Full wwPDB EM Validation Report ⓘ

Apr 21, 2024 – 02:17 am BST

PDB ID	:	7O7Z
EMDB ID	:	EMD-12757
Title	:	Rabbit 80S ribosome stalled close to the mutated SARS-CoV-2 slippery site by a pseudoknot (classified for pseudoknot)
Authors	:	Bhatt, P.R.; Scaiola, A.; Leibundgut, M.A.; Atkins, J.F.; Ban, N.
Deposited on	:	2021-04-14
Resolution	:	2.40 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

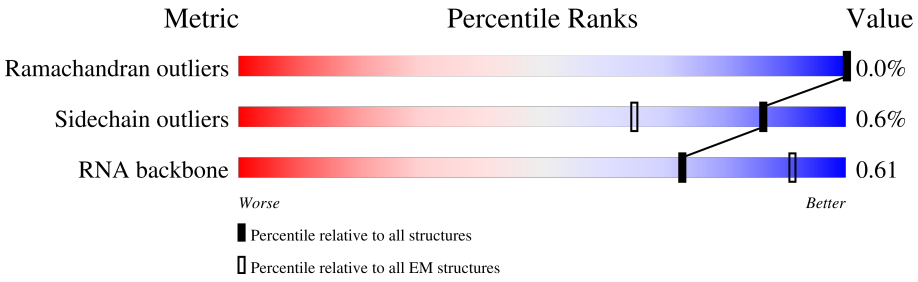
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



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

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

Mol	Chain	Length	Quality of chain
1	A2	1870	6% 78% 16% 5%
2	AA	84	7% 98%
3	AB	69	7% 90% 9%
4	AC	156	24% 47% 53%
5	AD	133	7% 42% 57%
6	AE	115	87% 12%
7	AF	317	9% 97%
8	AG	56	98%

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Mol	Chain	Length	Quality of chain
9	AH	220	22% 30% 14% 57%
10	AI	76	46% 99%
11	AT	76	5% 70% 26%
12	AZ	295	5% 73% 25%
13	Aa	264	84% 15%
14	Ab	293	74% 25%
15	Ac	281	6% 79% 20%
16	Ad	263	100%
17	Ae	204	5% 94% 6%
18	Af	249	8% 94% 5%
19	Ag	432	7% 44% 56%
20	Ah	208	99%
21	Ai	194	5% 95% 5%
22	Aj	165	58% 42%
23	Ak	158	11% 97%
24	Al	132	57% 92% 6%
25	Am	151	99%
26	An	151	89% 10%
27	Ao	145	88% 12%
28	Ap	172	81% 18%
29	Aq	135	8% 99%
30	Ar	152	6% 95%
31	As	145	99%
32	At	119	7% 86% 13%
33	Au	83	99%

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Mol	Chain	Length	Quality of chain
34	Av	130	99%
35	Aw	143	97%
36	Ax	130	96%
37	Ay	124	8% 69% 31%
38	Az	25	100%
39	B5	4808	5% 66% 12% 22%
40	B7	120	92% 8%
41	B8	158	85% 13%
42	BA	257	98%
43	BB	403	99%
44	BC	413	87% 12%
45	BD	297	99%
46	BE	291	8% 84% 16%
47	BF	247	91% 9%
48	BG	266	7% 87% 12%
49	BH	192	99%
50	BI	214	99%
51	BJ	178	95%
52	BK	1071	97%
53	BL	211	98%
54	BM	218	63% 37%
55	BN	204	100%
56	BO	203	98%
57	BP	184	86% 14%
58	BQ	188	99%

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Mol	Chain	Length	Quality of chain
59	BR	196	91% 8%
60	BS	176	100%
61	BT	160	99%
62	BU	128	77% 23%
63	BV	140	6% 99%
64	BW	157	38% 76% 23%
65	BX	156	76% 24%
66	BY	145	92% 8%
67	BZ	136	99%
68	Ba	148	98%
69	Bb	245	7% 44% 56%
70	Bc	115	11% 94% 6%
71	Bd	125	5% 86% 14%
72	Be	135	96%
73	Bf	110	100%
74	Bg	117	97%
75	Bh	123	99%
76	Bi	105	96%
77	Bj	97	89% 11%
78	Bk	70	99%
79	Bl	51	94%
80	Bm	128	41% 59%
81	Bo	106	98%
82	Bp	92	99%
83	Br	137	91% 8%

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Mol	Chain	Length	Quality of chain
84	Bs	318	62% 62% 38%
85	Bt	165	95% 94% 5%
86	Bv	217	95% 95%

2 Entry composition

There are 92 unique types of molecules in this entry. The entry contains 229742 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	74	610	385	117	101	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
6	AE	101	Total	C	N	O	S	0	0
			814	507	170	132	5		

- Molecule 7 is a protein called RACK1.

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

- Molecule 8 is a protein called uS14.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	AH	95	Total	C	N	O	P	0	0
			2018	901	349	673	95		

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
10	AI	76	Total	C	N	O	P	0	0
			939	393	11	459	76		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	AT	76	Total	C	N	O	P	0	0
			1652	746	294	536	76		

- 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 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
25	Am	150	Total	C	N	O	S	0	0
			1208	773	229	205	1		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Ao	128	Total	C	N	O	S	0	0
			1048	665	197	179	7		

- Molecule 28 is a protein called uS9.

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Ar	148	Total	C	N	O	S	0	0
			1217	763	245	208	1		

- Molecule 31 is a protein called Ribosomal protein eS19.

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

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

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

- Molecule 33 is a protein called Ribosomal protein eS21.

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

- Molecule 34 is a protein called Ribosomal protein S15a.

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

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

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

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

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

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

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

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

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

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

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

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.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	B7	120	Total	C	N	O	P	0	0
			2570	1141	456	851	122		

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

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

- Molecule 42 is a protein called Ribosomal protein uL2.

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

- Molecule 43 is a protein called Ribosomal protein L3.

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

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

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

- Molecule 45 is a protein called Ribosomal_L18_c domain-containing protein.

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

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
46	BE	243	Total	C	N	O	S	0	0
			1960	1258	378	321	3		

- Molecule 47 is a protein called Ribosomal Protein uL30.

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

- Molecule 48 is a protein called Ribosomal protein eL8.

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

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

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

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

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

- 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	35	Total	C	N	O	S	0	0
			265	163	45	51	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 uL13.

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 eL18.

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 eL20.

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
65	BX	118	Total	C	N	O	S	0	0
			967	618	181	167	1		

- Molecule 66 is a protein called Ribosomal protein L26.

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

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

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

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

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

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

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

- Molecule 70 is a protein called eL30.

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

- Molecule 71 is a protein called eL31.

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

- Molecule 72 is a protein called eL32.

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

- Molecule 73 is a protein called eL33.

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

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

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

- Molecule 75 is a protein called uL29.

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

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

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

- Molecule 77 is a protein called Ribosomal protein L37.

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

- Molecule 78 is a protein called eL38.

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

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
79	Bl	50	Total	C	N	O	S	0	0
			447	286	96	64	1		

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

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

- Molecule 81 is a protein called eL42.

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

- Molecule 82 is a protein called eL43.

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

- Molecule 83 is a protein called Ribosomal protein eL28.

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

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

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

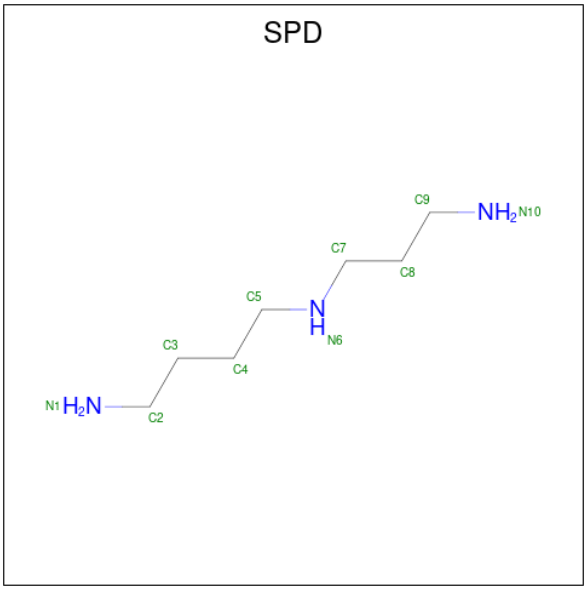
- Molecule 85 is a protein called Ribosomal protein L12.

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

- Molecule 86 is a protein called Ribosomal protein uL1.

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

- Molecule 87 is SPERMIDINE (three-letter code: SPD) (formula: $C_7H_{19}N_3$).



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

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Mol	Chain	Residues	Atoms	AltConf
87	B5	1	Total C N 10 7 3	0
87	B5	1	Total C N 10 7 3	0
87	B5	1	Total C N 10 7 3	0
87	B5	1	Total C N 10 7 3	0
87	B5	1	Total C N 10 7 3	0
87	B5	1	Total C N 10 7 3	0
87	B5	1	Total C N 10 7 3	0
87	B5	1	Total C N 10 7 3	0
87	B5	1	Total C N 10 7 3	0
87	B5	1	Total C N 10 7 3	0
87	B5	1	Total C N 10 7 3	0
87	B5	1	Total C N 10 7 3	0
87	B5	1	Total C N 10 7 3	0
87	B5	1	Total C N 10 7 3	0
87	B5	1	Total C N 10 7 3	0
87	B5	1	Total C N 10 7 3	0
87	B5	1	Total C N 10 7 3	0
87	B5	1	Total C N 10 7 3	0
87	B5	1	Total C N 10 7 3	0
87	B5	1	Total C N 10 7 3	0

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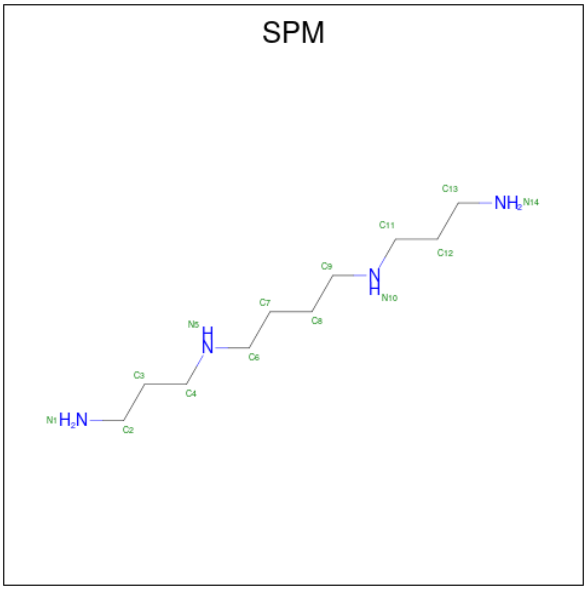
Mol	Chain	Residues	Atoms	AltConf
87	B5	1	Total C N 10 7 3	0

- Molecule 88 is SPERMINE (three-letter code: SPM) (formula: $C_{10}H_{26}N_4$).



Mol	Chain	Residues	Atoms	AltConf
88	A2	1	Total C N 14 10 4	0
88	B5	1	Total C N 14 10 4	0
88	B5	1	Total C N 14 10 4	0

- Molecule 89 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
89	A2	109	Total Mg 109 109	0
89	AH	1	Total Mg 1 1	0
89	AT	3	Total Mg 3 3	0
89	Af	1	Total Mg 1 1	0
89	B5	284	Total Mg 284 284	0

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Mol	Chain	Residues	Atoms	AltConf
89	B7	9	Total Mg 9 9	0
89	B8	9	Total Mg 9 9	0
89	BP	1	Total Mg 1 1	0
89	BR	1	Total Mg 1 1	0
89	BV	1	Total Mg 1 1	0
89	Ba	1	Total Mg 1 1	0

- Molecule 90 is UNKNOWN ATOM OR ION (three-letter code: UNX) (formula: X).

Mol	Chain	Residues	Atoms	AltConf
90	A2	60	Total X 60 60	0
90	AT	4	Total X 4 4	0
90	Ae	1	Total X 1 1	0
90	An	1	Total X 1 1	0
90	Ar	1	Total X 1 1	0
90	As	1	Total X 1 1	0
90	B5	225	Total X 225 225	0
90	B7	6	Total X 6 6	0
90	B8	8	Total X 8 8	0
90	BA	3	Total X 3 3	0
90	BB	4	Total X 4 4	0
90	BC	1	Total X 1 1	0
90	BH	1	Total X 1 1	0

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Mol	Chain	Residues	Atoms	AltConf
90	BI	1	Total X 1 1	0
90	BL	1	Total X 1 1	0
90	BN	1	Total X 1 1	0
90	BQ	2	Total X 2 2	0
90	BT	2	Total X 2 2	0
90	Bb	1	Total X 1 1	0
90	Be	1	Total X 1 1	0
90	Bf	1	Total X 1 1	0
90	Bg	1	Total X 1 1	0
90	Bl	1	Total X 1 1	0
90	Bo	1	Total X 1 1	0

- Molecule 91 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 92 is water.

Mol	Chain	Residues	Atoms	AltConf
92	A2	526	Total O 526 526	0
92	AH	9	Total O 9 9	0
92	AI	1	Total O 1 1	0
92	AT	12	Total O 12 12	0
92	Aa	1	Total O 1 1	0
92	Ac	1	Total O 1 1	0
92	Af	3	Total O 3 3	0
92	Ak	1	Total O 1 1	0
92	Am	1	Total O 1 1	0
92	An	2	Total O 2 2	0
92	Ap	3	Total O 3 3	0
92	As	2	Total O 2 2	0
92	At	1	Total O 1 1	0
92	Aw	3	Total O 3 3	0
92	B5	1391	Total O 1391 1391	0
92	B7	45	Total O 45 45	0
92	B8	50	Total O 50 50	0
92	BA	10	Total O 10 10	0
92	BB	5	Total O 5 5	0
92	BC	7	Total O 7 7	0
92	BD	1	Total O 1 1	0

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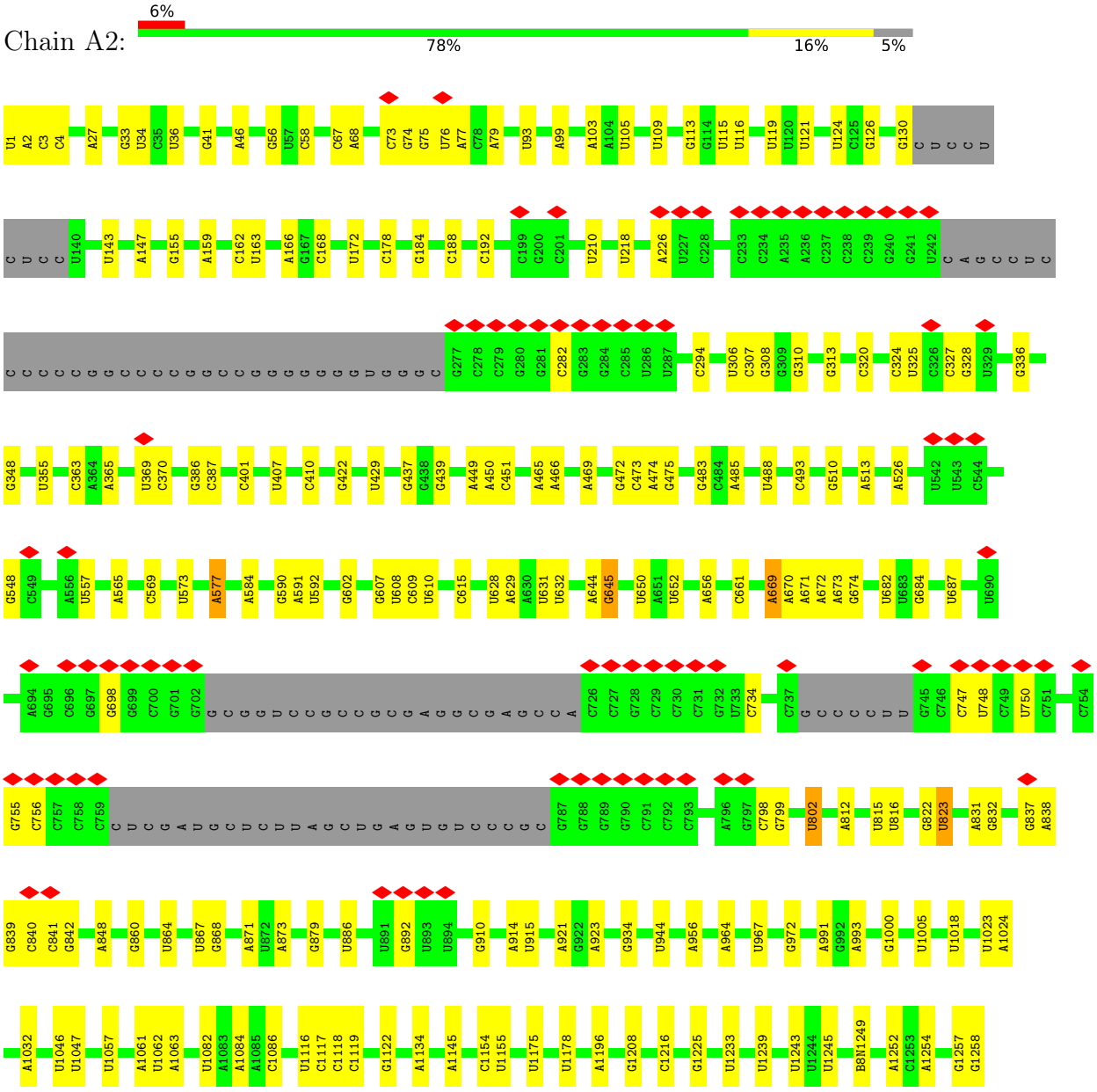
Mol	Chain	Residues	Atoms	AltConf
92	BF	1	Total O 1 1	0
92	BH	1	Total O 1 1	0
92	BI	4	Total O 4 4	0
92	BL	3	Total O 3 3	0
92	BN	3	Total O 3 3	0
92	BO	1	Total O 1 1	0
92	BP	2	Total O 2 2	0
92	BR	5	Total O 5 5	0
92	BV	2	Total O 2 2	0
92	BX	2	Total O 2 2	0
92	Ba	6	Total O 6 6	0
92	Bd	1	Total O 1 1	0
92	Be	4	Total O 4 4	0
92	Bg	2	Total O 2 2	0
92	Bj	3	Total O 3 3	0
92	Bl	1	Total O 1 1	0
92	Bo	1	Total O 1 1	0

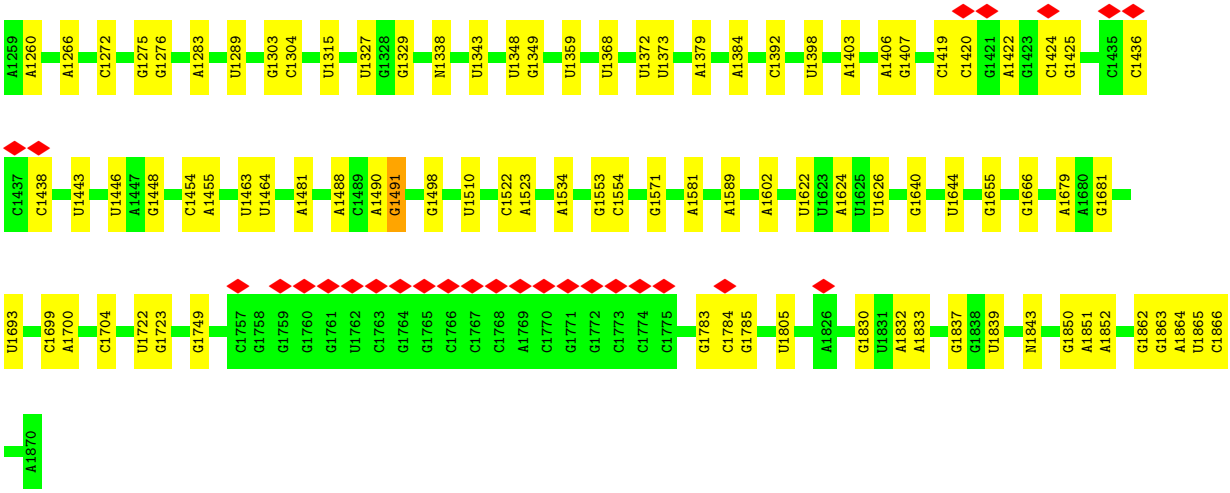
3 Residue-property plots (i)

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

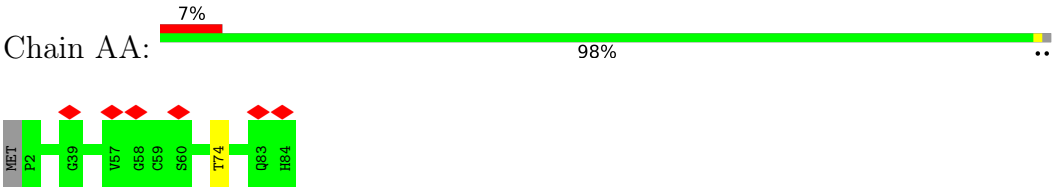
- Molecule 1: 18S rRNA

Chain A2:

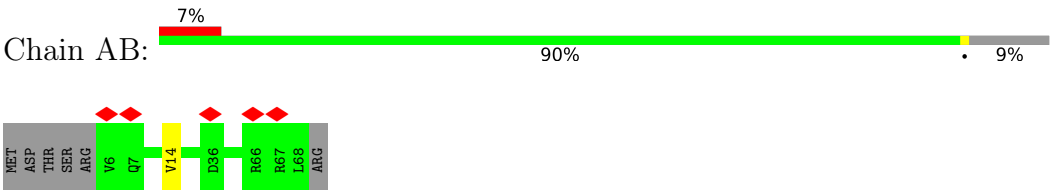




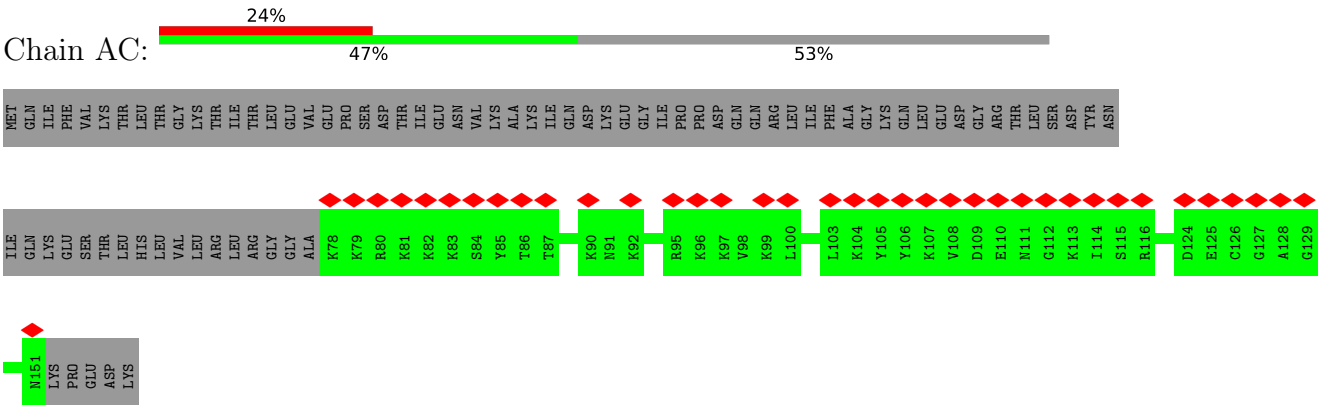
• Molecule 2: 40S ribosomal protein S27



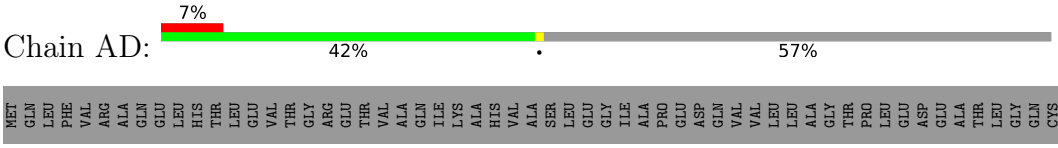
• Molecule 3: Ribosomal protein S28

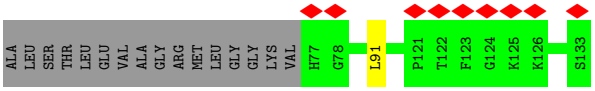


• Molecule 4: Ribosomal protein S27a



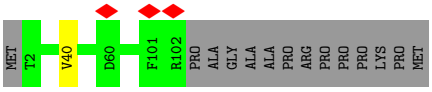
• Molecule 5: 40S ribosomal protein S30





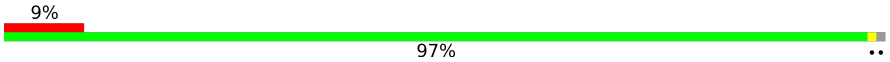
• Molecule 6: Ribosomal protein eS26

Chain AE:



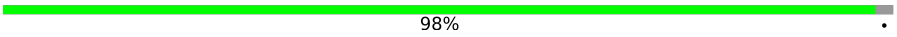
• Molecule 7: RACK1

Chain AF:



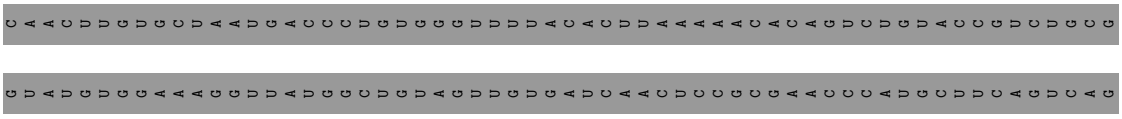
• Molecule 8: uS14

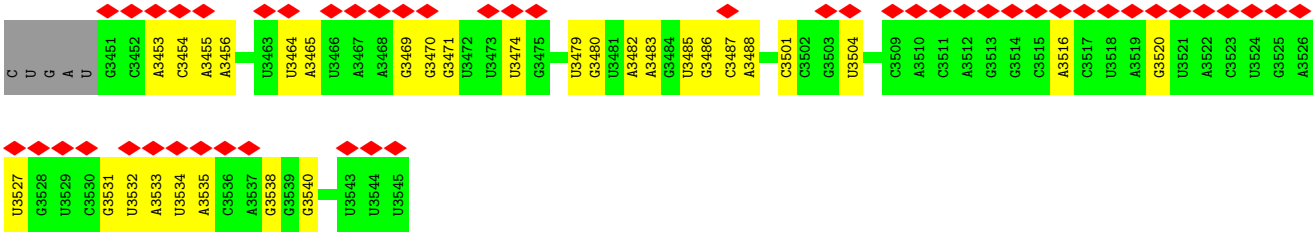
Chain AG:



• Molecule 9: mRNA containing SARS-CoV-2 sequence

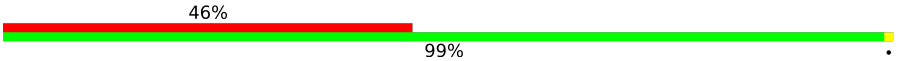
Chain AH:

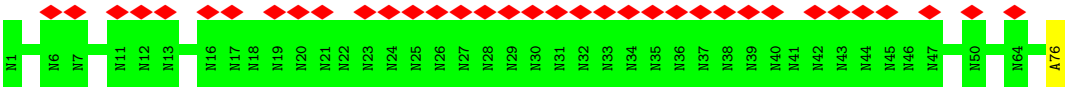




• Molecule 10: E-site tRNA

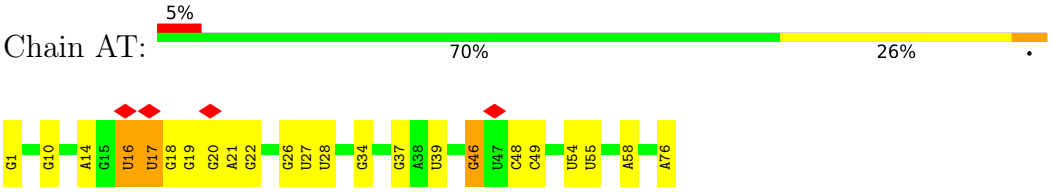
Chain AI:





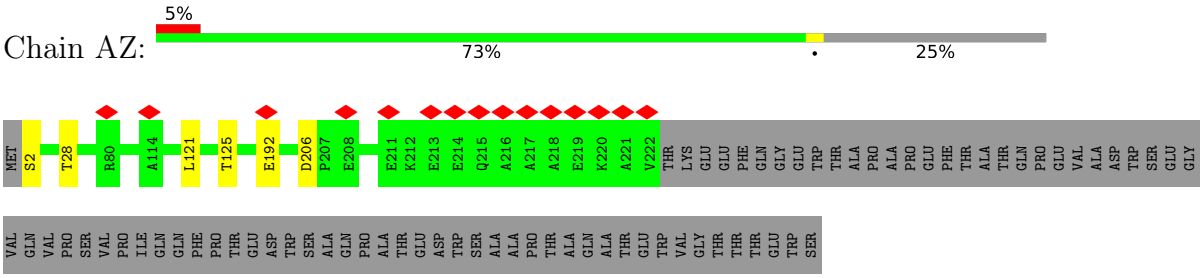
• Molecule 11: P-site Phe-tRNA(Phe)

Chain AT:



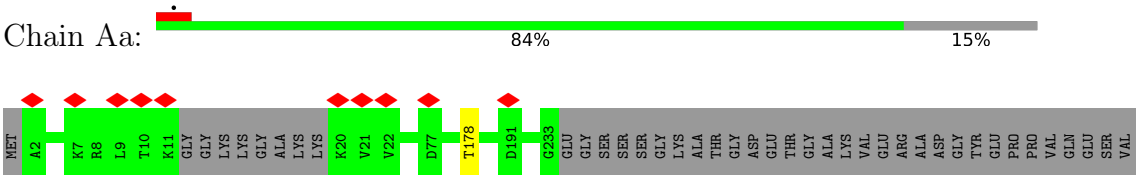
• Molecule 12: 40S ribosomal protein SA

Chain AZ:



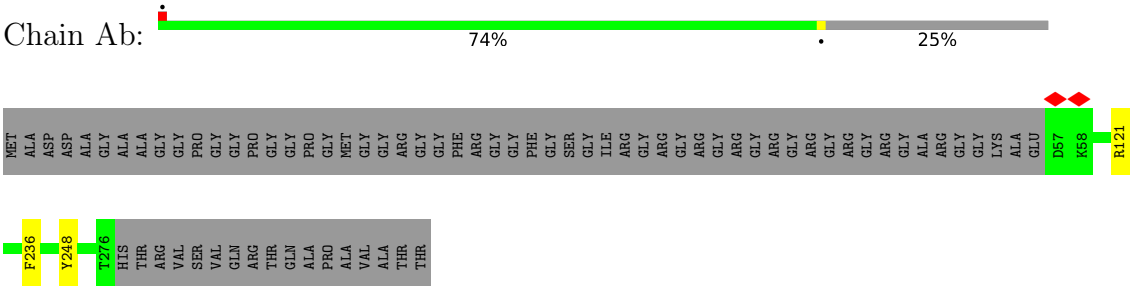
• Molecule 13: 40S ribosomal protein S3a

Chain Aa:



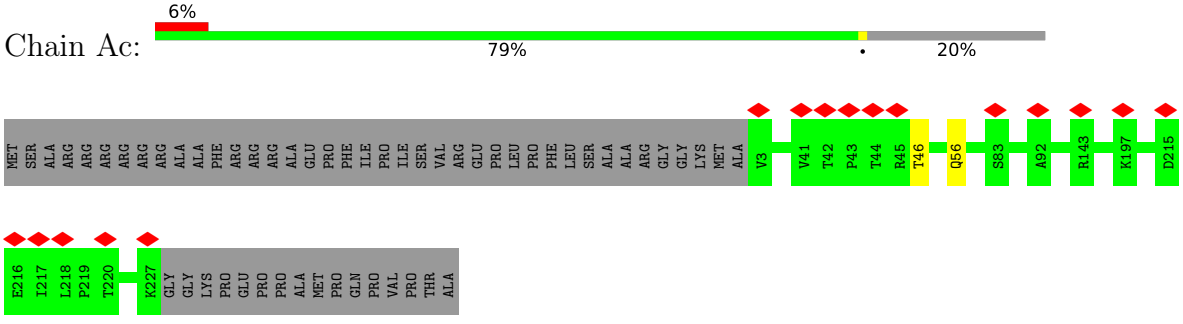
• Molecule 14: Ribosomal protein uS5

Chain Ab:



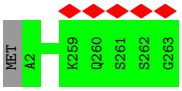
• Molecule 15: 40S ribosomal protein S3

Chain Ac:



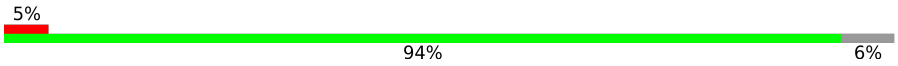
• Molecule 16: Ribosomal protein eS4

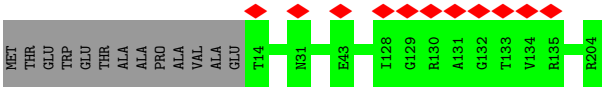
Chain Ad:



• Molecule 17: Ribosomal protein S5

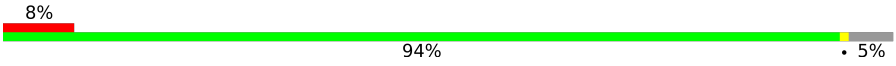
Chain Ae:

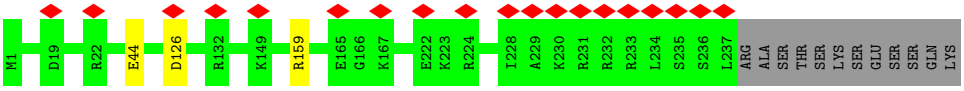




• Molecule 18: 40S ribosomal protein S6

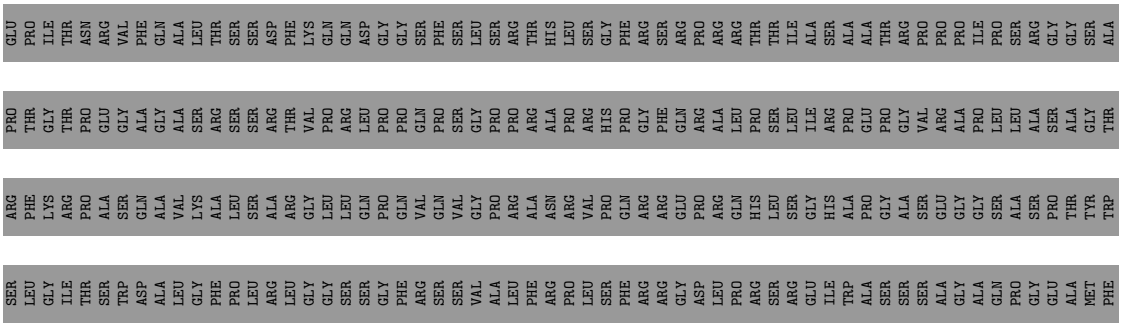
Chain Af:

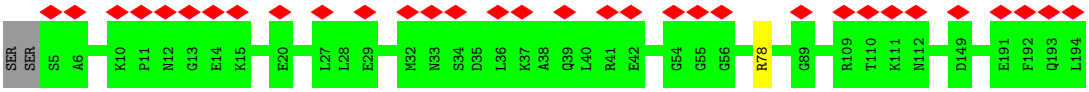




• Molecule 19: 40S ribosomal protein S7

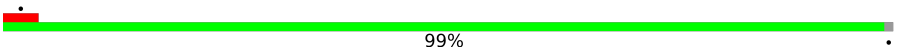
Chain Ag:

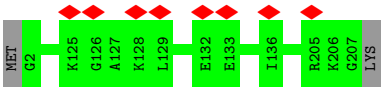




• Molecule 20: 40S ribosomal protein S8

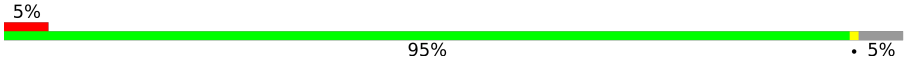
Chain Ah:

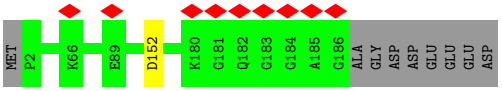




• Molecule 21: Ribosomal protein S9 (Predicted)

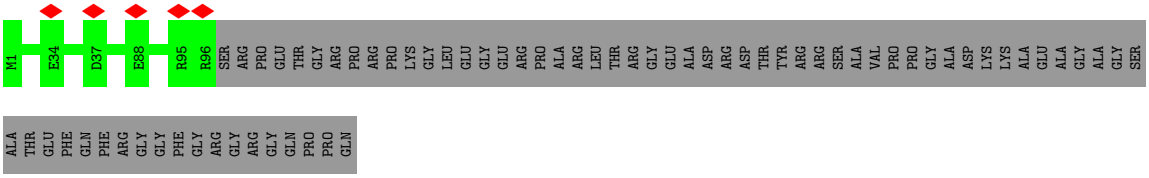
Chain Ai:





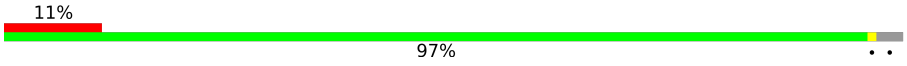
• Molecule 22: eS10

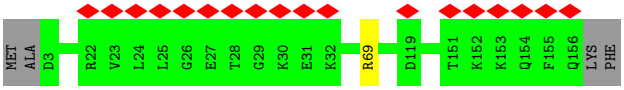
Chain Aj:



• Molecule 23: 40S ribosomal protein S11

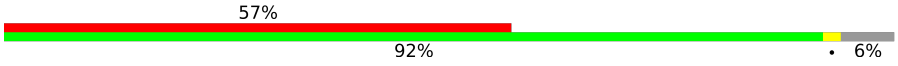
Chain Ak:

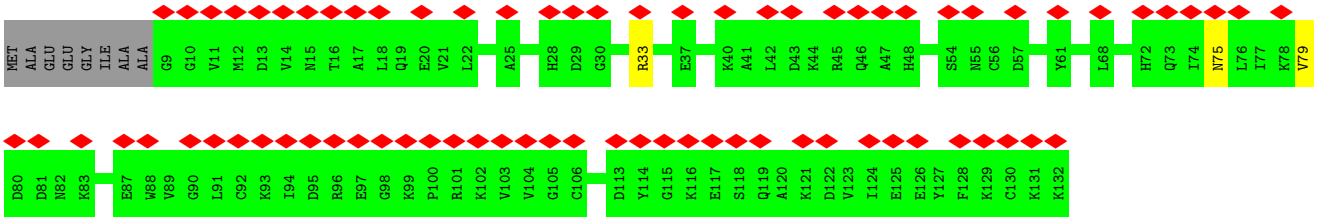




• Molecule 24: 40S ribosomal protein S12

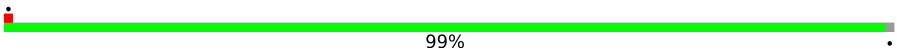
Chain Al:

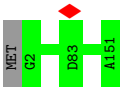




• Molecule 25: uS15

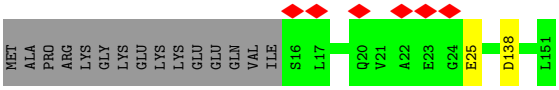
Chain Am:





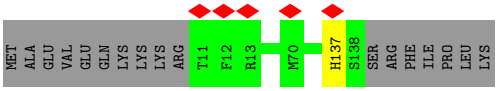
• Molecule 26: 40S ribosomal protein uS11

Chain An:

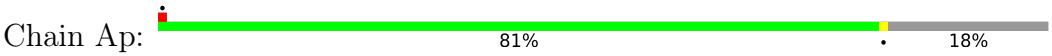


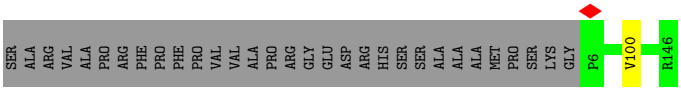
• Molecule 27: 40S ribosomal protein uS19

Chain Ao:

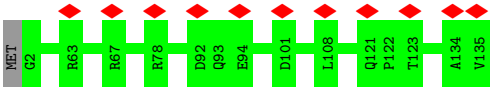


• Molecule 28: uS9

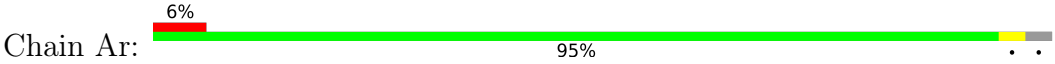


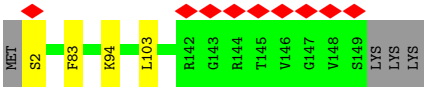


• Molecule 29: 40S ribosomal protein eS17

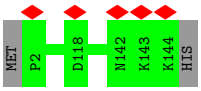


• Molecule 30: 40S ribosomal protein S18

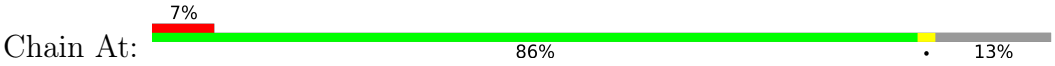


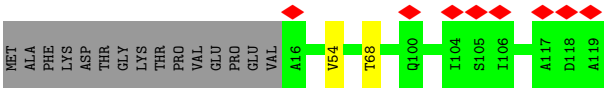


• Molecule 31: Ribosomal protein eS19

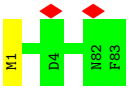


• Molecule 32: 40S ribosomal protein uS10



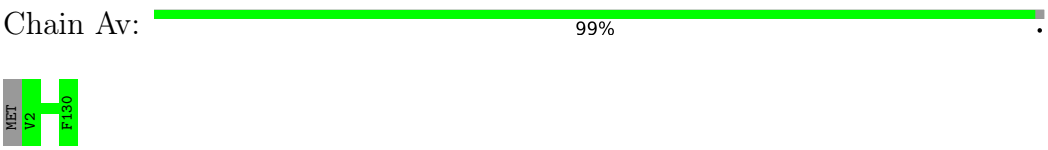


• Molecule 33: Ribosomal protein eS21



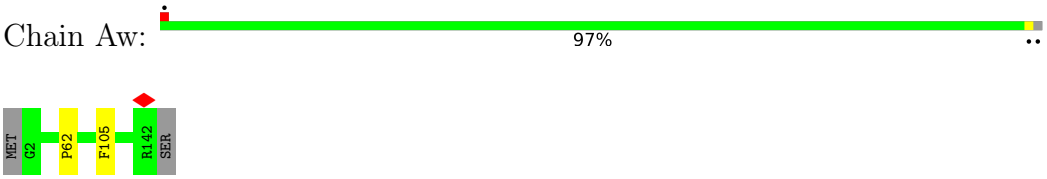
• Molecule 34: Ribosomal protein S15a

Chain Av:



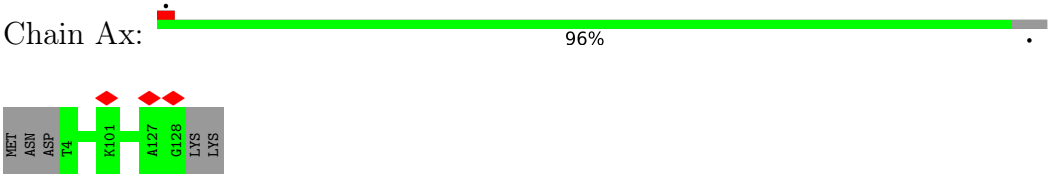
• Molecule 35: 40S ribosomal protein S23

Chain Aw:



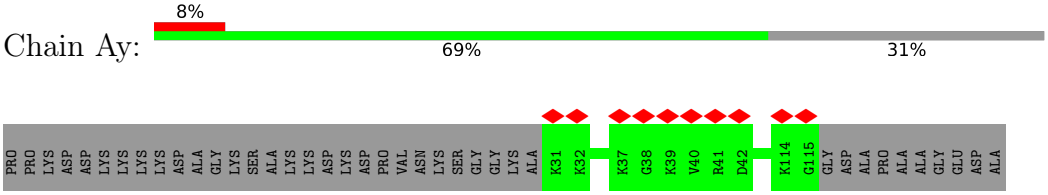
• Molecule 36: 40S ribosomal protein S24

Chain Ax:



• Molecule 37: 40S ribosomal protein S25

Chain Ay:



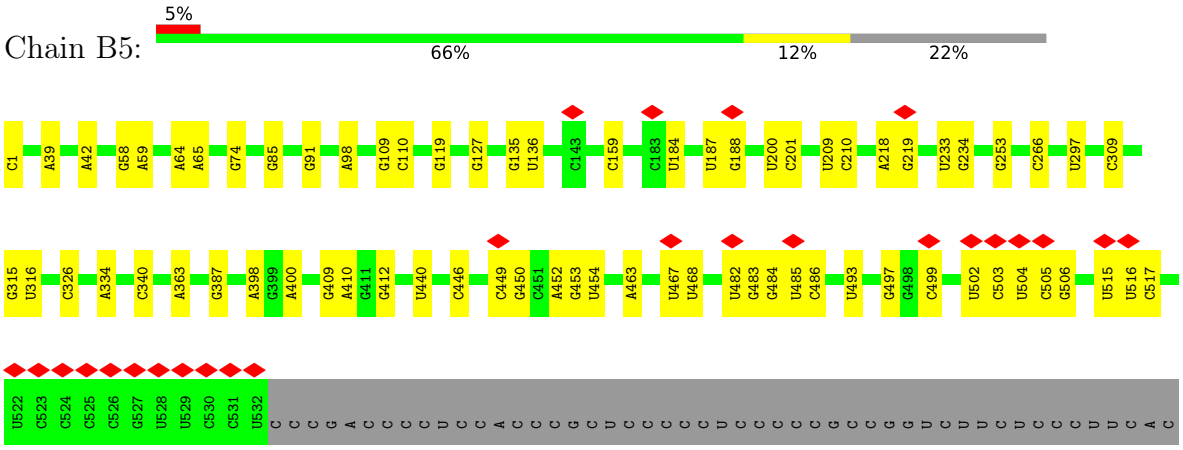
• Molecule 38: 60s ribosomal protein l41

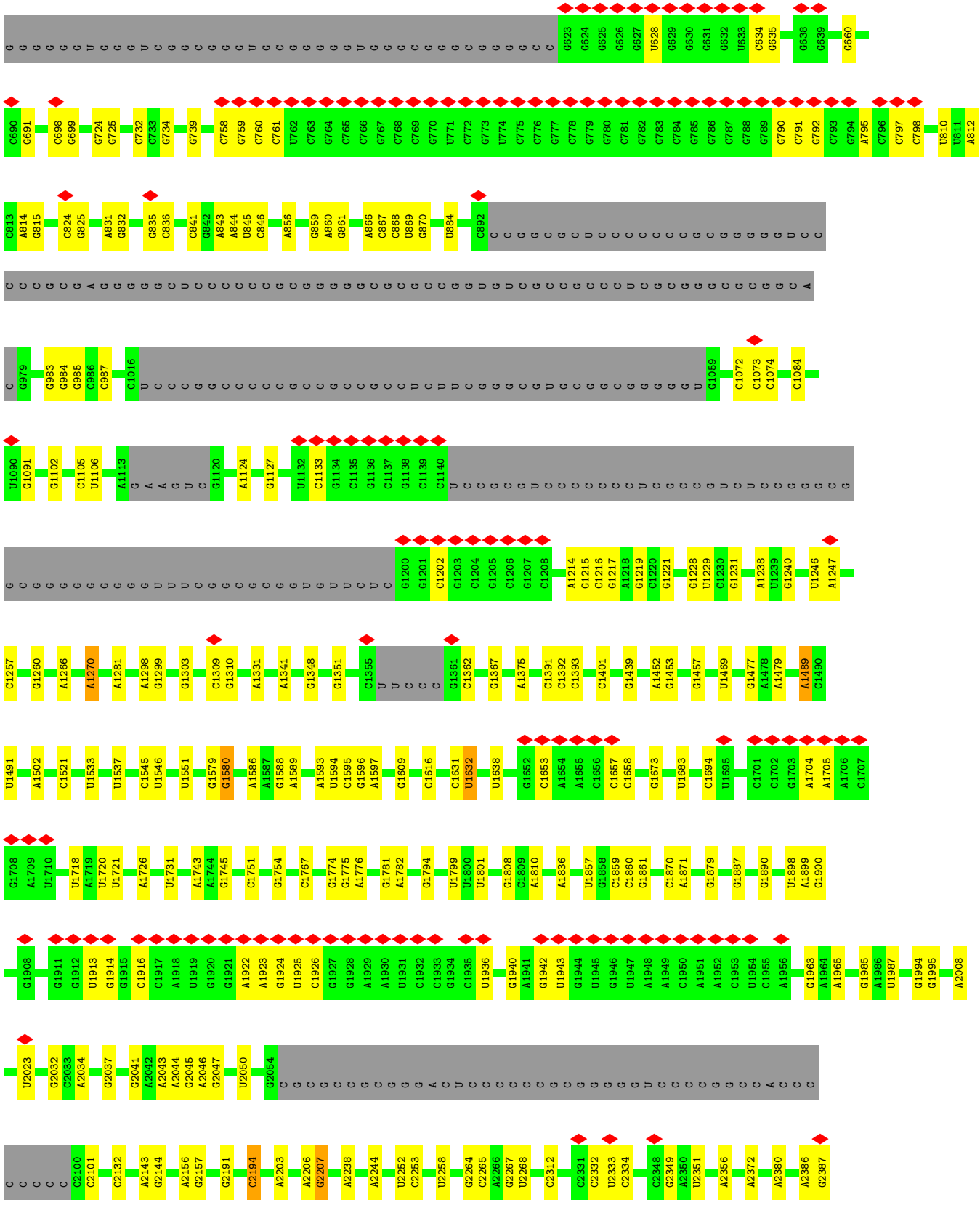
Chain Az:

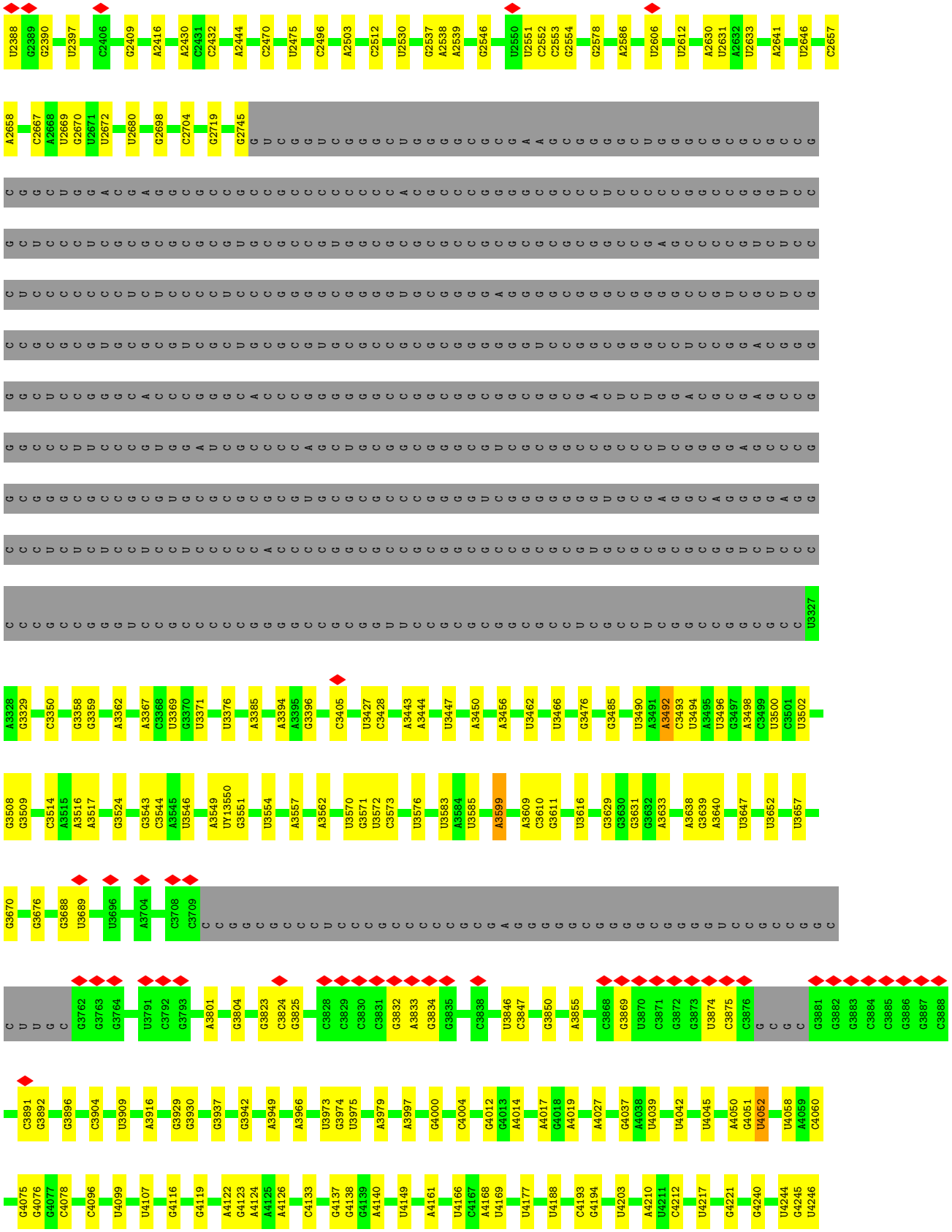
There are no outlier residues recorded for this chain.

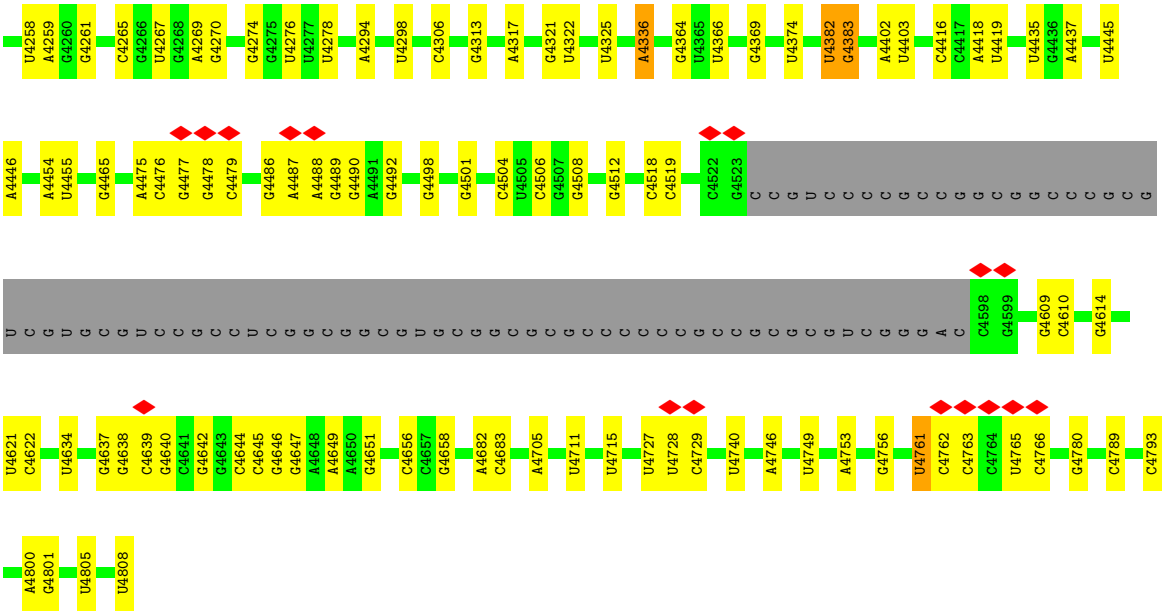
• Molecule 39: 28S rRNA

Chain B5:







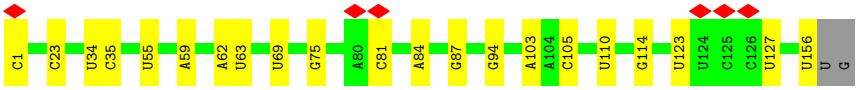


• Molecule 40: 5S

Chain B7:

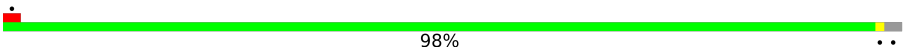
• Molecule 41: 5.8S rRNA

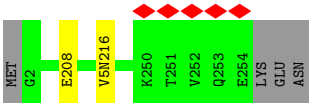
Chain B8:



• Molecule 42: Ribosomal protein uL2

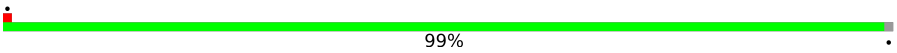
Chain BA:

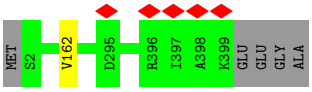




• Molecule 43: Ribosomal protein L3

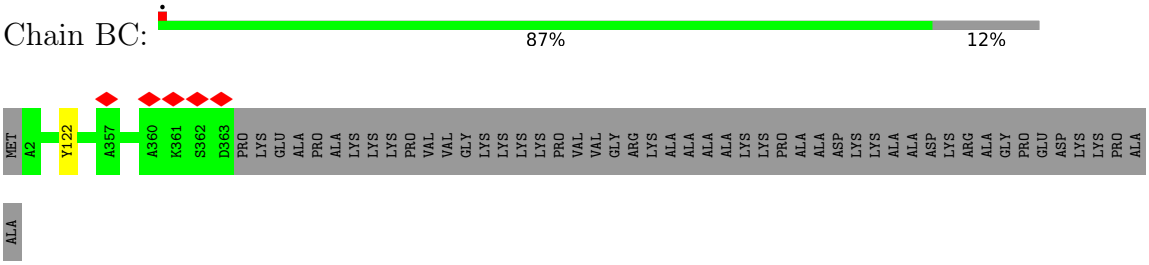
Chain BB:





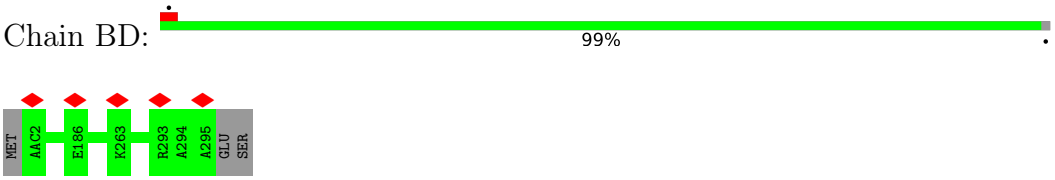
• Molecule 44: 60S ribosomal protein L4

Chain BC:



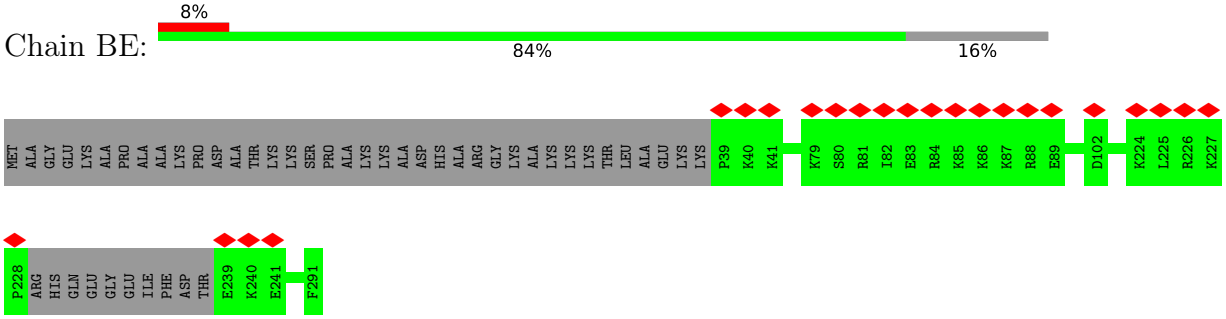
• Molecule 45: Ribosomal_L18_c domain-containing protein

Chain BD:



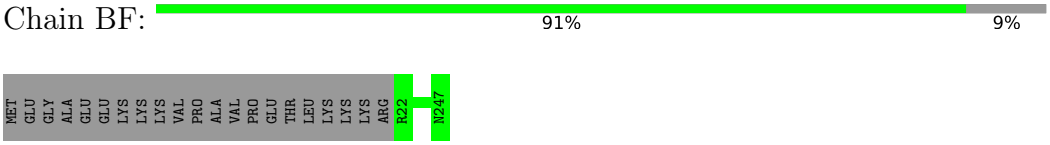
• Molecule 46: 60S ribosomal protein L6

Chain BE:



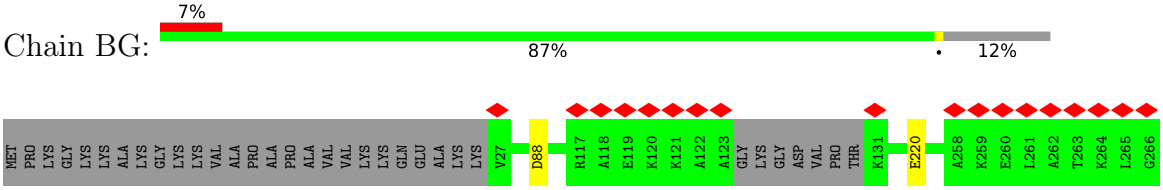
• Molecule 47: Ribosomal Protein uL30

Chain BF:



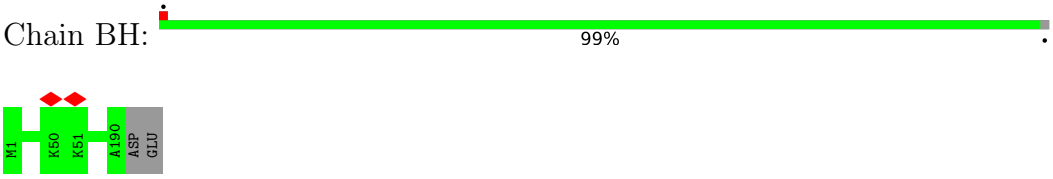
• Molecule 48: Ribosomal protein eL8

Chain BG:



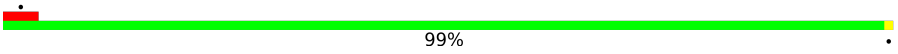
• Molecule 49: 60S ribosomal protein L9

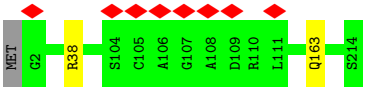
Chain BH:



• Molecule 50: 60S ribosomal protein L10

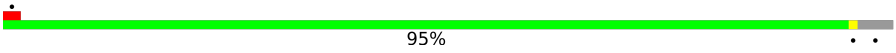
Chain BI:

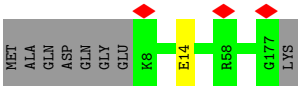




• Molecule 51: Ribosomal protein L11

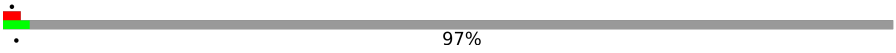
Chain BJ:

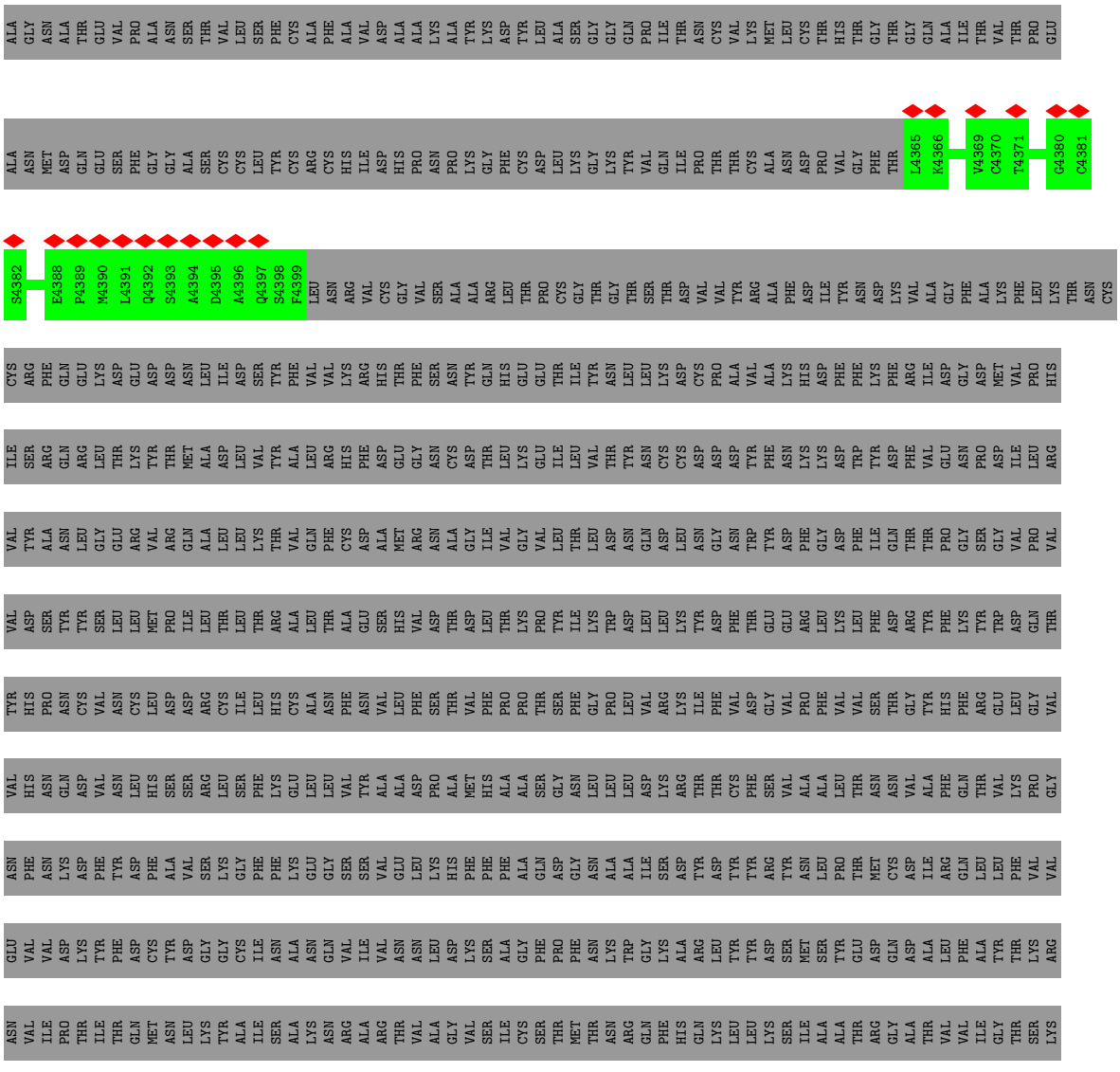


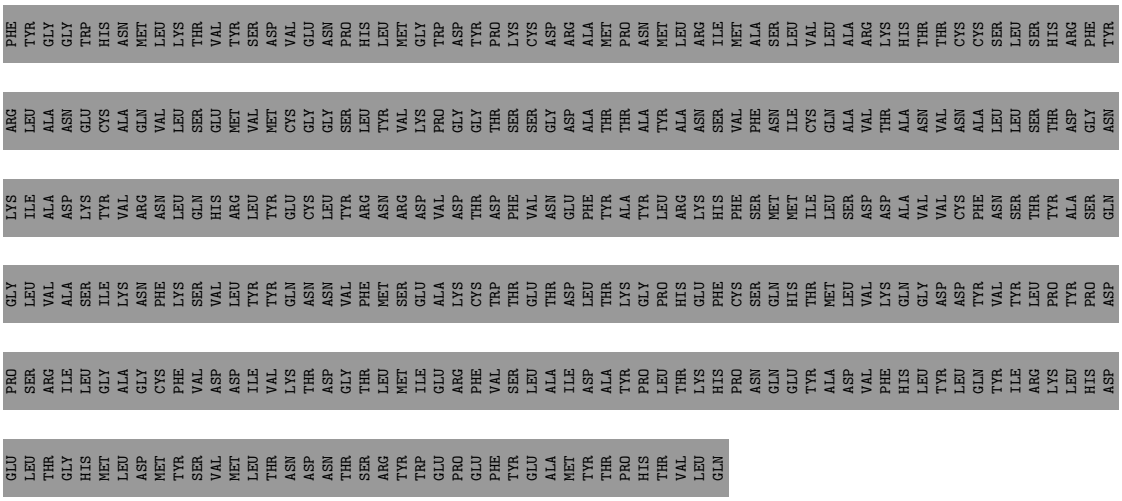


• Molecule 52: Replicase polyprotein 1ab

Chain BK:

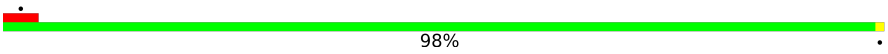


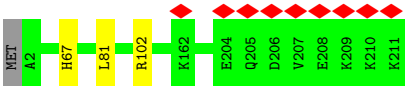




• Molecule 53: Ribosomal protein eL13

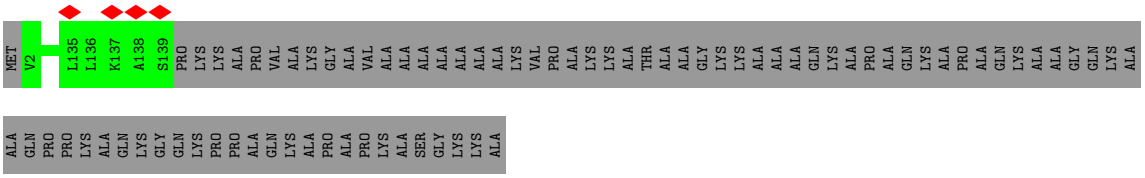
Chain BL:





• Molecule 54: Ribosomal protein L14

Chain BM:

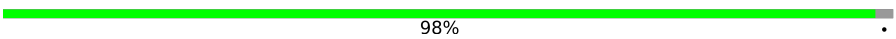


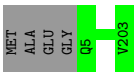
• Molecule 55: Ribosomal protein L15

Chain BN:

• Molecule 56: Ribosomal protein uL13

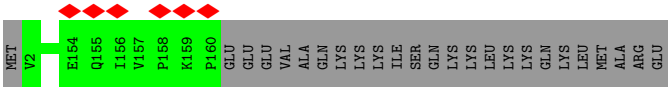
Chain BO:



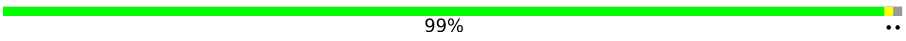


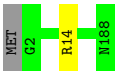
• Molecule 57: uL22

Chain BP:



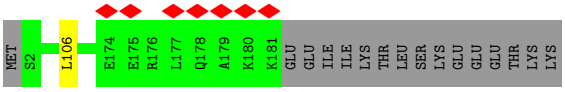
• Molecule 58: Ribosomal Protein eL18

Chain BQ: 

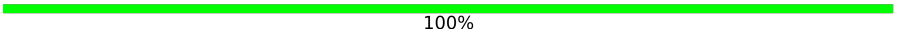


• Molecule 59: 60S ribosomal protein L19

Chain BR:

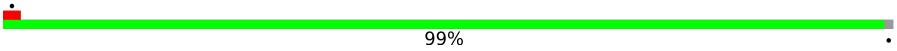


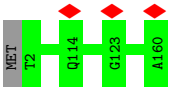
• Molecule 60: Ribosomal protein eL20

Chain BS: 

There are no outlier residues recorded for this chain.

