



wwPDB EM Validation Summary Report ⓘ

Jun 19, 2026 – 06:41 am BST

PDB ID : 9F1D / pdb_00009f1d
EMDB ID : EMD-50126
Title : Mammalian quaternary complex of a translating 80S ribosome, NAC, MetAP1 and NatA/E-HYPK
Authors : Yudin, D.; Scaiola, A.; Ban, N.
Deposited on : 2024-04-18
Resolution : 3.26 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

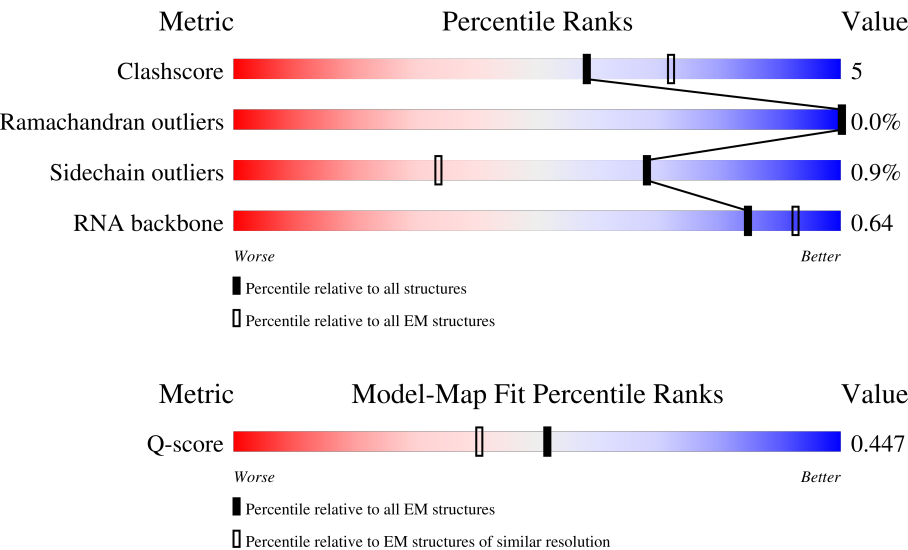
EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.26 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	14557 (2.76 - 3.76)

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

Mol	Chain	Length	Quality of chain
1	B5	4808	7% 55% 20% 23%
2	BT	160	85% 14%
3	Bb	245	8% 38% 6% 56%

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Mol	Chain	Length	Quality of chain
4	Bt	165	
5	AH	3	
6	Aq	135	
7	B7	120	
8	AT	76	
9	Ar	151	
10	B8	158	
11	BU	128	
12	As	145	
13	BA	257	
14	BV	140	
15	At	119	
16	BB	403	
17	BP	184	
18	BY	145	
19	Av	130	
20	B	297	
21	BX	156	
22	BQ	188	
23	BZ	136	
24	Aw	143	
25	BE	291	
26	BW	157	
27	Au	83	
28	Ba	148	

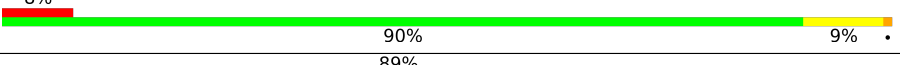
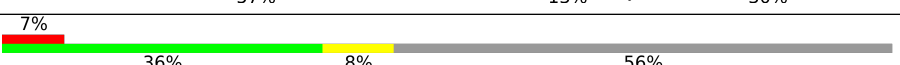
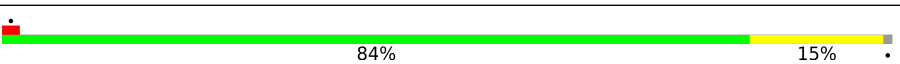
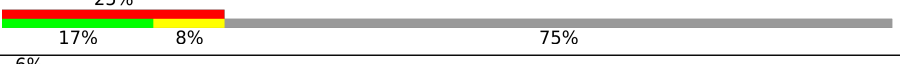
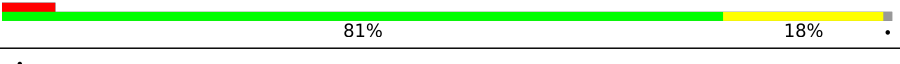
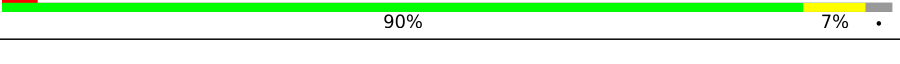
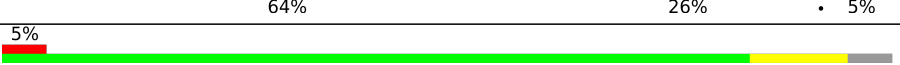
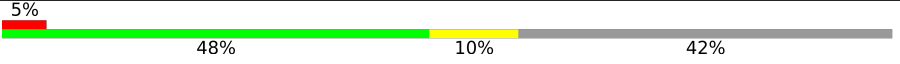
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Mol	Chain	Length	Quality of chain
29	Ax	130	
30	BF	247	
31	BR	196	
32	AZ	294	
33	Ay	124	
34	BG	266	
35	BC	412	
36	BS	176	
37	Aa	264	
38	Az	25	
39	BH	192	
40	EA	386	
41	Ab	293	
42	Bc	115	
43	BI	214	
44	Ct	238	
45	Ac	281	
46	Bd	125	
47	BJ	178	
48	Cu	162	
49	Ad	263	
50	Be	135	
51	BK	27	
52	DA	403	
53	Ae	204	

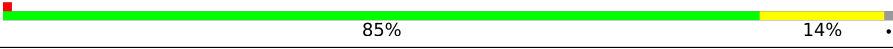
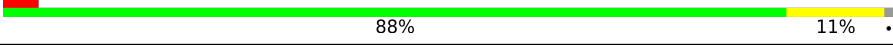
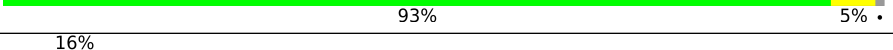
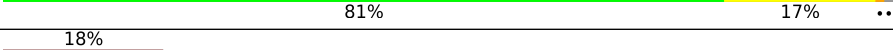
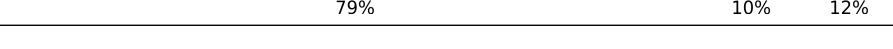
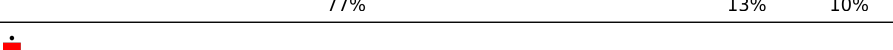
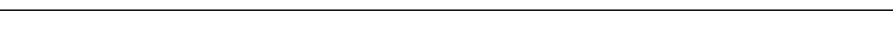
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Mol	Chain	Length	Quality of chain
54	Bf	110	
55	BL	211	
56	DB	915	
57	Af	249	
58	Bg	117	
59	BM	218	
60	DC	235	
61	Ag	432	
62	Bh	123	
63	BN	204	
64	DD	228	
65	Ah	208	
66	Bi	105	
67	BO	203	
68	A2	1870	
69	Ai	194	
70	Bj	97	
71	AA	84	
72	Aj	165	
73	Bk	70	
74	AB	69	
75	Ak	158	
76	Bl	51	
77	AC	156	
78	Al	132	

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Mol	Chain	Length	Quality of chain
79	Bm	128	
80	AD	133	
81	Am	151	
82	Bo	106	
83	AE	115	
84	An	151	
85	Bp	92	
86	AF	317	
87	Ao	145	
88	Br	136	
89	AG	56	
90	Ap	172	
91	Bs	318	

2 Entry composition

There are 99 unique types of molecules in this entry. The entry contains 237089 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
1	B5	3706	Total	C	N	O	P	0	0
			79525	35447	14532	25840	3706		

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 2 is a protein called 60S ribosomal protein L21.

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

- Molecule 3 is a protein called 60S ribosomal protein L29.

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

- Molecule 4 is a protein called 60S ribosomal protein L12.

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

- Molecule 5 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	AH	3	Total	C	O	P	0	0
			36	15	18	3		

- Molecule 6 is a protein called 40S ribosomal protein eS17.

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

- Molecule 7 is a RNA chain called 5S rRNA.

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

- Molecule 8 is a RNA chain called P-site tRNA.

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

- Molecule 9 is a protein called Small ribosomal subunit protein uS13.

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

- Molecule 10 is a RNA chain called 5.8S rRNA.

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

- Molecule 11 is a protein called 60S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	BU	102	Total	C	N	O	S	0	0
			831	531	146	152	2		

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BU	32	GLY	ARG	variant	UNP G1TSG1
BU	36	ALA	GLU	variant	UNP G1TSG1
BU	39	PHE	SER	variant	UNP G1TSG1
BU	54	GLY	ARG	variant	UNP G1TSG1
BU	97	ARG	HIS	variant	UNP G1TSG1

- Molecule 12 is a protein called 40S ribosomal protein S19.

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

There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 13 is a protein called Large ribosomal subunit protein uL2.

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

- Molecule 14 is a protein called Ribosomal protein L23.

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

- Molecule 15 is a protein called 40S ribosomal protein uS10.

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

- Molecule 16 is a protein called Ribosomal protein L3.

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

- Molecule 17 is a protein called Large ribosomal subunit protein uL22.

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

- Molecule 18 is a protein called Ribosomal protein L26.

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

- Molecule 19 is a protein called Ribosomal protein S15a.

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

- Molecule 20 is a protein called Large ribosomal subunit protein uL18.

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	176	SER	GLY	variant	UNP G1SZF4
B	248	ARG	GLN	variant	UNP G1SZF4

- Molecule 21 is a protein called Large ribosomal subunit protein uL23.

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

- Molecule 22 is a protein called Large ribosomal subunit protein eL18.

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

- Molecule 23 is a protein called 60S ribosomal protein L27.

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

- Molecule 24 is a protein called 40S ribosomal protein S23.

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

- Molecule 25 is a protein called 60S ribosomal protein L6.

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

- Molecule 26 is a protein called Ribosomal protein L24.

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

- Molecule 27 is a protein called Small ribosomal subunit protein eS21.

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

- Molecule 28 is a protein called 60S ribosomal protein L27a.

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

- Molecule 29 is a protein called 40S ribosomal protein S24.

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

- Molecule 30 is a protein called Ribosomal Protein uL30.

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

There are 4 discrepancies between the modelled and reference sequences:

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

- Molecule 31 is a protein called Ribosomal protein L19.

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

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BR	38	ARG	CYS	variant	UNP G1TJR3
BR	64	ARG	GLN	variant	UNP G1TJR3
BR	94	THR	LYS	variant	UNP G1TJR3

- Molecule 32 is a protein called Small ribosomal subunit protein uS2.

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

- Molecule 33 is a protein called 40S ribosomal protein S25.

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

- Molecule 34 is a protein called Large ribosomal subunit protein eL8.

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

- Molecule 35 is a protein called Large ribosomal subunit protein uL4.

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

- Molecule 36 is a protein called Large ribosomal subunit protein eL20.

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

- Molecule 37 is a protein called 40S ribosomal protein S3a.

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

- Molecule 38 is a protein called 60S ribosomal protein L41.

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

- Molecule 39 is a protein called 60S ribosomal protein L9.

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

- Molecule 40 is a protein called Methionine aminopeptidase 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	EA	304	Total	C	N	O	S	0	0
			2395	1505	430	442	18		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
EA	220	ASN	ASP	engineered mutation	UNP P53582

- Molecule 41 is a protein called Small ribosomal subunit protein uS5.

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

- Molecule 42 is a protein called 60S ribosomal protein L30.

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

- Molecule 43 is a protein called 60S ribosomal protein L10.

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

- Molecule 44 is a protein called Nascent polypeptide-associated complex subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	Ct	117	Total	C	N	O	S	0	0
			908	568	166	170	4		

There are 23 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Ct	-22	MET	-	initiating methionine	UNP Q13765
Ct	-21	GLY	-	expression tag	UNP Q13765
Ct	-20	SER	-	expression tag	UNP Q13765
Ct	-19	SER	-	expression tag	UNP Q13765
Ct	-18	HIS	-	expression tag	UNP Q13765
Ct	-17	HIS	-	expression tag	UNP Q13765
Ct	-16	HIS	-	expression tag	UNP Q13765
Ct	-15	HIS	-	expression tag	UNP Q13765
Ct	-14	HIS	-	expression tag	UNP Q13765
Ct	-13	HIS	-	expression tag	UNP Q13765
Ct	-12	SER	-	expression tag	UNP Q13765
Ct	-11	SER	-	expression tag	UNP Q13765
Ct	-10	GLY	-	expression tag	UNP Q13765
Ct	-9	LEU	-	expression tag	UNP Q13765
Ct	-8	GLU	-	expression tag	UNP Q13765
Ct	-7	VAL	-	expression tag	UNP Q13765
Ct	-6	LEU	-	expression tag	UNP Q13765
Ct	-5	PHE	-	expression tag	UNP Q13765
Ct	-4	GLN	-	expression tag	UNP Q13765
Ct	-3	GLY	-	expression tag	UNP Q13765
Ct	-2	PRO	-	expression tag	UNP Q13765
Ct	-1	SER	-	expression tag	UNP Q13765
Ct	0	GLY	-	expression tag	UNP Q13765

- Molecule 45 is a protein called 40S ribosomal protein S3.

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

- Molecule 46 is a protein called 60S ribosomal protein L31.

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

- Molecule 47 is a protein called 60S ribosomal protein L11.

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

- Molecule 48 is a protein called Isoform 2 of Transcription factor BTF3.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	Cu	107	Total	C	N	O	S	0	0
			828	518	154	153	3		

- Molecule 49 is a protein called 40S ribosomal protein S4.

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

There are 4 discrepancies between the modelled and reference sequences:

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

- Molecule 50 is a protein called Ribosomal protein L32.

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

- Molecule 51 is a protein called Nascent chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
51	BK	27	Total	C	N	O	0	0
			135	81	27	27		

- Molecule 52 is a protein called Glutathione S-transferase class-mu 26 kDa isozyme,N-alpha-acetyltransferase 50,N-alpha-acetyltransferase 50.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	DA	155	Total	C	N	O	S	0	0
			1260	808	221	225	6		

- Molecule 53 is a protein called Ribosomal protein S5.

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

- Molecule 54 is a protein called 60S ribosomal protein L35a.

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

- Molecule 55 is a protein called Large ribosomal subunit protein eL13.

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

There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 56 is a protein called N-alpha-acetyltransferase 15, NatA auxiliary subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	DB	837	Total	C	N	O	S	0	0
			6900	4391	1192	1276	41		

There are 49 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DB	-48	MET	-	initiating methionine	UNP Q9BXJ9
DB	-47	GLY	-	expression tag	UNP Q9BXJ9
DB	-46	SER	-	expression tag	UNP Q9BXJ9
DB	-45	SER	-	expression tag	UNP Q9BXJ9
DB	-44	HIS	-	expression tag	UNP Q9BXJ9
DB	-43	HIS	-	expression tag	UNP Q9BXJ9
DB	-42	HIS	-	expression tag	UNP Q9BXJ9
DB	-41	HIS	-	expression tag	UNP Q9BXJ9
DB	-40	HIS	-	expression tag	UNP Q9BXJ9
DB	-39	HIS	-	expression tag	UNP Q9BXJ9
DB	-38	SER	-	expression tag	UNP Q9BXJ9
DB	-37	SER	-	expression tag	UNP Q9BXJ9
DB	-36	GLY	-	expression tag	UNP Q9BXJ9
DB	-35	LEU	-	expression tag	UNP Q9BXJ9
DB	-34	VAL	-	expression tag	UNP Q9BXJ9
DB	-33	PRO	-	expression tag	UNP Q9BXJ9
DB	-32	ARG	-	expression tag	UNP Q9BXJ9
DB	-31	GLY	-	expression tag	UNP Q9BXJ9
DB	-30	SER	-	expression tag	UNP Q9BXJ9
DB	-29	HIS	-	expression tag	UNP Q9BXJ9
DB	-28	MET	-	expression tag	UNP Q9BXJ9
DB	-27	ALA	-	expression tag	UNP Q9BXJ9
DB	-26	SER	-	expression tag	UNP Q9BXJ9
DB	-25	MET	-	expression tag	UNP Q9BXJ9
DB	-24	THR	-	expression tag	UNP Q9BXJ9
DB	-23	GLY	-	expression tag	UNP Q9BXJ9
DB	-22	GLY	-	expression tag	UNP Q9BXJ9
DB	-21	GLN	-	expression tag	UNP Q9BXJ9
DB	-20	GLN	-	expression tag	UNP Q9BXJ9
DB	-19	MET	-	expression tag	UNP Q9BXJ9
DB	-18	GLY	-	expression tag	UNP Q9BXJ9
DB	-17	ARG	-	expression tag	UNP Q9BXJ9
DB	-16	ALA	-	expression tag	UNP Q9BXJ9
DB	-15	ARG	-	expression tag	UNP Q9BXJ9
DB	-14	GLY	-	expression tag	UNP Q9BXJ9
DB	-13	ILE	-	expression tag	UNP Q9BXJ9
DB	-12	GLN	-	expression tag	UNP Q9BXJ9
DB	-11	ARG	-	expression tag	UNP Q9BXJ9
DB	-10	PRO	-	expression tag	UNP Q9BXJ9
DB	-9	THR	-	expression tag	UNP Q9BXJ9
DB	-8	SER	-	expression tag	UNP Q9BXJ9
DB	-7	THR	-	expression tag	UNP Q9BXJ9
DB	-6	SER	-	expression tag	UNP Q9BXJ9

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Chain	Residue	Modelled	Actual	Comment	Reference
DB	-5	SER	-	expression tag	UNP Q9BXJ9
DB	-4	LEU	-	expression tag	UNP Q9BXJ9
DB	-3	VAL	-	expression tag	UNP Q9BXJ9
DB	-2	ALA	-	expression tag	UNP Q9BXJ9
DB	-1	ALA	-	expression tag	UNP Q9BXJ9
DB	0	ALA	-	expression tag	UNP Q9BXJ9

- Molecule 57 is a protein called 40S ribosomal protein S6.

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

- Molecule 58 is a protein called 60S ribosomal protein L34.

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

- Molecule 59 is a protein called 60S ribosomal protein L14.

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

- Molecule 60 is a protein called N-alpha-acetyltransferase 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	DC	165	Total	C	N	O	S	0	0
			1339	844	242	242	11		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DC	24	GLN	GLU	engineered mutation	UNP P41227
DC	26	PHE	TYR	engineered mutation	UNP P41227

- Molecule 61 is a protein called 40S ribosomal protein S7.

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

- Molecule 62 is a protein called 60S ribosomal protein L35.

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

- Molecule 63 is a protein called Ribosomal protein L15.

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

- Molecule 64 is a protein called Isoform 2 of Huntingtin-interacting protein K.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	DD	57	Total	C	N	O	S	0	0
			439	269	78	89	3		

There are 107 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DD	-106	MET	-	initiating methionine	UNP Q9NX55
DD	-105	LYS	-	expression tag	UNP Q9NX55
DD	-104	HIS	-	expression tag	UNP Q9NX55
DD	-103	HIS	-	expression tag	UNP Q9NX55
DD	-102	HIS	-	expression tag	UNP Q9NX55
DD	-101	HIS	-	expression tag	UNP Q9NX55
DD	-100	HIS	-	expression tag	UNP Q9NX55
DD	-99	HIS	-	expression tag	UNP Q9NX55
DD	-98	PRO	-	expression tag	UNP Q9NX55
DD	-97	MET	-	expression tag	UNP Q9NX55
DD	-96	SER	-	expression tag	UNP Q9NX55
DD	-95	ASP	-	expression tag	UNP Q9NX55
DD	-94	SER	-	expression tag	UNP Q9NX55
DD	-93	GLU	-	expression tag	UNP Q9NX55
DD	-92	VAL	-	expression tag	UNP Q9NX55
DD	-91	ASN	-	expression tag	UNP Q9NX55
DD	-90	GLN	-	expression tag	UNP Q9NX55
DD	-89	GLU	-	expression tag	UNP Q9NX55
DD	-88	ALA	-	expression tag	UNP Q9NX55

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Chain	Residue	Modelled	Actual	Comment	Reference
DD	-87	LYS	-	expression tag	UNP Q9NX55
DD	-86	PRO	-	expression tag	UNP Q9NX55
DD	-85	GLU	-	expression tag	UNP Q9NX55
DD	-84	VAL	-	expression tag	UNP Q9NX55
DD	-83	LYS	-	expression tag	UNP Q9NX55
DD	-82	PRO	-	expression tag	UNP Q9NX55
DD	-81	GLU	-	expression tag	UNP Q9NX55
DD	-80	VAL	-	expression tag	UNP Q9NX55
DD	-79	LYS	-	expression tag	UNP Q9NX55
DD	-78	PRO	-	expression tag	UNP Q9NX55
DD	-77	GLU	-	expression tag	UNP Q9NX55
DD	-76	THR	-	expression tag	UNP Q9NX55
DD	-75	HIS	-	expression tag	UNP Q9NX55
DD	-74	ILE	-	expression tag	UNP Q9NX55
DD	-73	ASN	-	expression tag	UNP Q9NX55
DD	-72	LEU	-	expression tag	UNP Q9NX55
DD	-71	LYS	-	expression tag	UNP Q9NX55
DD	-70	VAL	-	expression tag	UNP Q9NX55
DD	-69	SER	-	expression tag	UNP Q9NX55
DD	-68	ASP	-	expression tag	UNP Q9NX55
DD	-67	GLY	-	expression tag	UNP Q9NX55
DD	-66	SER	-	expression tag	UNP Q9NX55
DD	-65	SER	-	expression tag	UNP Q9NX55
DD	-64	GLU	-	expression tag	UNP Q9NX55
DD	-63	ILE	-	expression tag	UNP Q9NX55
DD	-62	PHE	-	expression tag	UNP Q9NX55
DD	-61	PHE	-	expression tag	UNP Q9NX55
DD	-60	LYS	-	expression tag	UNP Q9NX55
DD	-59	ILE	-	expression tag	UNP Q9NX55
DD	-58	LYS	-	expression tag	UNP Q9NX55
DD	-57	LYS	-	expression tag	UNP Q9NX55
DD	-56	THR	-	expression tag	UNP Q9NX55
DD	-55	THR	-	expression tag	UNP Q9NX55
DD	-54	PRO	-	expression tag	UNP Q9NX55
DD	-53	LEU	-	expression tag	UNP Q9NX55
DD	-52	ARG	-	expression tag	UNP Q9NX55
DD	-51	ARG	-	expression tag	UNP Q9NX55
DD	-50	LEU	-	expression tag	UNP Q9NX55
DD	-49	MET	-	expression tag	UNP Q9NX55
DD	-48	GLU	-	expression tag	UNP Q9NX55
DD	-47	ALA	-	expression tag	UNP Q9NX55
DD	-46	PHE	-	expression tag	UNP Q9NX55

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Chain	Residue	Modelled	Actual	Comment	Reference
DD	-45	ALA	-	expression tag	UNP Q9NX55
DD	-44	LYS	-	expression tag	UNP Q9NX55
DD	-43	ARG	-	expression tag	UNP Q9NX55
DD	-42	GLN	-	expression tag	UNP Q9NX55
DD	-41	GLY	-	expression tag	UNP Q9NX55
DD	-40	LYS	-	expression tag	UNP Q9NX55
DD	-39	GLU	-	expression tag	UNP Q9NX55
DD	-38	MET	-	expression tag	UNP Q9NX55
DD	-37	ASP	-	expression tag	UNP Q9NX55
DD	-36	SER	-	expression tag	UNP Q9NX55
DD	-35	LEU	-	expression tag	UNP Q9NX55
DD	-34	ARG	-	expression tag	UNP Q9NX55
DD	-33	PHE	-	expression tag	UNP Q9NX55
DD	-32	LEU	-	expression tag	UNP Q9NX55
DD	-31	TYR	-	expression tag	UNP Q9NX55
DD	-30	ASP	-	expression tag	UNP Q9NX55
DD	-29	GLY	-	expression tag	UNP Q9NX55
DD	-28	ILE	-	expression tag	UNP Q9NX55
DD	-27	ARG	-	expression tag	UNP Q9NX55
DD	-26	ILE	-	expression tag	UNP Q9NX55
DD	-25	GLN	-	expression tag	UNP Q9NX55
DD	-24	ALA	-	expression tag	UNP Q9NX55
DD	-23	ASP	-	expression tag	UNP Q9NX55
DD	-22	GLN	-	expression tag	UNP Q9NX55
DD	-21	THR	-	expression tag	UNP Q9NX55
DD	-20	PRO	-	expression tag	UNP Q9NX55
DD	-19	GLU	-	expression tag	UNP Q9NX55
DD	-18	ASP	-	expression tag	UNP Q9NX55
DD	-17	LEU	-	expression tag	UNP Q9NX55
DD	-16	ASP	-	expression tag	UNP Q9NX55
DD	-15	MET	-	expression tag	UNP Q9NX55
DD	-14	GLU	-	expression tag	UNP Q9NX55
DD	-13	ASP	-	expression tag	UNP Q9NX55
DD	-12	ASN	-	expression tag	UNP Q9NX55
DD	-11	ASP	-	expression tag	UNP Q9NX55
DD	-10	ILE	-	expression tag	UNP Q9NX55
DD	-9	ILE	-	expression tag	UNP Q9NX55
DD	-8	GLU	-	expression tag	UNP Q9NX55
DD	-7	ALA	-	expression tag	UNP Q9NX55
DD	-6	HIS	-	expression tag	UNP Q9NX55
DD	-5	ARG	-	expression tag	UNP Q9NX55
DD	-4	GLU	-	expression tag	UNP Q9NX55

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Chain	Residue	Modelled	Actual	Comment	Reference
DD	-3	GLN	-	expression tag	UNP Q9NX55
DD	-2	ILE	-	expression tag	UNP Q9NX55
DD	-1	GLY	-	expression tag	UNP Q9NX55
DD	0	GLY	-	expression tag	UNP Q9NX55

- Molecule 65 is a protein called 40S ribosomal protein S8.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 66 is a protein called 60S ribosomal protein L36.

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

- Molecule 67 is a protein called Large ribosomal subunit protein uL13.

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

- Molecule 68 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	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 69 is a protein called 40S ribosomal protein S9.

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

- Molecule 70 is a protein called Ribosomal protein L37.

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

- Molecule 71 is a protein called 40S ribosomal protein S27.

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

- Molecule 72 is a protein called S10_pectin domain-containing protein.

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

- Molecule 73 is a protein called 60S ribosomal protein L38.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 74 is a protein called 40S ribosomal protein S28.

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

- Molecule 75 is a protein called 40S ribosomal protein S11.

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

- Molecule 76 is a protein called 60S ribosomal protein L39-like.

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

- Molecule 77 is a protein called Ribosomal protein S27a.

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

- Molecule 78 is a protein called 40S ribosomal protein S12.

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

- Molecule 79 is a protein called Ubiquitin-ribosomal protein eL40 fusion protein.

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

- Molecule 80 is a protein called 40S ribosomal protein S30.

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

- Molecule 81 is a protein called 40S ribosomal protein S13.

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

- Molecule 82 is a protein called Large ribosomal subunit protein eL42.

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

- Molecule 83 is a protein called Small ribosomal subunit protein eS26.

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

- Molecule 84 is a protein called Small ribosomal subunit protein uS11.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
An	165	IAS	ASP	conflict	UNP A0AAA9WYR1

- Molecule 85 is a protein called 60S ribosomal protein L37a.

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

- Molecule 86 is a protein called Small ribosomal subunit protein RACK1.

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

- Molecule 87 is a protein called 40S ribosomal protein uS19.

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

- Molecule 88 is a protein called Large ribosomal subunit protein eL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
88	Br	123	Total	C	N	O	S	0	0
			990	613	205	167	5		

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 89 is a protein called 40S ribosomal protein S29.

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

- Molecule 90 is a protein called Small ribosomal subunit protein uS9.

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

- Molecule 91 is a protein called Large ribosomal subunit protein uL10.

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

- Molecule 92 is UNKNOWN LIGAND (CCD ID: UNX) (formula: X).

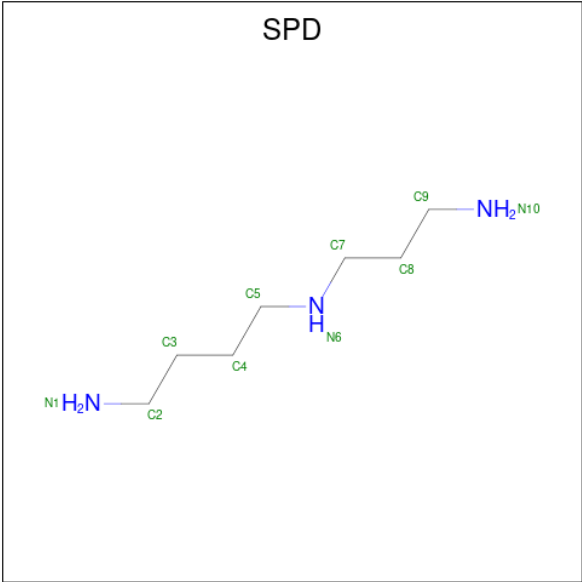
Mol	Chain	Residues	Atoms		AltConf
92	B5	200	Total	X	0
			200	200	
92	BT	2	Total	X	0
			2	2	
92	Bb	2	Total	X	0
			2	2	
92	B7	6	Total	X	0
			6	6	
92	AT	2	Total	X	0
			2	2	
92	B8	6	Total	X	0
			6	6	
92	BA	4	Total	X	0
			4	4	

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Mol	Chain	Residues	Atoms		AltConf
92	BB	3	Total 3	X 3	0
92	BY	1	Total 1	X 1	0
92	BQ	2	Total 2	X 2	0
92	BH	1	Total 1	X 1	0
92	BI	1	Total 1	X 1	0
92	Ad	1	Total 1	X 1	0
92	Be	3	Total 3	X 3	0
92	Bf	1	Total 1	X 1	0
92	BL	1	Total 1	X 1	0
92	BN	1	Total 1	X 1	0
92	A2	54	Total 54	X 54	0
92	Ak	1	Total 1	X 1	0
92	Bo	1	Total 1	X 1	0
92	AE	1	Total 1	X 1	0
92	An	1	Total 1	X 1	0

- Molecule 93 is SPERMIDINE (CCD ID: SPD) (formula: $C_7H_{19}N_3$).



