1810	A2M	C3'-C2'-O2'-CM'
39	B5	2667	OMC	C3'-C2'-O2'-CM2
39	B5	3557	A2M	C3'-C2'-O2'-CM'
39	B5	1489	A2M	O4'-C4'-C5'-O5'
39	B5	3599	A2M	O4'-C4'-C5'-O5'
1	A2	1833	6MZ	N1-C6-N6-C9
39	B5	3433	OMC	O4'-C1'-N1-C2
1	A2	628	OMU	O4'-C1'-N1-C6
1	A2	510	OMG	O4'-C4'-C5'-O5'
39	B5	4278	PSU	C3'-C4'-C5'-O5'
1	A2	1704	OMC	C3'-C4'-C5'-O5'
39	B5	1284	OMC	C1'-C2'-O2'-CM2
39	B5	1810	A2M	C1'-C2'-O2'-CM'
39	B5	1284	OMC	C3'-C2'-O2'-CM2
39	B5	3619	OMC	C4'-C5'-O5'-P
39	B5	4278	PSU	O4'-C4'-C5'-O5'
35	Aw	62	HY3	O-C-CA-C3
39	B5	1632	PSU	O4'-C1'-C5-C6
39	B5	2194	OMC	C2'-C1'-N1-C2
1	A2	429	OMU	O4'-C1'-N1-C2
1	A2	628	OMU	O4'-C1'-N1-C2
1	A2	1289	OMU	C4'-C5'-O5'-P
39	B5	2194	OMC	O4'-C4'-C5'-O5'
39	B5	3517	A2M	O4'-C4'-C5'-O5'
1	A2	469	A2M	C3'-C2'-O2'-CM'
39	B5	2265	OMC	C3'-C2'-O2'-CM2
39	B5	3476	OMG	C3'-C2'-O2'-CM2
39	B5	4383	OMG	C3'-C2'-O2'-CM2
41	B8	75	OMG	C3'-C2'-O2'-CM2
39	B5	4269	A2M	C3'-C4'-C5'-O5'
1	A2	429	OMU	C3'-C4'-C5'-O5'
39	B5	3450	A2M	O4'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry

Of 741 ligands modelled in this entry, 363 are monoatomic and 374 are unknown - leaving 4 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
94	SF4	Bz	1000	88	0,12,12	-	-	-	-	-
89	SPD	A2	1901	-	9,9,9	0.16	0	8,8,8	0.16	0
93	GTP	B7	201	40	26,34,34	0.95	2 (7%)	32,54,54	0.79	0
94	SF4	Bz	1001	88	0,12,12	-	-	-	-	-

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
94	SF4	Bz	1000	88	-	-	0/6/5/5
89	SPD	A2	1901	-	-	0/7/7/7	-
93	GTP	B7	201	40	-	0/18/38/38	0/3/3/3
94	SF4	Bz	1001	88	-	-	0/6/5/5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
93	B7	201	GTP	C5-C6	-2.61	1.42	1.47
93	B7	201	GTP	C8-N7	-2.08	1.31	1.35

There are no bond angle outliers.

There are no chirality outliers.

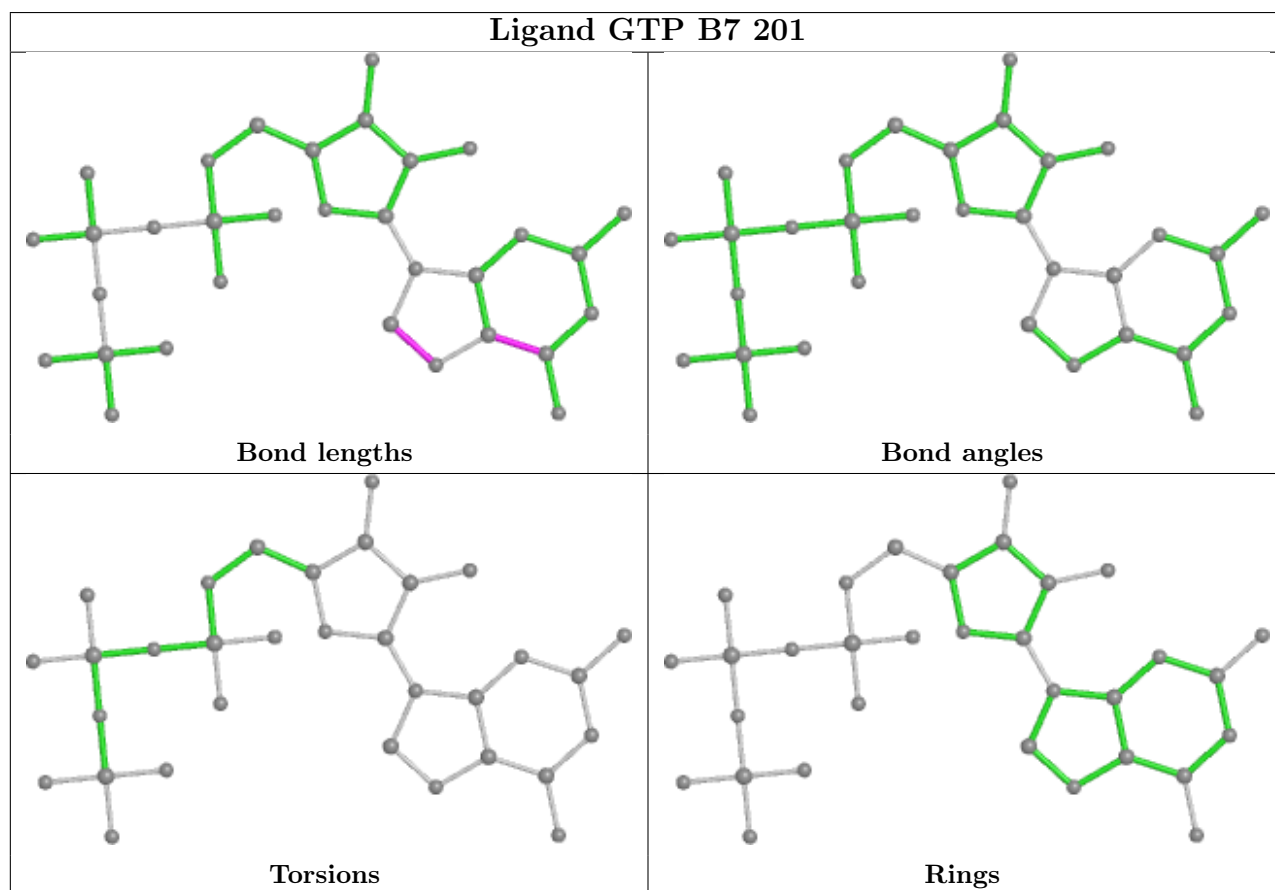
There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

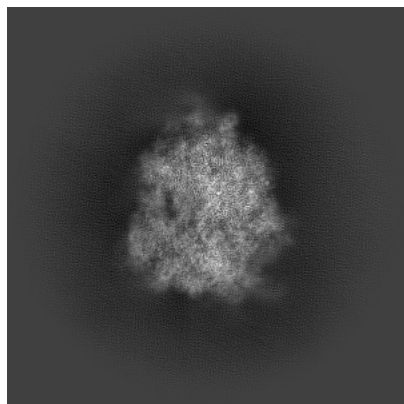
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12758. These allow visual inspection of the internal detail of the map and identification of artifacts.

