wwPDB EM Validation Summary Report ⓘ

Apr 16, 2024 – 05:41 pm BST

PDB ID	:	8P2K
EMDB ID	:	EMD-17367
Title	:	Ternary complex of translating ribosome, NAC and METAP1
Authors	:	Jia, M.; Jaskolowski, M.; Scaiola, A.; Jomaa, A.; Ban, N.
Deposited on	:	2023-05-16
Resolution	:	2.90 Å(reported)
Based on initial models	:	7O7Y, 2B3K, 7QWR

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

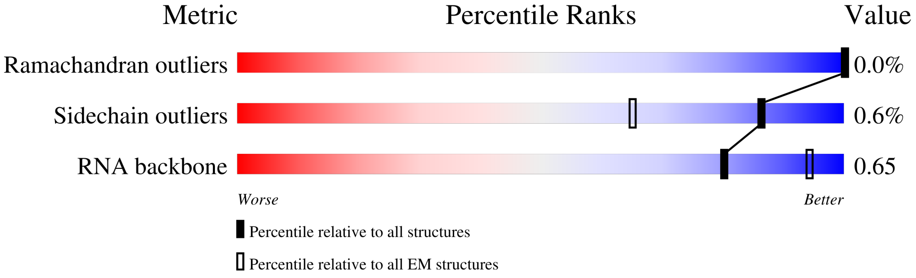
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance ⓘ

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

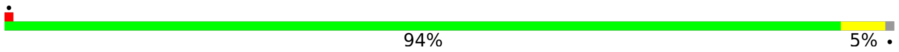
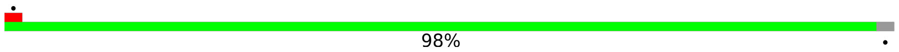
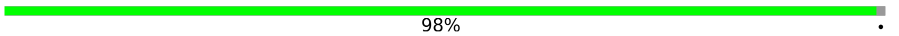
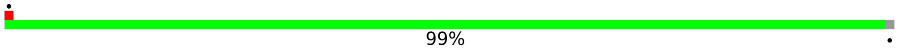
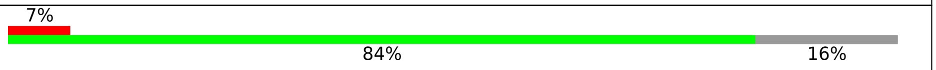
The reported resolution of this entry is 2.90 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=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	B5	4808	
2	B7	120	
3	B8	158	
4	BA	257	
5	BB	403	
6	BC	413	
7	BD	297	
8	BE	291	

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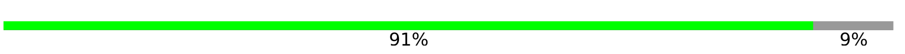
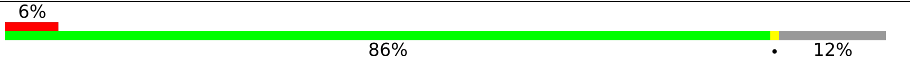
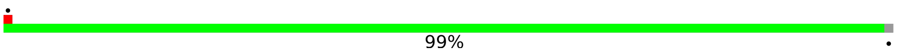
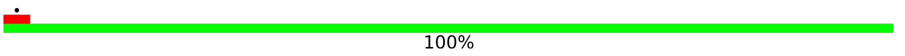
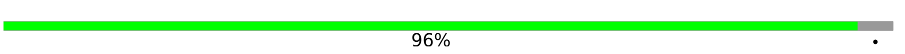
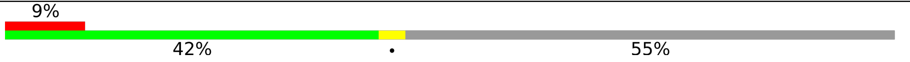
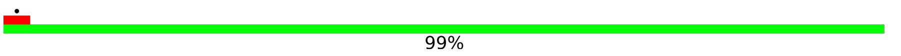
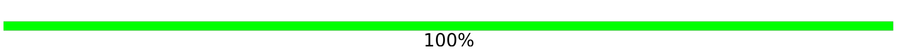
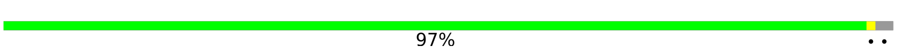
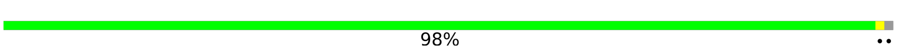
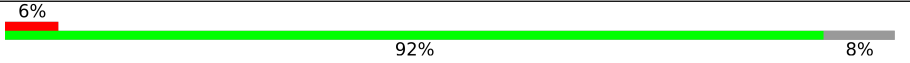
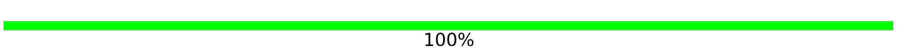
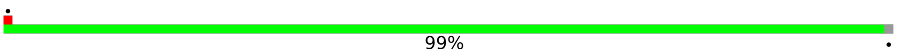
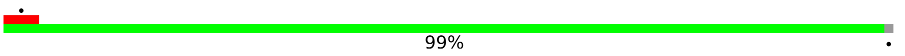
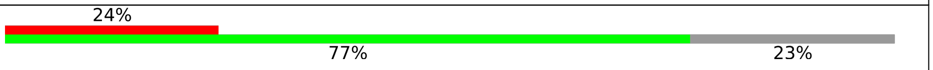
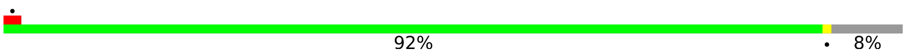
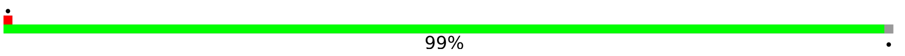
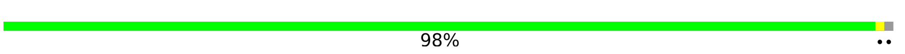
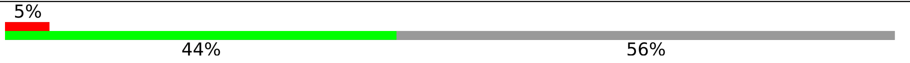
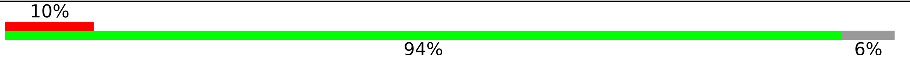
Mol	Chain	Length	Quality of chain
9	BF	247	
10	BG	266	
11	BH	192	
12	BI	214	
13	BJ	178	
14	BK	65	
15	BL	211	
16	BM	218	
17	BN	204	
18	BO	203	
19	BP	184	
20	BQ	188	
21	BR	196	
22	BS	176	
23	BT	160	
24	BU	128	
25	BV	140	
26	BW	157	
27	BX	156	
28	BY	145	
29	BZ	136	
30	Ba	148	
31	Bb	245	
32	Bc	115	
33	Bd	125	

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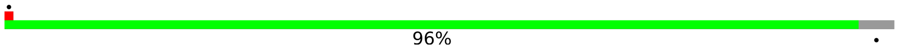
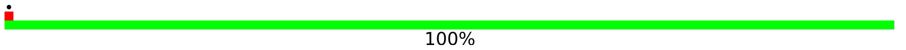
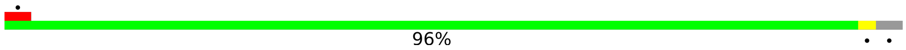
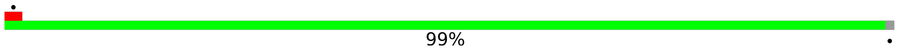
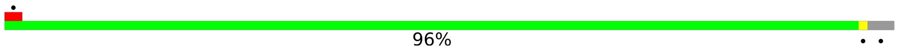
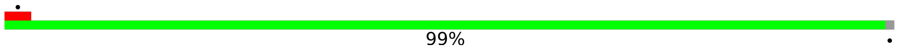
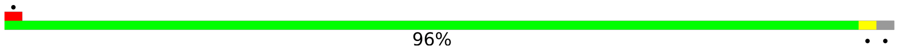
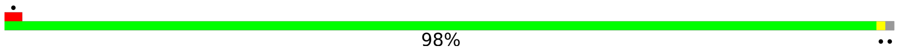
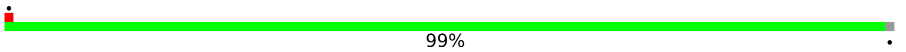
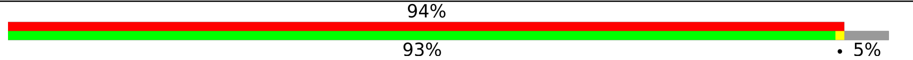
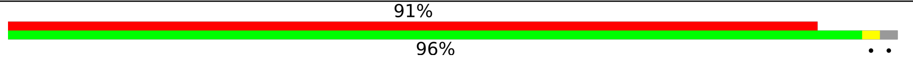
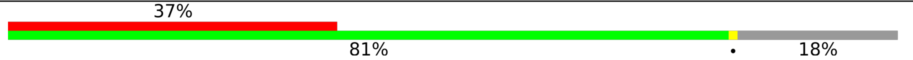
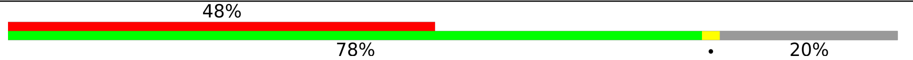
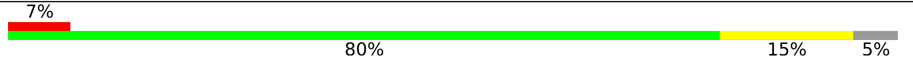
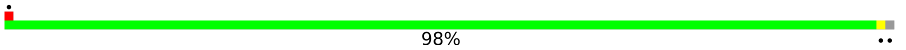
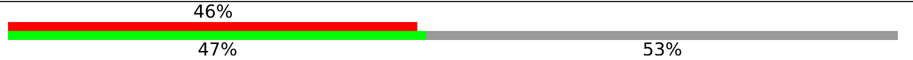
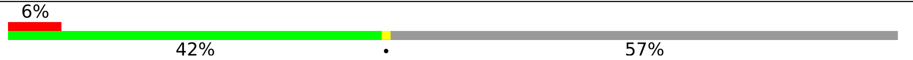
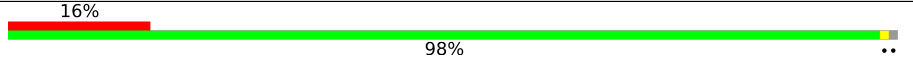
Mol	Chain	Length	Quality of chain
34	Be	135	
35	Bf	110	
36	Bg	117	
37	Bh	123	
38	Bi	105	
39	Bj	97	
40	Bk	70	
41	Bl	51	
42	Bm	128	
43	Bo	106	
44	Bp	92	
45	Br	137	
46	Bs	318	
47	Bt	165	
48	Bv	217	
49	MA	386	
50	Na	215	
51	Nb	132	
52	A2	1870	
53	AA	84	
54	AB	69	
55	AC	156	
56	AD	133	
57	AE	115	
58	AF	317	

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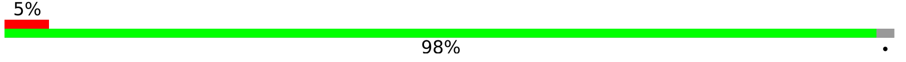
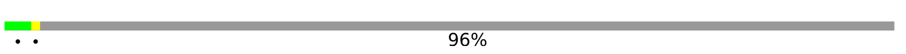
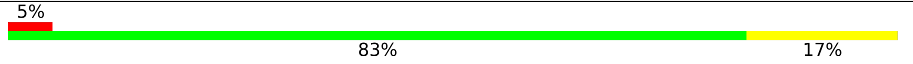
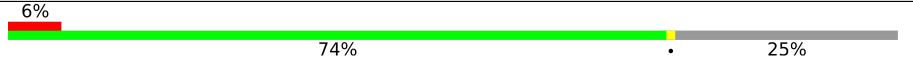
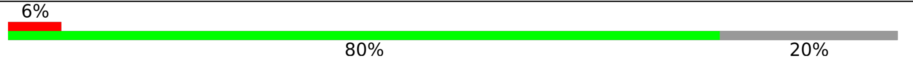
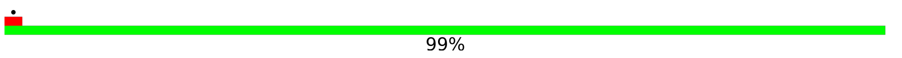
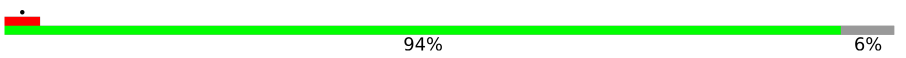
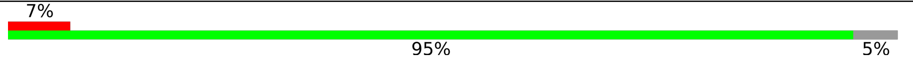
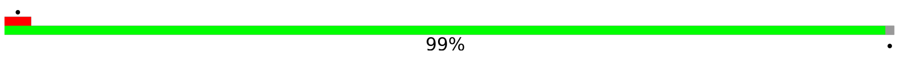
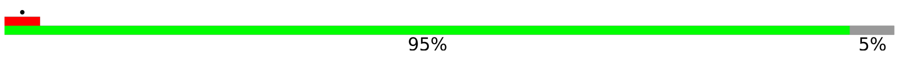
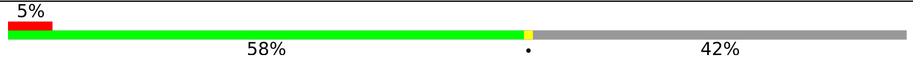
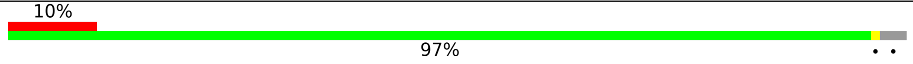
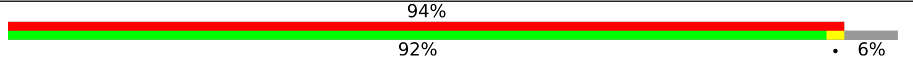
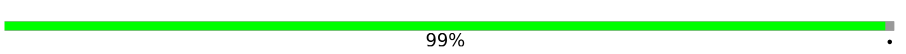
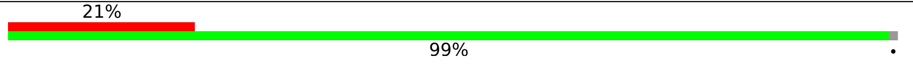
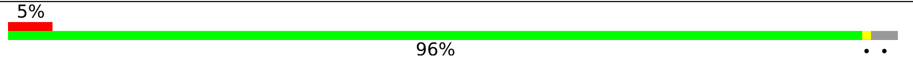
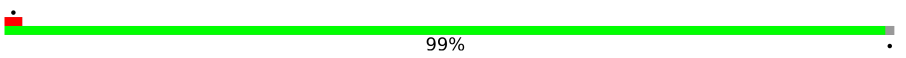
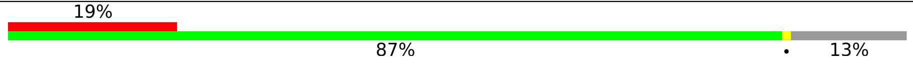
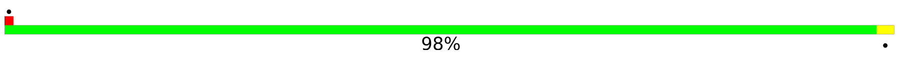
Mol	Chain	Length	Quality of chain
59	AG	56	 5% 98%
60	AI	76	 96%
61	AT	76	 5% 83% 17%
62	AZ	295	 6% 74% 25%
63	Aa	264	 84% 15%
64	Ab	293	 74% 25%
65	Ac	281	 6% 80% 20%
66	Ad	263	 99%
67	Ae	204	 94% 6%
68	Af	249	 7% 95% 5%
69	Ag	432	 14% 44% 56%
70	Ah	208	 99%
71	Ai	194	 95% 5%
72	Aj	165	 5% 58% 42%
73	Ak	158	 10% 97%
74	Al	132	 94% 92% 6%
75	Am	151	 99%
76	An	151	 88% 10%
77	Ao	145	 88% 12%
78	Ap	172	 82% 18%
79	Aq	135	 21% 99%
80	Ar	152	 5% 96%
81	As	145	 99%
82	At	119	 19% 87% 13%
83	Au	83	 98%

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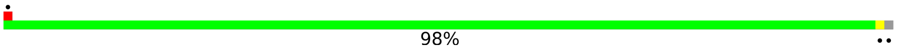
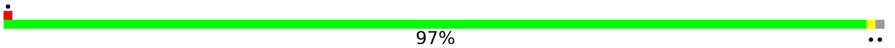
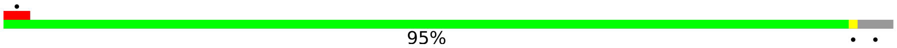
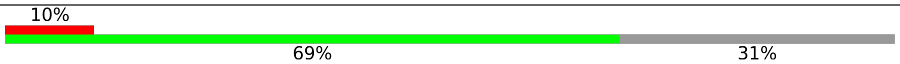
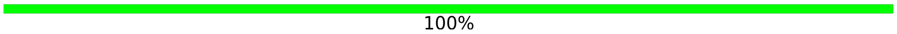
Mol	Chain	Length	Quality of chain
84	Av	130	
85	Aw	143	
86	Ax	130	
87	Ay	124	
88	Az	25	

2 Entry composition

There are 97 unique types of molecules in this entry. The entry contains 231486 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 28S rRNA.

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

- Molecule 2 is a RNA chain called 5S rRNA.

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

- Molecule 3 is a RNA chain called 5.8S rRNA.

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

- Molecule 4 is a protein called 60S ribosomal protein L8.

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

- Molecule 5 is a protein called Ribosomal protein L3.

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

- Molecule 6 is a protein called 60S ribosomal protein L4.

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

- Molecule 7 is a protein called Ribosomal protein L5 eukaryotic C-terminal domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	BD	293	2391	1512	438	427	14	0	0

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 8 is a protein called 60S ribosomal protein L6.

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

- Molecule 9 is a protein called Ribosomal Protein uL30.

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

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BF	61	ARG	GLY	conflict	UNP G1TUB1
BF	93	ARG	GLY	conflict	UNP G1TUB1
BF	131	MET	VAL	conflict	UNP G1TUB1
BF	153	ILE	VAL	conflict	UNP G1TUB1

- Molecule 10 is a protein called 60S ribosomal protein L7a.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BG	184	LEU	ILE	conflict	UNP P62424

- Molecule 11 is a protein called 60S ribosomal protein L9.

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

- Molecule 12 is a protein called 60S ribosomal protein L10.

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

- Molecule 13 is a protein called 60S ribosomal protein L11.

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

- Molecule 14 is a protein called Glucose-6-phosphate isomerase.

Mol	Chain	Residues	Atoms	AltConf	Trace
14	BK	29	Total C N O S 237 152 40 40 5	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BK	60	MET	VAL	conflict	UNP P06744
BK	61	MET	-	expression tag	UNP P06744
BK	62	MET	-	expression tag	UNP P06744
BK	63	MET	-	expression tag	UNP P06744
BK	64	MET	-	expression tag	UNP P06744
BK	65	VAL	-	expression tag	UNP P06744

- Molecule 15 is a protein called 60S ribosomal protein L13.

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BL	74	ARG	HIS	conflict	UNP G1TKB3
BL	190	ARG	HIS	conflict	UNP G1TKB3

- Molecule 16 is a protein called 60S ribosomal protein L14.

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

- Molecule 17 is a protein called Ribosomal protein L15.

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

- Molecule 18 is a protein called 60S ribosomal protein L13a.

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BO	174	LEU	ILE	conflict	UNP A0A0N8ETI8
BO	194	ASP	GLU	conflict	UNP A0A0N8ETI8

- Molecule 19 is a protein called uL22.

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

- Molecule 20 is a protein called eL18.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BQ	134	ARG	CYS	conflict	UNP F6QKI9

- Molecule 21 is a protein called Ribosomal protein L19.

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BR	38	ARG	HIS	conflict	UNP G1TYL6
BR	151	ARG	HIS	conflict	UNP G1TYL6

- Molecule 22 is a protein called 60S ribosomal protein L18a.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BS	36	ASN	ILE	conflict	UNP A0A1Z5LHJ5

- Molecule 23 is a protein called 60S ribosomal protein L21.

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

- Molecule 24 is a protein called 60S ribosomal protein L22.

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

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BU	32	GLY	ARG	conflict	UNP G1TSG1
BU	36	ALA	GLU	conflict	UNP G1TSG1

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Chain	Residue	Modelled	Actual	Comment	Reference
BU	39	PHE	SER	conflict	UNP G1TSG1
BU	54	GLY	ARG	conflict	UNP G1TSG1
BU	97	ARG	HIS	conflict	UNP G1TSG1

- Molecule 25 is a protein called Ribosomal protein L23.

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

- Molecule 26 is a protein called Ribosomal protein L24.

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

- Molecule 27 is a protein called Ribosomal_L23eN domain-containing protein.

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

- Molecule 28 is a protein called Ribosomal protein L26.

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

- Molecule 29 is a protein called 60S ribosomal protein L27.

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

- Molecule 30 is a protein called 60S ribosomal protein L27a.

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

- Molecule 31 is a protein called 60S ribosomal protein L29.

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

- Molecule 32 is a protein called 60S ribosomal protein L30.

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

- Molecule 33 is a protein called 60S ribosomal protein L31.

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

- Molecule 34 is a protein called Ribosomal protein L32.

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

- Molecule 35 is a protein called 60S ribosomal protein L35a.

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

- Molecule 36 is a protein called 60S ribosomal protein L34.

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

- Molecule 37 is a protein called 60S ribosomal protein L35.

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

- Molecule 38 is a protein called 60S ribosomal protein L36.

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

- Molecule 39 is a protein called Ribosomal protein L37.

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

- Molecule 40 is a protein called 60S ribosomal protein L38.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 41 is a protein called 60S ribosomal protein L39-like.

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

- Molecule 42 is a protein called Ubiquitin-60S ribosomal protein L40.

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

- Molecule 43 is a protein called eL42.

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

- Molecule 44 is a protein called 60S ribosomal protein L37a.

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

- Molecule 45 is a protein called 60S ribosomal protein L28.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Br	103	ARG	HIS	conflict	UNP G1U7L1

- Molecule 46 is a protein called 60S acidic ribosomal protein P0.

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

- Molecule 47 is a protein called 60S ribosomal protein L12.

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

- Molecule 48 is a protein called Ribosomal protein uL1.

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

- Molecule 49 is a protein called Methionine aminopeptidase 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
49	MA	315	2485	1562	444	461	18	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
MA	220	ASN	ASP	conflict	UNP P53582

- Molecule 50 is a protein called Nascent polypeptide-associated complex subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	Na	67	Total	C	N	O	S	0	0
			531	335	97	98	1		

- Molecule 51 is a protein called Transcription factor BTF3.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	Nb	106	Total	C	N	O	S	0	0
			821	514	153	151	3		

- Molecule 52 is a RNA chain called 18s rRNA.

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

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 53 is a protein called 40S ribosomal protein S27.

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

- Molecule 54 is a protein called 40S ribosomal protein S28.

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

- Molecule 55 is a protein called Ribosomal protein S27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	AC	74	Total	C	N	O	S	0	0
			610	385	117	101	7		

- Molecule 56 is a protein called 40S ribosomal protein S30.

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

- Molecule 57 is a protein called eS26.

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

- Molecule 58 is a protein called RACK1.

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

- Molecule 59 is a protein called 40S ribosomal protein S29.

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

- Molecule 60 is a RNA chain called E-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	AI	3	Total	C	N	O	P	0	0
			62	28	11	20	3		

- Molecule 61 is a RNA chain called P-site Val-tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	AT	76	Total	C	N	O	P	0	0
			1621	724	290	531	76		

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

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

- Molecule 63 is a protein called 40S ribosomal protein S3a.

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

- Molecule 64 is a protein called 40S ribosomal protein S2.

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Ab	33	ILE	VAL	conflict	UNP O18789
Ab	101	ALA	SER	conflict	UNP O18789

- Molecule 65 is a protein called 40S ribosomal protein S3.

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

- Molecule 66 is a protein called 40S ribosomal protein S4.

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

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Ad	25	GLY	SER	conflict	UNP G1TK17
Ad	51	ARG	LYS	conflict	UNP G1TK17
Ad	78	THR	ALA	conflict	UNP G1TK17
Ad	156	VAL	MET	conflict	UNP G1TK17

- Molecule 67 is a protein called Ribosomal protein S5.

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

- Molecule 68 is a protein called 40S ribosomal protein S6.

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

- Molecule 69 is a protein called 40S ribosomal protein S7.

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

- Molecule 70 is a protein called 40S ribosomal protein S8.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 71 is a protein called 40S ribosomal protein S9.

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

- Molecule 72 is a protein called S10_plectin domain-containing protein.

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

- Molecule 73 is a protein called 40S ribosomal protein S11.

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

- Molecule 74 is a protein called 40S ribosomal protein S12.

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

- Molecule 75 is a protein called 40S ribosomal protein S13.

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

- Molecule 76 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	An	136	Total 1017	C 622	N 199	O 190	S 6	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
An	138	5F0	ASP	conflict	UNP G1U472

- Molecule 77 is a protein called 40S ribosomal protein uS19.

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

- Molecule 78 is a protein called uS9.

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

- Molecule 79 is a protein called 40S ribosomal protein eS17.

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

- Molecule 80 is a protein called 40S ribosomal protein S18.

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

- Molecule 81 is a protein called 40S ribosomal protein S19.

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
As	119	GLY	TRP	conflict	UNP G1TN62
As	142	ASN	LYS	conflict	UNP G1TN62

- Molecule 82 is a protein called 40S ribosomal protein uS10.

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

- Molecule 83 is a protein called 40S ribosomal protein S21.

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

- Molecule 84 is a protein called Ribosomal protein S15a.

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

- Molecule 85 is a protein called 40S ribosomal protein S23.

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

- Molecule 86 is a protein called 40S ribosomal protein S24.

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

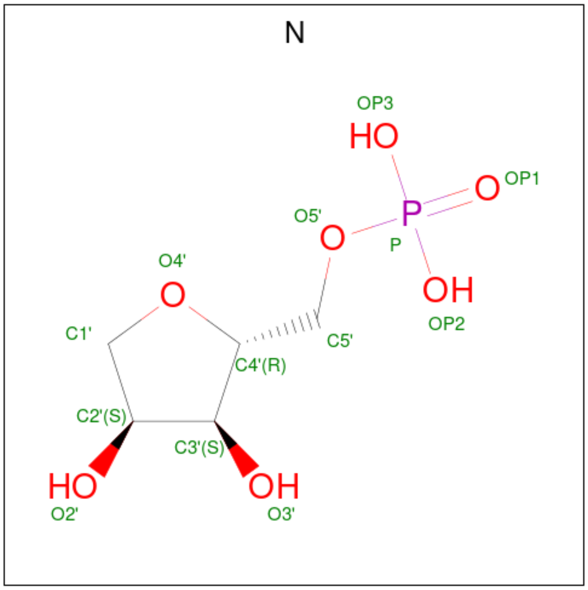
- Molecule 87 is a protein called 40S ribosomal protein S25.

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

- Molecule 88 is a protein called 60S ribosomal protein L41.

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

- Molecule 89 is ANY 5'-MONOPHOSPHATE NUCLEOTIDE (three-letter code: N) (formula: $C_5H_{11}O_7P$).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
89	B5	1	12	5	6	1	0
89	B5	1	12	5	6	1	0
89	B5	1	12	5	6	1	0
89	B5	1	12	5	6	1	0

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Mol	Chain	Residues	Atoms	AltConf
89	B5	1	Total C O P 12 5 6 1	0
89	B5	1	Total C O P 12 5 6 1	0
89	B5	1	Total C O P 12 5 6 1	0
89	B5	1	Total C O P 12 5 6 1	0
89	B5	1	Total C O P 12 5 6 1	0
89	B5	1	Total C O P 12 5 6 1	0
89	B5	1	Total C O P 12 5 6 1	0
89	B5	1	Total C O P 12 5 6 1	0
89	B5	1	Total C O P 12 5 6 1	0
89	B5	1	Total C O P 12 5 6 1	0
89	B5	1	Total C O P 12 5 6 1	0
89	B5	1	Total C O P 12 5 6 1	0
89	B5	1	Total C O P 12 5 6 1	0
89	B5	1	Total C O P 12 5 6 1	0
89	B5	1	Total C O P 12 5 6 1	0
89	B5	1	Total C O P 12 5 6 1	0
89	Bo	1	Total C O P 13 5 7 1	0
89	Bo	1	Total C O P 12 5 6 1	0
89	Bo	1	Total C O P 12 5 6 1	0
89	Bo	1	Total C O P 12 5 6 1	0
89	Bo	1	Total C O P 12 5 6 1	0

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Mol	Chain	Residues	Atoms	AltConf
89	Bo	1	Total C O P 12 5 6 1	0
89	Bo	1	Total C O P 12 5 6 1	0
89	Bo	1	Total C O P 12 5 6 1	0
89	Bo	1	Total C O P 12 5 6 1	0
89	Bo	1	Total C O P 12 5 6 1	0
89	Bo	1	Total C O P 12 5 6 1	0
89	Bv	1	Total C O P 12 5 6 1	0
89	Bv	1	Total C O P 12 5 6 1	0
89	Bv	1	Total C O P 12 5 6 1	0
89	Bv	1	Total C O P 12 5 6 1	0
89	Bv	1	Total C O P 12 5 6 1	0
89	Bv	1	Total C O P 12 5 6 1	0
89	Bv	1	Total C O P 12 5 6 1	0
89	A2	1	Total C O P 12 5 6 1	0
89	A2	1	Total C O P 12 5 6 1	0
89	A2	1	Total C O P 12 5 6 1	0
89	AI	1	Total C O P 12 5 6 1	0
89	AT	1	Total C O P 12 5 6 1	0
89	AT	1	Total C O P 12 5 6 1	0
89	AT	1	Total C O P 12 5 6 1	0
89	AT	1	Total C O P 12 5 6 1	0

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Mol	Chain	Residues	Atoms	AltConf
89	AT	1	Total C O P 12 5 6 1	0
89	AT	1	Total C O P 12 5 6 1	0
89	Aa	1	Total C O P 12 5 6 1	0
89	Aa	1	Total C O P 12 5 6 1	0
89	Aa	1	Total C O P 12 5 6 1	0
89	Aa	1	Total C O P 12 5 6 1	0
89	Aa	1	Total C O P 12 5 6 1	0
89	Aa	1	Total C O P 12 5 6 1	0
89	Aa	1	Total C O P 12 5 6 1	0
89	Aa	1	Total C O P 12 5 6 1	0
89	Aa	1	Total C O P 12 5 6 1	0
89	Aa	1	Total C O P 12 5 6 1	0
89	Ae	1	Total C O P 12 5 6 1	0
89	Ae	1	Total C O P 12 5 6 1	0
89	Ae	1	Total C O P 12 5 6 1	0
89	Ae	1	Total C O P 12 5 6 1	0
89	Ae	1	Total C O P 12 5 6 1	0
89	Ae	1	Total C O P 12 5 6 1	0
89	Ae	1	Total C O P 12 5 6 1	0
89	Ae	1	Total C O P 12 5 6 1	0
89	Ae	1	Total C O P 12 5 6 1	0

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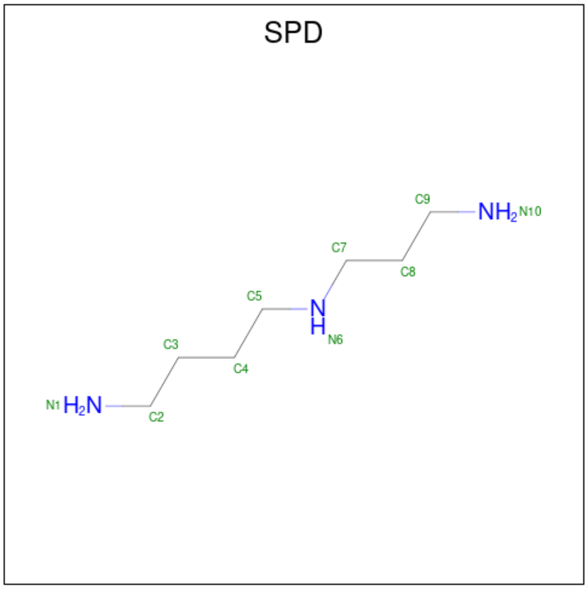
Mol	Chain	Residues	Atoms	AltConf
89	Ae	1	Total C O P 12 5 6 1	0
89	Ay	1	Total C O P 12 5 6 1	0
89	Ay	1	Total C O P 12 5 6 1	0
89	Ay	1	Total C O P 12 5 6 1	0
89	Ay	1	Total C O P 12 5 6 1	0
89	Ay	1	Total C O P 12 5 6 1	0

- Molecule 90 is SPERMIDINE (three-letter code: SPD) (formula: $C_7H_{19}N_3$).



