



wwPDB EM Validation Summary Report ⓘ

Sep 22, 2026 – 10:35 pm BST

PDB ID : 29IZ / pdb_000029iz
EMDB ID : EMD-57204
Title : Dormant 80S:eEF2:SERBP1:tRNA complex from human cells treated with toxin NT-2
Authors : Rabl, J.; Karousis, E.D.
Deposited on : 2026-03-16
Resolution : 2.08 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.dev133
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) : 2.50

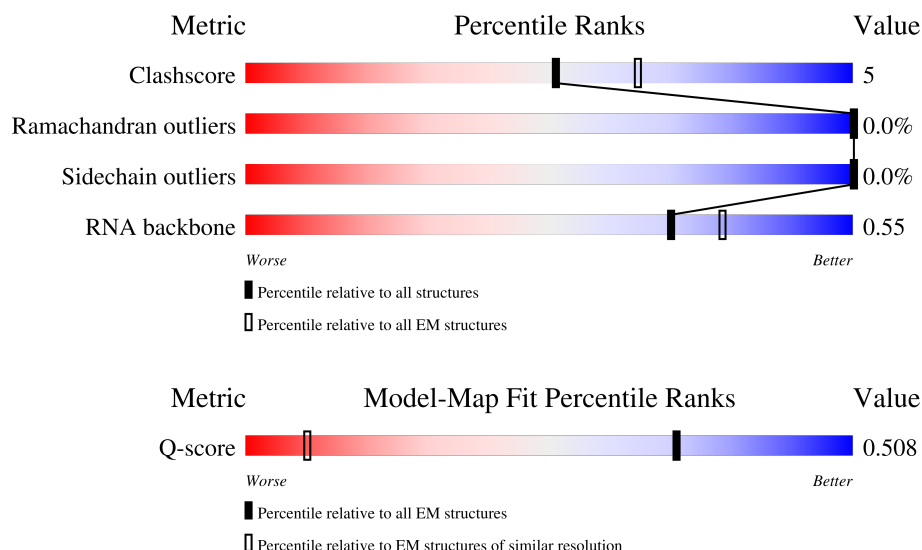
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.08 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	1976 (1.58 - 2.58)

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

Mol	Chain	Length	Quality of chain
1	AA	248	
2	AB	266	
3	AC	192	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	AD	214	
5	AE	178	
6	AF	211	
7	AG	215	
8	AH	204	
9	AI	203	
10	AJ	184	
11	AK	188	
12	AL	196	
13	AM	176	
14	AN	160	
15	AO	128	
16	AP	140	
17	AQ	157	
18	AR	156	
19	AS	145	
20	AT	136	
21	AU	148	
22	AV	159	
23	AW	115	
24	AX	125	
25	AY	135	
26	AZ	110	
27	Aa	117	
28	Ab	123	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
29	Ac	105	
30	Ad	97	
31	Ae	70	
32	Af	51	
33	Ag	128	
34	Ah	106	
35	Ai	92	
36	Aj	137	
37	BA	5069	
38	BB	120	
39	BC	157	
40	BD	257	
41	CA	403	
42	CB	427	
43	CC	297	
44	CD	288	
45	DA	77	
46	ER	858	
47	GF	408	
48	Hi	25	
49	HA	1868	
50	HC	264	
51	HF	263	
52	HI	194	
53	HJ	208	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
54	HM	158	
55	HS	135	
56	A	84	
57	HY	143	
58	Hb	115	
59	HD	293	
60	HH	249	
61	HK	194	
62	HO	151	
63	HP	151	
64	HX	130	
65	HZ	133	
66	Hc	84	
67	Hf	133	
68	B	207	
69	HE	243	
70	HG	204	
71	HL	165	
72	HQ	145	
73	HR	146	
74	HT	152	
75	HU	145	
76	HV	119	
77	Hd	69	
78	He	56	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
79	HN	132	
80	Ha	125	
81	Hg	156	
82	Hh	317	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
84	PUT	BA	5101	-	-	X	-
84	PUT	BB	201	-	-	X	-
87	SPD	BA	5108	-	-	X	-