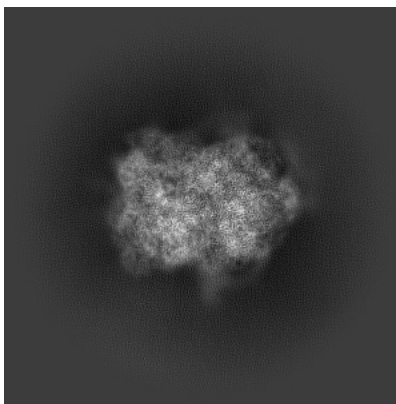
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

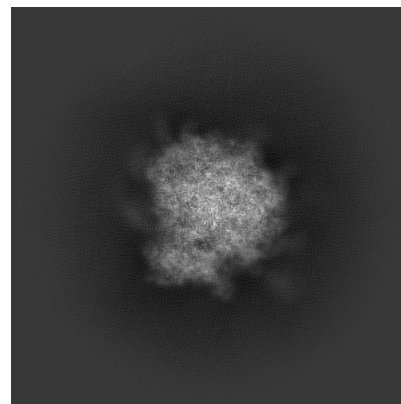
#### 6.1.1 Primary map



X

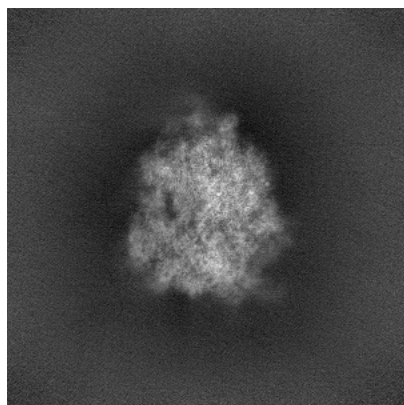


Y

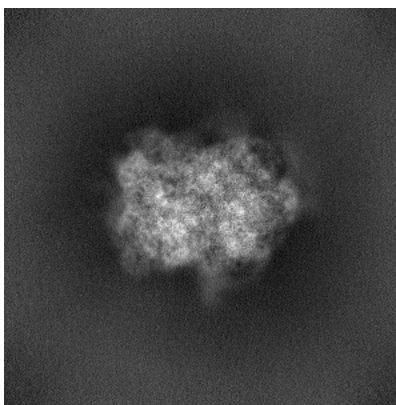


Z

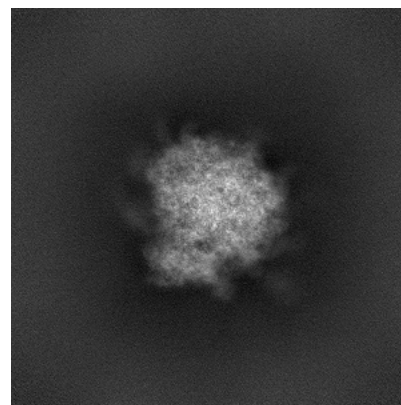
#### 6.1.2 Raw map



X



Y

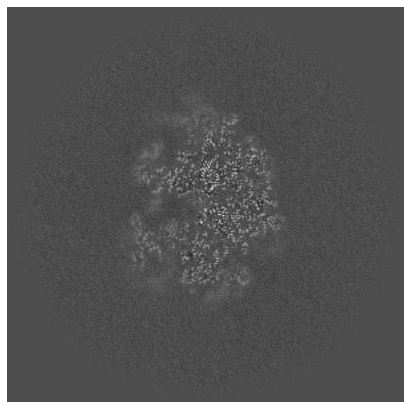


Z

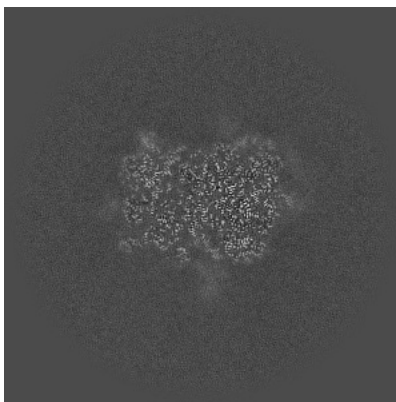
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