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

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

- Molecule 94 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

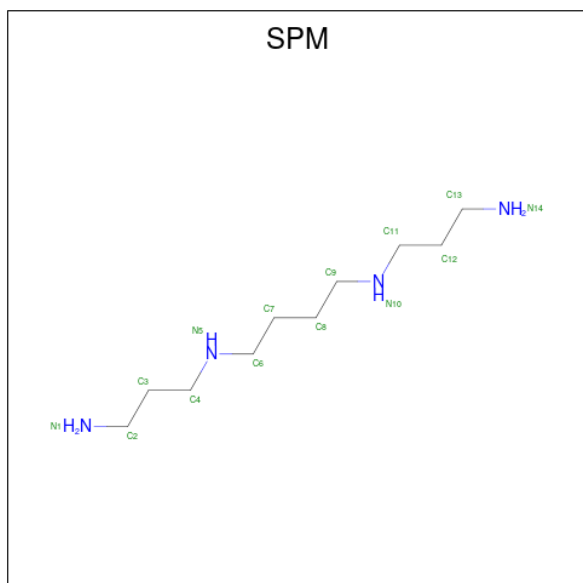
Mol	Chain	Residues	Atoms		AltConf
94	B5	283	Total	Mg	0
			283	283	
94	B7	9	Total	Mg	0
			9	9	
94	AT	2	Total	Mg	0
			2	2	

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Mol	Chain	Residues	Atoms		AltConf
94	B8	8	Total	Mg	0
			8	8	
94	BV	1	Total	Mg	0
			1	1	
94	BP	1	Total	Mg	0
			1	1	
94	Ba	1	Total	Mg	0
			1	1	
94	BI	1	Total	Mg	0
			1	1	
94	Ct	1	Total	Mg	0
			1	1	
94	Be	1	Total	Mg	0
			1	1	
94	A2	110	Total	Mg	0
			110	110	
94	Bj	1	Total	Mg	0
			1	1	
94	An	1	Total	Mg	0
			1	1	

- Molecule 95 is SPERMINE (CCD ID: SPM) (formula: $C_{10}H_{26}N_4$).



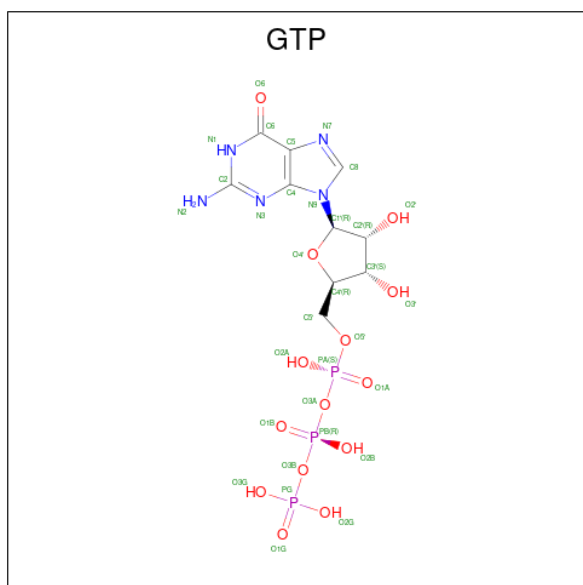
Mol	Chain	Residues	Atoms			AltConf
95	B5	1	Total	C	N	0
			14	10	4	

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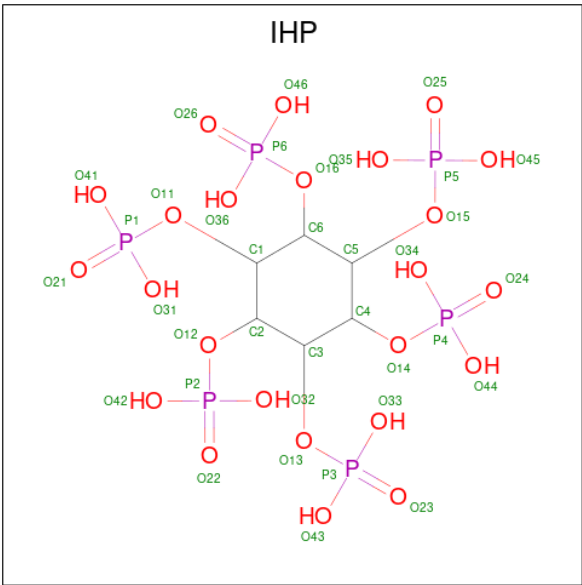
Mol	Chain	Residues	Atoms			AltConf
95	B5	1	Total	C	N	0
			14	10	4	
95	A2	1	Total	C	N	0
			14	10	4	

- Molecule 96 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



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

- Molecule 97 is INOSITOL HEXAKISPHOSPHATE (CCD ID: IHP) (formula: $C_6H_{18}O_{24}P_6$).



Mol	Chain	Residues	Atoms				AltConf
97	DB	1	Total	C	O	P	0
			36	6	24	6	

- Molecule 98 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 99 is water.

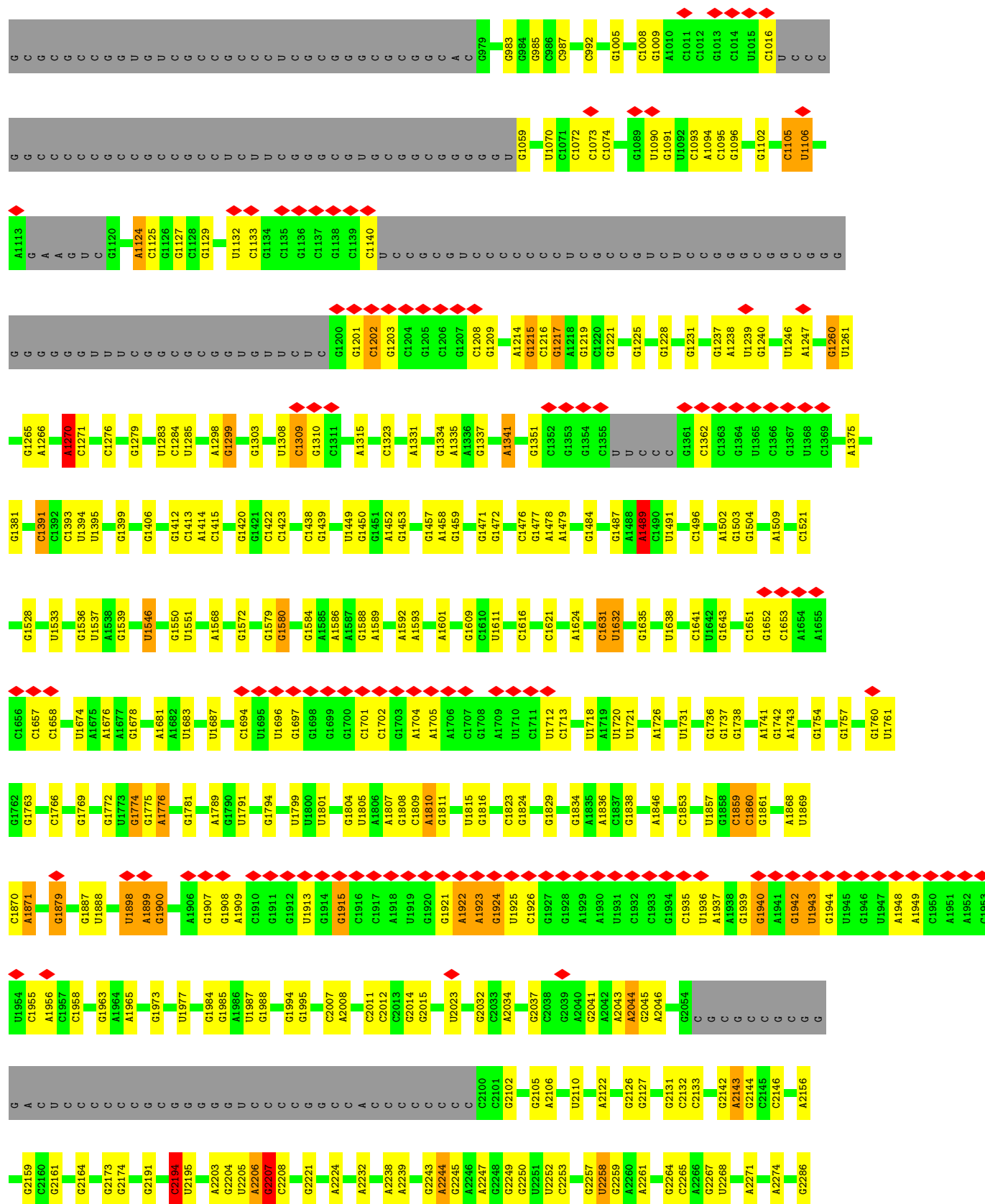
Mol	Chain	Residues	Atoms		AltConf
99	B5	1383	Total 1383	O 1383	0
99	BT	2	Total 2	O 2	0
99	Bb	1	Total 1	O 1	0
99	AH	3	Total 3	O 3	0
99	B7	45	Total 45	O 45	0
99	AT	12	Total 12	O 12	0
99	Ar	2	Total 2	O 2	0
99	B8	48	Total 48	O 48	0
99	As	1	Total 1	O 1	0
99	BA	7	Total 7	O 7	0
99	BV	3	Total 3	O 3	0
99	BB	8	Total 8	O 8	0
99	BP	3	Total 3	O 3	0
99	B	1	Total 1	O 1	0
99	BX	1	Total 1	O 1	0
99	Aw	4	Total 4	O 4	0
99	Ba	7	Total 7	O 7	0
99	BR	5	Total 5	O 5	0
99	BC	6	Total 6	O 6	0
99	Aa	3	Total 3	O 3	0
99	BH	2	Total 2	O 2	0
99	BI	1	Total 1	O 1	0

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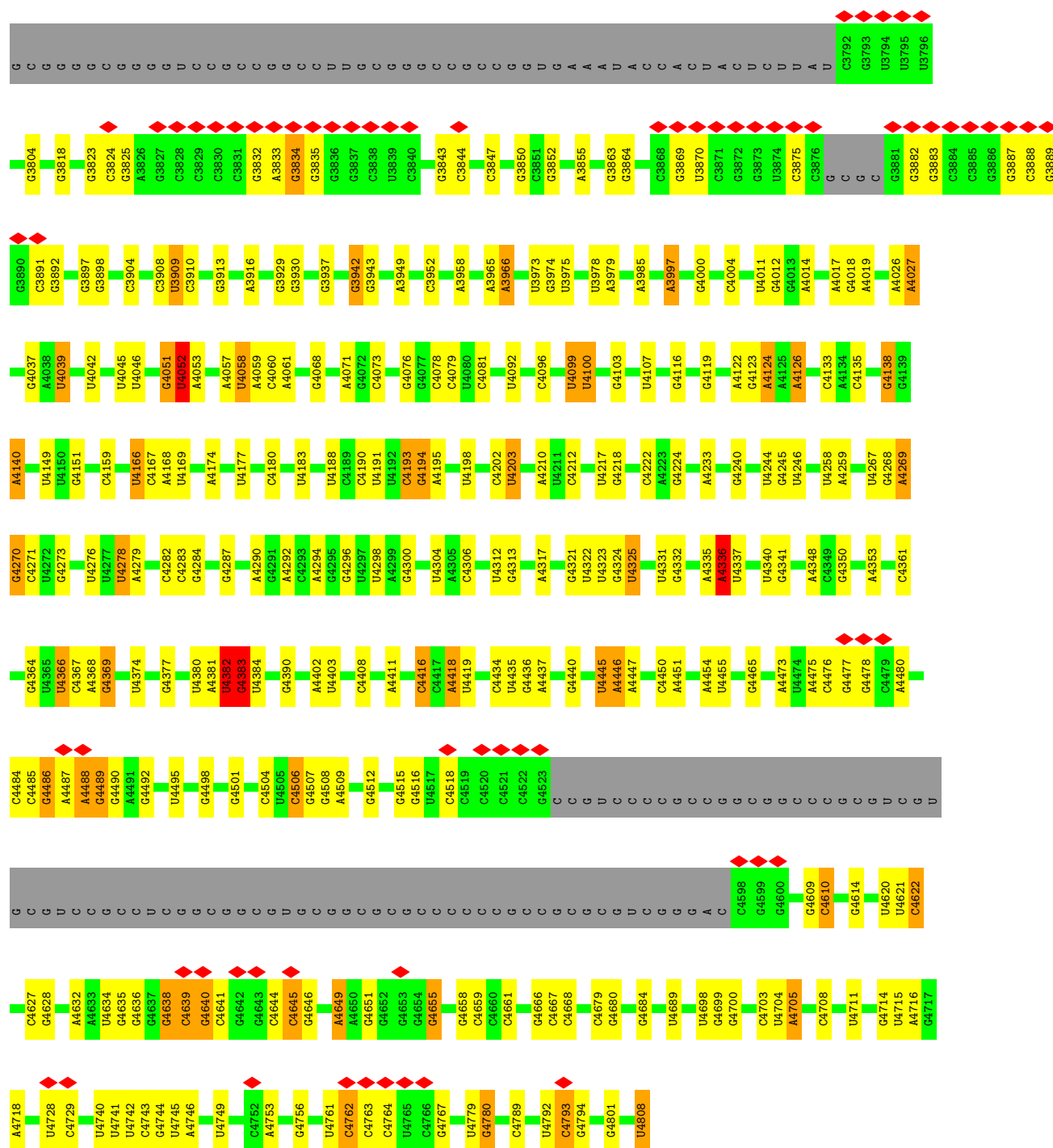
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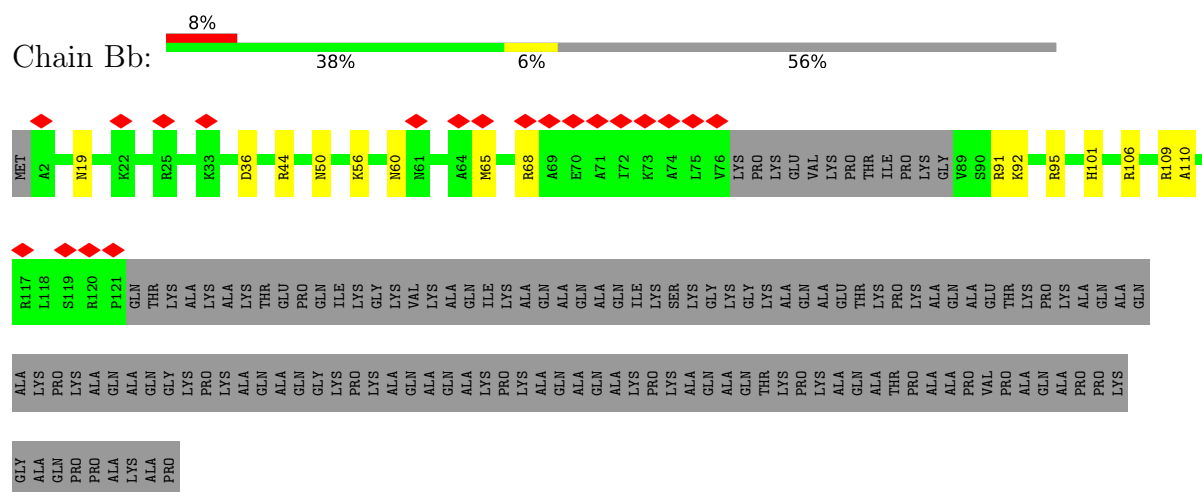
Mol	Chain	Residues	Atoms		AltConf
99	Ct	3	Total 3	O 3	0
99	Bd	1	Total 1	O 1	0
99	Ad	2	Total 2	O 2	0
99	Be	4	Total 4	O 4	0
99	BL	1	Total 1	O 1	0
99	Af	1	Total 1	O 1	0
99	Bg	3	Total 3	O 3	0
99	BN	6	Total 6	O 6	0
99	A2	531	Total 531	O 531	0
99	Bj	6	Total 6	O 6	0
99	Ak	2	Total 2	O 2	0
99	Bl	3	Total 3	O 3	0
99	Bm	1	Total 1	O 1	0
99	Bo	1	Total 1	O 1	0
99	AE	1	Total 1	O 1	0
99	An	1	Total 1	O 1	0
99	Ap	2	Total 2	O 2	0



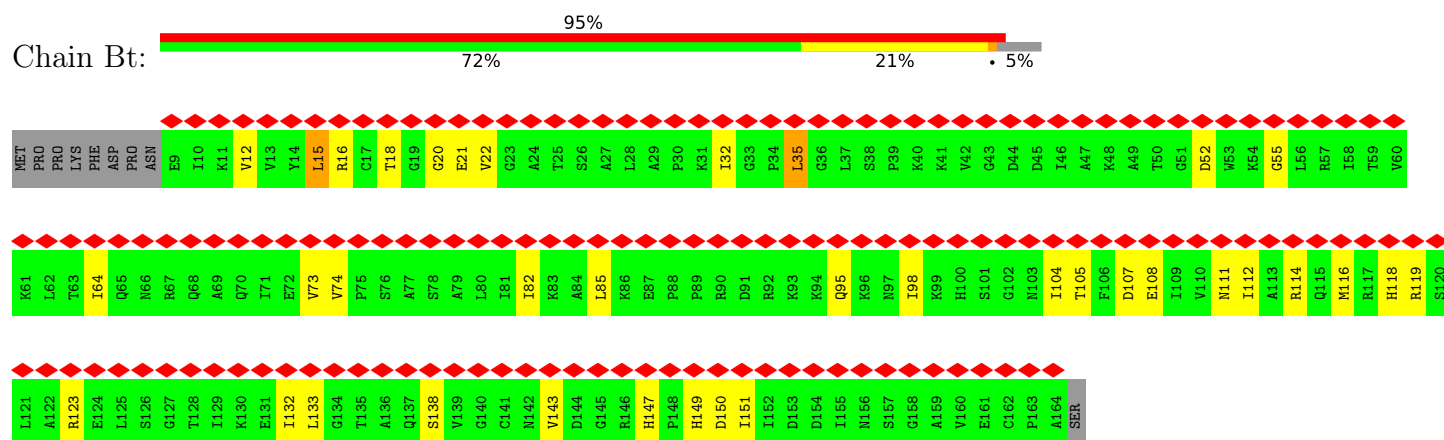




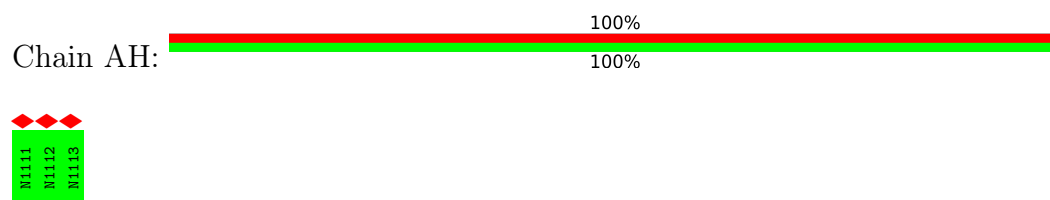




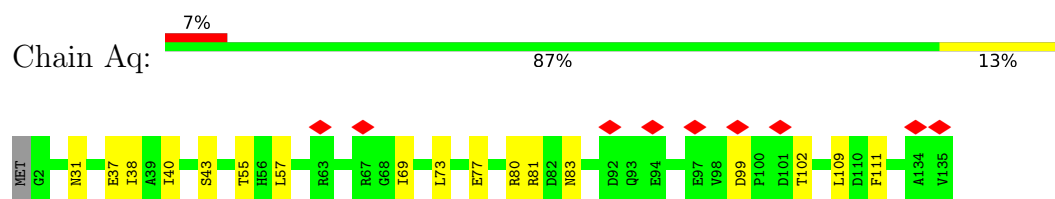
- Molecule 4: 60S ribosomal protein L12



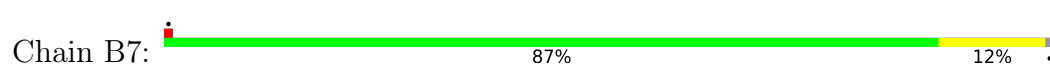
- Molecule 5: mRNA



- Molecule 6: 40S ribosomal protein eS17

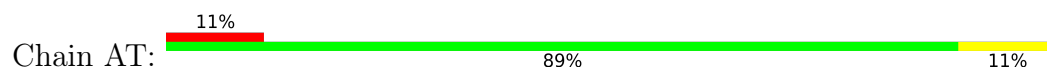


- Molecule 7: 5S rRNA

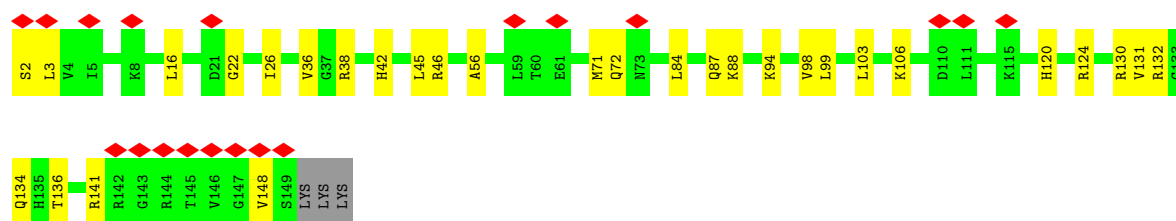
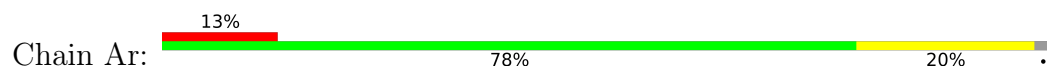




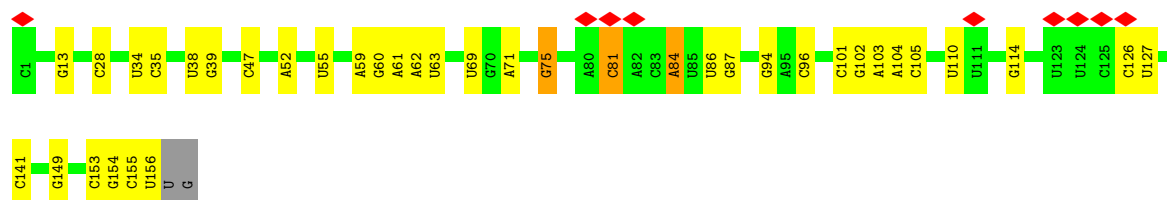
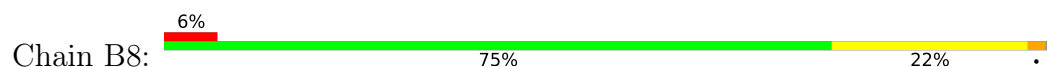
- Molecule 8: P-site tRNA



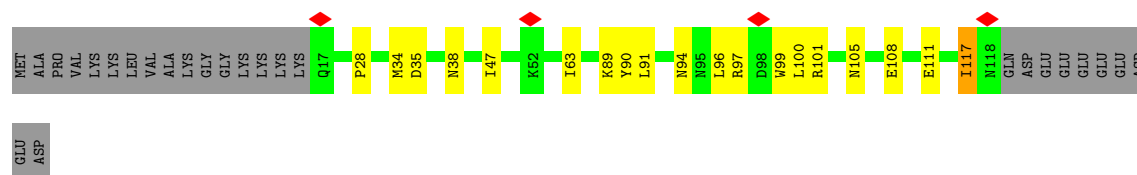
- Molecule 9: Small ribosomal subunit protein uS13



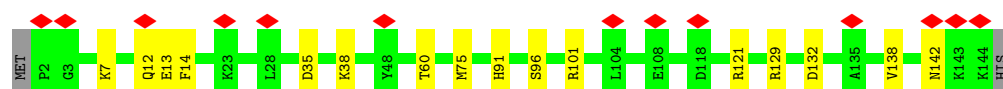
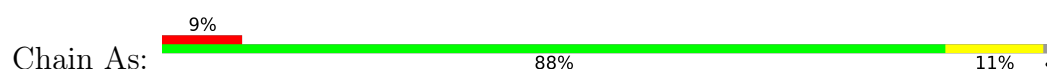
- Molecule 10: 5.8S rRNA

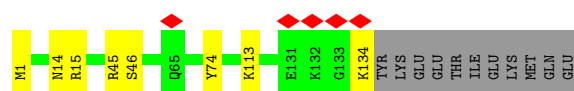
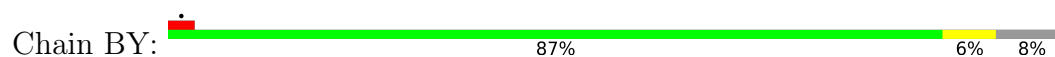


- Molecule 11: 60S ribosomal protein L22

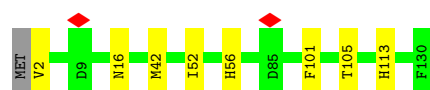


- Molecule 12: 40S ribosomal protein S19

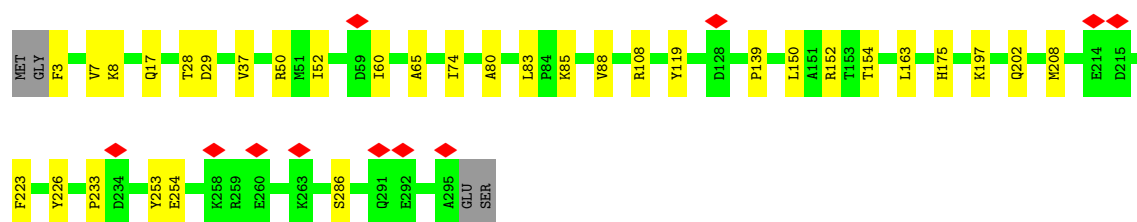
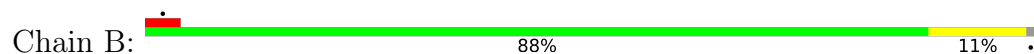




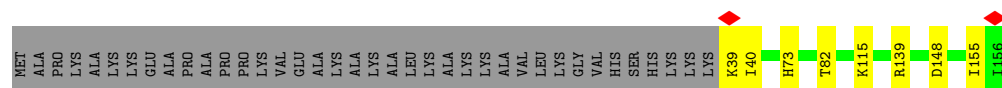
- Molecule 19: Ribosomal protein S15a



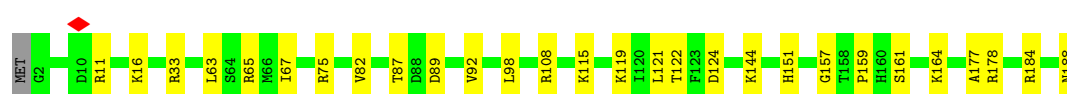
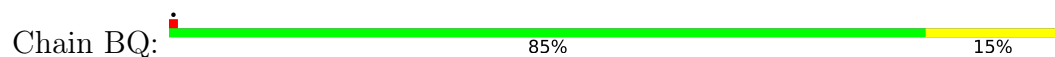
- Molecule 20: Large ribosomal subunit protein uL18



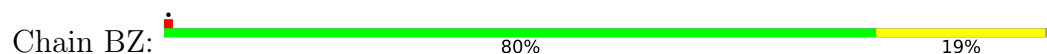
- Molecule 21: Large ribosomal subunit protein uL23



- Molecule 22: Large ribosomal subunit protein eL18

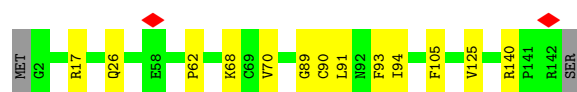


- Molecule 23: 60S ribosomal protein L27

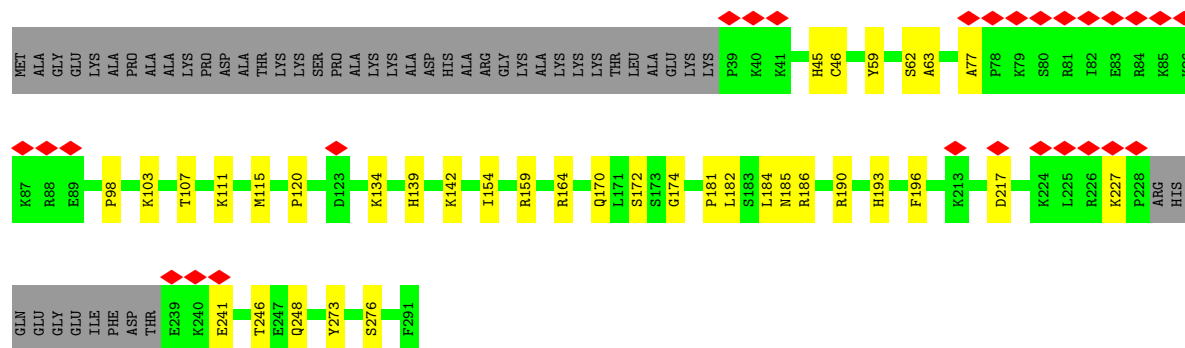
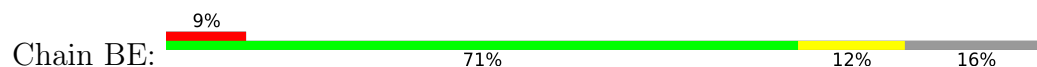


- Molecule 24: 40S ribosomal protein S23

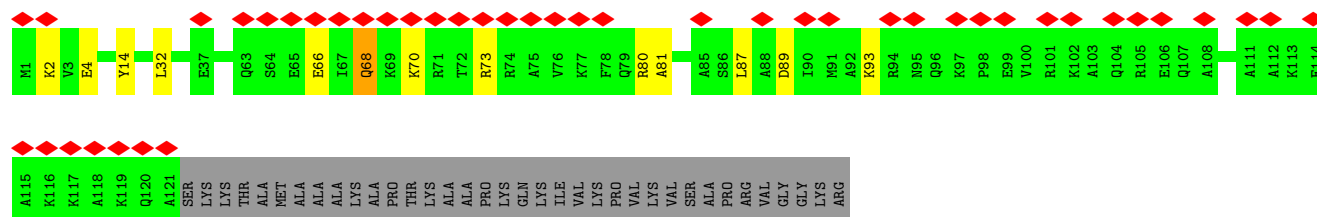
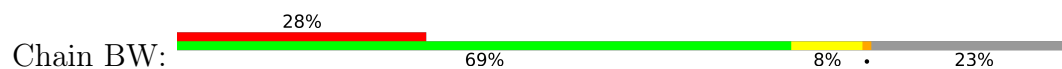