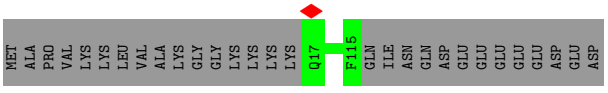
• Molecule 61: eL21

Chain BT: 

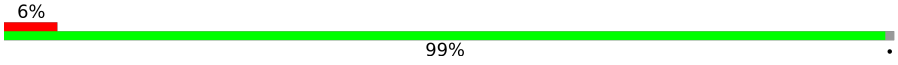


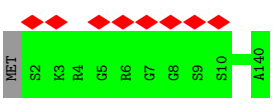
• Molecule 62: Ribosomal protein eL22

Chain BU:



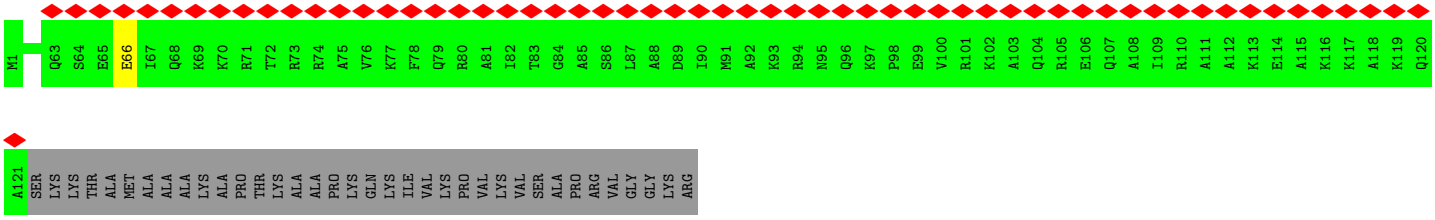
• Molecule 63: Ribosomal protein L23

Chain BV: 



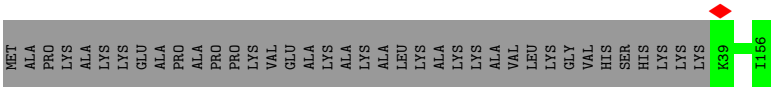
• Molecule 64: eL24

Chain BW:



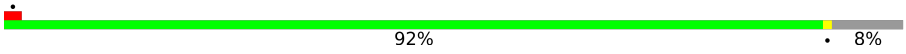
• Molecule 65: uL23

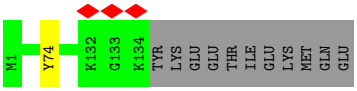
Chain BX:



• Molecule 66: Ribosomal protein L26

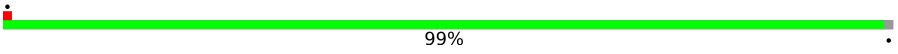
Chain BY:

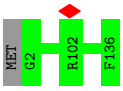




• Molecule 67: 60S ribosomal protein L27

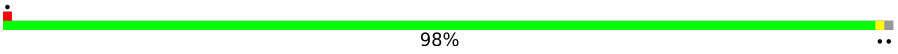
Chain BZ:

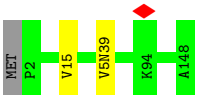




• Molecule 68: 60S ribosomal protein L27a

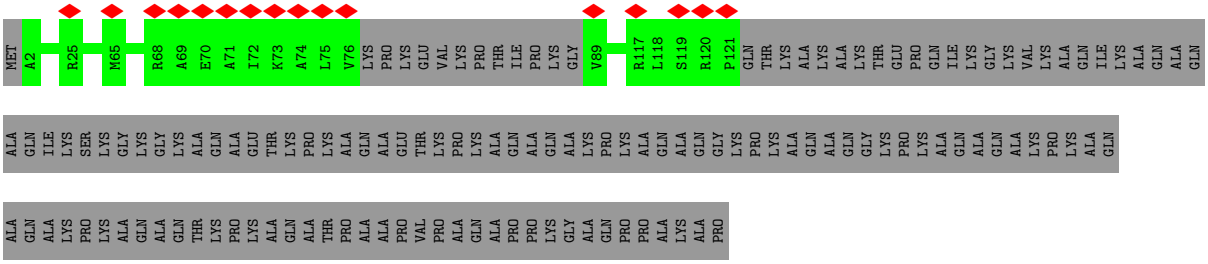
Chain Ba:





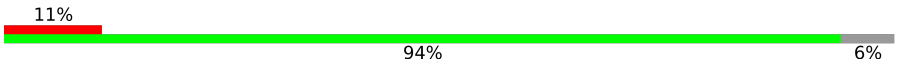
• Molecule 69: 60S ribosomal protein L29

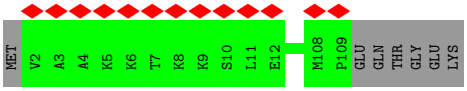
Chain Bb:



• Molecule 70: eL30

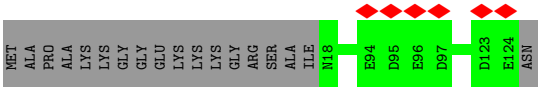
Chain Bc:





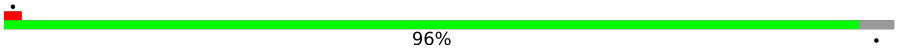
• Molecule 71: eL31

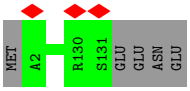
Chain Bd:



• Molecule 72: eL32

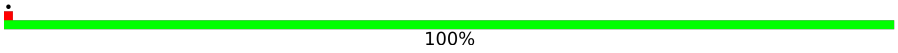
Chain Be:





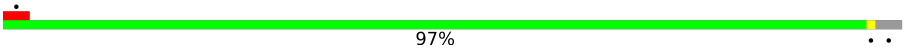
• Molecule 73: eL33

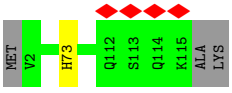
Chain Bf:



• Molecule 74: 60S ribosomal protein L34

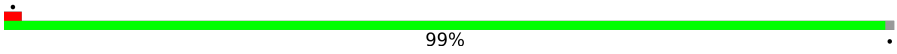
Chain Bg:





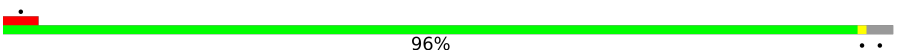
• Molecule 75: uL29

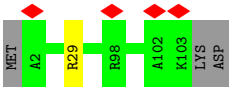
Chain Bh:



• Molecule 76: 60S ribosomal protein L36

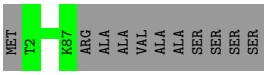
Chain Bi:





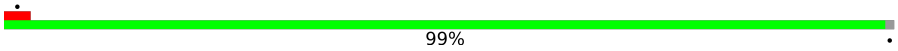
• Molecule 77: Ribosomal protein L37

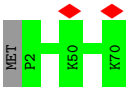
Chain Bj:



• Molecule 78: eL38

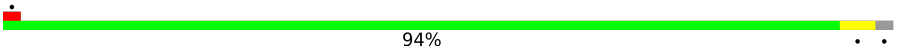
Chain Bk:

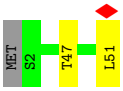




• Molecule 79: eL39

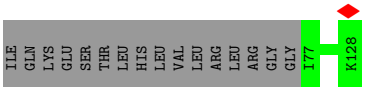
Chain Bl:





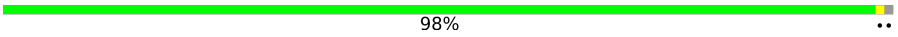
• Molecule 80: 60S ribosomal protein L40

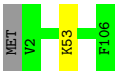
Chain Bm:



• Molecule 81: eL42

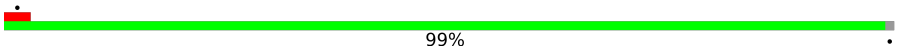
Chain Bo:

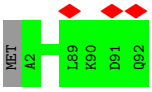




• Molecule 82: eL43

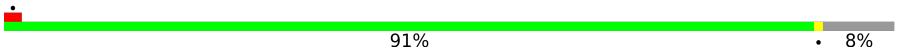
Chain Bp:

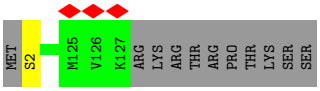




• Molecule 83: Ribosomal protein eL28

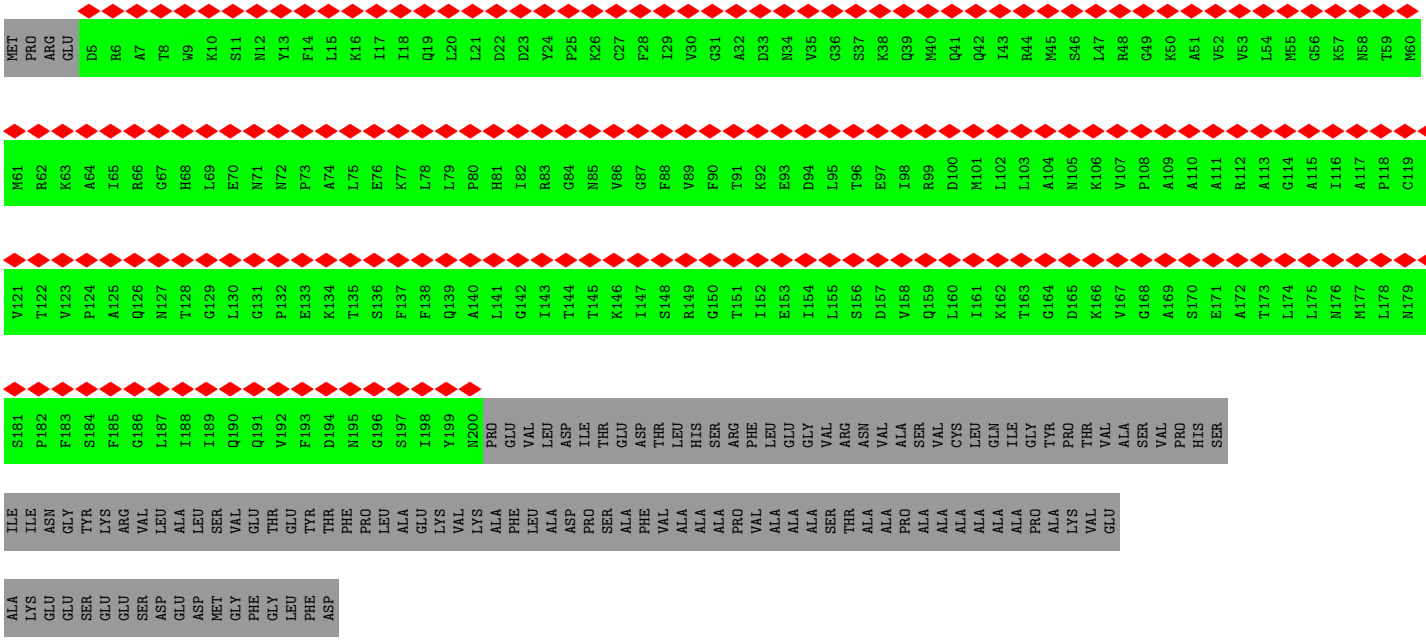
Chain Br:





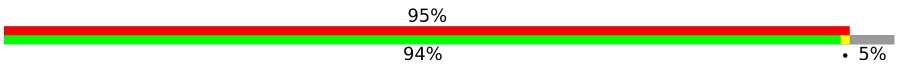
• Molecule 84: 60S acidic ribosomal protein P0

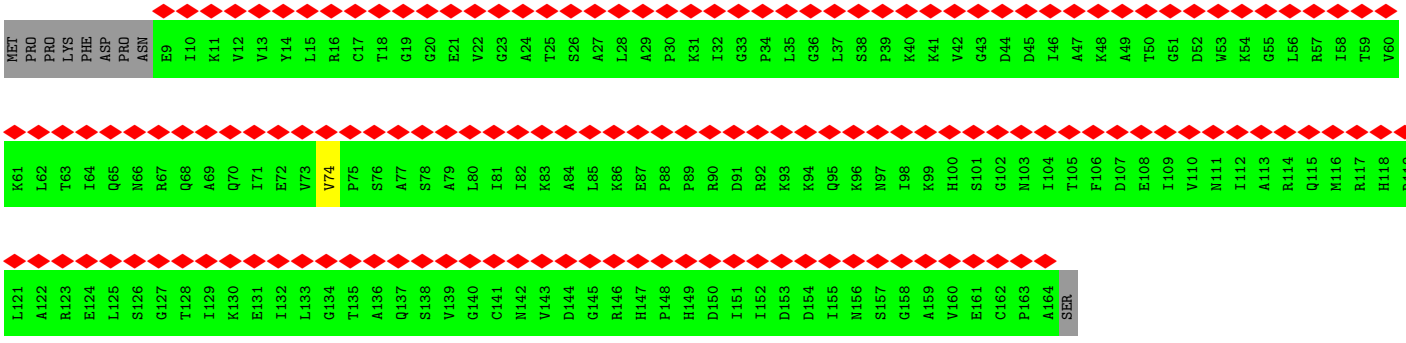
Chain Bs:



• Molecule 85: Ribosomal protein L12

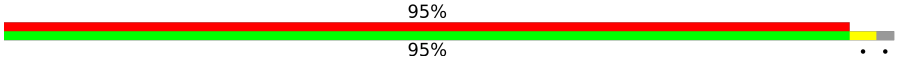
Chain Bt:

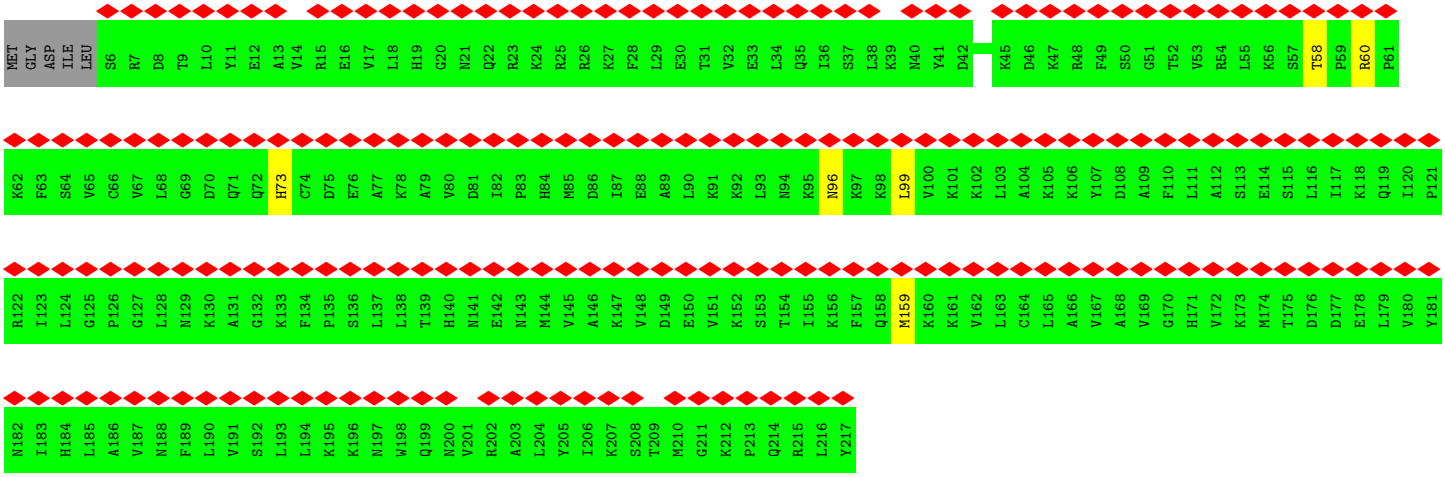




• Molecule 86: Ribosomal protein uL1

Chain Bv:




MET GLY ASP ILE LEU S6 R7 D8 T9 L10 Y11 E12 A13 V14 R15 E16 V17 L18 H19 G20 N21 Q22 R23 K24 R25 R26 K27 F28 L29 E30 T31 V32 E33 L34 Q35 I36 S37 L38 K39 N40 Y41 D42 K45 D46 K47 R48 F49 S50 G51 T52 V53 R54 L55 K56 S57 T58 P59 R60 P61
K62 F63 S64 V65 C66 V67 L68 G69 D70 Q71 Q72 H73 C74 D75 E76 A77 K78 A79 V80 D81 I82 P83 H84 M85 D86 I87 E88 A89 L90 K91 K92 L93 N94 K95 N96 K97 K98 L99 V100 K101 K102 L103 A104 K105 K106 Y107 D108 A109 F110 L111 A112 S113 E114 S115 L116 I117 K118 Q119 I120 P121
R122 I123 L124 G125 P126 G127 L128 N129 K130 A131 G132 K133 F134 P135 S136 L137 L138 T139 H140 N141 E142 N143 M144 V145 A146 K147 V148 D149 E150 V151 K152 S153 T154 I155 K156 F157 Q158 M159 K160 K161 V162 L163 C164 L165 A166 V167 A168 V169 G170 H171 V172 K173 M174 T175 D176 D177 E178 L179 V180 Y181
N182 I183 H184 L185 A186 V187 N188 F189 L190 V191 S192 L193 L194 K195 K196 N197 W198 Q199 N200 V201 R202 A203 L204 Y205 I206 K207 S208 T209 M210 G211 K212 P213 Q214 R215 L216 Y217

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	171706	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 ($e^-/Å^2$)	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	45.454	Depositor
Minimum map value	-18.107	Depositor
Average map value	-0.006	Depositor
Map value standard deviation	0.952	Depositor
Recommended contour level	5.0	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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 2MG, V5N, M3L, SPM, AYA, OMG, OMU, HIC, MLZ, MA6, PSU, OMC, UR3, G7M, H2U, M2G, 5MU, ZN, YYG, 4AC, A2M, 1MA, B8N, 6MZ, UNX, SAC, SPD, UY1, GTP, MG, 5MC, AAC, HY3, AME, NMM

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	0.22	1/40342 (0.0%)	0.70	11/62877 (0.0%)
2	AA	0.24	0/665	0.46	0/891
3	AB	0.25	0/497	0.56	0/666
4	AC	0.24	0/622	0.48	0/822
5	AD	0.25	0/462	0.53	0/607
6	AE	0.25	0/828	0.54	0/1109
7	AF	0.23	0/2493	0.46	0/3394
8	AG	0.24	0/470	0.52	0/623
9	AH	0.13	0/2253	0.69	3/3508 (0.1%)
10	AI	0.29	0/68	0.70	0/103
11	AT	0.36	1/1440 (0.1%)	0.68	0/2242
12	AZ	0.24	0/1771	0.47	0/2406
13	Aa	0.24	0/1841	0.46	0/2459
14	Ab	0.25	0/1742	0.46	0/2354
15	Ac	0.25	0/1779	0.49	0/2395
16	Ad	0.25	0/2118	0.51	0/2849
17	Ae	0.24	0/1531	0.48	0/2059
18	Af	0.24	0/1946	0.52	0/2590
19	Ag	0.25	0/1552	0.48	0/2079
20	Ah	0.24	0/1715	0.52	0/2287
21	Ai	0.24	0/1550	0.53	0/2069
22	Aj	0.24	0/834	0.43	0/1125
23	Ak	0.26	0/1284	0.51	0/1717
24	Al	0.22	0/968	0.42	0/1296
25	Am	0.23	0/1232	0.48	0/1656
26	An	0.25	0/1029	0.55	0/1380
27	Ao	0.25	0/1069	0.49	0/1429
28	Ap	0.24	0/1142	0.51	0/1528
29	Aq	0.23	0/1094	0.49	0/1469
30	Ar	0.24	0/1226	0.54	0/1643

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
31	As	0.23	0/1119	0.46	0/1498
32	At	0.23	0/831	0.52	0/1115
33	Au	0.25	0/636	0.49	0/852
34	Av	0.24	0/1051	0.49	0/1406
35	Aw	0.25	0/1107	0.51	0/1475
36	Ax	0.24	0/1032	0.51	0/1371
37	Ay	0.23	0/691	0.46	0/922
38	Az	0.22	0/240	0.66	0/305
39	B5	0.25	3/87403 (0.0%)	0.70	12/136359 (0.0%)
40	B7	0.24	0/2835	0.69	0/4418
41	B8	0.30	1/3635 (0.0%)	0.70	0/5661
42	BA	0.26	0/1965	0.55	0/2633
43	BB	0.25	0/3261	0.50	0/4364
44	BC	0.24	0/2932	0.51	0/3939
45	BD	0.25	0/2437	0.48	0/3264
46	BE	0.25	0/1998	0.50	0/2673
47	BF	0.25	0/1922	0.50	0/2563
48	BG	0.24	0/1908	0.48	0/2566
49	BH	0.24	0/1535	0.50	0/2063
50	BI	0.25	0/1756	0.51	0/2346
51	BJ	0.25	0/1385	0.51	0/1852
52	BK	0.25	0/269	0.46	0/361
53	BL	0.25	0/1733	0.54	0/2316
54	BM	0.24	0/1158	0.50	0/1547
55	BN	0.25	0/1746	0.55	0/2338
56	BO	0.25	0/1662	0.49	0/2222
57	BP	0.24	0/1317	0.49	0/1768
58	BQ	0.25	0/1539	0.56	0/2054
59	BR	0.23	0/1524	0.54	0/2013
60	BS	0.26	0/1497	0.53	0/2008
61	BT	0.26	0/1326	0.50	0/1770
62	BU	0.25	0/820	0.48	0/1100
63	BV	0.26	0/1048	0.53	0/1402
64	BW	0.25	0/1006	0.50	0/1334
65	BX	0.25	0/984	0.49	0/1323
66	BY	0.24	0/1132	0.52	0/1504
67	BZ	0.26	0/1130	0.49	0/1507
68	Ba	0.25	0/1179	0.50	0/1572
69	Bb	0.23	0/884	0.52	0/1169
70	Bc	0.24	0/847	0.44	0/1134
71	Bd	0.25	0/903	0.53	0/1216
72	Be	0.24	0/1088	0.53	0/1451
73	Bf	0.27	0/903	0.54	0/1208

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
74	Bg	0.25	0/916	0.55	0/1220
75	Bh	0.23	0/1021	0.49	0/1348
76	Bi	0.24	0/841	0.52	0/1112
77	Bj	0.25	0/720	0.56	0/952
78	Bk	0.25	0/575	0.45	0/761
79	Bl	0.23	0/459	0.50	0/608
80	Bm	0.23	0/426	0.51	0/564
81	Bo	0.26	0/866	0.52	0/1141
82	Bp	0.24	0/718	0.50	0/953
83	Br	0.24	0/1020	0.54	0/1366
84	Bs	0.24	0/1530	0.45	0/2064
85	Bt	0.23	0/1193	0.48	0/1609
86	Bv	0.23	0/1735	0.45	0/2328
All	All	0.24	6/236957 (0.0%)	0.63	26/347620 (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	12.83	1.33	1.23
41	B8	1	C	OP3-P	-10.68	1.48	1.61
1	A2	1	U	OP3-P	-10.67	1.48	1.61
39	B5	1	C	OP3-P	-10.59	1.48	1.61
11	AT	1	G	OP3-P	-10.58	1.48	1.61
39	B5	4761	U	N3-C4	-5.24	1.33	1.38

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	B5	4761	U	N3-C4-C5	12.53	122.12	114.60
39	B5	4761	U	C2-N3-C4	-11.85	119.89	127.00
39	B5	4761	U	C5-C4-O4	-9.84	120.00	125.90
1	A2	1454	C	C2-N1-C1'	7.45	126.99	118.80
39	B5	4761	U	N1-C2-N3	7.12	119.17	114.90
39	B5	2312	C	C2-N1-C1'	7.02	126.53	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A2	1454	C	N1-C2-O2	7.01	123.11	118.90
1	A2	294	C	N1-C2-O2	6.82	122.99	118.90
39	B5	2252	U	C2-N1-C1'	6.78	125.84	117.70
1	A2	294	C	C2-N1-C1'	6.71	126.18	118.80
39	B5	2312	C	N1-C2-O2	6.67	122.90	118.90
39	B5	1594	U	C2-N1-C1'	6.46	125.45	117.70
1	A2	631	U	C2-N1-C1'	6.32	125.28	117.70
9	AH	3464	U	C2-N1-C1'	6.25	125.20	117.70
39	B5	2252	U	N1-C2-O2	6.04	127.03	122.80
9	AH	3464	U	N1-C2-O2	5.56	126.69	122.80
1	A2	1023	U	C2-N1-C1'	5.50	124.30	117.70
1	A2	294	C	N3-C2-O2	-5.45	118.08	121.90
1	A2	1454	C	N3-C2-O2	-5.40	118.12	121.90
39	B5	1594	U	N1-C2-O2	5.39	126.57	122.80
39	B5	2312	C	N3-C2-O2	-5.38	118.14	121.90
39	B5	2252	U	N3-C2-O2	-5.37	118.44	122.20
1	A2	631	U	N1-C2-O2	5.34	126.54	122.80
1	A2	1315	U	C2-N1-C1'	5.29	124.05	117.70
1	A2	1454	C	C6-N1-C1'	-5.28	114.46	120.80
9	AH	3464	U	N3-C2-O2	-5.18	118.57	122.20

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	72/156 (46%)	70 (97%)	2 (3%)	0	100	100
5	AD	55/133 (41%)	54 (98%)	1 (2%)	0	100	100
6	AE	99/115 (86%)	99 (100%)	0	0	100	100
7	AF	311/317 (98%)	302 (97%)	9 (3%)	0	100	100
8	AG	53/56 (95%)	53 (100%)	0	0	100	100
12	AZ	219/295 (74%)	214 (98%)	5 (2%)	0	100	100
13	Aa	220/264 (83%)	218 (99%)	2 (1%)	0	100	100
14	Ab	218/293 (74%)	217 (100%)	1 (0%)	0	100	100
15	Ac	223/281 (79%)	222 (100%)	1 (0%)	0	100	100
16	Ad	260/263 (99%)	257 (99%)	3 (1%)	0	100	100
17	Ae	189/204 (93%)	186 (98%)	3 (2%)	0	100	100
18	Af	235/249 (94%)	234 (100%)	1 (0%)	0	100	100
19	Ag	188/432 (44%)	186 (99%)	2 (1%)	0	100	100
20	Ah	204/208 (98%)	201 (98%)	3 (2%)	0	100	100
21	Ai	183/194 (94%)	180 (98%)	3 (2%)	0	100	100
22	Aj	94/165 (57%)	91 (97%)	3 (3%)	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%)	148 (100%)	0	0	100	100
26	An	134/151 (89%)	131 (98%)	3 (2%)	0	100	100
27	Ao	126/145 (87%)	125 (99%)	0	1 (1%)	19	29
28	Ap	139/172 (81%)	135 (97%)	3 (2%)	1 (1%)	22	32
29	Aq	132/135 (98%)	132 (100%)	0	0	100	100
30	Ar	146/152 (96%)	143 (98%)	3 (2%)	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
35	Aw	138/143 (96%)	136 (99%)	2 (1%)	0	100	100
36	Ax	123/130 (95%)	123 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	Ay	83/124 (67%)	81 (98%)	2 (2%)	0	100	100
38	Az	23/25 (92%)	23 (100%)	0	0	100	100
42	BA	250/257 (97%)	242 (97%)	8 (3%)	0	100	100
43	BB	395/403 (98%)	391 (99%)	4 (1%)	0	100	100
44	BC	360/413 (87%)	356 (99%)	4 (1%)	0	100	100
45	BD	291/297 (98%)	289 (99%)	2 (1%)	0	100	100
46	BE	239/291 (82%)	233 (98%)	6 (2%)	0	100	100
47	BF	224/247 (91%)	218 (97%)	6 (3%)	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%)	206 (98%)	5 (2%)	0	100	100
51	BJ	168/178 (94%)	168 (100%)	0	0	100	100
52	BK	33/1071 (3%)	33 (100%)	0	0	100	100
53	BL	208/211 (99%)	205 (99%)	3 (1%)	0	100	100
54	BM	136/218 (62%)	134 (98%)	2 (2%)	0	100	100
55	BN	201/204 (98%)	197 (98%)	4 (2%)	0	100	100
56	BO	197/203 (97%)	195 (99%)	2 (1%)	0	100	100
57	BP	157/184 (85%)	155 (99%)	2 (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%)	156 (99%)	1 (1%)	0	100	100
62	BU	97/128 (76%)	96 (99%)	1 (1%)	0	100	100
63	BV	137/140 (98%)	136 (99%)	1 (1%)	0	100	100
64	BW	119/157 (76%)	119 (100%)	0	0	100	100
65	BX	116/156 (74%)	115 (99%)	1 (1%)	0	100	100
66	BY	132/145 (91%)	131 (99%)	1 (1%)	0	100	100
67	BZ	133/136 (98%)	132 (99%)	1 (1%)	0	100	100
68	Ba	144/148 (97%)	138 (96%)	5 (4%)	1 (1%)	22	32
69	Bb	103/245 (42%)	99 (96%)	4 (4%)	0	100	100
70	Bc	106/115 (92%)	106 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	119 (99%)	1 (1%)	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%)	86 (97%)	3 (3%)	0	100	100
83	Br	124/137 (90%)	122 (98%)	2 (2%)	0	100	100
84	Bs	194/318 (61%)	189 (97%)	5 (3%)	0	100	100
85	Bt	154/165 (93%)	152 (99%)	2 (1%)	0	100	100
86	Bv	210/217 (97%)	197 (94%)	13 (6%)	0	100	100
All	All	11943/14908 (80%)	11780 (99%)	160 (1%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
27	Ao	137	HIS
28	Ap	100	VAL
68	Ba	15	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AA	75/76 (99%)	74 (99%)	1 (1%)	69	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	AB	56/62 (90%)	55 (98%)	1 (2%)	59 76
4	AC	67/140 (48%)	67 (100%)	0	100 100
5	AD	47/106 (44%)	46 (98%)	1 (2%)	53 72
6	AE	88/98 (90%)	87 (99%)	1 (1%)	73 87
7	AF	272/275 (99%)	268 (98%)	4 (2%)	65 80
8	AG	48/49 (98%)	48 (100%)	0	100 100
12	AZ	182/243 (75%)	177 (97%)	5 (3%)	44 65
13	Aa	203/231 (88%)	202 (100%)	1 (0%)	88 95
14	Ab	185/223 (83%)	182 (98%)	3 (2%)	62 79
15	Ac	189/232 (82%)	187 (99%)	2 (1%)	73 87
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%)	204 (99%)	3 (1%)	67 82
19	Ag	170/360 (47%)	169 (99%)	1 (1%)	86 94
20	Ah	178/180 (99%)	178 (100%)	0	100 100
21	Ai	161/168 (96%)	160 (99%)	1 (1%)	86 94
22	Aj	87/136 (64%)	87 (100%)	0	100 100
23	Ak	139/142 (98%)	138 (99%)	1 (1%)	84 92
24	Al	104/108 (96%)	101 (97%)	3 (3%)	42 62
25	Am	130/131 (99%)	130 (100%)	0	100 100
26	An	106/119 (89%)	104 (98%)	2 (2%)	57 75
27	Ao	114/130 (88%)	114 (100%)	0	100 100
28	Ap	117/140 (84%)	117 (100%)	0	100 100
29	Aq	120/121 (99%)	120 (100%)	0	100 100
30	Ar	127/131 (97%)	124 (98%)	3 (2%)	49 68
31	As	112/114 (98%)	112 (100%)	0	100 100
32	At	94/107 (88%)	92 (98%)	2 (2%)	53 72
33	Au	67/67 (100%)	67 (100%)	0	100 100
34	Av	112/113 (99%)	112 (100%)	0	100 100
35	Aw	112/114 (98%)	111 (99%)	1 (1%)	78 90
36	Ax	107/112 (96%)	107 (100%)	0	100 100

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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	95
43	BB	344/347 (99%)	343 (100%)	1 (0%)	92	97
44	BC	302/337 (90%)	301 (100%)	1 (0%)	92	97
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%)	197 (100%)	0	100	100
48	BG	199/223 (89%)	197 (99%)	2 (1%)	76	88
49	BH	169/171 (99%)	169 (100%)	0	100	100
50	BI	180/181 (99%)	178 (99%)	2 (1%)	73	87
51	BJ	143/149 (96%)	142 (99%)	1 (1%)	84	92
52	BK	30/936 (3%)	30 (100%)	0	100	100
53	BL	175/176 (99%)	172 (98%)	3 (2%)	60	78
54	BM	117/161 (73%)	117 (100%)	0	100	100
55	BN	171/172 (99%)	171 (100%)	0	100	100
56	BO	171/173 (99%)	171 (100%)	0	100	100
57	BP	140/163 (86%)	140 (100%)	0	100	100
58	BQ	164/165 (99%)	163 (99%)	1 (1%)	86	94
59	BR	159/175 (91%)	158 (99%)	1 (1%)	86	94
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%)	106 (100%)	0	100	100
64	BW	100/126 (79%)	99 (99%)	1 (1%)	76	88
65	BX	106/134 (79%)	106 (100%)	0	100	100
66	BY	124/135 (92%)	123 (99%)	1 (1%)	81	91
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 88
75	Bh	109/110 (99%)	109 (100%)	0	100 100
76	Bi	86/89 (97%)	85 (99%)	1 (1%)	71 85
77	Bj	73/80 (91%)	73 (100%)	0	100 100
78	Bk	64/65 (98%)	64 (100%)	0	100 100
79	Bl	47/48 (98%)	45 (96%)	2 (4%)	29 46
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%)	164 (100%)	0	100 100
85	Bt	128/137 (93%)	127 (99%)	1 (1%)	81 91
86	Bv	191/195 (98%)	185 (97%)	6 (3%)	40 60
All	All	10394/12642 (82%)	10332 (99%)	62 (1%)	86 94

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	AA	74	THR
3	AB	14	VAL
5	AD	91	LEU
6	AE	40	VAL
7	AF	107	ASP
7	AF	113	PHE
7	AF	159	ASN
7	AF	231	ASP
12	AZ	28	THR
12	AZ	121	LEU
12	AZ	125	THR
12	AZ	192	GLU
12	AZ	206	ASP
13	Aa	178	THR
14	Ab	121	ARG

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Mol	Chain	Res	Type
14	Ab	236	PHE
14	Ab	248	TYR
15	Ac	46	THR
15	Ac	56	GLN
18	Af	44	GLU
18	Af	126	ASP
18	Af	159	ARG
19	Ag	78	ARG
21	Ai	152	ASP
23	Ak	69	ARG
24	Al	33	ARG
24	Al	75	ASN
24	Al	79	VAL
26	An	25	GLU
26	An	138	ASP
30	Ar	83	PHE
30	Ar	94	LYS
30	Ar	103	LEU
32	At	54	VAL
32	At	68	THR
35	Aw	105	PHE
42	BA	208	GLU
43	BB	162	VAL
44	BC	122	TYR
48	BG	88	ASP
48	BG	220	GLU
50	BI	38	ARG
50	BI	163	GLN
51	BJ	14	GLU
53	BL	67	HIS
53	BL	81	LEU
53	BL	102	ARG
58	BQ	14	ARG
59	BR	106	LEU
64	BW	66	GLU
66	BY	74	TYR
74	Bg	73	HIS
76	Bi	29	ARG
79	Bl	47	THR
79	Bl	51	LEU
85	Bt	74	VAL
86	Bv	58	THR

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Mol	Chain	Res	Type
86	Bv	60	ARG
86	Bv	73	HIS
86	Bv	96	ASN
86	Bv	99	LEU
86	Bv	159	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (65) 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	147	HIS
12	AZ	141	ASN
12	AZ	193	HIS
16	Ad	98	ASN
16	Ad	142	HIS
17	Ae	65	GLN
17	Ae	83	ASN
19	Ag	91	HIS
20	Ah	7	ASN
20	Ah	167	GLN
22	Aj	32	HIS
22	Aj	61	GLN
22	Aj	66	HIS
22	Aj	77	GLN
24	Al	72	HIS
26	An	113	GLN
27	Ao	104	GLN
28	Ap	24	HIS
28	Ap	86	GLN
28	Ap	97	GLN
28	Ap	114	GLN
29	Aq	121	GLN
30	Ar	72	GLN
31	As	12	GLN
34	Av	90	GLN
42	BA	140	ASN
42	BA	205	ASN
43	BB	184	GLN
43	BB	289	GLN

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Mol	Chain	Res	Type
44	BC	38	ASN
44	BC	50	GLN
44	BC	310	HIS
45	BD	202	GLN
46	BE	269	GLN
48	BG	64	GLN
48	BG	81	ASN
54	BM	33	GLN
56	BO	180	GLN
59	BR	75	HIS
59	BR	143	HIS
61	BT	131	GLN
63	BV	50	ASN
64	BW	120	GLN
66	BY	14	ASN
68	Ba	93	ASN
69	Bb	17	HIS
74	Bg	28	ASN
77	Bj	13	ASN
78	Bk	58	GLN
79	Bl	4	HIS
80	Bm	117	HIS
81	Bo	102	GLN
83	Br	6	GLN
84	Bs	34	ASN
84	Bs	41	GLN
84	Bs	179	ASN
84	Bs	191	GLN
85	Bt	70	GLN
85	Bt	147	HIS
86	Bv	44	GLN
86	Bv	96	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A2	1758/1870 (94%)	225 (12%)	0
10	AI	2/76 (2%)	1 (50%)	0
11	AT	75/76 (98%)	10 (13%)	0
39	B5	3750/4808 (77%)	489 (13%)	3 (0%)
40	B7	118/120 (98%)	8 (6%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
41	B8	155/158 (98%)	17 (10%)	0
9	AH	94/220 (42%)	29 (30%)	0
All	All	5952/7328 (81%)	779 (13%)	3 (0%)

All (779) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A2	2	A
1	A2	3	C
1	A2	4	C
1	A2	33	G
1	A2	41	G
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	75	G
1	A2	76	U
1	A2	77	A
1	A2	79	A
1	A2	103	A
1	A2	113	G
1	A2	115	U
1	A2	124	U
1	A2	126	G
1	A2	130	G
1	A2	143	U
1	A2	147	A
1	A2	155	G
1	A2	162	C
1	A2	163	U
1	A2	168	C
1	A2	178	C
1	A2	184	G
1	A2	188	C
1	A2	192	C
1	A2	226	A
1	A2	282	C
1	A2	306	U

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Mol	Chain	Res	Type
1	A2	307	C
1	A2	308	G
1	A2	310	G
1	A2	313	G
1	A2	320	C
1	A2	324	C
1	A2	325	U
1	A2	327	C
1	A2	328	G
1	A2	336	G
1	A2	348	G
1	A2	363	C
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	422	G
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	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	526	A
1	A2	548	G
1	A2	557	U
1	A2	565	A
1	A2	569	C
1	A2	577	A2M
1	A2	584	A
1	A2	590	G
1	A2	592	U

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Mol	Chain	Res	Type
1	A2	607	G
1	A2	608	U
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	671	A
1	A2	672	A
1	A2	673	A
1	A2	674	G
1	A2	698	G
1	A2	734	C
1	A2	747	C
1	A2	748	U
1	A2	750	U
1	A2	755	G
1	A2	756	C
1	A2	798	C
1	A2	799	G
1	A2	802	PSU
1	A2	812	A
1	A2	822	G
1	A2	823	PSU
1	A2	831	A
1	A2	832	G
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	860	G
1	A2	871	A
1	A2	873	A
1	A2	879	G

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Mol	Chain	Res	Type
1	A2	886	U
1	A2	892	G
1	A2	910	G
1	A2	914	A
1	A2	915	U
1	A2	921	A
1	A2	923	A
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	1018	U
1	A2	1024	A
1	A2	1061	A
1	A2	1062	U
1	A2	1063	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
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	1266	A

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Mol	Chain	Res	Type
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	1349	G
1	A2	1359	U
1	A2	1372	U
1	A2	1373	U
1	A2	1379	A
1	A2	1398	U
1	A2	1403	A
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	1425	G
1	A2	1436	C
1	A2	1438	C
1	A2	1455	A
1	A2	1463	U
1	A2	1464	U
1	A2	1481	A
1	A2	1488	A
1	A2	1490	A
1	A2	1491	OMG
1	A2	1498	G
1	A2	1510	U
1	A2	1522	C
1	A2	1523	A
1	A2	1534	A
1	A2	1553	G
1	A2	1554	C
1	A2	1571	G
1	A2	1581	A
1	A2	1589	A
1	A2	1602	A
1	A2	1622	U