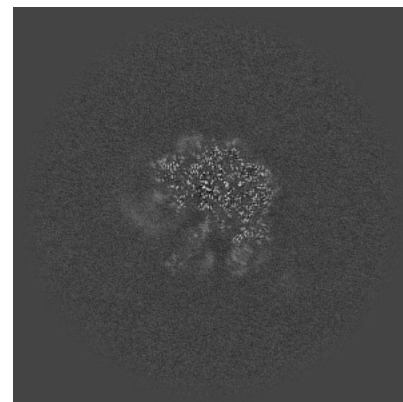
### 6.2.1 Primary map



X Index: 280

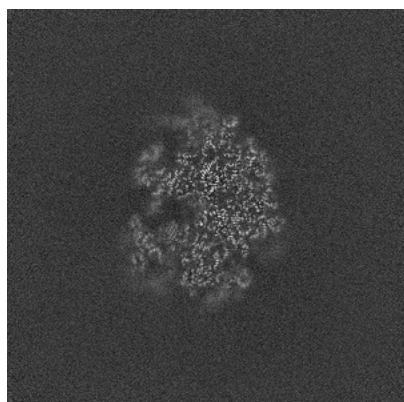


Y Index: 280

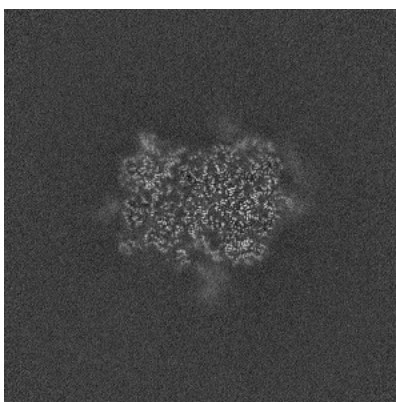


Z Index: 280

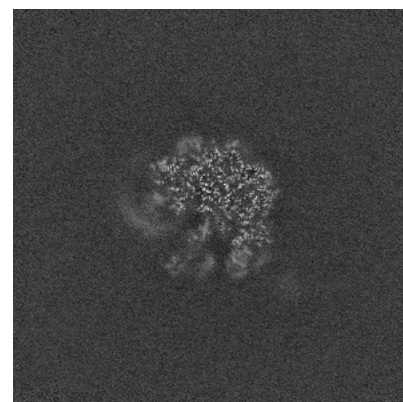
### 6.2.2 Raw map



X Index: 280



Y Index: 280

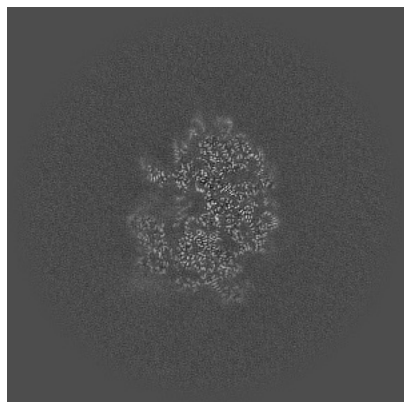


Z Index: 280

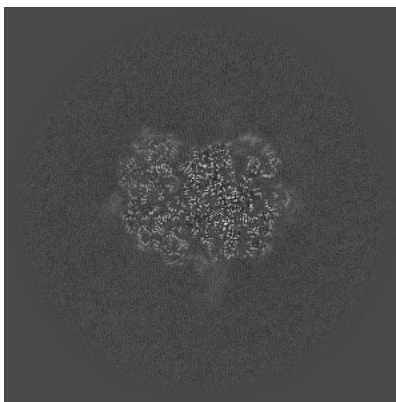
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