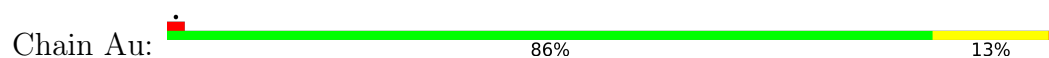
- Molecule 25: 60S ribosomal protein L6



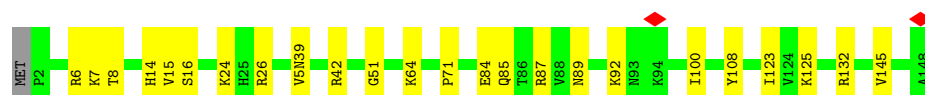
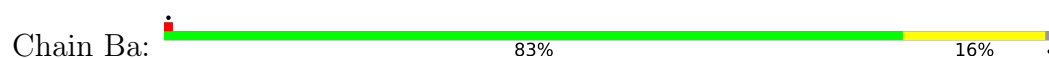
- Molecule 26: Ribosomal protein L24



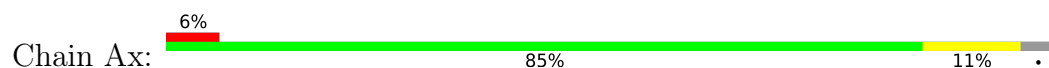
- Molecule 27: Small ribosomal subunit protein eS21

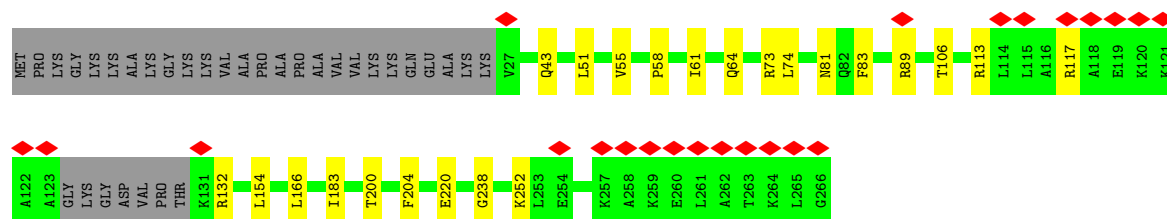
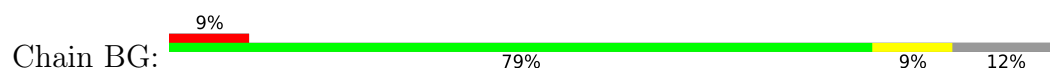


- Molecule 28: 60S ribosomal protein L27a

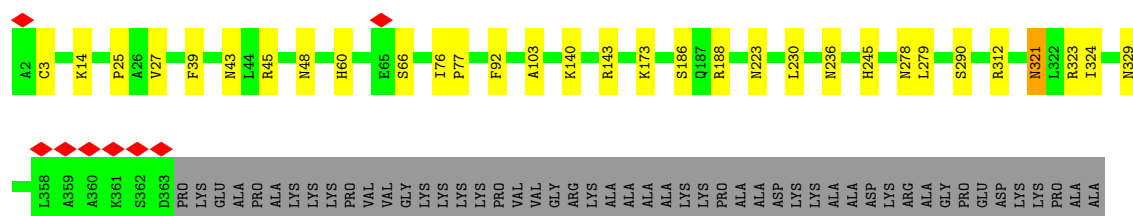
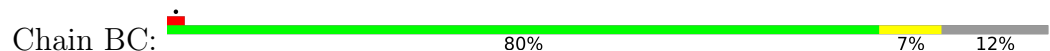


- Molecule 29: 40S ribosomal protein S24





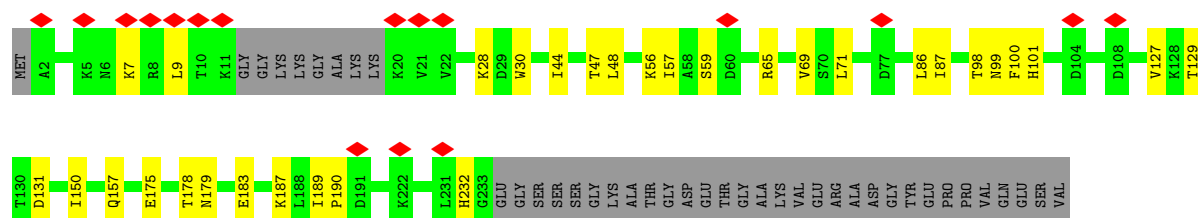
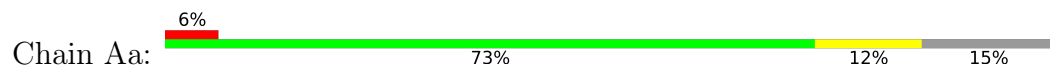
- Molecule 35: Large ribosomal subunit protein uL4



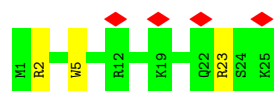
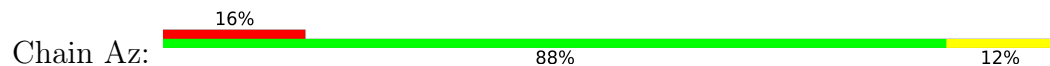
- Molecule 36: Large ribosomal subunit protein eL20



- Molecule 37: 40S ribosomal protein S3a



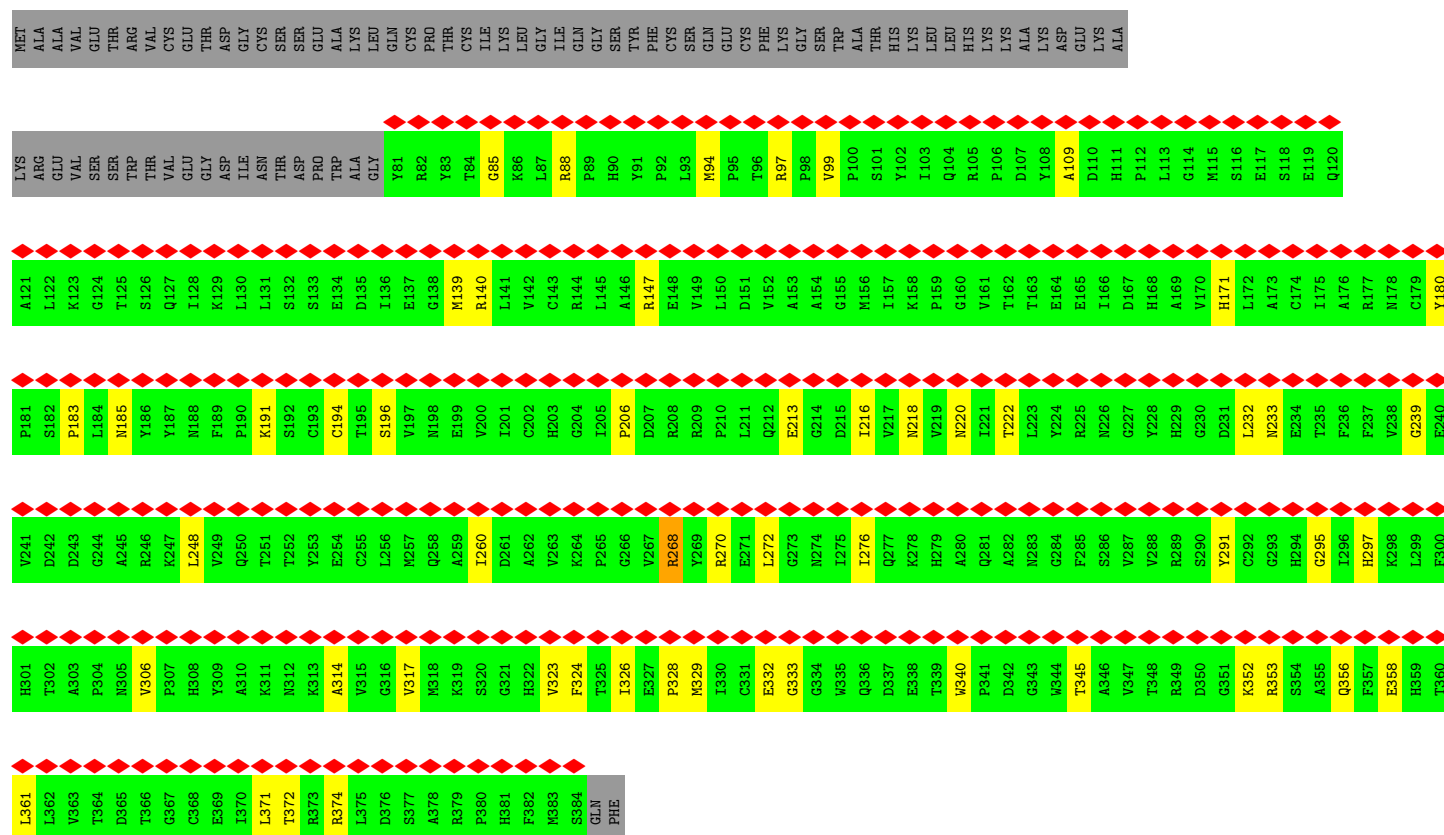
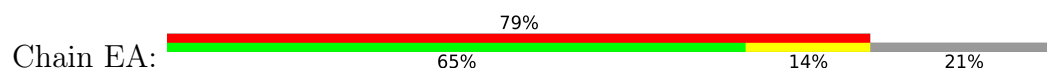
- Molecule 38: 60S ribosomal protein L41



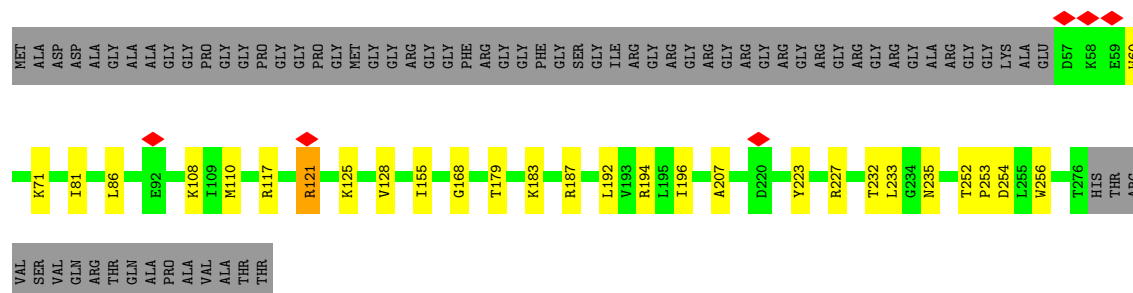
- Molecule 39: 60S ribosomal protein L9



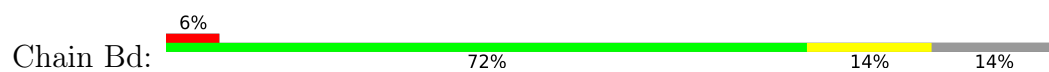
- Molecule 40: Methionine aminopeptidase 1



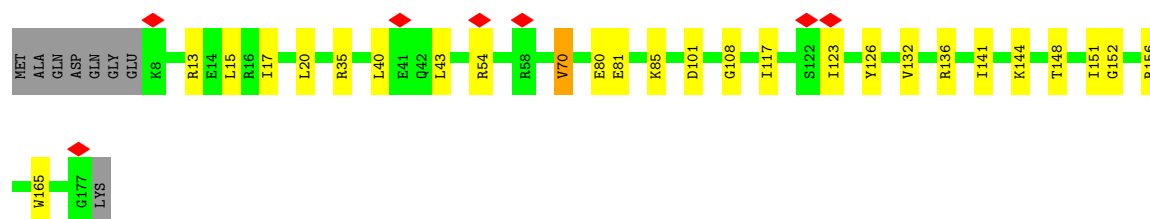
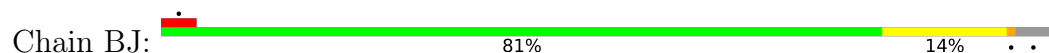
- Molecule 41: Small ribosomal subunit protein uS5



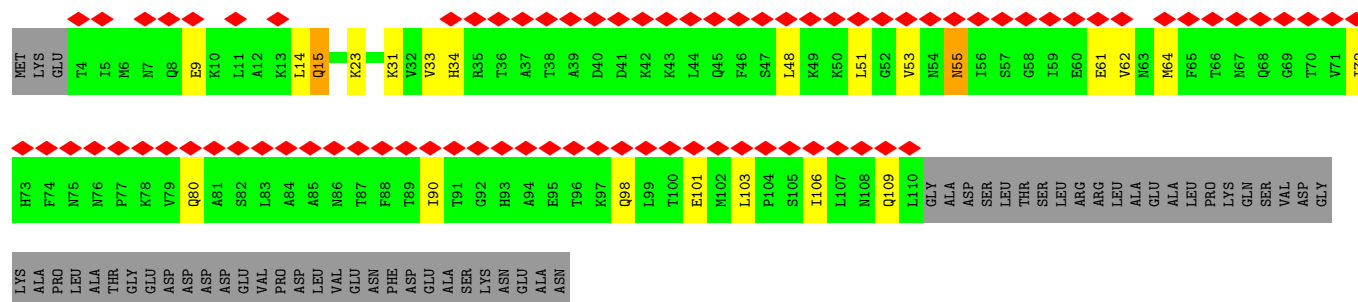
- Molecule 42: 60S ribosomal protein L30



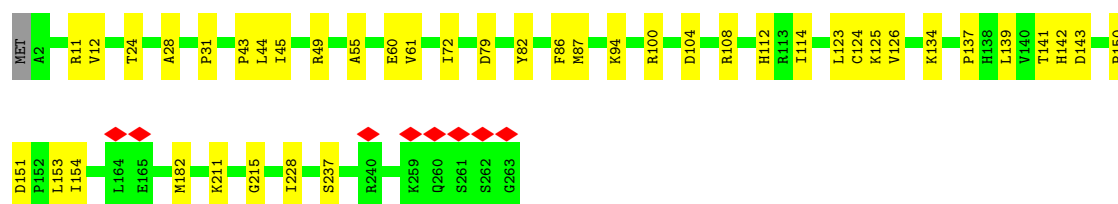
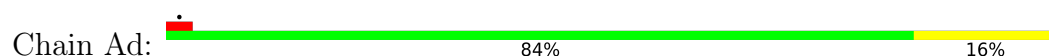
- Molecule 47: 60S ribosomal protein L11



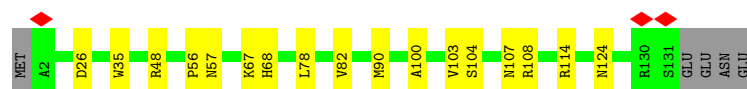
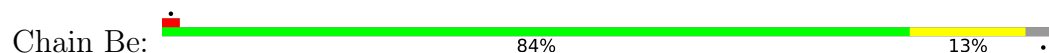
- Molecule 48: Isoform 2 of Transcription factor BTF3



- Molecule 49: 40S ribosomal protein S4



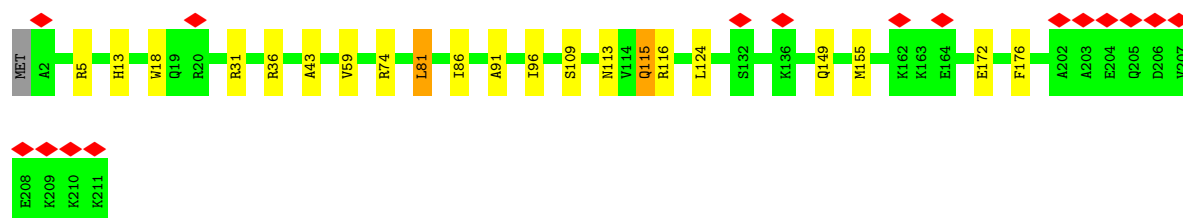
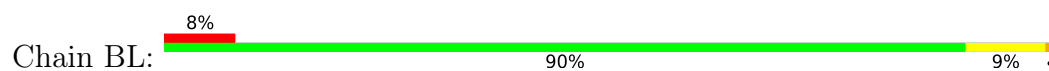
- Molecule 50: Ribosomal protein L32



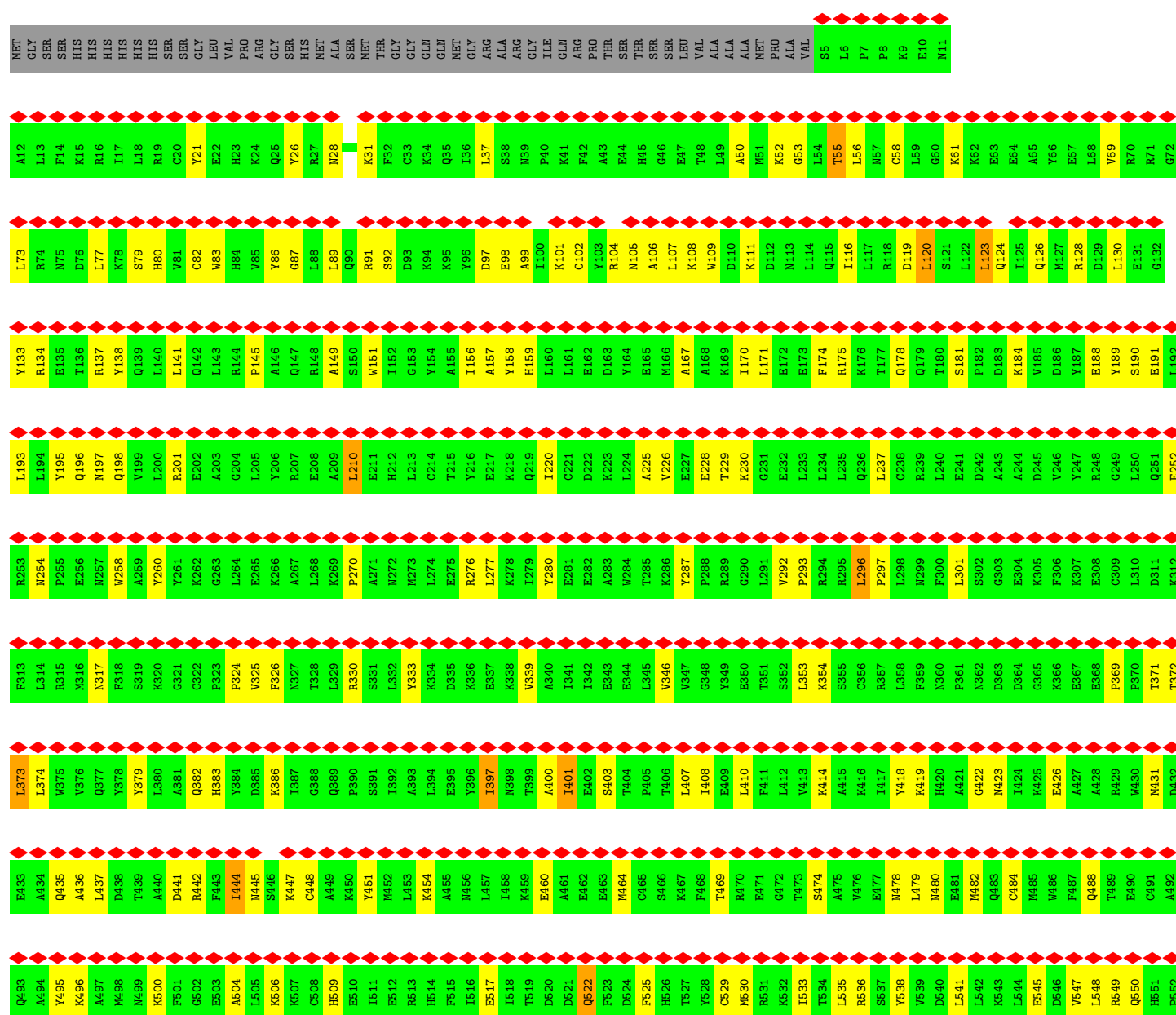
- Molecule 51: Nascent chain

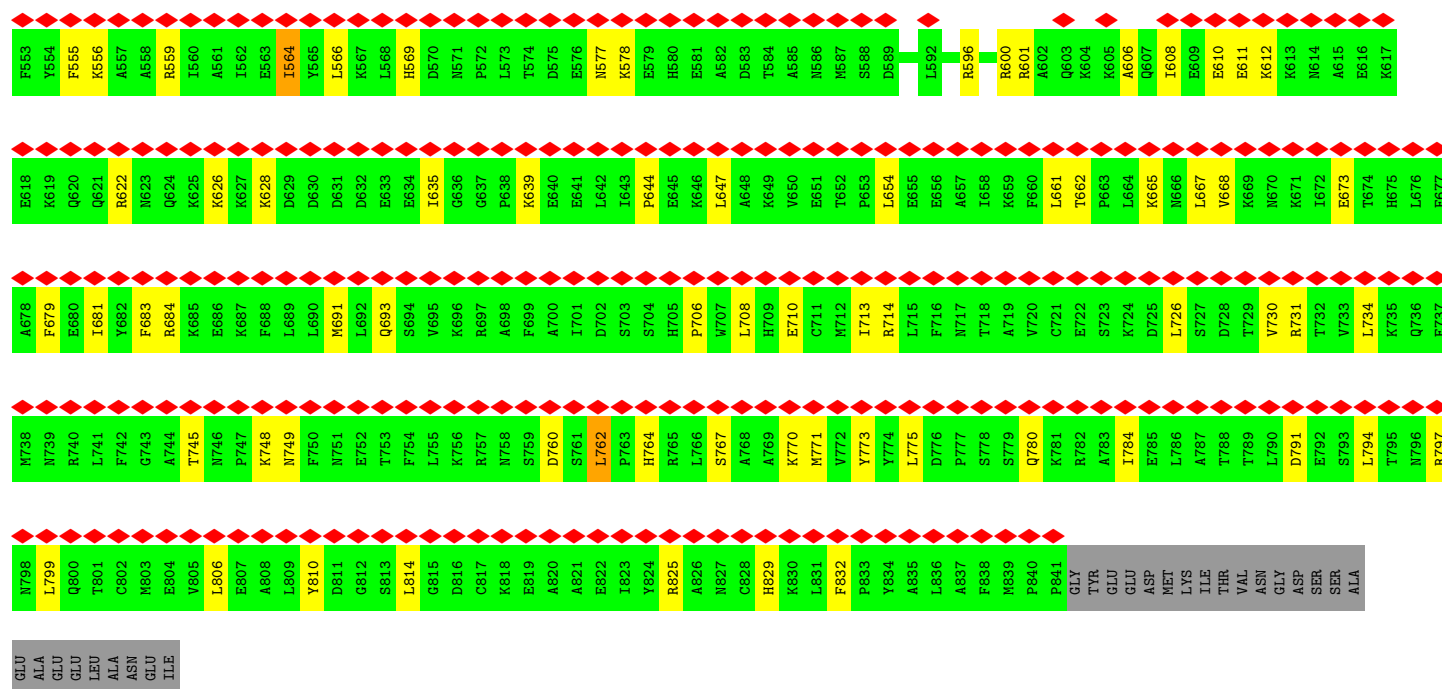
Chain BK:

• Molecule 55: Large ribosomal subunit protein eL13

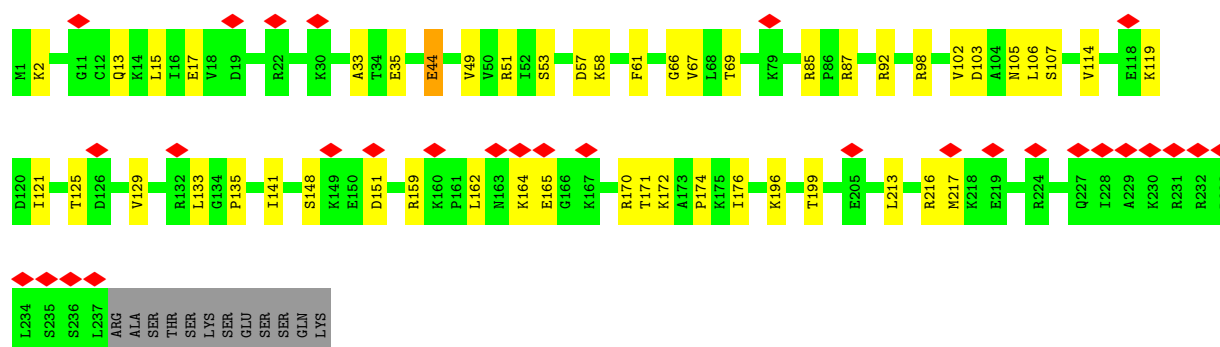
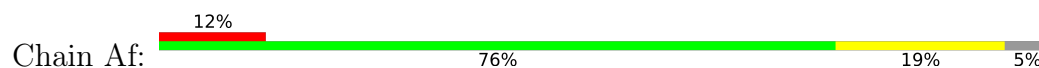


• Molecule 56: N-alpha-acetyltransferase 15, NatA auxiliary subunit

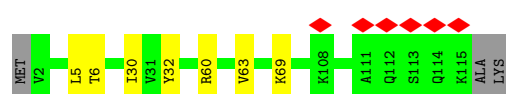
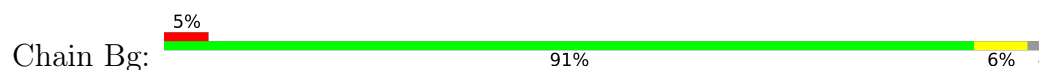




- Molecule 57: 40S ribosomal protein S6



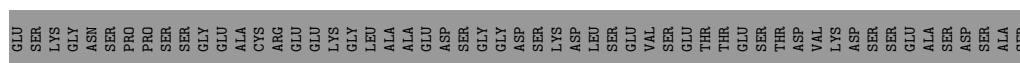
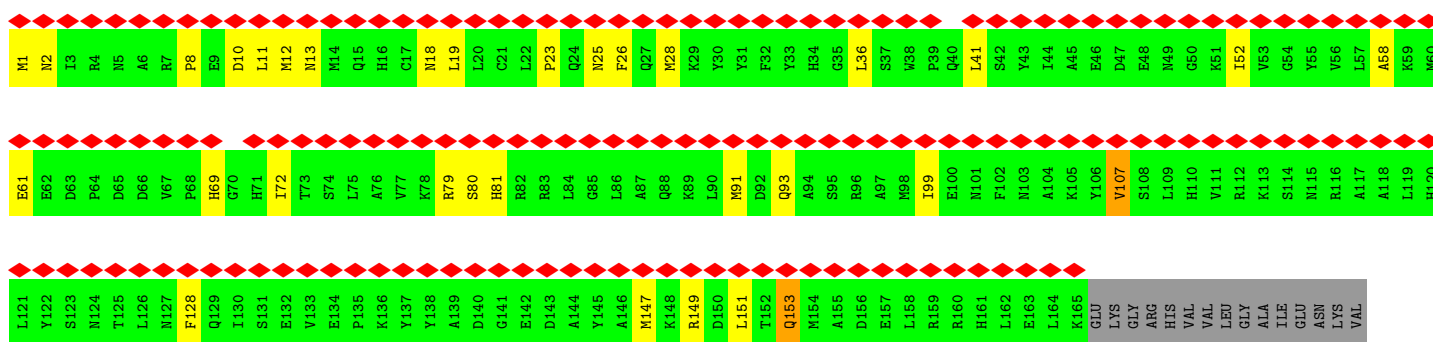
- Molecule 58: 60S ribosomal protein L34



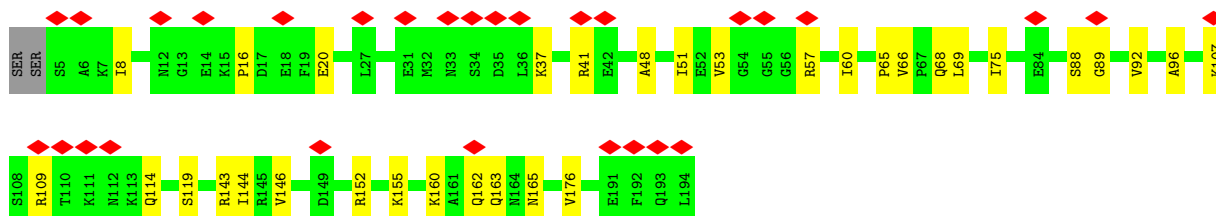
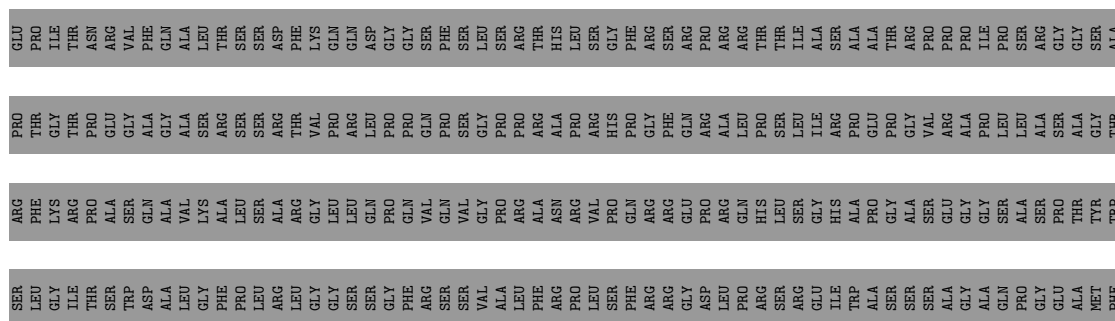
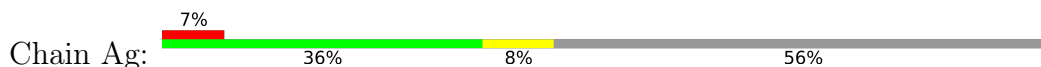
- Molecule 59: 60S ribosomal protein L14



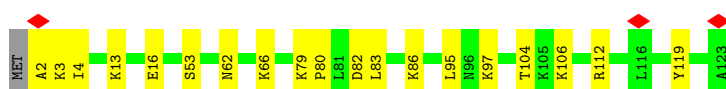
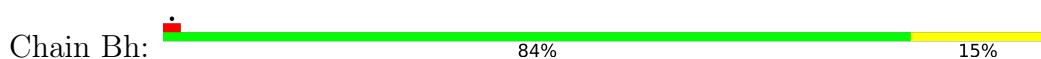
- Molecule 60: N-alpha-acetyltransferase 10



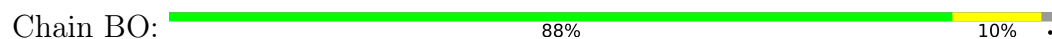
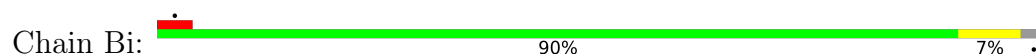
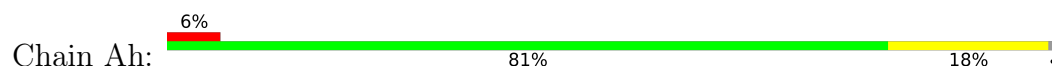
- Molecule 61: 40S ribosomal protein S7