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Mol	Chain	Res	Type
1	A2	1624	A
1	A2	1655	G
1	A2	1666	G
1	A2	1681	G
1	A2	1699	C
1	A2	1700	A
1	A2	1722	U
1	A2	1723	G
1	A2	1749	G
1	A2	1783	G
1	A2	1784	C
1	A2	1785	G
1	A2	1830	G
1	A2	1832	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	1865	U
1	A2	1866	C
9	AH	3453	A
9	AH	3454	C
9	AH	3455	A
9	AH	3456	A
9	AH	3465	A
9	AH	3469	G
9	AH	3470	G
9	AH	3471	G
9	AH	3474	U
9	AH	3479	U
9	AH	3480	G
9	AH	3482	A
9	AH	3483	A
9	AH	3485	U
9	AH	3486	G
9	AH	3487	C
9	AH	3488	A
9	AH	3501	C
9	AH	3504	U
9	AH	3516	A

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Mol	Chain	Res	Type
9	AH	3520	G
9	AH	3527	U
9	AH	3531	G
9	AH	3532	U
9	AH	3533	A
9	AH	3534	U
9	AH	3535	A
9	AH	3538	G
9	AH	3540	G
10	AI	76	A
11	AT	16	H2U
11	AT	17	H2U
11	AT	18	G
11	AT	19	G
11	AT	20	G
11	AT	21	A
11	AT	22	G
11	AT	46	G7M
11	AT	48	C
11	AT	76	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	74	G
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	127	G
39	B5	135	G
39	B5	136	U
39	B5	159	C
39	B5	184	U
39	B5	187	U
39	B5	188	G
39	B5	200	U
39	B5	201	C

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Mol	Chain	Res	Type
39	B5	209	U
39	B5	210	C
39	B5	218	A
39	B5	219	G
39	B5	233	U
39	B5	234	G
39	B5	253	G
39	B5	266	C
39	B5	297	U
39	B5	309	C
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	409	G
39	B5	410	A
39	B5	412	G
39	B5	440	U
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	484	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

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Mol	Chain	Res	Type
39	B5	506	G
39	B5	515	U
39	B5	516	U
39	B5	517	C
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	739	G
39	B5	758	C
39	B5	759	G
39	B5	760	C
39	B5	761	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	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	836	C
39	B5	841	C
39	B5	843	A
39	B5	844	A
39	B5	845	U
39	B5	846	C
39	B5	856	A

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Mol	Chain	Res	Type
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
39	B5	884	U
39	B5	983	G
39	B5	984	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	1133	C
39	B5	1202	C
39	B5	1214	A
39	B5	1215	G
39	B5	1216	C
39	B5	1217	G
39	B5	1219	G
39	B5	1221	G
39	B5	1228	G
39	B5	1229	U
39	B5	1231	G
39	B5	1238	A
39	B5	1240	G
39	B5	1246	U
39	B5	1247	A
39	B5	1257	C
39	B5	1270	A2M
39	B5	1281	A
39	B5	1298	A

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Mol	Chain	Res	Type
39	B5	1299	G
39	B5	1303	G
39	B5	1309	C
39	B5	1310	G
39	B5	1331	A
39	B5	1341	A
39	B5	1348	G
39	B5	1351	G
39	B5	1362	C
39	B5	1367	G
39	B5	1375	A
39	B5	1391	C
39	B5	1392	C
39	B5	1393	C
39	B5	1401	C
39	B5	1439	G
39	B5	1452	A
39	B5	1453	G
39	B5	1457	G
39	B5	1469	U
39	B5	1489	A2M
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	1595	C
39	B5	1596	G
39	B5	1597	A
39	B5	1609	G
39	B5	1616	C
39	B5	1631	C
39	B5	1632	PSU
39	B5	1653	C
39	B5	1657	C
39	B5	1658	C

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Mol	Chain	Res	Type
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	1751	C
39	B5	1754	G
39	B5	1767	C
39	B5	1774	G
39	B5	1775	G
39	B5	1776	A
39	B5	1781	G
39	B5	1782	A
39	B5	1794	G
39	B5	1808	G
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	1899	A
39	B5	1900	G
39	B5	1913	U
39	B5	1914	G
39	B5	1916	C
39	B5	1922	A
39	B5	1923	A
39	B5	1924	G
39	B5	1925	U
39	B5	1926	C
39	B5	1936	U
39	B5	1940	G
39	B5	1942	G
39	B5	1943	U

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Mol	Chain	Res	Type
39	B5	1963	G
39	B5	1965	A
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	2034	A
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	2047	G
39	B5	2050	U
39	B5	2101	C
39	B5	2132	C
39	B5	2143	A
39	B5	2144	G
39	B5	2156	A
39	B5	2157	G
39	B5	2191	G
39	B5	2194	OMC
39	B5	2203	A
39	B5	2207	OMG
39	B5	2238	A
39	B5	2253	C
39	B5	2264	G
39	B5	2268	U
39	B5	2332	C
39	B5	2333	U
39	B5	2334	C
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

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Mol	Chain	Res	Type
39	B5	2390	G
39	B5	2397	U
39	B5	2409	G
39	B5	2416	A
39	B5	2430	A
39	B5	2432	C
39	B5	2444	A
39	B5	2470	C
39	B5	2496	C
39	B5	2503	A
39	B5	2512	C
39	B5	2530	U
39	B5	2537	G
39	B5	2538	A
39	B5	2539	A
39	B5	2546	G
39	B5	2551	U
39	B5	2552	C
39	B5	2553	C
39	B5	2554	G
39	B5	2578	G
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	2646	U
39	B5	2657	C
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	3376	U
39	B5	3385	A
39	B5	3394	A

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Mol	Chain	Res	Type
39	B5	3396	G
39	B5	3405	C
39	B5	3428	C
39	B5	3443	A
39	B5	3444	A
39	B5	3485	G
39	B5	3492	A2M
39	B5	3493	C
39	B5	3498	A
39	B5	3508	G
39	B5	3509	G
39	B5	3516	A
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	3571	G
39	B5	3572	U
39	B5	3599	A2M
39	B5	3609	A
39	B5	3610	C
39	B5	3611	G
39	B5	3629	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	3801	A
39	B5	3804	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	3846	U

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Mol	Chain	Res	Type
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	3896	G
39	B5	3904	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	3975	U
39	B5	3979	A
39	B5	3997	A
39	B5	4000	G
39	B5	4004	C
39	B5	4012	G
39	B5	4014	A
39	B5	4017	A
39	B5	4019	A
39	B5	4027	A
39	B5	4037	G
39	B5	4050	A
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	4119	G
39	B5	4122	A
39	B5	4123	G
39	B5	4124	A
39	B5	4126	A
39	B5	4133	C
39	B5	4137	G

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Mol	Chain	Res	Type
39	B5	4140	A
39	B5	4161	A
39	B5	4168	A
39	B5	4194	G
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	4270	G
39	B5	4274	G
39	B5	4294	A
39	B5	4306	C
39	B5	4313	G
39	B5	4321	G
39	B5	4336	A2M
39	B5	4382	PSU
39	B5	4383	OMG
39	B5	4402	A
39	B5	4403	U
39	B5	4416	C
39	B5	4418	A
39	B5	4437	A
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	4479	C
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

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Mol	Chain	Res	Type
39	B5	4504	C
39	B5	4506	C
39	B5	4508	G
39	B5	4512	G
39	B5	4518	C
39	B5	4519	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	4637	G
39	B5	4638	G
39	B5	4639	C
39	B5	4640	G
39	B5	4642	G
39	B5	4644	C
39	B5	4645	C
39	B5	4646	G
39	B5	4647	G
39	B5	4649	A
39	B5	4651	G
39	B5	4656	C
39	B5	4658	G
39	B5	4682	A
39	B5	4683	C
39	B5	4705	A
39	B5	4715	U
39	B5	4727	U
39	B5	4728	U
39	B5	4729	C
39	B5	4746	A
39	B5	4753	A
39	B5	4756	G
39	B5	4761	U
39	B5	4762	C
39	B5	4763	C
39	B5	4765	U
39	B5	4766	C
39	B5	4780	G
39	B5	4789	C

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Mol	Chain	Res	Type
39	B5	4793	C
39	B5	4800	A
39	B5	4801	G
39	B5	4805	U
39	B5	4808	U
40	B7	7	G
40	B7	42	A
40	B7	50	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
41	B8	110	U
41	B8	114	G
41	B8	123	U
41	B8	127	U
41	B8	156	U

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
39	B5	1545	C
39	B5	1588	G
39	B5	4445	U

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	OMC	A2	1704	1	19,22,23	0.81	0	26,31,34	0.83	1 (3%)
39	PSU	B5	3616	39	18,21,22	1.36	2 (11%)	22,30,33	1.87	3 (13%)
1	OMG	A2	602	1	18,26,27	0.94	1 (5%)	19,38,41	1.07	2 (10%)
39	PSU	B5	4740	39	18,21,22	1.36	2 (11%)	22,30,33	1.89	3 (13%)
1	A2M	A2	99	1,89	18,25,26	1.02	1 (5%)	18,36,39	1.26	2 (11%)
1	PSU	A2	1626	1	18,21,22	1.36	2 (11%)	22,30,33	1.89	3 (13%)
39	A2M	B5	2206	39,89	18,25,26	0.99	1 (5%)	18,36,39	1.19	2 (11%)
1	PSU	A2	210	1	18,21,22	1.36	2 (11%)	22,30,33	1.86	3 (13%)
1	PSU	A2	1233	1	18,21,22	1.36	2 (11%)	22,30,33	1.90	3 (13%)
39	OMG	B5	4116	39	18,26,27	0.92	1 (5%)	19,38,41	1.10	2 (10%)
39	PSU	B5	3500	39	18,21,22	1.37	2 (11%)	22,30,33	1.91	3 (13%)
39	A2M	B5	3456	39	18,25,26	1.02	1 (5%)	18,36,39	1.25	2 (11%)
11	PSU	AT	28	11	18,21,22	1.36	2 (11%)	22,30,33	1.90	4 (18%)
39	PSU	B5	4278	39	18,21,22	1.37	2 (11%)	22,30,33	1.88	3 (13%)
11	OMG	AT	34	11,9	18,26,27	0.92	1 (5%)	19,38,41	1.09	2 (10%)
39	PSU	B5	4382	39	18,21,22	1.37	2 (11%)	22,30,33	1.89	4 (18%)
39	OMG	B5	3631	39	18,26,27	0.92	1 (5%)	19,38,41	1.13	2 (10%)
39	PSU	B5	1683	39	18,21,22	1.35	2 (11%)	22,30,33	1.91	4 (18%)
39	OMC	B5	2647	39	19,22,23	0.81	0	26,31,34	0.82	0
11	G7M	AT	46	11	20,26,27	2.63	4 (20%)	17,39,42	0.95	1 (5%)
1	PSU	A2	119	1	18,21,22	1.35	2 (11%)	22,30,33	1.86	3 (13%)
39	A2M	B5	1489	39,89	18,25,26	1.00	1 (5%)	18,36,39	1.37	2 (11%)
1	A2M	A2	513	1	18,25,26	1.02	1 (5%)	18,36,39	1.23	2 (11%)
39	PSU	B5	1801	39	18,21,22	1.36	2 (11%)	22,30,33	1.92	4 (18%)
39	OMC	B5	3619	39	19,22,23	0.81	0	26,31,34	0.84	0
1	OMU	A2	1443	1,89	19,22,23	1.22	3 (15%)	26,31,34	1.69	4 (15%)
39	PSU	B5	1638	39	18,21,22	1.38	2 (11%)	22,30,33	1.90	3 (13%)
39	PSU	B5	4149	39	18,21,22	1.36	2 (11%)	22,30,33	1.94	4 (18%)
39	A2M	B5	3492	39,1	18,25,26	1.01	1 (5%)	18,36,39	1.28	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	OMC	A2	1392	1	19,22,23	0.84	0	26,31,34	0.95	1 (3%)
39	PSU	B5	1491	39	18,21,22	1.37	2 (11%)	22,30,33	1.93	4 (18%)
39	OMU	B5	3973	39	19,22,23	1.24	3 (15%)	26,31,34	1.69	4 (15%)
39	PSU	B5	4749	39	18,21,22	1.36	2 (11%)	22,30,33	1.89	3 (13%)
39	A2M	B5	3557	39	18,25,26	1.00	1 (5%)	18,36,39	1.23	2 (11%)
1	OMG	A2	645	1	18,26,27	0.94	1 (5%)	19,38,41	1.10	2 (10%)
39	OMG	B5	4245	39	18,26,27	0.92	1 (5%)	19,38,41	1.07	2 (10%)
39	A2M	B5	2630	39,89	18,25,26	0.97	1 (5%)	18,36,39	1.27	2 (11%)
1	PSU	A2	34	1	18,21,22	1.36	2 (11%)	22,30,33	1.91	4 (18%)
1	PSU	A2	573	1	18,21,22	1.33	2 (11%)	22,30,33	1.91	4 (18%)
1	PSU	A2	802	1	18,21,22	1.37	2 (11%)	22,30,33	1.88	3 (13%)
39	PSU	B5	4419	39	18,21,22	1.36	2 (11%)	22,30,33	1.92	4 (18%)
1	OMC	A2	518	1	19,22,23	0.81	0	26,31,34	0.80	0
1	PSU	A2	1245	1	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
39	PSU	B5	2351	39	18,21,22	1.36	2 (11%)	22,30,33	1.92	4 (18%)
39	OMC	B5	4282	39,89	19,22,23	0.82	0	26,31,34	0.83	0
1	A2M	A2	669	1,89	18,25,26	0.93	1 (5%)	18,36,39	1.34	2 (11%)
39	5MC	B5	4193	39	18,22,23	1.00	2 (11%)	26,32,35	1.24	2 (7%)
43	HIC	BB	245	43	8,11,12	0.85	0	6,14,16	0.82	0
11	H2U	AT	17	11	18,21,22	1.00	2 (11%)	21,30,33	1.72	2 (9%)
11	1MA	AT	58	11	16,25,26	1.58	2 (12%)	18,37,40	1.05	2 (11%)
39	OMG	B5	1260	39	18,26,27	0.94	1 (5%)	19,38,41	1.17	2 (10%)
1	A2M	A2	577	1	18,25,26	1.00	1 (5%)	18,36,39	1.24	2 (11%)
1	G7M	A2	1640	11,1	20,26,27	2.64	4 (20%)	17,39,42	0.91	1 (5%)
1	OMG	A2	868	1	18,26,27	0.93	1 (5%)	19,38,41	1.09	2 (10%)
1	PSU	A2	650	1	18,21,22	1.37	2 (11%)	22,30,33	1.94	4 (18%)
1	PSU	A2	1644	1,89	18,21,22	1.36	2 (11%)	22,30,33	1.90	3 (13%)
39	OMG	B5	4138	39	18,26,27	0.91	1 (5%)	19,38,41	1.09	2 (10%)
1	PSU	A2	1348	1	18,21,22	1.36	2 (11%)	22,30,33	1.91	3 (13%)
11	5MU	AT	54	11	19,22,23	1.41	6 (31%)	28,32,35	2.05	7 (25%)
39	PSU	B5	3369	39	18,21,22	1.38	3 (16%)	22,30,33	1.94	4 (18%)
39	PSU	B5	4298	39	18,21,22	1.37	2 (11%)	22,30,33	1.94	4 (18%)
1	A2M	A2	1679	1	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	1.91	3 (13%)
39	PSU	B5	1720	39	18,21,22	1.37	2 (11%)	22,30,33	1.88	3 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
39	UR3	B5	4276	39	19,22,23	0.99	1 (5%)	26,32,35	1.42	1 (3%)
39	PSU	B5	4107	39	18,21,22	1.37	2 (11%)	22,30,33	1.89	3 (13%)
39	OMG	B5	2719	39	18,26,27	0.94	1 (5%)	19,38,41	1.07	2 (10%)
11	PSU	AT	55	11	18,21,22	1.34	2 (11%)	22,30,33	1.91	4 (18%)
1	OMG	A2	1329	1	18,26,27	0.92	1 (5%)	19,38,41	1.10	2 (10%)
39	PSU	B5	4325	39	18,21,22	1.37	2 (11%)	22,30,33	1.92	3 (13%)
39	OMC	B5	3573	39	19,22,23	0.81	0	26,31,34	0.87	1 (3%)
39	OMU	B5	4244	39	19,22,23	1.21	2 (10%)	26,31,34	1.70	4 (15%)
39	PSU	B5	3447	39	18,21,22	1.36	2 (11%)	22,30,33	1.92	3 (13%)
11	M2G	AT	26	11	20,27,28	1.40	3 (15%)	22,40,43	0.98	2 (9%)
1	PSU	A2	1047	1	18,21,22	1.36	2 (11%)	22,30,33	1.91	3 (13%)
1	A2M	A2	485	1	18,25,26	0.98	1 (5%)	18,36,39	1.27	2 (11%)
1	OMC	A2	174	1,89	19,22,23	0.80	0	26,31,34	0.78	0
39	PSU	B5	3496	39	18,21,22	1.37	2 (11%)	22,30,33	1.92	3 (13%)
39	PSU	B5	4374	39	18,21,22	1.37	2 (11%)	22,30,33	1.93	3 (13%)
39	PSU	B5	4217	39	18,21,22	1.39	2 (11%)	22,30,33	1.87	3 (13%)
1	OMU	A2	121	1	19,22,23	1.22	3 (15%)	26,31,34	1.69	4 (15%)
68	V5N	Ba	39	68	4,11,12	0.76	0	5,14,16	1.56	1 (20%)
41	PSU	B8	55	41	18,21,22	1.36	2 (11%)	22,30,33	1.93	4 (18%)
39	OMC	B5	3540	39	19,22,23	0.79	0	26,31,34	0.77	0
1	PSU	A2	1005	1	18,21,22	1.38	2 (11%)	22,30,33	1.87	3 (13%)
39	A2M	B5	4317	39	18,25,26	1.01	1 (5%)	18,36,39	1.23	2 (11%)
39	PSU	B5	1731	39	18,21,22	1.35	2 (11%)	22,30,33	1.85	4 (18%)
11	2MG	AT	10	11	18,26,27	0.90	1 (5%)	16,38,41	1.10	2 (12%)
1	PSU	A2	687	1	18,21,22	1.35	2 (11%)	22,30,33	1.90	3 (13%)
39	A2M	B5	1270	39	18,25,26	0.94	1 (5%)	18,36,39	1.26	2 (11%)
39	PSU	B5	4435	39	18,21,22	1.38	2 (11%)	22,30,33	1.91	3 (13%)
11	OMC	AT	32	11	19,22,23	0.81	0	26,31,34	0.80	0
39	A2M	B5	3599	39	18,25,26	0.96	1 (5%)	18,36,39	1.23	2 (11%)
1	PSU	A2	652	1	18,21,22	1.35	2 (11%)	22,30,33	1.91	3 (13%)
39	PSU	B5	1537	39	18,21,22	1.37	2 (11%)	22,30,33	1.89	3 (13%)
1	PSU	A2	1057	1	18,21,22	1.37	2 (11%)	22,30,33	1.90	3 (13%)
39	PSU	B5	3427	39	18,21,22	1.34	2 (11%)	22,30,33	1.92	3 (13%)
39	OMC	B5	1820	39,89	19,22,23	0.81	0	26,31,34	0.84	0
1	OMC	A2	463	1	19,22,23	0.81	0	26,31,34	0.81	0
1	OMU	A2	116	1	19,22,23	1.21	3 (15%)	26,31,34	1.69	5 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	PSU	A2	1046	1	18,21,22	1.35	2 (11%)	22,30,33	1.89	3 (13%)
39	A2M	B5	2244	39,89	18,25,26	0.99	1 (5%)	18,36,39	1.24	2 (11%)
39	PSU	B5	4099	39	18,21,22	1.37	2 (11%)	22,30,33	1.92	3 (13%)
39	PSU	B5	4042	39	18,21,22	1.35	2 (11%)	22,30,33	1.93	4 (18%)
39	A2M	B5	4269	39,89	18,25,26	1.01	1 (5%)	18,36,39	1.28	2 (11%)
1	PSU	A2	1368	1	18,21,22	1.34	2 (11%)	22,30,33	1.91	3 (13%)
1	MA6	A2	1851	1	18,26,27	0.90	1 (5%)	19,38,41	1.49	3 (15%)
80	M3L	Bm	98	80	10,11,12	0.82	0	9,14,16	0.50	0
39	PSU	B5	3583	39	18,21,22	1.38	2 (11%)	22,30,33	1.93	3 (13%)
39	PSU	B5	4045	39	18,21,22	1.36	2 (11%)	22,30,33	1.90	3 (13%)
11	5MC	AT	49	11	18,22,23	0.95	2 (11%)	26,32,35	1.13	2 (7%)
1	OMG	A2	510	1,89	18,26,27	0.93	1 (5%)	19,38,41	1.08	2 (10%)
39	A2M	B5	4336	39	18,25,26	1.03	1 (5%)	18,36,39	1.25	2 (11%)
1	PSU	A2	823	1	18,21,22	1.37	2 (11%)	22,30,33	1.90	4 (18%)
1	PSU	A2	1693	1	18,21,22	1.37	2 (11%)	22,30,33	1.90	4 (18%)
39	OMC	B5	1284	39	19,22,23	0.80	0	26,31,34	0.77	0
39	PSU	B5	4177	39	18,21,22	1.36	2 (11%)	22,30,33	1.88	3 (13%)
1	A2M	A2	27	1,89	18,25,26	1.00	1 (5%)	18,36,39	1.22	2 (11%)
1	A2M	A2	1384	1	18,25,26	1.03	1 (5%)	18,36,39	1.23	2 (11%)
39	5MC	B5	3514	39,89	18,22,23	0.94	2 (11%)	26,32,35	1.18	3 (11%)
39	PSU	B5	4267	39,89	18,21,22	1.37	2 (11%)	22,30,33	1.89	5 (22%)
1	OMU	A2	1805	1	19,22,23	1.23	3 (15%)	26,31,34	1.71	4 (15%)
1	A2M	A2	1032	1	18,25,26	0.97	1 (5%)	18,36,39	1.27	2 (11%)
39	6MZ	B5	3966	39	18,25,26	0.86	1 (5%)	16,36,39	2.01	4 (25%)
11	1MA	AT	14	11	16,25,26	1.56	2 (12%)	18,37,40	1.03	3 (16%)
39	PSU	B5	4203	39	18,21,22	1.36	2 (11%)	22,30,33	1.88	3 (13%)
39	PSU	B5	4058	39	18,21,22	1.36	2 (11%)	22,30,33	1.91	3 (13%)
1	B8N	A2	1249	1	24,29,30	1.29	3 (12%)	29,42,45	1.26	3 (10%)
1	PSU	A2	407	1	18,21,22	1.36	2 (11%)	22,30,33	1.90	3 (13%)
39	PSU	B5	4246	39	18,21,22	1.35	2 (11%)	22,30,33	1.93	3 (13%)
39	OMC	B5	2704	39	19,22,23	0.81	0	26,31,34	0.83	1 (3%)
39	PSU	B5	4169	39	18,21,22	1.37	2 (11%)	22,30,33	1.88	3 (13%)
39	PSU	B5	3585	39,89	18,21,22	1.39	2 (11%)	22,30,33	1.89	3 (13%)
39	OMC	B5	4202	39	19,22,23	0.81	0	26,31,34	0.80	0
1	OMU	A2	628	1	19,22,23	1.18	2 (10%)	26,31,34	1.70	5 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	PSU	A2	218	1	18,21,22	1.35	2 (11%)	22,30,33	1.91	3 (13%)
1	PSU	A2	1178	1	18,21,22	1.36	2 (11%)	22,30,33	1.94	3 (13%)
1	PSU	A2	105	1	18,21,22	1.37	2 (11%)	22,30,33	1.92	3 (13%)
1	PSU	A2	1239	1	18,21,22	1.36	2 (11%)	22,30,33	1.90	4 (18%)
39	OMC	B5	2265	39,89	19,22,23	0.82	0	26,31,34	0.86	1 (3%)
39	PSU	B5	1799	39	18,21,22	1.38	2 (11%)	22,30,33	1.90	3 (13%)
39	PSU	B5	4322	39	18,21,22	1.35	2 (11%)	22,30,33	1.89	3 (13%)
39	OMG	B5	3676	39	18,26,27	0.93	1 (5%)	19,38,41	1.11	2 (10%)
1	OMU	A2	1327	1,89	19,22,23	1.19	2 (10%)	26,31,34	1.71	5 (19%)
1	PSU	A2	1446	1	18,21,22	1.35	2 (11%)	22,30,33	1.90	3 (13%)
39	PSU	B5	4711	39	18,21,22	1.36	2 (11%)	22,30,33	1.91	4 (18%)
83	SAC	Br	2	83	7,8,9	0.51	0	8,9,11	0.86	1 (12%)
1	PSU	A2	816	1	18,21,22	1.34	2 (11%)	22,30,33	1.91	4 (18%)
1	PSU	A2	682	1	18,21,22	1.38	2 (11%)	22,30,33	1.89	3 (13%)
39	OMU	B5	2680	39	19,22,23	1.22	2 (10%)	26,31,34	1.74	5 (19%)
1	OMU	A2	172	1	19,22,23	1.20	3 (15%)	26,31,34	1.72	4 (15%)
39	PSU	B5	4188	39	18,21,22	1.36	2 (11%)	22,30,33	1.91	3 (13%)
39	UY1	B5	3550	39	19,22,23	1.31	3 (15%)	22,31,34	2.02	5 (22%)
41	OMG	B8	75	41	18,26,27	0.92	1 (5%)	19,38,41	1.09	2 (10%)
1	OMG	A2	437	1	18,26,27	0.93	1 (5%)	19,38,41	1.09	2 (10%)
39	OMU	B5	4052	39	19,22,23	1.23	3 (15%)	26,31,34	1.71	5 (19%)
1	A2M	A2	159	1	18,25,26	1.00	1 (5%)	18,36,39	1.25	2 (11%)
39	PSU	B5	3466	39	18,21,22	1.35	2 (11%)	22,30,33	1.91	4 (18%)
39	OMU	B5	3657	39	19,22,23	1.24	2 (10%)	26,31,34	1.76	5 (19%)
1	4AC	A2	1843	1	21,24,25	1.01	1 (4%)	29,34,37	1.04	3 (10%)
11	H2U	AT	16	11	18,21,22	0.99	2 (11%)	21,30,33	1.38	2 (9%)
39	OMG	B5	1477	39	18,26,27	0.92	1 (5%)	19,38,41	1.09	2 (10%)
1	OMU	A2	429	1	19,22,23	1.19	2 (10%)	26,31,34	1.69	5 (19%)
39	PSU	B5	3494	39	18,21,22	1.37	2 (11%)	22,30,33	1.89	3 (13%)
39	OMG	B5	4383	39	18,26,27	0.95	1 (5%)	19,38,41	1.10	2 (10%)
1	OMG	A2	684	1	18,26,27	0.92	1 (5%)	19,38,41	1.12	2 (10%)
1	PSU	A2	1082	1	18,21,22	1.39	3 (16%)	22,30,33	1.85	3 (13%)
39	PSU	B5	1721	39	18,21,22	1.36	2 (11%)	22,30,33	1.91	4 (18%)
81	MLZ	Bo	53	81	8,9,10	0.48	0	4,9,11	0.10	0
41	PSU	B8	69	41	18,21,22	1.38	2 (11%)	22,30,33	1.93	4 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
33	AME	Au	1	33	9,10,11	0.47	0	9,11,13	0.88	1 (11%)
1	A2M	A2	469	1	18,25,26	1.03	1 (5%)	18,36,39	1.30	2 (11%)
1	PSU	A2	610	1	18,21,22	1.36	2 (11%)	22,30,33	1.90	3 (13%)
39	OMU	B5	4366	39	19,22,23	1.23	3 (15%)	26,31,34	1.71	4 (15%)
39	OMG	B5	4364	39	18,26,27	0.92	1 (5%)	19,38,41	1.10	2 (10%)
1	OMG	A2	1448	1	18,26,27	0.94	1 (5%)	19,38,41	1.09	2 (10%)
39	A2M	B5	2658	39,89	18,25,26	1.00	1 (5%)	18,36,39	1.24	2 (11%)
31	NMM	As	67	31	9,11,12	0.59	0	6,12,14	0.46	0
1	A2M	A2	591	1	18,25,26	1.03	1 (5%)	18,36,39	1.19	2 (11%)
39	A2M	B5	398	39	18,25,26	1.02	1 (5%)	18,36,39	1.23	2 (11%)
1	PSU	A2	1175	1	18,21,22	1.36	2 (11%)	22,30,33	1.88	3 (13%)
39	OMG	B5	4369	39	18,26,27	0.94	1 (5%)	19,38,41	1.13	2 (10%)
11	YYG	AT	37	11	31,42,43	1.68	4 (12%)	33,62,65	2.12	10 (30%)
1	PSU	A2	109	1	18,21,22	1.36	2 (11%)	22,30,33	1.90	3 (13%)
1	PSU	A2	967	1	18,21,22	1.37	2 (11%)	22,30,33	1.89	3 (13%)
39	OMG	B5	3524	39	18,26,27	0.90	1 (5%)	19,38,41	1.06	2 (10%)
1	PSU	A2	815	1	18,21,22	1.36	2 (11%)	22,30,33	1.89	3 (13%)
1	4AC	A2	1338	1	21,24,25	1.09	2 (9%)	29,34,37	1.31	3 (10%)
1	PSU	A2	867	1	18,21,22	1.35	2 (11%)	22,30,33	1.92	4 (18%)
39	PSU	B5	1718	39	18,21,22	1.35	2 (11%)	22,30,33	1.89	3 (13%)
39	OMG	B5	3476	39	18,26,27	0.93	1 (5%)	19,38,41	1.08	2 (10%)
39	PSU	B5	3371	39	18,21,22	1.37	2 (11%)	22,30,33	1.88	3 (13%)
11	PSU	AT	27	11	18,21,22	1.35	2 (11%)	22,30,33	1.92	3 (13%)
39	OMG	B5	3974	39	18,26,27	0.89	1 (5%)	19,38,41	1.13	2 (10%)
39	A2M	B5	3517	39	18,25,26	0.93	1 (5%)	18,36,39	1.37	2 (11%)
1	MA6	A2	1852	1	18,26,27	0.94	1 (5%)	19,38,41	1.42	3 (15%)
39	OMG	B5	4240	39	18,26,27	0.92	1 (5%)	19,38,41	1.07	2 (10%)
39	OMC	B5	3433	39	19,22,23	0.79	0	26,31,34	0.76	0
30	SAC	Ar	2	30	7,8,9	0.53	0	8,9,11	0.89	1 (12%)
39	1MA	B5	1266	39,89	16,25,26	1.52	2 (12%)	18,37,40	1.06	3 (16%)
39	PSU	B5	1632	39	18,21,22	1.38	2 (11%)	22,30,33	1.89	4 (18%)
1	PSU	A2	36	1	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
39	OMU	B5	2258	39	19,22,23	1.22	2 (10%)	26,31,34	1.68	4 (15%)
44	AYA	BC	2	44	6,7,8	0.75	0	5,8,10	0.24	0
35	HY3	Aw	62	35	6,8,9	1.90	1 (16%)	5,10,12	1.13	1 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	PSU	A2	93	1	18,21,22	1.37	2 (11%)	22,30,33	1.90	3 (13%)
39	OMG	B5	2207	39	18,26,27	0.92	1 (5%)	19,38,41	1.08	2 (10%)
39	OMG	B5	1580	39	18,26,27	0.94	1 (5%)	19,38,41	1.08	2 (10%)
12	SAC	AZ	2	12	7,8,9	0.52	0	8,9,11	0.86	1 (12%)
39	OMG	B5	3359	39	18,26,27	0.94	1 (5%)	19,38,41	1.11	2 (10%)
39	PSU	B5	4166	39	18,21,22	1.37	2 (11%)	22,30,33	1.86	4 (18%)
1	A2M	A2	166	1	18,25,26	1.04	1 (5%)	18,36,39	1.27	2 (11%)
39	A2M	B5	1810	39,89	18,25,26	1.01	1 (5%)	18,36,39	1.34	2 (11%)
39	OMC	B5	2194	39,89	19,22,23	0.81	0	26,31,34	0.94	2 (7%)
39	PSU	B5	2475	39	18,21,22	1.36	2 (11%)	22,30,33	1.87	3 (13%)
39	PSU	B5	3490	39	18,21,22	1.36	2 (11%)	22,30,33	1.88	4 (18%)
39	PSU	B5	3502	39	18,21,22	1.37	2 (11%)	22,30,33	1.95	4 (18%)
39	A2M	B5	400	39	18,25,26	1.02	1 (5%)	18,36,39	1.23	2 (11%)
39	PSU	B5	3652	39,89	18,21,22	1.38	2 (11%)	22,30,33	1.91	3 (13%)
39	OMC	B5	3601	39	19,22,23	0.81	0	26,31,34	0.80	0
39	PSU	B5	3554	39	18,21,22	1.36	2 (11%)	22,30,33	1.86	3 (13%)
39	PSU	B5	4039	39	18,21,22	1.37	2 (11%)	22,30,33	1.88	3 (13%)
39	OMG	B5	2267	39	18,26,27	0.94	1 (5%)	19,38,41	1.03	2 (10%)
42	V5N	BA	216	42	4,11,12	0.77	0	5,14,16	1.55	1 (20%)
1	OMU	A2	355	1	19,22,23	1.24	3 (15%)	26,31,34	1.74	4 (15%)
1	6MZ	A2	1833	1,89	18,25,26	0.94	1 (5%)	16,36,39	1.77	3 (18%)
40	GTP	B7	1	40	26,34,34	0.94	2 (7%)	32,54,54	0.80	0
11	PSU	AT	39	11	18,21,22	1.36	2 (11%)	22,30,33	1.91	3 (13%)
39	OMC	B5	2208	39,89	19,22,23	0.79	0	26,31,34	0.78	0
39	A2M	B5	1479	39	18,25,26	0.98	1 (5%)	18,36,39	1.27	2 (11%)
69	MLZ	Bb	5	69	8,9,10	0.48	0	4,9,11	0.07	0
1	OMG	A2	1491	1,89	18,26,27	0.90	1 (5%)	19,38,41	1.17	3 (15%)
39	OMC	B5	2667	39	19,22,23	0.81	0	26,31,34	0.82	1 (3%)
39	PSU	B5	3462	39	18,21,22	1.34	2 (11%)	22,30,33	1.89	3 (13%)
39	A2M	B5	3562	39	18,25,26	1.01	1 (5%)	18,36,39	1.27	2 (11%)
39	A2M	B5	3450	39	18,25,26	1.00	1 (5%)	18,36,39	1.19	2 (11%)
39	PSU	B5	3576	39	18,21,22	1.38	2 (11%)	22,30,33	1.87	3 (13%)
1	OMU	A2	1289	1	19,22,23	1.24	3 (15%)	26,31,34	1.69	5 (19%)
39	OMG	B5	3942	11,39	18,26,27	0.94	1 (5%)	19,38,41	1.10	2 (10%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMC	A2	1704	1	-	2/9/27/28	0/2/2/2
39	PSU	B5	3616	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	4740	39	-	0/7/25/26	0/2/2/2
1	A2M	A2	99	1,89	-	2/5/27/28	0/3/3/3
1	PSU	A2	1626	1	-	0/7/25/26	0/2/2/2
39	A2M	B5	2206	39,89	-	0/5/27/28	0/3/3/3
1	PSU	A2	210	1	-	0/7/25/26	0/2/2/2
1	PSU	A2	1233	1	-	0/7/25/26	0/2/2/2
39	OMG	B5	4116	39	-	0/5/27/28	0/3/3/3
39	PSU	B5	3500	39	-	0/7/25/26	0/2/2/2
39	A2M	B5	3456	39	-	0/5/27/28	0/3/3/3
11	PSU	AT	28	11	-	0/7/25/26	0/2/2/2
39	PSU	B5	4278	39	-	0/7/25/26	0/2/2/2
11	OMG	AT	34	11,9	-	0/5/27/28	0/3/3/3
39	PSU	B5	4382	39	-	3/7/25/26	0/2/2/2
39	OMG	B5	3631	39	-	0/5/27/28	0/3/3/3
39	PSU	B5	1683	39	-	0/7/25/26	0/2/2/2
39	OMC	B5	2647	39	-	1/9/27/28	0/2/2/2
11	G7M	AT	46	11	-	1/3/25/26	0/3/3/3
1	PSU	A2	119	1	-	0/7/25/26	0/2/2/2
39	A2M	B5	1489	39,89	-	1/5/27/28	0/3/3/3
1	A2M	A2	513	1	-	4/5/27/28	0/3/3/3
39	PSU	B5	1801	39	-	0/7/25/26	0/2/2/2
39	OMC	B5	3619	39	-	2/9/27/28	0/2/2/2
1	OMU	A2	1443	1,89	-	1/9/27/28	0/2/2/2
39	PSU	B5	1638	39	-	0/7/25/26	0/2/2/2
39	PSU	B5	4149	39	-	0/7/25/26	0/2/2/2
39	A2M	B5	3492	39,1	-	2/5/27/28	0/3/3/3
1	OMC	A2	1392	1	-	1/9/27/28	0/2/2/2
39	PSU	B5	1491	39	-	0/7/25/26	0/2/2/2
39	OMU	B5	3973	39	-	1/9/27/28	0/2/2/2
39	PSU	B5	4749	39	-	0/7/25/26	0/2/2/2
39	A2M	B5	3557	39	-	1/5/27/28	0/3/3/3
1	OMG	A2	645	1	-	4/5/27/28	0/3/3/3
39	OMG	B5	4245	39	-	0/5/27/28	0/3/3/3
39	A2M	B5	2630	39,89	-	0/5/27/28	0/3/3/3
1	PSU	A2	34	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	A2	573	1	-	0/7/25/26	0/2/2/2
1	PSU	A2	802	1	-	2/7/25/26	0/2/2/2
39	PSU	B5	4419	39	-	0/7/25/26	0/2/2/2
1	OMC	A2	518	1	-	0/9/27/28	0/2/2/2
1	PSU	A2	1245	1	-	0/7/25/26	0/2/2/2
39	PSU	B5	2351	39	-	0/7/25/26	0/2/2/2
39	OMC	B5	4282	39,89	-	0/9/27/28	0/2/2/2
1	A2M	A2	669	1,89	-	2/5/27/28	0/3/3/3
39	5MC	B5	4193	39	-	4/7/25/26	0/2/2/2
43	HIC	BB	245	43	-	1/5/6/8	0/1/1/1
11	H2U	AT	17	11	-	6/7/38/39	0/2/2/2
11	1MA	AT	58	11	-	0/3/25/26	0/3/3/3
39	OMG	B5	1260	39	-	1/5/27/28	0/3/3/3
1	A2M	A2	577	1	-	2/5/27/28	0/3/3/3
1	G7M	A2	1640	11,1	-	0/3/25/26	0/3/3/3
1	OMG	A2	868	1	-	0/5/27/28	0/3/3/3
1	PSU	A2	650	1	-	0/7/25/26	0/2/2/2
1	PSU	A2	1644	1,89	-	0/7/25/26	0/2/2/2
39	OMG	B5	4138	39	-	0/5/27/28	0/3/3/3
1	PSU	A2	1348	1	-	0/7/25/26	0/2/2/2
11	5MU	AT	54	11	-	0/7/25/26	0/2/2/2
39	PSU	B5	3369	39	-	0/7/25/26	0/2/2/2
39	PSU	B5	4298	39	-	0/7/25/26	0/2/2/2
1	A2M	A2	1679	1	-	0/5/27/28	0/3/3/3
1	PSU	A2	864	1	-	0/7/25/26	0/2/2/2
39	PSU	B5	1720	39	-	0/7/25/26	0/2/2/2
39	UR3	B5	4276	39	-	0/7/25/26	0/2/2/2
39	PSU	B5	4107	39	-	0/7/25/26	0/2/2/2
39	OMG	B5	2719	39	-	0/5/27/28	0/3/3/3
11	PSU	AT	55	11	-	0/7/25/26	0/2/2/2
1	OMG	A2	1329	1	-	1/5/27/28	0/3/3/3
39	PSU	B5	4325	39	-	0/7/25/26	0/2/2/2
39	OMC	B5	3573	39	-	0/9/27/28	0/2/2/2
39	OMU	B5	4244	39	-	0/9/27/28	0/2/2/2
39	PSU	B5	3447	39	-	0/7/25/26	0/2/2/2
11	M2G	AT	26	11	-	0/7/29/30	0/3/3/3
1	PSU	A2	1047	1	-	0/7/25/26	0/2/2/2
1	A2M	A2	485	1	-	0/5/27/28	0/3/3/3
1	OMC	A2	174	1,89	-	0/9/27/28	0/2/2/2
39	PSU	B5	3496	39	-	0/7/25/26	0/2/2/2
39	PSU	B5	4374	39	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	PSU	B5	4217	39	-	0/7/25/26	0/2/2/2
1	OMU	A2	121	1	-	1/9/27/28	0/2/2/2
68	V5N	Ba	39	68	-	0/5/10/12	0/1/1/1
41	PSU	B8	55	41	-	0/7/25/26	0/2/2/2
39	OMC	B5	3540	39	-	0/9/27/28	0/2/2/2
1	PSU	A2	1005	1	-	0/7/25/26	0/2/2/2
39	A2M	B5	4317	39	-	0/5/27/28	0/3/3/3
39	PSU	B5	1731	39	-	0/7/25/26	0/2/2/2
11	2MG	AT	10	11	-	0/5/27/28	0/3/3/3
1	PSU	A2	687	1	-	0/7/25/26	0/2/2/2
39	A2M	B5	1270	39	-	0/5/27/28	0/3/3/3
39	PSU	B5	4435	39	-	0/7/25/26	0/2/2/2
11	OMC	AT	32	11	-	0/9/27/28	0/2/2/2
39	A2M	B5	3599	39	-	2/5/27/28	0/3/3/3
1	PSU	A2	652	1	-	0/7/25/26	0/2/2/2
39	PSU	B5	1537	39	-	0/7/25/26	0/2/2/2
1	PSU	A2	1057	1	-	0/7/25/26	0/2/2/2
39	PSU	B5	3427	39	-	0/7/25/26	0/2/2/2
39	OMC	B5	1820	39,89	-	1/9/27/28	0/2/2/2
1	OMC	A2	463	1	-	0/9/27/28	0/2/2/2
1	OMU	A2	116	1	-	1/9/27/28	0/2/2/2
1	PSU	A2	1046	1	-	0/7/25/26	0/2/2/2
39	A2M	B5	2244	39,89	-	0/5/27/28	0/3/3/3
39	PSU	B5	4099	39	-	0/7/25/26	0/2/2/2
39	PSU	B5	4042	39	-	0/7/25/26	0/2/2/2
39	A2M	B5	4269	39,89	-	0/5/27/28	0/3/3/3
1	PSU	A2	1368	1	-	0/7/25/26	0/2/2/2
1	MA6	A2	1851	1	-	0/7/29/30	0/3/3/3
80	M3L	Bm	98	80	-	0/9/10/12	-
39	PSU	B5	3583	39	-	1/7/25/26	0/2/2/2
39	PSU	B5	4045	39	-	0/7/25/26	0/2/2/2
11	5MC	AT	49	11	-	0/7/25/26	0/2/2/2
1	OMG	A2	510	1,89	-	0/5/27/28	0/3/3/3
39	A2M	B5	4336	39	-	1/5/27/28	0/3/3/3
1	PSU	A2	823	1	-	1/7/25/26	0/2/2/2
1	PSU	A2	1693	1	-	0/7/25/26	0/2/2/2
39	OMC	B5	1284	39	-	2/9/27/28	0/2/2/2
39	PSU	B5	4177	39	-	0/7/25/26	0/2/2/2
1	A2M	A2	27	1,89	-	2/5/27/28	0/3/3/3
1	A2M	A2	1384	1	-	0/5/27/28	0/3/3/3
39	5MC	B5	3514	39,89	-	0/7/25/26	0/2/2/2
39	PSU	B5	4267	39,89	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMU	A2	1805	1	-	2/9/27/28	0/2/2/2
1	A2M	A2	1032	1	-	0/5/27/28	0/3/3/3
39	6MZ	B5	3966	39	-	0/5/27/28	0/3/3/3
11	1MA	AT	14	11	-	0/3/25/26	0/3/3/3
39	PSU	B5	4203	39	-	0/7/25/26	0/2/2/2
39	PSU	B5	4058	39	-	0/7/25/26	0/2/2/2
1	B8N	A2	1249	1	-	4/16/34/35	0/2/2/2
1	PSU	A2	407	1	-	0/7/25/26	0/2/2/2
39	PSU	B5	4246	39	-	1/7/25/26	0/2/2/2
39	OMC	B5	2704	39	-	1/9/27/28	0/2/2/2
39	PSU	B5	4169	39	-	0/7/25/26	0/2/2/2
39	PSU	B5	3585	39,89	-	0/7/25/26	0/2/2/2
39	OMC	B5	4202	39	-	1/9/27/28	0/2/2/2
1	OMU	A2	628	1	-	2/9/27/28	0/2/2/2
1	PSU	A2	218	1	-	0/7/25/26	0/2/2/2
1	PSU	A2	1178	1	-	0/7/25/26	0/2/2/2
1	PSU	A2	105	1	-	0/7/25/26	0/2/2/2
1	PSU	A2	1239	1	-	0/7/25/26	0/2/2/2
39	OMC	B5	2265	39,89	-	1/9/27/28	0/2/2/2
39	PSU	B5	1799	39	-	0/7/25/26	0/2/2/2
39	PSU	B5	4322	39	-	0/7/25/26	0/2/2/2
39	OMG	B5	3676	39	-	1/5/27/28	0/3/3/3
1	OMU	A2	1327	1,89	-	0/9/27/28	0/2/2/2
1	PSU	A2	1446	1	-	0/7/25/26	0/2/2/2
39	PSU	B5	4711	39	-	0/7/25/26	0/2/2/2
83	SAC	Br	2	83	-	0/7/8/10	-
1	PSU	A2	816	1	-	0/7/25/26	0/2/2/2
1	PSU	A2	682	1	-	0/7/25/26	0/2/2/2
39	OMU	B5	2680	39	-	1/9/27/28	0/2/2/2
1	OMU	A2	172	1	-	0/9/27/28	0/2/2/2
39	PSU	B5	4188	39	-	0/7/25/26	0/2/2/2
39	UY1	B5	3550	39	-	4/9/27/28	0/2/2/2
41	OMG	B8	75	41	-	0/5/27/28	0/3/3/3
1	OMG	A2	437	1	-	0/5/27/28	0/3/3/3
39	OMU	B5	4052	39	-	0/9/27/28	0/2/2/2
1	A2M	A2	159	1	-	0/5/27/28	0/3/3/3
39	PSU	B5	3466	39	-	0/7/25/26	0/2/2/2
39	OMU	B5	3657	39	-	0/9/27/28	0/2/2/2
1	4AC	A2	1843	1	-	2/11/29/30	0/2/2/2
11	H2U	AT	16	11	-	1/7/38/39	0/2/2/2
39	OMG	B5	1477	39	-	1/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMU	A2	429	1	-	4/9/27/28	0/2/2/2
39	PSU	B5	3494	39	-	1/7/25/26	0/2/2/2
39	OMG	B5	4383	39	-	0/5/27/28	0/3/3/3
1	OMG	A2	684	1	-	4/5/27/28	0/3/3/3
1	PSU	A2	1082	1	-	1/7/25/26	0/2/2/2
39	PSU	B5	1721	39	-	0/7/25/26	0/2/2/2
81	MLZ	Bo	53	81	-	0/7/8/10	-
41	PSU	B8	69	41	-	0/7/25/26	0/2/2/2
33	AME	Au	1	33	-	2/9/10/12	-
1	A2M	A2	469	1	-	1/5/27/28	0/3/3/3
1	PSU	A2	610	1	-	0/7/25/26	0/2/2/2
39	OMU	B5	4366	39	-	0/9/27/28	0/2/2/2
39	OMG	B5	4364	39	-	0/5/27/28	0/3/3/3
1	OMG	A2	1448	1	-	2/5/27/28	0/3/3/3
39	A2M	B5	2658	39,89	-	0/5/27/28	0/3/3/3
31	NMM	As	67	31	-	1/9/11/13	-
1	A2M	A2	591	1	-	0/5/27/28	0/3/3/3
39	A2M	B5	398	39	-	2/5/27/28	0/3/3/3
1	PSU	A2	1175	1	-	0/7/25/26	0/2/2/2
39	OMG	B5	4369	39	-	1/5/27/28	0/3/3/3
11	YYG	AT	37	11	-	0/20/42/43	0/3/4/4
1	PSU	A2	109	1	-	0/7/25/26	0/2/2/2
1	PSU	A2	967	1	-	0/7/25/26	0/2/2/2
39	OMG	B5	3524	39	-	1/5/27/28	0/3/3/3
1	PSU	A2	815	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	867	1	-	0/7/25/26	0/2/2/2
39	PSU	B5	1718	39	-	0/7/25/26	0/2/2/2
39	OMG	B5	3476	39	-	0/5/27/28	0/3/3/3
39	PSU	B5	3371	39	-	0/7/25/26	0/2/2/2
11	PSU	AT	27	11	-	0/7/25/26	0/2/2/2
39	OMG	B5	3974	39	-	0/5/27/28	0/3/3/3
39	A2M	B5	3517	39	-	2/5/27/28	0/3/3/3
1	MA6	A2	1852	1	-	2/7/29/30	0/3/3/3
39	OMG	B5	4240	39	-	0/5/27/28	0/3/3/3
39	OMC	B5	3433	39	-	4/9/27/28	0/2/2/2
30	SAC	Ar	2	30	-	0/7/8/10	-
39	1MA	B5	1266	39,89	-	0/3/25/26	0/3/3/3
39	PSU	B5	1632	39	-	0/7/25/26	0/2/2/2
1	PSU	A2	36	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	OMU	B5	2258	39	-	0/9/27/28	0/2/2/2
44	AYA	BC	2	44	-	0/4/6/8	-
35	HY3	Aw	62	35	-	0/1/12/14	0/1/1/1
1	PSU	A2	93	1	-	0/7/25/26	0/2/2/2
39	OMG	B5	2207	39	-	2/5/27/28	0/3/3/3
39	OMG	B5	1580	39	-	0/5/27/28	0/3/3/3
12	SAC	AZ	2	12	-	2/7/8/10	-
39	OMG	B5	3359	39	-	0/5/27/28	0/3/3/3
39	PSU	B5	4166	39	-	0/7/25/26	0/2/2/2
1	A2M	A2	166	1	-	0/5/27/28	0/3/3/3
39	A2M	B5	1810	39,89	-	0/5/27/28	0/3/3/3
39	OMC	B5	2194	39,89	-	2/9/27/28	0/2/2/2
39	PSU	B5	2475	39	-	0/7/25/26	0/2/2/2
39	PSU	B5	3490	39	-	0/7/25/26	0/2/2/2
39	PSU	B5	3502	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	3652	39,89	-	0/7/25/26	0/2/2/2
39	OMC	B5	3601	39	-	0/9/27/28	0/2/2/2
39	PSU	B5	3554	39	-	0/7/25/26	0/2/2/2
39	PSU	B5	4039	39	-	0/7/25/26	0/2/2/2
39	OMG	B5	2267	39	-	0/5/27/28	0/3/3/3
42	V5N	BA	216	42	-	1/5/10/12	0/1/1/1
1	OMU	A2	355	1	-	0/9/27/28	0/2/2/2
1	6MZ	A2	1833	1,89	-	2/5/27/28	0/3/3/3
40	GTP	B7	1	40	-	0/18/38/38	0/3/3/3
11	PSU	AT	39	11	-	0/7/25/26	0/2/2/2
39	OMC	B5	2208	39,89	-	0/9/27/28	0/2/2/2
39	A2M	B5	1479	39	-	0/5/27/28	0/3/3/3
69	MLZ	Bb	5	69	-	2/7/8/10	-
1	OMG	A2	1491	1,89	-	2/5/27/28	0/3/3/3
39	OMC	B5	2667	39	-	0/9/27/28	0/2/2/2
39	PSU	B5	3462	39	-	0/7/25/26	0/2/2/2
39	A2M	B5	3562	39	-	0/5/27/28	0/3/3/3
39	A2M	B5	3450	39	-	1/5/27/28	0/3/3/3
39	PSU	B5	3576	39	-	1/7/25/26	0/2/2/2
1	OMU	A2	1289	1	-	0/9/27/28	0/2/2/2
39	OMG	B5	3942	11,39	-	0/5/27/28	0/3/3/3