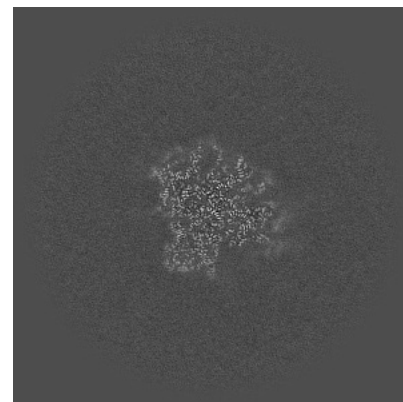
### 6.3.1 Primary map



X Index: 263

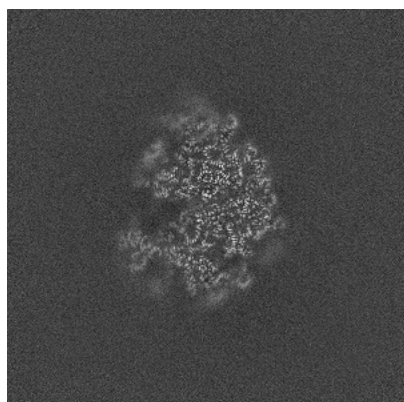


Y Index: 289

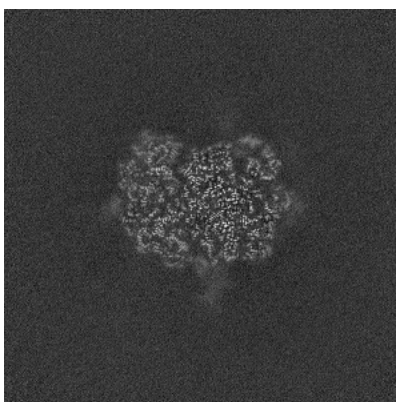


Z Index: 323

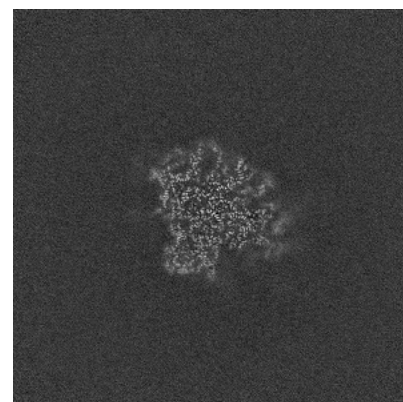
### 6.3.2 Raw map



X Index: 285



Y Index: 289

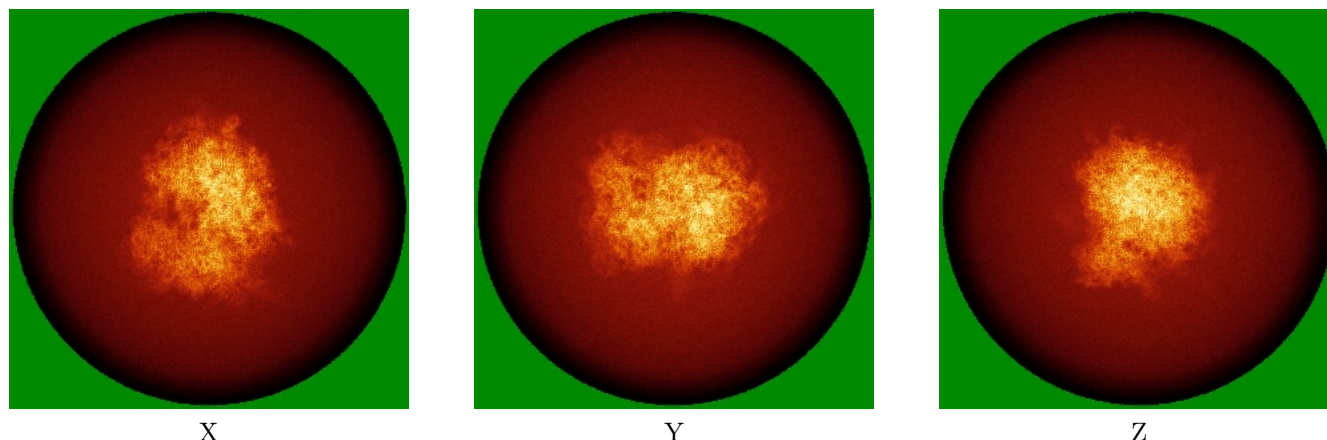


Z Index: 323

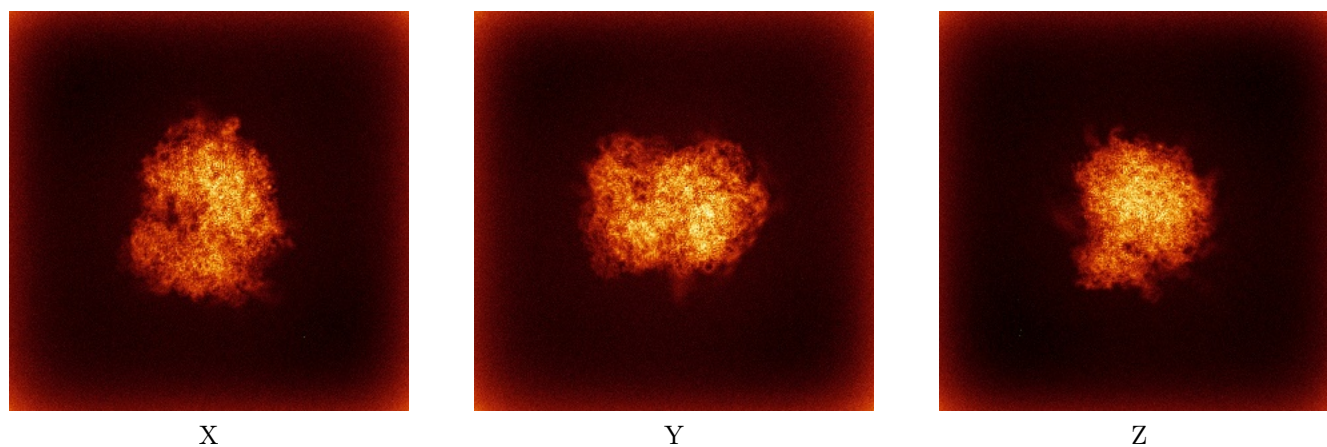
The images above show the largest variance slices of the map in three orthogonal directions.

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

### 6.4.1 Primary map



### 6.4.2 Raw map



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



## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.7. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



X



Y



Z

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

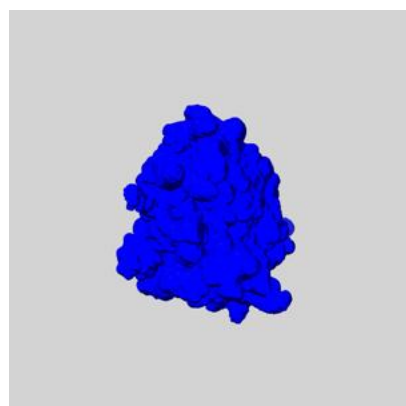
## 6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

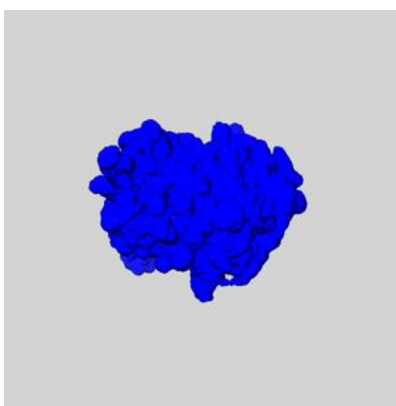
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

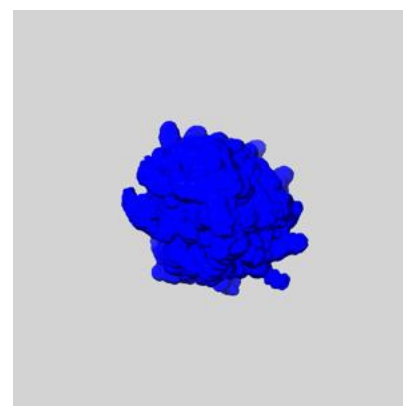
### 6.6.1 emd\_12758\_msk\_1.map [i](#)



X

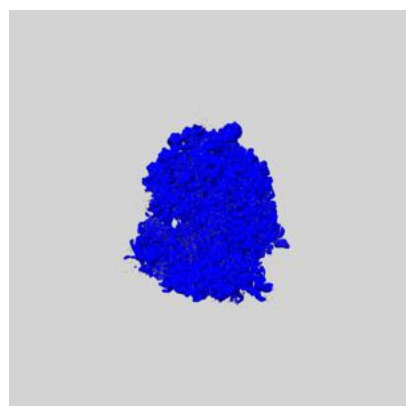


Y

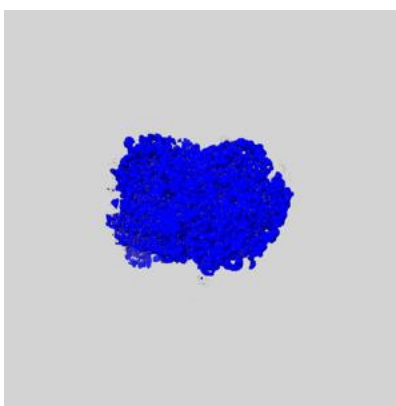


Z

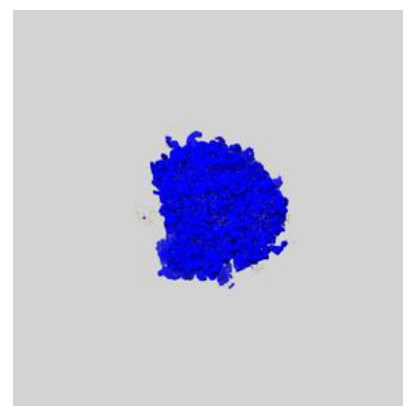
### 6.6.2 emd\_12758\_msk\_2.map [i](#)