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

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Mol	Chain	Residues	Atoms	AltConf
90	B5	1	Total C N 10 7 3	0
90	B5	1	Total C N 10 7 3	0
90	B5	1	Total C N 10 7 3	0
90	B5	1	Total C N 10 7 3	0
90	B5	1	Total C N 10 7 3	0
90	B5	1	Total C N 10 7 3	0
90	B5	1	Total C N 10 7 3	0
90	B5	1	Total C N 10 7 3	0
90	B5	1	Total C N 10 7 3	0
90	B5	1	Total C N 10 7 3	0
90	B5	1	Total C N 10 7 3	0
90	B5	1	Total C N 10 7 3	0
90	B5	1	Total C N 10 7 3	0
90	B5	1	Total C N 10 7 3	0
90	B5	1	Total C N 10 7 3	0
90	B5	1	Total C N 10 7 3	0
90	B5	1	Total C N 10 7 3	0
90	A2	1	Total C N 10 7 3	0
90	A2	1	Total C N 10 7 3	0
90	A2	1	Total C N 10 7 3	0
90	A2	1	Total C N 10 7 3	0

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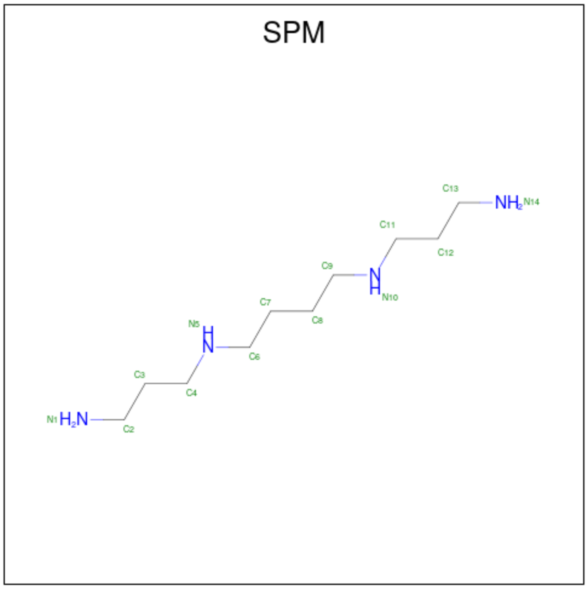
Mol	Chain	Residues	Atoms	AltConf
90	A2	1	Total C N 10 7 3	0
90	A2	1	Total C N 10 7 3	0
90	A2	1	Total C N 10 7 3	0
90	A2	1	Total C N 10 7 3	0

- Molecule 91 is SPERMINE (three-letter code: SPM) (formula: $C_{10}H_{26}N_4$).



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

- Molecule 92 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
92	B5	282	Total Mg 282 282	0
92	B7	9	Total Mg 9 9	0

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Mol	Chain	Residues	Atoms	AltConf
92	B8	9	Total Mg 9 9	0
92	BI	1	Total Mg 1 1	0
92	BP	1	Total Mg 1 1	0
92	BR	1	Total Mg 1 1	0
92	BV	1	Total Mg 1 1	0
92	Ba	1	Total Mg 1 1	0
92	Bj	1	Total Mg 1 1	0
92	Na	1	Total Mg 1 1	0
92	A2	108	Total Mg 108 108	0
92	AT	3	Total Mg 3 3	0
92	Af	1	Total Mg 1 1	0
92	An	1	Total Mg 1 1	0

- Molecule 93 is UNKNOWN ATOM OR ION (three-letter code: UNX) (formula: X).

Mol	Chain	Residues	Atoms	AltConf
93	B5	214	Total X 214 214	0
93	B7	6	Total X 6 6	0
93	B8	6	Total X 6 6	0
93	BA	3	Total X 3 3	0
93	BB	2	Total X 2 2	0
93	BH	1	Total X 1 1	0
93	BI	1	Total X 1 1	0

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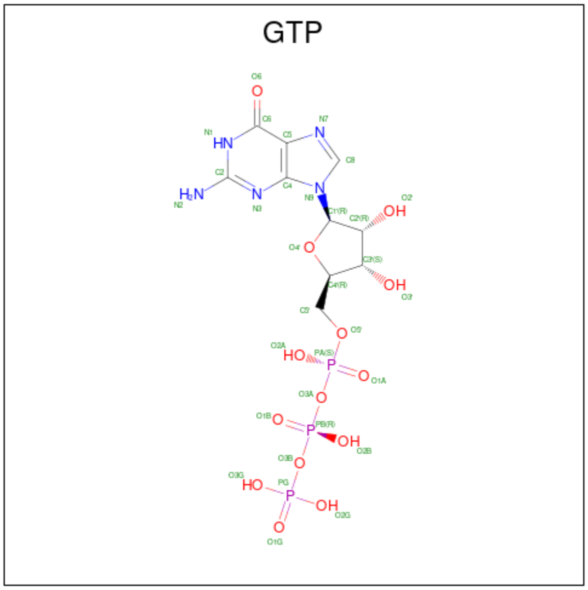
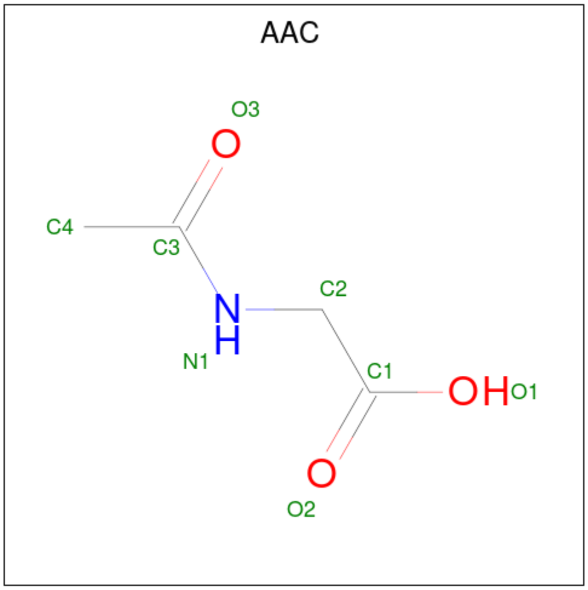
Mol	Chain	Residues	Atoms	AltConf
93	BL	1	Total X 1 1	0
93	BN	1	Total X 1 1	0
93	BP	1	Total X 1 1	0
93	BQ	2	Total X 2 2	0
93	BT	1	Total X 1 1	0
93	Bb	2	Total X 2 2	0
93	Be	3	Total X 3 3	0
93	Bf	1	Total X 1 1	0
93	Bl	2	Total X 2 2	0
93	Bo	1	Total X 1 1	0
93	A2	56	Total X 56 56	0
93	AE	1	Total X 1 1	0
93	AT	2	Total X 2 2	0
93	Ae	1	Total X 1 1	0
93	Ak	1	Total X 1 1	0
93	An	1	Total X 1 1	0
93	Ar	1	Total X 1 1	0
93	Az	1	Total X 1 1	0

- Molecule 94 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



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

- Molecule 95 is ACETYLAMINO-ACETIC ACID (three-letter code: AAC) (formula: $C_4H_7NO_3$).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
95	BD	1	7	4	1	2	0

- Molecule 96 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 97 is water.

Mol	Chain	Residues	Atoms	AltConf
97	B5	1388	Total O 1388 1388	0
97	B7	44	Total O 44 44	0
97	B8	49	Total O 49 49	0
97	BA	9	Total O 9 9	0
97	BB	6	Total O 6 6	0
97	BC	7	Total O 7 7	0
97	BD	1	Total O 1 1	0
97	BF	1	Total O 1 1	0
97	BH	2	Total O 2 2	0
97	BI	1	Total O 1 1	0
97	BL	3	Total O 3 3	0
97	BN	5	Total O 5 5	0

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Mol	Chain	Residues	Atoms	AltConf
97	BP	2	Total O 2 2	0
97	BR	5	Total O 5 5	0
97	BT	1	Total O 1 1	0
97	BV	3	Total O 3 3	0
97	BX	1	Total O 1 1	0
97	Ba	7	Total O 7 7	0
97	Bb	1	Total O 1 1	0
97	Bd	1	Total O 1 1	0
97	Be	5	Total O 5 5	0
97	Bg	2	Total O 2 2	0
97	Bj	2	Total O 2 2	0
97	Bl	1	Total O 1 1	0
97	Bo	1	Total O 1 1	0
97	Na	3	Total O 3 3	0
97	A2	530	Total O 530 530	0
97	AI	1	Total O 1 1	0
97	AT	13	Total O 13 13	0
97	Aa	2	Total O 2 2	0
97	Ad	1	Total O 1 1	0
97	Af	1	Total O 1 1	0
97	Ak	2	Total O 2 2	0

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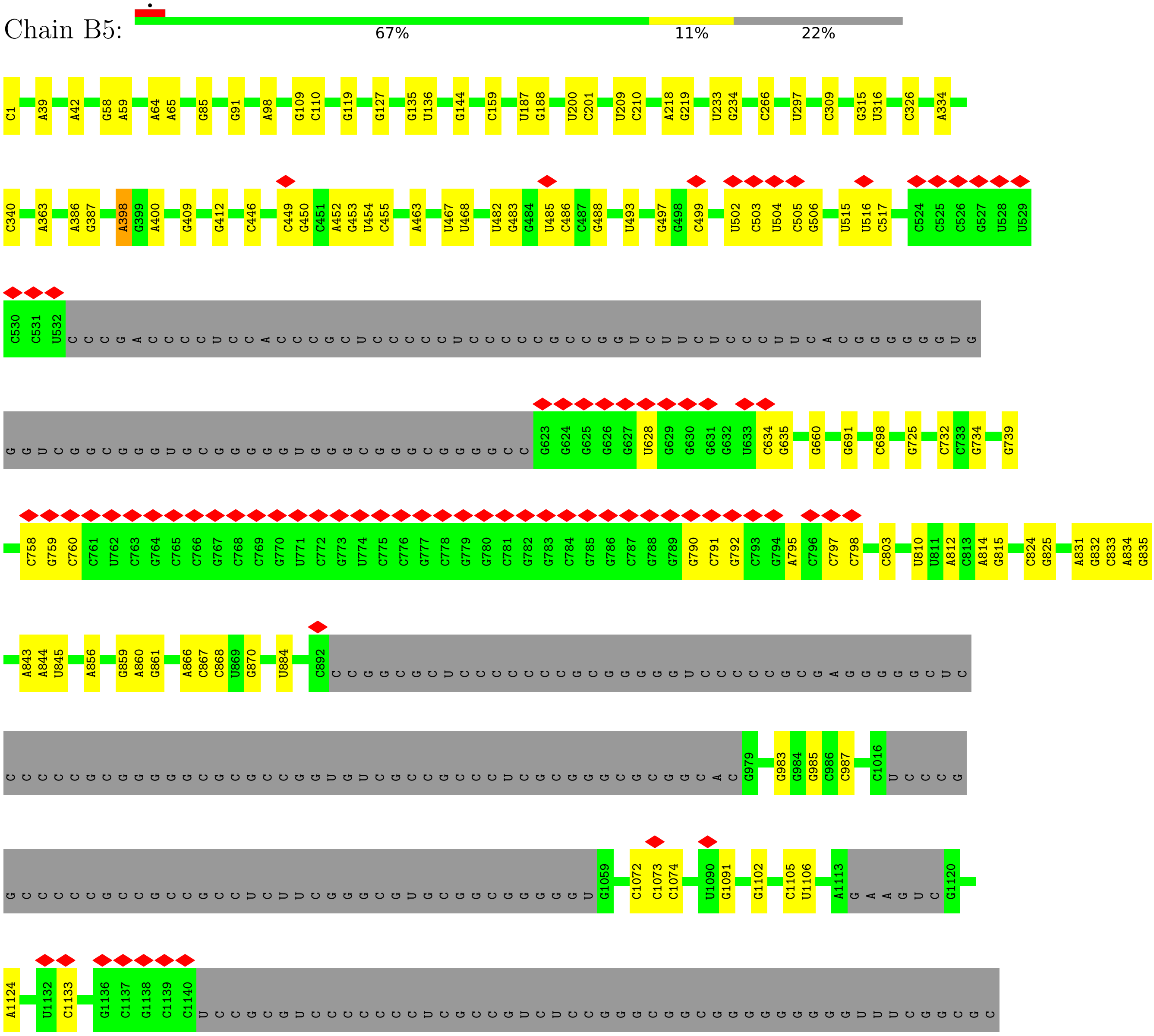
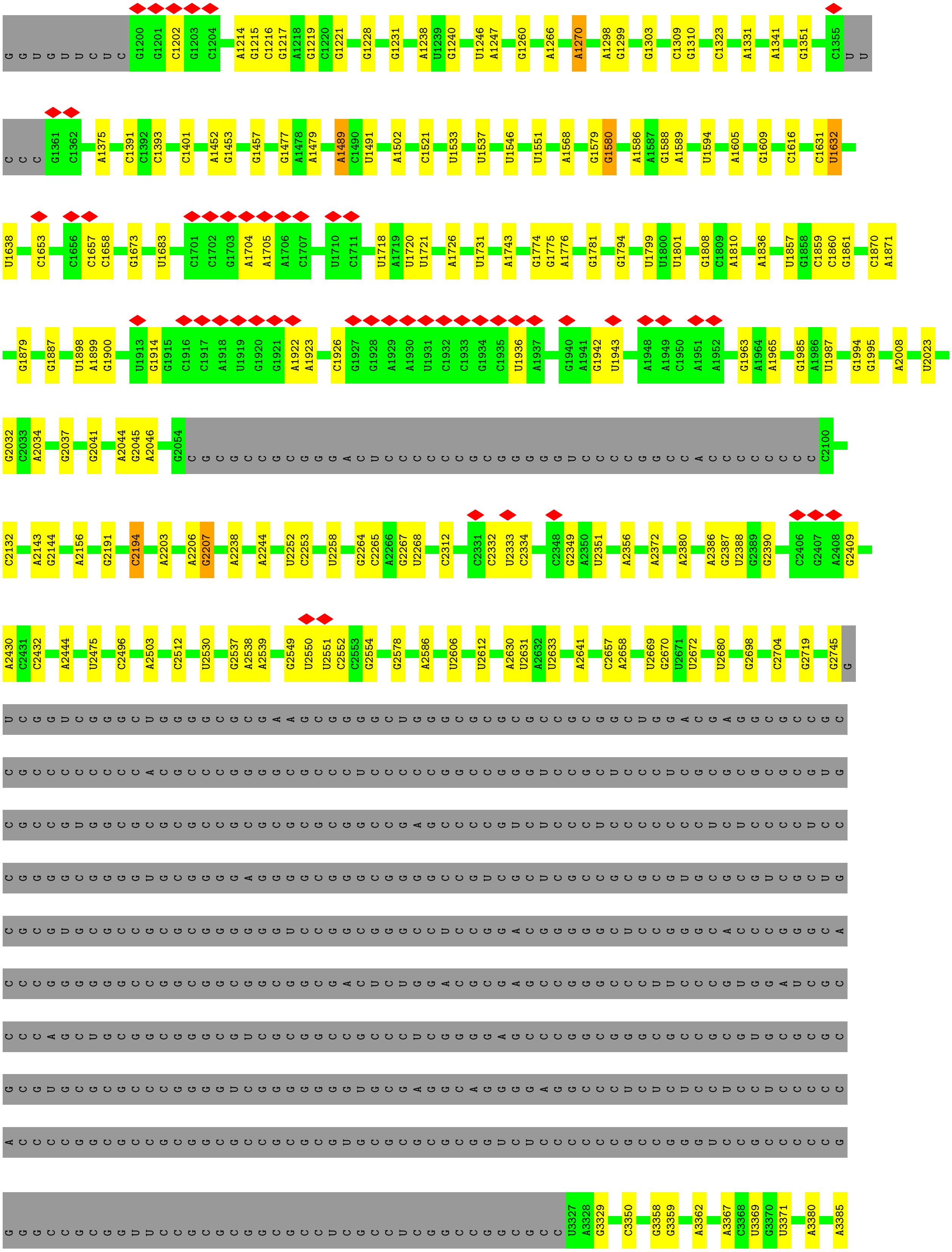
Mol	Chain	Residues	Atoms	AltConf
97	Am	1	Total O 1 1	0
97	An	3	Total O 3 3	0
97	Ap	2	Total O 2 2	0
97	Ar	2	Total O 2 2	0
97	As	2	Total O 2 2	0
97	At	1	Total O 1 1	0
97	Aw	5	Total O 5 5	0

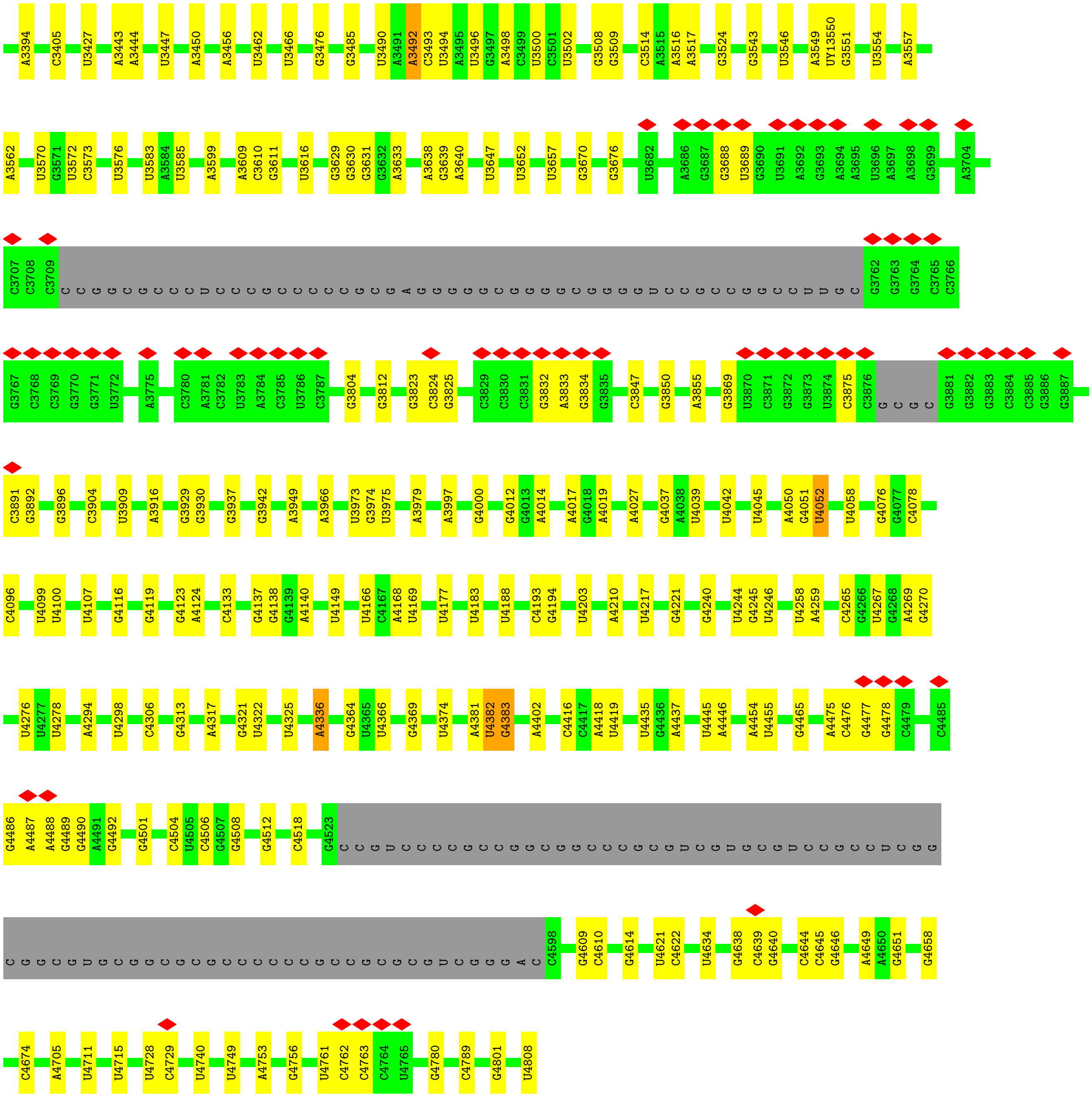
3 Residue-property plots ⓘ

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: 28S rRNA

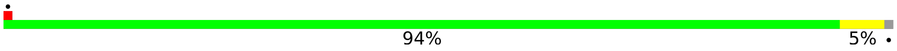


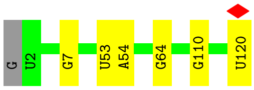

G G U G U U C U C G1200 G1201 C1202 G1203 C1204 A1214 G1215 C1216 G1217 A1218 G1219 C1220 G1221 G1228 G1231 A1238 U1239 G1240 U1246 A1247 G1260 A1266 A1270 A1298 G1299 G1303 C1309 G1310 C1323 A1331 A1341 G1351 C1355 U U
C C C G1361 C1362 A1375 C1391 C1392 C1393 C1401 A1452 G1453 G1457 G1477 A1478 A1479 A1489 C1490 U1491 A1502 C1521 U1533 U1537 U1546 U1551 A1568 G1579 G1580 A1586 A1587 G1588 A1589 U1594 A1605 G1609 C1616 C1631 U1632
U1638 C1653 C1656 C1657 C1658 G1673 U1683 C1701 C1702 G1703 A1704 A1705 A1706 C1707 U1710 C1711 U1718 A1719 U1720 U1721 A1726 U1731 A1743 G1774 G1775 A1776 G1781 G1794 U1799 U1800 U1801 G1808 C1809 A1810 A1836 U1857 G1858 C1859 C1860 G1861 C1870 A1871
G1879 G1887 U1898 A1899 G1900 U1913 G1914 G1915 C1916 C1917 A1918 U1919 G1920 G1921 A1922 A1923 C1926 G1927 G1928 A1929 A1930 U1931 C1932 C1933 G1934 C1935 U1936 A1937 G1940 A1941 G1942 U1943 A1948 A1949 C1950 A1951 A1952 G1963 A1964 A1965 G1985 A1986 U1987 G1994 G1995 A2008 U2023
G2032 C2033 A2034 G2037 G2041 A2044 G2045 A2046 G2054 C G C G C C G C G G G A C U C C C C C C G C G G G G G U C C C C G G C C A C C C C C C C C C2100
C2132 A2143 G2144 A2156 G2191 C2194 A2203 A2206 G2207 A2238 A2244 U2252 C2253 U2258 G2264 C2265 A2266 G2267 U2268 C2312 C2331 C2332 U2333 C2334 C2348 G2349 A2350 U2351 A2356 A2372 A2380 A2386 G2387 U2388 G2389 G2390 C2406 G2407 A2408 G2409
A2430 C2431 C2432 A2444 U2475 C2496 A2503 C2512 U2530 G2537 A2538 A2539 G2549 U2550 U2551 C2552 C2553 G2554 G2578 A2586 U2606 U2612 A2630 U2631 A2632 U2633 A2641 C2657 A2658 U2669 G2670 U2671 U2672 U2680 G2698 C2704 G2719 G2745 G
U C G G U C G G G C U G G G G C G C G A A G C G G G C U G G G C G C G C G C C G C G G C U G G A C G A G G C G C C G C
C G C C C C C C C C A C G C C C G G G G C G C C C U C C C C C G G C C G G G U C C G C U C C C U C G C G C G C G C G U G
C G C C G U G G C G C G C G C C G C G C G C G C G G C C G A G C C C C G U C U C C C U C C C C C C C U C U C C C C U C C
C G G G G C G G G G U G C G G G G A G G G G C G G G C G G G G C C G U C G C U C G C C G C G C G U G C G C G U C G C U G
C G C G U G C G C C G C G C G G G G G G U C C G G C G G G C C U C C G G A C G G G G G C U C C G G G C A C C C G G G C A
C C C G G G G G G C C G G C G G C G G C G G C G A C U C U G G A C G C G A G C C G G G C C C U U C C C G U G G A U C G C
C C C A G C U G C G G C G G G C G U C G C G G C C G C C C U C G G G G A G C C C G G C G G G C G C C G C G U G C G C G C
G C G U G C G C G C C C G G G G U C G G G G G G U G C G A G G C A G G G G A G G C C C U C U C U C C U C C U C C C C C
A C C C C G G C G C C G C G G C G C C G C G C G U G C G C G C G C G G U C U C C C C C C G C C G G G U C C G C C C C C G
G G G C C G C G G U U C C G C G C G G C G C C U C G C C U C G G C C G G C G C C U3327 A3328 G3329 C3350 G3358 G3359 A3362 A3367 C3368 U3369 G3370 U3371 A3380 A3385



- Molecule 2: 5S rRNA

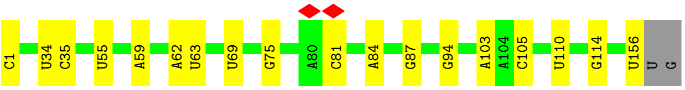
Chain B7:





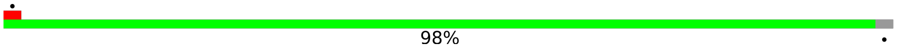
- Molecule 3: 5.8S rRNA

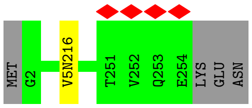
Chain B8:



- Molecule 4: 60S ribosomal protein L8

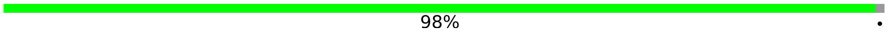
Chain BA:

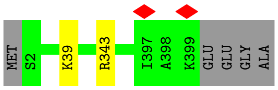




- Molecule 5: Ribosomal protein L3

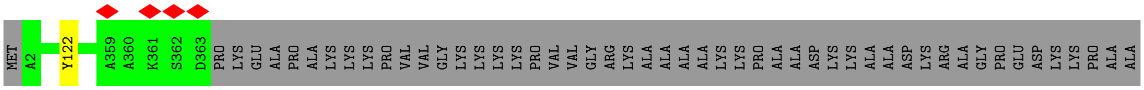
Chain BB:





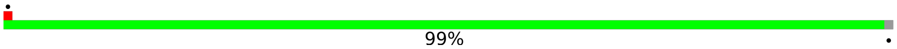
- Molecule 6: 60S ribosomal protein L4

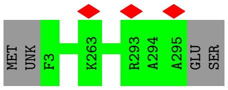
Chain BC:



- Molecule 7: Ribosomal protein L5 eukaryotic C-terminal domain-containing protein

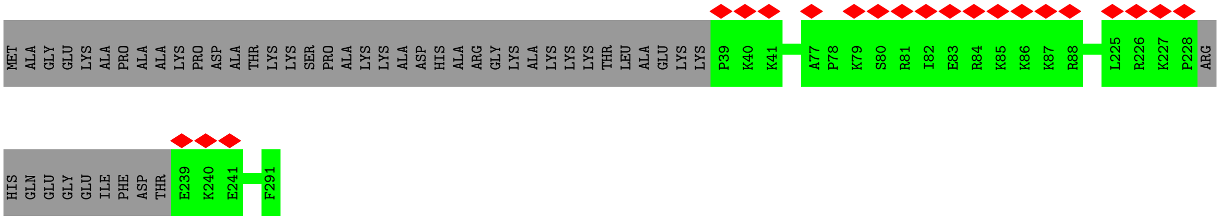
Chain BD:





- Molecule 8: 60S ribosomal protein L6

Chain BE:

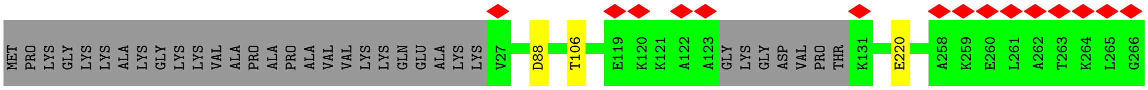


- Molecule 9: Ribosomal Protein uL30

Chain BF:

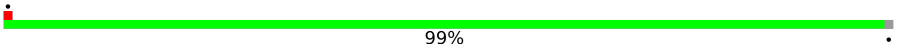
- Molecule 10: 60S ribosomal protein L7a

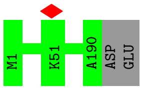
Chain BG:



- Molecule 11: 60S ribosomal protein L9

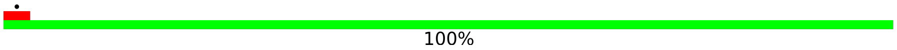
Chain BH:

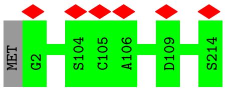




- Molecule 12: 60S ribosomal protein L10

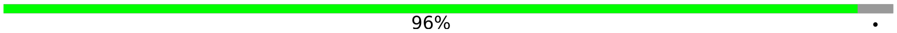
Chain BI:

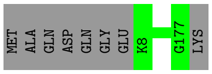




- Molecule 13: 60S ribosomal protein L11

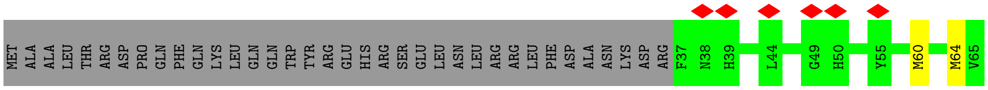
Chain BJ:





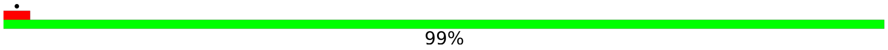
- Molecule 14: Glucose-6-phosphate isomerase

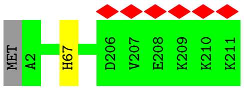
Chain BK:



- Molecule 15: 60S ribosomal protein L13

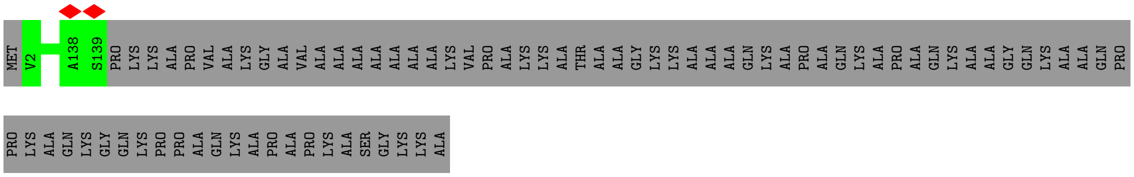
Chain BL:





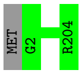
- Molecule 16: 60S ribosomal protein L14

Chain BM:

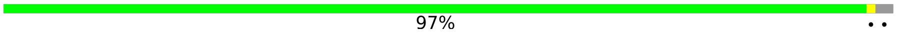



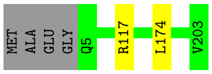
- Molecule 17: Ribosomal protein L15

Chain BN:

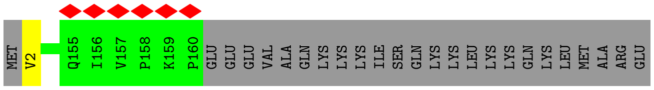
- Molecule 18: 60S ribosomal protein L13a

Chain BO:


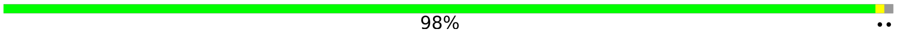


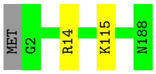
- Molecule 19: uL22

Chain BP:

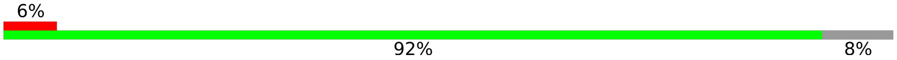



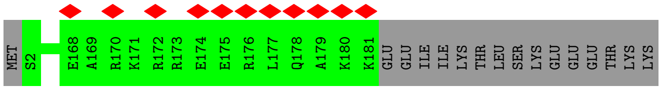
- Molecule 20: eL18

Chain BQ:


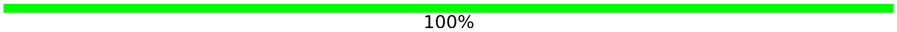


- Molecule 21: Ribosomal protein L19

Chain BR:




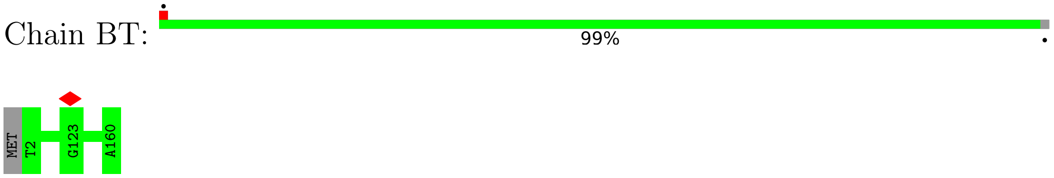
- Molecule 22: 60S ribosomal protein L18a

Chain BS:


There are no outlier residues recorded for this chain.