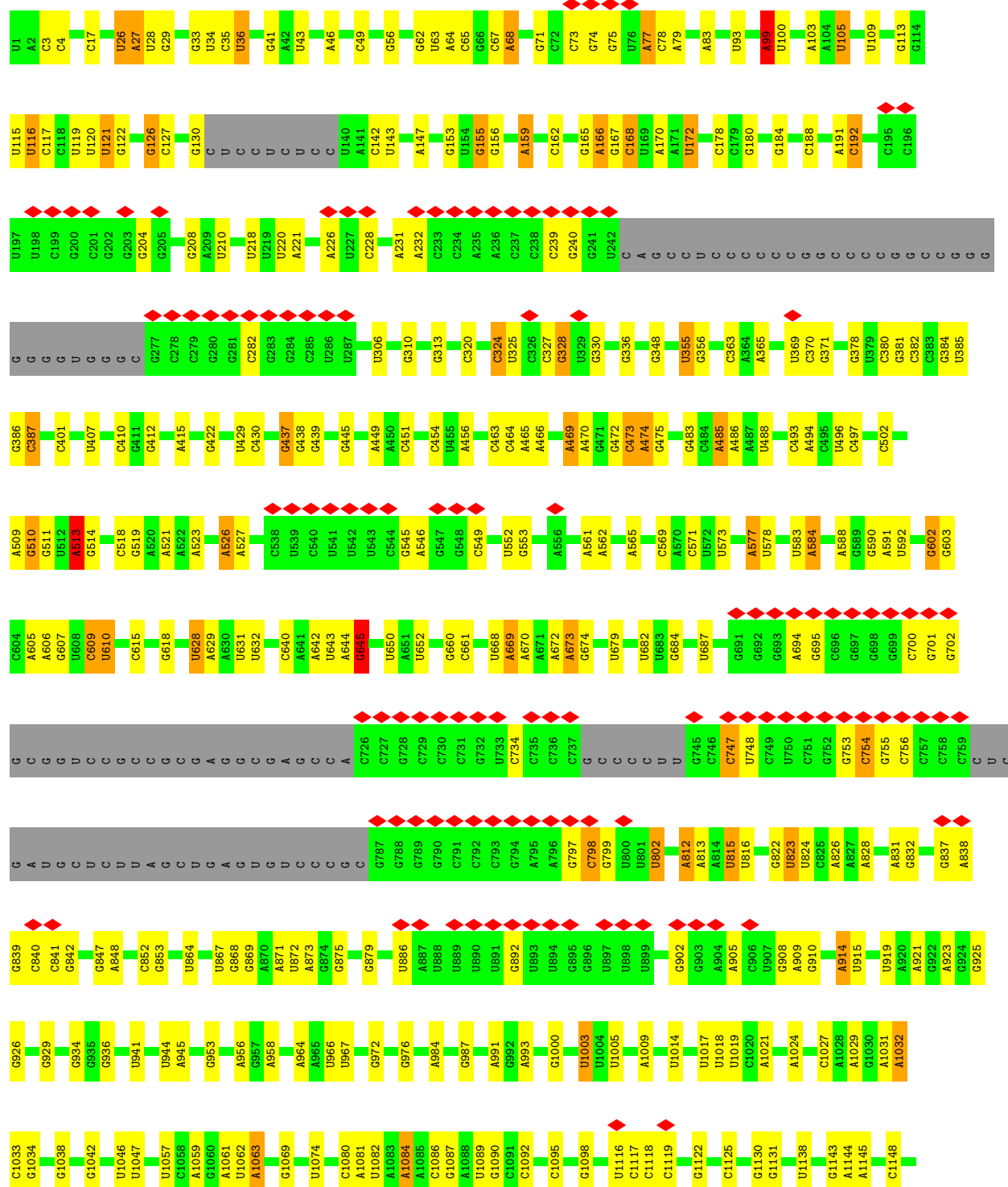


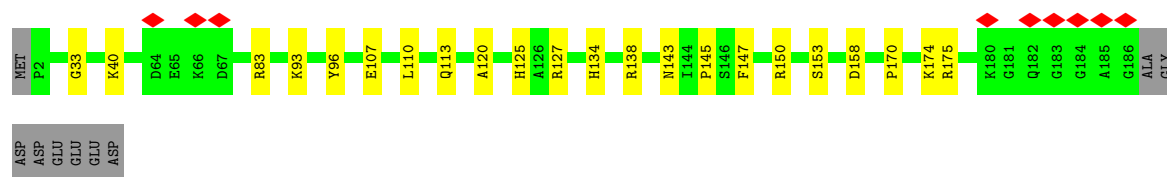
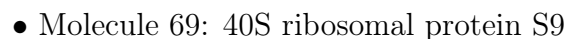
- Molecule 62: 60S ribosomal protein L35



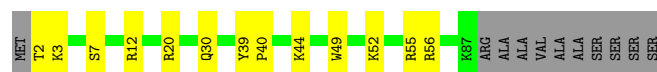
Chain BN: 86% 14%



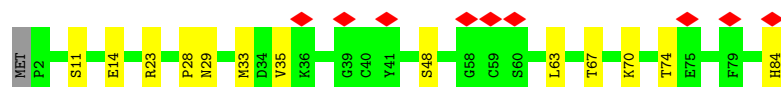




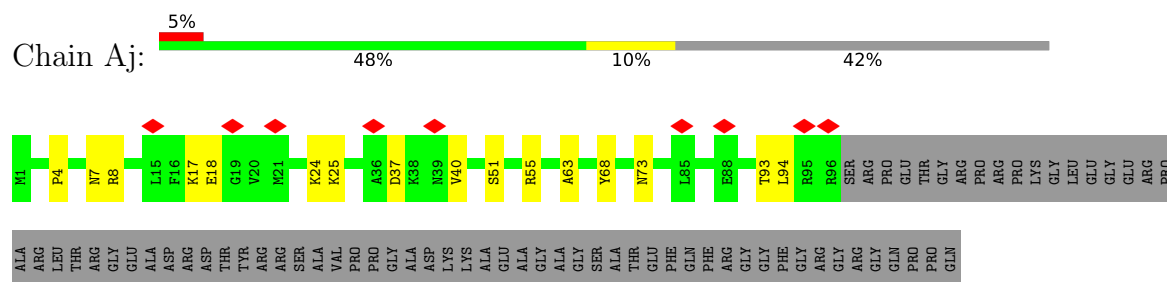
- Molecule 70: Ribosomal protein L37



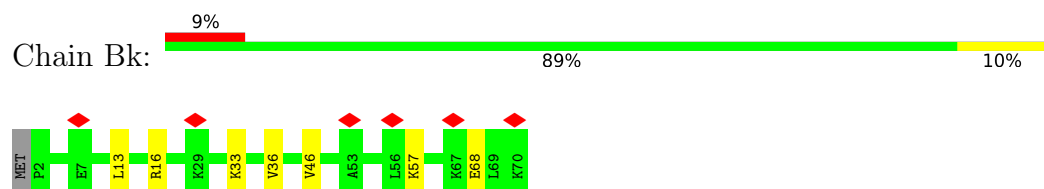
- Molecule 71: 40S ribosomal protein S27



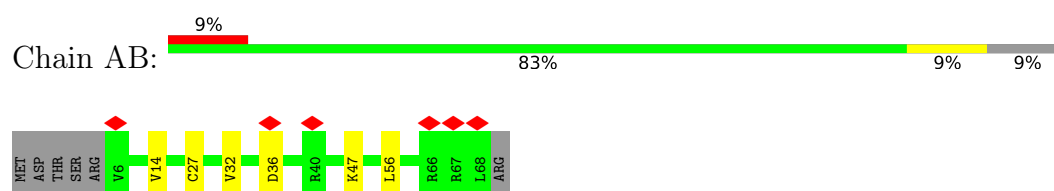
- Molecule 72: S10_pectin domain-containing protein



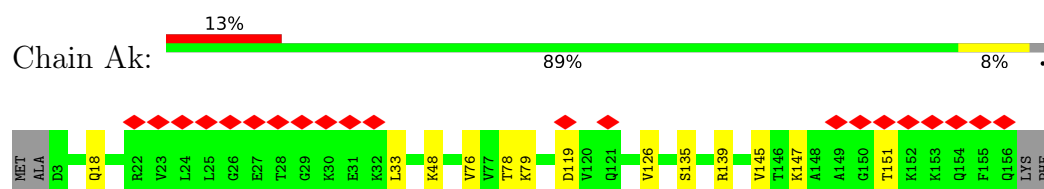
- Molecule 73: 60S ribosomal protein L38



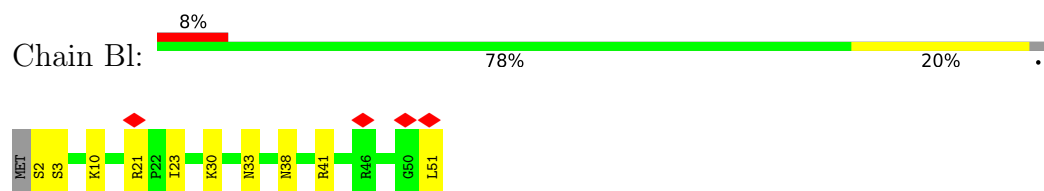
- Molecule 74: 40S ribosomal protein S28



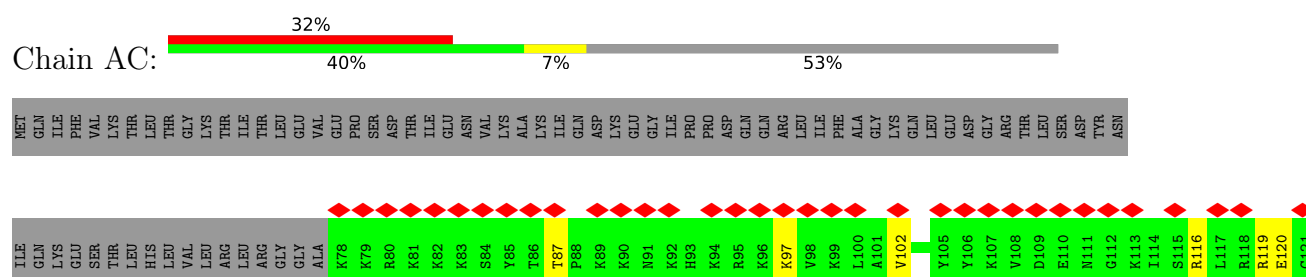
- Molecule 75: 40S ribosomal protein S11

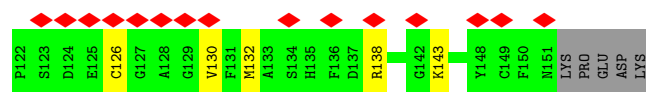


- Molecule 76: 60S ribosomal protein L39-like

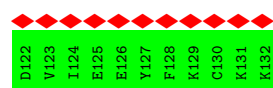
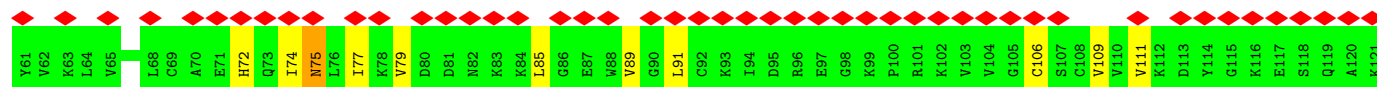
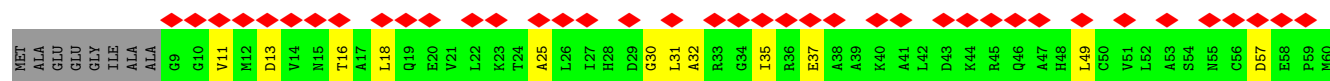
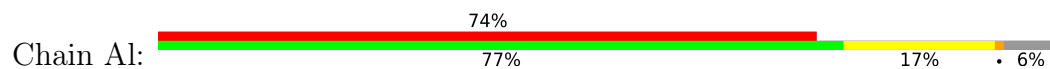


- Molecule 77: Ribosomal protein S27a

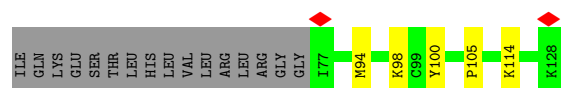
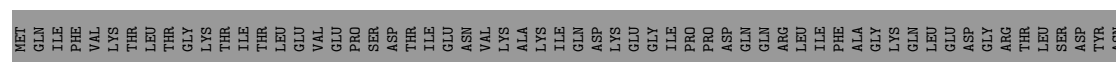




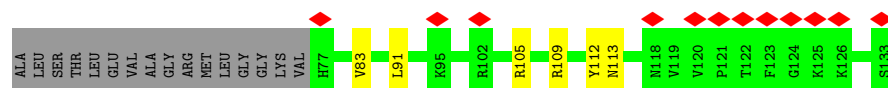
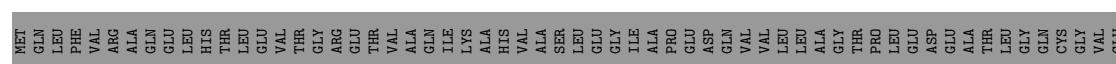
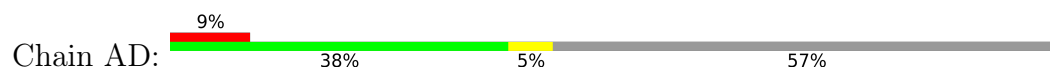
- Molecule 78: 40S ribosomal protein S12



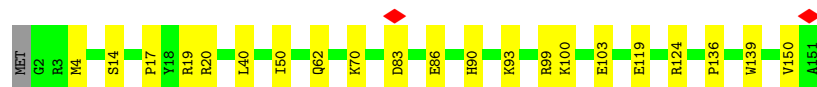
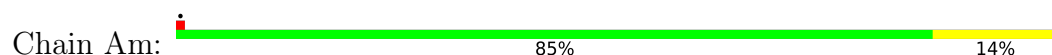
- Molecule 79: Ubiquitin-ribosomal protein eL40 fusion protein



- Molecule 80: 40S ribosomal protein S30

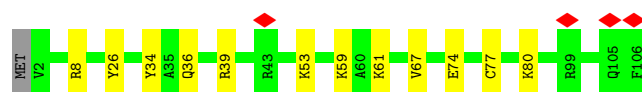


- Molecule 81: 40S ribosomal protein S13

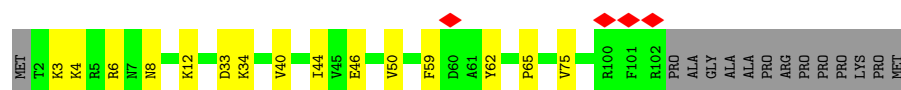
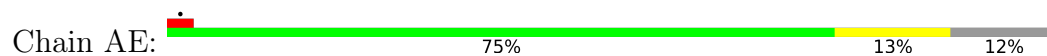


- Molecule 82: Large ribosomal subunit protein eL42

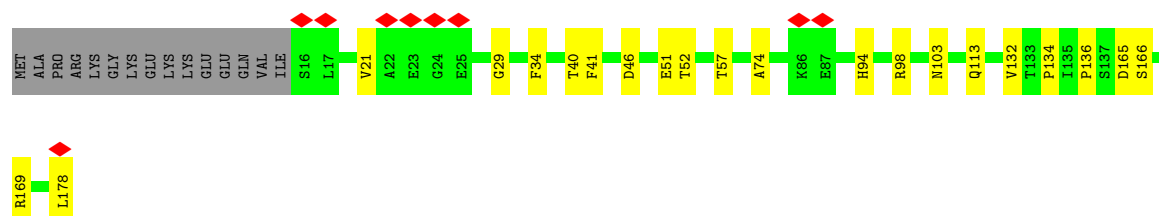
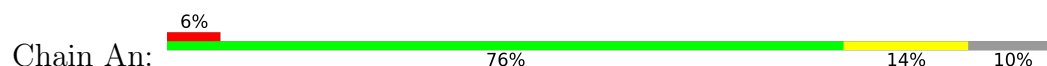




- Molecule 83: Small ribosomal subunit protein eS26



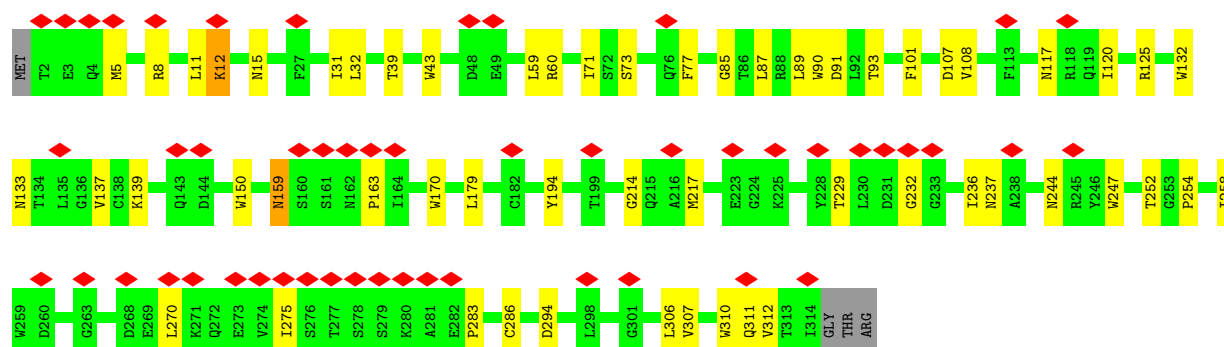
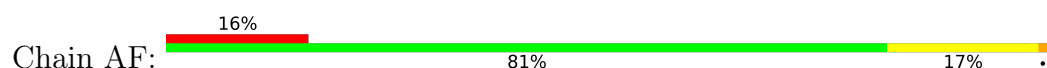
- Molecule 84: Small ribosomal subunit protein uS11



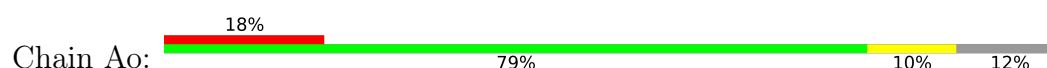
- Molecule 85: 60S ribosomal protein L37a

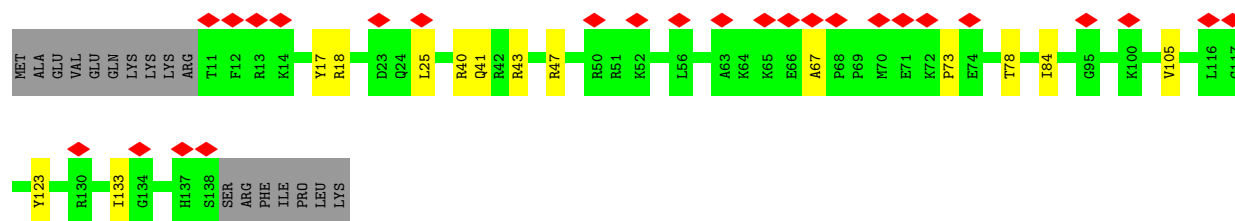


- Molecule 86: Small ribosomal subunit protein RACK1

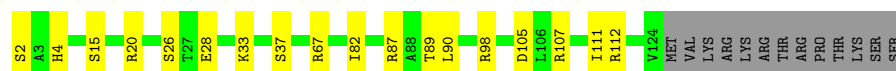
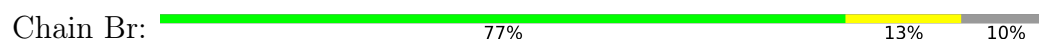


- Molecule 87: 40S ribosomal protein uS19

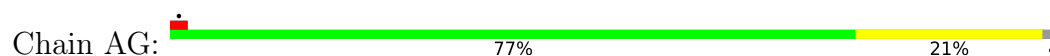




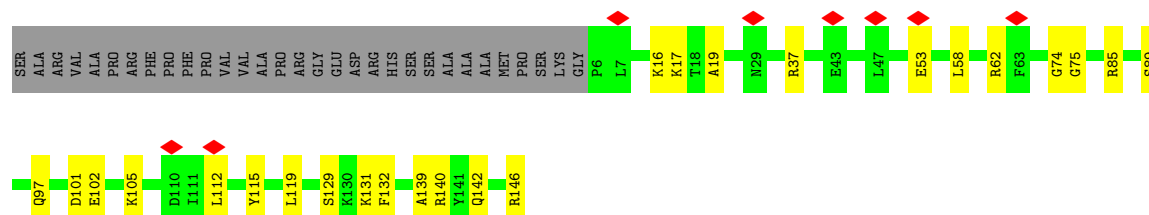
- Molecule 88: Large ribosomal subunit protein eL28



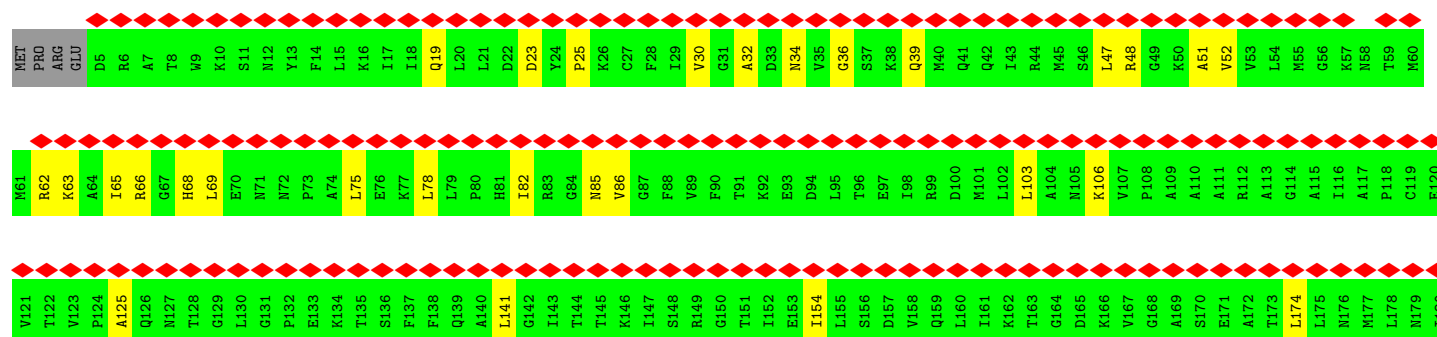
- Molecule 89: 40S ribosomal protein S29



- Molecule 90: Small ribosomal subunit protein uS9



- Molecule 91: Large ribosomal subunit protein uL10



[illegible]

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	23034	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.400	Depositor
Minimum map value	-0.732	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.058	Depositor
Recommended contour level	0.25	Depositor
Map size (Å)	593.6, 593.6, 593.6	wwPDB
Map dimensions	560, 560, 560	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	B5	0.11	3/86006 (0.0%)	0.12	0/134179
2	BT	0.07	0/1326	0.18	0/1770
3	Bb	0.07	0/884	0.18	0/1169
4	Bt	0.07	0/1193	0.21	0/1609
6	Aq	0.06	0/1094	0.18	0/1469
7	B7	0.06	0/2835	0.09	0/4418
8	AT	0.05	0/68	0.15	0/103
9	Ar	0.06	0/1226	0.19	0/1643
10	B8	0.06	0/3635	0.11	0/5661
11	BU	0.08	0/845	0.21	0/1134
12	As	0.06	0/1119	0.16	0/1498
13	BA	0.09	0/1965	0.22	0/2633
14	BV	0.08	0/1048	0.20	0/1402
15	At	0.07	0/831	0.20	0/1115
16	BB	0.08	0/3261	0.20	0/4364
17	BP	0.08	0/1317	0.21	0/1768
18	BY	0.07	0/1132	0.20	0/1504
19	Av	0.09	0/1051	0.19	0/1406
20	B	0.07	0/2437	0.20	0/3264
21	BX	0.07	0/984	0.19	0/1323
22	BQ	0.08	0/1539	0.20	0/2054
23	BZ	0.07	0/1130	0.19	0/1507
24	Aw	0.07	0/1107	0.19	0/1475
25	BE	0.09	0/1998	0.22	0/2673
26	BW	0.07	0/1006	0.19	0/1334
27	Au	0.07	0/636	0.17	0/852
28	Ba	0.07	0/1179	0.20	0/1572
29	Ax	0.06	0/1032	0.18	0/1371
30	BF	0.08	0/1922	0.20	0/2563
31	BR	0.07	0/1524	0.17	0/2013
32	AZ	0.08	0/1771	0.20	0/2406

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	Ay	0.07	0/691	0.19	0/922
34	BG	0.07	0/1908	0.19	0/2566
35	BC	0.08	0/2932	0.19	0/3939
36	BS	0.07	0/1497	0.19	0/2008
37	Aa	0.08	0/1841	0.22	0/2459
38	Az	0.06	0/240	0.14	0/305
39	BH	0.08	0/1535	0.20	0/2063
40	EA	0.07	0/2455	0.21	0/3333
41	Ab	0.08	0/1742	0.21	0/2354
42	Bc	0.07	0/847	0.17	0/1134
43	BI	0.07	0/1756	0.19	0/2346
44	Ct	0.08	0/913	0.22	0/1219
45	Ac	0.07	0/1779	0.20	0/2395
46	Bd	0.07	0/903	0.18	0/1216
47	BJ	0.07	0/1385	0.20	0/1852
48	Cu	0.09	0/836	0.28	0/1122
49	Ad	0.07	0/2118	0.20	0/2849
50	Be	0.07	0/1088	0.20	0/1451
52	DA	0.07	0/1284	0.21	0/1728
53	Ae	0.07	0/1531	0.23	0/2059
54	Bf	0.08	0/903	0.19	0/1208
55	BL	0.07	0/1733	0.19	0/2316
56	DB	0.12	0/7038	0.28	1/9468 (0.0%)
57	Af	0.06	0/1946	0.18	0/2590
58	Bg	0.07	0/916	0.20	0/1220
59	BM	0.07	0/1158	0.18	0/1547
60	DC	0.09	0/1368	0.24	0/1843
61	Ag	0.07	0/1552	0.19	0/2079
62	Bh	0.06	0/1021	0.16	0/1348
63	BN	0.07	0/1746	0.19	0/2338
64	DD	0.42	0/439	0.55	0/587
65	Ah	0.07	0/1715	0.19	0/2287
66	Bi	0.06	0/841	0.18	0/1112
67	BO	0.08	0/1662	0.19	0/2222
68	A2	0.13	2/40342 (0.0%)	0.12	0/62877
69	Ai	0.07	0/1550	0.19	0/2069
70	Bj	0.07	0/720	0.22	0/952
71	AA	0.06	0/665	0.19	0/891
72	Aj	0.07	0/834	0.19	0/1125
73	Bk	0.08	0/575	0.19	0/761
74	AB	0.07	0/497	0.18	0/666
75	Ak	0.07	0/1284	0.20	0/1717
76	Bl	0.07	0/459	0.17	0/608

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
77	AC	0.06	0/622	0.20	0/822
78	Al	0.07	0/968	0.22	0/1296
79	Bm	0.08	0/426	0.21	0/564
80	AD	0.06	0/462	0.18	0/607
81	Am	0.06	0/1232	0.18	0/1656
82	Bo	0.07	0/866	0.19	0/1141
83	AE	0.07	0/828	0.19	0/1109
84	An	0.12	0/1020	0.21	0/1366
85	Bp	0.08	0/718	0.22	0/953
86	AF	0.07	0/2493	0.21	0/3394
87	Ao	0.06	0/1069	0.19	0/1429
88	Br	0.08	0/996	0.21	0/1335
89	AG	0.08	0/470	0.21	0/623
90	Ap	0.09	0/1142	0.26	0/1528
91	Bs	0.07	0/1530	0.19	0/2064
All	All	0.10	5/244188 (0.0%)	0.16	1/356290 (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
82	Bo	0	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B5	4269	A2M	O3'-P	5.07	1.61	1.56
1	B5	1270	A2M	O3'-P	5.04	1.61	1.56
68	A2	1679	A2M	O3'-P	5.04	1.61	1.56
1	B5	3517	A2M	O3'-P	5.02	1.61	1.56
68	A2	485	A2M	O3'-P	5.01	1.61	1.56

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	DB	116	ILE	N-CA-C	-5.06	107.87	112.12

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
82	Bo	53	MLZ	Mainchain

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B5	79525	0	40255	554	0
2	BT	1298	0	1365	21	0
3	Bb	881	0	957	13	0
4	Bt	1178	0	1235	24	0
5	AH	36	0	25	0	0
6	Aq	1080	0	1135	12	0
7	B7	2538	0	1283	7	0
8	AT	939	0	617	6	0
9	Ar	1217	0	1279	20	0
10	B8	3319	0	1684	24	0
11	BU	831	0	852	12	0
12	As	1113	0	1145	14	0
13	BA	1940	0	2028	31	0
14	BV	1034	0	1097	14	0
15	At	821	0	883	9	0
16	BB	3206	0	3353	32	0
17	BP	1289	0	1329	18	0
18	BY	1115	0	1205	8	0
19	Av	1034	0	1080	7	0
20	B	2391	0	2424	21	0
21	BX	967	0	1040	4	0
22	BQ	1515	0	1634	19	0
23	BZ	1107	0	1182	14	0
24	Aw	1099	0	1162	9	0
25	BE	1960	0	2153	25	0
26	BW	991	0	1048	10	0
27	Au	640	0	633	7	0
28	Ba	1163	0	1202	19	0
29	Ax	1015	0	1086	9	0
30	BF	1886	0	2008	19	0
31	BR	1508	0	1664	14	0
32	AZ	1743	0	1748	24	0
33	Ay	683	0	761	11	0

Continued on next page...