X



Y

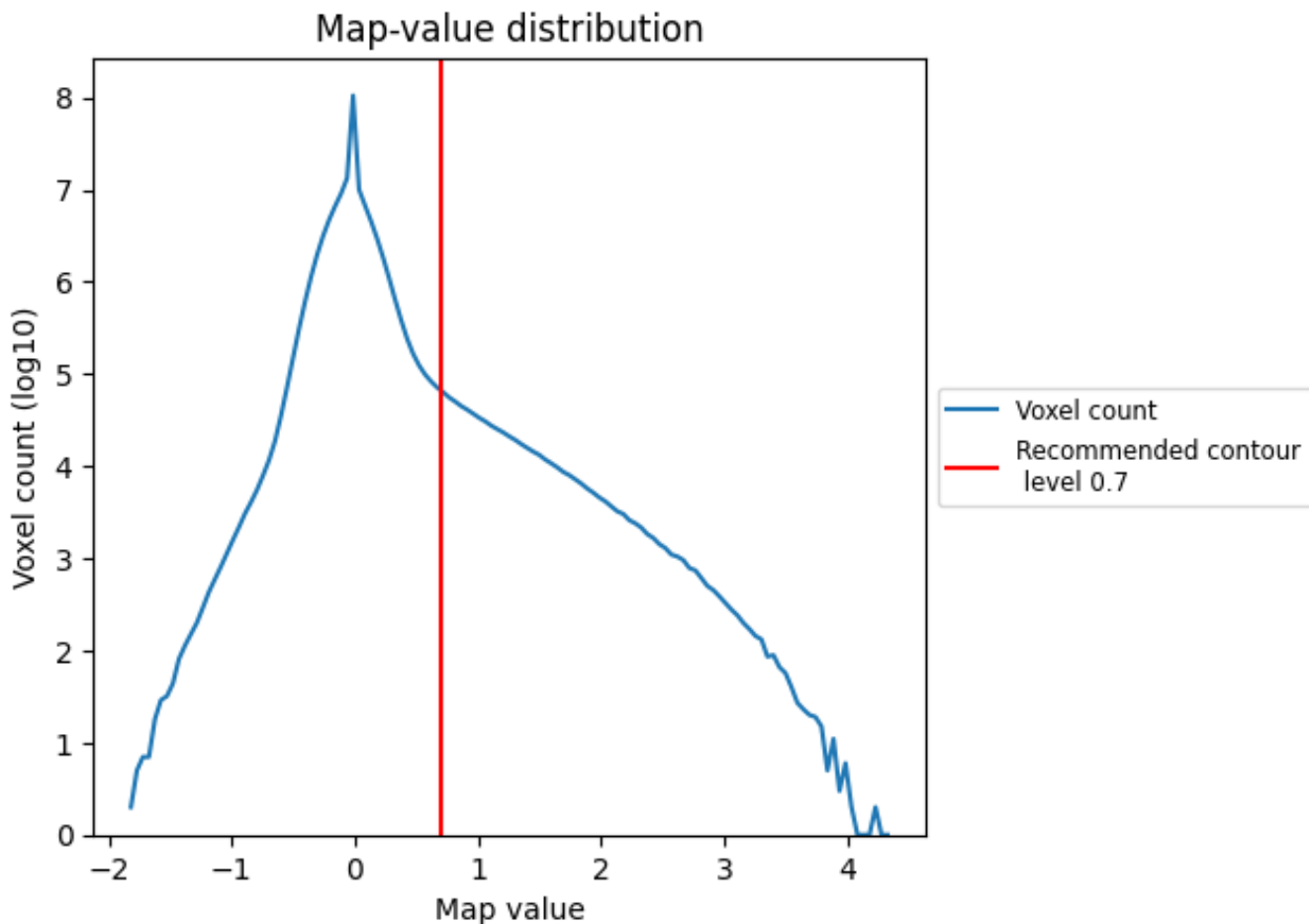


Z

## 7 Map analysis [i](#)

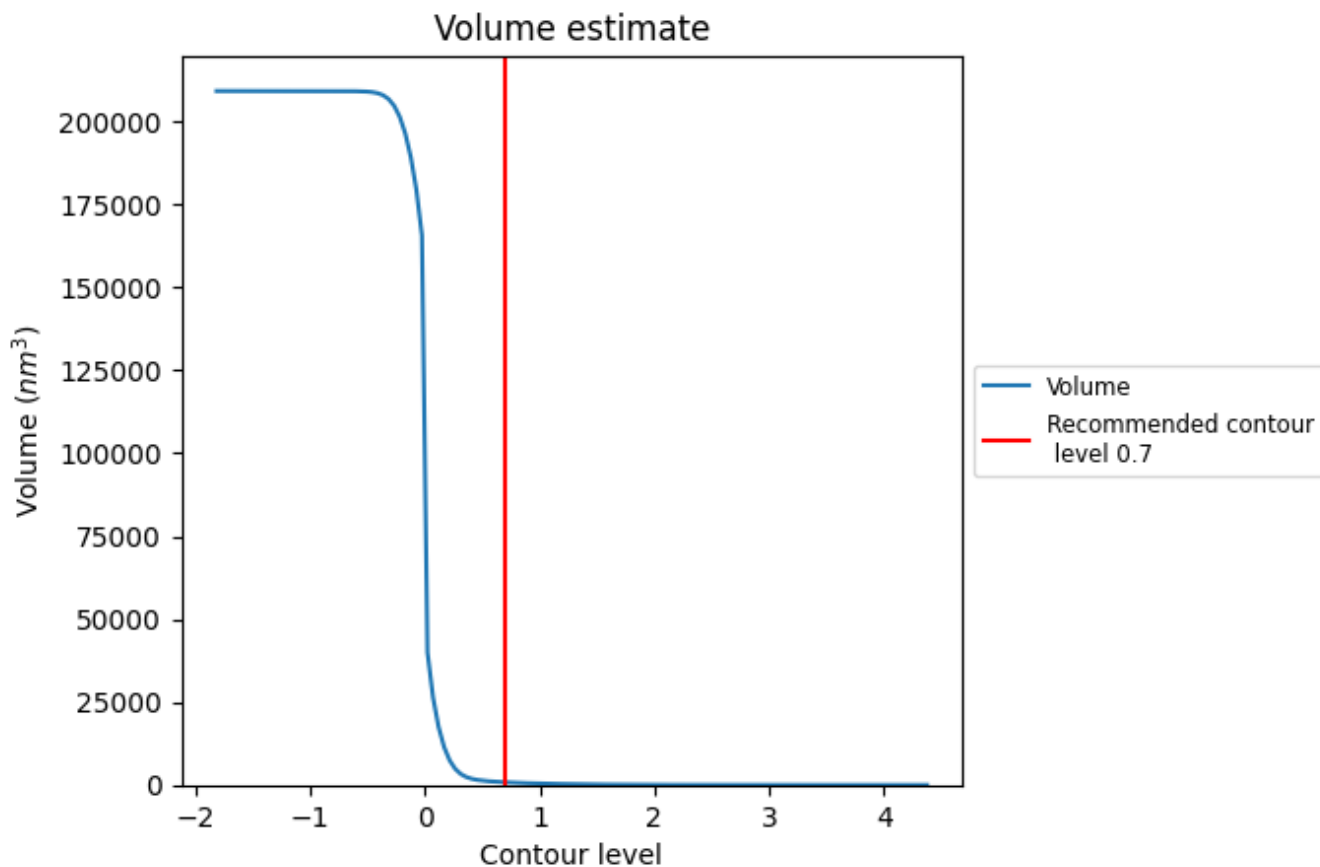
This section contains the results of statistical analysis of the map.