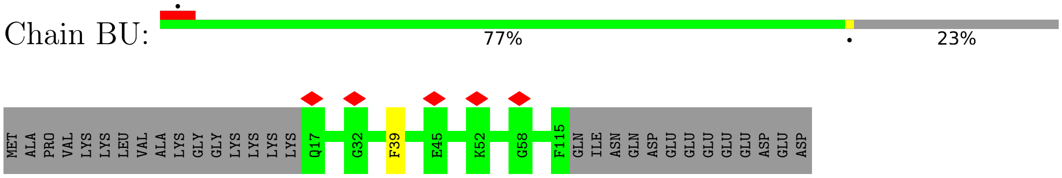
- Molecule 23: 60S ribosomal protein L21

Chain BT:



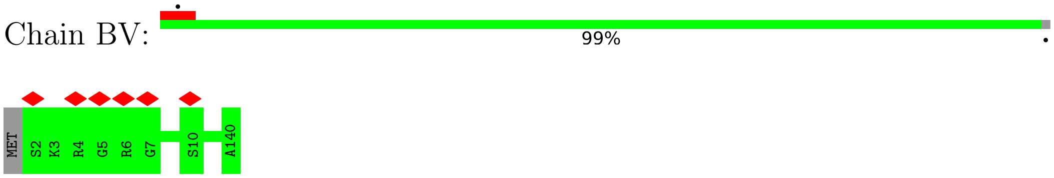
- Molecule 24: 60S ribosomal protein L22

Chain BU:



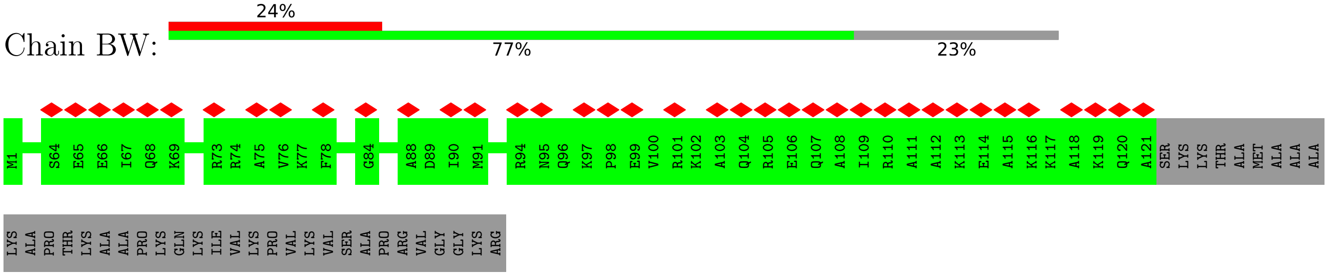
- Molecule 25: Ribosomal protein L23

Chain BV:



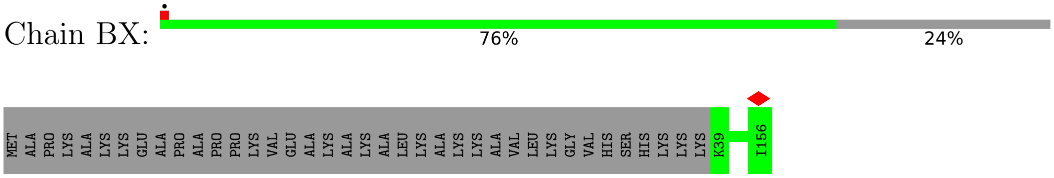
- Molecule 26: Ribosomal protein L24

Chain BW:



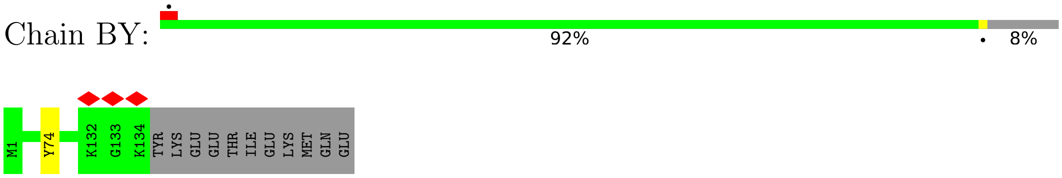
- Molecule 27: Ribosomal_L23eN domain-containing protein

Chain BX:

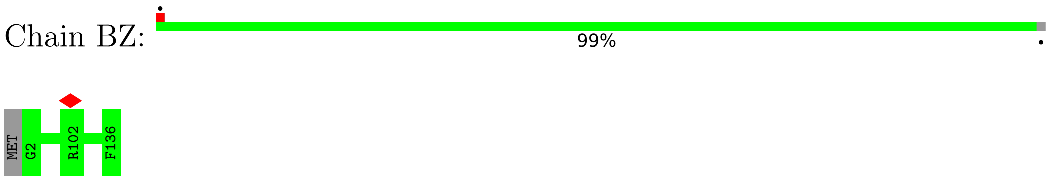


- Molecule 28: Ribosomal protein L26

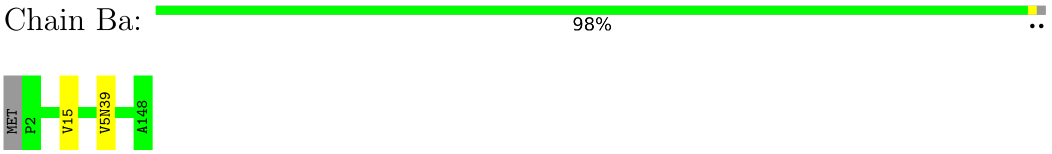
Chain BY:



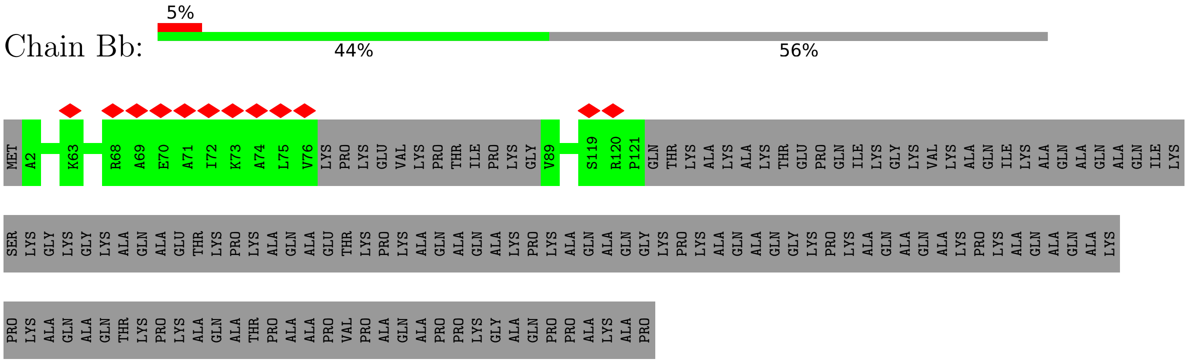
- Molecule 29: 60S ribosomal protein L27



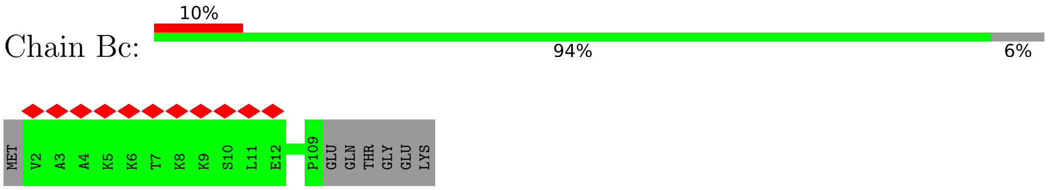
- Molecule 30: 60S ribosomal protein L27a



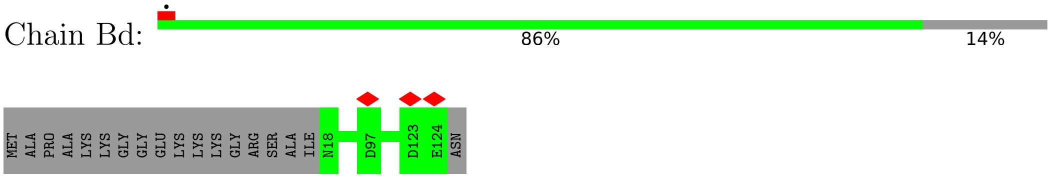
- Molecule 31: 60S ribosomal protein L29



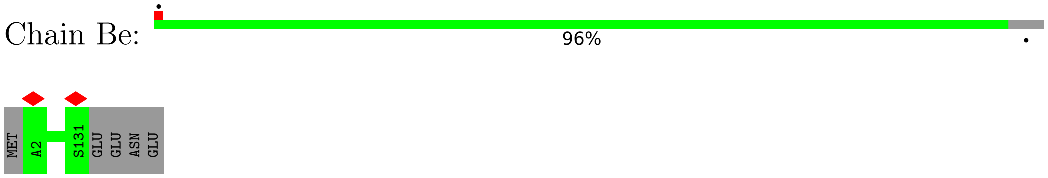
- Molecule 32: 60S ribosomal protein L30



- Molecule 33: 60S ribosomal protein L31

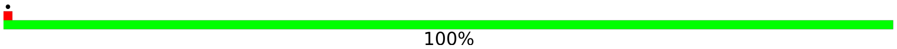


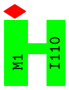
- Molecule 34: Ribosomal protein L32



- Molecule 35: 60S ribosomal protein L35a

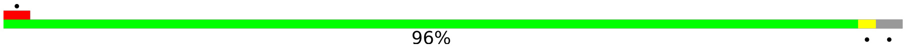
Chain Bf:

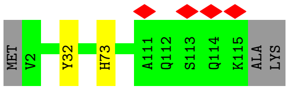




- Molecule 36: 60S ribosomal protein L34

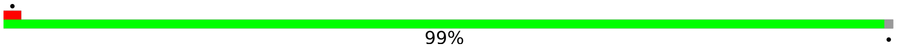
Chain Bg:

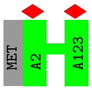




- Molecule 37: 60S ribosomal protein L35

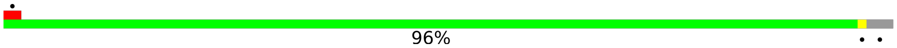
Chain Bh:

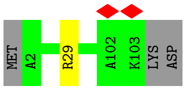




- Molecule 38: 60S ribosomal protein L36

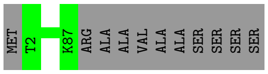
Chain Bi:





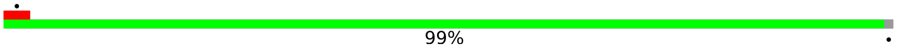
- Molecule 39: Ribosomal protein L37

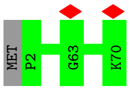
Chain Bj:



- Molecule 40: 60S ribosomal protein L38

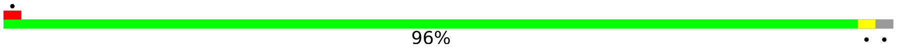
Chain Bk:

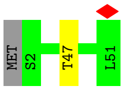




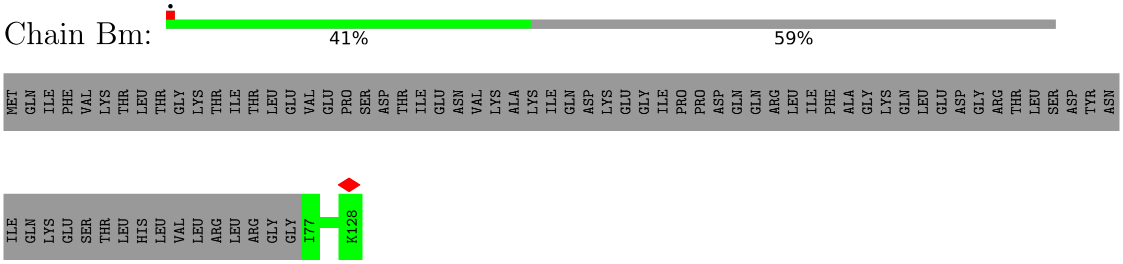
- Molecule 41: 60S ribosomal protein L39-like

Chain Bl:

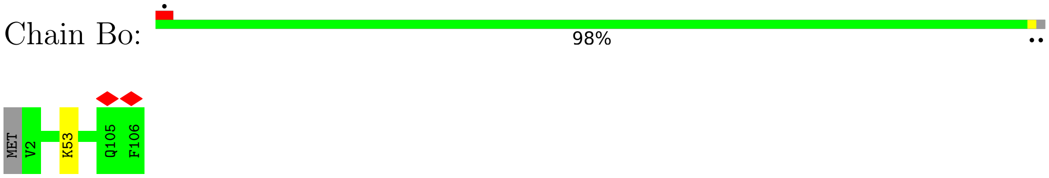




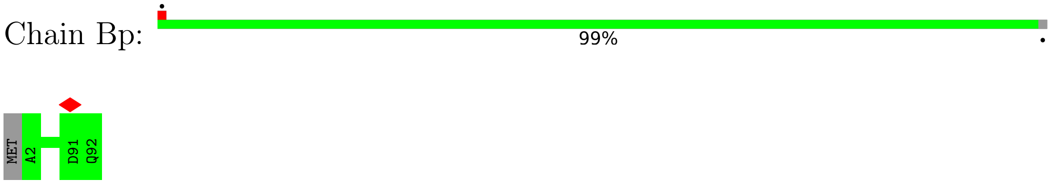
- Molecule 42: Ubiquitin-60S ribosomal protein L40



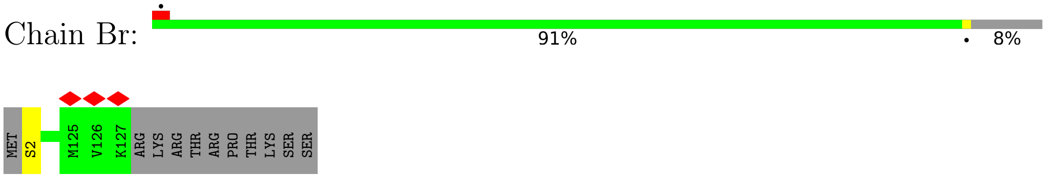
- Molecule 43: eL42



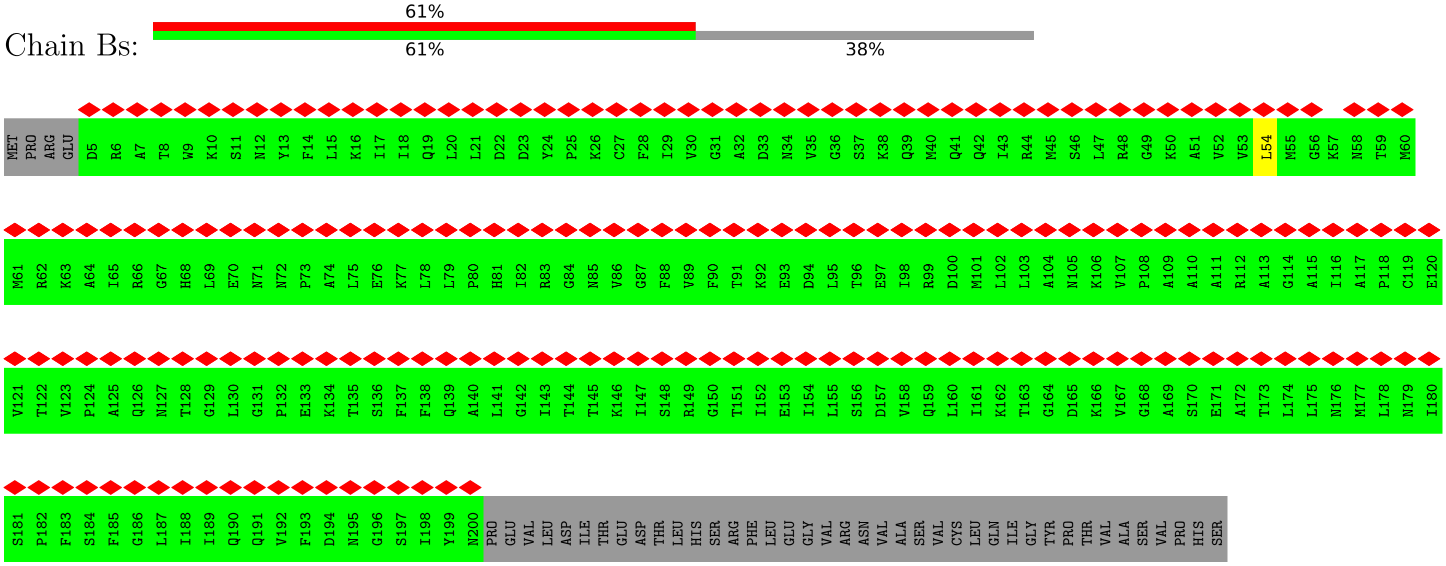
- Molecule 44: 60S ribosomal protein L37a

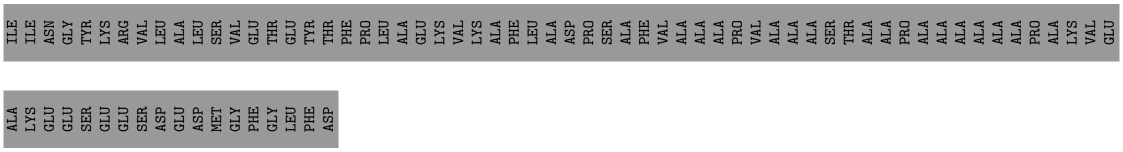


- Molecule 45: 60S ribosomal protein L28



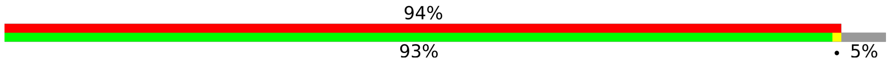
- Molecule 46: 60S acidic ribosomal protein P0

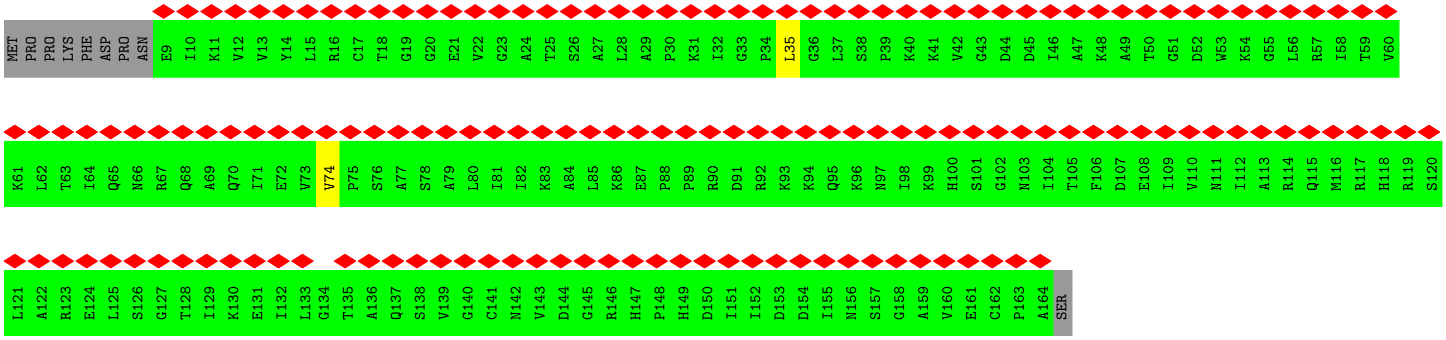




- Molecule 47: 60S ribosomal protein L12

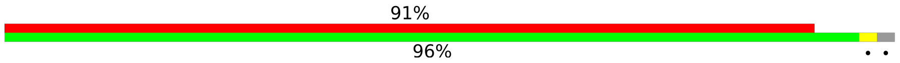
Chain Bt:

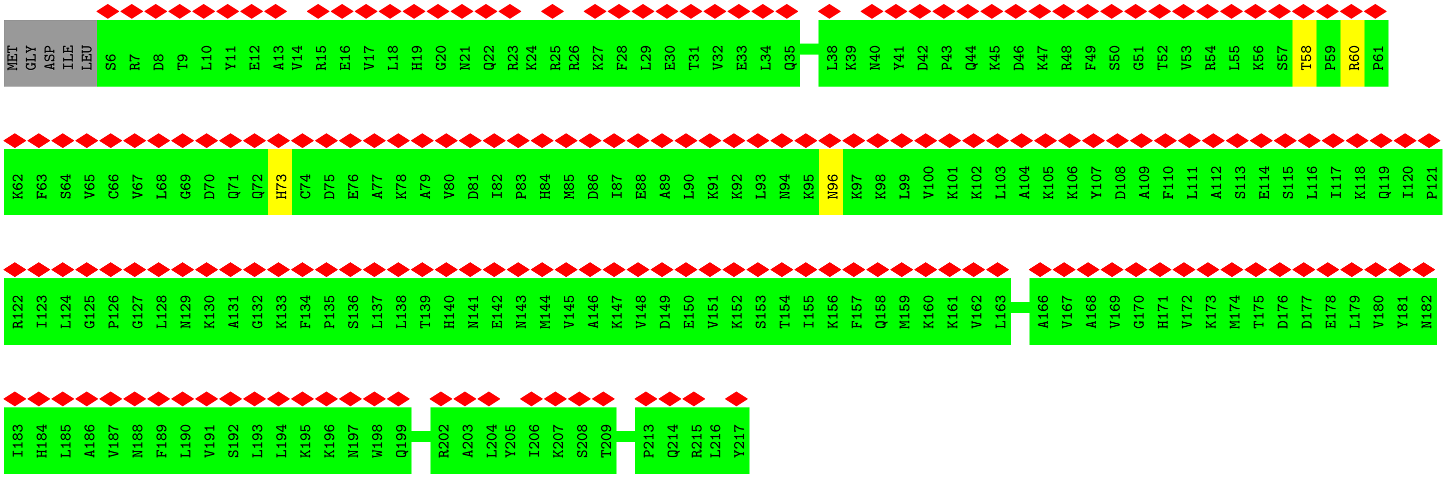




- Molecule 48: Ribosomal protein uL1

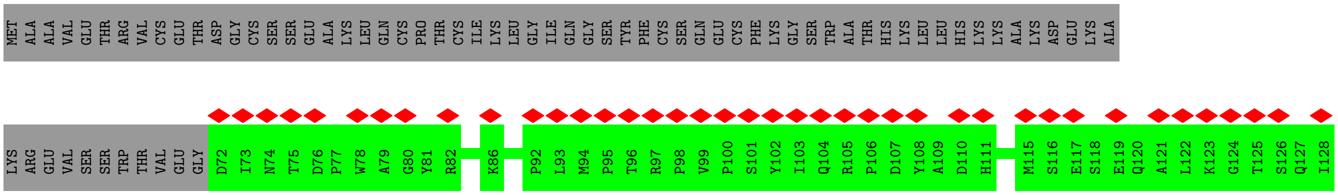
Chain Bv:

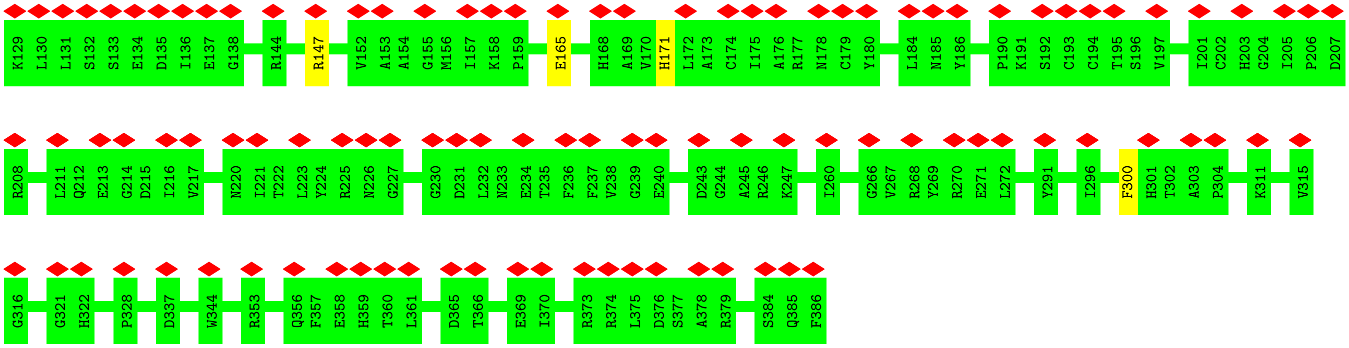




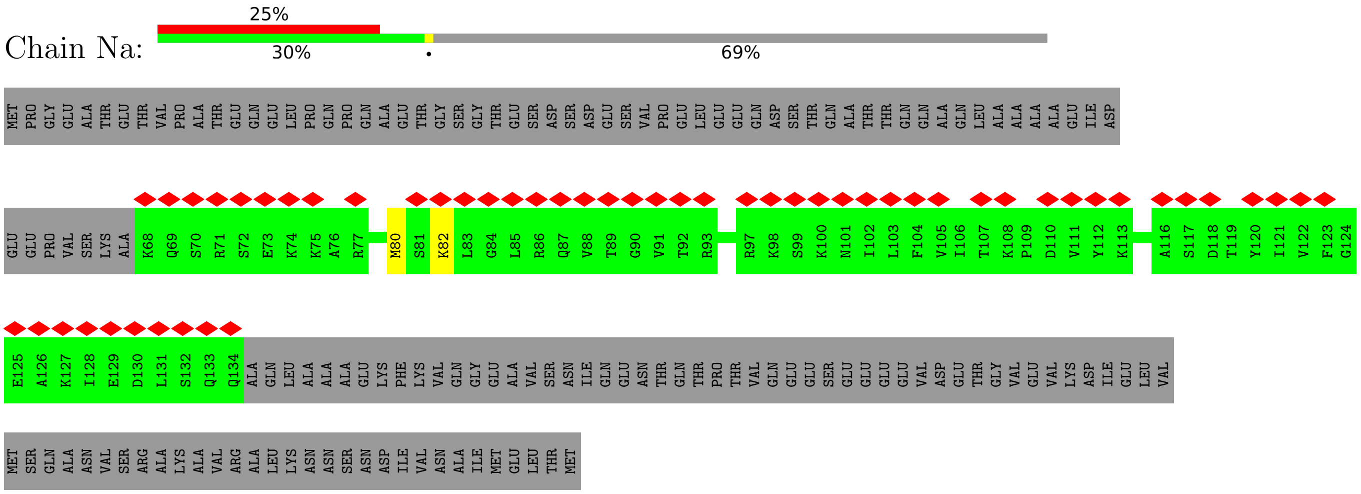
- Molecule 49: Methionine aminopeptidase 1

Chain MA:

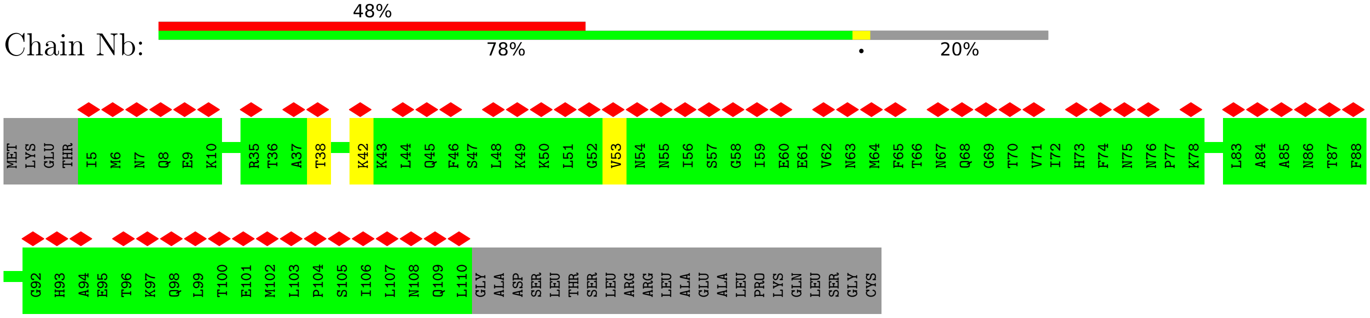




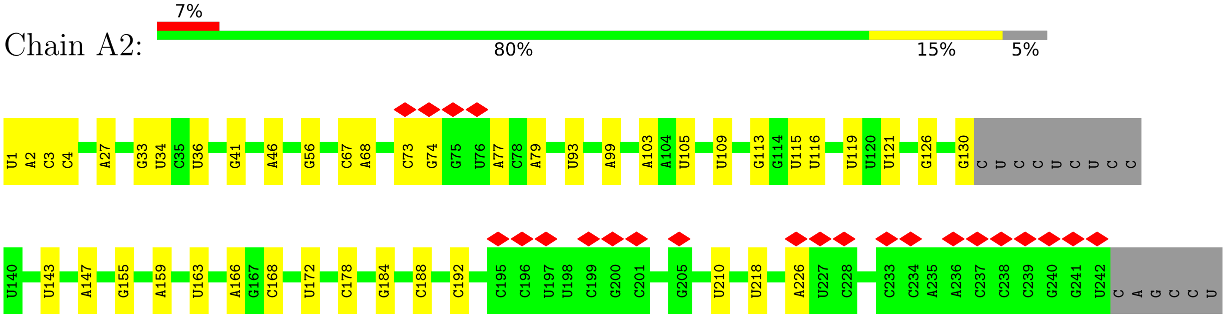
- Molecule 50: Nascent polypeptide-associated complex subunit alpha

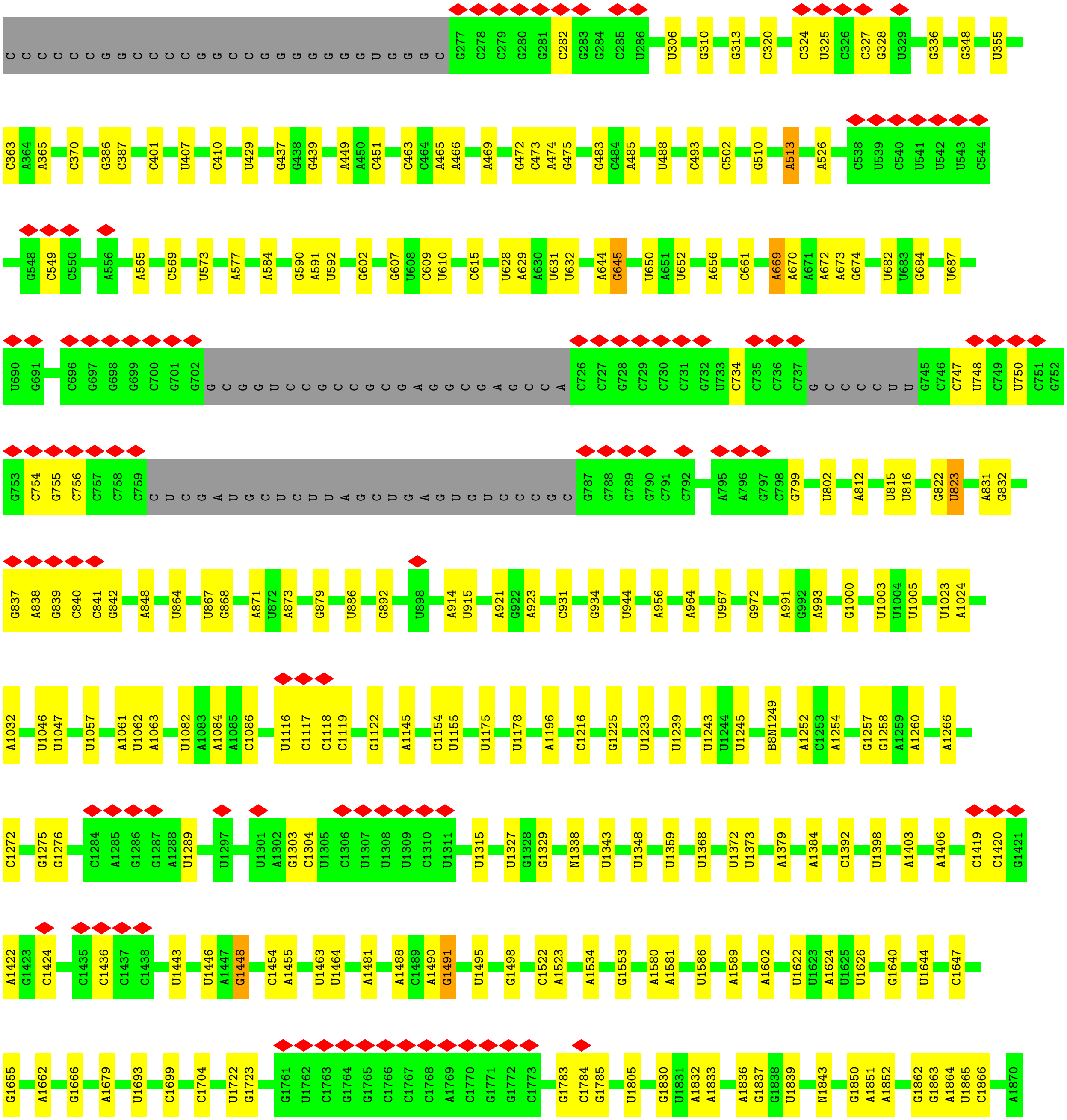


- Molecule 51: Transcription factor BTF3



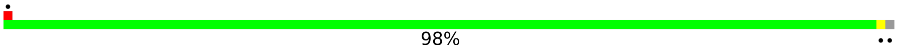
- Molecule 52: 18s rRNA

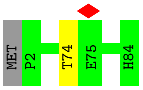




- Molecule 53: 40S ribosomal protein S27

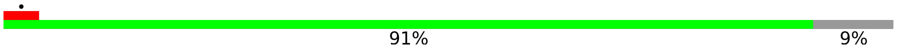
Chain AA:

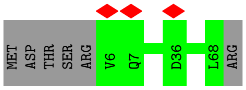




- Molecule 54: 40S ribosomal protein S28

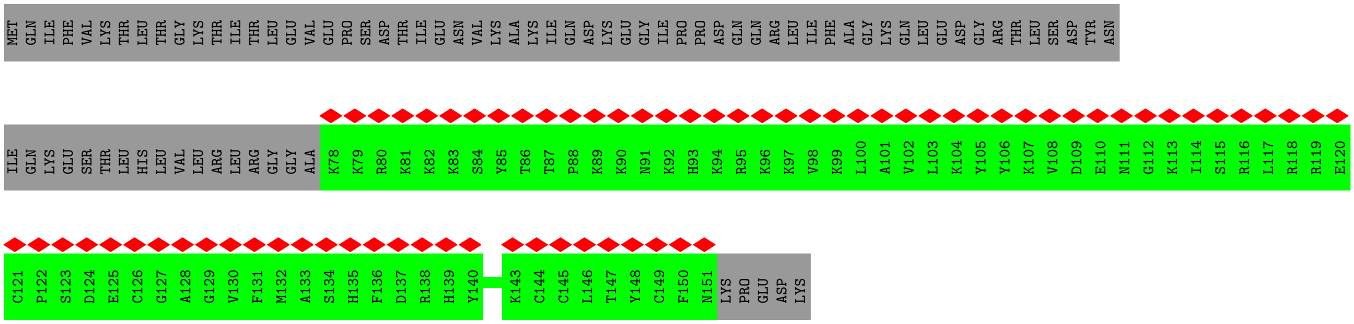
Chain AB:





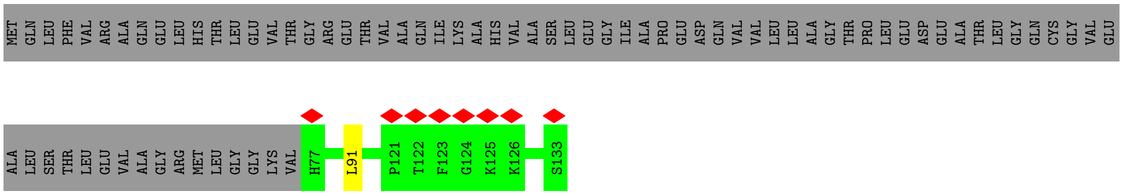
- Molecule 55: Ribosomal protein S27a

Chain AC:



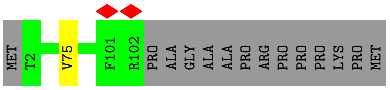
- Molecule 56: 40S ribosomal protein S30

Chain AD:



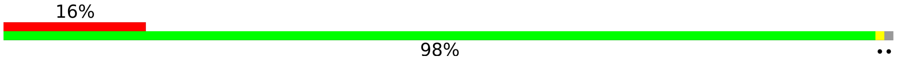
- Molecule 57: eS26

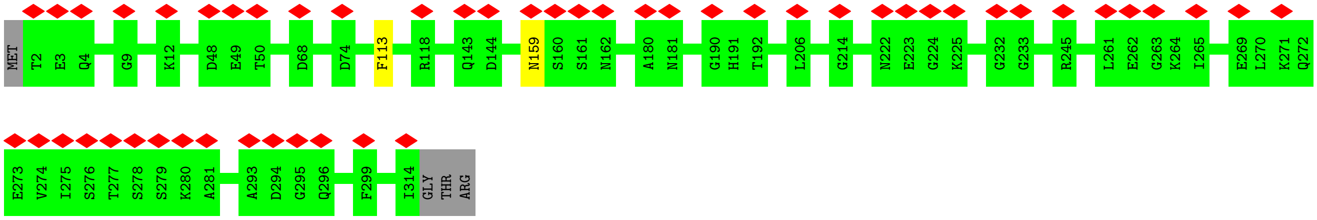
Chain AE:



- Molecule 58: RACK1

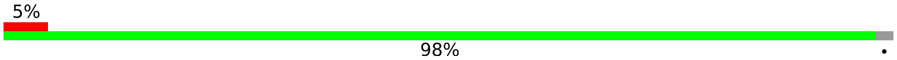
Chain AF:

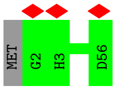




- Molecule 59: 40S ribosomal protein S29

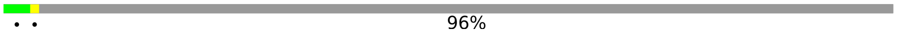
Chain AG:

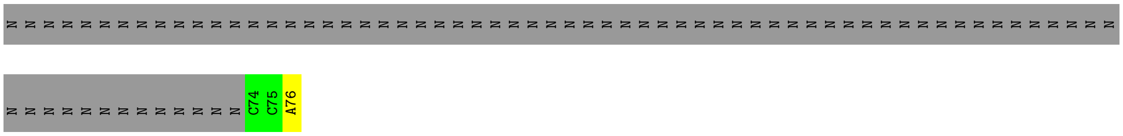




- Molecule 60: E-site tRNA

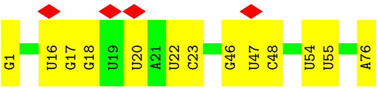
Chain AI:





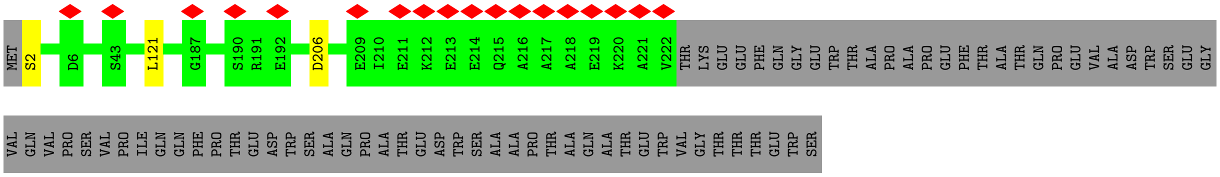
- Molecule 61: P-site Val-tRNA

Chain AT:



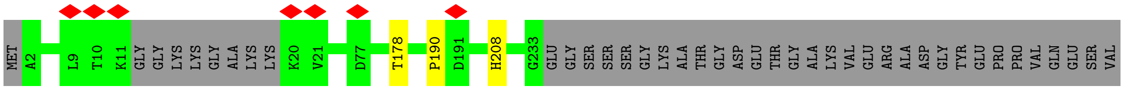
- Molecule 62: 40S ribosomal protein SA

Chain AZ:



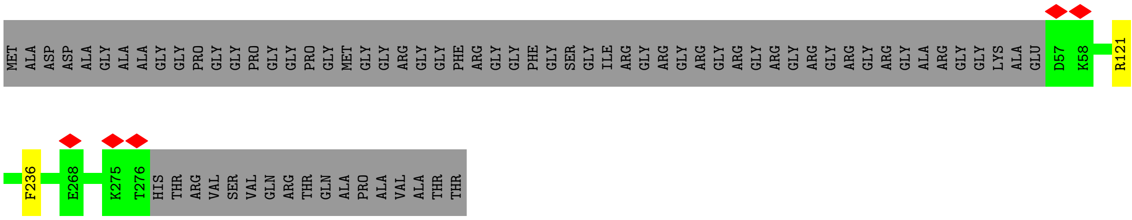
- Molecule 63: 40S ribosomal protein S3a

Chain Aa:

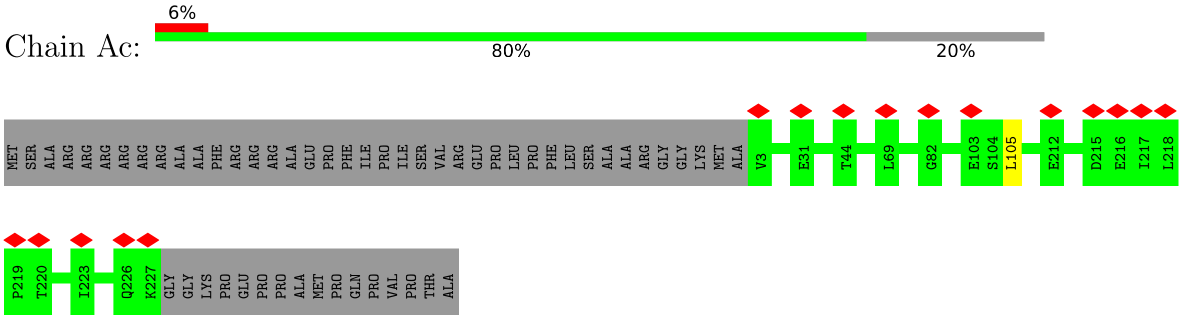


- Molecule 64: 40S ribosomal protein S2

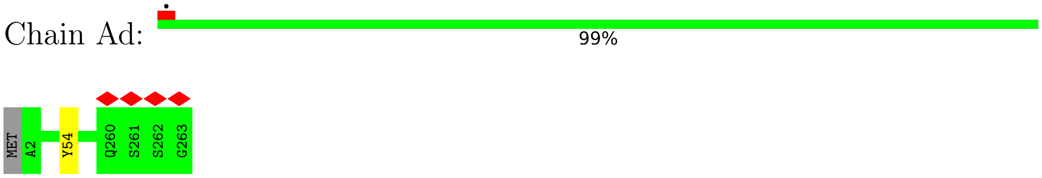
Chain Ab:



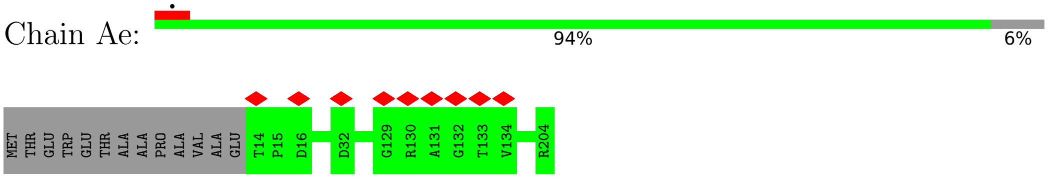
- Molecule 65: 40S ribosomal protein S3



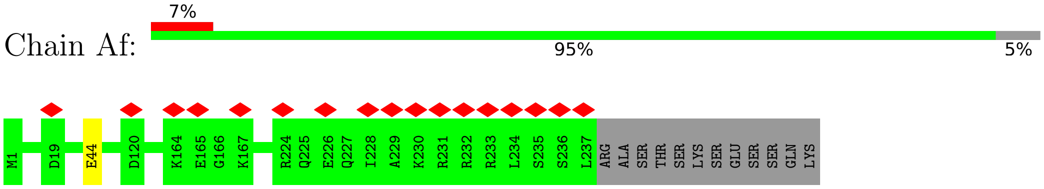
- Molecule 66: 40S ribosomal protein S4



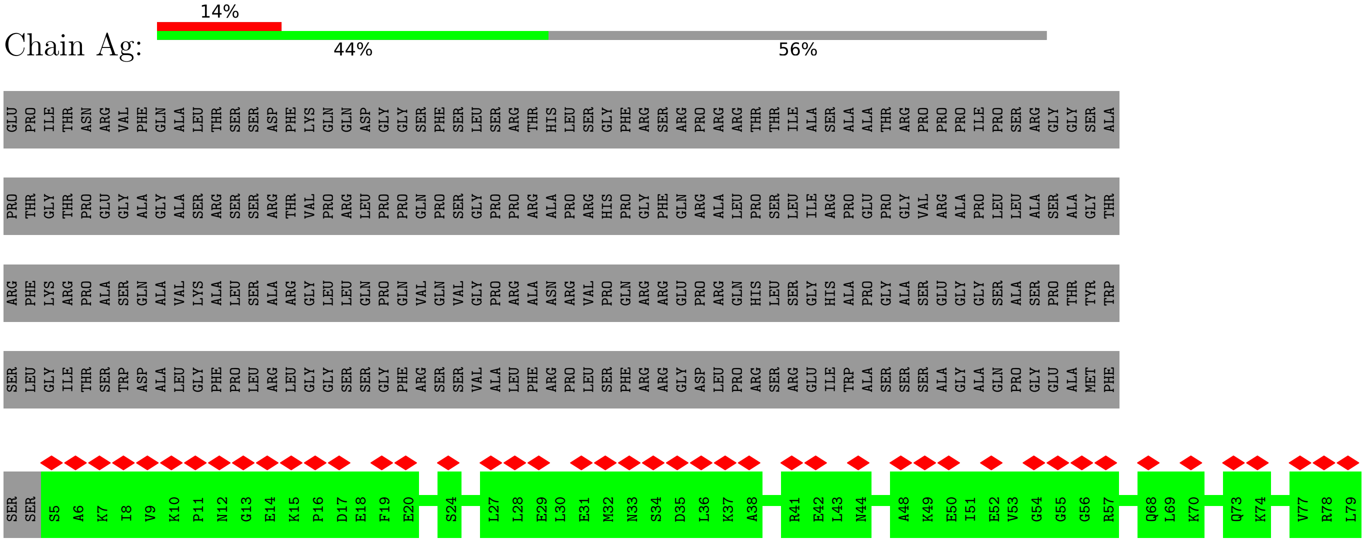
- Molecule 67: Ribosomal protein S5

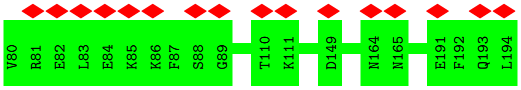


- Molecule 68: 40S ribosomal protein S6

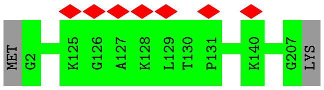


- Molecule 69: 40S ribosomal protein S7

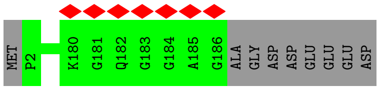




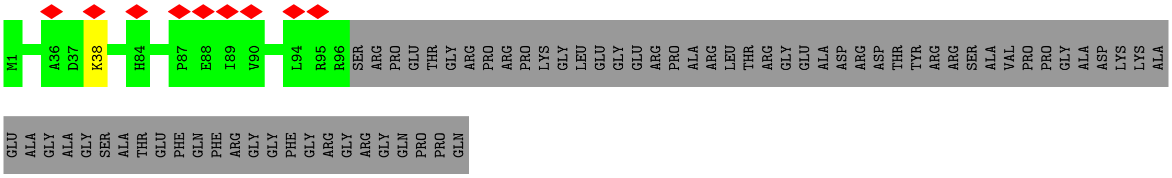
- Molecule 70: 40S ribosomal protein S8



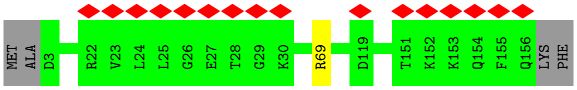
- Molecule 71: 40S ribosomal protein S9



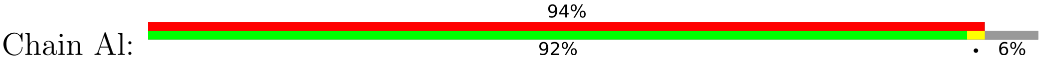
- Molecule 72: S10_plectin domain-containing protein

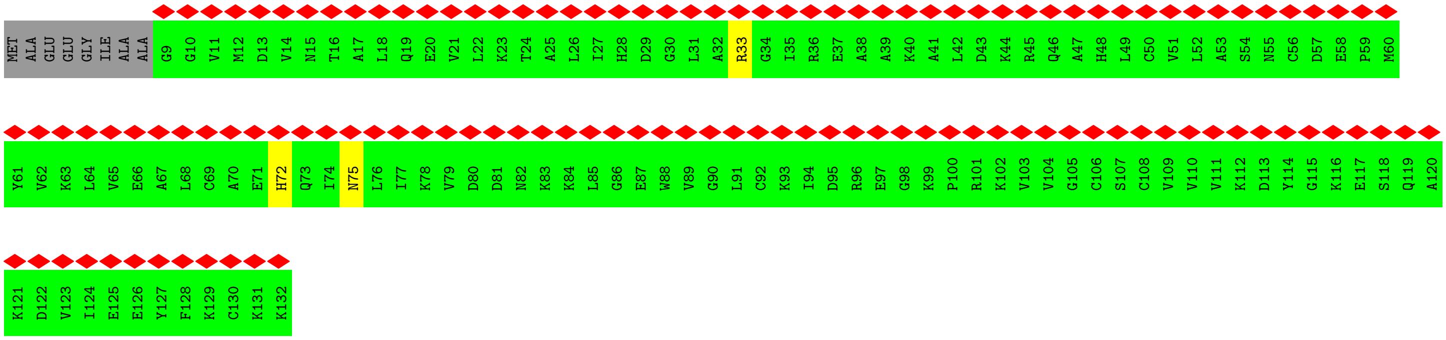


- Molecule 73: 40S ribosomal protein S11



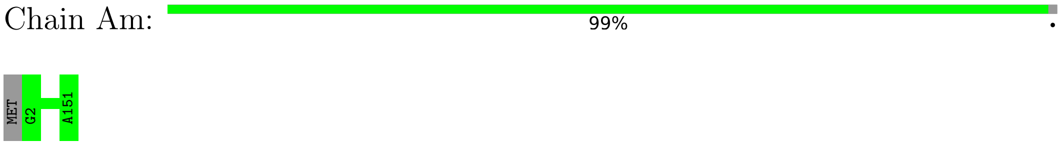
- Molecule 74: 40S ribosomal protein S12





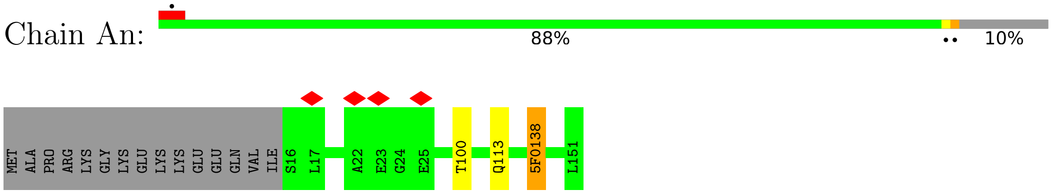
- Molecule 75: 40S ribosomal protein S13

Chain Am:



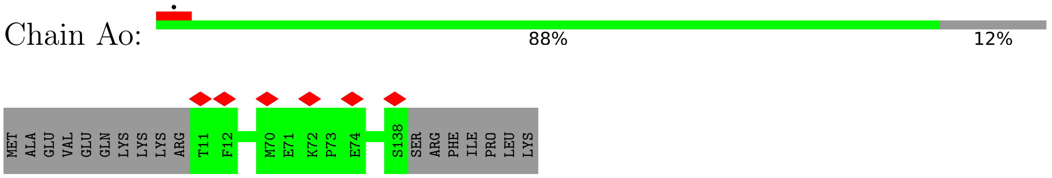
- Molecule 76: 40S ribosomal protein S14

Chain An:



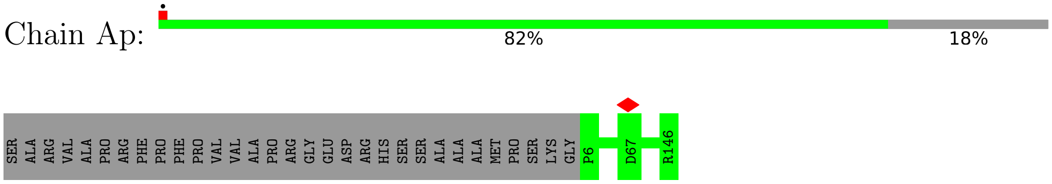
- Molecule 77: 40S ribosomal protein uS19

Chain Ao:



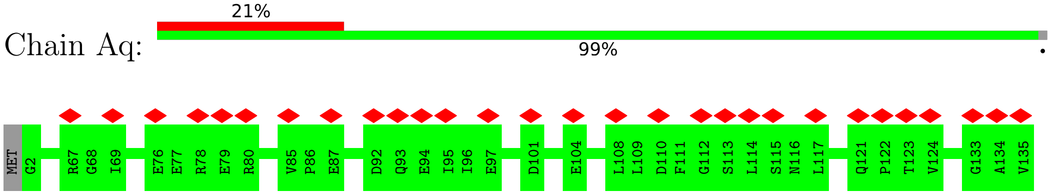
- Molecule 78: uS9

Chain Ap:



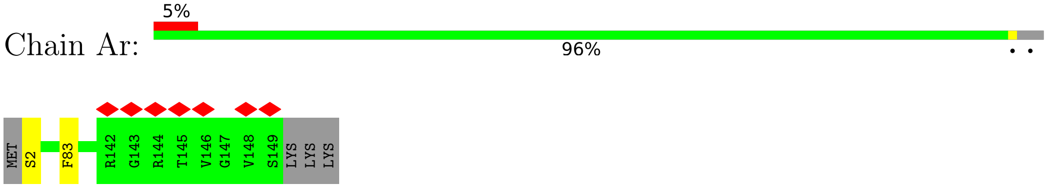
- Molecule 79: 40S ribosomal protein eS17

Chain Aq:



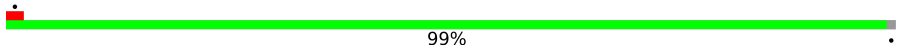
- Molecule 80: 40S ribosomal protein S18

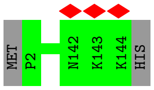
Chain Ar:



- Molecule 81: 40S ribosomal protein S19

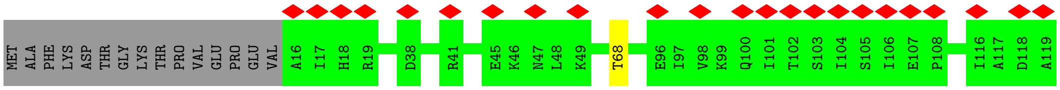
Chain As:





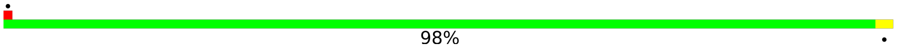
- Molecule 82: 40S ribosomal protein uS10

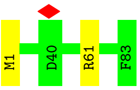
Chain At:



- Molecule 83: 40S ribosomal protein S21

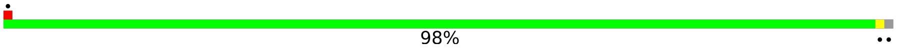
Chain Au:

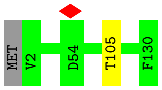




- Molecule 84: Ribosomal protein S15a

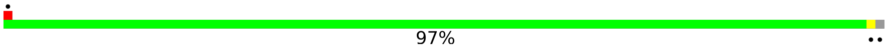
Chain Av:

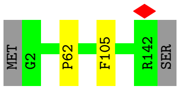




- Molecule 85: 40S ribosomal protein S23

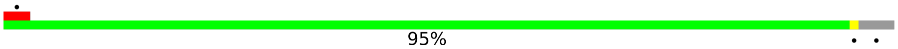
Chain Aw:

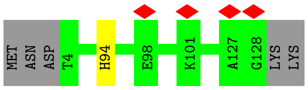




- Molecule 86: 40S ribosomal protein S24

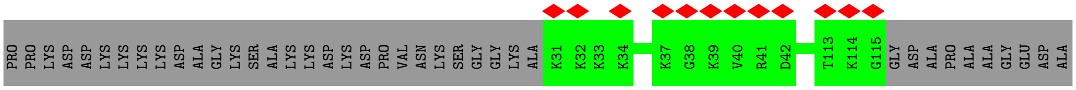
Chain Ax:





- Molecule 87: 40S ribosomal protein S25

Chain Ay:



- Molecule 88: 60S ribosomal protein L41

Chain Az: 

There are no outlier residues recorded for this chain.