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	BG	1877	0	2023	15	0
35	BC	2886	0	3057	21	0
36	BS	1457	0	1492	8	0
37	Aa	1815	0	1908	20	0
38	Az	239	0	289	2	0
39	BH	1516	0	1597	16	0
40	EA	2395	0	2344	29	0
41	Ab	1706	0	1796	17	0
42	Bc	836	0	888	5	0
43	BI	1717	0	1764	19	0
44	Ct	908	0	971	16	0
45	Ac	1751	0	1846	13	0
46	Bd	888	0	930	12	0
47	BJ	1362	0	1399	16	0
48	Cu	828	0	874	17	0
49	Ad	2076	0	2177	27	0
50	Be	1070	0	1165	13	0
51	BK	135	0	33	0	0
52	DA	1260	0	1282	24	0
53	Ae	1509	0	1563	17	0
54	Bf	884	0	923	9	0
55	BL	1702	0	1820	16	0
56	DB	6900	0	6944	178	0
57	Af	1923	0	2089	37	0
58	Bg	906	0	998	5	0
59	BM	1137	0	1211	16	0
60	DC	1339	0	1315	22	0
61	Ag	1529	0	1627	19	0
62	Bh	1013	0	1147	19	0
63	BN	1701	0	1749	23	0
64	DD	439	0	441	17	0
65	Ah	1686	0	1772	24	0
66	Bi	830	0	916	7	0
67	BO	1630	0	1778	15	0
68	A2	37833	0	19165	284	0
69	Ai	1525	0	1640	15	0
70	Bj	705	0	737	14	0
71	AA	651	0	672	7	0
72	Aj	810	0	836	11	0
73	Bk	569	0	637	3	0
74	AB	495	0	523	4	0
75	Ak	1262	0	1335	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
76	Bl	447	0	480	8	0
77	AC	610	0	634	9	0
78	Al	958	0	993	18	0
79	Bm	432	0	470	4	0
80	AD	457	0	502	8	0
81	Am	1208	0	1294	16	0
82	Bo	863	0	929	7	0
83	AE	814	0	863	11	0
84	An	1016	0	1038	14	0
85	Bp	708	0	756	4	0
86	AF	2436	0	2393	33	0
87	Ao	1048	0	1093	10	0
88	Br	990	0	1052	14	0
89	AG	459	0	448	13	0
90	Ap	1124	0	1193	20	0
91	Bs	1507	0	1564	25	0
92	A2	54	0	0	2	0
92	AE	1	0	0	0	0
92	AT	2	0	0	0	0
92	Ad	1	0	0	0	0
92	Ak	1	0	0	0	0
92	An	1	0	0	0	0
92	B5	200	0	0	2	0
92	B7	6	0	0	1	0
92	B8	6	0	0	0	0
92	BA	4	0	0	0	0
92	BB	3	0	0	0	0
92	BH	1	0	0	0	0
92	BI	1	0	0	0	0
92	BL	1	0	0	0	0
92	BN	1	0	0	0	0
92	BQ	2	0	0	1	0
92	BT	2	0	0	0	0
92	BY	1	0	0	0	0
92	Bb	2	0	0	0	0
92	Be	3	0	0	0	0
92	Bf	1	0	0	0	0
92	Bo	1	0	0	0	0
93	A2	80	0	152	6	0
93	B5	220	0	418	11	0
94	A2	110	0	0	0	0
94	AT	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
94	An	1	0	0	0	0
94	B5	283	0	0	0	0
94	B7	9	0	0	0	0
94	B8	8	0	0	0	0
94	BI	1	0	0	0	0
94	BP	1	0	0	0	0
94	BV	1	0	0	0	0
94	Ba	1	0	0	0	0
94	Be	1	0	0	0	0
94	Bj	1	0	0	0	0
94	Ct	1	0	0	0	0
95	A2	14	0	26	3	0
95	B5	28	0	52	1	0
96	B7	32	0	11	0	0
97	DB	36	0	6	1	0
98	AC	1	0	0	0	0
98	AE	1	0	0	0	0
98	AG	1	0	0	0	0
98	Bg	1	0	0	0	0
98	Bj	1	0	0	0	0
98	Bm	1	0	0	0	0
98	Bo	1	0	0	0	0
98	Bp	1	0	0	0	0
99	A2	531	0	0	25	0
99	AE	1	0	0	0	0
99	AH	3	0	0	0	0
99	AT	12	0	0	1	0
99	Aa	3	0	0	1	0
99	Ad	2	0	0	0	0
99	Af	1	0	0	0	0
99	Ak	2	0	0	0	0
99	An	1	0	0	0	0
99	Ap	2	0	0	0	0
99	Ar	2	0	0	1	0
99	As	1	0	0	0	0
99	Aw	4	0	0	1	0
99	B	1	0	0	0	0
99	B5	1383	0	0	49	0
99	B7	45	0	0	2	0
99	B8	48	0	0	0	0
99	BA	7	0	0	0	0
99	BB	8	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
99	BC	6	0	0	0	0
99	BH	2	0	0	0	0
99	BI	1	0	0	0	0
99	BL	1	0	0	0	0
99	BN	6	0	0	0	0
99	BP	3	0	0	0	0
99	BR	5	0	0	0	0
99	BT	2	0	0	0	0
99	BV	3	0	0	0	0
99	BX	1	0	0	0	0
99	Ba	7	0	0	1	0
99	Bb	1	0	0	0	0
99	Bd	1	0	0	0	0
99	Be	4	0	0	0	0
99	Bg	3	0	0	0	0
99	Bj	6	0	0	1	0
99	Bl	3	0	0	0	0
99	Bm	1	0	0	0	0
99	Bo	1	0	0	0	0
99	Ct	3	0	0	0	0
All	All	237089	0	178592	1861	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

The worst 5 of 1861 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
92:A2:2002:UNX:UNK	99:A2:2415:HOH:O	1.01	1.27
92:B5:4955:UNX:UNK	99:B5:6243:HOH:O	1.10	1.26
19:Av:2:VAL:N	68:A2:1092:C:HO2'	1.58	1.01
1:B5:3374:A:HO2'	70:Bj:2:THR:N	1.69	0.90
92:B7:212:UNX:UNK	99:B7:321:HOH:O	1.58	0.84

There are no symmetry-related clashes.

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	
2	BT	157/160 (98%)	155 (99%)	2 (1%)	0	100	100
3	Bb	103/245 (42%)	98 (95%)	5 (5%)	0	100	100
4	Bt	154/165 (93%)	153 (99%)	1 (1%)	0	100	100
6	Aq	132/135 (98%)	132 (100%)	0	0	100	100
9	Ar	146/151 (97%)	143 (98%)	3 (2%)	0	100	100
11	BU	100/128 (78%)	98 (98%)	2 (2%)	0	100	100
12	As	140/145 (97%)	140 (100%)	0	0	100	100
13	BA	250/257 (97%)	241 (96%)	9 (4%)	0	100	100
14	BV	137/140 (98%)	136 (99%)	1 (1%)	0	100	100
15	At	102/119 (86%)	100 (98%)	2 (2%)	0	100	100
16	BB	395/403 (98%)	392 (99%)	3 (1%)	0	100	100
17	BP	157/184 (85%)	155 (99%)	2 (1%)	0	100	100
18	BY	132/145 (91%)	131 (99%)	1 (1%)	0	100	100
19	Av	127/130 (98%)	127 (100%)	0	0	100	100
20	B	291/297 (98%)	287 (99%)	4 (1%)	0	100	100
21	BX	116/156 (74%)	114 (98%)	2 (2%)	0	100	100
22	BQ	185/188 (98%)	182 (98%)	3 (2%)	0	100	100
23	BZ	133/136 (98%)	132 (99%)	1 (1%)	0	100	100
24	Aw	138/143 (96%)	136 (99%)	2 (1%)	0	100	100
25	BE	239/291 (82%)	235 (98%)	4 (2%)	0	100	100
26	BW	119/157 (76%)	118 (99%)	1 (1%)	0	100	100
27	Au	81/83 (98%)	79 (98%)	2 (2%)	0	100	100
28	Ba	144/148 (97%)	138 (96%)	5 (4%)	1 (1%)	18	48
29	Ax	123/130 (95%)	123 (100%)	0	0	100	100
30	BF	224/247 (91%)	218 (97%)	6 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
31	BR	178/196 (91%)	178 (100%)	0	0	100	100
32	AZ	219/294 (74%)	215 (98%)	4 (2%)	0	100	100
33	Ay	83/124 (67%)	81 (98%)	2 (2%)	0	100	100
34	BG	229/266 (86%)	226 (99%)	3 (1%)	0	100	100
35	BC	360/412 (87%)	358 (99%)	2 (1%)	0	100	100
36	BS	174/176 (99%)	172 (99%)	2 (1%)	0	100	100
37	Aa	220/264 (83%)	218 (99%)	2 (1%)	0	100	100
38	Az	23/25 (92%)	23 (100%)	0	0	100	100
39	BH	188/192 (98%)	188 (100%)	0	0	100	100
40	EA	302/386 (78%)	297 (98%)	4 (1%)	1 (0%)	36	66
41	Ab	218/293 (74%)	218 (100%)	0	0	100	100
42	Bc	106/115 (92%)	104 (98%)	2 (2%)	0	100	100
43	BI	211/214 (99%)	208 (99%)	3 (1%)	0	100	100
44	Ct	113/238 (48%)	110 (97%)	3 (3%)	0	100	100
45	Ac	223/281 (79%)	221 (99%)	2 (1%)	0	100	100
46	Bd	105/125 (84%)	105 (100%)	0	0	100	100
47	BJ	168/178 (94%)	167 (99%)	1 (1%)	0	100	100
48	Cu	105/162 (65%)	100 (95%)	5 (5%)	0	100	100
49	Ad	260/263 (99%)	257 (99%)	3 (1%)	0	100	100
50	Be	128/135 (95%)	128 (100%)	0	0	100	100
52	DA	153/403 (38%)	150 (98%)	3 (2%)	0	100	100
53	Ae	189/204 (93%)	185 (98%)	4 (2%)	0	100	100
54	Bf	108/110 (98%)	107 (99%)	1 (1%)	0	100	100
55	BL	208/211 (99%)	205 (99%)	3 (1%)	0	100	100
56	DB	835/915 (91%)	823 (99%)	10 (1%)	2 (0%)	43	70
57	Af	235/249 (94%)	234 (100%)	1 (0%)	0	100	100
58	Bg	112/117 (96%)	111 (99%)	1 (1%)	0	100	100
59	BM	136/218 (62%)	134 (98%)	2 (2%)	0	100	100
60	DC	163/235 (69%)	162 (99%)	1 (1%)	0	100	100
61	Ag	188/432 (44%)	185 (98%)	3 (2%)	0	100	100
62	Bh	120/123 (98%)	119 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
63	BN	201/204 (98%)	199 (99%)	2 (1%)	0	100	100
64	DD	55/228 (24%)	50 (91%)	5 (9%)	0	100	100
65	Ah	204/208 (98%)	201 (98%)	3 (2%)	0	100	100
66	Bi	100/105 (95%)	98 (98%)	2 (2%)	0	100	100
67	BO	197/203 (97%)	196 (100%)	1 (0%)	0	100	100
69	Ai	183/194 (94%)	181 (99%)	2 (1%)	0	100	100
70	Bj	84/97 (87%)	83 (99%)	1 (1%)	0	100	100
71	AA	81/84 (96%)	79 (98%)	2 (2%)	0	100	100
72	Aj	94/165 (57%)	90 (96%)	4 (4%)	0	100	100
73	Bk	67/70 (96%)	67 (100%)	0	0	100	100
74	AB	61/69 (88%)	61 (100%)	0	0	100	100
75	Ak	152/158 (96%)	150 (99%)	2 (1%)	0	100	100
76	Bl	48/51 (94%)	48 (100%)	0	0	100	100
77	AC	72/156 (46%)	71 (99%)	1 (1%)	0	100	100
78	Al	122/132 (92%)	119 (98%)	3 (2%)	0	100	100
79	Bm	49/128 (38%)	49 (100%)	0	0	100	100
80	AD	55/133 (41%)	54 (98%)	1 (2%)	0	100	100
81	Am	148/151 (98%)	147 (99%)	1 (1%)	0	100	100
82	Bo	102/106 (96%)	100 (98%)	2 (2%)	0	100	100
83	AE	99/115 (86%)	98 (99%)	1 (1%)	0	100	100
84	An	132/151 (87%)	129 (98%)	3 (2%)	0	100	100
85	Bp	89/92 (97%)	87 (98%)	2 (2%)	0	100	100
86	AF	311/317 (98%)	304 (98%)	7 (2%)	0	100	100
87	Ao	126/145 (87%)	123 (98%)	3 (2%)	0	100	100
88	Br	121/136 (89%)	120 (99%)	1 (1%)	0	100	100
89	AG	53/56 (95%)	53 (100%)	0	0	100	100
90	Ap	139/172 (81%)	133 (96%)	6 (4%)	0	100	100
91	Bs	194/318 (61%)	188 (97%)	6 (3%)	0	100	100
All	All	13424/16183 (83%)	13230 (99%)	190 (1%)	4 (0%)	100	100

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
40	EA	297	HIS
56	DB	577	ASN
56	DB	578	LYS
28	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	
2	BT	139/140 (99%)	139 (100%)	0	100	100
3	Bb	87/183 (48%)	87 (100%)	0	100	100
4	Bt	128/137 (93%)	122 (95%)	6 (5%)	23	51
6	Aq	120/121 (99%)	119 (99%)	1 (1%)	73	78
9	Ar	127/130 (98%)	125 (98%)	2 (2%)	55	70
11	BU	91/113 (80%)	88 (97%)	3 (3%)	33	57
12	As	112/114 (98%)	112 (100%)	0	100	100
13	BA	194/198 (98%)	194 (100%)	0	100	100
14	BV	106/107 (99%)	106 (100%)	0	100	100
15	At	94/107 (88%)	92 (98%)	2 (2%)	47	66
16	BB	344/347 (99%)	341 (99%)	3 (1%)	70	76
17	BP	140/163 (86%)	140 (100%)	0	100	100
18	BY	124/135 (92%)	124 (100%)	0	100	100
19	Av	112/113 (99%)	111 (99%)	1 (1%)	70	76
20	B	247/250 (99%)	247 (100%)	0	100	100
21	BX	106/134 (79%)	105 (99%)	1 (1%)	70	76
22	BQ	164/165 (99%)	162 (99%)	2 (1%)	63	74
23	BZ	117/118 (99%)	117 (100%)	0	100	100
24	Aw	112/114 (98%)	110 (98%)	2 (2%)	51	69
25	BE	216/251 (86%)	216 (100%)	0	100	100
26	BW	100/126 (79%)	99 (99%)	1 (1%)	68	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
27	Au	67/67 (100%)	65 (97%)	2 (3%)	36	59
28	Ba	118/119 (99%)	118 (100%)	0	100	100
29	Ax	107/112 (96%)	106 (99%)	1 (1%)	70	76
30	BF	197/215 (92%)	197 (100%)	0	100	100
31	BR	159/175 (91%)	158 (99%)	1 (1%)	78	81
32	AZ	182/242 (75%)	180 (99%)	2 (1%)	65	75
33	Ay	75/102 (74%)	74 (99%)	1 (1%)	61	73
34	BG	199/223 (89%)	197 (99%)	2 (1%)	68	75
35	BC	302/336 (90%)	301 (100%)	1 (0%)	86	86
36	BS	154/154 (100%)	154 (100%)	0	100	100
37	Aa	203/231 (88%)	200 (98%)	3 (2%)	57	71
38	Az	24/24 (100%)	24 (100%)	0	100	100
39	BH	169/171 (99%)	169 (100%)	0	100	100
40	EA	261/330 (79%)	259 (99%)	2 (1%)	73	78
41	Ab	185/223 (83%)	184 (100%)	1 (0%)	81	82
42	Bc	92/98 (94%)	91 (99%)	1 (1%)	65	75
43	BI	180/181 (99%)	179 (99%)	1 (1%)	78	81
44	Ct	100/202 (50%)	99 (99%)	1 (1%)	68	75
45	Ac	189/232 (82%)	186 (98%)	3 (2%)	55	70
46	Bd	98/110 (89%)	98 (100%)	0	100	100
47	BJ	143/149 (96%)	142 (99%)	1 (1%)	76	79
48	Cu	91/136 (67%)	86 (94%)	5 (6%)	19	46
49	Ad	224/225 (100%)	224 (100%)	0	100	100
50	Be	116/121 (96%)	116 (100%)	0	100	100
52	DA	137/355 (39%)	136 (99%)	1 (1%)	76	79
53	Ae	161/170 (95%)	161 (100%)	0	100	100
54	Bf	89/89 (100%)	89 (100%)	0	100	100
55	BL	175/176 (99%)	173 (99%)	2 (1%)	65	75
56	DB	746/806 (93%)	724 (97%)	22 (3%)	37	60
57	Af	207/218 (95%)	206 (100%)	1 (0%)	81	82
58	Bg	98/100 (98%)	97 (99%)	1 (1%)	68	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
59	BM	117/161 (73%)	117 (100%)	0	100	100
60	DC	141/202 (70%)	139 (99%)	2 (1%)	59	72
61	Ag	170/360 (47%)	168 (99%)	2 (1%)	63	74
62	Bh	109/110 (99%)	109 (100%)	0	100	100
63	BN	171/172 (99%)	171 (100%)	0	100	100
64	DD	45/201 (22%)	44 (98%)	1 (2%)	45	65
65	Ah	178/180 (99%)	177 (99%)	1 (1%)	78	81
66	Bi	86/89 (97%)	86 (100%)	0	100	100
67	BO	171/173 (99%)	169 (99%)	2 (1%)	63	74
69	Ai	161/168 (96%)	161 (100%)	0	100	100
70	Bj	73/80 (91%)	73 (100%)	0	100	100
71	AA	75/76 (99%)	74 (99%)	1 (1%)	61	73
72	Aj	87/136 (64%)	86 (99%)	1 (1%)	65	75
73	Bk	64/65 (98%)	63 (98%)	1 (2%)	55	70
74	AB	56/62 (90%)	55 (98%)	1 (2%)	51	69
75	Ak	139/142 (98%)	138 (99%)	1 (1%)	76	79
76	Bl	47/48 (98%)	47 (100%)	0	100	100
77	AC	67/140 (48%)	67 (100%)	0	100	100
78	Al	104/108 (96%)	103 (99%)	1 (1%)	68	75
79	Bm	47/115 (41%)	47 (100%)	0	100	100
80	AD	47/106 (44%)	47 (100%)	0	100	100
81	Am	130/131 (99%)	130 (100%)	0	100	100
82	Bo	92/93 (99%)	92 (100%)	0	100	100
83	AE	88/98 (90%)	86 (98%)	2 (2%)	44	65
84	An	105/118 (89%)	104 (99%)	1 (1%)	68	75
85	Bp	74/75 (99%)	73 (99%)	1 (1%)	59	72
86	AF	272/275 (99%)	269 (99%)	3 (1%)	65	75
87	Ao	114/130 (88%)	112 (98%)	2 (2%)	51	69
88	Br	106/119 (89%)	106 (100%)	0	100	100
89	AG	48/49 (98%)	48 (100%)	0	100	100
90	Ap	117/140 (84%)	117 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
91	Bs	164/258 (64%)	162 (99%)	2 (1%)	63	74
All	All	11693/13738 (85%)	11589 (99%)	104 (1%)	68	76

5 of 104 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
56	DB	123	LEU
56	DB	611	GLU
86	AF	275	ILE
56	DB	170	ILE
56	DB	401	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 153 such sidechains are listed below:

Mol	Chain	Res	Type
65	Ah	138	ASN
89	AG	28	HIS
66	Bi	36	HIS
76	Bl	25	GLN
91	Bs	39	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	B5	3694/4808 (76%)	428 (11%)	2 (0%)
10	B8	155/158 (98%)	15 (9%)	0
5	AH	0/3	-	-
68	A2	1764/1870 (94%)	219 (12%)	0
7	B7	118/120 (98%)	7 (5%)	0
8	AT	2/76 (2%)	1 (50%)	0
All	All	5733/7035 (81%)	670 (11%)	2 (0%)

5 of 670 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	B5	39	A
1	B5	42	A
1	B5	59	A
1	B5	64	A
1	B5	65	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