All (365) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A2	1640	G7M	C8-N9	7.54	1.47	1.33
11	AT	46	G7M	C8-N9	7.45	1.46	1.33
11	AT	46	G7M	C8-N7	7.17	1.46	1.33
1	A2	1640	G7M	C8-N7	7.15	1.46	1.33
11	AT	37	YYG	O23-C21	6.57	1.45	1.34
11	AT	37	YYG	O18-C16	5.16	1.45	1.33
11	AT	58	1MA	C2-N3	4.87	1.34	1.29
11	AT	14	1MA	C2-N3	4.80	1.34	1.29
39	B5	1266	1MA	C2-N3	4.63	1.34	1.29
11	AT	26	M2G	C2-N3	4.35	1.36	1.30
1	A2	1640	G7M	C5-C4	4.32	1.47	1.39
35	Aw	62	HY3	C3-CA	-4.29	1.50	1.55
11	AT	46	G7M	C5-C4	4.24	1.47	1.39
39	B5	3550	UY1	C6-C5	3.38	1.39	1.35
11	AT	58	1MA	C6-N6	3.24	1.35	1.27
1	A2	210	PSU	C6-C5	3.21	1.39	1.35
1	A2	867	PSU	C6-C5	3.20	1.39	1.35
39	B5	1266	1MA	C6-N6	3.20	1.35	1.27
1	A2	802	PSU	C6-C5	3.19	1.39	1.35
39	B5	4039	PSU	C6-C5	3.19	1.39	1.35
11	AT	14	1MA	C6-N6	3.19	1.35	1.27
41	B8	55	PSU	C6-C5	3.18	1.39	1.35
1	A2	1249	B8N	C4-N3	-3.18	1.34	1.40
39	B5	3494	PSU	C6-C5	3.17	1.39	1.35
39	B5	3616	PSU	C6-C5	3.17	1.39	1.35
39	B5	4166	PSU	C6-C5	3.16	1.39	1.35
1	A2	1005	PSU	C6-C5	3.15	1.39	1.35
1	A2	864	PSU	C6-C5	3.14	1.39	1.35
39	B5	1720	PSU	C6-C5	3.14	1.39	1.35
1	A2	610	PSU	C6-C5	3.14	1.39	1.35
1	A2	682	PSU	C6-C5	3.14	1.39	1.35
11	AT	28	PSU	C6-C5	3.14	1.39	1.35
39	B5	4042	PSU	C6-C5	3.14	1.39	1.35
1	A2	1178	PSU	C6-C5	3.13	1.39	1.35
39	B5	1632	PSU	C6-C5	3.13	1.39	1.35
39	B5	4099	PSU	C6-C5	3.13	1.39	1.35
39	B5	1799	PSU	C6-C5	3.13	1.39	1.35
39	B5	4325	PSU	C6-C5	3.13	1.39	1.35
39	B5	4711	PSU	C6-C5	3.13	1.39	1.35
39	B5	4749	PSU	C6-C5	3.13	1.39	1.35
39	B5	3496	PSU	C6-C5	3.12	1.39	1.35
1	A2	93	PSU	C6-C5	3.12	1.39	1.35
1	A2	1626	PSU	C6-C5	3.12	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A2	1239	PSU	C6-C5	3.12	1.39	1.35
39	B5	4217	PSU	C6-C5	3.12	1.39	1.35
39	B5	3576	PSU	C6-C5	3.12	1.39	1.35
1	A2	967	PSU	C6-C5	3.11	1.38	1.35
39	B5	4374	PSU	C6-C5	3.11	1.38	1.35
1	A2	34	PSU	C6-C5	3.11	1.38	1.35
1	A2	1047	PSU	C6-C5	3.11	1.38	1.35
39	B5	2475	PSU	C6-C5	3.10	1.38	1.35
1	A2	1233	PSU	C6-C5	3.10	1.38	1.35
1	A2	1348	PSU	C6-C5	3.10	1.38	1.35
39	B5	4740	PSU	C6-C5	3.10	1.38	1.35
39	B5	3466	PSU	C6-C5	3.09	1.38	1.35
39	B5	1638	PSU	C6-C5	3.09	1.38	1.35
39	B5	1721	PSU	C6-C5	3.09	1.38	1.35
1	A2	105	PSU	C6-C5	3.09	1.38	1.35
39	B5	1731	PSU	C6-C5	3.08	1.38	1.35
39	B5	3554	PSU	C6-C5	3.08	1.38	1.35
1	A2	1693	PSU	C6-C5	3.08	1.38	1.35
39	B5	4267	PSU	C6-C5	3.08	1.38	1.35
39	B5	4435	PSU	C6-C5	3.08	1.38	1.35
11	AT	55	PSU	C6-C5	3.08	1.38	1.35
1	A2	650	PSU	C6-C5	3.08	1.38	1.35
39	B5	3500	PSU	C6-C5	3.08	1.38	1.35
1	A2	1057	PSU	C6-C5	3.07	1.38	1.35
1	A2	1082	PSU	C6-C5	3.07	1.38	1.35
39	B5	4322	PSU	C6-C5	3.07	1.38	1.35
39	B5	3583	PSU	C6-C5	3.07	1.38	1.35
39	B5	4169	PSU	C6-C5	3.07	1.38	1.35
1	A2	119	PSU	C6-C5	3.07	1.38	1.35
1	A2	1446	PSU	C6-C5	3.06	1.38	1.35
39	B5	1801	PSU	C6-C5	3.06	1.38	1.35
39	B5	1537	PSU	C6-C5	3.06	1.38	1.35
39	B5	3585	PSU	C6-C5	3.06	1.38	1.35
39	B5	4177	PSU	C6-C5	3.06	1.38	1.35
11	AT	27	PSU	C6-C5	3.06	1.38	1.35
1	A2	815	PSU	C6-C5	3.06	1.38	1.35
39	B5	3502	PSU	C6-C5	3.06	1.38	1.35
11	AT	39	PSU	C6-C5	3.06	1.38	1.35
39	B5	4107	PSU	C6-C5	3.05	1.38	1.35
1	A2	823	PSU	C6-C5	3.05	1.38	1.35
1	A2	218	PSU	C6-C5	3.05	1.38	1.35
39	B5	4382	PSU	C6-C5	3.04	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	B5	3447	PSU	C6-C5	3.04	1.38	1.35
1	A2	687	PSU	C6-C5	3.04	1.38	1.35
1	A2	816	PSU	C6-C5	3.04	1.38	1.35
39	B5	4278	PSU	C6-C5	3.04	1.38	1.35
39	B5	4246	PSU	C6-C5	3.04	1.38	1.35
1	A2	1046	PSU	C6-C5	3.04	1.38	1.35
1	A2	573	PSU	C6-C5	3.03	1.38	1.35
39	B5	1683	PSU	C6-C5	3.03	1.38	1.35
39	B5	2351	PSU	C6-C5	3.03	1.38	1.35
39	B5	4045	PSU	C6-C5	3.03	1.38	1.35
39	B5	3490	PSU	C6-C5	3.03	1.38	1.35
1	A2	1175	PSU	C6-C5	3.03	1.38	1.35
1	A2	109	PSU	C6-C5	3.03	1.38	1.35
41	B8	69	PSU	C6-C5	3.02	1.38	1.35
1	A2	652	PSU	C6-C5	3.02	1.38	1.35
39	B5	4298	PSU	C6-C5	3.02	1.38	1.35
39	B5	1491	PSU	C6-C5	3.02	1.38	1.35
1	A2	1644	PSU	C6-C5	3.02	1.38	1.35
1	A2	1368	PSU	C6-C5	3.01	1.38	1.35
39	B5	4149	PSU	C6-C5	3.01	1.38	1.35
39	B5	1718	PSU	C6-C5	3.01	1.38	1.35
39	B5	4058	PSU	C6-C5	3.01	1.38	1.35
39	B5	3427	PSU	C6-C5	3.00	1.38	1.35
39	B5	3462	PSU	C6-C5	3.00	1.38	1.35
39	B5	3652	PSU	C6-C5	2.99	1.38	1.35
1	A2	407	PSU	C6-C5	2.98	1.38	1.35
39	B5	4419	PSU	C6-C5	2.98	1.38	1.35
39	B5	3371	PSU	C6-C5	2.98	1.38	1.35
1	A2	1245	PSU	C6-C5	2.98	1.38	1.35
39	B5	4188	PSU	C6-C5	2.97	1.38	1.35
39	B5	4203	PSU	C6-C5	2.97	1.38	1.35
1	A2	36	PSU	C6-C5	2.96	1.38	1.35
1	A2	1249	B8N	C6-C5	2.92	1.39	1.34
39	B5	3369	PSU	C6-C5	2.92	1.38	1.35
39	B5	4193	5MC	C6-C5	2.91	1.39	1.34
39	B5	1491	PSU	C4-N3	-2.90	1.33	1.38
1	A2	1338	4AC	C4-N4	-2.90	1.35	1.39
39	B5	3369	PSU	C4-N3	-2.89	1.33	1.38
39	B5	4217	PSU	C4-N3	-2.85	1.33	1.38
39	B5	1799	PSU	C4-N3	-2.84	1.33	1.38
39	B5	3583	PSU	C4-N3	-2.84	1.33	1.38
39	B5	4419	PSU	C4-N3	-2.83	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	B5	4298	PSU	C4-N3	-2.83	1.33	1.38
1	A2	407	PSU	C4-N3	-2.82	1.33	1.38
1	A2	1693	PSU	C4-N3	-2.82	1.33	1.38
39	B5	3585	PSU	C4-N3	-2.81	1.33	1.38
39	B5	4435	PSU	C4-N3	-2.81	1.33	1.38
1	A2	864	PSU	C4-N3	-2.81	1.33	1.38
39	B5	1638	PSU	C4-N3	-2.81	1.33	1.38
1	A2	1348	PSU	C4-N3	-2.81	1.33	1.38
39	B5	3490	PSU	C4-N3	-2.81	1.33	1.38
39	B5	3500	PSU	C4-N3	-2.81	1.33	1.38
39	B5	3652	PSU	C4-N3	-2.81	1.33	1.38
1	A2	682	PSU	C4-N3	-2.80	1.33	1.38
1	A2	1175	PSU	C4-N3	-2.80	1.33	1.38
39	B5	4058	PSU	C4-N3	-2.80	1.33	1.38
41	B8	69	PSU	C4-N3	-2.80	1.33	1.38
39	B5	4107	PSU	C4-N3	-2.80	1.33	1.38
39	B5	4740	PSU	C4-N3	-2.79	1.33	1.38
39	B5	1801	PSU	C4-N3	-2.79	1.33	1.38
39	B5	3576	PSU	C4-N3	-2.79	1.33	1.38
39	B5	4045	PSU	C4-N3	-2.79	1.33	1.38
39	B5	2351	PSU	C4-N3	-2.79	1.33	1.38
39	B5	3427	PSU	C4-N3	-2.79	1.33	1.38
39	B5	1731	PSU	C4-N3	-2.79	1.33	1.38
1	A2	1082	PSU	C4-N3	-2.78	1.33	1.38
39	B5	4374	PSU	C4-N3	-2.78	1.33	1.38
1	A2	1005	PSU	C4-N3	-2.78	1.33	1.38
39	B5	4267	PSU	C4-N3	-2.78	1.33	1.38
1	A2	650	PSU	C4-N3	-2.77	1.33	1.38
1	A2	967	PSU	C4-N3	-2.77	1.33	1.38
1	A2	815	PSU	C4-N3	-2.77	1.33	1.38
39	B5	4149	PSU	C4-N3	-2.77	1.33	1.38
39	B5	4203	PSU	C4-N3	-2.77	1.33	1.38
39	B5	4325	PSU	C4-N3	-2.77	1.33	1.38
39	B5	4188	PSU	C4-N3	-2.76	1.33	1.38
39	B5	3502	PSU	C4-N3	-2.76	1.33	1.38
39	B5	1721	PSU	C4-N3	-2.76	1.33	1.38
11	AT	27	PSU	C4-N3	-2.76	1.33	1.38
39	B5	3371	PSU	C4-N3	-2.76	1.33	1.38
1	A2	1245	PSU	C4-N3	-2.76	1.33	1.38
39	B5	4382	PSU	C4-N3	-2.75	1.33	1.38
39	B5	4099	PSU	C4-N3	-2.75	1.33	1.38
1	A2	105	PSU	C4-N3	-2.75	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	B5	3616	PSU	C4-N3	-2.75	1.33	1.38
1	A2	1233	PSU	C4-N3	-2.75	1.33	1.38
39	B5	4169	PSU	C4-N3	-2.75	1.33	1.38
1	A2	93	PSU	C4-N3	-2.75	1.33	1.38
39	B5	1683	PSU	C4-N3	-2.75	1.33	1.38
39	B5	3447	PSU	C4-N3	-2.75	1.33	1.38
39	B5	1720	PSU	C4-N3	-2.75	1.33	1.38
1	A2	1047	PSU	C4-N3	-2.75	1.33	1.38
1	A2	109	PSU	C4-N3	-2.75	1.33	1.38
1	A2	34	PSU	C4-N3	-2.75	1.33	1.38
1	A2	652	PSU	C4-N3	-2.75	1.33	1.38
39	B5	1537	PSU	C4-N3	-2.75	1.33	1.38
1	A2	1446	PSU	C4-N3	-2.74	1.33	1.38
11	AT	28	PSU	C4-N3	-2.74	1.33	1.38
39	B5	3496	PSU	C4-N3	-2.74	1.33	1.38
1	A2	1057	PSU	C4-N3	-2.74	1.33	1.38
11	AT	55	PSU	C4-N3	-2.74	1.33	1.38
1	A2	1046	PSU	C4-N3	-2.74	1.33	1.38
1	A2	1239	PSU	C4-N3	-2.74	1.33	1.38
39	B5	4278	PSU	C4-N3	-2.74	1.33	1.38
39	B5	3466	PSU	C4-N3	-2.74	1.33	1.38
1	A2	1178	PSU	C4-N3	-2.74	1.33	1.38
39	B5	4711	PSU	C4-N3	-2.74	1.33	1.38
39	B5	4042	PSU	C4-N3	-2.73	1.33	1.38
39	B5	2475	PSU	C4-N3	-2.73	1.33	1.38
1	A2	687	PSU	C4-N3	-2.73	1.33	1.38
1	A2	218	PSU	C4-N3	-2.72	1.33	1.38
39	B5	4039	PSU	C4-N3	-2.72	1.33	1.38
39	B5	4749	PSU	C4-N3	-2.72	1.33	1.38
1	A2	610	PSU	C4-N3	-2.72	1.33	1.38
39	B5	3462	PSU	C4-N3	-2.72	1.33	1.38
1	A2	1368	PSU	C4-N3	-2.72	1.33	1.38
11	AT	39	PSU	C4-N3	-2.72	1.33	1.38
39	B5	4322	PSU	C4-N3	-2.72	1.33	1.38
1	A2	816	PSU	C4-N3	-2.72	1.33	1.38
41	B8	55	PSU	C4-N3	-2.71	1.33	1.38
1	A2	1644	PSU	C4-N3	-2.71	1.33	1.38
39	B5	3514	5MC	C6-C5	2.71	1.39	1.34
11	AT	26	M2G	C2-N2	2.71	1.40	1.35
1	A2	867	PSU	C4-N3	-2.70	1.33	1.38
1	A2	119	PSU	C4-N3	-2.70	1.33	1.38
1	A2	1626	PSU	C4-N3	-2.70	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	B5	4246	PSU	C4-N3	-2.70	1.33	1.38
11	AT	49	5MC	C6-C5	2.70	1.39	1.34
39	B5	3554	PSU	C4-N3	-2.69	1.33	1.38
39	B5	4166	PSU	C4-N3	-2.69	1.33	1.38
39	B5	4177	PSU	C4-N3	-2.69	1.33	1.38
1	A2	802	PSU	C4-N3	-2.69	1.33	1.38
39	B5	1718	PSU	C4-N3	-2.69	1.33	1.38
1	A2	36	PSU	C4-N3	-2.68	1.33	1.38
39	B5	2267	OMG	C6-N1	-2.67	1.33	1.37
11	AT	54	5MU	C6-C5	2.67	1.39	1.34
11	AT	54	5MU	C4-N3	-2.67	1.33	1.38
1	A2	573	PSU	C4-N3	-2.67	1.33	1.38
39	B5	4244	OMU	C4-N3	-2.66	1.33	1.38
39	B5	3657	OMU	C4-N3	-2.66	1.33	1.38
39	B5	4366	OMU	C4-N3	-2.66	1.33	1.38
39	B5	3494	PSU	C4-N3	-2.64	1.33	1.38
39	B5	3550	UY1	C2-N1	2.64	1.40	1.36
39	B5	3942	OMG	C6-N1	-2.64	1.33	1.37
1	A2	355	OMU	C4-N3	-2.63	1.33	1.38
39	B5	2719	OMG	C6-N1	-2.63	1.33	1.37
1	A2	823	PSU	C4-N3	-2.63	1.34	1.38
39	B5	3973	OMU	C4-N3	-2.62	1.33	1.38
1	A2	1843	4AC	C4-N4	-2.62	1.35	1.39
39	B5	4052	OMU	C4-N3	-2.61	1.33	1.38
39	B5	1580	OMG	C6-N1	-2.61	1.34	1.37
39	B5	3359	OMG	C6-N1	-2.61	1.34	1.37
39	B5	2680	OMU	C4-N3	-2.61	1.33	1.38
1	A2	210	PSU	C4-N3	-2.60	1.34	1.38
1	A2	602	OMG	C6-N1	-2.59	1.34	1.37
40	B7	1	GTP	C5-C6	-2.59	1.42	1.47
39	B5	1632	PSU	C4-N3	-2.58	1.34	1.38
39	B5	2207	OMG	C6-N1	-2.58	1.34	1.37
1	A2	1491	OMG	C6-N1	-2.58	1.34	1.37
39	B5	4116	OMG	C6-N1	-2.58	1.34	1.37
39	B5	2258	OMU	C4-N3	-2.57	1.34	1.38
1	A2	437	OMG	C6-N1	-2.56	1.34	1.37
1	A2	510	OMG	C6-N1	-2.56	1.34	1.37
1	A2	121	OMU	C4-N3	-2.55	1.34	1.38
1	A2	172	OMU	C4-N3	-2.55	1.34	1.38
39	B5	4364	OMG	C6-N1	-2.55	1.34	1.37
11	AT	17	H2U	C2-N3	-2.55	1.33	1.38
39	B5	1260	OMG	C6-N1	-2.54	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	B5	4245	OMG	C6-N1	-2.54	1.34	1.37
1	A2	645	OMG	C6-N1	-2.54	1.34	1.37
39	B5	3476	OMG	C6-N1	-2.54	1.34	1.37
39	B5	4138	OMG	C6-N1	-2.54	1.34	1.37
1	A2	1443	OMU	C4-N3	-2.54	1.34	1.38
39	B5	4383	OMG	C6-N1	-2.53	1.34	1.37
1	A2	429	OMU	C4-N3	-2.53	1.34	1.38
1	A2	1805	OMU	C4-N3	-2.53	1.34	1.38
1	A2	1249	B8N	C2-N3	-2.52	1.34	1.38
1	A2	1289	OMU	C4-N3	-2.52	1.34	1.38
1	A2	1448	OMG	C6-N1	-2.51	1.34	1.37
39	B5	1477	OMG	C6-N1	-2.51	1.34	1.37
39	B5	4369	OMG	C6-N1	-2.51	1.34	1.37
11	AT	16	H2U	C2-N3	-2.50	1.33	1.38
39	B5	4240	OMG	C6-N1	-2.50	1.34	1.37
1	A2	1329	OMG	C6-N1	-2.50	1.34	1.37
1	A2	1327	OMU	C4-N3	-2.49	1.34	1.38
1	A2	591	A2M	C5-C4	2.49	1.47	1.40
39	B5	3524	OMG	C6-N1	-2.49	1.34	1.37
39	B5	3492	A2M	C5-C4	2.48	1.47	1.40
39	B5	3631	OMG	C6-N1	-2.48	1.34	1.37
11	AT	10	2MG	C6-N1	-2.48	1.34	1.37
1	A2	116	OMU	C4-N3	-2.47	1.34	1.38
1	A2	1852	MA6	C5-C4	2.46	1.47	1.40
11	AT	26	M2G	C6-N1	-2.46	1.34	1.37
11	AT	37	YYG	C4-N3	-2.46	1.35	1.40
39	B5	3676	OMG	C6-N1	-2.46	1.34	1.37
1	A2	1851	MA6	C5-C4	2.45	1.47	1.40
39	B5	3974	OMG	C6-N1	-2.45	1.34	1.37
11	AT	34	OMG	C6-N1	-2.44	1.34	1.37
39	B5	398	A2M	C5-C4	2.44	1.47	1.40
1	A2	868	OMG	C6-N1	-2.43	1.34	1.37
41	B8	75	OMG	C6-N1	-2.43	1.34	1.37
39	B5	400	A2M	C5-C4	2.43	1.47	1.40
1	A2	628	OMU	C4-N3	-2.43	1.34	1.38
39	B5	4317	A2M	C5-C4	2.43	1.47	1.40
39	B5	3599	A2M	C5-C4	2.43	1.47	1.40
1	A2	1384	A2M	C5-C4	2.43	1.47	1.40
1	A2	684	OMG	C6-N1	-2.42	1.34	1.37
39	B5	3456	A2M	C5-C4	2.42	1.47	1.40
1	A2	27	A2M	C5-C4	2.42	1.47	1.40
1	A2	513	A2M	C5-C4	2.42	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A2	166	A2M	C5-C4	2.42	1.47	1.40
1	A2	1640	G7M	C6-N1	-2.42	1.34	1.37
39	B5	4336	A2M	C5-C4	2.42	1.47	1.40
1	A2	159	A2M	C5-C4	2.42	1.47	1.40
1	A2	577	A2M	C5-C4	2.41	1.47	1.40
1	A2	99	A2M	C5-C4	2.41	1.47	1.40
39	B5	2658	A2M	C5-C4	2.40	1.47	1.40
1	A2	469	A2M	C5-C4	2.40	1.47	1.40
39	B5	4269	A2M	C5-C4	2.40	1.47	1.40
39	B5	3562	A2M	C5-C4	2.39	1.47	1.40
39	B5	3557	A2M	C5-C4	2.39	1.47	1.40
39	B5	3966	6MZ	C5-C4	2.39	1.47	1.40
1	A2	485	A2M	C5-C4	2.38	1.47	1.40
1	A2	1833	6MZ	C5-C4	2.38	1.47	1.40
39	B5	3657	OMU	C2-N3	-2.37	1.33	1.38
39	B5	1489	A2M	C5-C4	2.37	1.47	1.40
39	B5	2206	A2M	C5-C4	2.37	1.47	1.40
1	A2	1679	A2M	C5-C4	2.37	1.47	1.40
39	B5	3450	A2M	C5-C4	2.37	1.47	1.40
39	B5	2244	A2M	C5-C4	2.36	1.47	1.40
39	B5	1810	A2M	C5-C4	2.36	1.47	1.40
39	B5	2630	A2M	C5-C4	2.36	1.47	1.40
39	B5	1270	A2M	C5-C4	2.36	1.47	1.40
39	B5	1479	A2M	C5-C4	2.34	1.47	1.40
11	AT	54	5MU	C6-N1	-2.33	1.34	1.38
1	A2	669	A2M	C5-C4	2.32	1.47	1.40
1	A2	1032	A2M	C5-C4	2.32	1.47	1.40
39	B5	3973	OMU	C2-N3	-2.31	1.33	1.38
39	B5	4193	5MC	C6-N1	-2.30	1.34	1.38
11	AT	17	H2U	C4-N3	-2.30	1.33	1.37
11	AT	54	5MU	C4-C5	2.29	1.48	1.44
11	AT	49	5MC	C6-N1	-2.29	1.34	1.38
11	AT	46	G7M	C6-N1	-2.29	1.34	1.37
39	B5	4244	OMU	C2-N3	-2.27	1.33	1.38
1	A2	116	OMU	C2-N3	-2.26	1.33	1.38
39	B5	3550	UY1	C6-N1	-2.24	1.32	1.36
39	B5	2680	OMU	C2-N3	-2.24	1.34	1.38
1	A2	1327	OMU	C2-N3	-2.24	1.34	1.38
39	B5	3514	5MC	C6-N1	-2.23	1.34	1.38
39	B5	4366	OMU	C2-N3	-2.23	1.34	1.38
39	B5	2258	OMU	C2-N3	-2.22	1.34	1.38
1	A2	1289	OMU	C2-N1	2.22	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	B5	3517	A2M	C5-C4	2.22	1.46	1.40
1	A2	355	OMU	C2-N3	-2.22	1.34	1.38
1	A2	121	OMU	C2-N3	-2.21	1.34	1.38
39	B5	4052	OMU	C2-N3	-2.20	1.34	1.38
1	A2	1805	OMU	C2-N3	-2.20	1.34	1.38
1	A2	628	OMU	C2-N3	-2.19	1.34	1.38
1	A2	429	OMU	C2-N3	-2.17	1.34	1.38
1	A2	1443	OMU	C2-N3	-2.17	1.34	1.38
1	A2	1289	OMU	C2-N3	-2.17	1.34	1.38
11	AT	16	H2U	C4-N3	-2.15	1.33	1.37
39	B5	3369	PSU	C2-N3	-2.14	1.33	1.37
11	AT	54	5MU	C2-N1	2.13	1.41	1.38
1	A2	172	OMU	C2-N3	-2.13	1.34	1.38
1	A2	1805	OMU	C2-N1	2.08	1.41	1.38
1	A2	116	OMU	C5-C4	-2.07	1.39	1.43
39	B5	4052	OMU	C5-C4	-2.07	1.39	1.43
40	B7	1	GTP	C8-N7	-2.06	1.31	1.35
11	AT	37	YYG	O6-C6	2.06	1.25	1.22
1	A2	121	OMU	C5-C4	-2.05	1.39	1.43
1	A2	172	OMU	C5-C4	-2.05	1.39	1.43
1	A2	1338	4AC	C7-N4	-2.05	1.33	1.37
1	A2	1443	OMU	C5-C4	-2.05	1.39	1.43
39	B5	3973	OMU	C2-N1	2.04	1.41	1.38
11	AT	54	5MU	C2-N3	-2.03	1.34	1.38
1	A2	1082	PSU	C2-N3	-2.03	1.34	1.37
39	B5	4366	OMU	C5-C4	-2.03	1.39	1.43
1	A2	355	OMU	C5-C4	-2.02	1.39	1.43
39	B5	4276	UR3	C2-N1	2.01	1.41	1.38