4 Experimental information ⓘ

Property	**Value**	**Source**
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	21221	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{Å}^2)$	60	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	5.350	Depositor
Minimum map value	-1.922	Depositor
Average map value	0.010	Depositor
Map value standard deviation	0.221	Depositor
Recommended contour level	0.75	Depositor
Map size (Å)	542.717, 542.717, 542.717	wwPDB
Map dimensions	434, 434, 434	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.2505, 1.2505, 1.2505	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, A2M, AYA, MA6, 5F0, G7M, V5N, GTP, ZN, HIC, SPD, OMG, PSU, MLZ, OMU, SAC, M3L, 4AC, UR3, 6MZ, 1MA, OMC, UY1, AAC, 5MU, HY3, AME, UNX, B8N, NMM, 5MC, SPM

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	B5	0.17	1/87403 (0.0%)	0.67	10/136359 (0.0%)
2	B7	0.16	0/2835	0.66	0/4418
3	B8	0.24	1/3635 (0.0%)	0.67	0/5661
4	BA	0.25	0/1965	0.55	0/2633
5	BB	0.24	0/3261	0.49	0/4364
6	BC	0.23	0/2932	0.50	0/3939
7	BD	0.24	0/2437	0.48	0/3264
8	BE	0.24	0/1998	0.50	0/2673
9	BF	0.24	0/1922	0.49	0/2563
10	BG	0.24	0/1908	0.47	0/2566
11	BH	0.24	0/1535	0.49	0/2063
12	BI	0.24	0/1756	0.50	0/2346
13	BJ	0.24	0/1385	0.50	0/1852
14	BK	0.26	0/242	0.49	0/324
15	BL	0.24	0/1733	0.53	0/2316
16	BM	0.24	0/1158	0.48	0/1547
17	BN	0.24	0/1746	0.54	0/2338
18	BO	0.24	0/1662	0.48	0/2222
19	BP	0.23	0/1317	0.48	0/1768
20	BQ	0.24	0/1539	0.56	0/2054
21	BR	0.22	0/1524	0.53	0/2013
22	BS	0.25	0/1497	0.52	0/2008
23	BT	0.25	0/1326	0.49	0/1770
24	BU	0.24	0/820	0.47	0/1100
25	BV	0.25	0/1048	0.51	0/1402
26	BW	0.24	0/1006	0.49	0/1334
27	BX	0.24	0/984	0.49	0/1323
28	BY	0.23	0/1132	0.51	0/1504
29	BZ	0.25	0/1130	0.49	0/1507
30	Ba	0.24	0/1179	0.50	0/1572
31	Bb	0.23	0/884	0.51	0/1169

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	Bc	0.24	0/847	0.43	0/1134
33	Bd	0.24	0/903	0.51	0/1216
34	Be	0.23	0/1088	0.51	0/1451
35	Bf	0.25	0/903	0.53	0/1208
36	Bg	0.23	0/916	0.54	0/1220
37	Bh	0.23	0/1021	0.48	0/1348
38	Bi	0.23	0/841	0.51	0/1112
39	Bj	0.24	0/720	0.57	0/952
40	Bk	0.24	0/575	0.45	0/761
41	Bl	0.22	0/459	0.51	0/608
42	Bm	0.23	0/426	0.50	0/564
43	Bo	0.25	0/866	0.51	0/1141
44	Bp	0.23	0/718	0.49	0/953
45	Br	0.23	0/1020	0.53	0/1366
46	Bs	0.24	0/1530	0.45	0/2064
47	Bt	0.23	0/1193	0.47	0/1609
48	Bv	0.23	0/1735	0.45	0/2328
49	MA	0.23	0/2549	0.47	0/3462
50	Na	0.24	0/536	0.49	0/715
51	Nb	0.25	0/829	0.47	0/1112
52	A2	0.16	1/40342 (0.0%)	0.68	14/62877 (0.0%)
53	AA	0.23	0/665	0.46	0/891
54	AB	0.23	0/497	0.56	0/666
55	AC	0.24	0/622	0.48	0/822
56	AD	0.24	0/462	0.53	0/607
57	AE	0.23	0/828	0.53	0/1109
58	AF	0.23	0/2493	0.46	0/3394
59	AG	0.24	0/470	0.50	0/623
60	AI	0.16	0/68	0.65	0/103
61	AT	0.28	1/1766 (0.1%)	0.65	0/2749
62	AZ	0.23	0/1771	0.46	0/2406
63	Aa	0.23	0/1841	0.46	0/2459
64	Ab	0.24	0/1742	0.45	0/2354
65	Ac	0.24	0/1779	0.49	0/2395
66	Ad	0.24	0/2118	0.50	0/2849
67	Ae	0.23	0/1531	0.48	0/2059
68	Af	0.24	0/1946	0.52	0/2590
69	Ag	0.24	0/1552	0.46	0/2079
70	Ah	0.24	0/1715	0.51	0/2287
71	Ai	0.23	0/1550	0.52	0/2069
72	Aj	0.23	0/834	0.42	0/1125
73	Ak	0.25	0/1284	0.51	0/1717
74	Al	0.23	0/968	0.41	0/1296

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
75	Am	0.23	0/1232	0.47	0/1656
76	An	0.24	0/1020	0.53	0/1366
77	Ao	0.25	0/1069	0.47	0/1429
78	Ap	0.23	0/1142	0.50	0/1528
79	Aq	0.23	0/1094	0.48	0/1469
80	Ar	0.24	0/1226	0.53	0/1643
81	As	0.23	0/1119	0.45	0/1498
82	At	0.23	0/831	0.51	0/1115
83	Au	0.24	0/636	0.48	0/852
84	Av	0.24	0/1051	0.48	0/1406
85	Aw	0.24	0/1107	0.50	0/1475
86	Ax	0.24	0/1032	0.51	0/1371
87	Ay	0.23	0/691	0.46	0/922
88	Az	0.22	0/240	0.65	0/305
All	All	0.20	4/238908 (0.0%)	0.61	24/349857 (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
43	Bo	0	1
76	An	0	1
All	All	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B8	1	C	OP3-P	-10.67	1.48	1.61
52	A2	1	U	OP3-P	-10.65	1.48	1.61
1	B5	1	C	OP3-P	-10.53	1.48	1.61
61	AT	1	G	OP3-P	-10.50	1.48	1.61

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
52	A2	1454	C	C2-N1-C1’	8.98	128.68	118.80
52	A2	1454	C	N1-C2-O2	8.85	124.21	118.90
1	B5	2312	C	N1-C2-O2	8.26	123.86	118.90
1	B5	2312	C	C2-N1-C1’	8.23	127.85	118.80
52	A2	631	U	C2-N1-C1’	7.79	127.05	117.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
76	An	138	5F0	Peptide
43	Bo	53	MLZ	Mainchain

5.2 Too-close contacts ⓘ

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

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	BA	250/257 (97%)	242 (97%)	8 (3%)	0	100	100
5	BB	395/403 (98%)	390 (99%)	5 (1%)	0	100	100
6	BC	360/413 (87%)	356 (99%)	4 (1%)	0	100	100
7	BD	291/297 (98%)	286 (98%)	5 (2%)	0	100	100
8	BE	239/291 (82%)	235 (98%)	4 (2%)	0	100	100
9	BF	224/247 (91%)	219 (98%)	4 (2%)	1 (0%)	34	66
10	BG	229/266 (86%)	227 (99%)	2 (1%)	0	100	100
11	BH	188/192 (98%)	188 (100%)	0	0	100	100
12	BI	211/214 (99%)	209 (99%)	2 (1%)	0	100	100
13	BJ	168/178 (94%)	167 (99%)	1 (1%)	0	100	100
14	BK	27/65 (42%)	25 (93%)	2 (7%)	0	100	100
15	BL	208/211 (99%)	205 (99%)	3 (1%)	0	100	100
16	BM	136/218 (62%)	134 (98%)	2 (2%)	0	100	100
17	BN	201/204 (98%)	198 (98%)	3 (2%)	0	100	100
18	BO	197/203 (97%)	197 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	BP	157/184 (85%)	155 (99%)	2 (1%)	0	100	100
20	BQ	185/188 (98%)	182 (98%)	3 (2%)	0	100	100
21	BR	178/196 (91%)	178 (100%)	0	0	100	100
22	BS	174/176 (99%)	173 (99%)	1 (1%)	0	100	100
23	BT	157/160 (98%)	155 (99%)	2 (1%)	0	100	100
24	BU	97/128 (76%)	96 (99%)	1 (1%)	0	100	100
25	BV	137/140 (98%)	134 (98%)	3 (2%)	0	100	100
26	BW	119/157 (76%)	118 (99%)	1 (1%)	0	100	100
27	BX	116/156 (74%)	115 (99%)	1 (1%)	0	100	100
28	BY	132/145 (91%)	131 (99%)	1 (1%)	0	100	100
29	BZ	133/136 (98%)	131 (98%)	2 (2%)	0	100	100
30	Ba	144/148 (97%)	137 (95%)	6 (4%)	1 (1%)	22	54
31	Bb	103/245 (42%)	100 (97%)	3 (3%)	0	100	100
32	Bc	106/115 (92%)	106 (100%)	0	0	100	100
33	Bd	105/125 (84%)	105 (100%)	0	0	100	100
34	Be	128/135 (95%)	126 (98%)	2 (2%)	0	100	100
35	Bf	108/110 (98%)	108 (100%)	0	0	100	100
36	Bg	112/117 (96%)	111 (99%)	1 (1%)	0	100	100
37	Bh	120/123 (98%)	119 (99%)	1 (1%)	0	100	100
38	Bi	100/105 (95%)	98 (98%)	2 (2%)	0	100	100
39	Bj	84/97 (87%)	84 (100%)	0	0	100	100
40	Bk	67/70 (96%)	67 (100%)	0	0	100	100
41	Bl	48/51 (94%)	48 (100%)	0	0	100	100
42	Bm	49/128 (38%)	49 (100%)	0	0	100	100
43	Bo	102/106 (96%)	102 (100%)	0	0	100	100
44	Bp	89/92 (97%)	89 (100%)	0	0	100	100
45	Br	124/137 (90%)	123 (99%)	1 (1%)	0	100	100
46	Bs	194/318 (61%)	190 (98%)	4 (2%)	0	100	100
47	Bt	154/165 (93%)	152 (99%)	2 (1%)	0	100	100
48	Bv	210/217 (97%)	202 (96%)	8 (4%)	0	100	100
49	MA	313/386 (81%)	309 (99%)	4 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
50	Na	65/215 (30%)	63 (97%)	2 (3%)	0	100	100
51	Nb	104/132 (79%)	100 (96%)	4 (4%)	0	100	100
53	AA	81/84 (96%)	81 (100%)	0	0	100	100
54	AB	61/69 (88%)	61 (100%)	0	0	100	100
55	AC	72/156 (46%)	71 (99%)	1 (1%)	0	100	100
56	AD	55/133 (41%)	54 (98%)	1 (2%)	0	100	100
57	AE	99/115 (86%)	98 (99%)	1 (1%)	0	100	100
58	AF	311/317 (98%)	305 (98%)	6 (2%)	0	100	100
59	AG	53/56 (95%)	53 (100%)	0	0	100	100
62	AZ	219/295 (74%)	218 (100%)	1 (0%)	0	100	100
63	Aa	220/264 (83%)	217 (99%)	3 (1%)	0	100	100
64	Ab	218/293 (74%)	218 (100%)	0	0	100	100
65	Ac	223/281 (79%)	222 (100%)	1 (0%)	0	100	100
66	Ad	260/263 (99%)	257 (99%)	3 (1%)	0	100	100
67	Ae	189/204 (93%)	188 (100%)	1 (0%)	0	100	100
68	Af	235/249 (94%)	235 (100%)	0	0	100	100
69	Ag	188/432 (44%)	186 (99%)	2 (1%)	0	100	100
70	Ah	204/208 (98%)	202 (99%)	2 (1%)	0	100	100
71	Ai	183/194 (94%)	180 (98%)	3 (2%)	0	100	100
72	Aj	94/165 (57%)	93 (99%)	1 (1%)	0	100	100
73	Ak	152/158 (96%)	150 (99%)	2 (1%)	0	100	100
74	Al	122/132 (92%)	121 (99%)	1 (1%)	0	100	100
75	Am	148/151 (98%)	147 (99%)	1 (1%)	0	100	100
76	An	133/151 (88%)	129 (97%)	4 (3%)	0	100	100
77	Ao	126/145 (87%)	124 (98%)	2 (2%)	0	100	100
78	Ap	139/172 (81%)	134 (96%)	5 (4%)	0	100	100
79	Aq	132/135 (98%)	132 (100%)	0	0	100	100
80	Ar	146/152 (96%)	144 (99%)	2 (1%)	0	100	100
81	As	140/145 (97%)	140 (100%)	0	0	100	100
82	At	102/119 (86%)	99 (97%)	3 (3%)	0	100	100
83	Au	81/83 (98%)	79 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
84	Av	127/130 (98%)	127 (100%)	0	0	100	100
85	Aw	138/143 (96%)	136 (99%)	2 (1%)	0	100	100
86	Ax	123/130 (95%)	122 (99%)	1 (1%)	0	100	100
87	Ay	83/124 (67%)	82 (99%)	1 (1%)	0	100	100
88	Az	23/25 (92%)	23 (100%)	0	0	100	100
All	All	12418/14635 (85%)	12262 (99%)	154 (1%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	BF	196	VAL
30	Ba	15	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	BA	194/198 (98%)	194 (100%)	0	100	100
5	BB	344/347 (99%)	342 (99%)	2 (1%)	86	96
6	BC	302/337 (90%)	301 (100%)	1 (0%)	92	98
7	BD	247/250 (99%)	247 (100%)	0	100	100
8	BE	216/251 (86%)	216 (100%)	0	100	100
9	BF	197/215 (92%)	197 (100%)	0	100	100
10	BG	199/223 (89%)	196 (98%)	3 (2%)	65	87
11	BH	169/171 (99%)	169 (100%)	0	100	100
12	BI	180/181 (99%)	180 (100%)	0	100	100
13	BJ	143/149 (96%)	143 (100%)	0	100	100
14	BK	28/61 (46%)	26 (93%)	2 (7%)	14	40
15	BL	175/176 (99%)	174 (99%)	1 (1%)	86	96
16	BM	117/161 (73%)	117 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	BN	171/172 (99%)	171 (100%)	0	100	100
18	BO	171/173 (99%)	169 (99%)	2 (1%)	71	91
19	BP	140/163 (86%)	139 (99%)	1 (1%)	84	95
20	BQ	164/165 (99%)	162 (99%)	2 (1%)	71	91
21	BR	159/175 (91%)	159 (100%)	0	100	100
22	BS	154/154 (100%)	154 (100%)	0	100	100
23	BT	139/140 (99%)	139 (100%)	0	100	100
24	BU	88/113 (78%)	87 (99%)	1 (1%)	73	92
25	BV	106/107 (99%)	106 (100%)	0	100	100
26	BW	100/126 (79%)	100 (100%)	0	100	100
27	BX	106/134 (79%)	106 (100%)	0	100	100
28	BY	124/135 (92%)	123 (99%)	1 (1%)	81	94
29	BZ	117/118 (99%)	117 (100%)	0	100	100
30	Ba	118/119 (99%)	118 (100%)	0	100	100
31	Bb	87/183 (48%)	87 (100%)	0	100	100
32	Bc	92/98 (94%)	92 (100%)	0	100	100
33	Bd	98/110 (89%)	98 (100%)	0	100	100
34	Be	116/121 (96%)	116 (100%)	0	100	100
35	Bf	89/89 (100%)	89 (100%)	0	100	100
36	Bg	98/100 (98%)	96 (98%)	2 (2%)	55	82
37	Bh	109/110 (99%)	109 (100%)	0	100	100
38	Bi	86/89 (97%)	85 (99%)	1 (1%)	71	91
39	Bj	73/80 (91%)	73 (100%)	0	100	100
40	Bk	64/65 (98%)	64 (100%)	0	100	100
41	Bl	47/48 (98%)	46 (98%)	1 (2%)	53	81
42	Bm	47/115 (41%)	47 (100%)	0	100	100
43	Bo	92/93 (99%)	92 (100%)	0	100	100
44	Bp	74/75 (99%)	74 (100%)	0	100	100
45	Br	109/120 (91%)	109 (100%)	0	100	100
46	Bs	164/258 (64%)	163 (99%)	1 (1%)	86	96
47	Bt	128/137 (93%)	126 (98%)	2 (2%)	62	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
48	Bv	191/195 (98%)	187 (98%)	4 (2%)	53	81
49	MA	270/330 (82%)	266 (98%)	4 (2%)	65	87
50	Na	60/183 (33%)	58 (97%)	2 (3%)	38	72
51	Nb	90/111 (81%)	87 (97%)	3 (3%)	38	72
53	AA	75/76 (99%)	74 (99%)	1 (1%)	69	90
54	AB	56/62 (90%)	56 (100%)	0	100	100
55	AC	67/140 (48%)	67 (100%)	0	100	100
56	AD	47/106 (44%)	46 (98%)	1 (2%)	53	81
57	AE	88/98 (90%)	87 (99%)	1 (1%)	73	92
58	AF	272/275 (99%)	270 (99%)	2 (1%)	84	95
59	AG	48/49 (98%)	48 (100%)	0	100	100
62	AZ	182/243 (75%)	180 (99%)	2 (1%)	73	92
63	Aa	203/231 (88%)	200 (98%)	3 (2%)	65	87
64	Ab	185/223 (83%)	183 (99%)	2 (1%)	73	92
65	Ac	189/232 (82%)	188 (100%)	1 (0%)	88	96
66	Ad	224/225 (100%)	223 (100%)	1 (0%)	91	97
67	Ae	161/170 (95%)	161 (100%)	0	100	100
68	Af	207/218 (95%)	206 (100%)	1 (0%)	88	96
69	Ag	170/360 (47%)	170 (100%)	0	100	100
70	Ah	178/180 (99%)	178 (100%)	0	100	100
71	Ai	161/168 (96%)	161 (100%)	0	100	100
72	Aj	87/136 (64%)	86 (99%)	1 (1%)	73	92
73	Ak	139/142 (98%)	138 (99%)	1 (1%)	84	95
74	Al	104/108 (96%)	101 (97%)	3 (3%)	42	76
75	Am	130/131 (99%)	130 (100%)	0	100	100
76	An	105/118 (89%)	103 (98%)	2 (2%)	57	84
77	Ao	114/130 (88%)	114 (100%)	0	100	100
78	Ap	117/140 (84%)	117 (100%)	0	100	100
79	Aq	120/121 (99%)	120 (100%)	0	100	100
80	Ar	127/131 (97%)	126 (99%)	1 (1%)	81	94
81	As	112/114 (98%)	112 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
82	At	94/107 (88%)	93 (99%)	1 (1%)	73	92
83	Au	67/67 (100%)	66 (98%)	1 (2%)	65	87
84	Av	112/113 (99%)	111 (99%)	1 (1%)	78	93
85	Aw	112/114 (98%)	111 (99%)	1 (1%)	78	93
86	Ax	107/112 (96%)	106 (99%)	1 (1%)	78	93
87	Ay	75/102 (74%)	75 (100%)	0	100	100
88	Az	24/24 (100%)	24 (100%)	0	100	100
All	All	10811/12390 (87%)	10747 (99%)	64 (1%)	86	96

5 of 64 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
76	An	113	GLN
82	At	68	THR
48	Bv	60	ARG
48	Bv	58	THR
83	Au	61	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 95 such sidechains are listed below:

Mol	Chain	Res	Type
47	Bt	70	GLN
58	AF	159	ASN
48	Bv	188	ASN
51	Nb	7	ASN
66	Ad	98	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	B5	3750/4808 (77%)	422 (11%)	2 (0%)
2	B7	118/120 (98%)	6 (5%)	0
3	B8	155/158 (98%)	14 (9%)	0
52	A2	1758/1870 (94%)	204 (11%)	0
60	AI	2/76 (2%)	1 (50%)	0
61	AT	75/76 (98%)	10 (13%)	0
All	All	5858/7108 (82%)	657 (11%)	2 (0%)

5 of 657 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	B5	39	A
1	B5	42	A
1	B5	58	G
1	B5	59	A
1	B5	64	A

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	B5	1588	G
1	B5	4445	U

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

225 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	A2M	B5	1489	92,1	18,25,26	1.00	1 (5%)	18,36,39	1.36	2 (11%)
52	OMU	A2	1805	52	19,22,23	1.22	3 (15%)	26,31,34	1.69	4 (15%)
1	PSU	B5	4169	1	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
1	A2M	B5	3557	1	18,25,26	1.03	1 (5%)	18,36,39	1.22	2 (11%)
1	OMU	B5	3973	1	19,22,23	1.23	3 (15%)	26,31,34	1.70	4 (15%)
1	PSU	B5	4246	1	18,21,22	1.33	2 (11%)	22,30,33	1.91	3 (13%)
1	PSU	B5	4749	1	18,21,22	1.34	2 (11%)	22,30,33	1.89	3 (13%)
52	PSU	A2	1239	52	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
52	PSU	A2	210	52	18,21,22	1.34	2 (11%)	22,30,33	1.85	3 (13%)
52	PSU	A2	1047	52	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
1	PSU	B5	3583	1	18,21,22	1.35	2 (11%)	22,30,33	1.85	3 (13%)
1	OMG	B5	2267	1	18,26,27	0.92	1 (5%)	19,38,41	1.07	2 (10%)
52	PSU	A2	687	52	18,21,22	1.34	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
3	PSU	B8	55	3	18,21,22	1.35	2 (11%)	22,30,33	1.89	3 (13%)
1	PSU	B5	3652	92,1	18,21,22	1.36	2 (11%)	22,30,33	1.87	3 (13%)
1	5MC	B5	3514	92,1	18,22,23	0.95	2 (11%)	26,32,35	1.13	3 (11%)
52	PSU	A2	867	52	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
1	PSU	B5	4435	1	18,21,22	1.35	2 (11%)	22,30,33	1.89	3 (13%)
52	PSU	A2	816	52	18,21,22	1.34	2 (11%)	22,30,33	1.89	3 (13%)
1	PSU	B5	4058	1	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
1	6MZ	B5	3966	1	18,25,26	0.89	1 (5%)	16,36,39	2.03	4 (25%)
85	HY3	Aw	62	85	6,8,9	2.01	1 (16%)	5,10,12	1.14	1 (20%)
1	A2M	B5	3456	1	18,25,26	1.04	1 (5%)	18,36,39	1.21	2 (11%)
52	PSU	A2	109	52	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
1	PSU	B5	4166	1	18,21,22	1.37	2 (11%)	22,30,33	1.85	3 (13%)
52	A2M	A2	591	52	18,25,26	1.04	1 (5%)	18,36,39	1.24	2 (11%)
52	OMG	A2	1448	52	18,26,27	0.93	1 (5%)	19,38,41	1.07	2 (10%)
52	OMU	A2	355	52	19,22,23	1.22	2 (10%)	26,31,34	1.71	4 (15%)
1	PSU	B5	1721	1	18,21,22	1.34	2 (11%)	22,30,33	1.89	3 (13%)
1	OMG	B5	4116	1	18,26,27	0.92	1 (5%)	19,38,41	1.07	2 (10%)
1	A2M	B5	2658	92,1	18,25,26	1.02	1 (5%)	18,36,39	1.21	2 (11%)
52	A2M	A2	485	52	18,25,26	1.01	1 (5%)	18,36,39	1.26	2 (11%)
61	PSU	AT	55	61	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
1	PSU	B5	4203	1	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
1	OMG	B5	1580	1	18,26,27	0.93	1 (5%)	19,38,41	1.10	2 (10%)
1	PSU	B5	3502	1	18,21,22	1.34	2 (11%)	22,30,33	1.89	3 (13%)
52	4AC	A2	1338	52	21,24,25	1.07	1 (4%)	29,34,37	1.21	3 (10%)
52	PSU	A2	1245	52	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
1	PSU	B5	3490	1	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
1	A2M	B5	3599	1	18,25,26	0.99	1 (5%)	18,36,39	1.24	2 (11%)
1	OMG	B5	4364	1	18,26,27	0.92	1 (5%)	19,38,41	1.09	2 (10%)
52	OMU	A2	1289	52	19,22,23	1.21	3 (15%)	26,31,34	1.67	4 (15%)
1	A2M	B5	1479	1	18,25,26	1.01	1 (5%)	18,36,39	1.26	2 (11%)
1	PSU	B5	4188	1	18,21,22	1.35	2 (11%)	22,30,33	1.90	3 (13%)
1	PSU	B5	4177	1	18,21,22	1.35	2 (11%)	22,30,33	1.86	3 (13%)
1	OMG	B5	2719	1	18,26,27	0.93	1 (5%)	19,38,41	1.07	2 (10%)
52	MA6	A2	1852	52	18,26,27	1.09	2 (11%)	19,38,41	1.97	3 (15%)
1	OMG	B5	3359	1	18,26,27	0.93	1 (5%)	19,38,41	1.09	2 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
1	OMG	B5	3974	1	18,26,27	0.91	1 (5%)	19,38,41	1.12	2 (10%)
1	PSU	B5	4325	1	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)
1	OMG	B5	4383	1	18,26,27	0.94	1 (5%)	19,38,41	1.09	2 (10%)
1	A2M	B5	2206	92,1	18,25,26	1.03	1 (5%)	18,36,39	1.19	2 (11%)
1	PSU	B5	4419	1	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
1	PSU	B5	1731	1	18,21,22	1.34	2 (11%)	22,30,33	1.89	3 (13%)
1	PSU	B5	1683	1	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)
1	OMG	B5	4240	1	18,26,27	0.94	1 (5%)	19,38,41	1.08	2 (10%)
1	PSU	B5	1801	1	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
1	A2M	B5	3492	1,52	18,25,26	1.01	1 (5%)	18,36,39	1.37	2 (11%)
52	PSU	A2	1368	52	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
76	5F0	An	138	76	8,8,9	1.47	2 (25%)	7,9,11	1.74	1 (14%)
1	UY1	B5	3550	1	19,22,23	1.37	3 (15%)	22,31,34	1.90	5 (22%)
52	OMG	A2	437	52	18,26,27	0.92	1 (5%)	19,38,41	1.10	2 (10%)
52	B8N	A2	1249	52	24,29,30	1.29	3 (12%)	29,42,45	1.28	3 (10%)
52	A2M	A2	27	92,52	18,25,26	1.02	1 (5%)	18,36,39	1.19	2 (11%)
52	PSU	A2	1446	52	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
1	PSU	B5	3496	1	18,21,22	1.34	2 (11%)	22,30,33	1.90	3 (13%)
1	OMC	B5	2667	1	19,22,23	0.82	0	26,31,34	0.82	0
4	V5N	BA	216	4	4,11,12	0.78	0	5,14,16	1.54	1 (20%)
1	A2M	B5	1810	92,1	18,25,26	1.04	1 (5%)	18,36,39	1.24	2 (11%)
1	OMG	B5	4369	1	18,26,27	0.92	1 (5%)	19,38,41	1.11	2 (10%)
52	OMU	A2	121	52	19,22,23	1.21	3 (15%)	26,31,34	1.70	4 (15%)
52	PSU	A2	682	52	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
52	OMG	A2	1329	52	18,26,27	0.94	1 (5%)	19,38,41	1.07	2 (10%)
52	OMC	A2	1392	52	19,22,23	0.83	0	26,31,34	0.89	1 (3%)
52	PSU	A2	1178	52	18,21,22	1.35	2 (11%)	22,30,33	1.89	3 (13%)
1	OMG	B5	3676	1	18,26,27	0.93	1 (5%)	19,38,41	1.09	2 (10%)
52	PSU	A2	610	52	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
52	A2M	A2	1032	52	18,25,26	1.02	1 (5%)	18,36,39	1.24	2 (11%)
1	PSU	B5	4740	1	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
52	PSU	A2	1082	52	18,21,22	1.37	2 (11%)	22,30,33	1.85	3 (13%)
1	PSU	B5	3494	1	18,21,22	1.36	2 (11%)	22,30,33	1.88	3 (13%)
52	PSU	A2	407	52	18,21,22	1.34	2 (11%)	22,30,33	1.89	3 (13%)
1	PSU	B5	2351	1	18,21,22	1.34	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
80	SAC	Ar	2	80	7,8,9	0.53	0	8,9,11	0.91	1 (12%)
31	MLZ	Bb	5	31	8,9,10	0.49	0	4,9,11	0.13	0
52	PSU	A2	93	52	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
52	PSU	A2	1348	52	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
52	PSU	A2	1644	92,52	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
1	OMC	B5	4282	92,1	19,22,23	0.82	0	26,31,34	0.84	0
30	V5N	Ba	39	30	4,11,12	0.77	0	5,14,16	1.55	1 (20%)
1	OMC	B5	3601	1	19,22,23	0.81	0	26,31,34	0.85	0
52	PSU	A2	119	52	18,21,22	1.34	2 (11%)	22,30,33	1.85	3 (13%)
52	OMU	A2	429	52	19,22,23	1.20	3 (15%)	26,31,34	1.68	4 (15%)
1	OMC	B5	3573	1	19,22,23	0.82	0	26,31,34	0.88	1 (3%)
1	PSU	B5	3616	1	18,21,22	1.34	2 (11%)	22,30,33	1.90	3 (13%)
1	PSU	B5	4107	1	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
1	PSU	B5	4045	1	18,21,22	1.36	2 (11%)	22,30,33	1.87	3 (13%)
1	OMC	B5	1820	92,1	19,22,23	0.80	0	26,31,34	0.80	0
52	6MZ	A2	1833	92,52	18,25,26	0.93	1 (5%)	16,36,39	1.82	4 (25%)
1	A2M	B5	3517	1	18,25,26	0.96	1 (5%)	18,36,39	1.34	2 (11%)
1	PSU	B5	3576	1	18,21,22	1.37	2 (11%)	22,30,33	1.86	3 (13%)
3	OMG	B8	75	3	18,26,27	0.93	1 (5%)	19,38,41	1.06	2 (10%)
52	OMU	A2	116	52	19,22,23	1.20	3 (15%)	26,31,34	1.67	4 (15%)
52	PSU	A2	650	52	18,21,22	1.35	2 (11%)	22,30,33	1.90	3 (13%)
52	OMG	A2	868	52	18,26,27	0.92	1 (5%)	19,38,41	1.07	2 (10%)
42	M3L	Bm	98	42	10,11,12	0.83	0	9,14,16	0.55	0
52	PSU	A2	967	52	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
1	PSU	B5	1537	1	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
83	AME	Au	1	83	9,10,11	0.48	0	9,11,13	0.86	1 (11%)
1	OMU	B5	4366	1	19,22,23	1.21	2 (10%)	26,31,34	1.73	4 (15%)
1	PSU	B5	4278	1	18,21,22	1.36	2 (11%)	22,30,33	1.84	3 (13%)
52	PSU	A2	652	52	18,21,22	1.35	2 (11%)	22,30,33	1.89	3 (13%)
1	OMC	B5	1284	1	19,22,23	0.81	0	26,31,34	0.81	0
52	G7M	A2	1640	61,52	20,26,27	2.99	7 (35%)	17,39,42	0.94	1 (5%)
1	PSU	B5	3427	1	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
1	OMG	B5	4245	1	18,26,27	0.92	1 (5%)	19,38,41	1.07	2 (10%)
1	OMU	B5	3657	1	19,22,23	1.23	2 (10%)	26,31,34	1.75	5 (19%)
62	SAC	AZ	2	62	7,8,9	0.53	0	8,9,11	0.86	1 (12%)
52	PSU	A2	864	52	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$\lvert Z\rvert > 2$	Counts	RMSZ	#$\lvert Z\rvert > 2$
1	PSU	B5	4149	1	18,21,22	1.34	2 (11%)	22,30,33	1.91	3 (13%)
52	A2M	A2	577	52	18,25,26	1.02	1 (5%)	18,36,39	1.19	2 (11%)
1	OMU	B5	2680	1	19,22,23	1.21	2 (10%)	26,31,34	1.72	5 (19%)
45	SAC	Br	2	45	7,8,9	0.52	0	8,9,11	0.85	1 (12%)
52	PSU	A2	802	52	18,21,22	1.36	2 (11%)	22,30,33	1.87	3 (13%)
1	OMC	B5	2647	1	19,22,23	0.81	0	26,31,34	0.82	0
1	A2M	B5	1270	1	18,25,26	0.98	1 (5%)	18,36,39	1.24	2 (11%)
1	OMG	B5	4138	1	18,26,27	0.92	1 (5%)	19,38,41	1.09	2 (10%)
52	PSU	A2	823	52	18,21,22	1.36	2 (11%)	22,30,33	1.87	4 (18%)
52	PSU	A2	573	52	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
81	NMM	As	67	81	9,11,12	0.59	0	6,12,14	0.44	0
1	OMG	B5	1260	1	18,26,27	0.93	1 (5%)	19,38,41	1.12	2 (10%)
1	OMC	B5	2704	1	19,22,23	0.82	0	26,31,34	0.85	1 (3%)
1	A2M	B5	398	1	18,25,26	1.01	1 (5%)	18,36,39	1.25	2 (11%)
1	OMC	B5	2194	92,1	19,22,23	0.82	0	26,31,34	0.93	1 (3%)
52	PSU	A2	1626	52	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)
1	PSU	B5	4039	1	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
1	PSU	B5	4217	1	18,21,22	1.36	2 (11%)	22,30,33	1.86	3 (13%)
1	PSU	B5	1720	1	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
1	UR3	B5	4276	1	19,22,23	0.99	0	26,32,35	1.41	1 (3%)
52	PSU	A2	1046	52	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
3	PSU	B8	69	3	18,21,22	1.35	2 (11%)	22,30,33	1.89	3 (13%)
1	OMC	B5	3433	1	19,22,23	0.79	0	26,31,34	0.75	0
1	A2M	B5	3562	1	18,25,26	1.03	1 (5%)	18,36,39	1.22	2 (11%)
1	PSU	B5	3585	92,1	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
61	5MU	AT	54	61	19,22,23	1.41	5 (26%)	28,32,35	2.04	6 (21%)
1	OMG	B5	3942	61,1	18,26,27	0.93	1 (5%)	19,38,41	1.07	2 (10%)
1	PSU	B5	1718	1	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
1	PSU	B5	3447	1	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)
1	5MC	B5	4193	1	18,22,23	0.99	2 (11%)	26,32,35	1.17	2 (7%)
52	A2M	A2	1384	52	18,25,26	1.03	1 (5%)	18,36,39	1.21	2 (11%)
1	PSU	B5	4711	1	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
52	PSU	A2	105	52	18,21,22	1.35	2 (11%)	22,30,33	1.86	3 (13%)
52	OMG	A2	510	92,52	18,26,27	0.94	1 (5%)	19,38,41	1.09	2 (10%)
52	OMG	A2	684	52	18,26,27	0.93	1 (5%)	19,38,41	1.09	2 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	PSU	B5	4267	92,1	18,21,22	1.35	2 (11%)	22,30,33	1.91	3 (13%)
1	PSU	B5	1638	1	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
1	OMU	B5	2258	1	19,22,23	1.21	2 (10%)	26,31,34	1.68	4 (15%)
1	OMU	B5	4052	1	19,22,23	1.22	2 (10%)	26,31,34	1.67	4 (15%)
1	PSU	B5	3554	1	18,21,22	1.36	2 (11%)	22,30,33	1.86	3 (13%)
1	A2M	B5	400	1	18,25,26	1.02	1 (5%)	18,36,39	1.22	2 (11%)
1	OMC	B5	4202	1	19,22,23	0.81	0	26,31,34	0.79	0
1	A2M	B5	3450	1	18,25,26	1.02	1 (5%)	18,36,39	1.19	2 (11%)
1	OMC	B5	3540	1	19,22,23	0.82	0	26,31,34	0.82	0
1	1MA	B5	1266	92,1	16,25,26	1.57	2 (12%)	18,37,40	1.05	3 (16%)
1	OMC	B5	2208	92,1	19,22,23	0.81	0	26,31,34	0.80	0
1	OMC	B5	3619	1	19,22,23	0.80	0	26,31,34	0.84	0
52	OMU	A2	1327	92,52	19,22,23	1.18	2 (10%)	26,31,34	1.70	5 (19%)
1	PSU	B5	3500	1	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
1	PSU	B5	4042	1	18,21,22	1.34	2 (11%)	22,30,33	1.91	4 (18%)
1	OMG	B5	1477	1	18,26,27	0.93	1 (5%)	19,38,41	1.08	2 (10%)
1	PSU	B5	2475	1	18,21,22	1.35	2 (11%)	22,30,33	1.89	3 (13%)
52	OMG	A2	1491	92,52	18,26,27	0.94	1 (5%)	19,38,41	1.08	2 (10%)
52	OMG	A2	602	52	18,26,27	0.93	1 (5%)	19,38,41	1.07	2 (10%)
52	A2M	A2	1679	52	18,25,26	1.02	1 (5%)	18,36,39	1.28	2 (11%)
1	OMG	B5	3631	1	18,26,27	0.92	1 (5%)	19,38,41	1.10	2 (10%)
52	PSU	A2	1057	52	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
1	OMG	B5	2207	1	18,26,27	0.92	1 (5%)	19,38,41	1.08	2 (10%)
1	OMU	B5	4244	1	19,22,23	1.21	2 (10%)	26,31,34	1.70	5 (19%)
5	HIC	BB	245	5	8,11,12	0.87	0	6,14,16	0.83	0
1	PSU	B5	1491	1	18,21,22	1.35	2 (11%)	22,30,33	1.92	3 (13%)
52	OMU	A2	628	52	19,22,23	1.17	2 (10%)	26,31,34	1.69	5 (19%)
52	A2M	A2	469	52	18,25,26	1.03	1 (5%)	18,36,39	1.22	2 (11%)
52	A2M	A2	513	52	18,25,26	1.04	1 (5%)	18,36,39	1.20	2 (11%)
52	A2M	A2	669	92,52	18,25,26	0.98	1 (5%)	18,36,39	1.33	2 (11%)
52	PSU	A2	1175	52	18,21,22	1.34	2 (11%)	22,30,33	1.89	3 (13%)
1	PSU	B5	3462	1	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
1	OMG	B5	3524	1	18,26,27	0.92	1 (5%)	19,38,41	1.06	2 (10%)
1	OMC	B5	2265	92,1	19,22,23	0.82	0	26,31,34	0.86	1 (3%)
1	PSU	B5	4298	1	18,21,22	1.35	2 (11%)	22,30,33	1.90	3 (13%)
52	4AC	A2	1843	52	21,24,25	1.12	2 (9%)	29,34,37	1.32	3 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	PSU	B5	1632	1	18,21,22	1.35	2 (11%)	22,30,33	1.87	4 (18%)
1	PSU	B5	4382	1	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
52	OMC	A2	463	52	19,22,23	0.82	0	26,31,34	0.86	1 (3%)
1	PSU	B5	4374	1	18,21,22	1.36	2 (11%)	22,30,33	1.89	3 (13%)
52	PSU	A2	1233	52	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
52	OMG	A2	645	52	18,26,27	0.93	1 (5%)	19,38,41	1.10	2 (10%)
52	PSU	A2	1693	52	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
52	OMC	A2	1704	52	19,22,23	0.82	0	26,31,34	0.86	1 (3%)
1	OMG	B5	3476	1	18,26,27	0.93	1 (5%)	19,38,41	1.08	2 (10%)
6	AYA	BC	2	6	6,7,8	0.72	0	5,8,10	0.30	0
52	MA6	A2	1851	52	18,26,27	1.09	2 (11%)	19,38,41	2.00	3 (15%)
52	PSU	A2	815	52	18,21,22	1.35	2 (11%)	22,30,33	1.86	3 (13%)
1	A2M	B5	4336	1	18,25,26	1.02	1 (5%)	18,36,39	1.22	2 (11%)
1	A2M	B5	4269	92,1	18,25,26	1.03	1 (5%)	18,36,39	1.23	2 (11%)
52	OMU	A2	172	52	19,22,23	1.19	2 (10%)	26,31,34	1.70	4 (15%)
52	PSU	A2	34	52	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
52	PSU	A2	36	52	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)
1	PSU	B5	4322	1	18,21,22	1.35	2 (11%)	22,30,33	1.89	3 (13%)
52	A2M	A2	99	92,52	18,25,26	1.03	1 (5%)	18,36,39	1.21	2 (11%)
1	A2M	B5	2630	92,1	18,25,26	0.99	1 (5%)	18,36,39	1.32	2 (11%)
1	PSU	B5	1799	1	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
1	PSU	B5	3369	1	18,21,22	1.35	2 (11%)	22,30,33	1.90	4 (18%)
52	PSU	A2	1005	52	18,21,22	1.34	2 (11%)	22,30,33	1.86	3 (13%)
1	A2M	B5	4317	1	18,25,26	1.02	1 (5%)	18,36,39	1.23	2 (11%)
1	PSU	B5	3371	1	18,21,22	1.36	2 (11%)	22,30,33	1.86	3 (13%)
52	OMC	A2	174	92,52	19,22,23	0.82	0	26,31,34	0.81	0
52	OMC	A2	518	52	19,22,23	0.81	0	26,31,34	0.81	0
52	A2M	A2	159	52	18,25,26	1.01	1 (5%)	18,36,39	1.26	2 (11%)
1	A2M	B5	2244	92,1	18,25,26	1.01	1 (5%)	18,36,39	1.22	2 (11%)
1	PSU	B5	3466	1	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)
52	PSU	A2	218	52	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)
43	MLZ	Bo	53	43	8,9,10	0.48	0	4,9,11	0.09	0
1	PSU	B5	4099	1	18,21,22	1.35	2 (11%)	22,30,33	1.89	3 (13%)
52	A2M	A2	166	52	18,25,26	1.04	1 (5%)	18,36,39	1.24	2 (11%)
52	OMU	A2	1443	92,52	19,22,23	1.24	3 (15%)	26,31,34	1.69	5 (19%)