223 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	PSU	B5	1720	1	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
68	A2M	A2	159	68	22,25,26	1.47	4 (18%)	31,36,39	2.13	9 (29%)
1	PSU	B5	4217	1	18,21,22	1.34	2 (11%)	22,30,33	1.89	3 (13%)
1	PSU	B5	4203	1	18,21,22	1.36	2 (11%)	22,30,33	1.85	3 (13%)
1	PSU	B5	4325	1	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
1	PSU	B5	4149	1	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)
1	PSU	B5	3462	1	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
1	PSU	B5	3447	1	18,21,22	1.35	2 (11%)	22,30,33	1.86	3 (13%)
1	PSU	B5	4374	1	18,21,22	1.36	2 (11%)	22,30,33	1.90	3 (13%)
68	OMG	A2	1329	68	23,26,27	1.20	3 (13%)	33,38,41	1.94	6 (18%)
84	IAS	An	165	84	6,7,8	0.98	0	6,8,10	1.33	1 (16%)
10	PSU	B8	55	10	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)
68	PSU	A2	610	68	18,21,22	1.34	2 (11%)	22,30,33	1.86	3 (13%)
68	PSU	A2	650	68	18,21,22	1.33	2 (11%)	22,30,33	1.87	3 (13%)
1	OMC	B5	3573	1	19,22,23	0.80	0	26,31,34	0.87	1 (3%)
1	PSU	B5	1721	1	18,21,22	1.33	2 (11%)	22,30,33	1.88	3 (13%)
1	A2M	B5	2630	94,1	22,25,26	1.46	4 (18%)	31,36,39	2.19	9 (29%)
68	OMG	A2	510	94,68	23,26,27	1.19	3 (13%)	33,38,41	1.93	6 (18%)
68	PSU	A2	1644	94,68	18,21,22	1.33	2 (11%)	22,30,33	1.88	3 (13%)
68	PSU	A2	652	68	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
68	6MZ	A2	1833	94,68	22,25,26	1.45	4 (18%)	30,36,39	2.16	9 (30%)
68	4AC	A2	1338	68	21,24,25	1.06	2 (9%)	29,34,37	1.21	3 (10%)
1	OMG	B5	3524	1	23,26,27	1.19	3 (13%)	33,38,41	1.94	6 (18%)
1	PSU	B5	2475	1	18,21,22	1.34	2 (11%)	22,30,33	1.86	3 (13%)
68	A2M	A2	1032	68	22,25,26	1.46	4 (18%)	31,36,39	2.13	10 (32%)
1	5MC	B5	4193	1	18,22,23	0.99	2 (11%)	26,32,35	1.17	2 (7%)
1	OMU	B5	3657	1	19,22,23	1.22	3 (15%)	26,31,34	1.72	4 (15%)
1	OMC	B5	1284	1	19,22,23	0.82	0	26,31,34	0.81	0
68	PSU	A2	1233	68	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
1	PSU	B5	1632	1	18,21,22	1.38	2 (11%)	22,30,33	1.85	4 (18%)
68	PSU	A2	1693	68	18,21,22	1.36	2 (11%)	22,30,33	1.86	3 (13%)
1	PSU	B5	1491	1	18,21,22	1.36	2 (11%)	22,30,33	1.90	3 (13%)
1	PSU	B5	3369	1	18,21,22	1.35	2 (11%)	22,30,33	1.89	3 (13%)
3	MLZ	Bb	5	3	8,9,10	0.48	0	4,9,11	0.16	0
1	PSU	B5	3371	1	18,21,22	1.36	2 (11%)	22,30,33	1.83	3 (13%)
68	OMU	A2	116	68	19,22,23	1.19	2 (10%)	26,31,34	1.70	4 (15%)
68	4AC	A2	1843	68	21,24,25	1.10	2 (9%)	29,34,37	1.25	3 (10%)
1	6MZ	B5	3966	1	22,25,26	1.44	4 (18%)	30,36,39	2.17	9 (30%)
1	PSU	B5	4382	1	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
1	PSU	B5	3494	1	18,21,22	1.36	2 (11%)	22,30,33	1.87	3 (13%)
1	OMG	B5	3631	1	23,26,27	1.20	3 (13%)	33,38,41	1.94	6 (18%)
68	OMG	A2	645	68	23,26,27	1.19	3 (13%)	33,38,41	1.94	6 (18%)
68	PSU	A2	105	68	18,21,22	1.35	2 (11%)	22,30,33	1.86	3 (13%)
68	A2M	A2	485	68	22,25,26	1.47	4 (18%)	31,36,39	2.10	9 (29%)
1	OMG	B5	4116	1	23,26,27	1.20	3 (13%)	33,38,41	1.94	6 (18%)
1	OMC	B5	3433	1	19,22,23	0.80	0	26,31,34	0.75	0
1	PSU	B5	4435	1	18,21,22	1.34	2 (11%)	22,30,33	1.89	3 (13%)
1	OMC	B5	4282	94,1	19,22,23	0.82	0	26,31,34	0.85	0
1	PSU	B5	1718	1	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)
1	OMC	B5	2667	1	19,22,23	0.81	0	26,31,34	0.79	0
1	OMG	B5	3476	1	23,26,27	1.19	3 (13%)	33,38,41	1.94	6 (18%)
1	PSU	B5	1799	1	18,21,22	1.33	2 (11%)	22,30,33	1.87	3 (13%)
1	OMG	B5	4364	1	23,26,27	1.19	3 (13%)	33,38,41	1.95	6 (18%)
1	OMG	B5	4369	1	23,26,27	1.20	3 (13%)	33,38,41	1.95	6 (18%)
35	AYA	BC	2	35	6,7,8	0.70	0	5,8,10	0.32	0
88	SAC	Br	2	88	7,8,9	0.53	0	8,9,11	0.84	1 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
68	OMG	A2	602	68	23,26,27	1.19	3 (13%)	33,38,41	1.92	6 (18%)
1	PSU	B5	4166	1	18,21,22	1.39	2 (11%)	22,30,33	1.81	4 (18%)
1	PSU	B5	3554	1	18,21,22	1.34	2 (11%)	22,30,33	1.86	3 (13%)
1	OMG	B5	1260	1	23,26,27	1.20	3 (13%)	33,38,41	1.96	6 (18%)
1	PSU	B5	3576	1	18,21,22	1.36	2 (11%)	22,30,33	1.87	3 (13%)
68	PSU	A2	1239	68	18,21,22	1.35	2 (11%)	22,30,33	1.86	3 (13%)
1	OMG	B5	2719	1	23,26,27	1.21	3 (13%)	33,38,41	1.97	6 (18%)
1	A2M	B5	1810	94,1	22,25,26	1.47	4 (18%)	31,36,39	2.18	10 (32%)
1	A2M	B5	3492	1,68	22,25,26	1.46	4 (18%)	31,36,39	2.18	10 (32%)
1	OMU	B5	4366	1	19,22,23	1.23	3 (15%)	26,31,34	1.71	4 (15%)
68	PSU	A2	864	68	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
1	A2M	B5	3599	1	22,25,26	1.47	4 (18%)	31,36,39	2.11	9 (29%)
1	OMG	B5	1580	1	23,26,27	1.19	3 (13%)	33,38,41	1.93	6 (18%)
68	PSU	A2	93	68	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
9	SAC	Ar	2	9	7,8,9	0.53	0	8,9,11	0.90	1 (12%)
68	A2M	A2	577	68	22,25,26	1.48	4 (18%)	31,36,39	2.12	10 (32%)
68	A2M	A2	27	94,68	22,25,26	1.47	4 (18%)	31,36,39	2.12	9 (29%)
68	OMU	A2	1443	94,68	19,22,23	1.23	3 (15%)	26,31,34	1.69	4 (15%)
1	A2M	B5	2244	94,1	22,25,26	1.46	4 (18%)	31,36,39	2.12	9 (29%)
68	A2M	A2	1384	68	22,25,26	1.47	4 (18%)	31,36,39	2.10	10 (32%)
1	PSU	B5	3466	1	18,21,22	1.34	2 (11%)	22,30,33	1.86	3 (13%)
1	PSU	B5	1683	1	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
1	OMC	B5	3601	1	19,22,23	0.80	0	26,31,34	0.80	0
1	OMG	B5	4245	1	23,26,27	1.20	3 (13%)	33,38,41	1.91	6 (18%)
1	OMG	B5	3974	1	23,26,27	1.19	3 (13%)	33,38,41	1.93	6 (18%)
10	OMG	B8	75	10	23,26,27	1.20	3 (13%)	33,38,41	1.94	6 (18%)
68	A2M	A2	1679	68	22,25,26	1.46	4 (18%)	31,36,39	2.20	10 (32%)
68	PSU	A2	815	68	18,21,22	1.36	2 (11%)	22,30,33	1.86	3 (13%)
1	A2M	B5	3450	1	22,25,26	1.47	4 (18%)	31,36,39	2.11	10 (32%)
1	OMU	B5	2680	1	19,22,23	1.21	2 (10%)	26,31,34	1.71	4 (15%)
1	PSU	B5	4740	1	18,21,22	1.35	2 (11%)	22,30,33	1.86	3 (13%)
24	HY3	Aw	62	24	6,8,9	2.03	1 (16%)	5,10,12	1.11	1 (20%)
1	UR3	B5	4276	1	19,22,23	0.99	0	26,32,35	1.41	1 (3%)
68	OMC	A2	1704	68	19,22,23	0.82	0	26,31,34	0.79	0
1	OMU	B5	4244	1	19,22,23	1.21	2 (10%)	26,31,34	1.68	5 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	PSU	B5	3585	94,1	18,21,22	1.36	2 (11%)	22,30,33	1.86	3 (13%)
1	A2M	B5	3456	1	22,25,26	1.45	4 (18%)	31,36,39	2.16	10 (32%)
68	PSU	A2	407	68	18,21,22	1.34	2 (11%)	22,30,33	1.89	3 (13%)
68	PSU	A2	1047	68	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
1	OMG	B5	2207	1	23,26,27	1.20	3 (13%)	33,38,41	1.93	6 (18%)
1	OMG	B5	1477	1	23,26,27	1.20	3 (13%)	33,38,41	1.94	6 (18%)
1	OMC	B5	2194	94,1	19,22,23	0.82	0	26,31,34	0.92	1 (3%)
1	1MA	B5	1266	94,1	21,25,26	1.39	4 (19%)	31,37,40	1.71	5 (16%)
16	HIC	BB	245	16	10,11,12	0.61	0	8,14,16	0.38	0
68	OMU	A2	1805	68	19,22,23	1.22	3 (15%)	26,31,34	1.69	4 (15%)
1	A2M	B5	2206	94,1	22,25,26	1.46	4 (18%)	31,36,39	2.13	9 (29%)
1	OMG	B5	3676	1	23,26,27	1.19	3 (13%)	33,38,41	1.95	6 (18%)
1	A2M	B5	3562	1	22,25,26	1.47	4 (18%)	31,36,39	2.15	10 (32%)
68	PSU	A2	1175	68	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)
1	PSU	B5	3616	1	18,21,22	1.34	2 (11%)	22,30,33	1.89	3 (13%)
1	A2M	B5	4336	1	22,25,26	1.46	4 (18%)	31,36,39	2.15	10 (32%)
1	PSU	B5	4045	1	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
68	B8N	A2	1249	68	24,29,30	1.30	3 (12%)	29,42,45	1.29	3 (10%)
27	AME	Au	1	27	9,10,11	0.48	0	9,11,13	0.86	1 (11%)
1	OMC	B5	2265	94,1	19,22,23	0.83	0	26,31,34	0.89	1 (3%)
79	M3L	Bm	98	79	10,11,12	0.82	0	9,14,16	0.54	0
68	PSU	A2	1082	68	18,21,22	1.36	2 (11%)	22,30,33	1.86	3 (13%)
1	PSU	B5	3652	94,1	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)
1	OMC	B5	3540	1	19,22,23	0.81	0	26,31,34	0.85	0
68	PSU	A2	967	68	18,21,22	1.36	2 (11%)	22,30,33	1.85	3 (13%)
68	PSU	A2	109	68	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
1	OMC	B5	2208	94,1	19,22,23	0.82	0	26,31,34	0.78	0
1	PSU	B5	4711	1	18,21,22	1.33	2 (11%)	22,30,33	1.86	3 (13%)
1	PSU	B5	4107	1	18,21,22	1.36	2 (11%)	22,30,33	1.87	3 (13%)
13	V5N	BA	216	13	9,11,12	2.07	2 (22%)	9,14,16	1.71	2 (22%)
68	PSU	A2	36	68	18,21,22	1.33	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%)
68	PSU	A2	210	68	18,21,22	1.35	2 (11%)	22,30,33	1.84	3 (13%)
1	PSU	B5	1801	1	18,21,22	1.36	2 (11%)	22,30,33	1.88	3 (13%)
68	PSU	A2	1348	68	18,21,22	1.33	2 (11%)	22,30,33	1.87	3 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	PSU	B5	4419	1	18,21,22	1.34	2 (11%)	22,30,33	1.86	3 (13%)
1	PSU	B5	4246	1	18,21,22	1.33	2 (11%)	22,30,33	1.89	3 (13%)
1	A2M	B5	1489	94,1	22,25,26	1.45	4 (18%)	31,36,39	2.09	9 (29%)
1	PSU	B5	3502	1	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
68	PSU	A2	119	68	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)
68	OMC	A2	518	68	19,22,23	0.81	0	26,31,34	0.82	0
1	5MC	B5	3514	94,1	18,22,23	0.96	2 (11%)	26,32,35	1.15	3 (11%)
1	PSU	B5	4278	1	18,21,22	1.37	2 (11%)	22,30,33	1.87	3 (13%)
1	PSU	B5	3490	1	18,21,22	1.33	2 (11%)	22,30,33	1.85	3 (13%)
68	PSU	A2	802	68	18,21,22	1.35	2 (11%)	22,30,33	1.84	3 (13%)
1	PSU	B5	4058	1	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
68	A2M	A2	591	68	22,25,26	1.48	4 (18%)	31,36,39	2.21	7 (22%)
1	OMC	B5	2647	1	19,22,23	0.81	0	26,31,34	0.83	0
1	OMU	B5	4052	1	19,22,23	1.21	2 (10%)	26,31,34	1.68	4 (15%)
12	NMM	As	67	12	9,11,12	0.60	0	6,12,14	0.52	0
68	A2M	A2	469	68	22,25,26	1.47	4 (18%)	31,36,39	2.12	10 (32%)
68	OMU	A2	1327	94,68	19,22,23	1.19	2 (10%)	26,31,34	1.70	5 (19%)
1	A2M	B5	3557	1	22,25,26	1.46	4 (18%)	31,36,39	2.11	9 (29%)
1	PSU	B5	4039	1	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
32	SAC	AZ	2	32	7,8,9	0.52	0	8,9,11	0.86	1 (12%)
68	OMG	A2	437	68	23,26,27	1.20	3 (13%)	33,38,41	1.94	6 (18%)
68	PSU	A2	1446	68	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
68	PSU	A2	34	68	18,21,22	1.35	2 (11%)	22,30,33	1.86	3 (13%)
1	OMC	B5	1820	94,1	19,22,23	0.80	0	26,31,34	0.79	0
68	OMG	A2	684	68	23,26,27	1.19	3 (13%)	33,38,41	1.93	6 (18%)
1	A2M	B5	4317	1	22,25,26	1.46	4 (18%)	31,36,39	2.12	10 (32%)
1	PSU	B5	4749	1	18,21,22	1.35	2 (11%)	22,30,33	1.89	3 (13%)
68	OMG	A2	1491	94,68	23,26,27	1.20	3 (13%)	33,38,41	1.93	6 (18%)
68	PSU	A2	816	68	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
1	OMG	B5	4383	1	23,26,27	1.20	3 (13%)	33,38,41	1.94	6 (18%)
68	A2M	A2	99	94,68	22,25,26	1.46	4 (18%)	31,36,39	2.12	9 (29%)
68	OMG	A2	1448	68	23,26,27	1.21	3 (13%)	33,38,41	1.94	6 (18%)
1	OMU	B5	3973	1	19,22,23	1.21	2 (10%)	26,31,34	1.69	4 (15%)
1	OMG	B5	2267	1	23,26,27	1.19	3 (13%)	33,38,41	1.92	6 (18%)
1	OMU	B5	2258	1	19,22,23	1.22	4 (21%)	26,31,34	1.67	4 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	PSU	B5	3583	1	18,21,22	1.36	2 (11%)	22,30,33	1.87	3 (13%)
68	PSU	A2	1005	68	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
68	PSU	A2	1178	68	18,21,22	1.32	2 (11%)	22,30,33	1.84	3 (13%)
68	OMC	A2	1392	68	19,22,23	0.82	0	26,31,34	0.84	0
1	PSU	B5	4188	1	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
1	PSU	B5	1537	1	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
1	OMG	B5	4138	1	23,26,27	1.20	3 (13%)	33,38,41	1.94	6 (18%)
1	PSU	B5	4267	94,1	18,21,22	1.34	2 (11%)	22,30,33	1.90	3 (13%)
1	A2M	B5	2658	94,1	22,25,26	1.47	4 (18%)	31,36,39	2.11	9 (29%)
1	A2M	B5	400	1	22,25,26	1.47	4 (18%)	31,36,39	2.11	10 (32%)
68	A2M	A2	669	94,68	22,25,26	1.45	4 (18%)	31,36,39	2.12	10 (32%)
68	PSU	A2	1057	68	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
1	PSU	B5	4298	1	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
1	PSU	B5	3500	1	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)
68	PSU	A2	573	68	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
1	OMC	B5	2704	1	19,22,23	0.82	0	26,31,34	0.84	1 (3%)
68	PSU	A2	682	68	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
68	MA6	A2	1851	68	23,26,27	2.28	5 (21%)	34,38,41	3.69	13 (38%)
68	OMU	A2	172	68	19,22,23	1.19	2 (10%)	26,31,34	1.70	4 (15%)
1	A2M	B5	1479	1	22,25,26	1.47	4 (18%)	31,36,39	2.09	8 (25%)
1	PSU	B5	1638	1	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)
1	PSU	B5	4169	1	18,21,22	1.33	2 (11%)	22,30,33	1.87	3 (13%)
68	PSU	A2	687	68	18,21,22	1.34	2 (11%)	22,30,33	1.86	3 (13%)
68	OMU	A2	121	68	19,22,23	1.21	2 (10%)	26,31,34	1.68	4 (15%)
68	PSU	A2	1245	68	18,21,22	1.34	2 (11%)	22,30,33	1.86	3 (13%)
68	OMU	A2	429	68	19,22,23	1.20	3 (15%)	26,31,34	1.68	4 (15%)
1	PSU	B5	4099	1	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
68	OMU	A2	1289	68	19,22,23	1.22	3 (15%)	26,31,34	1.67	5 (19%)
68	MA6	A2	1852	68	23,26,27	2.25	5 (21%)	34,38,41	3.66	14 (41%)
68	PSU	A2	1046	68	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
1	UY1	B5	3550	1	19,22,23	1.39	3 (15%)	22,31,34	1.87	5 (22%)
1	A2M	B5	398	1	22,25,26	1.47	4 (18%)	31,36,39	2.17	10 (32%)
1	OMG	B5	3359	1	23,26,27	1.19	3 (13%)	33,38,41	1.95	6 (18%)
1	OMC	B5	3619	1	19,22,23	0.81	0	26,31,34	0.82	0
1	OMG	B5	4240	1	23,26,27	1.19	3 (13%)	33,38,41	1.94	6 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
68	PSU	A2	1368	68	18,21,22	1.33	2 (11%)	22,30,33	1.86	3 (13%)
68	OMU	A2	355	68	19,22,23	1.21	2 (10%)	26,31,34	1.68	4 (15%)
1	OMC	B5	4202	1	19,22,23	0.81	0	26,31,34	0.82	0
68	G7M	A2	1640	68	23,26,27	3.12	9 (39%)	35,39,42	3.31	13 (37%)
68	PSU	A2	1626	68	18,21,22	1.36	2 (11%)	22,30,33	1.87	3 (13%)
1	PSU	B5	4042	1	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
68	PSU	A2	867	68	18,21,22	1.34	2 (11%)	22,30,33	1.89	3 (13%)
28	V5N	Ba	39	28	9,11,12	2.09	2 (22%)	9,14,16	1.67	2 (22%)
68	PSU	A2	823	68	18,21,22	1.36	2 (11%)	22,30,33	1.85	3 (13%)
68	A2M	A2	513	68	22,25,26	1.47	4 (18%)	31,36,39	2.13	10 (32%)
68	OMG	A2	868	68	23,26,27	1.18	3 (13%)	33,38,41	1.92	6 (18%)
1	PSU	B5	3427	1	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
1	PSU	B5	2351	1	18,21,22	1.33	2 (11%)	22,30,33	1.88	3 (13%)
1	A2M	B5	3517	1	22,25,26	1.44	4 (18%)	31,36,39	2.19	11 (35%)
10	PSU	B8	69	10	18,21,22	1.35	2 (11%)	22,30,33	1.85	3 (13%)
1	PSU	B5	3496	1	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
68	OMC	A2	174	94,68	19,22,23	0.82	0	26,31,34	0.81	0
68	A2M	A2	166	68	22,25,26	1.48	4 (18%)	31,36,39	2.16	10 (32%)
1	OMG	B5	3942	1,8	23,26,27	1.20	3 (13%)	33,38,41	1.93	6 (18%)
82	MLZ	Bo	53	82	8,9,10	0.48	0	4,9,11	0.12	0
68	OMC	A2	463	68	19,22,23	0.82	0	26,31,34	0.85	0
68	PSU	A2	218	68	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)
1	PSU	B5	4322	1	18,21,22	1.33	2 (11%)	22,30,33	1.86	3 (13%)
68	OMU	A2	628	68	19,22,23	1.17	2 (10%)	26,31,34	1.70	5 (19%)
1	A2M	B5	4269	94,1	22,25,26	1.46	4 (18%)	31,36,39	2.14	10 (32%)
1	A2M	B5	1270	1	22,25,26	1.45	4 (18%)	31,36,39	2.11	10 (32%)
1	PSU	B5	4177	1	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	B5	1720	1	-	0/7/25/26	0/2/2/2
68	A2M	A2	159	68	-	0/9/27/28	0/3/3/3
1	PSU	B5	4217	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	B5	4203	1	-	0/7/25/26	0/2/2/2
1	PSU	B5	4325	1	-	0/7/25/26	0/2/2/2
1	PSU	B5	4149	1	-	0/7/25/26	0/2/2/2
1	PSU	B5	3462	1	-	0/7/25/26	0/2/2/2
1	PSU	B5	3447	1	-	0/7/25/26	0/2/2/2
1	PSU	B5	4374	1	-	0/7/25/26	0/2/2/2
68	OMG	A2	1329	68	-	0/9/27/28	0/3/3/3
84	IAS	An	165	84	-	2/7/7/8	-
10	PSU	B8	55	10	-	0/7/25/26	0/2/2/2
68	PSU	A2	610	68	-	0/7/25/26	0/2/2/2
68	PSU	A2	650	68	-	0/7/25/26	0/2/2/2
1	OMC	B5	3573	1	-	1/9/27/28	0/2/2/2
1	PSU	B5	1721	1	-	0/7/25/26	0/2/2/2
1	A2M	B5	2630	94,1	-	2/9/27/28	0/3/3/3
68	OMG	A2	510	94,68	-	1/9/27/28	0/3/3/3
68	PSU	A2	1644	94,68	-	0/7/25/26	0/2/2/2
68	PSU	A2	652	68	-	0/7/25/26	0/2/2/2
68	6MZ	A2	1833	94,68	-	0/9/27/28	0/3/3/3
68	4AC	A2	1338	68	-	3/11/29/30	0/2/2/2
1	OMG	B5	3524	1	-	0/9/27/28	0/3/3/3
1	PSU	B5	2475	1	-	0/7/25/26	0/2/2/2
68	A2M	A2	1032	68	-	1/9/27/28	0/3/3/3
1	5MC	B5	4193	1	-	4/7/25/26	0/2/2/2
1	OMU	B5	3657	1	-	0/9/27/28	0/2/2/2
1	OMC	B5	1284	1	-	1/9/27/28	0/2/2/2
68	PSU	A2	1233	68	-	0/7/25/26	0/2/2/2
1	PSU	B5	1632	1	-	0/7/25/26	0/2/2/2
68	PSU	A2	1693	68	-	0/7/25/26	0/2/2/2
1	PSU	B5	1491	1	-	0/7/25/26	0/2/2/2
1	PSU	B5	3369	1	-	0/7/25/26	0/2/2/2
3	MLZ	Bb	5	3	-	1/7/8/10	-
1	PSU	B5	3371	1	-	0/7/25/26	0/2/2/2
68	OMU	A2	116	68	-	1/9/27/28	0/2/2/2
68	4AC	A2	1843	68	-	4/11/29/30	0/2/2/2
1	6MZ	B5	3966	1	-	0/9/27/28	0/3/3/3
1	PSU	B5	4382	1	-	4/7/25/26	0/2/2/2
1	PSU	B5	3494	1	-	0/7/25/26	0/2/2/2
1	OMG	B5	3631	1	-	2/9/27/28	0/3/3/3
68	OMG	A2	645	68	-	3/9/27/28	0/3/3/3
68	PSU	A2	105	68	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
68	A2M	A2	485	68	-	0/9/27/28	0/3/3/3
1	OMG	B5	4116	1	-	0/9/27/28	0/3/3/3
1	OMC	B5	3433	1	-	4/9/27/28	0/2/2/2
1	PSU	B5	4435	1	-	0/7/25/26	0/2/2/2
1	OMC	B5	4282	94,1	-	0/9/27/28	0/2/2/2
1	PSU	B5	1718	1	-	0/7/25/26	0/2/2/2
1	OMC	B5	2667	1	-	2/9/27/28	0/2/2/2
1	OMG	B5	3476	1	-	2/9/27/28	0/3/3/3
1	PSU	B5	1799	1	-	0/7/25/26	0/2/2/2
1	OMG	B5	4364	1	-	0/9/27/28	0/3/3/3
1	OMG	B5	4369	1	-	1/9/27/28	0/3/3/3
35	AYA	BC	2	35	-	0/4/6/8	-
88	SAC	Br	2	88	-	0/7/8/10	-
68	OMG	A2	602	68	-	0/9/27/28	0/3/3/3
1	PSU	B5	4166	1	-	4/7/25/26	0/2/2/2
1	PSU	B5	3554	1	-	0/7/25/26	0/2/2/2
1	OMG	B5	1260	1	-	1/9/27/28	0/3/3/3
1	PSU	B5	3576	1	-	1/7/25/26	0/2/2/2
68	PSU	A2	1239	68	-	0/7/25/26	0/2/2/2
1	OMG	B5	2719	1	-	0/9/27/28	0/3/3/3
1	A2M	B5	1810	94,1	-	1/9/27/28	0/3/3/3
1	A2M	B5	3492	1,68	-	1/9/27/28	0/3/3/3
1	OMU	B5	4366	1	-	0/9/27/28	0/2/2/2
68	PSU	A2	864	68	-	0/7/25/26	0/2/2/2
1	A2M	B5	3599	1	-	1/9/27/28	0/3/3/3
1	OMG	B5	1580	1	-	0/9/27/28	0/3/3/3
68	PSU	A2	93	68	-	0/7/25/26	0/2/2/2
9	SAC	Ar	2	9	-	0/7/8/10	-
68	A2M	A2	577	68	-	2/9/27/28	0/3/3/3
68	A2M	A2	27	94,68	-	2/9/27/28	0/3/3/3
68	OMU	A2	1443	94,68	-	1/9/27/28	0/2/2/2
1	A2M	B5	2244	94,1	-	0/9/27/28	0/3/3/3
68	A2M	A2	1384	68	-	0/9/27/28	0/3/3/3
1	PSU	B5	3466	1	-	0/7/25/26	0/2/2/2
1	PSU	B5	1683	1	-	0/7/25/26	0/2/2/2
1	OMC	B5	3601	1	-	0/9/27/28	0/2/2/2
1	OMG	B5	4245	1	-	0/9/27/28	0/3/3/3
1	OMG	B5	3974	1	-	0/9/27/28	0/3/3/3
10	OMG	B8	75	10	-	0/9/27/28	0/3/3/3
68	A2M	A2	1679	68	-	0/9/27/28	0/3/3/3
68	PSU	A2	815	68	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	A2M	B5	3450	1	-	0/9/27/28	0/3/3/3
1	OMU	B5	2680	1	-	1/9/27/28	0/2/2/2
1	PSU	B5	4740	1	-	0/7/25/26	0/2/2/2
24	HY3	Aw	62	24	-	1/1/12/14	0/1/1/1
1	UR3	B5	4276	1	-	0/7/25/26	0/2/2/2
68	OMC	A2	1704	68	-	0/9/27/28	0/2/2/2
1	OMU	B5	4244	1	-	0/9/27/28	0/2/2/2
1	PSU	B5	3585	94,1	-	0/7/25/26	0/2/2/2
1	A2M	B5	3456	1	-	0/9/27/28	0/3/3/3
68	PSU	A2	407	68	-	0/7/25/26	0/2/2/2
68	PSU	A2	1047	68	-	0/7/25/26	0/2/2/2
1	OMG	B5	2207	1	-	2/9/27/28	0/3/3/3
1	OMG	B5	1477	1	-	0/9/27/28	0/3/3/3
1	OMC	B5	2194	94,1	-	2/9/27/28	0/2/2/2
1	1MA	B5	1266	94,1	-	0/7/25/26	0/3/3/3
16	HIC	BB	245	16	-	2/5/6/8	0/1/1/1
68	OMU	A2	1805	68	-	0/9/27/28	0/2/2/2
1	A2M	B5	2206	94,1	-	0/9/27/28	0/3/3/3
1	OMG	B5	3676	1	-	0/9/27/28	0/3/3/3
1	A2M	B5	3562	1	-	0/9/27/28	0/3/3/3
68	PSU	A2	1175	68	-	0/7/25/26	0/2/2/2
1	PSU	B5	3616	1	-	0/7/25/26	0/2/2/2
1	A2M	B5	4336	1	-	1/9/27/28	0/3/3/3
1	PSU	B5	4045	1	-	0/7/25/26	0/2/2/2
68	B8N	A2	1249	68	-	4/16/34/35	0/2/2/2
27	AME	Au	1	27	-	2/9/10/12	-
1	OMC	B5	2265	94,1	-	1/9/27/28	0/2/2/2
79	M3L	Bm	98	79	-	1/9/10/12	-
68	PSU	A2	1082	68	-	0/7/25/26	0/2/2/2
1	PSU	B5	3652	94,1	-	0/7/25/26	0/2/2/2
1	OMC	B5	3540	1	-	0/9/27/28	0/2/2/2
68	PSU	A2	967	68	-	0/7/25/26	0/2/2/2
68	PSU	A2	109	68	-	0/7/25/26	0/2/2/2
1	OMC	B5	2208	94,1	-	0/9/27/28	0/2/2/2
1	PSU	B5	4711	1	-	0/7/25/26	0/2/2/2
1	PSU	B5	4107	1	-	0/7/25/26	0/2/2/2
13	V5N	BA	216	13	-	3/9/10/12	0/1/1/1
68	PSU	A2	36	68	-	0/7/25/26	0/2/2/2
1	PSU	B5	1731	1	-	0/7/25/26	0/2/2/2
68	PSU	A2	210	68	-	0/7/25/26	0/2/2/2
1	PSU	B5	1801	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
68	PSU	A2	1348	68	-	0/7/25/26	0/2/2/2
1	PSU	B5	4419	1	-	0/7/25/26	0/2/2/2
1	PSU	B5	4246	1	-	1/7/25/26	0/2/2/2
1	A2M	B5	1489	94,1	-	2/9/27/28	0/3/3/3
1	PSU	B5	3502	1	-	0/7/25/26	0/2/2/2
68	PSU	A2	119	68	-	0/7/25/26	0/2/2/2
68	OMC	A2	518	68	-	0/9/27/28	0/2/2/2
1	5MC	B5	3514	94,1	-	0/7/25/26	0/2/2/2
1	PSU	B5	4278	1	-	0/7/25/26	0/2/2/2
1	PSU	B5	3490	1	-	0/7/25/26	0/2/2/2
68	PSU	A2	802	68	-	2/7/25/26	0/2/2/2
1	PSU	B5	4058	1	-	0/7/25/26	0/2/2/2
68	A2M	A2	591	68	-	3/9/27/28	0/3/3/3
1	OMC	B5	2647	1	-	1/9/27/28	0/2/2/2
1	OMU	B5	4052	1	-	0/9/27/28	0/2/2/2
12	NMM	As	67	12	-	0/9/11/13	-
68	A2M	A2	469	68	-	2/9/27/28	0/3/3/3
68	OMU	A2	1327	94,68	-	0/9/27/28	0/2/2/2
1	A2M	B5	3557	1	-	0/9/27/28	0/3/3/3
1	PSU	B5	4039	1	-	0/7/25/26	0/2/2/2
32	SAC	AZ	2	32	-	2/7/8/10	-
68	OMG	A2	437	68	-	0/9/27/28	0/3/3/3
68	PSU	A2	1446	68	-	0/7/25/26	0/2/2/2
68	PSU	A2	34	68	-	0/7/25/26	0/2/2/2
1	OMC	B5	1820	94,1	-	2/9/27/28	0/2/2/2
68	OMG	A2	684	68	-	2/9/27/28	0/3/3/3
1	A2M	B5	4317	1	-	1/9/27/28	0/3/3/3
1	PSU	B5	4749	1	-	0/7/25/26	0/2/2/2
68	OMG	A2	1491	94,68	-	0/9/27/28	0/3/3/3
68	PSU	A2	816	68	-	0/7/25/26	0/2/2/2
1	OMG	B5	4383	1	-	0/9/27/28	0/3/3/3
68	A2M	A2	99	94,68	-	2/9/27/28	0/3/3/3
68	OMG	A2	1448	68	-	3/9/27/28	0/3/3/3
1	OMU	B5	3973	1	-	0/9/27/28	0/2/2/2
1	OMG	B5	2267	1	-	1/9/27/28	0/3/3/3
1	OMU	B5	2258	1	-	1/9/27/28	0/2/2/2
1	PSU	B5	3583	1	-	0/7/25/26	0/2/2/2
68	PSU	A2	1005	68	-	0/7/25/26	0/2/2/2
68	PSU	A2	1178	68	-	0/7/25/26	0/2/2/2
68	OMC	A2	1392	68	-	0/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	B5	4188	1	-	0/7/25/26	0/2/2/2
1	PSU	B5	1537	1	-	0/7/25/26	0/2/2/2
1	OMG	B5	4138	1	-	1/9/27/28	0/3/3/3
1	PSU	B5	4267	94,1	-	0/7/25/26	0/2/2/2
1	A2M	B5	2658	94,1	-	0/9/27/28	0/3/3/3
1	A2M	B5	400	1	-	0/9/27/28	0/3/3/3
68	A2M	A2	669	94,68	-	2/9/27/28	0/3/3/3
68	PSU	A2	1057	68	-	0/7/25/26	0/2/2/2
1	PSU	B5	4298	1	-	0/7/25/26	0/2/2/2
1	PSU	B5	3500	1	-	0/7/25/26	0/2/2/2
68	PSU	A2	573	68	-	0/7/25/26	0/2/2/2
1	OMC	B5	2704	1	-	1/9/27/28	0/2/2/2
68	PSU	A2	682	68	-	0/7/25/26	0/2/2/2
68	MA6	A2	1851	68	-	0/11/29/30	0/3/3/3
68	OMU	A2	172	68	-	0/9/27/28	0/2/2/2
1	A2M	B5	1479	1	-	0/9/27/28	0/3/3/3
1	PSU	B5	1638	1	-	0/7/25/26	0/2/2/2
1	PSU	B5	4169	1	-	0/7/25/26	0/2/2/2
68	PSU	A2	687	68	-	0/7/25/26	0/2/2/2
68	OMU	A2	121	68	-	0/9/27/28	0/2/2/2
68	PSU	A2	1245	68	-	0/7/25/26	0/2/2/2
68	OMU	A2	429	68	-	5/9/27/28	0/2/2/2
1	PSU	B5	4099	1	-	0/7/25/26	0/2/2/2
68	OMU	A2	1289	68	-	0/9/27/28	0/2/2/2
68	MA6	A2	1852	68	-	3/11/29/30	0/3/3/3
68	PSU	A2	1046	68	-	0/7/25/26	0/2/2/2
1	UY1	B5	3550	1	-	1/9/27/28	0/2/2/2
1	A2M	B5	398	1	-	3/9/27/28	0/3/3/3
1	OMG	B5	3359	1	-	0/9/27/28	0/3/3/3
1	OMC	B5	3619	1	-	2/9/27/28	0/2/2/2
1	OMG	B5	4240	1	-	0/9/27/28	0/3/3/3
68	PSU	A2	1368	68	-	0/7/25/26	0/2/2/2
68	OMU	A2	355	68	-	1/9/27/28	0/2/2/2
1	OMC	B5	4202	1	-	0/9/27/28	0/2/2/2
68	G7M	A2	1640	68	-	2/7/25/26	0/3/3/3
68	PSU	A2	1626	68	-	0/7/25/26	0/2/2/2
1	PSU	B5	4042	1	-	0/7/25/26	0/2/2/2
68	PSU	A2	867	68	-	0/7/25/26	0/2/2/2
28	V5N	Ba	39	28	-	0/9/10/12	0/1/1/1
68	PSU	A2	823	68	-	0/7/25/26	0/2/2/2
68	A2M	A2	513	68	-	2/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
68	OMG	A2	868	68	-	0/9/27/28	0/3/3/3
1	PSU	B5	3427	1	-	0/7/25/26	0/2/2/2
1	PSU	B5	2351	1	-	0/7/25/26	0/2/2/2
1	A2M	B5	3517	1	-	2/9/27/28	0/3/3/3
10	PSU	B8	69	10	-	0/7/25/26	0/2/2/2
1	PSU	B5	3496	1	-	0/7/25/26	0/2/2/2
68	OMC	A2	174	94,68	-	0/9/27/28	0/2/2/2
68	A2M	A2	166	68	-	0/9/27/28	0/3/3/3
1	OMG	B5	3942	1,8	-	0/9/27/28	0/3/3/3
82	MLZ	Bo	53	82	-	0/7/8/10	-
68	OMC	A2	463	68	-	0/9/27/28	0/2/2/2
68	PSU	A2	218	68	-	0/7/25/26	0/2/2/2
1	PSU	B5	4322	1	-	0/7/25/26	0/2/2/2
68	OMU	A2	628	68	-	4/9/27/28	0/2/2/2
1	A2M	B5	4269	94,1	-	0/9/27/28	0/3/3/3
1	A2M	B5	1270	1	-	0/9/27/28	0/3/3/3
1	PSU	B5	4177	1	-	0/7/25/26	0/2/2/2

The worst 5 of 506 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
68	A2	1640	G7M	C4-N9	7.89	1.58	1.38
68	A2	1640	G7M	O6-C6	7.59	1.38	1.23
68	A2	1851	MA6	C5-N7	6.86	1.52	1.39
68	A2	1852	MA6	C5-N7	6.78	1.51	1.39
68	A2	1640	G7M	C5-C4	6.17	1.53	1.38

The worst 5 of 954 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
68	A2	1851	MA6	C4-N9-C8	14.61	121.56	105.73
68	A2	1852	MA6	C4-N9-C8	14.37	121.30	105.73
68	A2	1640	G7M	C8-N7-C5	11.39	122.03	107.78
68	A2	591	A2M	C5-C4-N3	-6.98	117.64	126.75
68	A2	1852	MA6	N3-C4-N9	6.85	138.36	127.08

There are no chirality outliers.

5 of 127 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B5	2207	OMG	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
1	B5	2207	OMG	C3'-C4'-C5'-O5'
1	B5	3433	OMC	C2'-C1'-N1-C2
1	B5	3433	OMC	C2'-C1'-N1-C6
1	B5	3599	A2M	C1'-C2'-O2'-CM'

There are no ring outliers.