### 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.

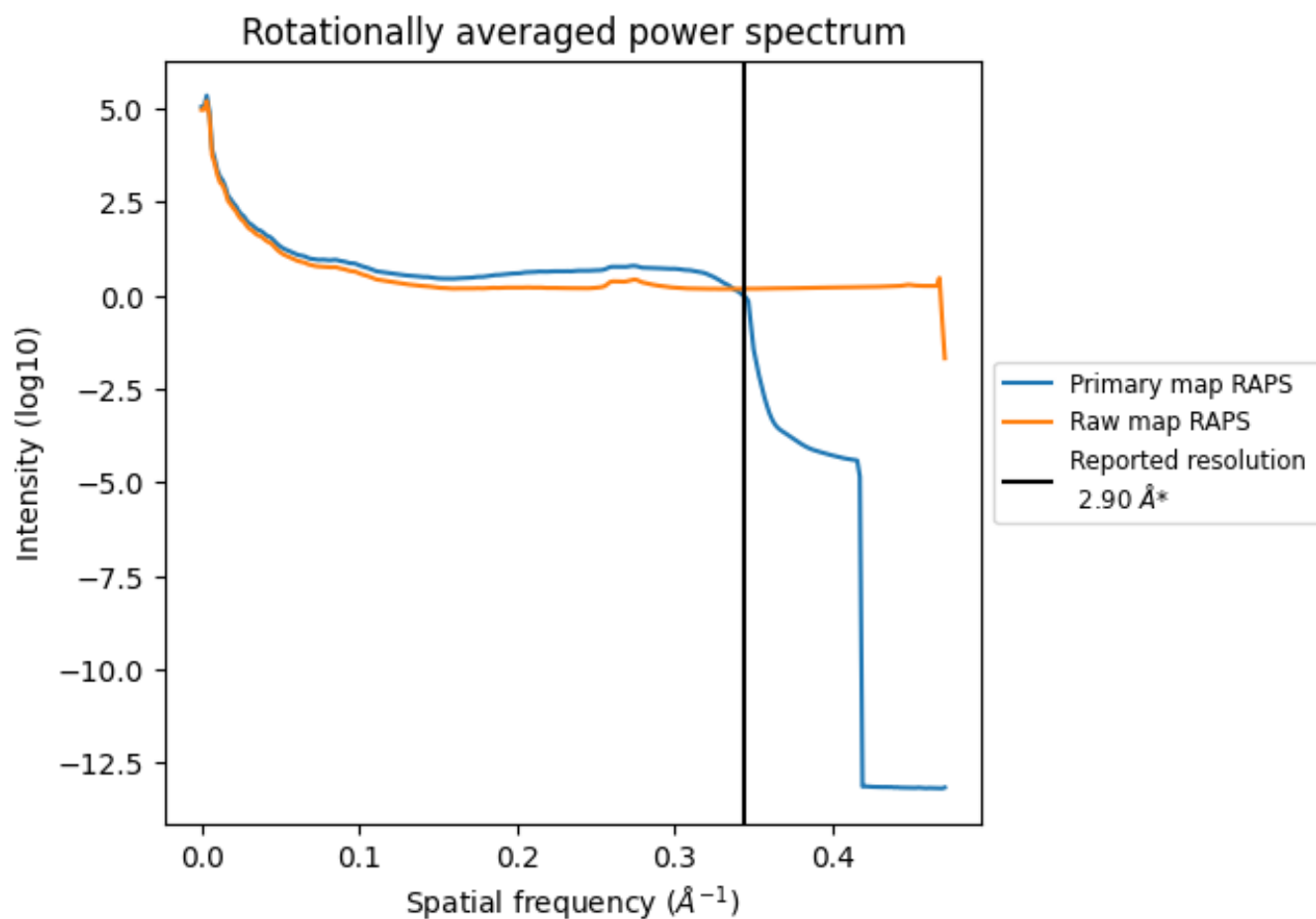
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is  $803 \text{ nm}^3$ ; this corresponds to an approximate mass of 726 kDa.