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	A2M	B5	1489	92,1	-	2/5/27/28	0/3/3/3
52	OMU	A2	1805	52	-	0/9/27/28	0/2/2/2
1	PSU	B5	4169	1	-	0/7/25/26	0/2/2/2
1	A2M	B5	3557	1	-	0/5/27/28	0/3/3/3
1	OMU	B5	3973	1	-	0/9/27/28	0/2/2/2
1	PSU	B5	4246	1	-	1/7/25/26	0/2/2/2
1	PSU	B5	4749	1	-	0/7/25/26	0/2/2/2
52	PSU	A2	1239	52	-	0/7/25/26	0/2/2/2
52	PSU	A2	210	52	-	0/7/25/26	0/2/2/2
52	PSU	A2	1047	52	-	0/7/25/26	0/2/2/2
1	PSU	B5	3583	1	-	0/7/25/26	0/2/2/2
1	OMG	B5	2267	1	-	0/5/27/28	0/3/3/3
52	PSU	A2	687	52	-	0/7/25/26	0/2/2/2
3	PSU	B8	55	3	-	0/7/25/26	0/2/2/2
1	PSU	B5	3652	92,1	-	0/7/25/26	0/2/2/2
1	5MC	B5	3514	92,1	-	0/7/25/26	0/2/2/2
52	PSU	A2	867	52	-	0/7/25/26	0/2/2/2
1	PSU	B5	4435	1	-	0/7/25/26	0/2/2/2
52	PSU	A2	816	52	-	0/7/25/26	0/2/2/2
1	PSU	B5	4058	1	-	0/7/25/26	0/2/2/2
1	6MZ	B5	3966	1	-	0/5/27/28	0/3/3/3
85	HY3	Aw	62	85	-	1/1/12/14	0/1/1/1
1	A2M	B5	3456	1	-	0/5/27/28	0/3/3/3
52	PSU	A2	109	52	-	0/7/25/26	0/2/2/2
1	PSU	B5	4166	1	-	0/7/25/26	0/2/2/2
52	A2M	A2	591	52	-	0/5/27/28	0/3/3/3
52	OMG	A2	1448	52	-	3/5/27/28	0/3/3/3
52	OMU	A2	355	52	-	1/9/27/28	0/2/2/2
1	PSU	B5	1721	1	-	0/7/25/26	0/2/2/2
1	OMG	B5	4116	1	-	0/5/27/28	0/3/3/3
1	A2M	B5	2658	92,1	-	0/5/27/28	0/3/3/3
52	A2M	A2	485	52	-	0/5/27/28	0/3/3/3
61	PSU	AT	55	61	-	0/7/25/26	0/2/2/2
1	PSU	B5	4203	1	-	0/7/25/26	0/2/2/2
1	OMG	B5	1580	1	-	0/5/27/28	0/3/3/3
1	PSU	B5	3502	1	-	0/7/25/26	0/2/2/2
52	4AC	A2	1338	52	-	4/11/29/30	0/2/2/2
52	PSU	A2	1245	52	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	B5	3490	1	-	0/7/25/26	0/2/2/2
1	A2M	B5	3599	1	-	1/5/27/28	0/3/3/3
1	OMG	B5	4364	1	-	0/5/27/28	0/3/3/3
52	OMU	A2	1289	52	-	0/9/27/28	0/2/2/2
1	A2M	B5	1479	1	-	0/5/27/28	0/3/3/3
1	PSU	B5	4188	1	-	0/7/25/26	0/2/2/2
1	PSU	B5	4177	1	-	0/7/25/26	0/2/2/2
1	OMG	B5	2719	1	-	0/5/27/28	0/3/3/3
52	MA6	A2	1852	52	-	2/7/29/30	0/3/3/3
1	OMG	B5	3359	1	-	0/5/27/28	0/3/3/3
1	OMG	B5	3974	1	-	0/5/27/28	0/3/3/3
1	PSU	B5	4325	1	-	0/7/25/26	0/2/2/2
1	OMG	B5	4383	1	-	1/5/27/28	0/3/3/3
1	A2M	B5	2206	92,1	-	0/5/27/28	0/3/3/3
1	PSU	B5	4419	1	-	0/7/25/26	0/2/2/2
1	PSU	B5	1731	1	-	0/7/25/26	0/2/2/2
1	PSU	B5	1683	1	-	0/7/25/26	0/2/2/2
1	OMG	B5	4240	1	-	0/5/27/28	0/3/3/3
1	PSU	B5	1801	1	-	0/7/25/26	0/2/2/2
1	A2M	B5	3492	1,52	-	1/5/27/28	0/3/3/3
52	PSU	A2	1368	52	-	0/7/25/26	0/2/2/2
76	5F0	An	138	76	-	1/9/9/10	-
1	UY1	B5	3550	1	-	1/9/27/28	0/2/2/2
52	OMG	A2	437	52	-	0/5/27/28	0/3/3/3
52	B8N	A2	1249	52	-	4/16/34/35	0/2/2/2
52	A2M	A2	27	92,52	-	1/5/27/28	0/3/3/3
52	PSU	A2	1446	52	-	0/7/25/26	0/2/2/2
1	PSU	B5	3496	1	-	0/7/25/26	0/2/2/2
1	OMC	B5	2667	1	-	1/9/27/28	0/2/2/2
4	V5N	BA	216	4	-	1/5/10/12	0/1/1/1
1	A2M	B5	1810	92,1	-	0/5/27/28	0/3/3/3
1	OMG	B5	4369	1	-	1/5/27/28	0/3/3/3
52	OMU	A2	121	52	-	0/9/27/28	0/2/2/2
52	PSU	A2	682	52	-	0/7/25/26	0/2/2/2
52	OMG	A2	1329	52	-	0/5/27/28	0/3/3/3
52	OMC	A2	1392	52	-	0/9/27/28	0/2/2/2
52	PSU	A2	1178	52	-	0/7/25/26	0/2/2/2
1	OMG	B5	3676	1	-	2/5/27/28	0/3/3/3
52	PSU	A2	610	52	-	0/7/25/26	0/2/2/2
52	A2M	A2	1032	52	-	0/5/27/28	0/3/3/3
1	PSU	B5	4740	1	-	0/7/25/26	0/2/2/2
52	PSU	A2	1082	52	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	B5	3494	1	-	1/7/25/26	0/2/2/2
52	PSU	A2	407	52	-	0/7/25/26	0/2/2/2
1	PSU	B5	2351	1	-	0/7/25/26	0/2/2/2
80	SAC	Ar	2	80	-	0/7/8/10	-
31	MLZ	Bb	5	31	-	2/7/8/10	-
52	PSU	A2	93	52	-	0/7/25/26	0/2/2/2
52	PSU	A2	1348	52	-	0/7/25/26	0/2/2/2
52	PSU	A2	1644	92,52	-	0/7/25/26	0/2/2/2
1	OMC	B5	4282	92,1	-	0/9/27/28	0/2/2/2
30	V5N	Ba	39	30	-	0/5/10/12	0/1/1/1
1	OMC	B5	3601	1	-	0/9/27/28	0/2/2/2
52	PSU	A2	119	52	-	0/7/25/26	0/2/2/2
52	OMU	A2	429	52	-	4/9/27/28	0/2/2/2
1	OMC	B5	3573	1	-	0/9/27/28	0/2/2/2
1	PSU	B5	3616	1	-	0/7/25/26	0/2/2/2
1	PSU	B5	4107	1	-	0/7/25/26	0/2/2/2
1	PSU	B5	4045	1	-	0/7/25/26	0/2/2/2
1	OMC	B5	1820	92,1	-	1/9/27/28	0/2/2/2
52	6MZ	A2	1833	92,52	-	0/5/27/28	0/3/3/3
1	A2M	B5	3517	1	-	2/5/27/28	0/3/3/3
1	PSU	B5	3576	1	-	1/7/25/26	0/2/2/2
3	OMG	B8	75	3	-	0/5/27/28	0/3/3/3
52	OMU	A2	116	52	-	1/9/27/28	0/2/2/2
52	PSU	A2	650	52	-	0/7/25/26	0/2/2/2
52	OMG	A2	868	52	-	0/5/27/28	0/3/3/3
42	M3L	Bm	98	42	-	0/9/10/12	-
52	PSU	A2	967	52	-	0/7/25/26	0/2/2/2
1	PSU	B5	1537	1	-	0/7/25/26	0/2/2/2
83	AME	Au	1	83	-	2/9/10/12	-
1	OMU	B5	4366	1	-	1/9/27/28	0/2/2/2
1	PSU	B5	4278	1	-	0/7/25/26	0/2/2/2
52	PSU	A2	652	52	-	0/7/25/26	0/2/2/2
1	OMC	B5	1284	1	-	0/9/27/28	0/2/2/2
52	G7M	A2	1640	61,52	-	2/3/25/26	0/3/3/3
1	PSU	B5	3427	1	-	0/7/25/26	0/2/2/2
1	OMG	B5	4245	1	-	0/5/27/28	0/3/3/3
1	OMU	B5	3657	1	-	1/9/27/28	0/2/2/2
62	SAC	AZ	2	62	-	2/7/8/10	-
52	PSU	A2	864	52	-	0/7/25/26	0/2/2/2
1	PSU	B5	4149	1	-	0/7/25/26	0/2/2/2
52	A2M	A2	577	52	-	2/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMU	B5	2680	1	-	1/9/27/28	0/2/2/2
45	SAC	Br	2	45	-	0/7/8/10	-
52	PSU	A2	802	52	-	0/7/25/26	0/2/2/2
1	OMC	B5	2647	1	-	0/9/27/28	0/2/2/2
1	A2M	B5	1270	1	-	0/5/27/28	0/3/3/3
1	OMG	B5	4138	1	-	1/5/27/28	0/3/3/3
52	PSU	A2	823	52	-	0/7/25/26	0/2/2/2
52	PSU	A2	573	52	-	0/7/25/26	0/2/2/2
81	NMM	As	67	81	-	1/9/11/13	-
1	OMG	B5	1260	1	-	1/5/27/28	0/3/3/3
1	OMC	B5	2704	1	-	0/9/27/28	0/2/2/2
1	A2M	B5	398	1	-	3/5/27/28	0/3/3/3
1	OMC	B5	2194	92,1	-	2/9/27/28	0/2/2/2
52	PSU	A2	1626	52	-	0/7/25/26	0/2/2/2
1	PSU	B5	4039	1	-	0/7/25/26	0/2/2/2
1	PSU	B5	4217	1	-	0/7/25/26	0/2/2/2
1	PSU	B5	1720	1	-	0/7/25/26	0/2/2/2
1	UR3	B5	4276	1	-	0/7/25/26	0/2/2/2
52	PSU	A2	1046	52	-	0/7/25/26	0/2/2/2
3	PSU	B8	69	3	-	0/7/25/26	0/2/2/2
1	OMC	B5	3433	1	-	4/9/27/28	0/2/2/2
1	A2M	B5	3562	1	-	0/5/27/28	0/3/3/3
1	PSU	B5	3585	92,1	-	0/7/25/26	0/2/2/2
61	5MU	AT	54	61	-	0/7/25/26	0/2/2/2
1	OMG	B5	3942	61,1	-	0/5/27/28	0/3/3/3
1	PSU	B5	1718	1	-	0/7/25/26	0/2/2/2
1	PSU	B5	3447	1	-	0/7/25/26	0/2/2/2
1	5MC	B5	4193	1	-	4/7/25/26	0/2/2/2
52	A2M	A2	1384	52	-	0/5/27/28	0/3/3/3
1	PSU	B5	4711	1	-	0/7/25/26	0/2/2/2
52	PSU	A2	105	52	-	0/7/25/26	0/2/2/2
52	OMG	A2	510	92,52	-	1/5/27/28	0/3/3/3
52	OMG	A2	684	52	-	2/5/27/28	0/3/3/3
1	PSU	B5	4267	92,1	-	0/7/25/26	0/2/2/2
1	PSU	B5	1638	1	-	0/7/25/26	0/2/2/2
1	OMU	B5	2258	1	-	0/9/27/28	0/2/2/2
1	OMU	B5	4052	1	-	0/9/27/28	0/2/2/2
1	PSU	B5	3554	1	-	0/7/25/26	0/2/2/2
1	A2M	B5	400	1	-	0/5/27/28	0/3/3/3
1	OMC	B5	4202	1	-	0/9/27/28	0/2/2/2
1	A2M	B5	3450	1	-	0/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMC	B5	3540	1	-	0/9/27/28	0/2/2/2
1	1MA	B5	1266	92,1	-	0/3/25/26	0/3/3/3
1	OMC	B5	2208	92,1	-	0/9/27/28	0/2/2/2
1	OMC	B5	3619	1	-	2/9/27/28	0/2/2/2
52	OMU	A2	1327	92,52	-	0/9/27/28	0/2/2/2
1	PSU	B5	3500	1	-	0/7/25/26	0/2/2/2
1	PSU	B5	4042	1	-	0/7/25/26	0/2/2/2
1	OMG	B5	1477	1	-	0/5/27/28	0/3/3/3
1	PSU	B5	2475	1	-	0/7/25/26	0/2/2/2
52	OMG	A2	1491	92,52	-	0/5/27/28	0/3/3/3
52	OMG	A2	602	52	-	0/5/27/28	0/3/3/3
52	A2M	A2	1679	52	-	0/5/27/28	0/3/3/3
1	OMG	B5	3631	1	-	1/5/27/28	0/3/3/3
52	PSU	A2	1057	52	-	0/7/25/26	0/2/2/2
1	OMG	B5	2207	1	-	3/5/27/28	0/3/3/3
1	OMU	B5	4244	1	-	0/9/27/28	0/2/2/2
5	HIC	BB	245	5	-	2/5/6/8	0/1/1/1
1	PSU	B5	1491	1	-	0/7/25/26	0/2/2/2
52	OMU	A2	628	52	-	4/9/27/28	0/2/2/2
52	A2M	A2	469	52	-	1/5/27/28	0/3/3/3
52	A2M	A2	513	52	-	2/5/27/28	0/3/3/3
52	A2M	A2	669	92,52	-	2/5/27/28	0/3/3/3
52	PSU	A2	1175	52	-	0/7/25/26	0/2/2/2
1	PSU	B5	3462	1	-	0/7/25/26	0/2/2/2
1	OMG	B5	3524	1	-	0/5/27/28	0/3/3/3
1	OMC	B5	2265	92,1	-	2/9/27/28	0/2/2/2
1	PSU	B5	4298	1	-	0/7/25/26	0/2/2/2
52	4AC	A2	1843	52	-	4/11/29/30	0/2/2/2
1	PSU	B5	1632	1	-	0/7/25/26	0/2/2/2
1	PSU	B5	4382	1	-	4/7/25/26	0/2/2/2
52	OMC	A2	463	52	-	0/9/27/28	0/2/2/2
1	PSU	B5	4374	1	-	0/7/25/26	0/2/2/2
52	PSU	A2	1233	52	-	0/7/25/26	0/2/2/2
52	OMG	A2	645	52	-	3/5/27/28	0/3/3/3
52	PSU	A2	1693	52	-	0/7/25/26	0/2/2/2
52	OMC	A2	1704	52	-	1/9/27/28	0/2/2/2
1	OMG	B5	3476	1	-	2/5/27/28	0/3/3/3
6	AYA	BC	2	6	-	3/4/6/8	-
52	MA6	A2	1851	52	-	0/7/29/30	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
52	PSU	A2	815	52	-	0/7/25/26	0/2/2/2
1	A2M	B5	4336	1	-	1/5/27/28	0/3/3/3
1	A2M	B5	4269	92,1	-	0/5/27/28	0/3/3/3
52	OMU	A2	172	52	-	0/9/27/28	0/2/2/2
52	PSU	A2	34	52	-	0/7/25/26	0/2/2/2
52	PSU	A2	36	52	-	0/7/25/26	0/2/2/2
1	PSU	B5	4322	1	-	0/7/25/26	0/2/2/2
52	A2M	A2	99	92,52	-	2/5/27/28	0/3/3/3
1	A2M	B5	2630	92,1	-	0/5/27/28	0/3/3/3
1	PSU	B5	1799	1	-	0/7/25/26	0/2/2/2
1	PSU	B5	3369	1	-	0/7/25/26	0/2/2/2
52	PSU	A2	1005	52	-	0/7/25/26	0/2/2/2
1	A2M	B5	4317	1	-	0/5/27/28	0/3/3/3
1	PSU	B5	3371	1	-	0/7/25/26	0/2/2/2
52	OMC	A2	174	92,52	-	0/9/27/28	0/2/2/2
52	OMC	A2	518	52	-	0/9/27/28	0/2/2/2
52	A2M	A2	159	52	-	1/5/27/28	0/3/3/3
1	A2M	B5	2244	92,1	-	0/5/27/28	0/3/3/3
1	PSU	B5	3466	1	-	0/7/25/26	0/2/2/2
52	PSU	A2	218	52	-	0/7/25/26	0/2/2/2
43	MLZ	Bo	53	43	-	0/7/8/10	-
1	PSU	B5	4099	1	-	0/7/25/26	0/2/2/2
52	A2M	A2	166	52	-	0/5/27/28	0/3/3/3
52	OMU	A2	1443	92,52	-	1/9/27/28	0/2/2/2

The worst 5 of 334 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	A2	1640	G7M	C5-C4	7.39	1.53	1.39
52	A2	1640	G7M	O6-C6	7.28	1.38	1.23
1	B5	1266	1MA	C2-N3	4.81	1.34	1.29
85	Aw	62	HY3	C3-CA	-4.55	1.50	1.55
52	A2	1640	G7M	C2-N2	4.45	1.44	1.34

The worst 5 of 554 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B5	1491	PSU	N1-C2-N3	6.08	122.02	115.13
1	B5	4267	PSU	N1-C2-N3	6.08	122.02	115.13
1	B5	3494	PSU	N1-C2-N3	6.06	122.00	115.13
1	B5	4042	PSU	N1-C2-N3	6.05	121.98	115.13
1	B5	4246	PSU	N1-C2-N3	6.04	121.98	115.13

There are no chirality outliers.