All (622) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	AT	17	H2U	C4-N3-C2	-7.02	119.97	125.79
39	B5	3369	PSU	N1-C2-N3	6.25	122.21	115.13
39	B5	4374	PSU	N1-C2-N3	6.22	122.18	115.13
39	B5	3502	PSU	N1-C2-N3	6.20	122.16	115.13
39	B5	4298	PSU	N1-C2-N3	6.19	122.14	115.13
1	A2	1178	PSU	N1-C2-N3	6.18	122.13	115.13
41	B8	69	PSU	N1-C2-N3	6.18	122.13	115.13
39	B5	4325	PSU	N1-C2-N3	6.16	122.11	115.13
39	B5	4246	PSU	N1-C2-N3	6.16	122.10	115.13
39	B5	3583	PSU	N1-C2-N3	6.15	122.10	115.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	B5	4188	PSU	N1-C2-N3	6.15	122.10	115.13
39	B5	4149	PSU	N1-C2-N3	6.15	122.10	115.13
1	A2	650	PSU	N1-C2-N3	6.15	122.09	115.13
39	B5	3496	PSU	N1-C2-N3	6.14	122.08	115.13
39	B5	3447	PSU	N1-C2-N3	6.14	122.08	115.13
39	B5	1801	PSU	N1-C2-N3	6.12	122.07	115.13
39	B5	4042	PSU	N1-C2-N3	6.12	122.06	115.13
39	B5	4711	PSU	N1-C2-N3	6.12	122.06	115.13
1	A2	105	PSU	N1-C2-N3	6.11	122.06	115.13
39	B5	4419	PSU	N1-C2-N3	6.11	122.06	115.13
39	B5	3427	PSU	N1-C2-N3	6.11	122.06	115.13
39	B5	3585	PSU	N1-C2-N3	6.11	122.06	115.13
39	B5	2351	PSU	N1-C2-N3	6.11	122.05	115.13
11	AT	39	PSU	N1-C2-N3	6.11	122.05	115.13
39	B5	4435	PSU	N1-C2-N3	6.11	122.05	115.13
1	A2	34	PSU	N1-C2-N3	6.11	122.05	115.13
39	B5	1491	PSU	N1-C2-N3	6.10	122.04	115.13
39	B5	3466	PSU	N1-C2-N3	6.10	122.04	115.13
39	B5	1721	PSU	N1-C2-N3	6.10	122.04	115.13
11	AT	27	PSU	N1-C2-N3	6.10	122.04	115.13
39	B5	1799	PSU	N1-C2-N3	6.10	122.04	115.13
11	AT	28	PSU	N1-C2-N3	6.10	122.04	115.13
41	B8	55	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	4058	PSU	N1-C2-N3	6.09	122.03	115.13
39	B5	4107	PSU	N1-C2-N3	6.09	122.03	115.13
39	B5	4045	PSU	N1-C2-N3	6.08	122.02	115.13
1	A2	816	PSU	N1-C2-N3	6.08	122.02	115.13
1	A2	1057	PSU	N1-C2-N3	6.08	122.02	115.13
39	B5	3500	PSU	N1-C2-N3	6.08	122.02	115.13
39	B5	4740	PSU	N1-C2-N3	6.08	122.02	115.13
1	A2	652	PSU	N1-C2-N3	6.08	122.01	115.13
1	A2	1047	PSU	N1-C2-N3	6.08	122.01	115.13
39	B5	1683	PSU	N1-C2-N3	6.07	122.01	115.13
39	B5	1632	PSU	N1-C2-N3	6.07	122.00	115.13
1	A2	1644	PSU	N1-C2-N3	6.07	122.00	115.13
39	B5	1638	PSU	N1-C2-N3	6.07	122.00	115.13
39	B5	3494	PSU	N1-C2-N3	6.07	122.00	115.13
1	A2	218	PSU	N1-C2-N3	6.06	122.00	115.13
1	A2	687	PSU	N1-C2-N3	6.06	122.00	115.13
1	A2	1693	PSU	N1-C2-N3	6.06	122.00	115.13
1	A2	967	PSU	N1-C2-N3	6.06	122.00	115.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	B5	1720	PSU	N1-C2-N3	6.06	121.99	115.13
1	A2	867	PSU	N1-C2-N3	6.06	121.99	115.13
39	B5	3371	PSU	N1-C2-N3	6.06	121.99	115.13
39	B5	1537	PSU	N1-C2-N3	6.05	121.99	115.13
1	A2	610	PSU	N1-C2-N3	6.05	121.99	115.13
1	A2	864	PSU	N1-C2-N3	6.05	121.98	115.13
1	A2	1233	PSU	N1-C2-N3	6.05	121.98	115.13
1	A2	1239	PSU	N1-C2-N3	6.05	121.98	115.13
1	A2	1626	PSU	N1-C2-N3	6.05	121.98	115.13
39	B5	3652	PSU	N1-C2-N3	6.05	121.98	115.13
39	B5	4382	PSU	N1-C2-N3	6.04	121.98	115.13
1	A2	407	PSU	N1-C2-N3	6.04	121.98	115.13
1	A2	1368	PSU	N1-C2-N3	6.04	121.98	115.13
39	B5	4322	PSU	N1-C2-N3	6.04	121.97	115.13
1	A2	1446	PSU	N1-C2-N3	6.04	121.97	115.13
1	A2	823	PSU	N1-C2-N3	6.04	121.97	115.13
1	A2	109	PSU	N1-C2-N3	6.03	121.97	115.13
1	A2	1348	PSU	N1-C2-N3	6.03	121.97	115.13
39	B5	4169	PSU	N1-C2-N3	6.03	121.96	115.13
1	A2	93	PSU	N1-C2-N3	6.03	121.96	115.13
39	B5	4217	PSU	N1-C2-N3	6.03	121.96	115.13
11	AT	55	PSU	N1-C2-N3	6.03	121.96	115.13
1	A2	573	PSU	N1-C2-N3	6.02	121.95	115.13
1	A2	815	PSU	N1-C2-N3	6.02	121.95	115.13
39	B5	4267	PSU	N1-C2-N3	6.01	121.94	115.13
1	A2	1046	PSU	N1-C2-N3	6.01	121.94	115.13
1	A2	682	PSU	N1-C2-N3	6.00	121.93	115.13
39	B5	4278	PSU	N1-C2-N3	6.00	121.93	115.13
1	A2	802	PSU	N1-C2-N3	6.00	121.93	115.13
39	B5	4177	PSU	N1-C2-N3	5.99	121.92	115.13
39	B5	2475	PSU	N1-C2-N3	5.99	121.92	115.13
1	A2	119	PSU	N1-C2-N3	5.99	121.91	115.13
39	B5	3576	PSU	N1-C2-N3	5.99	121.91	115.13
39	B5	4749	PSU	N1-C2-N3	5.98	121.91	115.13
39	B5	3490	PSU	N1-C2-N3	5.98	121.90	115.13
1	A2	36	PSU	N1-C2-N3	5.97	121.89	115.13
39	B5	4203	PSU	N1-C2-N3	5.97	121.89	115.13
1	A2	210	PSU	N1-C2-N3	5.96	121.89	115.13
1	A2	1245	PSU	N1-C2-N3	5.96	121.88	115.13
1	A2	1175	PSU	N1-C2-N3	5.96	121.88	115.13
39	B5	1718	PSU	N1-C2-N3	5.96	121.88	115.13
39	B5	4039	PSU	N1-C2-N3	5.95	121.88	115.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	B5	3462	PSU	N1-C2-N3	5.95	121.87	115.13
39	B5	3616	PSU	N1-C2-N3	5.93	121.85	115.13
1	A2	1005	PSU	N1-C2-N3	5.92	121.84	115.13
39	B5	3554	PSU	N1-C2-N3	5.92	121.83	115.13
1	A2	1082	PSU	N1-C2-N3	5.90	121.81	115.13
39	B5	3966	6MZ	C2-N1-C6	5.89	121.64	116.59
39	B5	4166	PSU	N1-C2-N3	5.87	121.78	115.13
39	B5	1731	PSU	N1-C2-N3	5.84	121.75	115.13
39	B5	4276	UR3	C4-N3-C2	-5.73	119.17	124.56
1	A2	1833	6MZ	C2-N1-C6	5.64	121.43	116.59
11	AT	37	YYG	C3-N3-C2	-5.60	114.89	120.13
39	B5	3550	UY1	C4-N3-C2	-5.36	118.62	126.34
11	AT	54	5MU	C4-N3-C2	-5.08	120.77	127.35
11	AT	16	H2U	C4-N3-C2	-4.82	121.80	125.79
11	AT	54	5MU	N3-C2-N1	4.78	121.24	114.89
1	A2	1338	4AC	N4-C4-N3	4.77	121.85	113.85
39	B5	3657	OMU	C4-N3-C2	-4.60	120.52	126.58
39	B5	2680	OMU	C4-N3-C2	-4.59	120.53	126.58
39	B5	4244	OMU	C4-N3-C2	-4.53	120.61	126.58
1	A2	355	OMU	C4-N3-C2	-4.51	120.63	126.58
1	A2	429	OMU	C4-N3-C2	-4.51	120.63	126.58
1	A2	628	OMU	C4-N3-C2	-4.51	120.64	126.58
1	A2	1327	OMU	C4-N3-C2	-4.50	120.64	126.58
11	AT	54	5MU	C5-C4-N3	4.50	119.15	115.31
11	AT	37	YYG	C3-N3-C4	4.50	124.69	116.71
1	A2	172	OMU	C4-N3-C2	-4.47	120.69	126.58
39	B5	3973	OMU	C4-N3-C2	-4.45	120.72	126.58
39	B5	2258	OMU	C4-N3-C2	-4.43	120.74	126.58
39	B5	4366	OMU	C4-N3-C2	-4.43	120.74	126.58
39	B5	3550	UY1	N1-C2-N3	4.42	120.14	115.13
1	A2	116	OMU	C4-N3-C2	-4.40	120.78	126.58
1	A2	1805	OMU	C4-N3-C2	-4.38	120.80	126.58
39	B5	4052	OMU	C4-N3-C2	-4.37	120.82	126.58
1	A2	1443	OMU	C4-N3-C2	-4.36	120.83	126.58
1	A2	121	OMU	C4-N3-C2	-4.33	120.87	126.58
1	A2	1289	OMU	C4-N3-C2	-4.28	120.94	126.58
1	A2	355	OMU	N3-C2-N1	4.24	120.52	114.89
39	B5	2680	OMU	N3-C2-N1	4.23	120.51	114.89
39	B5	3657	OMU	N3-C2-N1	4.23	120.50	114.89
39	B5	4366	OMU	N3-C2-N1	4.16	120.42	114.89
1	A2	116	OMU	N3-C2-N1	4.16	120.41	114.89
39	B5	4193	5MC	C5-C6-N1	-4.15	119.06	123.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	B5	4244	OMU	N3-C2-N1	4.15	120.39	114.89
39	B5	3973	OMU	N3-C2-N1	4.14	120.39	114.89
39	B5	4052	OMU	N3-C2-N1	4.11	120.34	114.89
39	B5	3502	PSU	C4-N3-C2	-4.11	120.42	126.34
11	AT	37	YYG	O23-C21-N20	4.09	117.98	110.80
39	B5	2258	OMU	N3-C2-N1	4.07	120.30	114.89
1	A2	429	OMU	N3-C2-N1	4.06	120.27	114.89
1	A2	1805	OMU	N3-C2-N1	4.06	120.27	114.89
39	B5	4149	PSU	C4-N3-C2	-4.05	120.50	126.34
1	A2	121	OMU	N3-C2-N1	4.05	120.27	114.89
41	B8	55	PSU	C4-N3-C2	-4.05	120.51	126.34
39	B5	4099	PSU	C4-N3-C2	-4.04	120.52	126.34
1	A2	1327	OMU	N3-C2-N1	4.04	120.25	114.89
39	B5	1491	PSU	C4-N3-C2	-4.04	120.52	126.34
1	A2	172	OMU	N3-C2-N1	4.04	120.25	114.89
39	B5	3369	PSU	C4-N3-C2	-4.03	120.53	126.34
1	A2	573	PSU	C4-N3-C2	-4.03	120.53	126.34
1	A2	650	PSU	C4-N3-C2	-4.03	120.53	126.34
1	A2	1443	OMU	N3-C2-N1	4.03	120.24	114.89
11	AT	55	PSU	C4-N3-C2	-4.03	120.54	126.34
1	A2	628	OMU	N3-C2-N1	4.02	120.23	114.89
39	B5	4298	PSU	C4-N3-C2	-4.02	120.54	126.34
39	B5	2351	PSU	C4-N3-C2	-4.02	120.55	126.34
39	B5	3583	PSU	C4-N3-C2	-4.02	120.55	126.34
39	B5	1721	PSU	C4-N3-C2	-4.01	120.55	126.34
39	B5	4419	PSU	C4-N3-C2	-4.01	120.56	126.34
1	A2	1178	PSU	C4-N3-C2	-4.01	120.56	126.34
1	A2	867	PSU	C4-N3-C2	-4.01	120.56	126.34
1	A2	1348	PSU	C4-N3-C2	-4.01	120.56	126.34
39	B5	3447	PSU	C4-N3-C2	-4.01	120.56	126.34
1	A2	105	PSU	C4-N3-C2	-4.01	120.57	126.34
1	A2	816	PSU	C4-N3-C2	-4.01	120.57	126.34
1	A2	34	PSU	C4-N3-C2	-4.00	120.58	126.34
39	B5	4042	PSU	C4-N3-C2	-3.98	120.60	126.34
11	AT	27	PSU	C4-N3-C2	-3.98	120.60	126.34
1	A2	1239	PSU	C4-N3-C2	-3.98	120.60	126.34
39	B5	3427	PSU	C4-N3-C2	-3.98	120.60	126.34
1	A2	218	PSU	C4-N3-C2	-3.98	120.61	126.34
39	B5	4325	PSU	C4-N3-C2	-3.98	120.61	126.34
11	AT	28	PSU	C4-N3-C2	-3.97	120.61	126.34
1	A2	1368	PSU	C4-N3-C2	-3.97	120.62	126.34
39	B5	1683	PSU	C4-N3-C2	-3.97	120.62	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A2	864	PSU	C4-N3-C2	-3.96	120.63	126.34
39	B5	3652	PSU	C4-N3-C2	-3.96	120.63	126.34
39	B5	4711	PSU	C4-N3-C2	-3.96	120.63	126.34
1	A2	687	PSU	C4-N3-C2	-3.96	120.63	126.34
39	B5	4058	PSU	C4-N3-C2	-3.96	120.63	126.34
1	A2	1233	PSU	C4-N3-C2	-3.96	120.64	126.34
39	B5	1801	PSU	C4-N3-C2	-3.96	120.64	126.34
39	B5	3500	PSU	C4-N3-C2	-3.96	120.64	126.34
1	A2	1446	PSU	C4-N3-C2	-3.95	120.64	126.34
41	B8	69	PSU	C4-N3-C2	-3.95	120.64	126.34
39	B5	4374	PSU	C4-N3-C2	-3.95	120.64	126.34
39	B5	1718	PSU	C4-N3-C2	-3.95	120.65	126.34
1	A2	652	PSU	C4-N3-C2	-3.95	120.65	126.34
1	A2	1289	OMU	N3-C2-N1	3.95	120.13	114.89
1	A2	1693	PSU	C4-N3-C2	-3.94	120.66	126.34
1	A2	93	PSU	C4-N3-C2	-3.94	120.66	126.34
1	A2	109	PSU	C4-N3-C2	-3.94	120.66	126.34
1	A2	1046	PSU	C4-N3-C2	-3.94	120.66	126.34
1	A2	407	PSU	C4-N3-C2	-3.94	120.66	126.34
39	B5	4188	PSU	C4-N3-C2	-3.93	120.67	126.34
1	A2	1644	PSU	C4-N3-C2	-3.93	120.68	126.34
39	B5	4267	PSU	C4-N3-C2	-3.93	120.68	126.34
39	B5	4740	PSU	C4-N3-C2	-3.93	120.68	126.34
39	B5	3462	PSU	C4-N3-C2	-3.93	120.68	126.34
39	B5	4749	PSU	C4-N3-C2	-3.92	120.68	126.34
11	AT	39	PSU	C4-N3-C2	-3.92	120.69	126.34
39	B5	4203	PSU	C4-N3-C2	-3.92	120.69	126.34
1	A2	1057	PSU	C4-N3-C2	-3.92	120.69	126.34
1	A2	1851	MA6	N1-C6-N6	3.92	121.18	117.06
39	B5	4246	PSU	C4-N3-C2	-3.92	120.70	126.34
1	A2	682	PSU	C4-N3-C2	-3.91	120.70	126.34
39	B5	3490	PSU	C4-N3-C2	-3.91	120.70	126.34
1	A2	967	PSU	C4-N3-C2	-3.91	120.70	126.34
39	B5	3466	PSU	C4-N3-C2	-3.91	120.70	126.34
39	B5	3496	PSU	C4-N3-C2	-3.91	120.70	126.34
39	B5	4177	PSU	C4-N3-C2	-3.91	120.70	126.34
1	A2	815	PSU	C4-N3-C2	-3.91	120.71	126.34
39	B5	4039	PSU	C4-N3-C2	-3.91	120.71	126.34
39	B5	1720	PSU	C4-N3-C2	-3.91	120.71	126.34
39	B5	3585	PSU	C4-N3-C2	-3.90	120.71	126.34
39	B5	1537	PSU	C4-N3-C2	-3.90	120.72	126.34
1	A2	1245	PSU	C4-N3-C2	-3.90	120.72	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A2	610	PSU	C4-N3-C2	-3.89	120.73	126.34
39	B5	4169	PSU	C4-N3-C2	-3.89	120.74	126.34
11	AT	54	5MU	O4-C4-C5	-3.89	120.40	124.90
39	B5	4435	PSU	C4-N3-C2	-3.89	120.74	126.34
39	B5	4322	PSU	C4-N3-C2	-3.88	120.74	126.34
1	A2	802	PSU	C4-N3-C2	-3.88	120.74	126.34
39	B5	1638	PSU	C4-N3-C2	-3.88	120.75	126.34
39	B5	1731	PSU	C4-N3-C2	-3.88	120.75	126.34
39	B5	4045	PSU	C4-N3-C2	-3.88	120.75	126.34
1	A2	1047	PSU	C4-N3-C2	-3.88	120.75	126.34
11	AT	37	YYG	O23-C21-O22	-3.87	118.89	124.58
1	A2	1626	PSU	C4-N3-C2	-3.87	120.76	126.34
39	B5	3576	PSU	C4-N3-C2	-3.87	120.77	126.34
1	A2	1005	PSU	C4-N3-C2	-3.86	120.77	126.34
39	B5	1799	PSU	C4-N3-C2	-3.86	120.78	126.34
39	B5	4107	PSU	C4-N3-C2	-3.86	120.78	126.34
1	A2	1175	PSU	C4-N3-C2	-3.84	120.81	126.34
39	B5	4278	PSU	C4-N3-C2	-3.83	120.82	126.34
39	B5	3371	PSU	C4-N3-C2	-3.83	120.82	126.34
1	A2	119	PSU	C4-N3-C2	-3.83	120.83	126.34
39	B5	3554	PSU	C4-N3-C2	-3.81	120.85	126.34
39	B5	3616	PSU	C4-N3-C2	-3.81	120.85	126.34
1	A2	823	PSU	C4-N3-C2	-3.81	120.86	126.34
39	B5	4217	PSU	C4-N3-C2	-3.80	120.86	126.34
39	B5	2475	PSU	C4-N3-C2	-3.80	120.86	126.34
1	A2	36	PSU	C4-N3-C2	-3.79	120.87	126.34
39	B5	3494	PSU	C4-N3-C2	-3.79	120.88	126.34
1	A2	1082	PSU	C4-N3-C2	-3.78	120.89	126.34
1	A2	210	PSU	C4-N3-C2	-3.78	120.89	126.34
39	B5	4166	PSU	C4-N3-C2	-3.76	120.91	126.34
39	B5	4382	PSU	C4-N3-C2	-3.75	120.94	126.34
11	AT	37	YYG	C24-O23-C21	3.74	120.08	115.66
39	B5	1632	PSU	C4-N3-C2	-3.74	120.96	126.34
39	B5	3657	OMU	C5-C4-N3	3.66	120.31	114.84
39	B5	4244	OMU	C5-C4-N3	3.65	120.30	114.84
1	A2	429	OMU	C5-C4-N3	3.65	120.30	114.84
39	B5	3494	PSU	O2-C2-N1	-3.63	118.80	122.79
39	B5	2258	OMU	C5-C4-N3	3.62	120.25	114.84
1	A2	1327	OMU	C5-C4-N3	3.62	120.25	114.84
39	B5	3973	OMU	C5-C4-N3	3.61	120.25	114.84
1	A2	628	OMU	C5-C4-N3	3.59	120.22	114.84
1	A2	116	OMU	C5-C4-N3	3.59	120.21	114.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A2	1805	OMU	C5-C4-N3	3.59	120.21	114.84
1	A2	1047	PSU	O2-C2-N1	-3.59	118.84	122.79
1	A2	1289	OMU	C5-C4-N3	3.59	120.20	114.84
39	B5	2680	OMU	C5-C4-N3	3.58	120.20	114.84
11	AT	54	5MU	C5-C6-N1	-3.58	119.66	123.34
39	B5	4246	PSU	O2-C2-N1	-3.56	118.87	122.79
1	A2	355	OMU	C5-C4-N3	3.56	120.16	114.84
39	B5	4366	OMU	C5-C4-N3	3.56	120.16	114.84
1	A2	121	OMU	C5-C4-N3	3.55	120.15	114.84
1	A2	1443	OMU	C5-C4-N3	3.55	120.15	114.84
39	B5	4052	OMU	C5-C4-N3	3.54	120.14	114.84
39	B5	4382	PSU	O2-C2-N1	-3.53	118.90	122.79
1	A2	172	OMU	C5-C4-N3	3.53	120.12	114.84
1	A2	36	PSU	O2-C2-N1	-3.52	118.91	122.79
39	B5	4149	PSU	O2-C2-N1	-3.52	118.91	122.79
1	A2	823	PSU	O2-C2-N1	-3.52	118.92	122.79
39	B5	3583	PSU	O2-C2-N1	-3.51	118.93	122.79
39	B5	4278	PSU	O2-C2-N1	-3.51	118.93	122.79
1	A2	650	PSU	O2-C2-N1	-3.49	118.95	122.79
11	AT	39	PSU	O2-C2-N1	-3.49	118.95	122.79
1	A2	1175	PSU	O2-C2-N1	-3.49	118.95	122.79
39	B5	3652	PSU	O2-C2-N1	-3.48	118.96	122.79
39	B5	1718	PSU	O2-C2-N1	-3.48	118.96	122.79
39	B5	4045	PSU	O2-C2-N1	-3.48	118.96	122.79
39	B5	3496	PSU	O2-C2-N1	-3.48	118.96	122.79
39	B5	1632	PSU	O2-C2-N1	-3.47	118.97	122.79
1	A2	1644	PSU	O2-C2-N1	-3.46	118.98	122.79
39	B5	4325	PSU	O2-C2-N1	-3.46	118.98	122.79
1	A2	610	PSU	O2-C2-N1	-3.46	118.98	122.79
39	B5	3514	5MC	C5-C6-N1	-3.46	119.78	123.34
41	B8	69	PSU	O2-C2-N1	-3.46	118.98	122.79
1	A2	210	PSU	O2-C2-N1	-3.45	118.99	122.79
1	A2	1368	PSU	O2-C2-N1	-3.45	118.99	122.79
1	A2	1626	PSU	O2-C2-N1	-3.45	119.00	122.79
1	A2	1178	PSU	O2-C2-N1	-3.44	119.00	122.79
11	AT	27	PSU	O2-C2-N1	-3.44	119.00	122.79
39	B5	1491	PSU	O2-C2-N1	-3.43	119.01	122.79
39	B5	4374	PSU	O2-C2-N1	-3.43	119.01	122.79
1	A2	218	PSU	O2-C2-N1	-3.43	119.02	122.79
1	A2	652	PSU	O2-C2-N1	-3.43	119.02	122.79
39	B5	3502	PSU	O2-C2-N1	-3.43	119.02	122.79
39	B5	3447	PSU	O2-C2-N1	-3.42	119.02	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	B5	3462	PSU	O2-C2-N1	-3.41	119.03	122.79
1	A2	573	PSU	O2-C2-N1	-3.41	119.03	122.79
1	A2	93	PSU	O2-C2-N1	-3.41	119.04	122.79
39	B5	4298	PSU	O2-C2-N1	-3.41	119.04	122.79
39	B5	4042	PSU	O2-C2-N1	-3.41	119.04	122.79
1	A2	407	PSU	O2-C2-N1	-3.40	119.04	122.79
1	A2	687	PSU	O2-C2-N1	-3.40	119.05	122.79
39	B5	4099	PSU	O2-C2-N1	-3.40	119.05	122.79
41	B8	55	PSU	O2-C2-N1	-3.39	119.05	122.79
39	B5	3371	PSU	O2-C2-N1	-3.39	119.06	122.79
1	A2	867	PSU	O2-C2-N1	-3.39	119.06	122.79
39	B5	1683	PSU	O2-C2-N1	-3.39	119.06	122.79
39	B5	4749	PSU	O2-C2-N1	-3.39	119.06	122.79
39	B5	2630	A2M	N3-C2-N1	-3.39	123.38	128.68
1	A2	34	PSU	O2-C2-N1	-3.38	119.06	122.79
1	A2	109	PSU	O2-C2-N1	-3.38	119.06	122.79
39	B5	4166	PSU	O2-C2-N1	-3.38	119.07	122.79
39	B5	4419	PSU	O2-C2-N1	-3.38	119.07	122.79
1	A2	1032	A2M	N3-C2-N1	-3.38	123.40	128.68
39	B5	3517	A2M	N3-C2-N1	-3.37	123.41	128.68
39	B5	1801	PSU	O2-C2-N1	-3.37	119.08	122.79
1	A2	815	PSU	O2-C2-N1	-3.37	119.08	122.79
39	B5	1537	PSU	O2-C2-N1	-3.37	119.08	122.79
39	B5	2351	PSU	O2-C2-N1	-3.37	119.08	122.79
39	B5	3466	PSU	O2-C2-N1	-3.36	119.09	122.79
39	B5	4188	PSU	O2-C2-N1	-3.36	119.09	122.79
11	AT	37	YYG	O18-C16-C15	3.36	120.12	111.52
39	B5	4169	PSU	O2-C2-N1	-3.36	119.09	122.79
1	A2	1249	B8N	C4-N3-C2	-3.36	121.21	125.46
1	A2	105	PSU	O2-C2-N1	-3.36	119.09	122.79
1	A2	1239	PSU	O2-C2-N1	-3.36	119.10	122.79
39	B5	4435	PSU	O2-C2-N1	-3.35	119.10	122.79
1	A2	802	PSU	O2-C2-N1	-3.35	119.10	122.79
1	A2	1446	PSU	O2-C2-N1	-3.35	119.10	122.79
1	A2	1851	MA6	C4-C5-N7	-3.35	105.91	109.40
11	AT	55	PSU	O2-C2-N1	-3.35	119.10	122.79
1	A2	864	PSU	O2-C2-N1	-3.35	119.11	122.79
39	B5	4058	PSU	O2-C2-N1	-3.35	119.11	122.79
39	B5	3550	UY1	CM2-O2'-C2'	-3.35	105.74	114.52
39	B5	4711	PSU	O2-C2-N1	-3.35	119.11	122.79
39	B5	3500	PSU	O2-C2-N1	-3.34	119.11	122.79
39	B5	2244	A2M	N3-C2-N1	-3.34	123.45	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	AT	49	5MC	C5-C6-N1	-3.34	119.90	123.34
39	B5	2658	A2M	N3-C2-N1	-3.34	123.46	128.68
39	B5	4039	PSU	O2-C2-N1	-3.34	119.11	122.79
39	B5	3554	PSU	O2-C2-N1	-3.34	119.12	122.79
1	A2	1693	PSU	O2-C2-N1	-3.33	119.12	122.79
1	A2	1245	PSU	O2-C2-N1	-3.33	119.12	122.79
39	B5	3576	PSU	O2-C2-N1	-3.32	119.14	122.79
39	B5	4177	PSU	O2-C2-N1	-3.32	119.14	122.79
39	B5	1810	A2M	N3-C2-N1	-3.31	123.50	128.68
39	B5	2475	PSU	O2-C2-N1	-3.31	119.14	122.79
39	B5	1799	PSU	O2-C2-N1	-3.31	119.14	122.79
1	A2	119	PSU	O2-C2-N1	-3.31	119.15	122.79
39	B5	1720	PSU	O2-C2-N1	-3.31	119.15	122.79
1	A2	485	A2M	N3-C2-N1	-3.31	123.51	128.68
1	A2	1046	PSU	O2-C2-N1	-3.30	119.15	122.79
39	B5	3456	A2M	N3-C2-N1	-3.30	123.52	128.68
1	A2	816	PSU	O2-C2-N1	-3.30	119.16	122.79
39	B5	3585	PSU	O2-C2-N1	-3.29	119.16	122.79
39	B5	3966	6MZ	C9-N6-C6	-3.29	120.04	122.87
1	A2	1679	A2M	N3-C2-N1	-3.29	123.53	128.68
39	B5	1721	PSU	O2-C2-N1	-3.29	119.17	122.79
39	B5	4217	PSU	O2-C2-N1	-3.29	119.17	122.79
39	B5	3427	PSU	O2-C2-N1	-3.29	119.17	122.79
1	A2	682	PSU	O2-C2-N1	-3.29	119.17	122.79
1	A2	1057	PSU	O2-C2-N1	-3.28	119.18	122.79
39	B5	1638	PSU	O2-C2-N1	-3.28	119.18	122.79
1	A2	1851	MA6	N3-C2-N1	-3.27	123.56	128.68
39	B5	4336	A2M	N3-C2-N1	-3.27	123.57	128.68
39	B5	4322	PSU	O2-C2-N1	-3.27	119.19	122.79
1	A2	1005	PSU	O2-C2-N1	-3.27	119.19	122.79
1	A2	1348	PSU	O2-C2-N1	-3.27	119.19	122.79
1	A2	577	A2M	N3-C2-N1	-3.26	123.58	128.68
39	B5	4203	PSU	O2-C2-N1	-3.26	119.20	122.79
39	B5	400	A2M	N3-C2-N1	-3.26	123.58	128.68
39	B5	2206	A2M	N3-C2-N1	-3.26	123.58	128.68
1	A2	967	PSU	O2-C2-N1	-3.26	119.20	122.79
39	B5	3490	PSU	O2-C2-N1	-3.26	119.20	122.79
1	A2	166	A2M	N3-C2-N1	-3.25	123.60	128.68
1	A2	1384	A2M	N3-C2-N1	-3.25	123.60	128.68
1	A2	1233	PSU	O2-C2-N1	-3.25	119.21	122.79
39	B5	1489	A2M	N3-C2-N1	-3.24	123.61	128.68
39	B5	4317	A2M	N3-C2-N1	-3.24	123.61	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	B5	4267	PSU	O2-C2-N1	-3.24	119.22	122.79
39	B5	3966	6MZ	N3-C2-N1	-3.24	123.62	128.68
39	B5	4107	PSU	O2-C2-N1	-3.24	119.23	122.79
39	B5	1270	A2M	N3-C2-N1	-3.23	123.62	128.68
1	A2	591	A2M	N3-C2-N1	-3.23	123.63	128.68
1	A2	469	A2M	N3-C2-N1	-3.22	123.64	128.68
1	A2	1852	MA6	C4-C5-N7	-3.22	106.05	109.40
39	B5	3557	A2M	N3-C2-N1	-3.21	123.65	128.68
1	A2	27	A2M	N3-C2-N1	-3.21	123.66	128.68
1	A2	99	A2M	N3-C2-N1	-3.21	123.67	128.68
39	B5	3616	PSU	O2-C2-N1	-3.21	119.26	122.79
1	A2	1852	MA6	N3-C2-N1	-3.20	123.67	128.68
39	B5	4740	PSU	O2-C2-N1	-3.20	119.27	122.79
11	AT	28	PSU	O2-C2-N1	-3.20	119.27	122.79
39	B5	1479	A2M	N3-C2-N1	-3.19	123.69	128.68
1	A2	513	A2M	N3-C2-N1	-3.19	123.70	128.68
1	A2	669	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	3492	A2M	N3-C2-N1	-3.16	123.75	128.68
39	B5	4269	A2M	N3-C2-N1	-3.15	123.75	128.68
39	B5	398	A2M	N3-C2-N1	-3.14	123.77	128.68
39	B5	3599	A2M	N3-C2-N1	-3.13	123.79	128.68
39	B5	3450	A2M	N3-C2-N1	-3.13	123.79	128.68
1	A2	159	A2M	N3-C2-N1	-3.12	123.80	128.68
39	B5	3369	PSU	O2-C2-N1	-3.10	119.38	122.79
1	A2	1249	B8N	N3-C2-N1	3.08	121.11	116.76
1	A2	1082	PSU	O2-C2-N1	-3.05	119.43	122.79
39	B5	1731	PSU	O2-C2-N1	-3.04	119.44	122.79
1	A2	172	OMU	O4-C4-C5	-3.04	119.81	125.16
1	A2	429	OMU	O4-C4-C5	-3.03	119.83	125.16
1	A2	628	OMU	O4-C4-C5	-3.01	119.87	125.16
39	B5	4052	OMU	O4-C4-C5	-3.01	119.87	125.16
1	A2	1289	OMU	O4-C4-C5	-2.99	119.90	125.16
39	B5	3657	OMU	O4-C4-C5	-2.98	119.92	125.16
1	A2	121	OMU	O4-C4-C5	-2.98	119.92	125.16
39	B5	3550	UY1	C6-C5-C4	2.98	120.28	118.20
1	A2	116	OMU	O4-C4-C5	-2.98	119.92	125.16
1	A2	1327	OMU	O4-C4-C5	-2.97	119.93	125.16
1	A2	355	OMU	O4-C4-C5	-2.97	119.94	125.16
1	A2	1833	6MZ	N3-C2-N1	-2.96	124.04	128.68
1	A2	1443	OMU	O4-C4-C5	-2.96	119.95	125.16
1	A2	1805	OMU	O4-C4-C5	-2.94	119.99	125.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	B5	2680	OMU	O4-C4-C5	-2.91	120.04	125.16
39	B5	2258	OMU	O4-C4-C5	-2.91	120.05	125.16
39	B5	4244	OMU	O4-C4-C5	-2.90	120.05	125.16
1	A2	1852	MA6	N1-C6-N6	2.90	120.11	117.06
39	B5	4366	OMU	O4-C4-C5	-2.84	120.17	125.16
39	B5	3973	OMU	O4-C4-C5	-2.83	120.18	125.16
11	AT	37	YYG	C5-C6-N1	2.83	118.17	113.96
39	B5	398	A2M	C4-C5-N7	-2.78	106.50	109.40
39	B5	1489	A2M	C4-C5-N7	-2.77	106.51	109.40
1	A2	1843	4AC	N4-C4-N3	2.77	118.50	113.85
39	B5	1810	A2M	C4-C5-N7	-2.73	106.56	109.40
39	B5	1479	A2M	C4-C5-N7	-2.71	106.58	109.40
1	A2	159	A2M	C4-C5-N7	-2.70	106.59	109.40
1	A2	513	A2M	C4-C5-N7	-2.69	106.59	109.40
1	A2	27	A2M	C4-C5-N7	-2.69	106.60	109.40
39	B5	4193	5MC	C5-C4-N3	-2.68	118.78	121.67
1	A2	469	A2M	C4-C5-N7	-2.68	106.61	109.40
1	A2	166	A2M	C4-C5-N7	-2.68	106.61	109.40
1	A2	1679	A2M	C4-C5-N7	-2.68	106.61	109.40
39	B5	3562	A2M	C4-C5-N7	-2.68	106.61	109.40
39	B5	2244	A2M	C4-C5-N7	-2.68	106.61	109.40
39	B5	2658	A2M	C4-C5-N7	-2.67	106.62	109.40
39	B5	4336	A2M	C4-C5-N7	-2.67	106.62	109.40
1	A2	669	A2M	C4-C5-N7	-2.66	106.62	109.40
39	B5	4269	A2M	C4-C5-N7	-2.66	106.63	109.40
1	A2	99	A2M	C4-C5-N7	-2.66	106.63	109.40
39	B5	400	A2M	C4-C5-N7	-2.65	106.63	109.40
1	A2	1491	OMG	C5-C6-N1	2.65	118.64	113.95
1	A2	577	A2M	C4-C5-N7	-2.65	106.64	109.40
11	AT	46	G7M	CN7-N7-C8	-2.63	112.76	125.43
39	B5	3456	A2M	C4-C5-N7	-2.62	106.67	109.40
1	A2	1338	4AC	C6-C5-C4	2.62	120.16	116.96
39	B5	3599	A2M	C4-C5-N7	-2.61	106.68	109.40
1	A2	1032	A2M	C4-C5-N7	-2.61	106.68	109.40
11	AT	37	YYG	O6-C6-C5	-2.60	119.56	124.17
1	A2	1640	G7M	CN7-N7-C8	-2.60	112.92	125.43
1	A2	1384	A2M	C4-C5-N7	-2.60	106.69	109.40
39	B5	3557	A2M	C4-C5-N7	-2.59	106.70	109.40
39	B5	3450	A2M	C4-C5-N7	-2.59	106.70	109.40
39	B5	3517	A2M	C4-C5-N7	-2.57	106.72	109.40
39	B5	3492	A2M	C4-C5-N7	-2.55	106.74	109.40
42	BA	216	V5N	O-C-CA	-2.55	118.10	124.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	B5	4317	A2M	C4-C5-N7	-2.54	106.75	109.40
39	B5	3966	6MZ	C4-C5-N7	-2.54	106.75	109.40
39	B5	1270	A2M	C4-C5-N7	-2.54	106.76	109.40
1	A2	1338	4AC	C5-C4-N4	-2.52	118.55	122.92
1	A2	485	A2M	C4-C5-N7	-2.51	106.78	109.40
33	Au	1	AME	O-C-CA	-2.51	118.20	124.78
1	A2	1843	4AC	C6-C5-C4	2.51	120.03	116.96
68	Ba	39	V5N	O-C-CA	-2.49	118.24	124.78
39	B5	2206	A2M	C4-C5-N7	-2.49	106.81	109.40
39	B5	3514	5MC	C5-C4-N3	-2.48	119.00	121.67
11	AT	49	5MC	C5-C4-N3	-2.48	119.00	121.67
1	A2	591	A2M	C4-C5-N7	-2.47	106.83	109.40
11	AT	37	YYG	O18-C16-O17	-2.46	119.03	123.84
39	B5	3514	5MC	O2-C2-N3	-2.43	118.37	122.33
39	B5	3631	OMG	C8-N7-C5	2.43	107.61	102.99
39	B5	2630	A2M	C4-C5-N7	-2.42	106.88	109.40
11	AT	16	H2U	C5-C6-N1	-2.41	103.67	111.61
30	Ar	2	SAC	O-C-CA	-2.41	118.46	124.78
39	B5	4369	OMG	C8-N7-C5	2.41	107.58	102.99
39	B5	3942	OMG	C5-C6-N1	2.41	118.20	113.95
1	A2	684	OMG	C8-N7-C5	2.40	107.57	102.99
1	A2	645	OMG	C8-N7-C5	2.40	107.55	102.99
39	B5	4383	OMG	C8-N7-C5	2.39	107.55	102.99
39	B5	2719	OMG	C5-C6-N1	2.39	118.18	113.95
1	A2	684	OMG	C5-C6-N1	2.39	118.17	113.95
39	B5	1260	OMG	C5-C6-N1	2.39	118.17	113.95
39	B5	4116	OMG	C5-C6-N1	2.39	118.17	113.95
1	A2	437	OMG	C8-N7-C5	2.38	107.52	102.99
39	B5	1260	OMG	C8-N7-C5	2.38	107.52	102.99
39	B5	2207	OMG	C8-N7-C5	2.38	107.52	102.99
1	A2	1491	OMG	O6-C6-C5	-2.38	119.73	124.37
39	B5	4240	OMG	C5-C6-N1	2.38	118.15	113.95
39	B5	4138	OMG	C5-C6-N1	2.38	118.15	113.95
1	A2	1329	OMG	C8-N7-C5	2.38	107.52	102.99
39	B5	3359	OMG	C8-N7-C5	2.37	107.51	102.99
1	A2	602	OMG	C5-C6-N1	2.37	118.14	113.95
39	B5	3676	OMG	C8-N7-C5	2.37	107.51	102.99
11	AT	58	1MA	C8-N7-C5	2.37	107.51	102.99
1	A2	510	OMG	C8-N7-C5	2.37	107.50	102.99
39	B5	4364	OMG	C8-N7-C5	2.37	107.50	102.99
11	AT	26	M2G	C8-N7-C5	2.36	107.49	102.99
39	B5	4116	OMG	C8-N7-C5	2.36	107.48	102.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	B5	1477	OMG	C5-C6-N1	2.36	118.11	113.95
39	B5	3631	OMG	C5-C6-N1	2.35	118.10	113.95
12	AZ	2	SAC	O-C-CA	-2.35	118.62	124.78
39	B5	1477	OMG	C8-N7-C5	2.35	107.46	102.99
39	B5	3974	OMG	C8-N7-C5	2.34	107.46	102.99
39	B5	3476	OMG	C5-C6-N1	2.34	118.09	113.95
11	AT	34	OMG	C5-C6-N1	2.34	118.09	113.95
39	B5	4245	OMG	C8-N7-C5	2.34	107.44	102.99
39	B5	2194	OMC	O2-C2-N3	-2.34	118.53	122.33
39	B5	3524	OMG	C5-C6-N1	2.33	118.07	113.95
1	A2	868	OMG	C8-N7-C5	2.33	107.43	102.99
41	B8	75	OMG	C8-N7-C5	2.33	107.43	102.99
41	B8	75	OMG	C5-C6-N1	2.32	118.05	113.95
39	B5	3476	OMG	C8-N7-C5	2.32	107.41	102.99
39	B5	3942	OMG	C8-N7-C5	2.32	107.41	102.99
39	B5	3676	OMG	C5-C6-N1	2.32	118.05	113.95
1	A2	602	OMG	C8-N7-C5	2.32	107.40	102.99
39	B5	4138	OMG	C8-N7-C5	2.32	107.40	102.99
39	B5	3359	OMG	C5-C6-N1	2.32	118.04	113.95
39	B5	4369	OMG	C5-C6-N1	2.32	118.04	113.95
1	A2	645	OMG	C5-C6-N1	2.32	118.04	113.95
11	AT	58	1MA	C5-C6-N1	2.31	117.34	113.90
39	B5	4383	OMG	C5-C6-N1	2.31	118.03	113.95
11	AT	10	2MG	C8-N7-C5	2.31	107.38	102.99
83	Br	2	SAC	O-C-CA	-2.31	118.73	124.78
39	B5	2719	OMG	C8-N7-C5	2.31	107.38	102.99
11	AT	26	M2G	C5-C6-N1	2.30	118.02	113.95
11	AT	34	OMG	C8-N7-C5	2.30	107.37	102.99
39	B5	4240	OMG	C8-N7-C5	2.30	107.37	102.99
39	B5	1266	1MA	C5-C6-N1	2.29	117.31	113.90
11	AT	14	1MA	C8-N7-C5	2.29	107.36	102.99
39	B5	1580	OMG	C5-C6-N1	2.29	118.00	113.95
39	B5	4245	OMG	C5-C6-N1	2.29	118.00	113.95
1	A2	1329	OMG	C5-C6-N1	2.29	117.99	113.95
1	A2	1448	OMG	C5-C6-N1	2.29	117.99	113.95
1	A2	868	OMG	C5-C6-N1	2.28	117.98	113.95
39	B5	4364	OMG	C5-C6-N1	2.28	117.98	113.95
1	A2	437	OMG	C5-C6-N1	2.28	117.98	113.95
39	B5	3550	UY1	O2-C2-N1	-2.28	120.28	122.79
11	AT	37	YYG	C8-N7-C5	2.28	107.33	102.99
11	AT	10	2MG	C5-C6-N1	2.28	117.97	113.95
1	A2	510	OMG	C5-C6-N1	2.27	117.96	113.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A2	1289	OMU	C1'-N1-C2	2.27	121.67	117.57
39	B5	2207	OMG	C5-C6-N1	2.26	117.94	113.95
1	A2	1448	OMG	C8-N7-C5	2.26	107.29	102.99
39	B5	3974	OMG	C5-C6-N1	2.25	117.93	113.95
11	AT	14	1MA	C5-C6-N1	2.25	117.26	113.90
39	B5	1266	1MA	C8-N7-C5	2.25	107.27	102.99
1	A2	1392	OMC	O2-C2-N3	-2.24	118.69	122.33
35	Aw	62	HY3	O-C-CA	-2.24	118.59	124.83
1	A2	1833	6MZ	C4-C5-N7	-2.22	107.08	109.40
39	B5	1580	OMG	C8-N7-C5	2.22	107.21	102.99
1	A2	628	OMU	O2-C2-N1	-2.22	119.84	122.79
11	AT	54	5MU	O2-C2-N1	-2.21	119.84	122.79
39	B5	3657	OMU	O2-C2-N1	-2.21	119.84	122.79
39	B5	2267	OMG	C5-C6-N1	2.21	117.85	113.95
1	A2	1327	OMU	O2-C2-N1	-2.20	119.86	122.79
39	B5	3524	OMG	C8-N7-C5	2.18	107.15	102.99
1	A2	823	PSU	O4'-C1'-C2'	2.17	108.20	105.14
1	A2	1491	OMG	C8-N7-C5	2.16	107.11	102.99
39	B5	2267	OMG	C8-N7-C5	2.16	107.11	102.99
39	B5	2265	OMC	O2-C2-N3	-2.16	118.82	122.33
1	A2	1704	OMC	O2-C2-N3	-2.15	118.83	122.33
39	B5	3573	OMC	O2-C2-N3	-2.15	118.84	122.33
39	B5	2194	OMC	C1'-N1-C2	2.13	123.16	118.42
11	AT	14	1MA	N1-C2-N3	-2.12	123.55	126.02
39	B5	2680	OMU	O2-C2-N1	-2.11	119.98	122.79
39	B5	3369	PSU	C5-C6-N1	-2.11	118.94	122.11
39	B5	3502	PSU	C5-C6-N1	-2.11	118.95	122.11
39	B5	4149	PSU	C5-C6-N1	-2.11	118.95	122.11
39	B5	4166	PSU	O4'-C1'-C2'	2.09	108.10	105.14
1	A2	429	OMU	O2-C2-N1	-2.09	120.00	122.79
39	B5	4267	PSU	C5-C6-N1	-2.09	118.97	122.11
1	A2	34	PSU	C5-C6-N1	-2.09	118.98	122.11
1	A2	1249	B8N	C5-C4-N3	2.09	120.03	116.17
39	B5	1632	PSU	O4'-C1'-C2'	2.08	108.08	105.14
39	B5	1721	PSU	C5-C6-N1	-2.08	118.99	122.11
11	AT	17	H2U	C5-C6-N1	-2.07	104.80	111.61
11	AT	55	PSU	C5-C6-N1	-2.07	119.01	122.11
39	B5	2704	OMC	O2-C2-N3	-2.07	118.97	122.33
39	B5	1266	1MA	N1-C2-N3	-2.06	123.62	126.02
39	B5	4711	PSU	C5-C6-N1	-2.06	119.02	122.11
39	B5	2351	PSU	C5-C6-N1	-2.05	119.03	122.11
39	B5	1491	PSU	C5-C6-N1	-2.05	119.03	122.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
41	B8	55	PSU	C5-C6-N1	-2.05	119.03	122.11
1	A2	573	PSU	C5-C6-N1	-2.05	119.04	122.11
41	B8	69	PSU	O4'-C1'-C2'	2.04	108.03	105.14
1	A2	1693	PSU	C5-C6-N1	-2.04	119.05	122.11
39	B5	1731	PSU	C5-C6-N1	-2.04	119.05	122.11
39	B5	3490	PSU	C5-C6-N1	-2.03	119.06	122.11
1	A2	867	PSU	C5-C6-N1	-2.03	119.06	122.11
39	B5	4267	PSU	O4'-C1'-C2'	2.03	108.01	105.14
1	A2	1843	4AC	C5-C4-N3	-2.03	119.33	122.59
1	A2	116	OMU	O2-C2-N1	-2.03	120.09	122.79
39	B5	4052	OMU	C1'-N1-C2	2.03	121.24	117.57
39	B5	4419	PSU	C5-C6-N1	-2.02	119.07	122.11
11	AT	28	PSU	C5-C6-N1	-2.02	119.08	122.11
1	A2	816	PSU	C5-C6-N1	-2.02	119.08	122.11
39	B5	4042	PSU	C5-C6-N1	-2.02	119.08	122.11
1	A2	1239	PSU	C5-C6-N1	-2.02	119.08	122.11
39	B5	4382	PSU	O4'-C1'-C2'	2.02	107.99	105.14
11	AT	54	5MU	C5M-C5-C4	2.01	120.98	118.77
39	B5	1801	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	4298	PSU	C5-C6-N1	-2.01	119.10	122.11
39	B5	1683	PSU	C5-C6-N1	-2.01	119.10	122.11
1	A2	650	PSU	C5-C6-N1	-2.00	119.10	122.11
39	B5	2667	OMC	O2-C2-N3	-2.00	119.08	122.33