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

### 7.3 Rotationally averaged power spectrum i

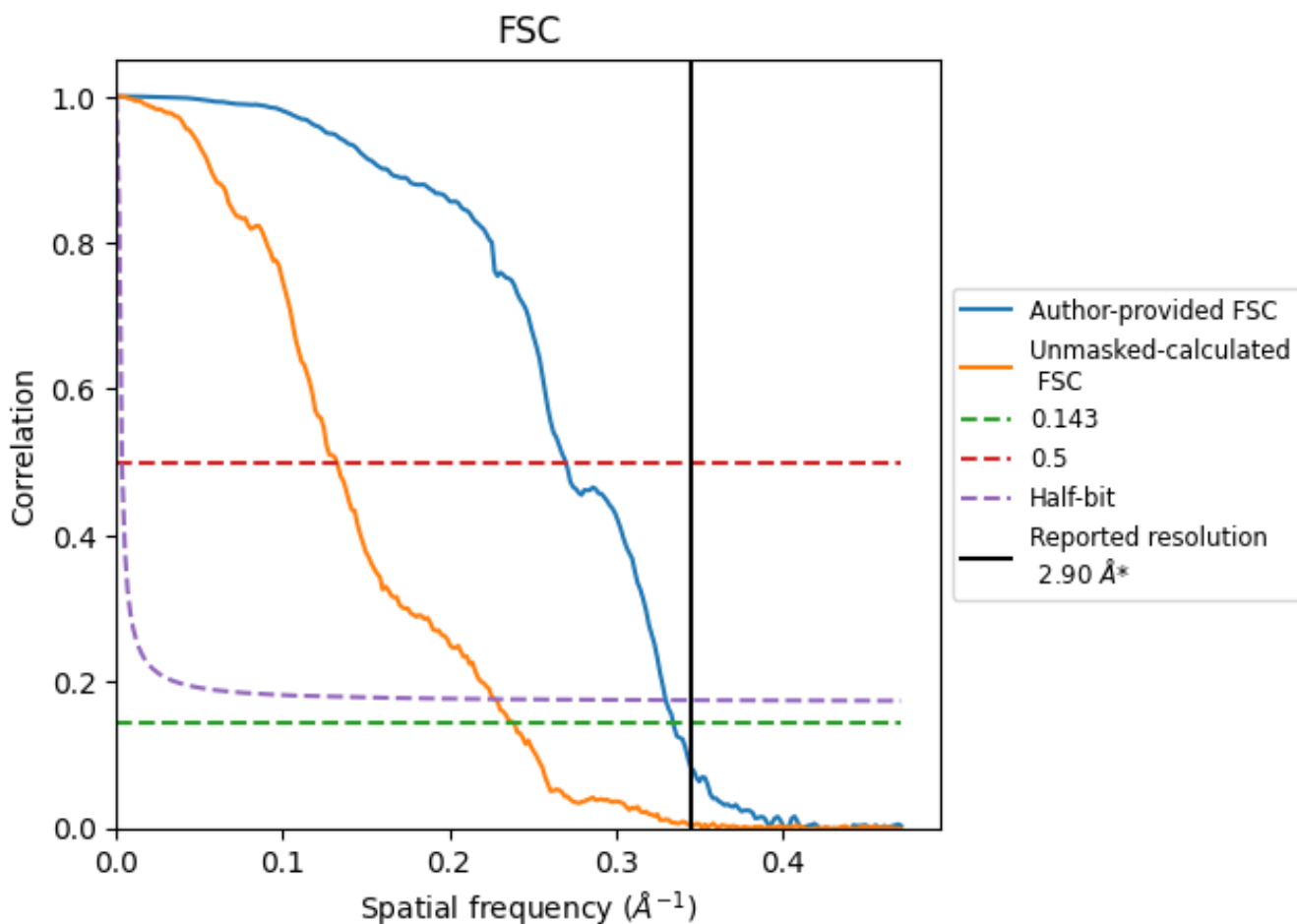


\*Reported resolution corresponds to spatial frequency of 0.345 Å<sup>-1</sup>

## 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 0.345 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

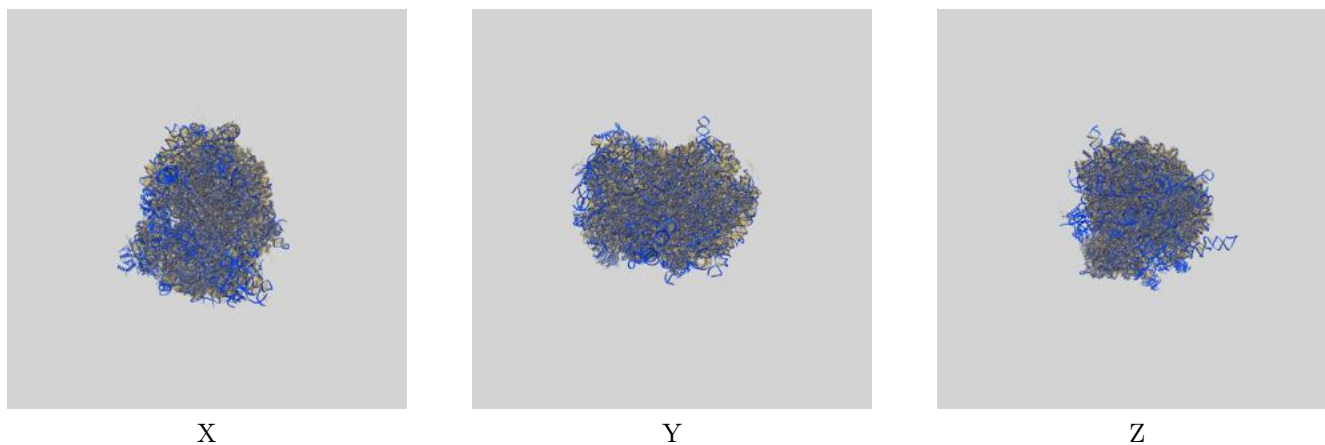
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	2.99	3.70	3.03
Unmasked-calculated*	4.18	7.56	4.39

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.18 differs from the reported value 2.9 by more than 10 %

## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-12758 and PDB model 7O80. Per-residue inclusion information can be found in section 3 on page 27.

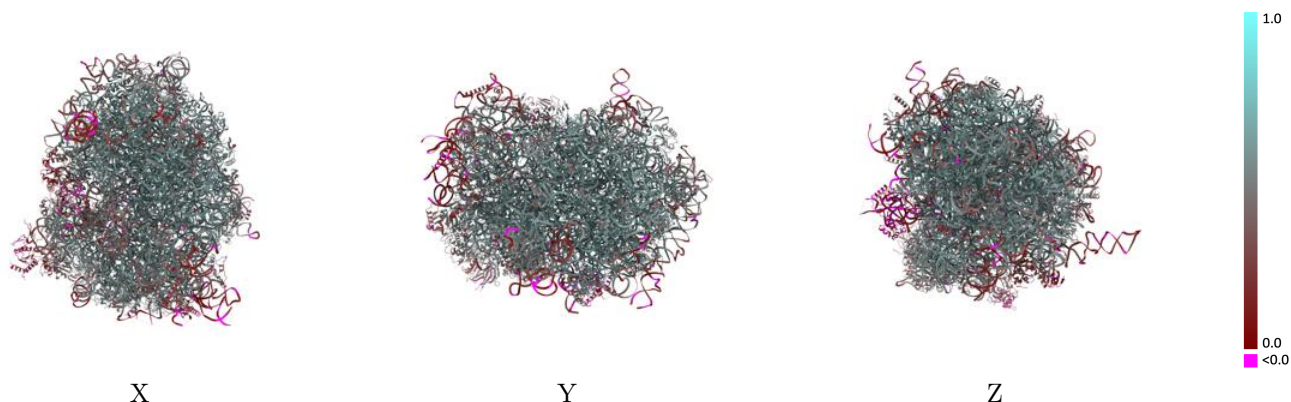
### 9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.7 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.