5 of 112 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	BA	216	V5N	O-C-CA-CB
5	BB	245	HIC	CA-CB-CG-ND1
6	BC	2	AYA	OT-CT-N-CA
6	BC	2	AYA	CM-CT-N-CA
31	Bb	5	MLZ	C-CA-CB-CG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 848 ligands modelled in this entry, 428 are monoatomic and 312 are unknown - leaving 108 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	$\#\|Z\| > 2$
90	SPD	B5	4923	-	9,9,9	0.15	0	8,8,8	0.18	0
89	N	AT	103	89	9,12,13	0.65	0	10,16,19	0.67	0
90	SPD	B5	4936	-	9,9,9	0.15	0	8,8,8	0.17	0
89	N	Bo	209	89	9,12,13	0.65	0	10,16,19	0.67	0
89	N	Ae	303	89	9,12,13	0.64	0	10,16,19	0.68	0
89	N	AI	101	60,89	9,12,13	0.65	0	10,16,19	0.68	0
89	N	Aa	307	89	9,12,13	0.65	0	10,16,19	0.64	0
89	N	Bv	302	89	9,12,13	0.66	0	10,16,19	0.68	0
90	SPD	B5	4925	-	9,9,9	0.15	0	8,8,8	0.19	0
89	N	B5	4915	89	9,12,13	0.65	0	10,16,19	0.64	0
89	N	Bo	210	89	9,12,13	0.66	0	10,16,19	0.67	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
89	N	B5	4904	89	9,12,13	0.65	0	10,16,19	0.68	0
89	N	Bv	303	89	9,12,13	0.66	0	10,16,19	0.67	0
90	SPD	B5	4940	-	9,9,9	0.15	0	8,8,8	0.20	0
89	N	B5	4909	89	9,12,13	0.66	0	10,16,19	0.66	0
90	SPD	B5	4941	-	9,9,9	0.15	0	8,8,8	0.18	0
89	N	B5	4902	89	9,12,13	0.66	0	10,16,19	0.66	0
89	N	B5	4918	89	9,12,13	0.65	0	10,16,19	0.67	0
89	N	Ae	307	89	9,12,13	0.65	0	10,16,19	0.67	0
90	SPD	B5	4926	-	9,9,9	0.16	0	8,8,8	0.18	0
89	N	Ae	304	89	9,12,13	0.65	0	10,16,19	0.67	0
90	SPD	A2	1906	-	9,9,9	0.15	0	8,8,8	0.19	0
90	SPD	A2	1904	-	9,9,9	0.15	0	8,8,8	0.18	0
90	SPD	B5	4933	-	9,9,9	0.15	0	8,8,8	0.20	0
89	N	Aa	305	89	9,12,13	0.65	0	10,16,19	0.65	0
89	N	B5	4905	89	9,12,13	0.65	0	10,16,19	0.67	0
89	N	Bo	212	89	9,12,13	0.66	0	10,16,19	0.68	0
90	SPD	B5	4939	-	9,9,9	0.15	0	8,8,8	0.17	0
90	SPD	B5	4921	-	9,9,9	0.15	0	8,8,8	0.14	0
90	SPD	B5	4922	-	9,9,9	0.15	0	8,8,8	0.18	0
89	N	B5	4914	89	9,12,13	0.64	0	10,16,19	0.70	0
89	N	Aa	301	89	9,12,13	0.65	0	10,16,19	0.67	0
89	N	Ay	205	89	9,12,13	0.65	0	10,16,19	0.66	0
90	SPD	A2	1907	-	9,9,9	0.15	0	8,8,8	0.20	0
89	N	AT	106	89	9,12,13	0.66	0	10,16,19	0.65	0
89	N	AT	101	89	9,12,13	0.66	0	10,16,19	0.65	0
89	N	B5	4917	89	9,12,13	0.66	0	10,16,19	0.69	0
90	SPD	B5	4924	-	9,9,9	0.15	0	8,8,8	0.21	0
89	N	B5	4916	89	9,12,13	0.65	0	10,16,19	0.68	0
95	AAC	BD	301	7	6,6,7	0.88	0	6,6,8	1.13	1 (16%)
89	N	AT	102	89	9,12,13	0.66	0	10,16,19	0.66	0
89	N	B5	4910	89	9,12,13	0.65	0	10,16,19	0.66	0
90	SPD	B5	4937	-	9,9,9	0.15	0	8,8,8	0.17	0
89	N	Ae	308	89	9,12,13	0.65	0	10,16,19	0.66	0
90	SPD	A2	1908	-	9,9,9	0.16	0	8,8,8	0.16	0
90	SPD	B5	4927	-	9,9,9	0.16	0	8,8,8	0.19	0
91	SPM	B5	4932	-	13,13,13	0.15	0	12,12,12	0.22	0
89	N	Aa	308	89	9,12,13	0.65	0	10,16,19	0.68	0
90	SPD	B5	4931	-	9,9,9	0.15	0	8,8,8	0.19	0
89	N	Bo	211	89	9,12,13	0.65	0	10,16,19	0.69	0
89	N	B5	4913	89	9,12,13	0.65	0	10,16,19	0.68	0
89	N	AT	104	89	9,12,13	0.65	0	10,16,19	0.65	0
89	N	B5	4903	89	9,12,13	0.66	0	10,16,19	0.69	0
89	N	Aa	306	89	9,12,13	0.66	0	10,16,19	0.66	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
89	N	B5	4901	89	9,12,13	0.65	0	10,16,19	0.69	0
89	N	Bo	206	89	9,12,13	0.65	0	10,16,19	0.69	0
90	SPD	A2	1910	-	9,9,9	0.15	0	8,8,8	0.19	0
90	SPD	B5	4938	-	9,9,9	0.15	0	8,8,8	0.18	0
89	N	Bv	306	89	9,12,13	0.65	0	10,16,19	0.68	0
89	N	Bv	301	89	9,12,13	0.65	0	10,16,19	0.66	0
89	N	Ay	201	89	9,12,13	0.66	0	10,16,19	0.68	0
89	N	Aa	303	89	9,12,13	0.64	0	10,16,19	0.66	0
89	N	Ae	305	89	9,12,13	0.65	0	10,16,19	0.67	0
90	SPD	B5	4943	-	9,9,9	0.15	0	8,8,8	0.21	0
90	SPD	B5	4928	-	9,9,9	0.15	0	8,8,8	0.16	0
94	GTP	B7	201	2	26,34,34	0.94	2 (7%)	32,54,54	0.78	0
89	N	Bo	205	89	9,12,13	0.66	0	10,16,19	0.67	0
89	N	Bo	204	89	9,12,13	0.65	0	10,16,19	0.65	0
89	N	B5	4908	89	9,12,13	0.66	0	10,16,19	0.64	0
89	N	Bo	207	89	9,12,13	0.64	0	10,16,19	0.66	0
89	N	Ae	310	89	9,12,13	0.65	0	10,16,19	0.66	0
89	N	Bo	202	89	13,13,13	0.80	0	17,19,19	0.87	1 (5%)
90	SPD	B5	4944	-	9,9,9	0.15	0	8,8,8	0.15	0
89	N	Bv	307	89	9,12,13	0.66	0	10,16,19	0.68	0
90	SPD	B5	4934	-	9,9,9	0.15	0	8,8,8	0.19	0
90	SPD	A2	1905	-	9,9,9	0.16	0	8,8,8	0.16	0
89	N	Ae	301	89	9,12,13	0.65	0	10,16,19	0.68	0
89	N	Bv	304	89	9,12,13	0.65	0	10,16,19	0.65	0
89	N	Ay	203	89	9,12,13	0.66	0	10,16,19	0.67	0
89	N	A2	1902	89	9,12,13	0.66	0	10,16,19	0.66	0
91	SPM	B5	4935	-	13,13,13	0.15	0	12,12,12	0.14	0
89	N	B5	4912	89	9,12,13	0.66	0	10,16,19	0.67	0
89	N	AT	105	89	9,12,13	0.66	0	10,16,19	0.65	0
89	N	Aa	302	89	9,12,13	0.66	0	10,16,19	0.66	0
89	N	Aa	309	89	9,12,13	0.65	0	10,16,19	0.67	0
89	N	B5	4906	89	9,12,13	0.64	0	10,16,19	0.64	0
89	N	Bo	203	89	9,12,13	0.65	0	10,16,19	0.63	0
89	N	Aa	304	89	9,12,13	0.66	0	10,16,19	0.66	0
90	SPD	B5	4942	-	9,9,9	0.15	0	8,8,8	0.18	0
90	SPD	A2	1911	-	9,9,9	0.15	0	8,8,8	0.17	0
90	SPD	A2	1909	-	9,9,9	0.15	0	8,8,8	0.18	0
89	N	Ay	204	89	9,12,13	0.65	0	10,16,19	0.67	0
89	N	Bo	208	89	9,12,13	0.64	0	10,16,19	0.68	0
89	N	B5	4907	89	9,12,13	0.65	0	10,16,19	0.66	0
89	N	Aa	310	89	9,12,13	0.65	0	10,16,19	0.68	0
89	N	Bv	305	89	9,12,13	0.66	0	10,16,19	0.68	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
89	N	B5	4919	89	9,12,13	0.65	0	10,16,19	0.66	0
91	SPM	A2	1912	-	13,13,13	0.15	0	12,12,12	0.16	0
89	N	Ae	309	89	9,12,13	0.65	0	10,16,19	0.69	0
90	SPD	B5	4929	-	9,9,9	0.16	0	8,8,8	0.17	0
89	N	B5	4920	89	9,12,13	0.64	0	10,16,19	0.68	0
89	N	A2	1901	89	9,12,13	0.65	0	10,16,19	0.69	0
90	SPD	B5	4930	-	9,9,9	0.15	0	8,8,8	0.20	0
89	N	A2	1903	89	9,12,13	0.65	0	10,16,19	0.64	0
89	N	Ay	202	89	9,12,13	0.65	0	10,16,19	0.68	0
89	N	Ae	306	89	9,12,13	0.65	0	10,16,19	0.68	0
89	N	Ae	302	89	9,12,13	0.66	0	10,16,19	0.68	0
89	N	B5	4911	89	9,12,13	0.65	0	10,16,19	0.65	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
90	SPD	B5	4923	-	-	1/7/7/7	-
89	N	AT	103	89	-	3/3/18/19	0/1/1/1
90	SPD	B5	4936	-	-	1/7/7/7	-
89	N	Bo	209	89	-	0/3/18/19	0/1/1/1
89	N	Ae	303	89	-	3/3/18/19	0/1/1/1
89	N	AI	101	60,89	-	1/3/18/19	0/1/1/1
89	N	Aa	307	89	-	0/3/18/19	0/1/1/1
89	N	Bv	302	89	-	3/3/18/19	0/1/1/1
90	SPD	B5	4925	-	-	1/7/7/7	-
89	N	B5	4915	89	-	1/3/18/19	0/1/1/1
89	N	Bo	210	89	-	0/3/18/19	0/1/1/1
89	N	B5	4904	89	-	0/3/18/19	0/1/1/1
89	N	Bv	303	89	-	0/3/18/19	0/1/1/1
90	SPD	B5	4940	-	-	1/7/7/7	-
89	N	B5	4909	89	-	1/3/18/19	0/1/1/1
90	SPD	B5	4941	-	-	0/7/7/7	-
89	N	B5	4902	89	-	2/3/18/19	0/1/1/1
89	N	B5	4918	89	-	2/3/18/19	0/1/1/1
89	N	Ae	307	89	-	0/3/18/19	0/1/1/1
90	SPD	B5	4926	-	-	1/7/7/7	-
89	N	Ae	304	89	-	3/3/18/19	0/1/1/1
90	SPD	A2	1906	-	-	0/7/7/7	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
90	SPD	A2	1904	-	-	1/7/7/7	-
90	SPD	B5	4933	-	-	0/7/7/7	-
89	N	Aa	305	89	-	1/3/18/19	0/1/1/1
89	N	B5	4905	89	-	1/3/18/19	0/1/1/1
89	N	Bo	212	89	-	2/3/18/19	0/1/1/1
90	SPD	B5	4939	-	-	0/7/7/7	-
90	SPD	B5	4921	-	-	1/7/7/7	-
90	SPD	B5	4922	-	-	1/7/7/7	-
89	N	B5	4914	89	-	1/3/18/19	0/1/1/1
89	N	Aa	301	89	-	0/3/18/19	0/1/1/1
89	N	Ay	205	89	-	2/3/18/19	0/1/1/1
90	SPD	A2	1907	-	-	0/7/7/7	-
89	N	AT	106	89	-	2/3/18/19	0/1/1/1
89	N	AT	101	89	-	3/3/18/19	0/1/1/1
89	N	B5	4917	89	-	3/3/18/19	0/1/1/1
90	SPD	B5	4924	-	-	0/7/7/7	-
89	N	B5	4916	89	-	3/3/18/19	0/1/1/1
95	AAC	BD	301	7	-	0/3/4/5	-
89	N	AT	102	89	-	0/3/18/19	0/1/1/1
89	N	B5	4910	89	-	2/3/18/19	0/1/1/1
90	SPD	B5	4937	-	-	0/7/7/7	-
89	N	Ae	308	89	-	0/3/18/19	0/1/1/1
90	SPD	A2	1908	-	-	0/7/7/7	-
90	SPD	B5	4927	-	-	0/7/7/7	-
91	SPM	B5	4932	-	-	0/11/11/11	-
89	N	Aa	308	89	-	3/3/18/19	0/1/1/1
90	SPD	B5	4931	-	-	0/7/7/7	-
89	N	Bo	211	89	-	2/3/18/19	0/1/1/1
89	N	B5	4913	89	-	3/3/18/19	0/1/1/1
89	N	AT	104	89	-	0/3/18/19	0/1/1/1
89	N	B5	4903	89	-	0/3/18/19	0/1/1/1
89	N	Aa	306	89	-	1/3/18/19	0/1/1/1
89	N	B5	4901	89	-	3/3/18/19	0/1/1/1
89	N	Bo	206	89	-	3/3/18/19	0/1/1/1
90	SPD	A2	1910	-	-	1/7/7/7	-
90	SPD	B5	4938	-	-	0/7/7/7	-
89	N	Bv	306	89	-	3/3/18/19	0/1/1/1
89	N	Bv	301	89	-	0/3/18/19	0/1/1/1
89	N	Ay	201	89	-	2/3/18/19	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
89	N	Aa	303	89	-	0/3/18/19	0/1/1/1
89	N	Ae	305	89	-	2/3/18/19	0/1/1/1
90	SPD	B5	4943	-	-	0/7/7/7	-
90	SPD	B5	4928	-	-	0/7/7/7	-
94	GTP	B7	201	2	-	0/18/38/38	0/3/3/3
89	N	Bo	205	89	-	0/3/18/19	0/1/1/1
89	N	Bo	204	89	-	0/3/18/19	0/1/1/1
89	N	B5	4908	89	-	2/3/18/19	0/1/1/1
89	N	Bo	207	89	-	3/3/18/19	0/1/1/1
89	N	Ae	310	89	-	0/3/18/19	0/1/1/1
89	N	Bo	202	89	-	0/6/19/19	0/1/1/1
90	SPD	B5	4944	-	-	1/7/7/7	-
89	N	Bv	307	89	-	3/3/18/19	0/1/1/1
90	SPD	B5	4934	-	-	0/7/7/7	-
90	SPD	A2	1905	-	-	0/7/7/7	-
89	N	Ae	301	89	-	3/3/18/19	0/1/1/1
89	N	Bv	304	89	-	1/3/18/19	0/1/1/1
89	N	Ay	203	89	-	2/3/18/19	0/1/1/1
89	N	A2	1902	89	-	2/3/18/19	0/1/1/1
91	SPM	B5	4935	-	-	0/11/11/11	-
89	N	B5	4912	89	-	0/3/18/19	0/1/1/1
89	N	AT	105	89	-	1/3/18/19	0/1/1/1
89	N	Aa	302	89	-	0/3/18/19	0/1/1/1
89	N	Aa	309	89	-	2/3/18/19	0/1/1/1
89	N	B5	4906	89	-	1/3/18/19	0/1/1/1
89	N	Bo	203	89	-	2/3/18/19	0/1/1/1
89	N	Aa	304	89	-	2/3/18/19	0/1/1/1
90	SPD	B5	4942	-	-	1/7/7/7	-
90	SPD	A2	1911	-	-	0/7/7/7	-
90	SPD	A2	1909	-	-	0/7/7/7	-
89	N	Ay	204	89	-	3/3/18/19	0/1/1/1
89	N	Bo	208	89	-	3/3/18/19	0/1/1/1
89	N	B5	4907	89	-	0/3/18/19	0/1/1/1
89	N	Aa	310	89	-	2/3/18/19	0/1/1/1
89	N	Bv	305	89	-	2/3/18/19	0/1/1/1
89	N	B5	4919	89	-	0/3/18/19	0/1/1/1
91	SPM	A2	1912	-	-	2/11/11/11	-
89	N	Ae	309	89	-	3/3/18/19	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
90	SPD	B5	4929	-	-	0/7/7/7	-
89	N	B5	4920	89	-	3/3/18/19	0/1/1/1
89	N	A2	1901	89	-	3/3/18/19	0/1/1/1
90	SPD	B5	4930	-	-	1/7/7/7	-
89	N	A2	1903	89	-	2/3/18/19	0/1/1/1
89	N	Ay	202	89	-	2/3/18/19	0/1/1/1
89	N	Ae	306	89	-	3/3/18/19	0/1/1/1
89	N	Ae	302	89	-	2/3/18/19	0/1/1/1
89	N	B5	4911	89	-	2/3/18/19	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
94	B7	201	GTP	C5-C6	-2.60	1.42	1.47
94	B7	201	GTP	C8-N7	-2.05	1.31	1.35

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
89	Bo	202	N	OP2-P-OP1	2.27	119.58	110.68
95	BD	301	AAC	O2-C1-C2	-2.25	118.92	125.42

There are no chirality outliers.

5 of 129 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
89	B5	4911	N	O4'-C4'-C5'-O5'
89	A2	1902	N	C3'-C4'-C5'-O5'
89	Aa	304	N	C3'-C4'-C5'-O5'
89	B5	4908	N	O4'-C4'-C5'-O5'
89	B5	4910	N	O4'-C4'-C5'-O5'

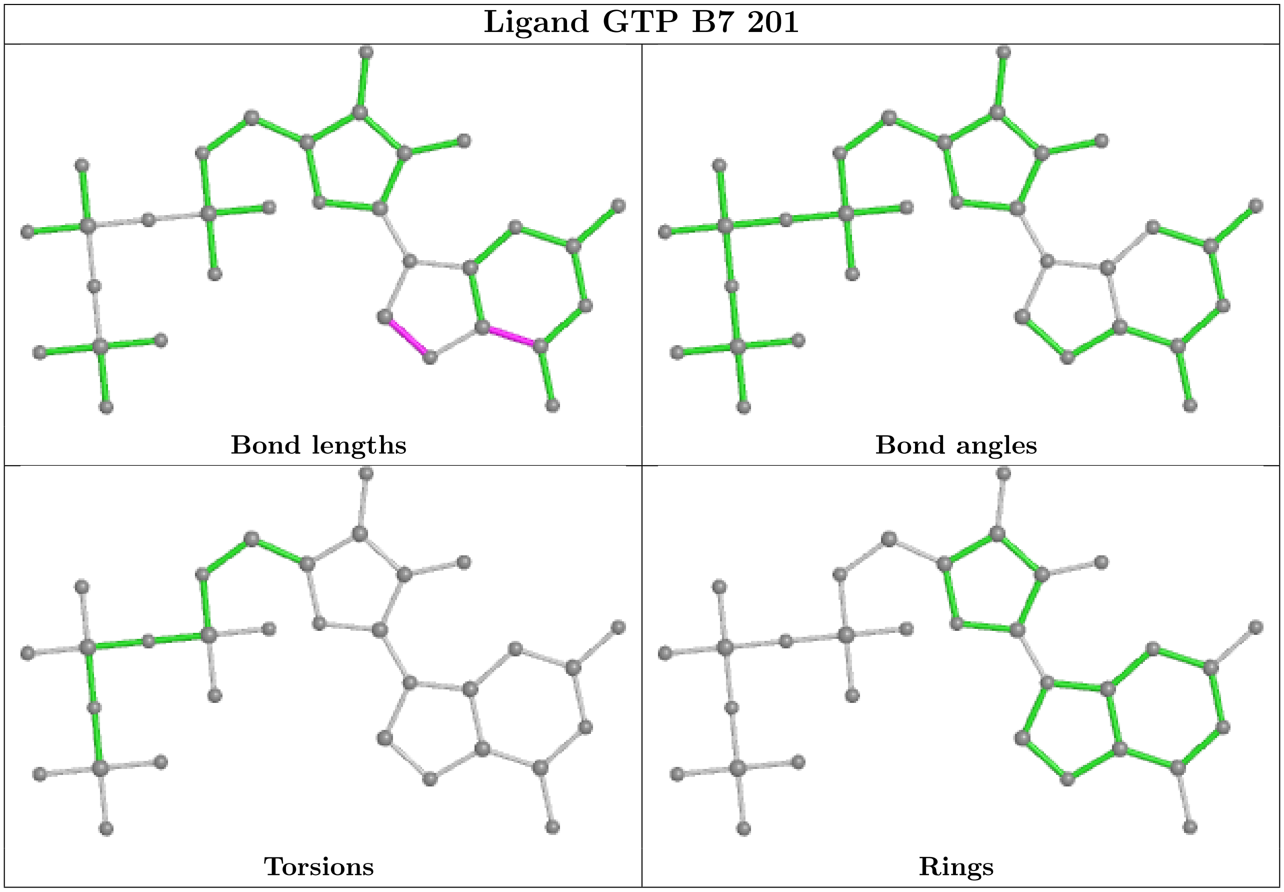
There are no ring outliers.

No monomer is involved in short contacts.

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

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

Ligand GTP B7 201



Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

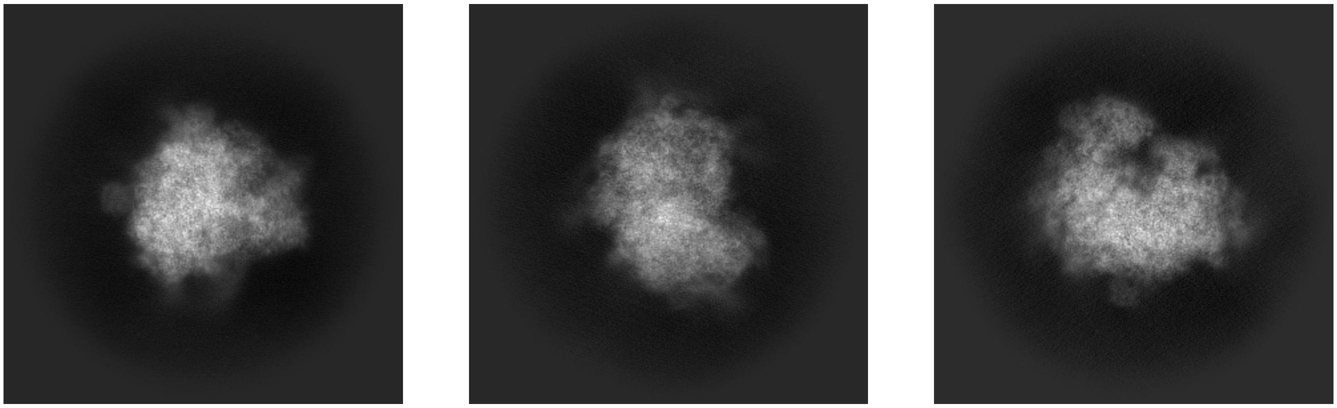
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-17367. 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.

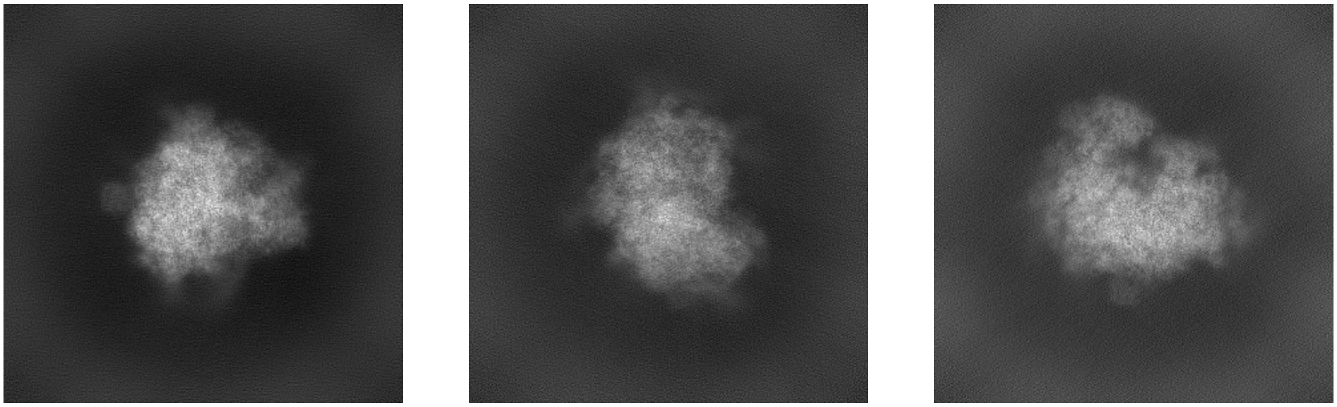
6.1 Orthogonal projections

6.1.1 Primary map



X Y Z

6.1.2 Raw map

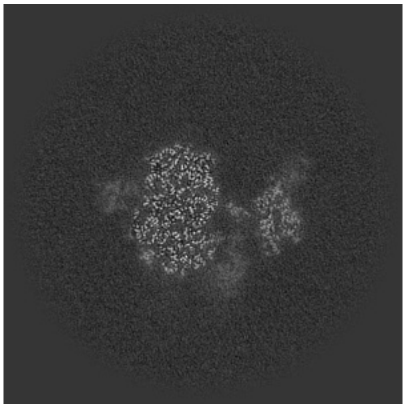


X Y Z

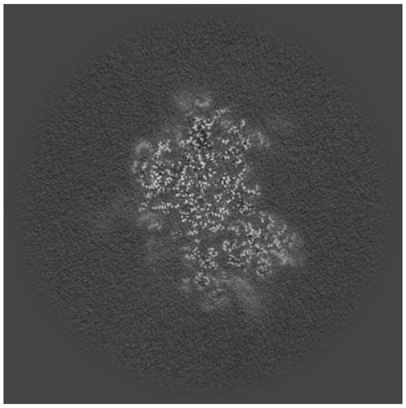
The images above show the map projected in three orthogonal directions.

6.2 Central slices

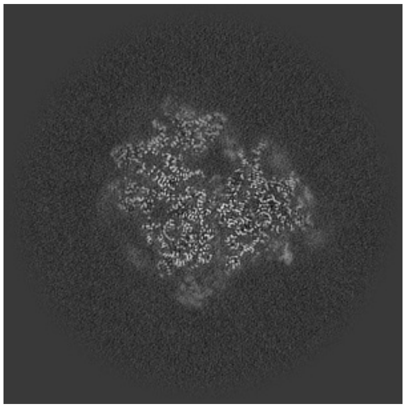
6.2.1 Primary map



X Index: 217

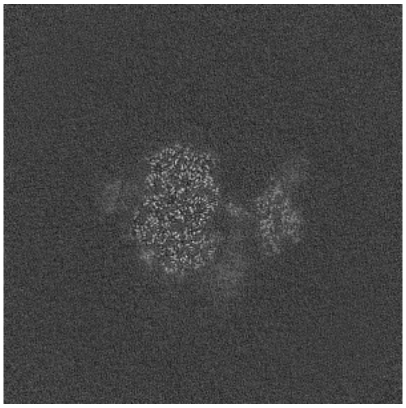


Y Index: 217

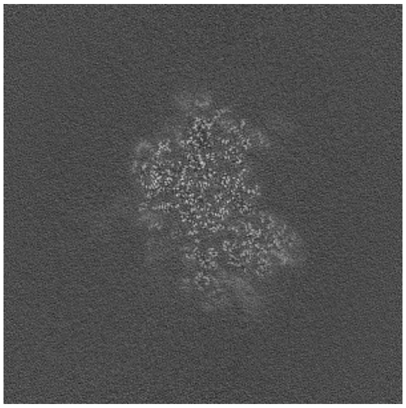


Z Index: 217

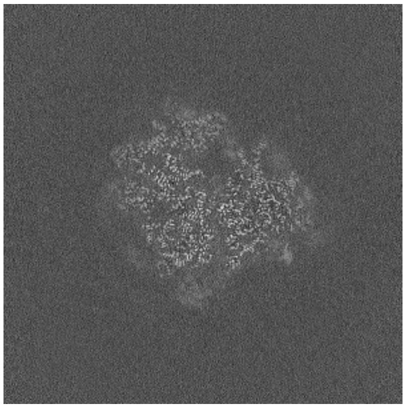
6.2.2 Raw map



X Index: 217



Y Index: 217

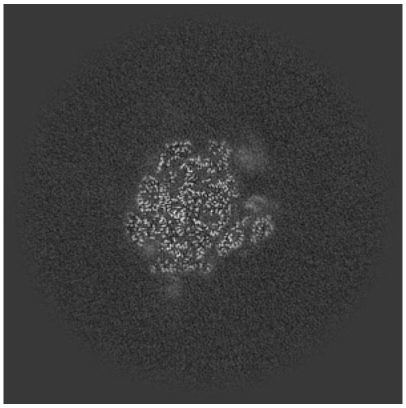


Z Index: 217

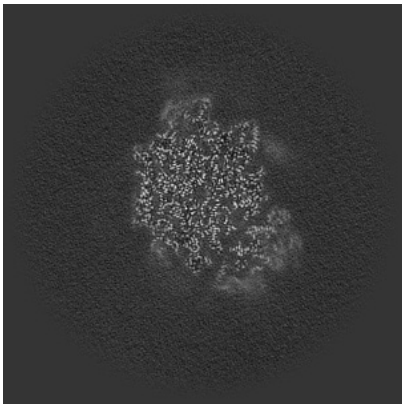
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

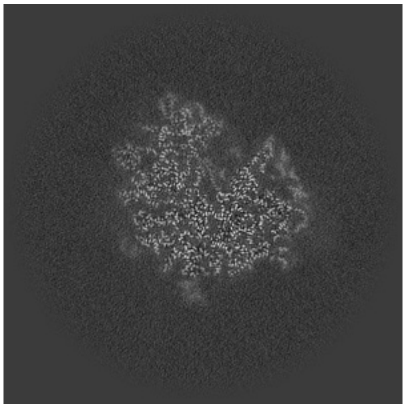
6.3.1 Primary map



X Index: 250

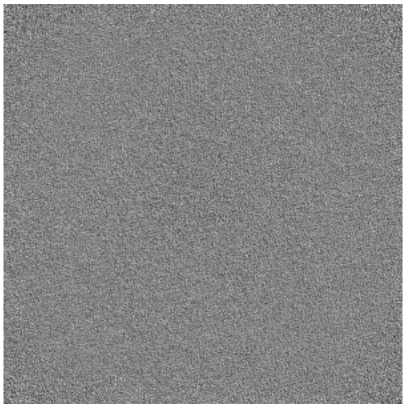


Y Index: 199

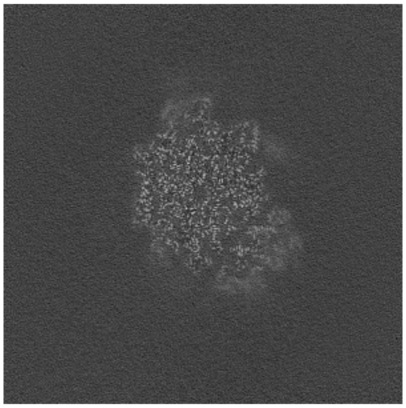


Z Index: 208

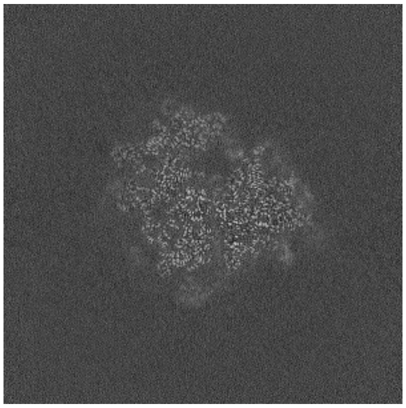
6.3.2 Raw map



X Index: 0



Y Index: 199

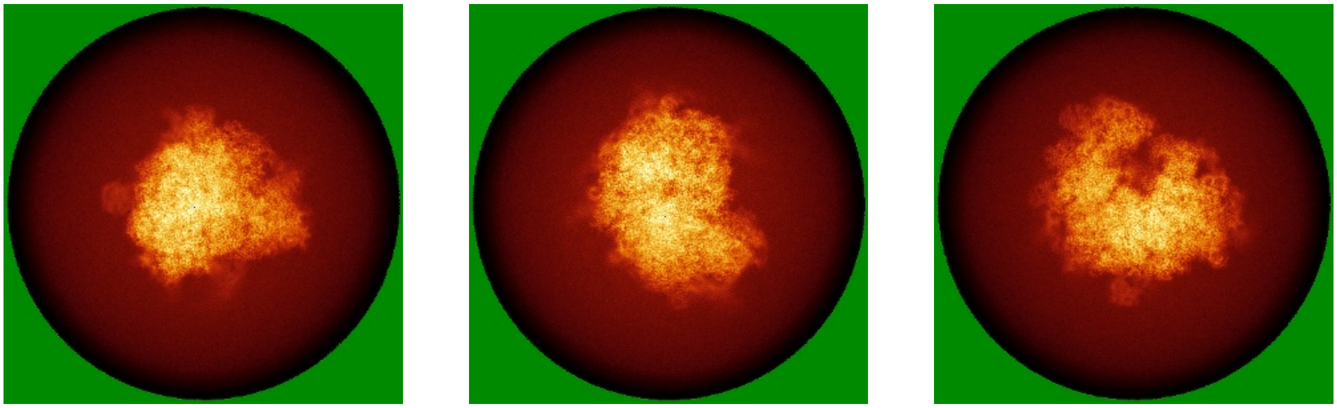


Z Index: 216

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

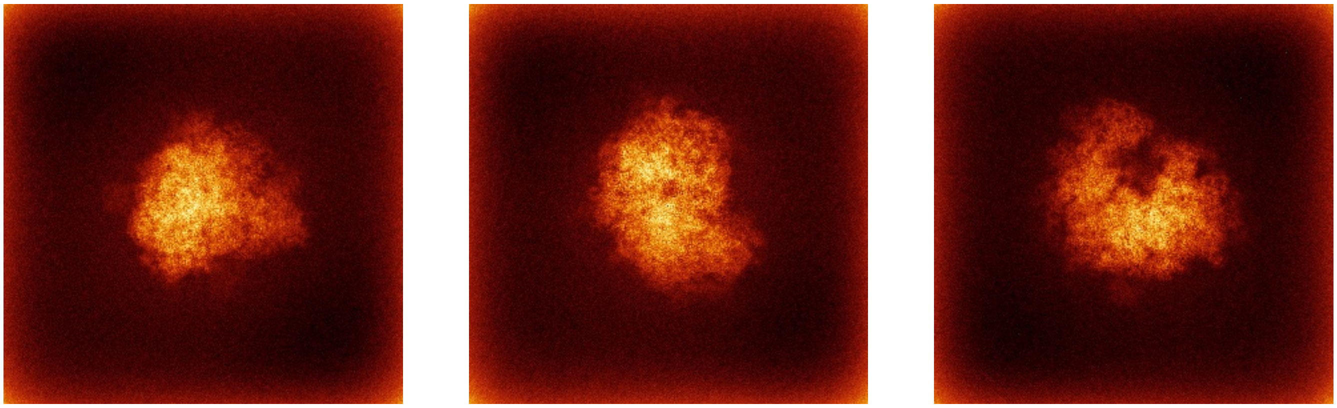
6.4 Orthogonal standard-deviation projections (False-color)

6.4.1 Primary map



X Y Z

6.4.2 Raw map



X Y Z

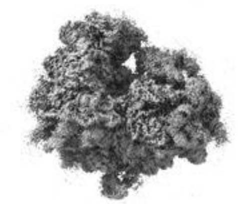
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views ⓘ

6.5.1 Primary map

X

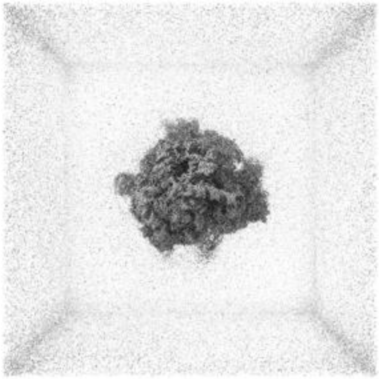
Y



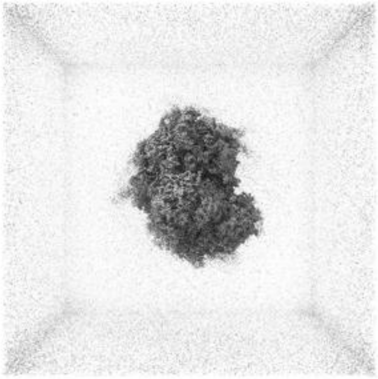
Z

The images above show the 3D surface view of the map at the recommended contour level 0.75. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

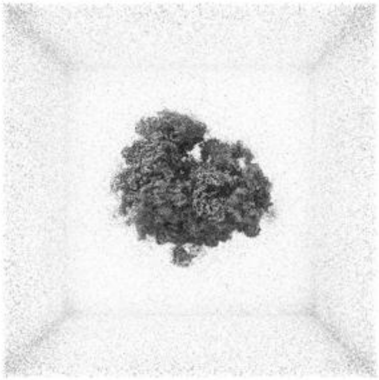
6.5.2 Raw map



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.