There are no chirality outliers.

All (126) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A2	429	OMU	C2'-C1'-N1-C2
1	A2	429	OMU	C2'-C1'-N1-C6
1	A2	645	OMG	O4'-C4'-C5'-O5'
1	A2	645	OMG	C3'-C4'-C5'-O5'
1	A2	1833	6MZ	N1-C6-N6-C9
39	B5	3433	OMC	C2'-C1'-N1-C2
39	B5	3433	OMC	C2'-C1'-N1-C6
39	B5	3517	A2M	O4'-C4'-C5'-O5'
39	B5	4336	A2M	C4'-C5'-O5'-P
39	B5	4382	PSU	C3'-C4'-C5'-O5'
39	B5	4382	PSU	O4'-C4'-C5'-O5'
43	BB	245	HIC	CA-CB-CG-ND1
1	A2	1249	B8N	N34-C33-C34-O35

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Mol	Chain	Res	Type	Atoms
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
11	AT	17	H2U	O4'-C4'-C5'-O5'
11	AT	17	H2U	O4'-C1'-N1-C6
11	AT	17	H2U	C2'-C1'-N1-C2
11	AT	17	H2U	C2'-C1'-N1-C6
31	As	67	NMM	O-C-CA-CB
42	BA	216	V5N	O-C-CA-CB
1	A2	513	A2M	O4'-C4'-C5'-O5'
1	A2	669	A2M	O4'-C4'-C5'-O5'
1	A2	669	A2M	C3'-C4'-C5'-O5'
1	A2	684	OMG	O4'-C4'-C5'-O5'
1	A2	1448	OMG	C3'-C4'-C5'-O5'
39	B5	2207	OMG	O4'-C4'-C5'-O5'
11	AT	17	H2U	C3'-C4'-C5'-O5'
33	Au	1	AME	CT2-CT1-N-CA
33	Au	1	AME	OT-CT1-N-CA
1	A2	577	A2M	O4'-C4'-C5'-O5'
1	A2	577	A2M	C3'-C4'-C5'-O5'
39	B5	398	A2M	O4'-C4'-C5'-O5'
39	B5	2207	OMG	C3'-C4'-C5'-O5'
39	B5	3492	A2M	C3'-C4'-C5'-O5'
39	B5	3517	A2M	C3'-C4'-C5'-O5'
1	A2	1249	B8N	N34-C33-C34-O36
1	A2	99	A2M	O4'-C4'-C5'-O5'
1	A2	513	A2M	C3'-C4'-C5'-O5'
39	B5	4193	5MC	C2'-C1'-N1-C6
1	A2	684	OMG	C3'-C4'-C5'-O5'
1	A2	802	PSU	C3'-C4'-C5'-O5'
39	B5	3492	A2M	O4'-C4'-C5'-O5'
39	B5	3599	A2M	C3'-C4'-C5'-O5'
1	A2	1448	OMG	O4'-C4'-C5'-O5'
1	A2	1704	OMC	O4'-C4'-C5'-O5'
1	A2	1852	MA6	C5-C6-N6-C9
1	A2	802	PSU	O4'-C4'-C5'-O5'
1	A2	1443	OMU	C3'-C2'-O2'-CM2
1	A2	1833	6MZ	C5-C6-N6-C9
39	B5	398	A2M	C3'-C4'-C5'-O5'
11	AT	17	H2U	O4'-C1'-N1-C2
12	AZ	2	SAC	C-CA-N-C1A

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Mol	Chain	Res	Type	Atoms
1	A2	1249	B8N	C32-C33-C34-O36
1	A2	121	OMU	C3'-C2'-O2'-CM2
1	A2	1491	OMG	C3'-C2'-O2'-CM2
1	A2	1805	OMU	C3'-C2'-O2'-CM2
39	B5	2680	OMU	C3'-C2'-O2'-CM2
39	B5	3676	OMG	C3'-C2'-O2'-CM2
39	B5	4193	5MC	O4'-C1'-N1-C6
1	A2	1843	4AC	N3-C4-N4-C7
1	A2	1843	4AC	C5-C4-N4-C7
39	B5	3576	PSU	C4'-C5'-O5'-P
39	B5	4246	PSU	C4'-C5'-O5'-P
39	B5	3599	A2M	O4'-C4'-C5'-O5'
69	Bb	5	MLZ	N-CA-CB-CG
39	B5	4193	5MC	O4'-C1'-N1-C2
39	B5	4193	5MC	C2'-C1'-N1-C2
1	A2	1249	B8N	C32-C33-C34-O35
1	A2	645	OMG	C4'-C5'-O5'-P
39	B5	3550	UY1	C4'-C5'-O5'-P
39	B5	3433	OMC	O4'-C1'-N1-C6
1	A2	1852	MA6	C4'-C5'-O5'-P
11	AT	16	H2U	C4'-C5'-O5'-P
1	A2	429	OMU	O4'-C1'-N1-C6
1	A2	645	OMG	C3'-C2'-O2'-CM2
39	B5	1260	OMG	C3'-C2'-O2'-CM2
39	B5	1477	OMG	C3'-C2'-O2'-CM2
39	B5	2647	OMC	C3'-C2'-O2'-CM2
39	B5	4202	OMC	C3'-C2'-O2'-CM2
39	B5	4369	OMG	C3'-C2'-O2'-CM2
39	B5	3550	UY1	C1'-C2'-O2'-CM2
1	A2	823	PSU	C3'-C4'-C5'-O5'
39	B5	3494	PSU	C3'-C4'-C5'-O5'
39	B5	3550	UY1	O4'-C1'-C5-C4
1	A2	116	OMU	C3'-C2'-O2'-CM2
1	A2	513	A2M	C3'-C2'-O2'-CM'
1	A2	684	OMG	C3'-C2'-O2'-CM2
1	A2	1329	OMG	C3'-C2'-O2'-CM2
39	B5	2265	OMC	C3'-C2'-O2'-CM2
39	B5	3524	OMG	C3'-C2'-O2'-CM2
39	B5	3557	A2M	C3'-C2'-O2'-CM'
1	A2	429	OMU	O4'-C1'-N1-C2
1	A2	628	OMU	C2'-C1'-N1-C6
39	B5	2194	OMC	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
1	A2	469	A2M	O4'-C4'-C5'-O5'
1	A2	1704	OMC	C3'-C4'-C5'-O5'
69	Bb	5	MLZ	C-CA-CB-CG
39	B5	3433	OMC	O4'-C1'-N1-C2
39	B5	3619	OMC	C4'-C5'-O5'-P
1	A2	99	A2M	C3'-C4'-C5'-O5'
1	A2	513	A2M	C1'-C2'-O2'-CM'
1	A2	684	OMG	C1'-C2'-O2'-CM2
39	B5	1284	OMC	C1'-C2'-O2'-CM2
1	A2	628	OMU	O4'-C1'-N1-C6
39	B5	3550	UY1	C3'-C2'-O2'-CM2
39	B5	4382	PSU	O4'-C1'-C5-C6
39	B5	2194	OMC	C2'-C1'-N1-C2
1	A2	27	A2M	O4'-C4'-C5'-O5'
1	A2	1805	OMU	O4'-C4'-C5'-O5'
39	B5	1489	A2M	O4'-C4'-C5'-O5'
39	B5	3450	A2M	O4'-C4'-C5'-O5'
12	AZ	2	SAC	CB-CA-N-C1A
1	A2	1491	OMG	C4'-C5'-O5'-P
1	A2	27	A2M	C3'-C2'-O2'-CM'
39	B5	1284	OMC	C3'-C2'-O2'-CM2
39	B5	1820	OMC	C3'-C2'-O2'-CM2
39	B5	2704	OMC	C3'-C2'-O2'-CM2
39	B5	3619	OMC	C3'-C2'-O2'-CM2
39	B5	3973	OMU	C3'-C2'-O2'-CM2
11	AT	46	G7M	O4'-C4'-C5'-O5'
1	A2	1392	OMC	C2'-C1'-N1-C2
1	A2	1082	PSU	C4'-C5'-O5'-P
39	B5	3583	PSU	C3'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 790 ligands modelled in this entry, 428 are monoatomic and 329 are unknown - leaving 33 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	$\#\|Z\| > 2$
87	SPD	B5	4909	-	9,9,9	0.16	0	8,8,8	0.19	0
87	SPD	B5	4918	-	9,9,9	0.15	0	8,8,8	0.17	0
87	SPD	A2	1901	-	9,9,9	0.16	0	8,8,8	0.18	0
87	SPD	B5	4904	-	9,9,9	0.15	0	8,8,8	0.19	0
87	SPD	B5	4905	-	9,9,9	0.16	0	8,8,8	0.21	0
87	SPD	B5	4922	-	9,9,9	0.15	0	8,8,8	0.17	0
88	SPM	A2	1909	-	13,13,13	0.14	0	12,12,12	0.18	0
87	SPD	B5	4902	-	9,9,9	0.15	0	8,8,8	0.23	0
87	SPD	B5	4906	-	9,9,9	0.15	0	8,8,8	0.16	0
87	SPD	A2	1903	-	9,9,9	0.15	0	8,8,8	0.19	0
87	SPD	B5	4910	-	9,9,9	0.15	0	8,8,8	0.18	0
87	SPD	B5	4923	-	9,9,9	0.15	0	8,8,8	0.20	0
87	SPD	B5	4907	-	9,9,9	0.16	0	8,8,8	0.18	0
87	SPD	A2	1906	-	9,9,9	0.16	0	8,8,8	0.18	0
87	SPD	B5	4920	-	9,9,9	0.15	0	8,8,8	0.23	0
87	SPD	A2	1908	-	9,9,9	0.15	0	8,8,8	0.20	0
87	SPD	B5	4911	-	9,9,9	0.15	0	8,8,8	0.17	0
88	SPM	B5	4915	-	13,13,13	0.16	0	12,12,12	0.22	0
87	SPD	A2	1904	-	9,9,9	0.15	0	8,8,8	0.19	0
87	SPD	B5	4914	-	9,9,9	0.15	0	8,8,8	0.17	0
87	SPD	B5	4903	-	9,9,9	0.16	0	8,8,8	0.20	0
87	SPD	A2	1905	-	9,9,9	0.16	0	8,8,8	0.17	0
87	SPD	B5	4921	-	9,9,9	0.16	0	8,8,8	0.18	0
87	SPD	B5	4913	-	9,9,9	0.16	0	8,8,8	0.17	0
87	SPD	B5	4908	-	9,9,9	0.16	0	8,8,8	0.16	0
87	SPD	B5	4919	-	9,9,9	0.15	0	8,8,8	0.21	0
87	SPD	A2	1902	-	9,9,9	0.15	0	8,8,8	0.15	0
87	SPD	B5	4924	-	9,9,9	0.16	0	8,8,8	0.14	0
87	SPD	A2	1907	-	9,9,9	0.15	0	8,8,8	0.18	0
87	SPD	B5	4917	-	9,9,9	0.15	0	8,8,8	0.18	0
87	SPD	B5	4916	-	9,9,9	0.15	0	8,8,8	0.22	0
87	SPD	B5	4901	-	9,9,9	0.14	0	8,8,8	0.15	0
88	SPM	B5	4912	-	13,13,13	0.15	0	12,12,12	0.23	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	SPD	B5	4909	-	-	0/7/7/7	-
87	SPD	B5	4918	-	-	0/7/7/7	-
87	SPD	A2	1901	-	-	1/7/7/7	-
87	SPD	B5	4904	-	-	0/7/7/7	-
87	SPD	B5	4905	-	-	0/7/7/7	-
87	SPD	B5	4922	-	-	1/7/7/7	-
88	SPM	A2	1909	-	-	1/11/11/11	-
87	SPD	B5	4902	-	-	1/7/7/7	-
87	SPD	B5	4906	-	-	1/7/7/7	-
87	SPD	A2	1903	-	-	0/7/7/7	-
87	SPD	B5	4910	-	-	1/7/7/7	-
87	SPD	B5	4923	-	-	0/7/7/7	-
87	SPD	B5	4907	-	-	0/7/7/7	-
87	SPD	A2	1906	-	-	1/7/7/7	-
87	SPD	B5	4920	-	-	0/7/7/7	-
87	SPD	A2	1908	-	-	0/7/7/7	-
87	SPD	B5	4911	-	-	0/7/7/7	-
88	SPM	B5	4915	-	-	0/11/11/11	-
87	SPD	A2	1904	-	-	0/7/7/7	-
87	SPD	B5	4914	-	-	0/7/7/7	-
87	SPD	B5	4903	-	-	2/7/7/7	-
87	SPD	A2	1905	-	-	0/7/7/7	-
87	SPD	B5	4921	-	-	1/7/7/7	-
87	SPD	B5	4913	-	-	0/7/7/7	-
87	SPD	B5	4908	-	-	0/7/7/7	-
87	SPD	B5	4919	-	-	0/7/7/7	-
87	SPD	A2	1902	-	-	0/7/7/7	-
87	SPD	B5	4924	-	-	1/7/7/7	-
87	SPD	A2	1907	-	-	1/7/7/7	-
87	SPD	B5	4917	-	-	0/7/7/7	-
87	SPD	B5	4916	-	-	0/7/7/7	-
87	SPD	B5	4901	-	-	1/7/7/7	-
88	SPM	B5	4912	-	-	1/11/11/11	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
88	A2	1909	SPM	C12-C11-N10-C9
87	B5	4901	SPD	C4-C5-N6-C7
87	B5	4902	SPD	C2-C3-C4-C5
87	B5	4924	SPD	C2-C3-C4-C5
87	B5	4903	SPD	C2-C3-C4-C5
87	B5	4906	SPD	C2-C3-C4-C5
87	A2	1906	SPD	C8-C7-N6-C5
87	A2	1907	SPD	C2-C3-C4-C5
87	B5	4910	SPD	C2-C3-C4-C5
87	B5	4922	SPD	C2-C3-C4-C5
87	B5	4921	SPD	C8-C7-N6-C5
88	B5	4912	SPM	C6-C7-C8-C9
87	B5	4903	SPD	C8-C7-N6-C5
87	A2	1901	SPD	C2-C3-C4-C5

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

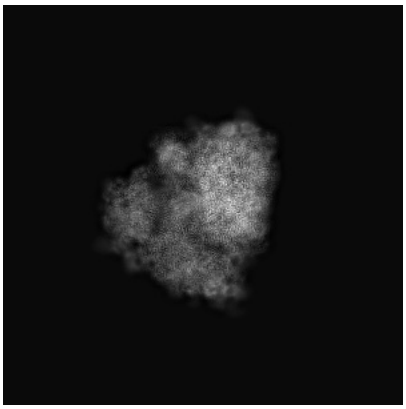
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-12757. These allow visual inspection of the internal detail of the map and identification of artifacts.

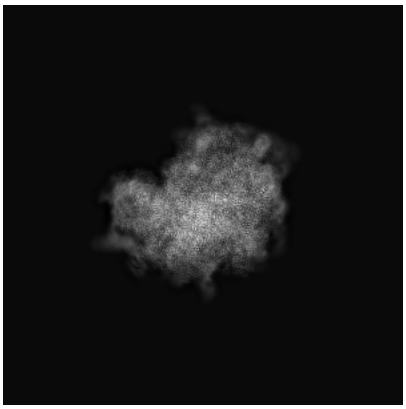
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

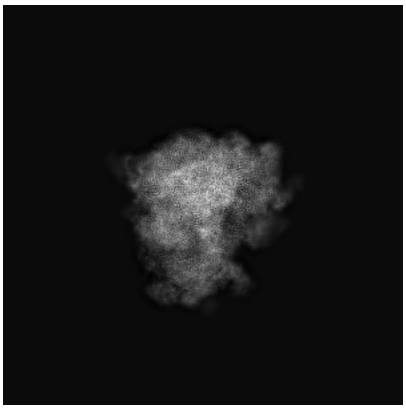
6.1.1 Primary map



X

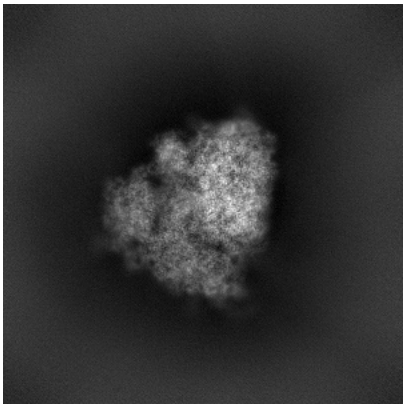


Y

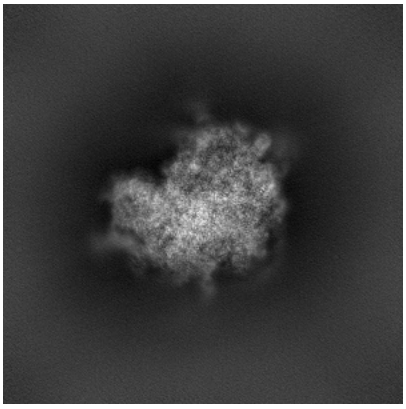


Z

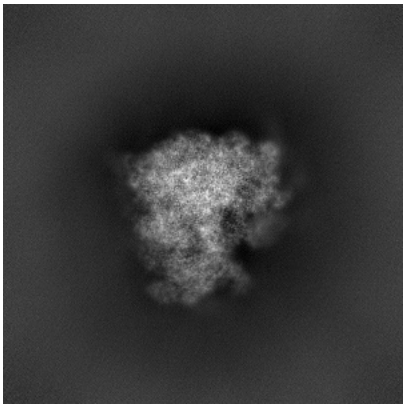
6.1.2 Raw map



X



Y

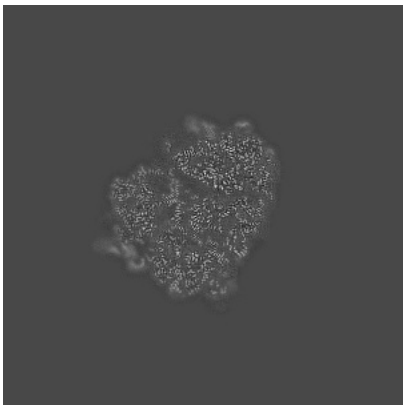


Z

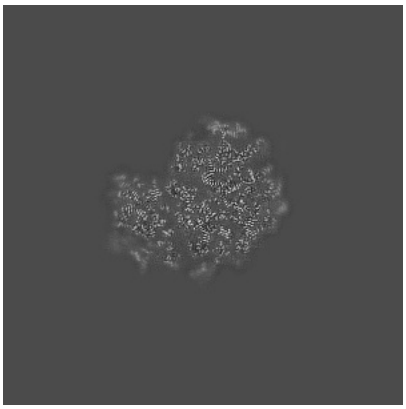
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

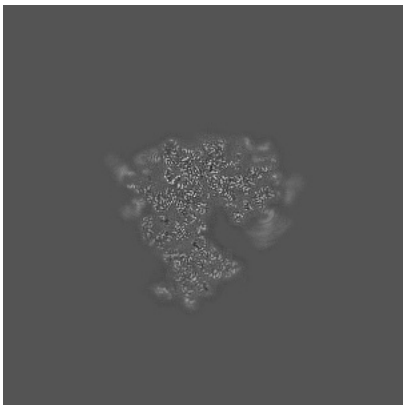
6.2.1 Primary map



X Index: 280

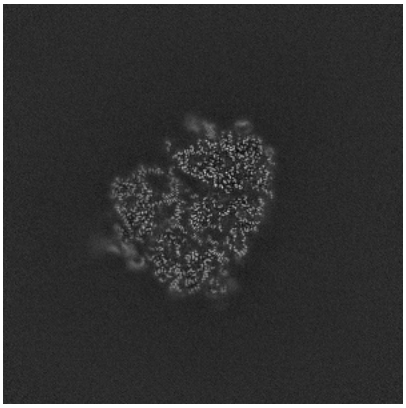


Y Index: 280

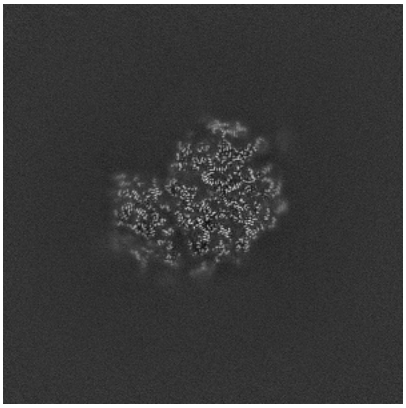


Z Index: 280

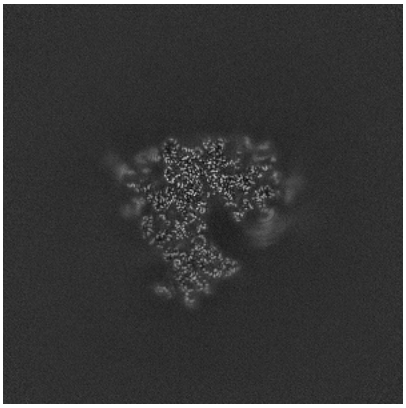
6.2.2 Raw map



X Index: 280



Y Index: 280

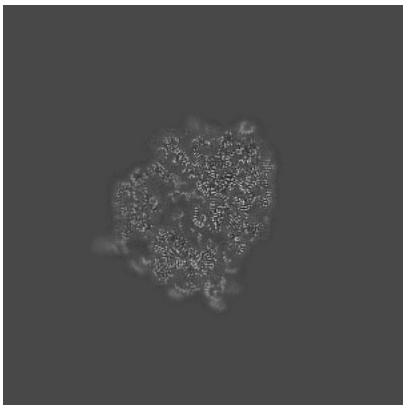


Z Index: 280

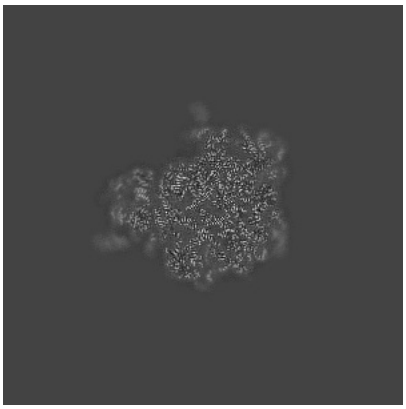
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