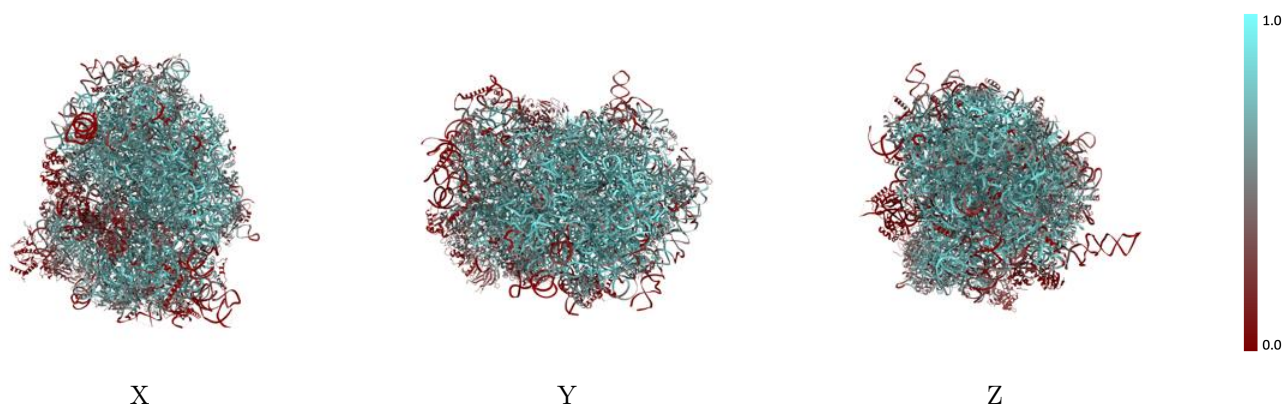


## 9.2 Q-score mapped to coordinate model [i](#)



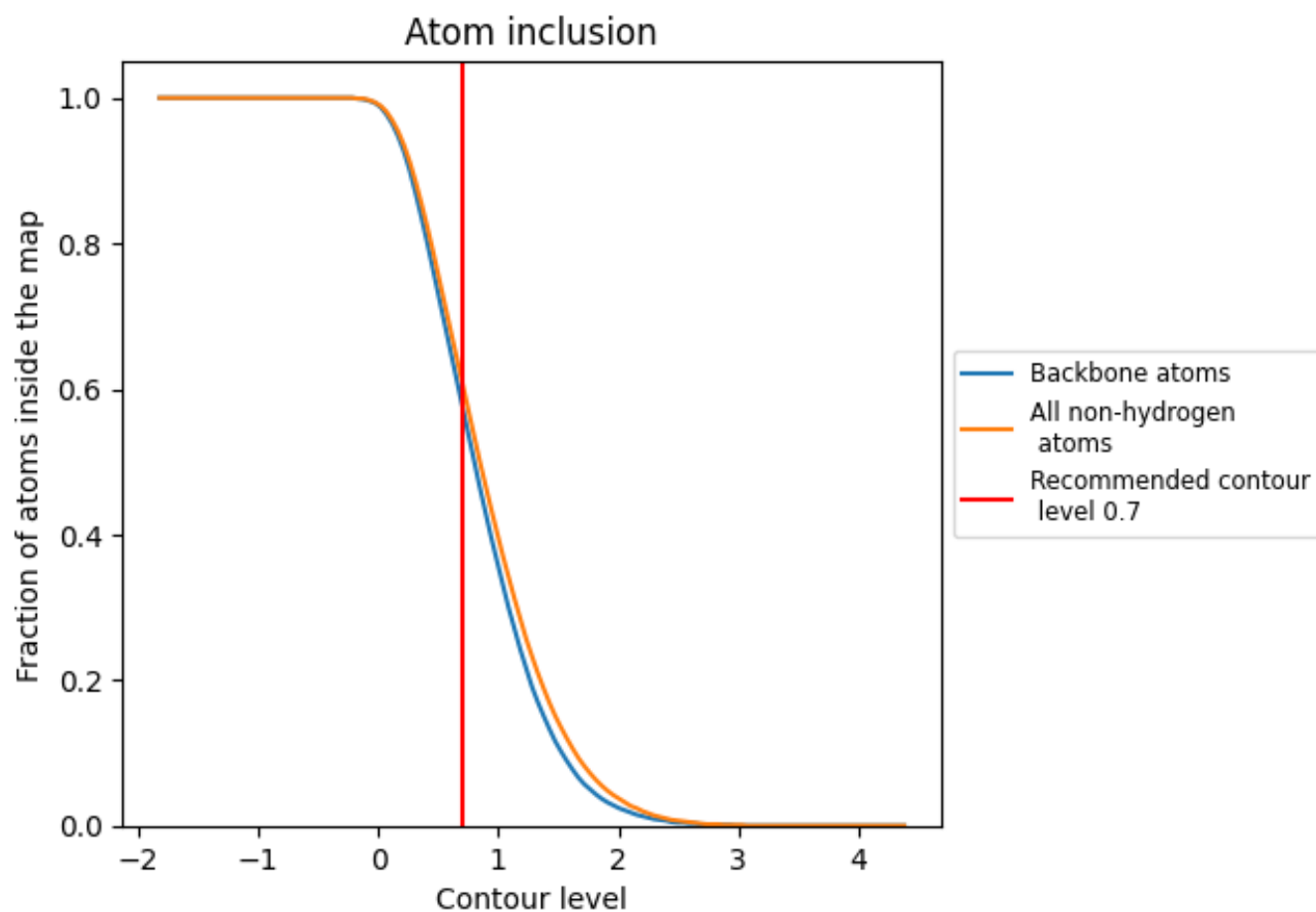
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.7).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 58% of all backbone atoms, 61% 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 (0.7) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6080	 0.4970
A2	 0.6790	 0.5030
AA	 0.4100	 0.4750
AB	 0.3560	 0.4680
AC	 0.0210	 0.1980
AD	 0.3750	 0.4330
AE	 0.5790	 0.5190
AF	 0.1850	 0.3450
AG	 0.5770	 0.5200
AH	 0.2650	 0.3280
AI	 0.0100	 0.1090
AT	 0.4490	 0.4340
AZ	 0.3900	 0.4760
Aa	 0.4740	 0.4800
Ab	 0.5260	 0.5200
Ac	 0.3110	 0.4240
Ad	 0.5380	 0.5060
Ae	 0.4370	 0.4700
Af	 0.3580	 0.4040
Ag	 0.2480	 0.3870
Ah	 0.5340	 0.4990
Ai	 0.5500	 0.4970
Aj	 0.2920	 0.3860
Ak	 0.5510	 0.4940
Al	 0.0050	 0.1510
Am	 0.5410	 0.5240
An	 0.5540	 0.5200
Ao	 0.3470	 0.4200
Ap	 0.4680	 0.4910
Aq	 0.2680	 0.4070
Ar	 0.4010	 0.4430
As	 0.4600	 0.4640
At	 0.2810	 0.4000
Au	 0.3950	 0.4780
Av	 0.6090	 0.5500



























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Chain	Atom inclusion	Q-score
Aw	0.5870	0.5400
Ax	0.4820	0.4650
Ay	0.3210	0.3960
Az	0.6560	0.5610
B5	0.7290	0.5210
B7	0.8580	0.5750
B8	0.7860	0.5590
BA	0.6980	0.5770
BB	0.6900	0.5650
BC	0.6970	0.5660
BD	0.5950	0.5100
BE	0.5100	0.4810
BF	0.7020	0.5670
BG	0.5180	0.4780
BH	0.5760	0.5180
BI	0.6030	0.5400
BJ	0.5070	0.4870
BK	0.0630	0.3010
BL	0.6260	0.5240
BM	0.6440	0.5360
BN	0.7770	0.5980
BO	0.7010	0.5720
BP	0.6800	0.5580
BQ	0.7070	0.5770
BR	0.6150	0.5190
BS	0.7060	0.5750
BT	0.6320	0.5470
BU	0.4380	0.4460
BV	0.6240	0.5550
BW	0.3690	0.3850
BX	0.6150	0.5370
BY	0.6650	0.5360
BZ	0.6100	0.5200
Ba	0.7550	0.5890
Bb	0.4760	0.4780
Bc	0.5350	0.4880
Bd	0.6380	0.5390
Be	0.7040	0.5740
Bf	0.7320	0.5880
Bg	0.6360	0.5480
Bh	0.6060	0.5260
Bi	0.5850	0.5210

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Chain	Atom inclusion	Q-score
Bj	 0.7770	 0.5920
Bk	 0.4340	 0.4540
Bl	 0.7070	 0.5710
Bm	 0.6160	 0.5460
Bo	 0.5960	 0.5370
Bp	 0.6310	 0.5550
Br	 0.6530	 0.5640
Bs	 0.0200	 0.1640
Bt	 0.0330	 0.2220
Bv	 0.0000	 0.0600
By	 0.2280	 0.4100
Bz	 0.2530	 0.3940