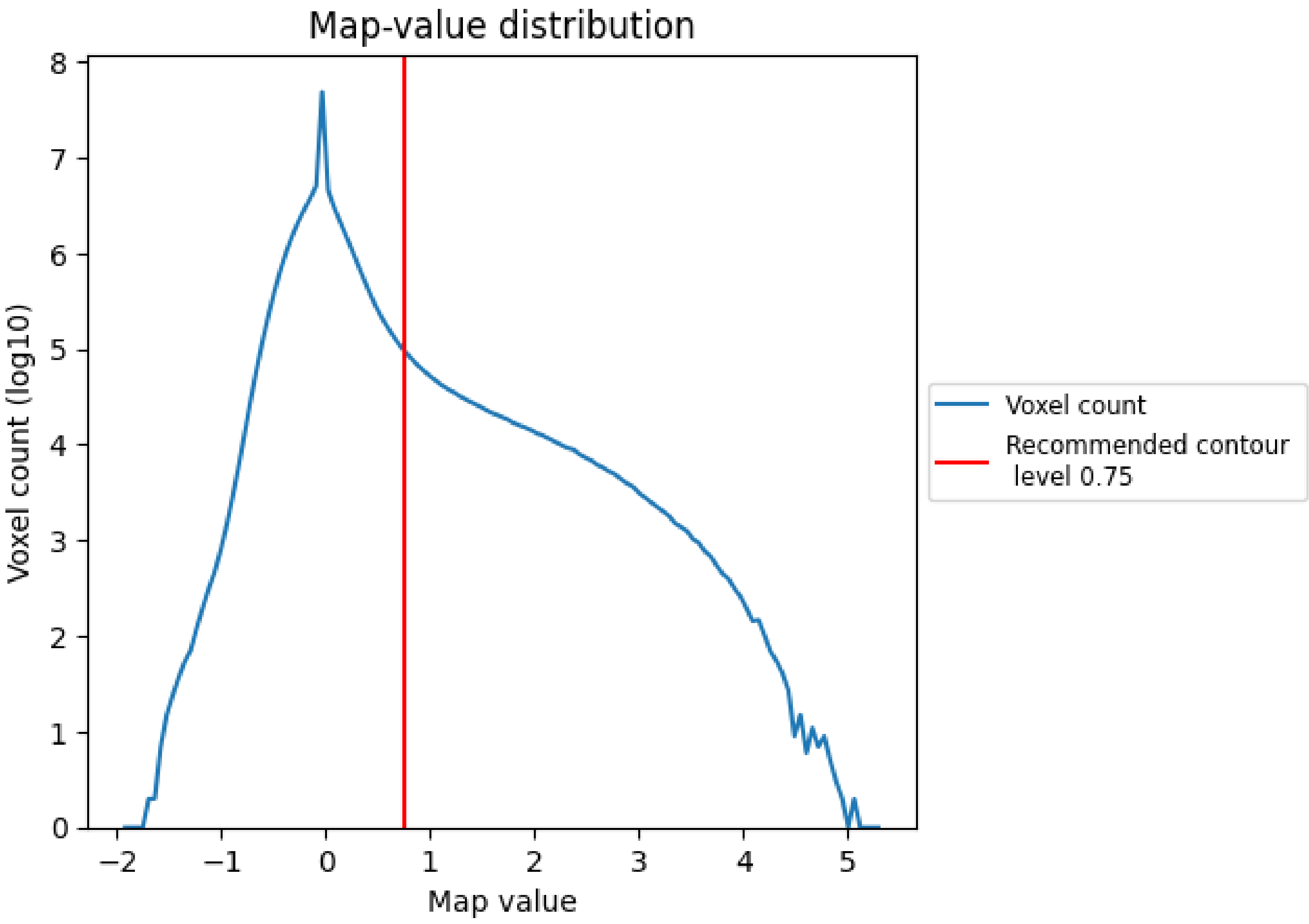
6.6 Mask visualisation ⓘ

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

7 Map analysis ⓘ

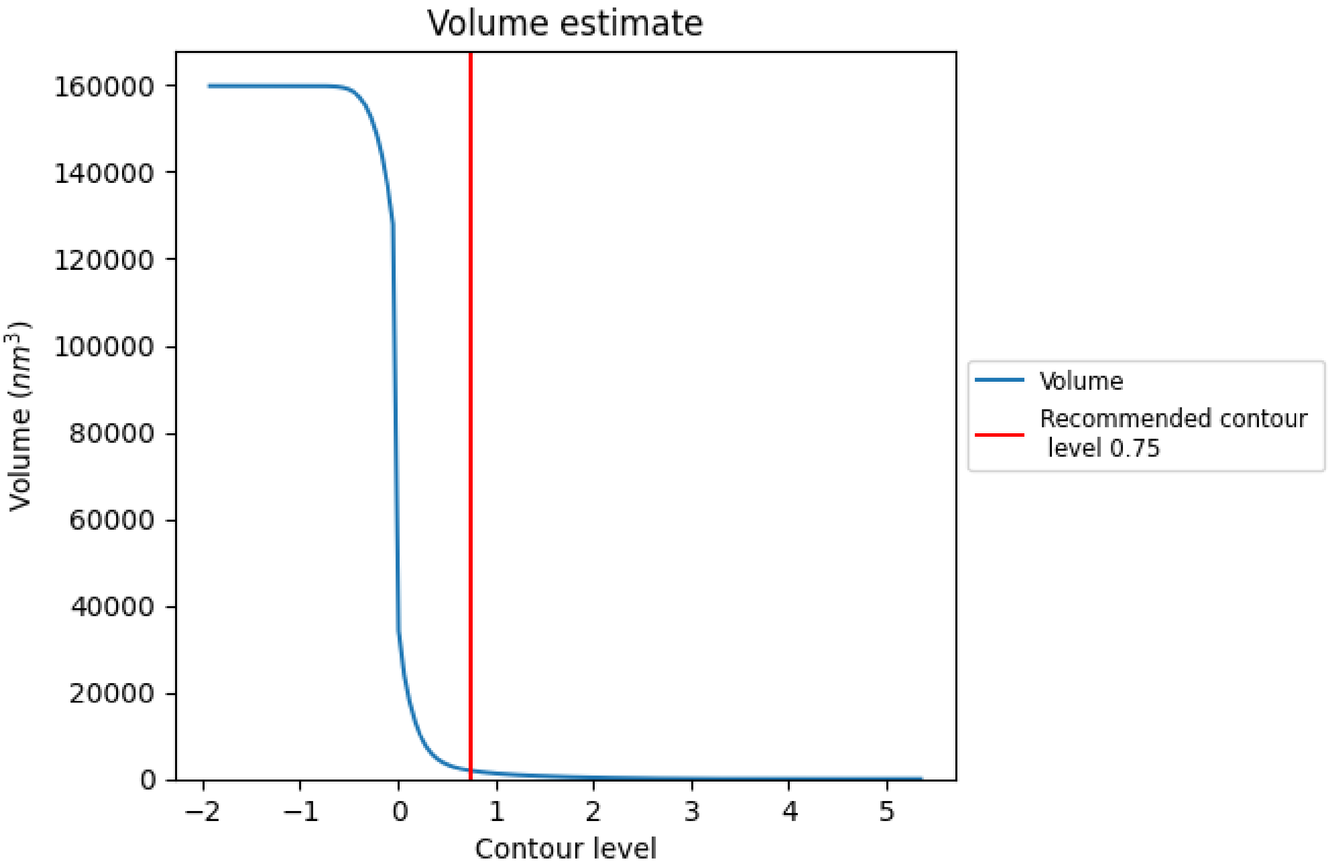
This section contains the results of statistical analysis of the map.

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.

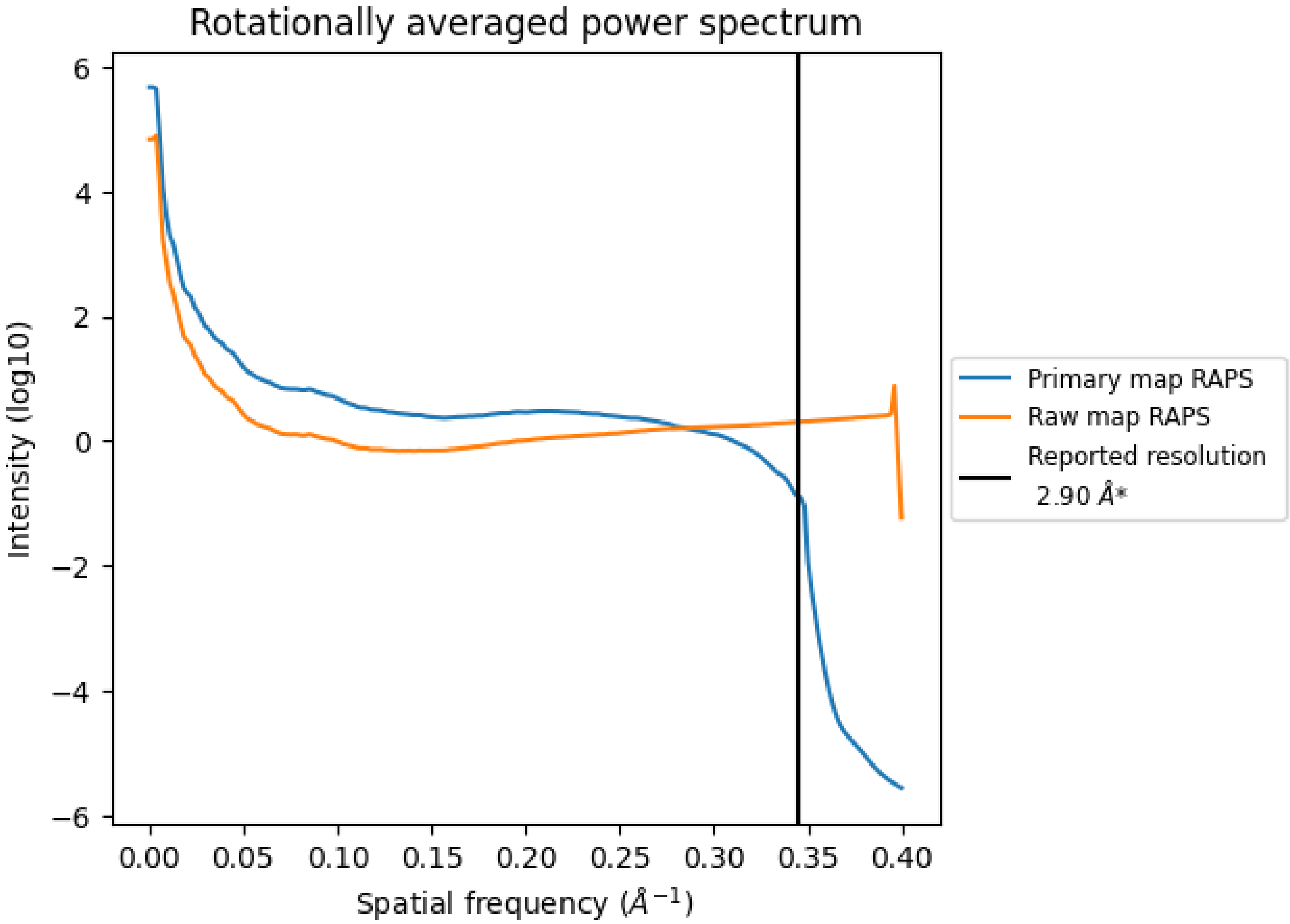
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 1923 nm^3; this corresponds to an approximate mass of 1737 kDa.

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

7.3 Rotationally averaged power spectrum (i)

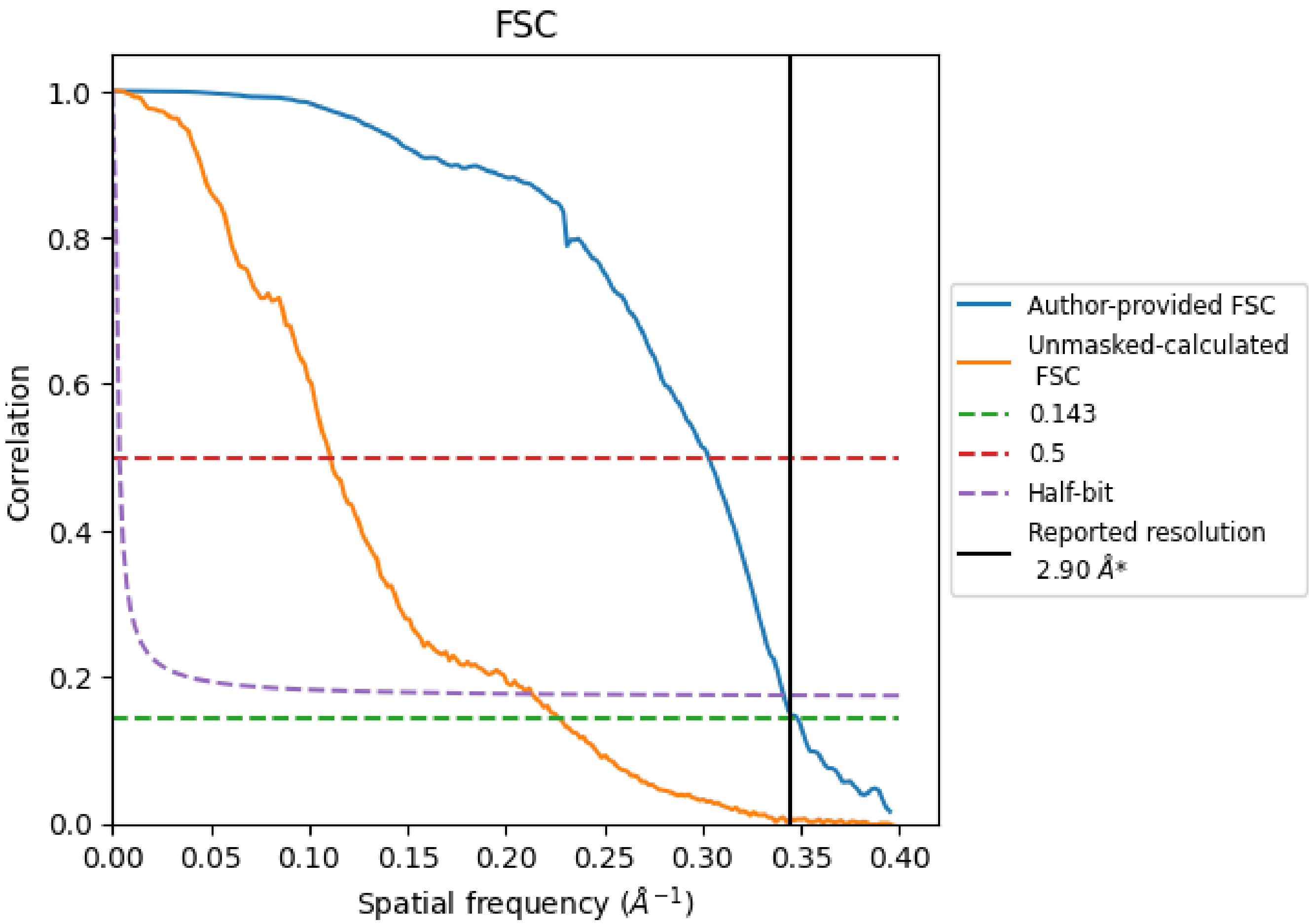


*Reported resolution corresponds to spatial frequency of 0.345 $Å^{-1}$

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 0.345 Å^{-1}

8.2 Resolution estimates ⓘ

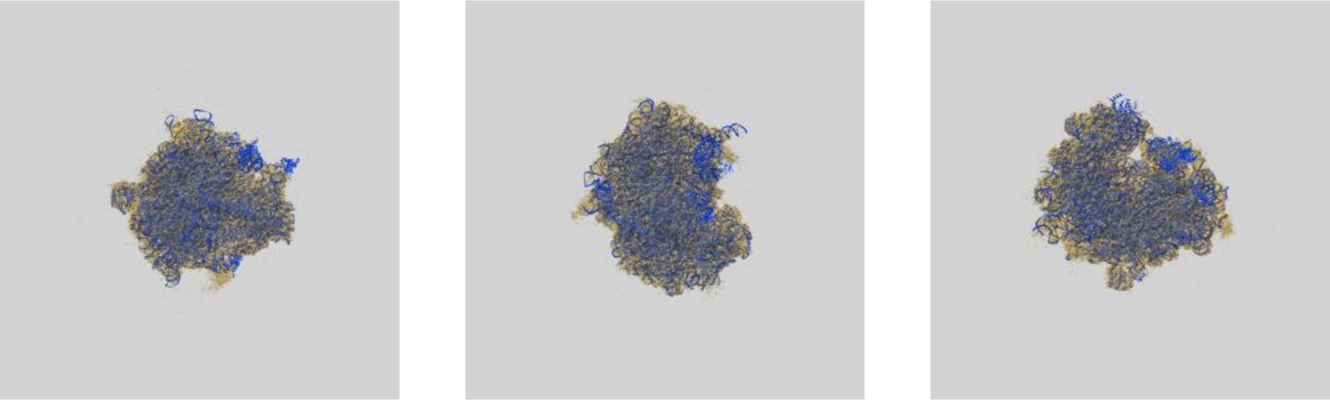
Resolution estimate (Å)	**Estimation criterion (FSC cut-off)**		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	2.87	3.30	2.93
Unmasked-calculated*	4.40	9.03	4.69

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.40 differs from the reported value 2.9 by more than 10 %

9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-17367 and PDB model 8P2K. Per-residue inclusion information can be found in section 3 on page 35.

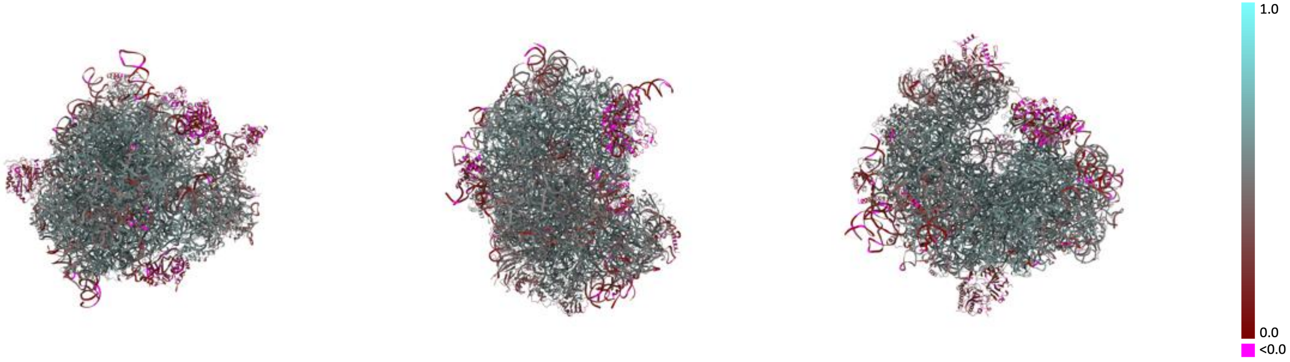
9.1 Map-model overlay



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.75 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.

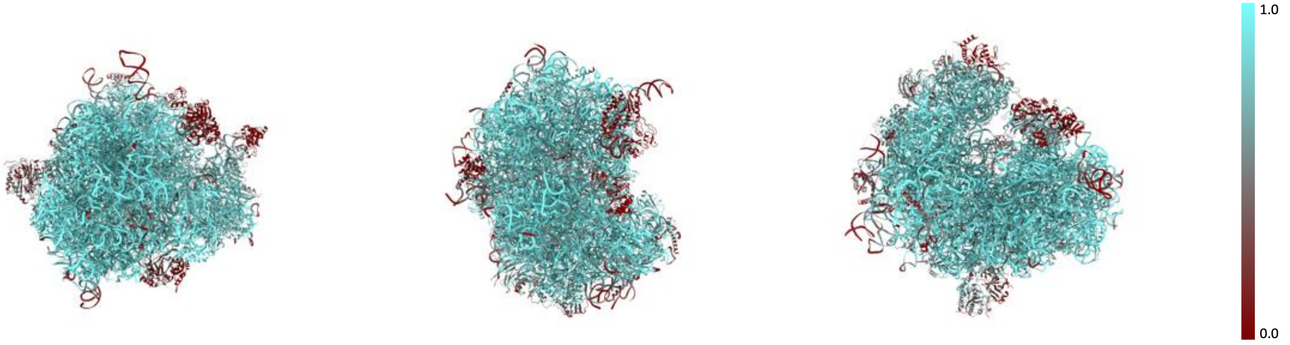
9.2 Q-score mapped to coordinate model



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.

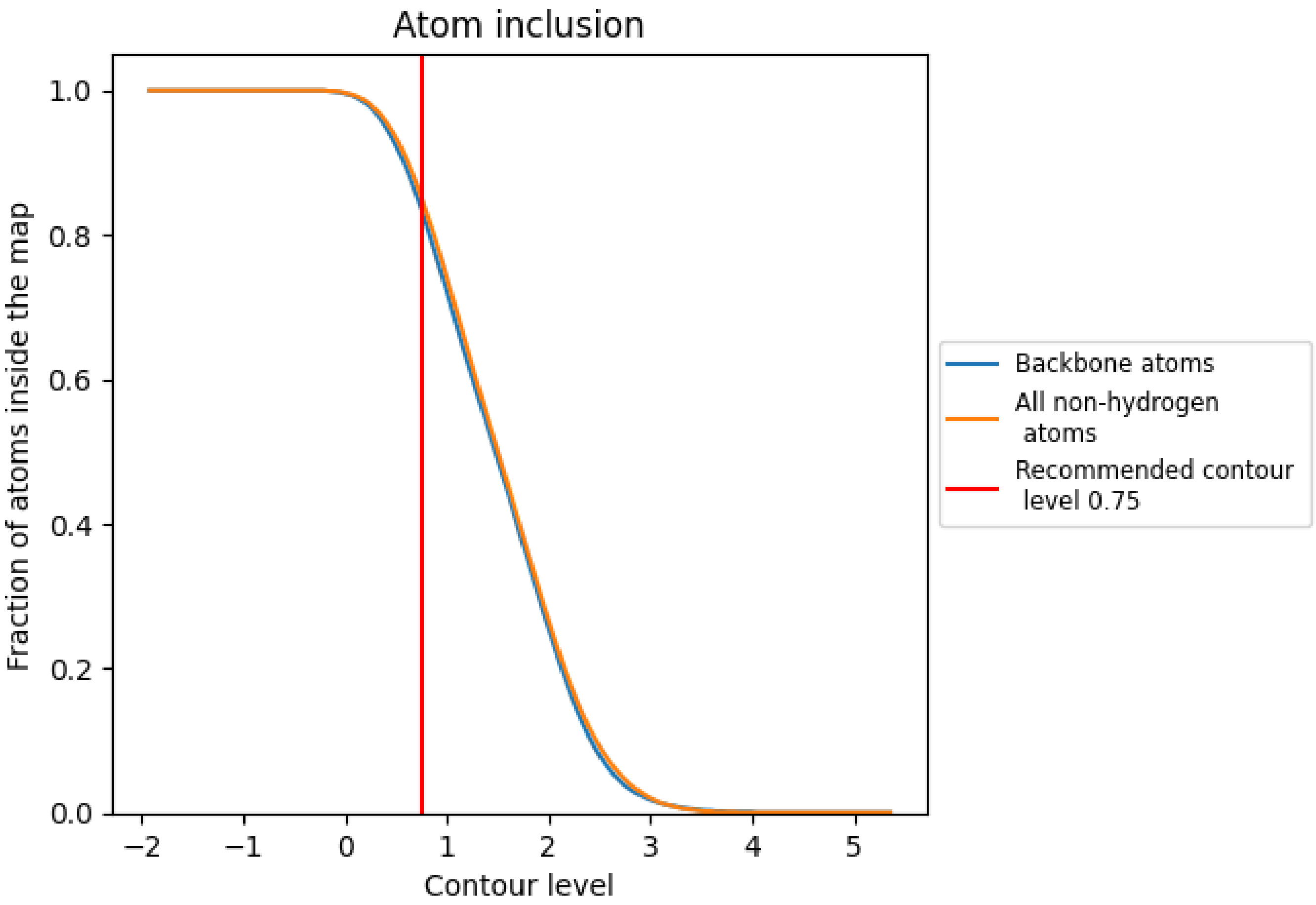
9.3 Atom inclusion mapped to coordinate model



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 (0.75).

9.4 Atom inclusion ⓘ



At the recommended contour level, 84% of all backbone atoms, 85% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.75) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8510	0.4830
A2	0.8920	0.4740
AA	0.8010	0.4780
AB	0.7860	0.4830
AC	0.0470	0.1220
AD	0.7250	0.4230
AE	0.8790	0.5200
AF	0.6310	0.3680
AG	0.8620	0.4800
AI	0.7840	0.4710
AT	0.7900	0.4410
AZ	0.7640	0.4670
Aa	0.8090	0.4860
Ab	0.8520	0.5200
Ac	0.7370	0.4370
Ad	0.8850	0.5090
Ae	0.7630	0.4660
Af	0.7590	0.4030
Ag	0.5680	0.3850
Ah	0.8530	0.4960
Ai	0.8540	0.4920
Aj	0.7280	0.3800
Ak	0.8270	0.4980
Al	0.0090	0.1370
Am	0.8810	0.5250
An	0.8760	0.5240
Ao	0.7610	0.4290
Ap	0.8370	0.4760
Aq	0.6590	0.4260
Ar	0.7960	0.4620
As	0.8330	0.4620
At	0.6550	0.3890
Au	0.7940	0.4790
Av	0.8920	0.5440
Aw	0.8910	0.5410

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Chain	Atom inclusion	Q-score
Ax	0.8200	0.4770
Ay	0.6560	0.4100
Az	0.9450	0.5650
B5	0.9130	0.5000
B7	0.9870	0.5590
B8	0.9570	0.5330
BA	0.9360	0.5690
BB	0.9190	0.5560
BC	0.9350	0.5540
BD	0.8950	0.5230
BE	0.8190	0.4910
BF	0.9180	0.5500
BG	0.8410	0.4870
BH	0.8900	0.5400
BI	0.8970	0.5470
BJ	0.8600	0.5040
BK	0.5890	0.3770
BL	0.8960	0.5310
BM	0.8930	0.5240
BN	0.9680	0.5820
BO	0.9380	0.5590
BP	0.9010	0.5560
BQ	0.9370	0.5670
BR	0.8560	0.5160
BS	0.9410	0.5600
BT	0.9030	0.5390
BU	0.8170	0.4400
BV	0.8960	0.5470
BW	0.6500	0.3800
BX	0.8940	0.5400
BY	0.9020	0.5420
BZ	0.9050	0.5290
Ba	0.9510	0.5770
Bb	0.7830	0.4580
Bc	0.8070	0.4920
Bd	0.8980	0.5430
Be	0.9270	0.5640
Bf	0.9380	0.5650
Bg	0.8970	0.5380
Bh	0.9010	0.5330
Bi	0.9120	0.5230
Bj	0.9660	0.5750

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Chain	Atom inclusion	Q-score
Bk	🟦 0.8040	⬛ 0.4830
Bl	🟦 0.9280	⬛ 0.5470
Bm	🟦 0.9120	⬛ 0.5390
Bo	🟦 0.8170	⬛ 0.5170
Bp	🟦 0.9100	⬛ 0.5540
Br	🟦 0.9240	⬛ 0.5440
Bs	🟥 0.0090	🟥 0.0580
Bt	🟥 0.0190	🟥 0.0570
Bv	🟥 0.1200	🟥 0.1370
MA	⬛ 0.4630	🟥 0.1940
Na	🟥 0.2130	🟥 0.1450
Nb	🟫 0.3510	🟫 0.2510