93 monomers are involved in 119 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
68	A2	159	A2M	1	0
1	B5	4203	PSU	1	0
1	B5	4325	PSU	1	0
68	A2	1329	OMG	1	0
68	A2	610	PSU	1	0
1	B5	2630	A2M	1	0
68	A2	510	OMG	1	0
68	A2	1833	6MZ	1	0
68	A2	1338	4AC	3	0
68	A2	1032	A2M	2	0
1	B5	4193	5MC	1	0
1	B5	1284	OMC	2	0
68	A2	116	OMU	1	0
68	A2	1843	4AC	1	0
1	B5	3966	6MZ	1	0
1	B5	4382	PSU	1	0
1	B5	3631	OMG	1	0
68	A2	645	OMG	1	0
68	A2	105	PSU	1	0
68	A2	485	A2M	1	0
1	B5	4282	OMC	1	0
1	B5	2667	OMC	1	0
1	B5	3476	OMG	1	0
1	B5	4369	OMG	1	0
68	A2	602	OMG	1	0
1	B5	4166	PSU	1	0
1	B5	1260	OMG	1	0
1	B5	1810	A2M	2	0
1	B5	4366	OMU	3	0
1	B5	3599	A2M	1	0
68	A2	577	A2M	1	0
68	A2	27	A2M	3	0
1	B5	2244	A2M	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
68	A2	1384	A2M	1	0
10	B8	75	OMG	1	0
68	A2	1679	A2M	2	0
68	A2	815	PSU	1	0
1	B5	3450	A2M	1	0
68	A2	1704	OMC	1	0
1	B5	3585	PSU	1	0
1	B5	3456	A2M	1	0
1	B5	2207	OMG	1	0
1	B5	2194	OMC	1	0
68	A2	1805	OMU	2	0
1	B5	2206	A2M	1	0
1	B5	3676	OMG	2	0
1	B5	3562	A2M	2	0
1	B5	3616	PSU	1	0
1	B5	4336	A2M	1	0
27	Au	1	AME	1	0
79	Bm	98	M3L	1	0
1	B5	3540	OMC	1	0
1	B5	2208	OMC	2	0
68	A2	36	PSU	2	0
1	B5	1489	A2M	1	0
68	A2	518	OMC	1	0
1	B5	4278	PSU	1	0
1	B5	4058	PSU	1	0
1	B5	2647	OMC	1	0
1	B5	4052	OMU	2	0
68	A2	469	A2M	1	0
1	B5	3557	A2M	1	0
1	B5	4039	PSU	1	0
68	A2	437	OMG	2	0
68	A2	1446	PSU	1	0
68	A2	1491	OMG	1	0
1	B5	4383	OMG	1	0
68	A2	99	A2M	2	0
68	A2	1448	OMG	2	0
1	B5	2258	OMU	2	0
68	A2	1392	OMC	1	0
1	B5	4138	OMG	2	0
1	B5	2658	A2M	3	0
1	B5	2704	OMC	1	0
68	A2	1851	MA6	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
68	A2	172	OMU	1	0
68	A2	121	OMU	2	0
1	B5	4099	PSU	1	0
68	A2	1289	OMU	2	0
1	B5	3550	UY1	2	0
1	B5	398	A2M	1	0
1	B5	3619	OMC	1	0
68	A2	355	OMU	1	0
1	B5	4202	OMC	1	0
68	A2	1640	G7M	1	0
68	A2	513	A2M	1	0
1	B5	3517	A2M	2	0
68	A2	166	A2M	1	0
1	B5	3942	OMG	2	0
68	A2	463	OMC	1	0
68	A2	628	OMU	1	0
1	B5	4269	A2M	2	0
1	B5	1270	A2M	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 758 ligands modelled in this entry, 295 are unknown and 428 are monoatomic - leaving 35 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	$\# Z > 2$
93	SPD	B5	5019	-	9,9,9	0.16	0	8,8,8	0.19	0
97	IHP	DB	901	-	36,36,36	1.55	6 (16%)	54,60,60	1.14	4 (7%)
93	SPD	B5	4902	-	9,9,9	0.16	0	8,8,8	0.17	0
93	SPD	B5	4922	-	9,9,9	0.15	0	8,8,8	0.19	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
93	SPD	A2	1915	-	9,9,9	0.16	0	8,8,8	0.17	0
93	SPD	B5	5241	-	9,9,9	0.16	0	8,8,8	0.16	0
93	SPD	B5	4982	-	9,9,9	0.15	0	8,8,8	0.19	0
93	SPD	B5	5120	-	9,9,9	0.15	0	8,8,8	0.18	0
93	SPD	A2	1947	-	9,9,9	0.15	0	8,8,8	0.18	0
93	SPD	A2	1930	-	9,9,9	0.15	0	8,8,8	0.18	0
93	SPD	B5	5222	-	9,9,9	0.15	0	8,8,8	0.18	0
93	SPD	B5	5079	-	9,9,9	0.15	0	8,8,8	0.19	0
93	SPD	B5	5202	-	9,9,9	0.16	0	8,8,8	0.19	0
93	SPD	B5	5162	-	9,9,9	0.15	0	8,8,8	0.19	0
93	SPD	A2	1908	-	9,9,9	0.15	0	8,8,8	0.18	0
93	SPD	A2	1939	-	9,9,9	0.16	0	8,8,8	0.17	0
93	SPD	B5	5141	-	9,9,9	0.15	0	8,8,8	0.20	0
95	SPM	A2	1962	-	13,13,13	0.15	0	12,12,12	0.16	0
93	SPD	B5	4941	-	9,9,9	0.15	0	8,8,8	0.18	0
93	SPD	B5	5000	-	9,9,9	0.15	0	8,8,8	0.17	0
93	SPD	B5	5387	-	9,9,9	0.15	0	8,8,8	0.19	0
95	SPM	B5	5059	-	13,13,13	0.15	0	12,12,12	0.14	0
93	SPD	A2	1955	-	9,9,9	0.15	0	8,8,8	0.17	0
93	SPD	B5	5366	-	9,9,9	0.16	0	8,8,8	0.22	0
93	SPD	A2	1922	-	9,9,9	0.16	0	8,8,8	0.18	0
93	SPD	A2	1929	-	9,9,9	0.15	0	8,8,8	0.17	0
93	SPD	B5	5323	-	9,9,9	0.15	0	8,8,8	0.18	0
93	SPD	B5	5303	-	9,9,9	0.15	0	8,8,8	0.15	0
93	SPD	B5	5039	-	9,9,9	0.15	0	8,8,8	0.19	0
95	SPM	B5	5194	-	13,13,13	0.15	0	12,12,12	0.21	0
93	SPD	B5	5182	-	9,9,9	0.15	0	8,8,8	0.18	0
93	SPD	B5	4962	-	9,9,9	0.16	0	8,8,8	0.18	0
93	SPD	B5	5344	-	9,9,9	0.16	0	8,8,8	0.18	0
93	SPD	B5	5100	-	9,9,9	0.15	0	8,8,8	0.17	0
96	GTP	B7	214	7	30,34,34	0.50	0	46,54,54	0.56	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
93	SPD	B5	5019	-	-	0/7/7/7	-
97	IHP	DB	901	-	-	10/30/54/54	0/1/1/1
93	SPD	B5	4902	-	-	1/7/7/7	-
93	SPD	B5	4922	-	-	0/7/7/7	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
93	SPD	A2	1915	-	-	0/7/7/7	-
93	SPD	B5	5241	-	-	1/7/7/7	-
93	SPD	B5	4982	-	-	1/7/7/7	-
93	SPD	B5	5120	-	-	0/7/7/7	-
93	SPD	A2	1947	-	-	1/7/7/7	-
93	SPD	A2	1930	-	-	0/7/7/7	-
93	SPD	B5	5222	-	-	0/7/7/7	-
93	SPD	B5	5079	-	-	0/7/7/7	-
93	SPD	B5	5202	-	-	1/7/7/7	-
93	SPD	B5	5162	-	-	0/7/7/7	-
93	SPD	A2	1908	-	-	1/7/7/7	-
93	SPD	A2	1939	-	-	0/7/7/7	-
93	SPD	B5	5141	-	-	0/7/7/7	-
95	SPM	A2	1962	-	-	1/11/11/11	-
93	SPD	B5	4941	-	-	0/7/7/7	-
93	SPD	B5	5000	-	-	0/7/7/7	-
93	SPD	B5	5387	-	-	1/7/7/7	-
95	SPM	B5	5059	-	-	0/11/11/11	-
93	SPD	A2	1955	-	-	0/7/7/7	-
93	SPD	B5	5366	-	-	0/7/7/7	-
93	SPD	A2	1922	-	-	0/7/7/7	-
93	SPD	A2	1929	-	-	0/7/7/7	-
93	SPD	B5	5323	-	-	1/7/7/7	-
93	SPD	B5	5303	-	-	1/7/7/7	-
93	SPD	B5	5039	-	-	0/7/7/7	-
95	SPM	B5	5194	-	-	1/11/11/11	-
93	SPD	B5	5182	-	-	0/7/7/7	-
93	SPD	B5	4962	-	-	0/7/7/7	-
93	SPD	B5	5344	-	-	1/7/7/7	-
93	SPD	B5	5100	-	-	0/7/7/7	-
96	GTP	B7	214	7	-	0/22/38/38	0/3/3/3

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
97	DB	901	IHP	P2-O12	3.51	1.65	1.59
97	DB	901	IHP	P5-O15	3.43	1.65	1.59
97	DB	901	IHP	P1-O11	3.27	1.65	1.59
97	DB	901	IHP	P6-O16	3.22	1.65	1.59
97	DB	901	IHP	P3-O13	3.20	1.65	1.59

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
97	DB	901	IHP	C6-C5-C4	4.35	119.94	110.41
97	DB	901	IHP	C5-C4-C3	3.62	118.33	110.41
97	DB	901	IHP	C5-C6-C1	3.52	118.12	110.41
97	DB	901	IHP	C4-C3-C2	2.19	115.21	110.41

There are no chirality outliers.

5 of 22 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
97	DB	901	IHP	C1-C2-O12-P2
97	DB	901	IHP	C4-C5-O15-P5
97	DB	901	IHP	C4-O14-P4-O24
95	A2	1962	SPM	C8-C9-N10-C11
97	DB	901	IHP	C2-O12-P2-O32

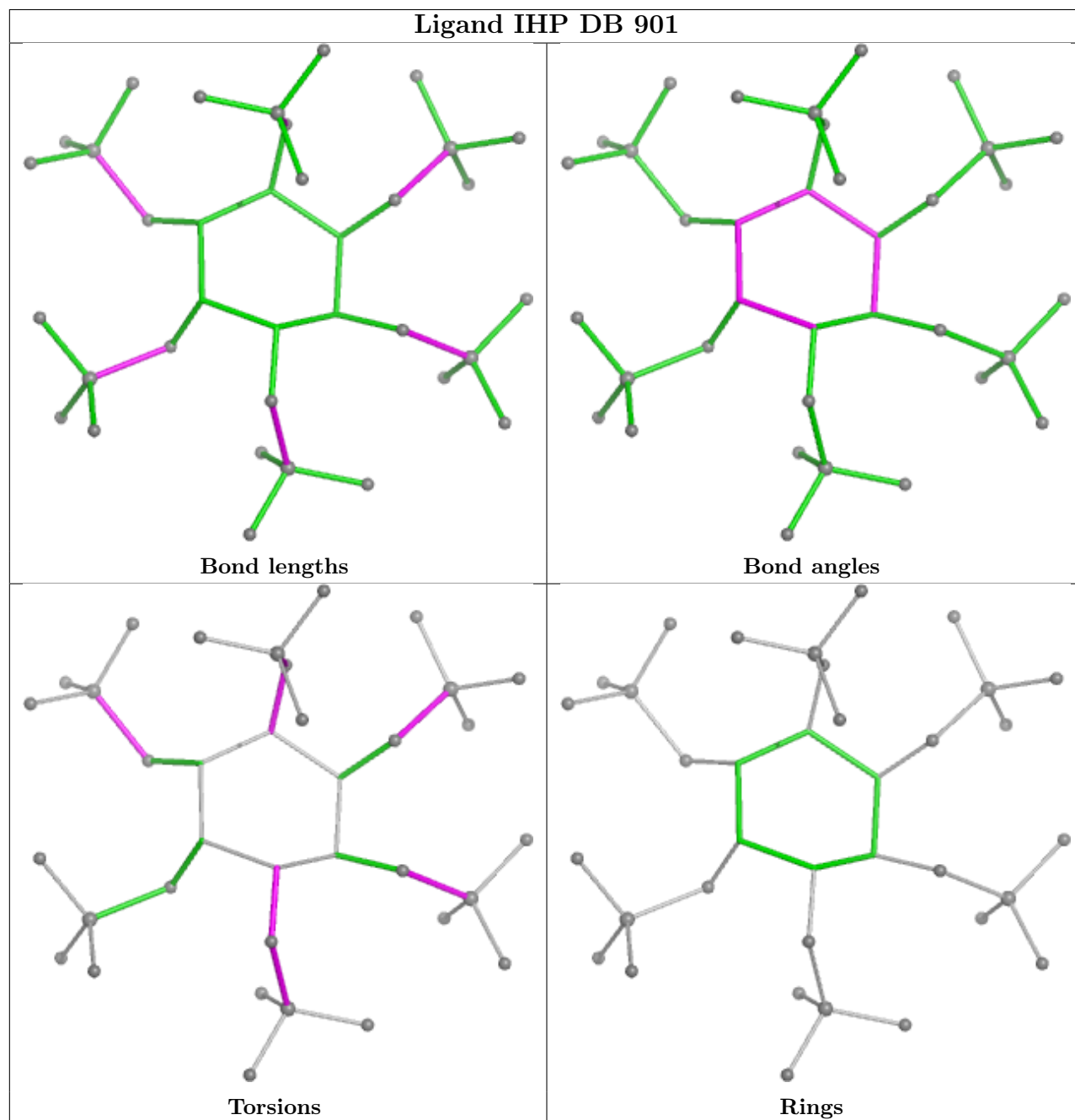
There are no ring outliers.

18 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
97	DB	901	IHP	1	0
93	B5	5241	SPD	1	0
93	A2	1947	SPD	1	0
93	A2	1930	SPD	1	0
93	B5	5079	SPD	2	0
93	B5	5202	SPD	1	0
93	A2	1908	SPD	1	0
93	A2	1939	SPD	1	0
93	B5	5141	SPD	1	0
95	A2	1962	SPM	3	0
93	B5	4941	SPD	1	0
93	A2	1955	SPD	1	0
93	B5	5366	SPD	1	0
93	A2	1922	SPD	1	0
95	B5	5194	SPM	1	0
93	B5	4962	SPD	1	0
93	B5	5344	SPD	1	0
93	B5	5100	SPD	2	0

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

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

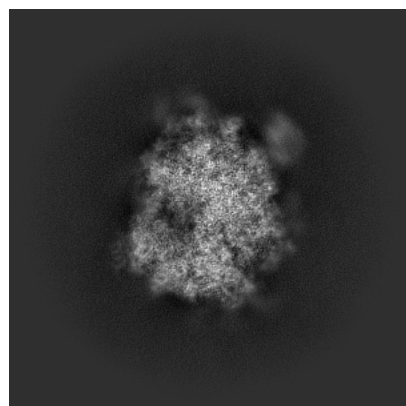
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-50126. These allow visual inspection of the internal detail of the map and identification of artifacts.

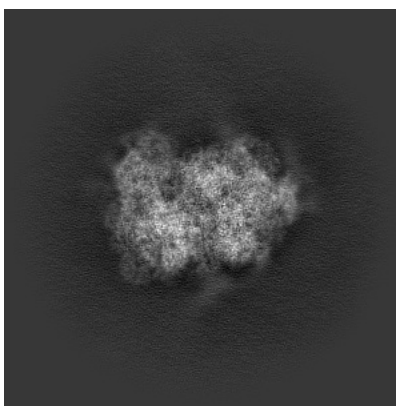
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

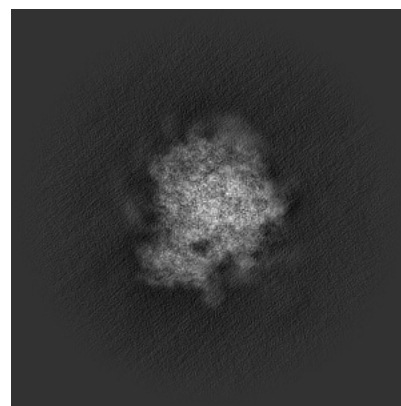
6.1.1 Primary map



X

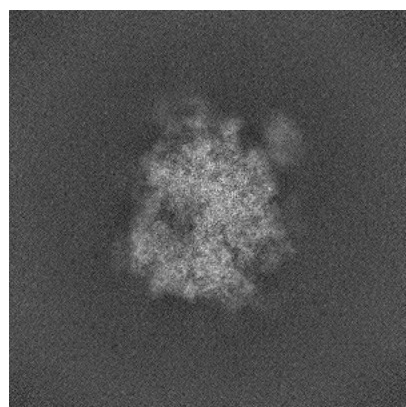


Y

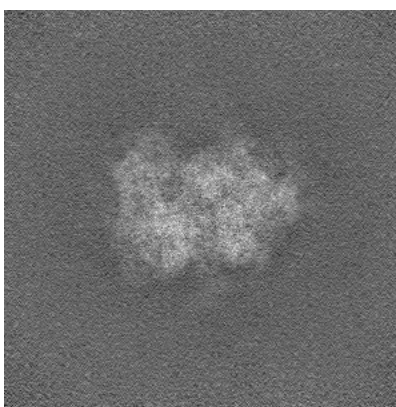


Z

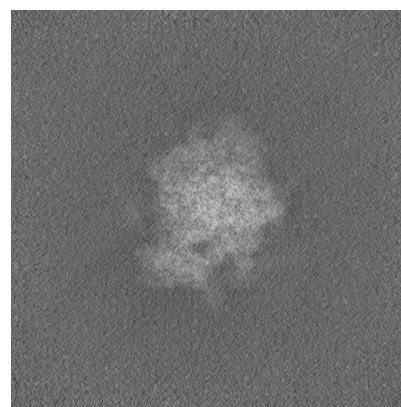
6.1.2 Raw map



X



Y

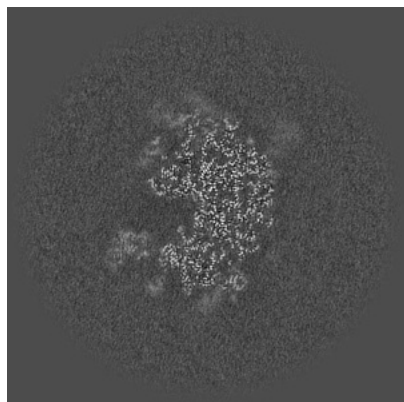


Z

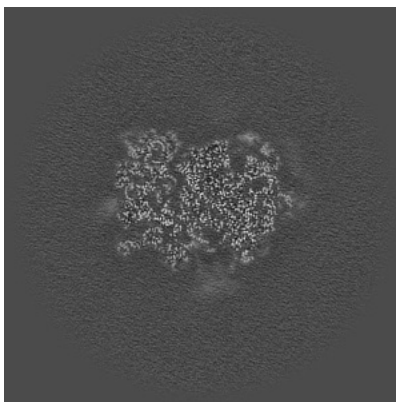
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

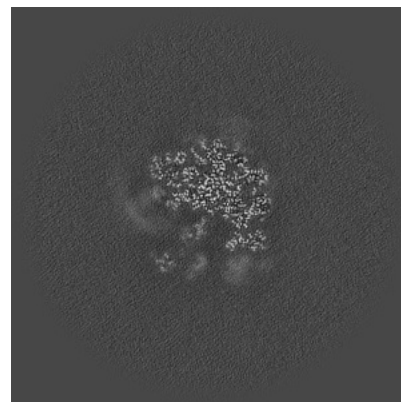
6.2.1 Primary map



X Index: 280

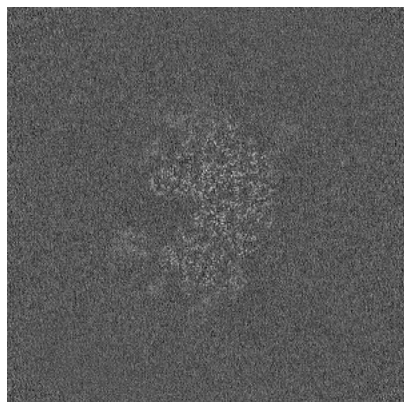


Y Index: 280

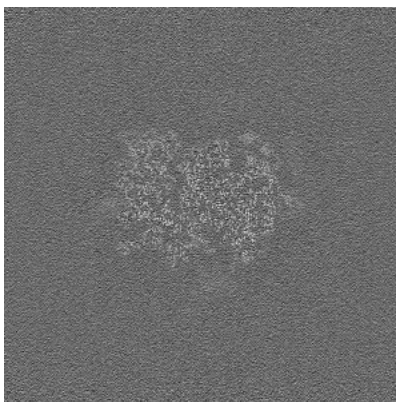


Z Index: 280

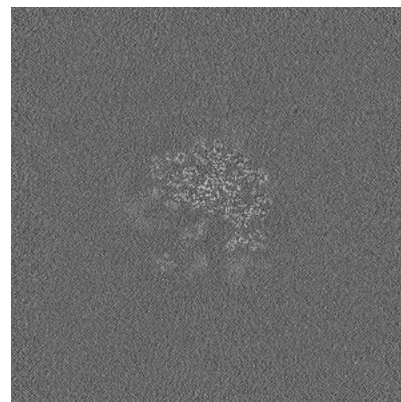
6.2.2 Raw map



X Index: 280



Y Index: 280

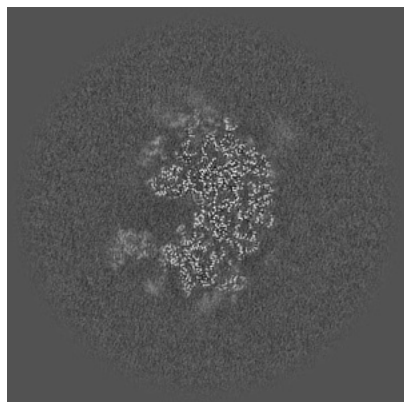


Z Index: 280

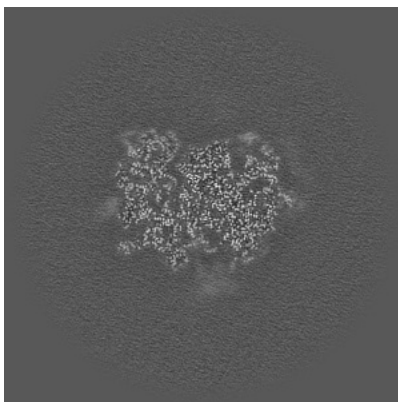
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

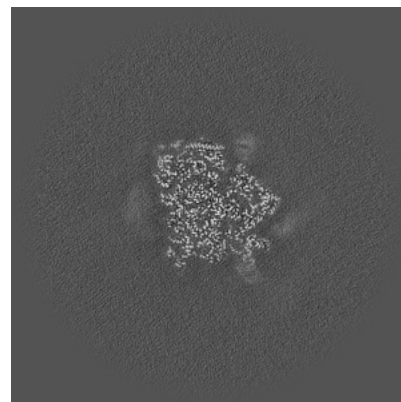
6.3.1 Primary map



X Index: 279

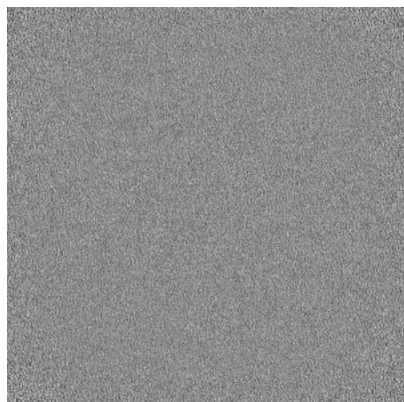


Y Index: 281

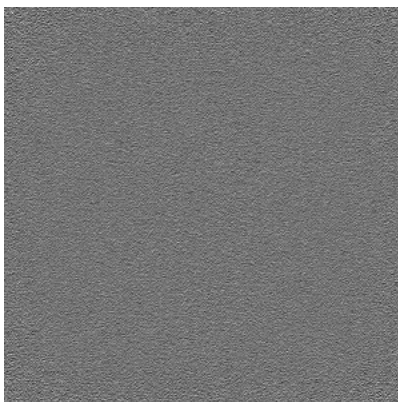


Z Index: 309

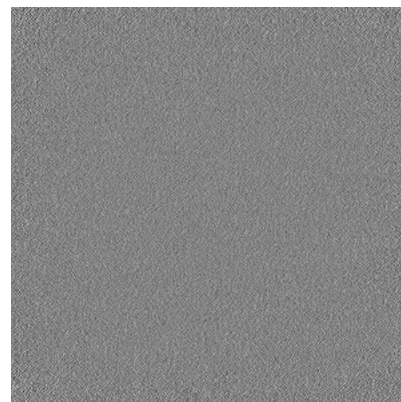
6.3.2 Raw map



X Index: 0



Y Index: 0

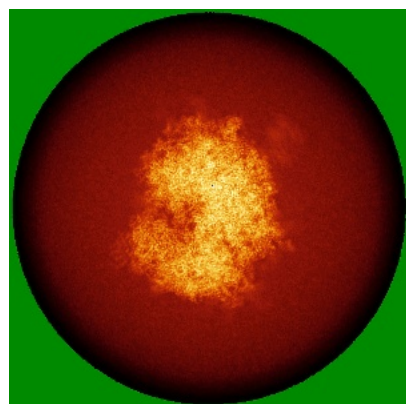


Z Index: 0

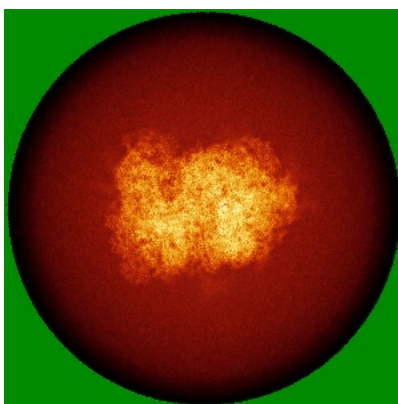
The images above show the largest variance slices of the map in three orthogonal directions.

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

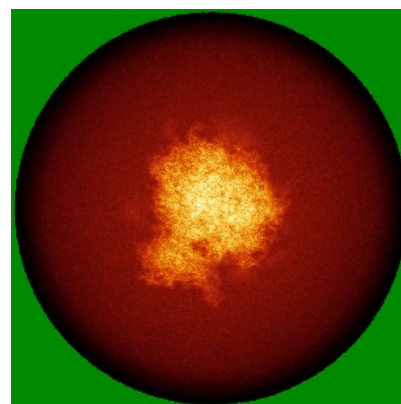
6.4.1 Primary map



X

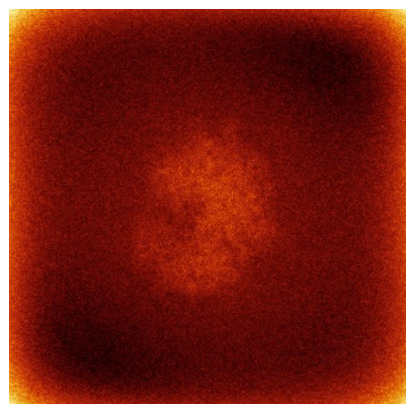


Y

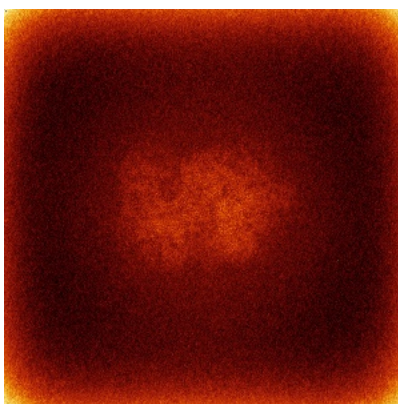


Z

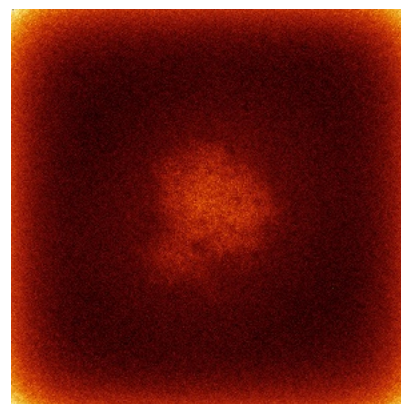
6.4.2 Raw map



X



Y

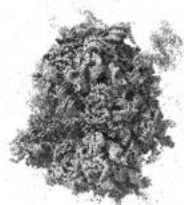


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



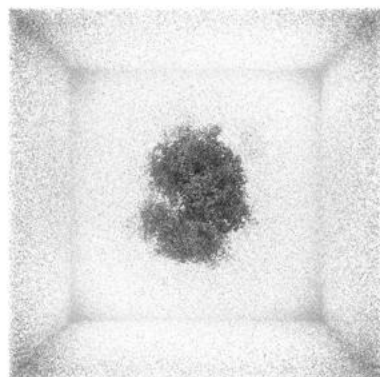
Y



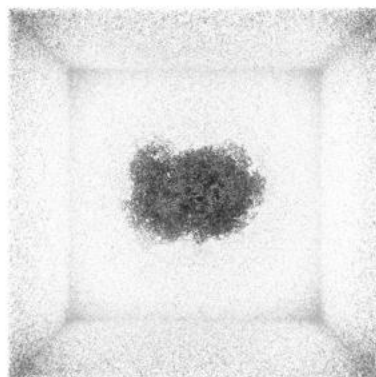
Z

The images above show the 3D surface view of the map at the recommended contour level 0.25. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

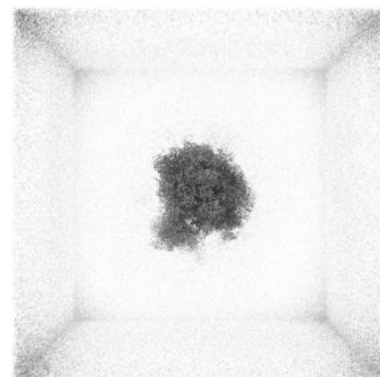
6.5.2 Raw map



X



Y



Z

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

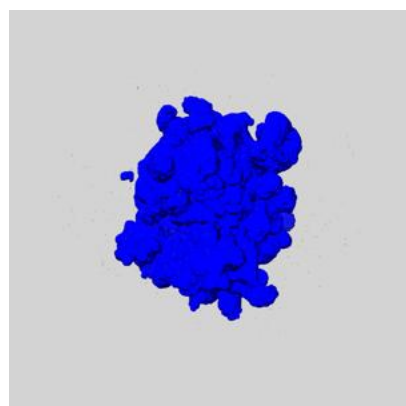
6.6 Mask visualisation [i](#)

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

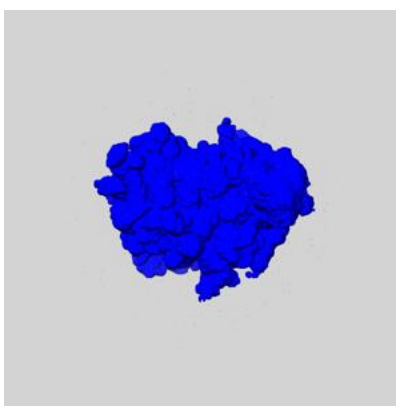
A mask typically either:

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

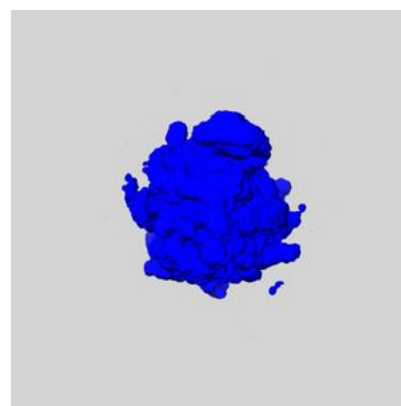
6.6.1 emd_50126_msk_1.map [i](#)



X

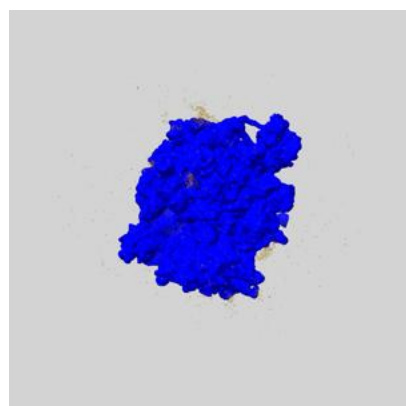


Y

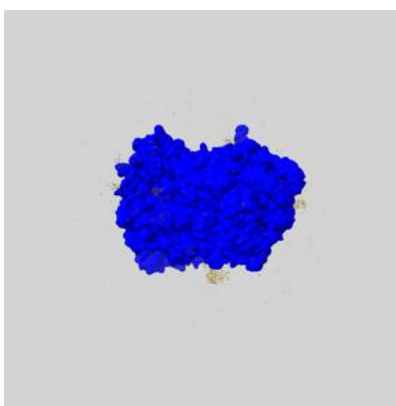


Z

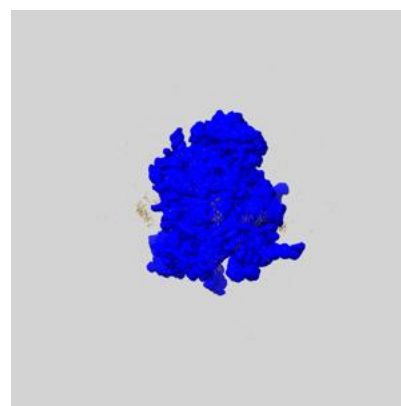
6.6.2 emd_50126_msk_2.map [i](#)



X



Y

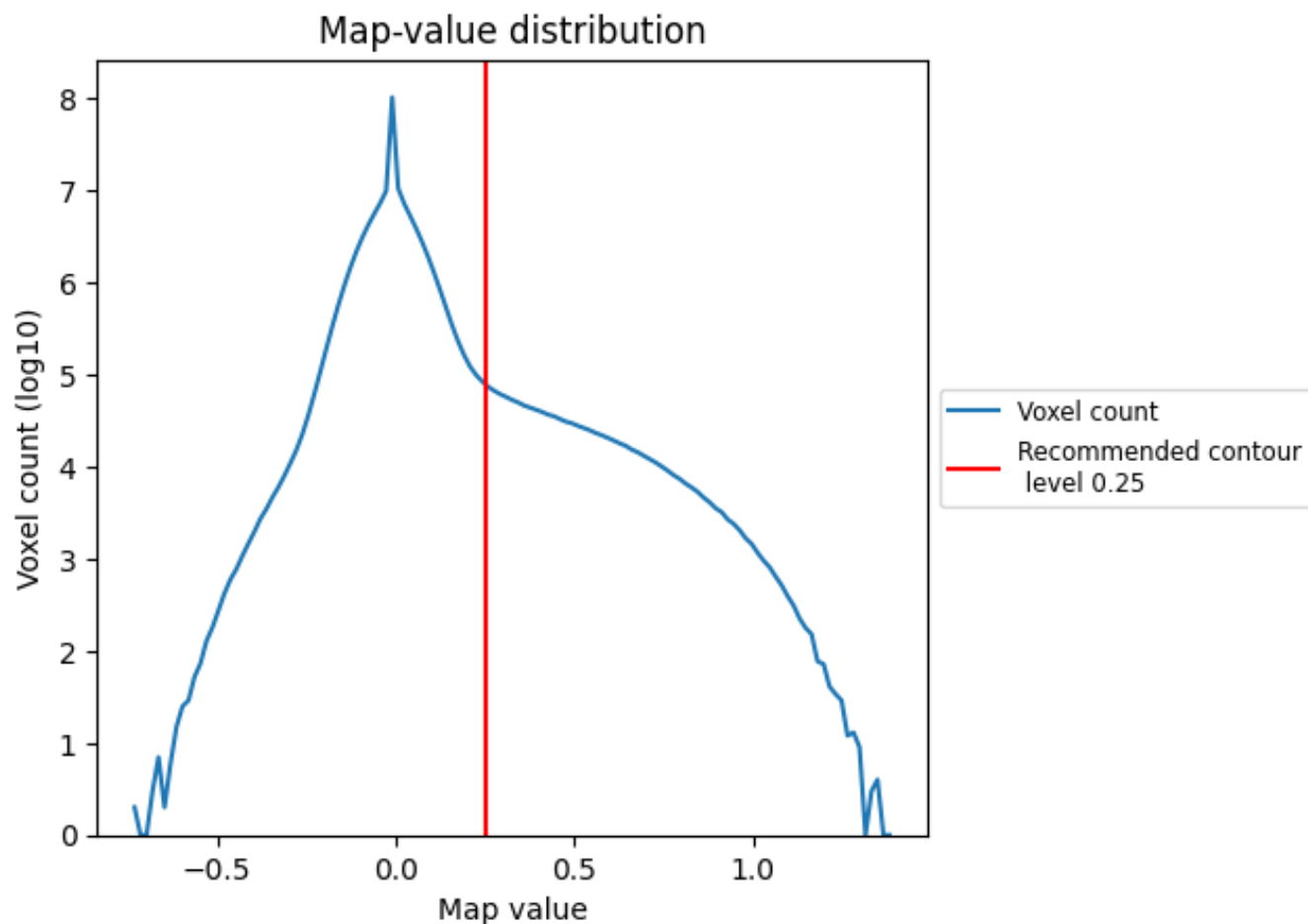


Z

7 Map analysis [i](#)

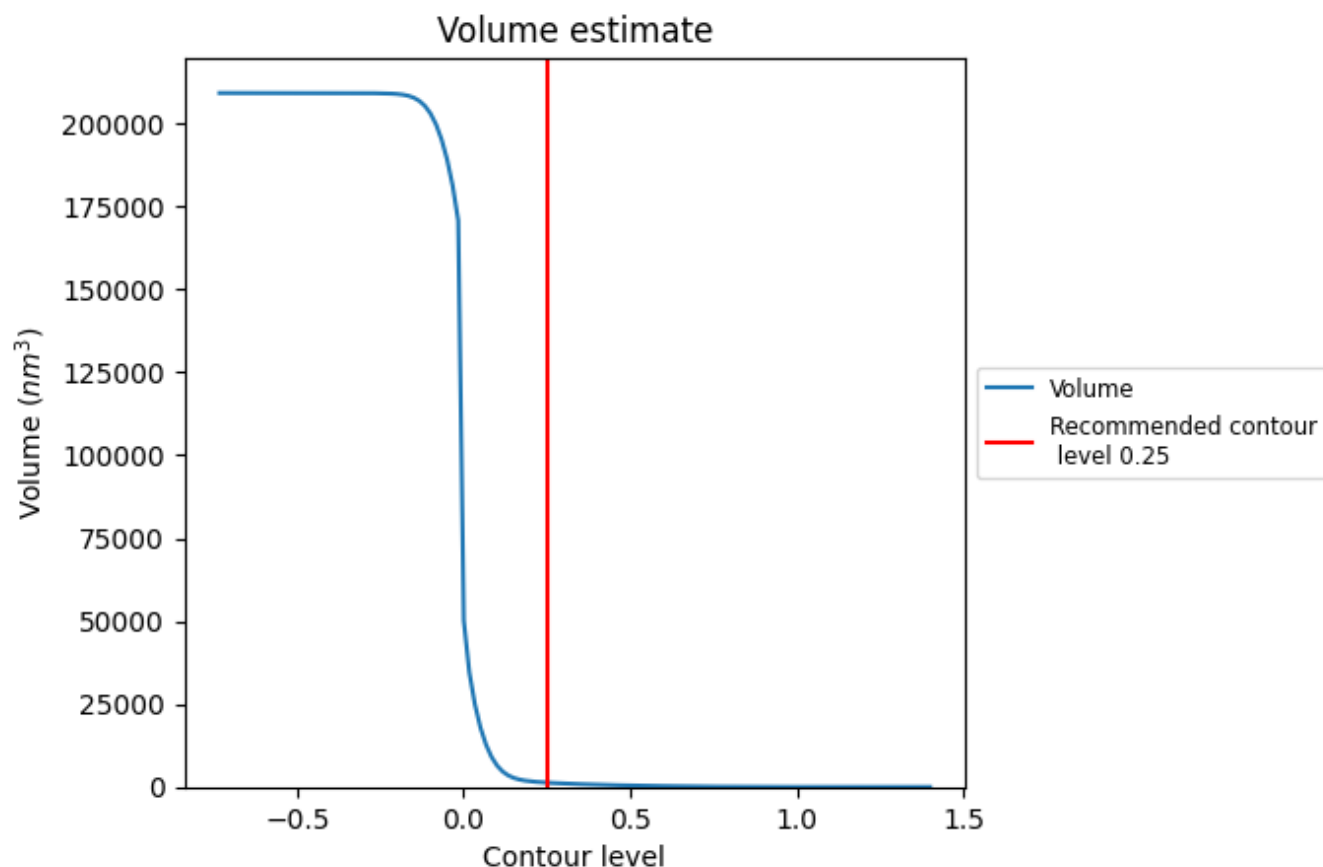
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

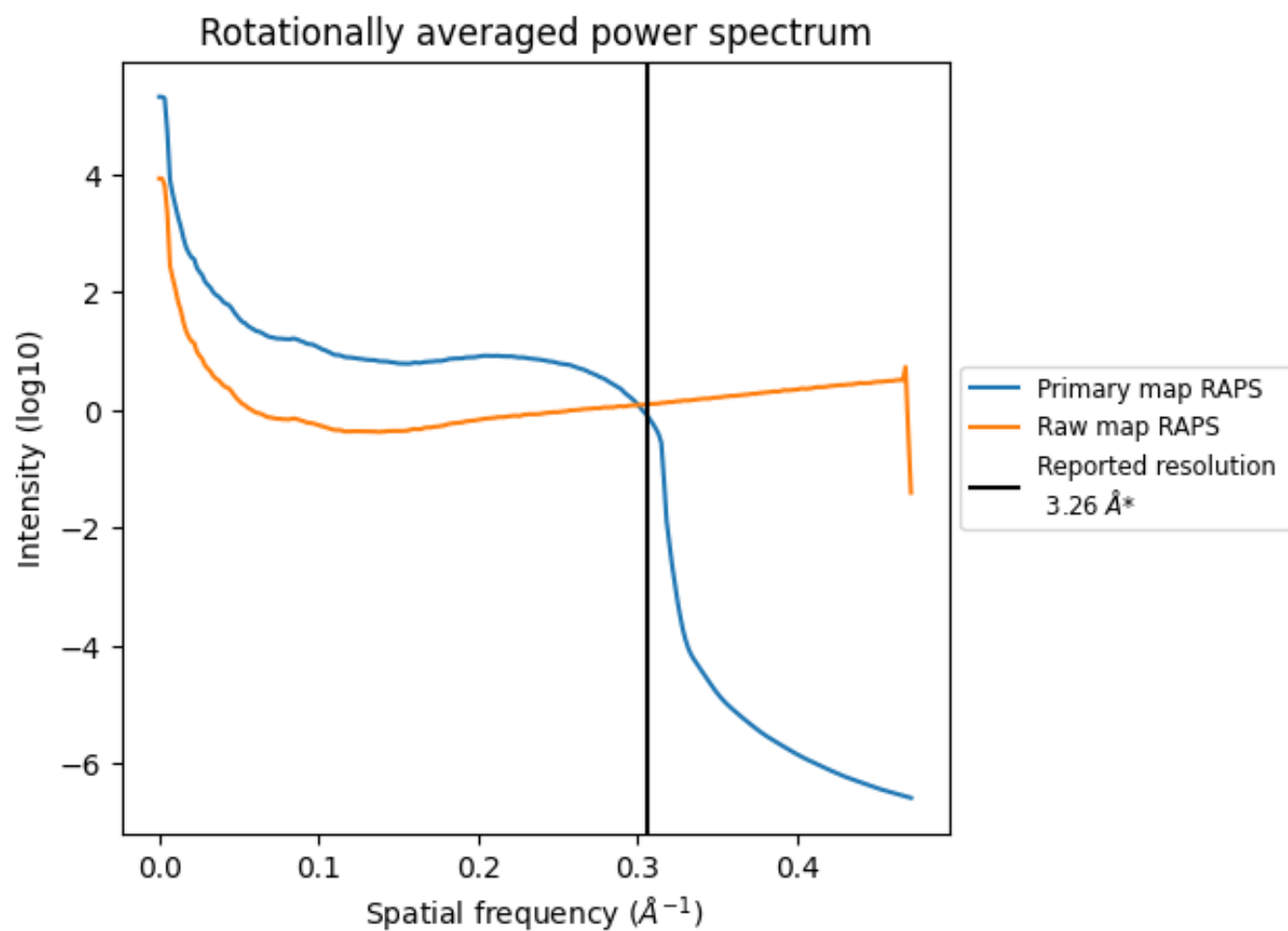
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1299 nm^3 ; this corresponds to an approximate mass of 1173 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

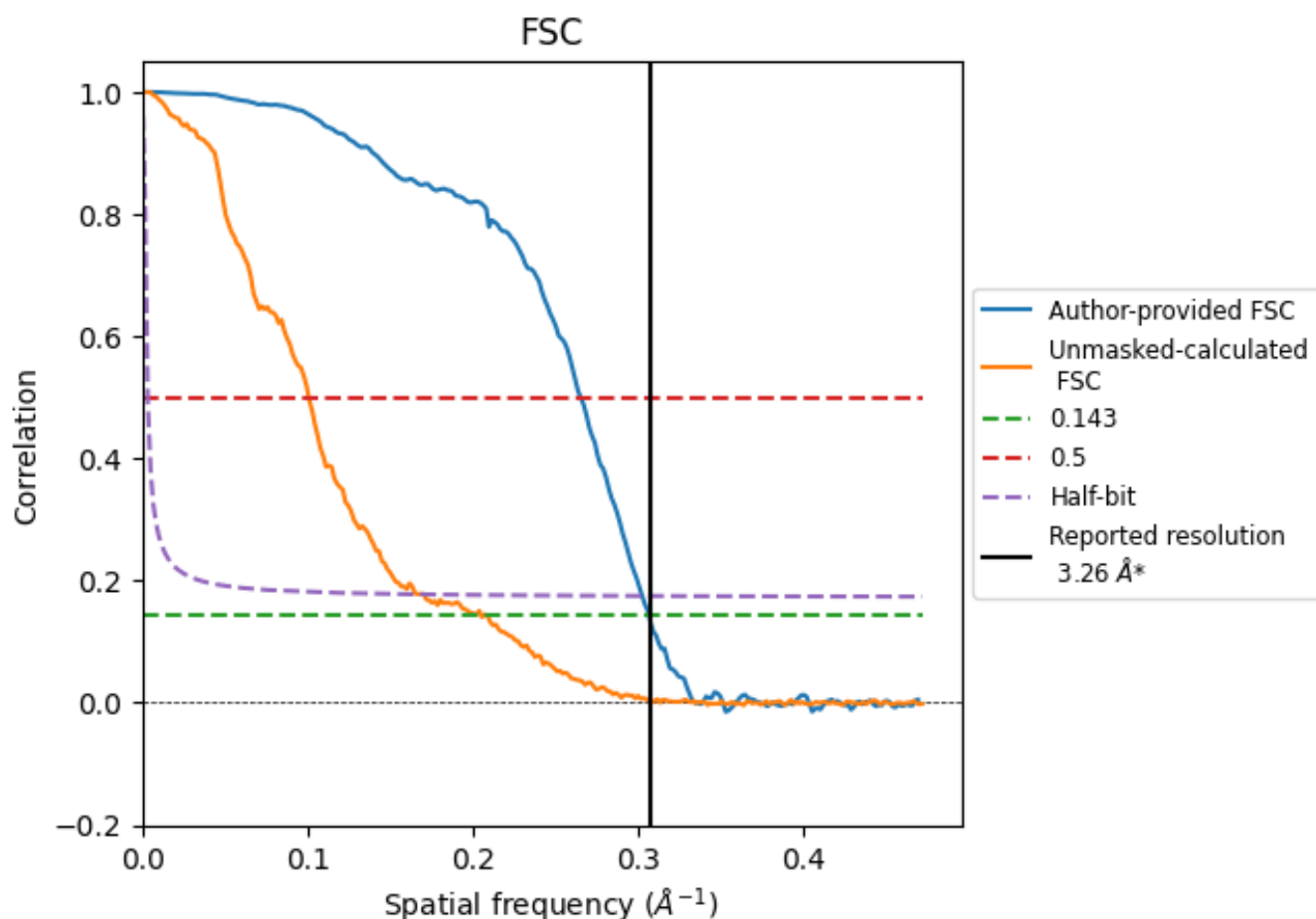


*Reported resolution corresponds to spatial frequency of 0.307 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.307 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

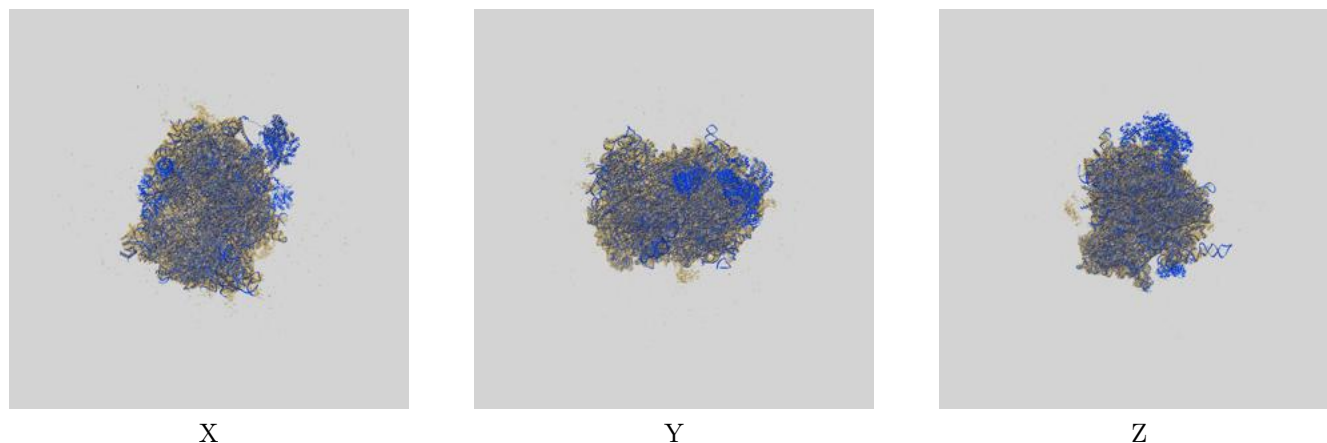
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.26	-	-
Author-provided FSC curve	3.26	3.77	3.31
Unmasked-calculated*	4.88	9.93	5.87

*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 4.88 differs from the reported value 3.26 by more than 10 %

9 Map-model fit [i](#)

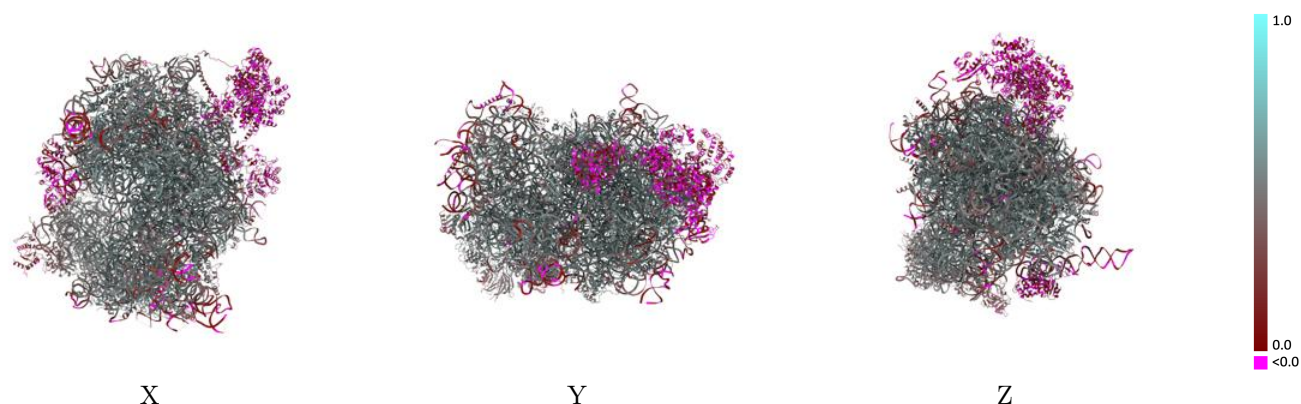
This section contains information regarding the fit between EMDB map EMD-50126 and PDB model 9F1D. Per-residue inclusion information can be found in section [3](#) on page [35](#).

9.1 Map-model overlay [i](#)



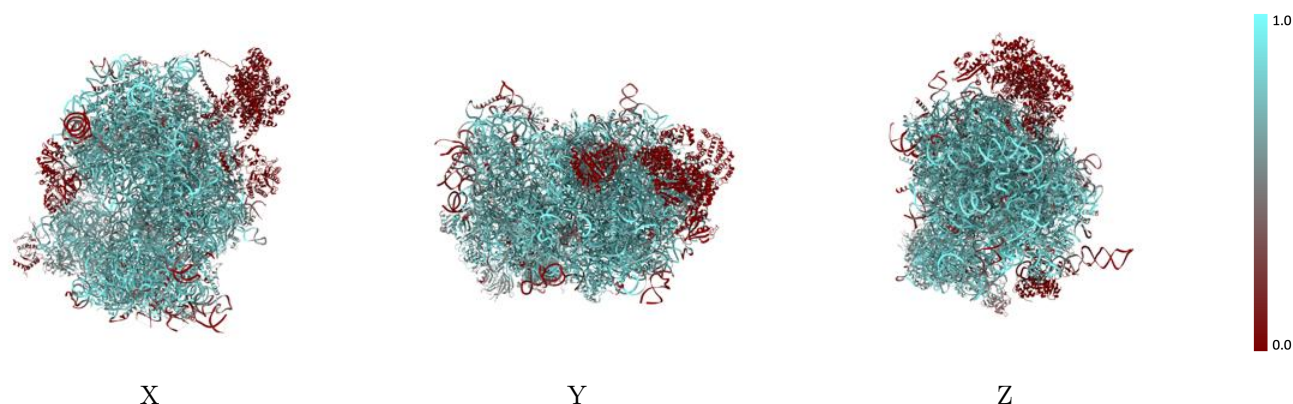
The images above show the 3D surface view of the map at the recommended contour level 0.25 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



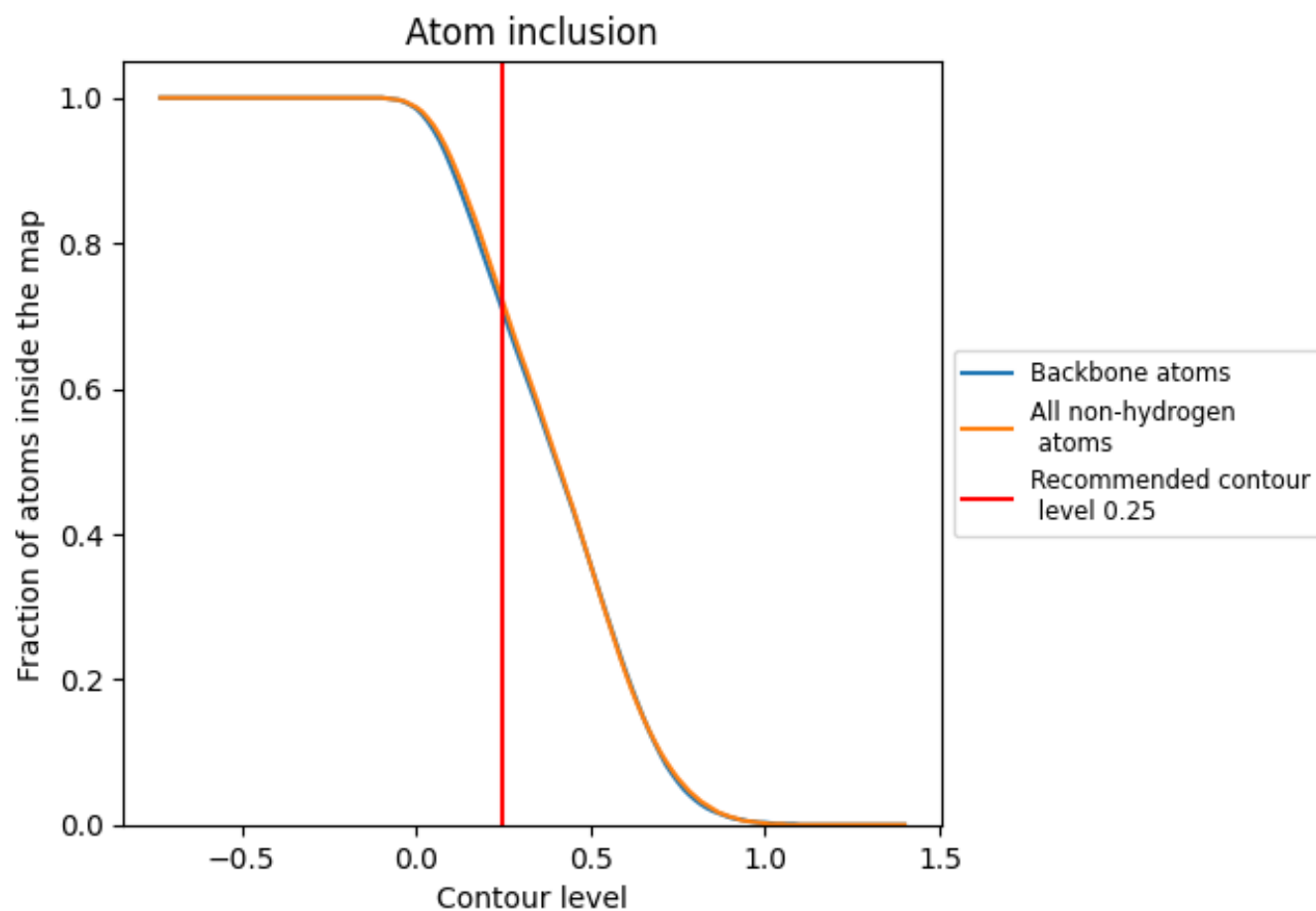
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.25).

9.4 Atom inclusion [i](#)



At the recommended contour level, 70% of all backbone atoms, 72% 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 (0.25) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7170	 0.4470
A2	 0.8080	 0.4530
AA	 0.6850	 0.4930
AB	 0.6560	 0.4740
AC	 0.3050	 0.2390
AD	 0.5910	 0.4330
AE	 0.7460	 0.5090
AF	 0.5890	 0.3900
AG	 0.7760	 0.4930
AH	 0.1390	 0.4330
AT	 0.6570	 0.4410
AZ	 0.7330	 0.4930
Aa	 0.6800	 0.4900
Ab	 0.7510	 0.5170
Ac	 0.6280	 0.4370
Ad	 0.7350	 0.5090
Ae	 0.6540	 0.4590
Af	 0.6250	 0.4190
Ag	 0.6330	 0.4300
Ah	 0.7210	 0.4960
Ai	 0.7410	 0.4910
Aj	 0.6380	 0.4050
Ak	 0.6870	 0.4880
Al	 0.2070	 0.1750
Am	 0.7440	 0.5220
An	 0.7090	 0.5030
Ao	 0.5990	 0.4060
Ap	 0.6840	 0.4750
Aq	 0.6850	 0.4660
Ar	 0.6320	 0.4270
As	 0.6770	 0.4480
At	 0.5950	 0.4170
Au	 0.7270	 0.5060
Av	 0.7710	 0.5370
Aw	 0.7310	 0.5300



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Chain	Atom inclusion	Q-score
Ax	 0.6910	 0.4590
Ay	 0.5290	 0.3970
Az	 0.6240	 0.5030
B	 0.7700	 0.5000
B5	 0.8200	 0.4700
B7	 0.9110	 0.5140
B8	 0.8540	 0.4930
BA	 0.7870	 0.5470
BB	 0.7850	 0.5380
BC	 0.7910	 0.5390
BE	 0.7060	 0.4750
BF	 0.7870	 0.5360
BG	 0.6950	 0.4820
BH	 0.7190	 0.5080
BI	 0.7680	 0.5320
BJ	 0.7060	 0.4860
BK	 0.1700	 0.4450
BL	 0.7420	 0.5090
BM	 0.7890	 0.5160
BN	 0.8280	 0.5550
BO	 0.7800	 0.5350
BP	 0.7600	 0.5320
BQ	 0.7910	 0.5450
BR	 0.7290	 0.4960
BS	 0.8040	 0.5420
BT	 0.7460	 0.5190
BU	 0.6880	 0.4870
BV	 0.7030	 0.5220
BW	 0.5320	 0.3540
BX	 0.7420	 0.5200
BY	 0.7450	 0.5230
BZ	 0.7650	 0.5120
Ba	 0.8140	 0.5480
Bb	 0.6580	 0.4560
Bc	 0.6700	 0.4790
Bd	 0.7210	 0.5170
Be	 0.7710	 0.5390
Bf	 0.8200	 0.5510
Bg	 0.7350	 0.5160
Bh	 0.7550	 0.5060
Bi	 0.7220	 0.5030
Bj	 0.8430	 0.5550

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Chain	Atom inclusion	Q-score
Bk	 0.6550	 0.4630
Bl	 0.7420	 0.5300
Bm	 0.7780	 0.5440
Bo	 0.7290	 0.5210
Bp	 0.7370	 0.5320
Br	 0.7970	 0.5410
Bs	 0.0190	 0.0810
Bt	 0.0130	 0.0520
Ct	 0.0360	 0.0630
Cu	 0.1890	 0.1950
DA	 0.0010	 0.0140
DB	 0.0490	 0.0560
DC	 0.0250	 0.0300
DD	 0.0000	 0.0100
EA	 0.0010	 0.0590