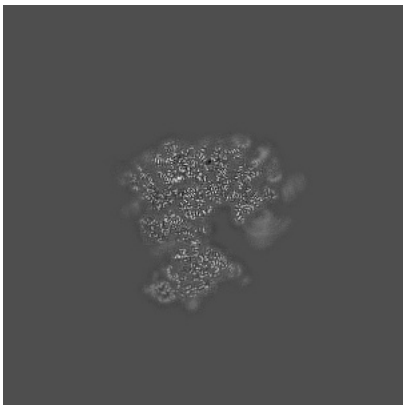
6.3.1 Primary map



X Index: 287

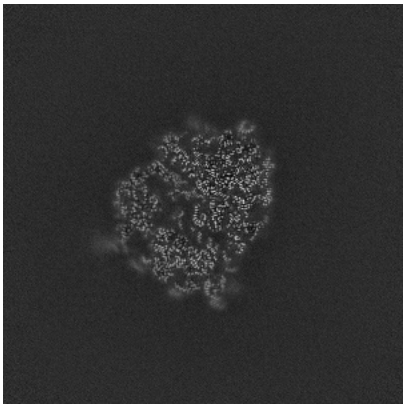


Y Index: 313

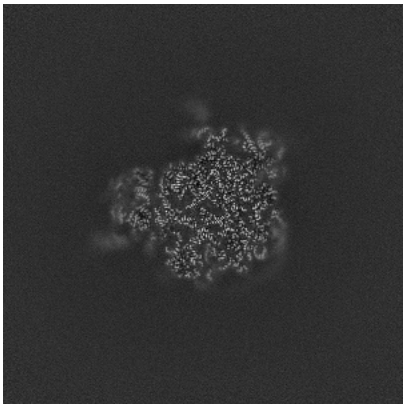


Z Index: 272

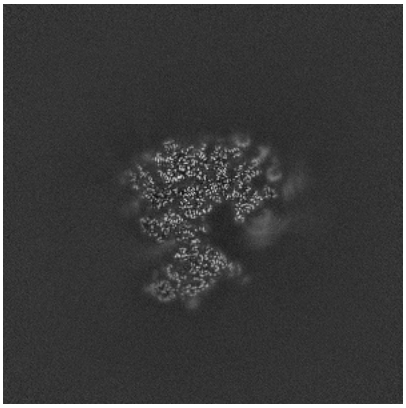
6.3.2 Raw map



X Index: 287



Y Index: 313

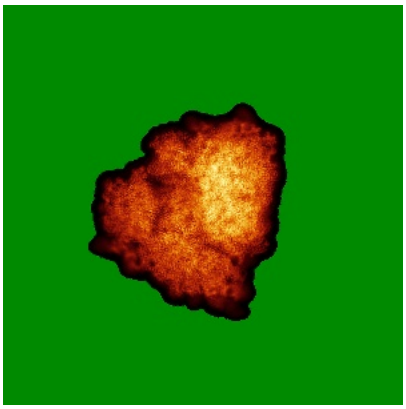


Z Index: 272

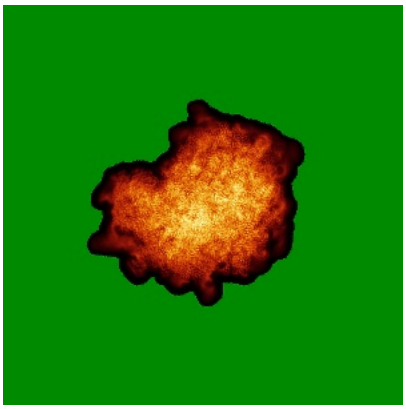
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

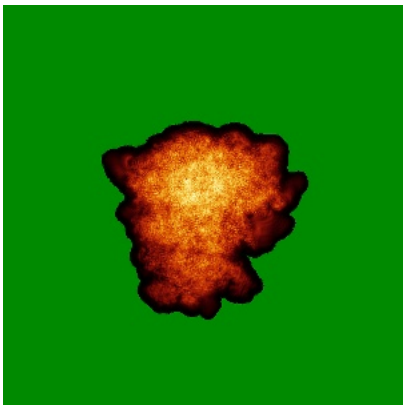
6.4.1 Primary map



X

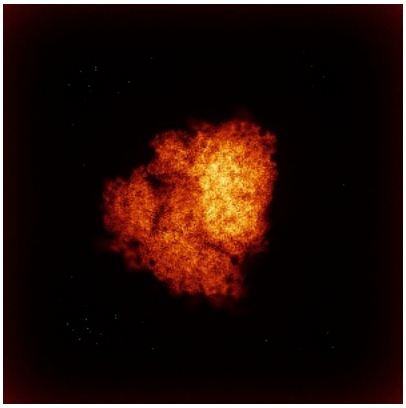


Y

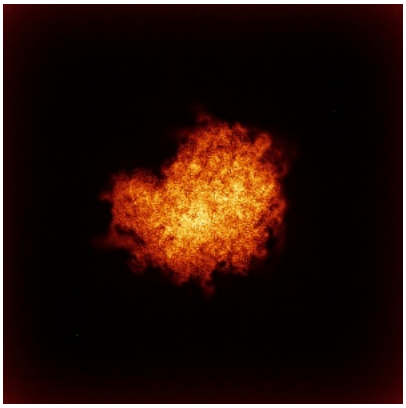


Z

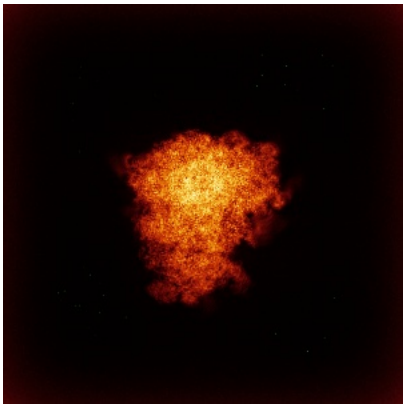
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 5.0. 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.

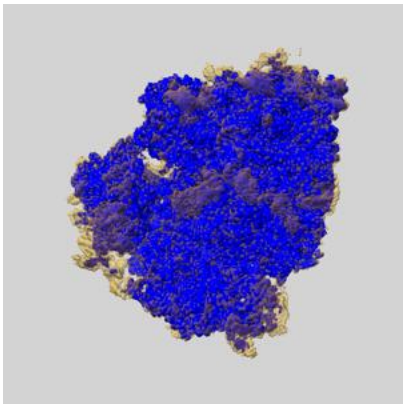
6.6 Mask visualisation

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

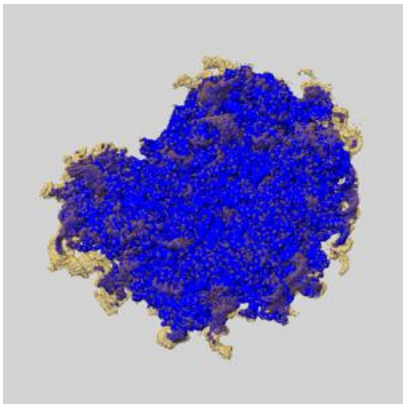
A mask typically either:

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

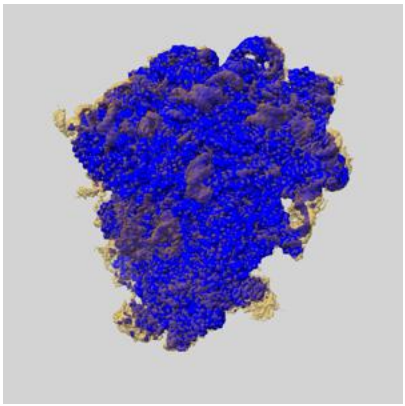
6.6.1 emd_12757_msk_1.map



X

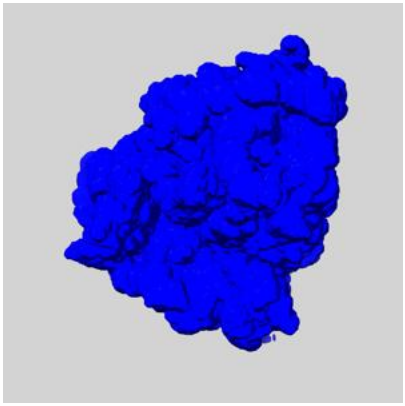


Y

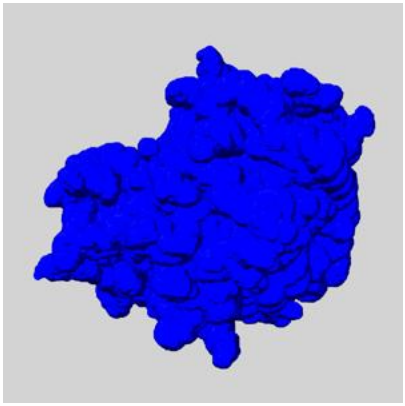


Z

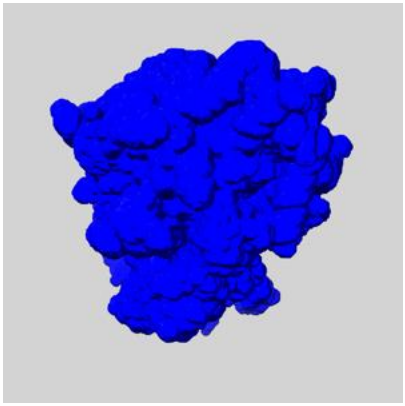
6.6.2 emd_12757_msk_2.map



X



Y

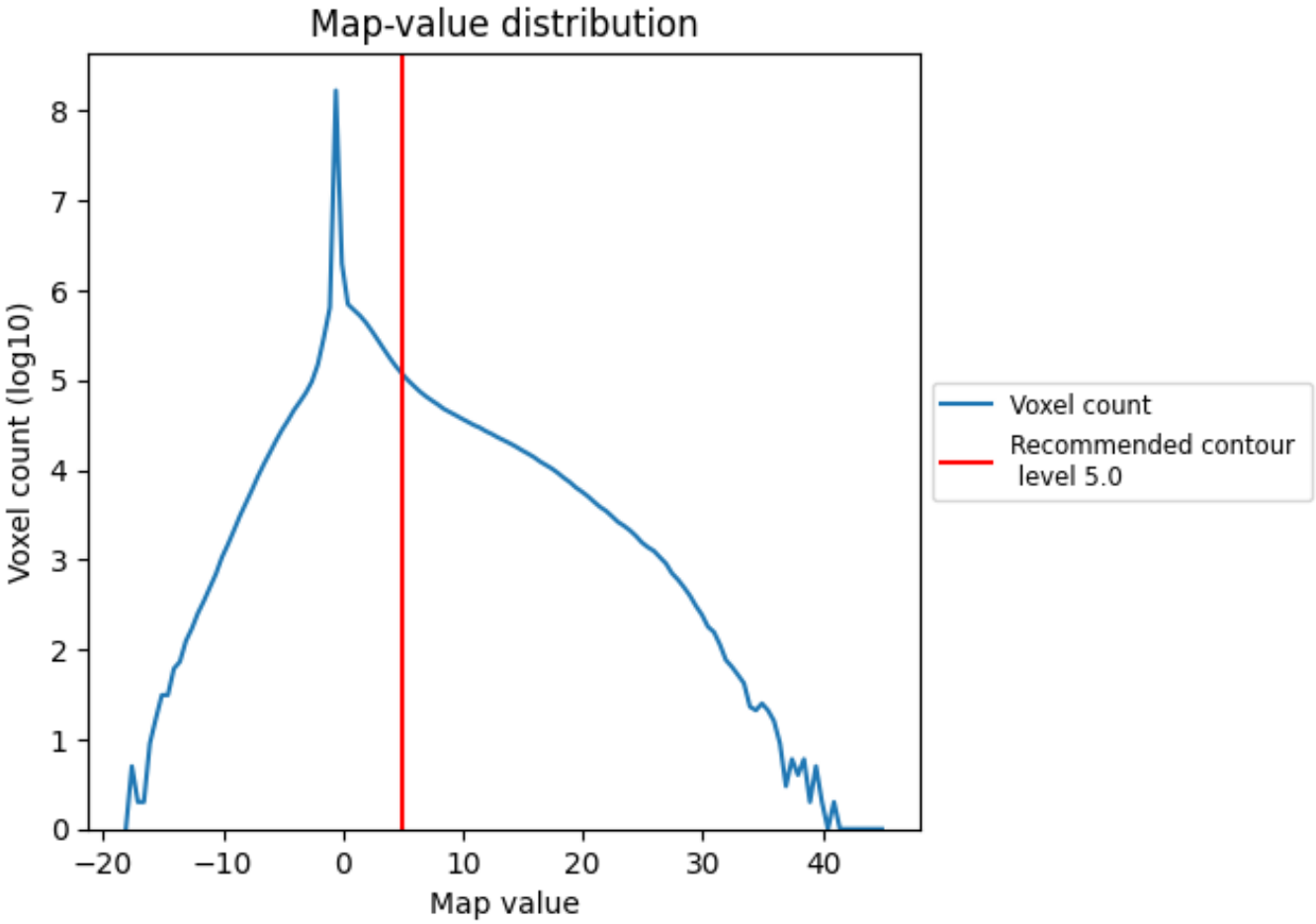


Z

7 Map analysis

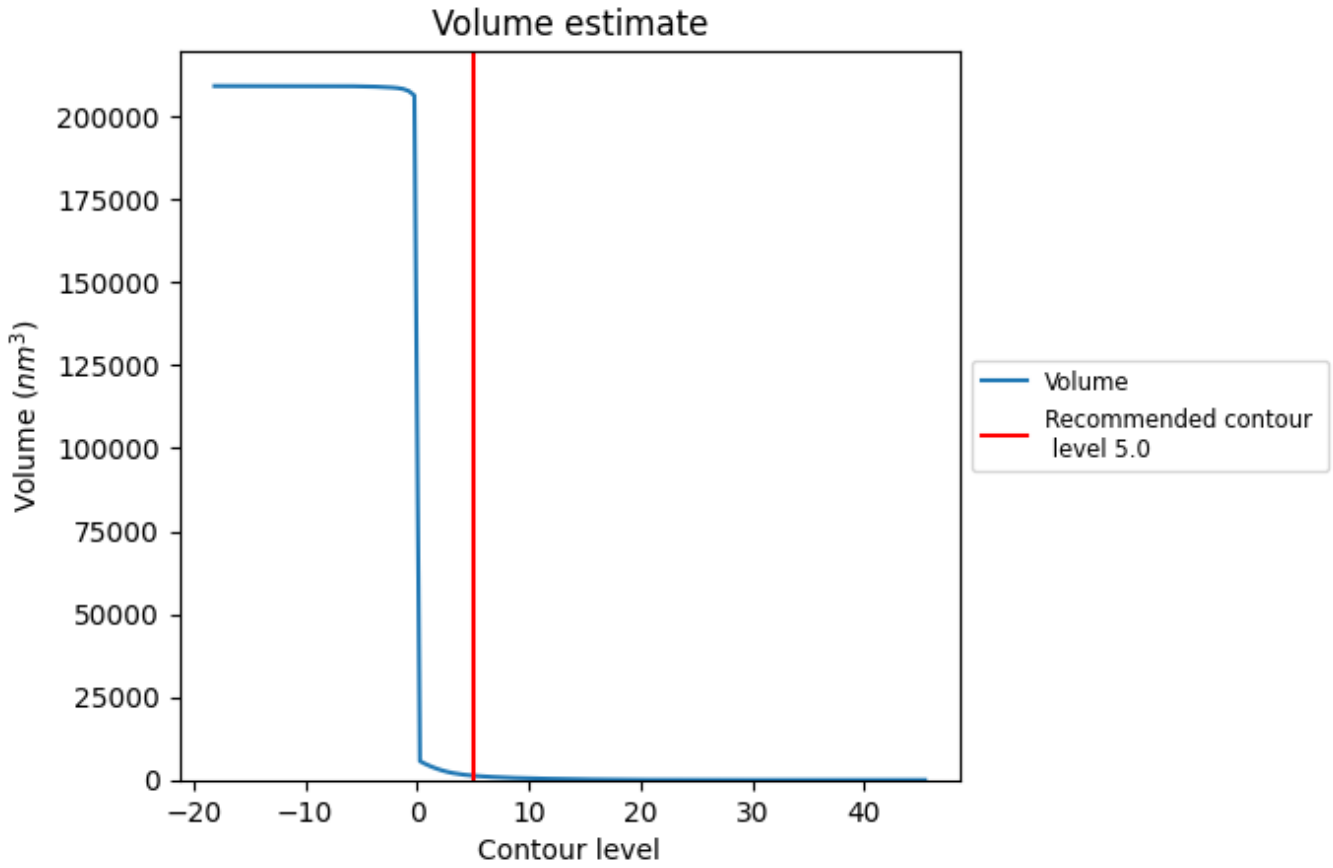
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

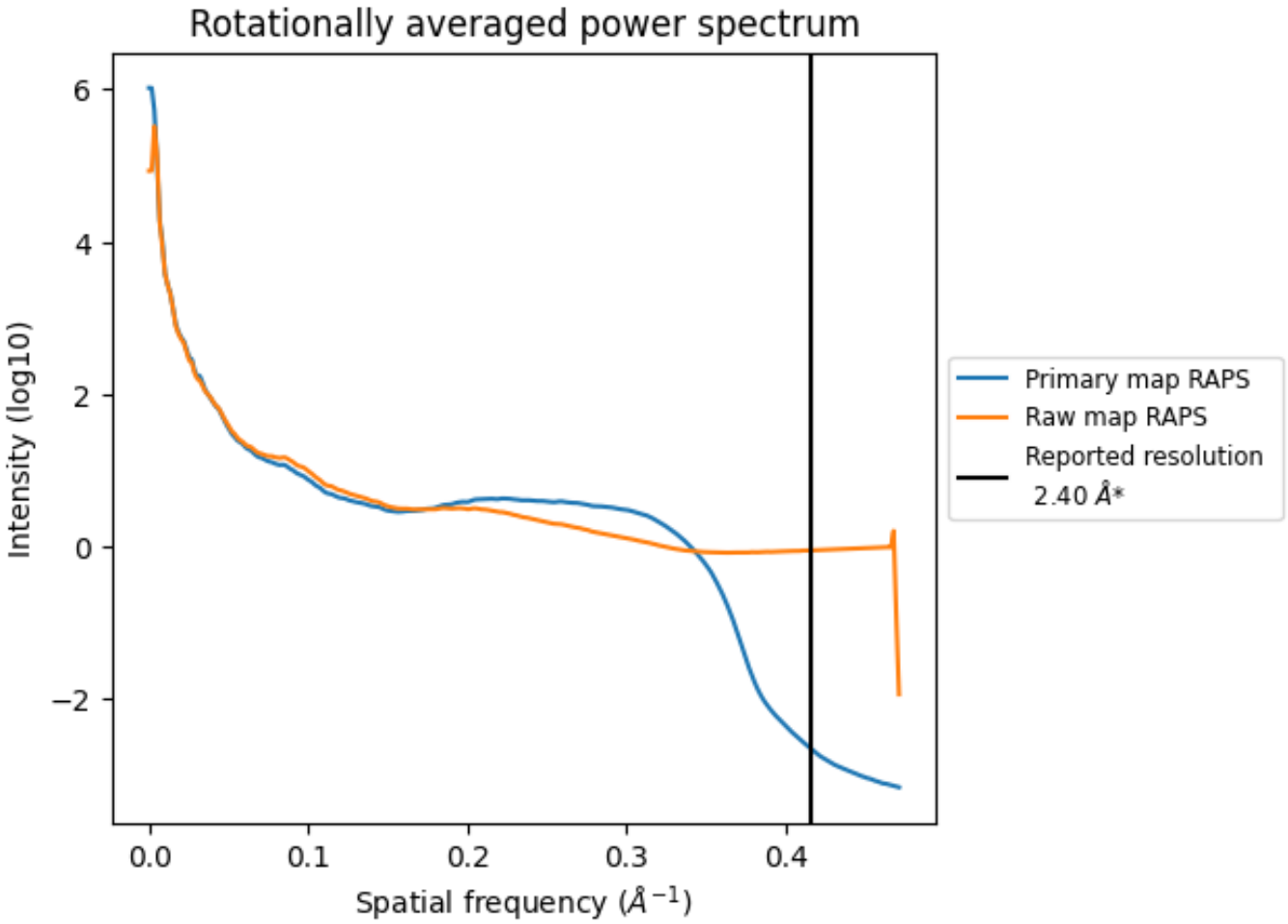
7.2 Volume estimate



The volume at the recommended contour level is 1298 nm^3; this corresponds to an approximate mass of 1172 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)

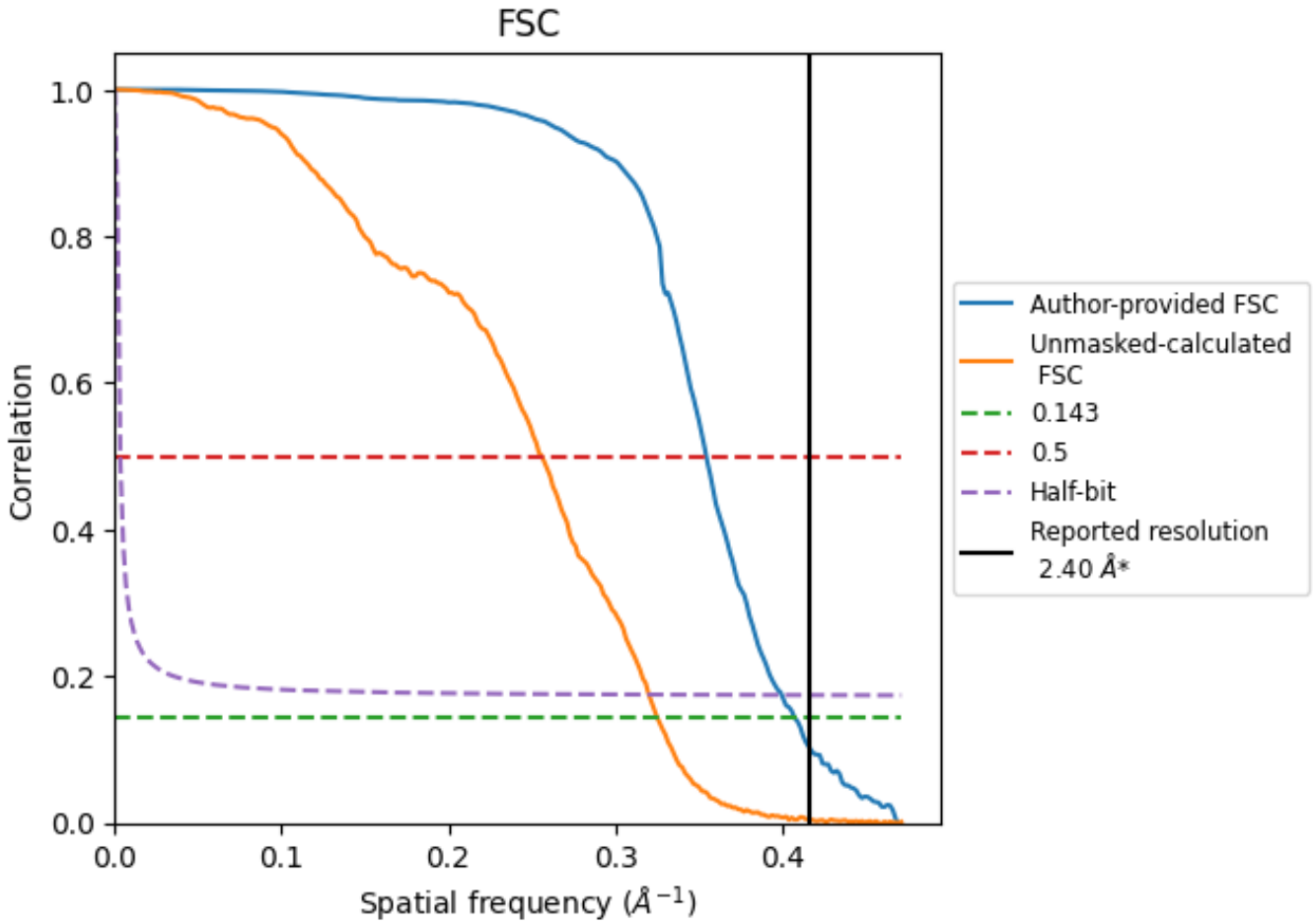


*Reported resolution corresponds to spatial frequency of 0.417 $Å^{-1}$

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.417 Å^{-1}

8.2 Resolution estimates (i)

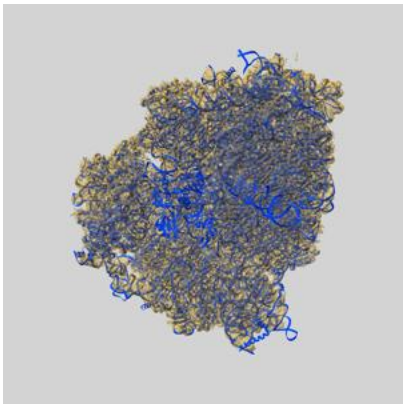
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.40	-	-
Author-provided FSC curve	2.45	2.82	2.50
Unmasked-calculated*	3.07	3.90	3.12

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.07 differs from the reported value 2.4 by more than 10 %

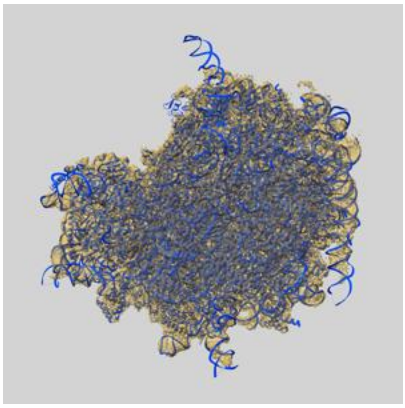
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-12757 and PDB model 7O7Z. Per-residue inclusion information can be found in section 3 on page 27.

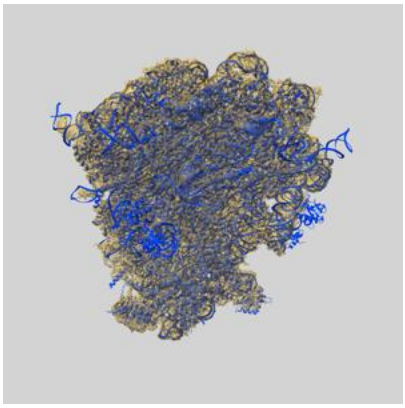
9.1 Map-model overlay



X



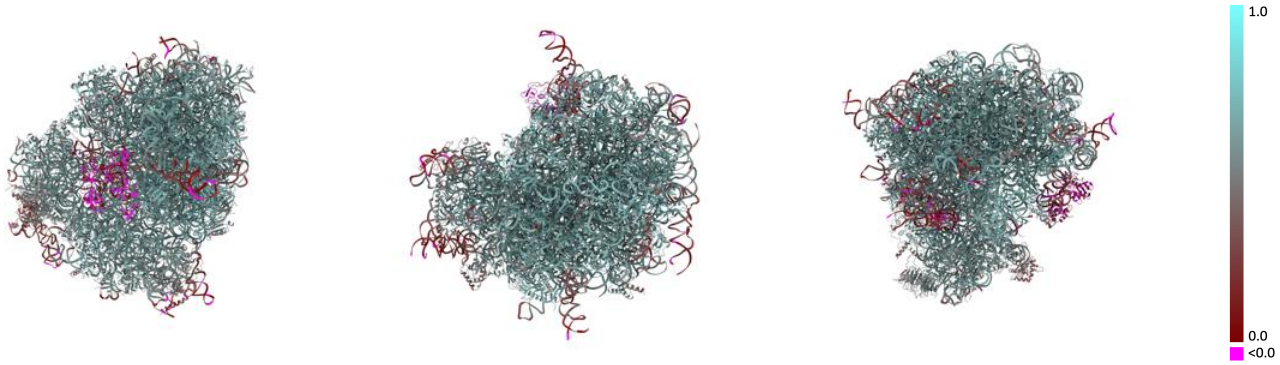
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 5.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

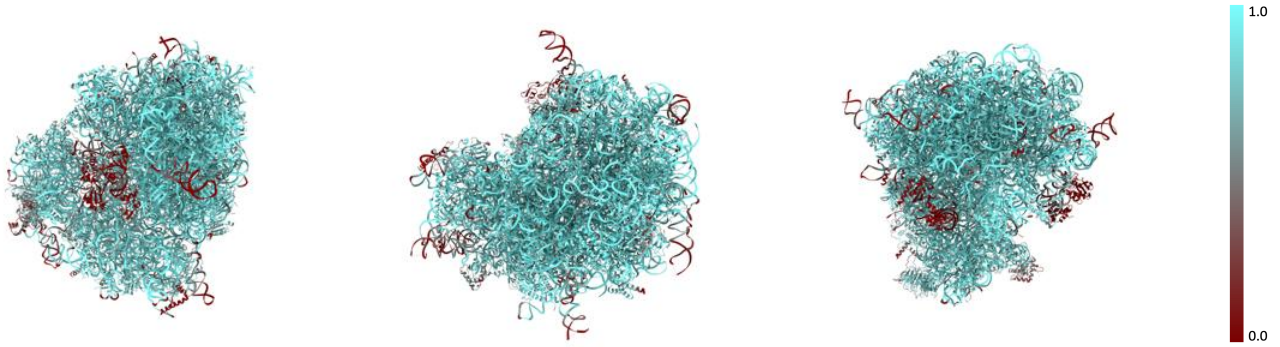
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

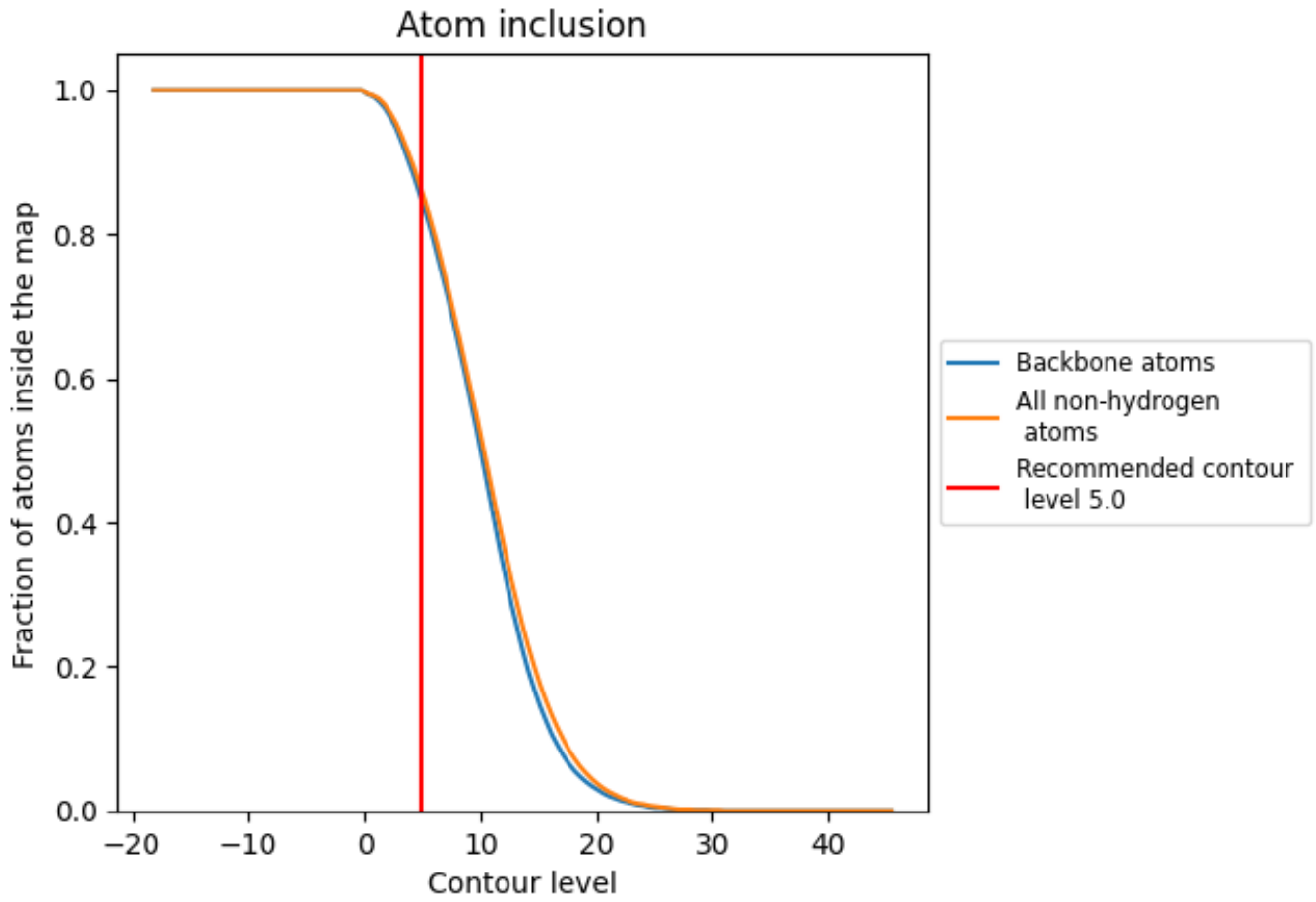
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (5.0).

9.4 Atom inclusion (i)



At the recommended contour level, 84% of all backbone atoms, 86% 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 (5.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8580	0.5760
A2	0.9060	0.5760
AA	0.7930	0.5730
AB	0.7670	0.5800
AC	0.4040	0.3600
AD	0.7460	0.5580
AE	0.8720	0.6130
AF	0.7090	0.4910
AG	0.9050	0.6280
AH	0.4400	0.2140
AI	0.4400	0.3250
AT	0.8960	0.6030
AZ	0.8340	0.6010
Aa	0.8400	0.6110
Ab	0.8900	0.6230
Ac	0.7440	0.5600
Ad	0.8750	0.5940
Ae	0.8290	0.6050
Af	0.7430	0.4900
Ag	0.6430	0.5080
Ah	0.8560	0.5960
Ai	0.8690	0.6040
Aj	0.7680	0.5230
Ak	0.8180	0.5960
Al	0.3160	0.2940
Am	0.8860	0.6270
An	0.8800	0.6310
Ao	0.7990	0.5420
Ap	0.8460	0.5760
Aq	0.7250	0.5510
Ar	0.8200	0.5640
As	0.8520	0.5830
At	0.7390	0.5270
Au	0.8530	0.6110
Av	0.9430	0.6510

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Chain	Atom inclusion	Q-score
Aw	0.9120	0.6380
Ax	0.8280	0.5500
Ay	0.7210	0.5460
Az	0.8850	0.6340
B5	0.9010	0.5820
B7	0.9860	0.6500
B8	0.9430	0.6250
BA	0.9330	0.6500
BB	0.9210	0.6470
BC	0.9370	0.6450
BD	0.9080	0.6190
BE	0.8130	0.5770
BF	0.9430	0.6560
BG	0.8290	0.5900
BH	0.8980	0.6340
BI	0.8850	0.6430
BJ	0.8680	0.6220
BK	0.4100	0.4710
BL	0.8760	0.6160
BM	0.9080	0.6220
BN	0.9750	0.6620
BO	0.9420	0.6520
BP	0.8990	0.6400
BQ	0.9400	0.6520
BR	0.8630	0.6040
BS	0.9460	0.6560
BT	0.8890	0.6210
BU	0.8210	0.5660
BV	0.8840	0.6410
BW	0.5050	0.4500
BX	0.9030	0.6360
BY	0.9010	0.6330
BZ	0.9090	0.6370
Ba	0.9630	0.6560
Bb	0.7560	0.5580
Bc	0.8070	0.5920
Bd	0.8820	0.6290
Be	0.9380	0.6460
Bf	0.9500	0.6570
Bg	0.9060	0.6290
Bh	0.8920	0.6290
Bi	0.8670	0.6150

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Chain	Atom inclusion	Q-score
Bj	0.9640	0.6530
Bk	0.7850	0.5750
Bl	0.9280	0.6400
Bm	0.9240	0.6420
Bo	0.8970	0.6490
Bp	0.8950	0.6420
Br	0.9360	0.6430
Bs	0.0060	0.0310
Bt	0.0020	0.0450
Bv	0.0720	0.1750