2 Entry composition

There are 90 unique types of molecules in this entry. The entry contains 374899 atoms, of which 160059 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Large ribosomal subunit protein uL30.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	AA	221	Total	C	H	N	O	S	1	0
			3828	1186	1983	356	294	9		

- Molecule 2 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	AB	225	Total	C	H	N	O	S	0	0
			3784	1163	1962	351	304	4		

- Molecule 3 is a protein called 60S ribosomal protein L9.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	AC	190	Total	C	H	N	O	S	0	0
			3119	956	1601	284	272	6		

- Molecule 4 is a protein called Ribosomal protein uL16-like.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	AD	205	Total	C	H	N	O	S	2	0
			3385	1059	1715	323	275	13		

- Molecule 5 is a protein called 60S ribosomal protein L11.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	AE	171	Total	C	H	N	O	S	0	0
			2783	867	1412	256	242	6		

- Molecule 6 is a protein called 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	AF	202	Total	C	H	N	O	S	0	0
			3377	1022	1746	340	265	4		

- Molecule 7 is a protein called 60S ribosomal protein L14.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	AG	136	Total	C	H	N	O	S	0	0
			2307	719	1187	215	179	7		

- Molecule 8 is a protein called 60S ribosomal protein L15.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	AH	203	Total	C	H	N	O	S	0	0
			3450	1072	1749	359	266	4		

- Molecule 9 is a protein called 60S ribosomal protein L13a.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	AI	201	Total	C	H	N	O	S	0	0
			3445	1063	1795	321	261	5		

- Molecule 10 is a protein called 60S ribosomal protein L17.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	AJ	151	Total	C	H	N	O	S	0	0
			2474	765	1250	238	212	9		

- Molecule 11 is a protein called 60S ribosomal protein L18.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	AK	187	Total	C	H	N	O	S	0	0
			3142	944	1629	314	250	5		

- Molecule 12 is a protein called 60S ribosomal protein L19.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	AL	161	Total	C	H	N	O	S	0	0
			2816	834	1475	288	210	9		

- Molecule 13 is a protein called 60S ribosomal protein L18a.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	AM	175	Total	C	H	N	O	S	0	0
			2943	925	1490	283	235	10		

- Molecule 14 is a protein called 60S ribosomal protein L21.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	AN	159	Total	C	H	N	O	S	1	0
			2684	828	1380	253	217	6		

- Molecule 15 is a protein called 60S ribosomal protein L22.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	AO	99	Total	C	H	N	O	S	0	0
			1639	518	831	141	147	2		

- Molecule 16 is a protein called 60S ribosomal protein L23.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	AP	131	Total	C	H	N	O	S	0	0
			2018	618	1039	184	172	5		

- Molecule 17 is a protein called 60S ribosomal protein L24.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	AQ	62	Total	C	H	N	O	S	0	0
			1052	332	533	101	83	3		

- Molecule 18 is a protein called 60S ribosomal protein L23a.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	AR	119	Total	C	H	N	O	S	0	0
			2029	624	1053	183	168	1		

- Molecule 19 is a protein called 60S ribosomal protein L26.

Mol	Chain	Residues	Atoms						AltConf	Trace
19	AS	134	Total	C	H	N	O	S	0	0
			2320	700	1205	226	186	3		

- Molecule 20 is a protein called 60S ribosomal protein L27.

Mol	Chain	Residues	Atoms						AltConf	Trace
20	AT	135	Total	C	H	N	O	S	0	0
			2289	714	1182	208	182	3		

- Molecule 21 is a protein called Large ribosomal subunit protein uL15.

Mol	Chain	Residues	Atoms						AltConf	Trace
21	AU	147	Total	C	H	N	O	S	0	0
			2373	736	1210	237	187	3		

- Molecule 22 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms						AltConf	Trace
22	AV	98	Total	C	H	N	O	S	0	0
			1660	497	862	175	123	3		

- Molecule 23 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms						AltConf	Trace
23	AW	98	Total	C	H	N	O	S	0	0
			1568	485	804	135	138	6		

- Molecule 24 is a protein called 60S ribosomal protein L31.

Mol	Chain	Residues	Atoms						AltConf	Trace
24	AX	109	Total	C	H	N	O	S	0	0
			1848	569	947	173	157	2		

- Molecule 25 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms						AltConf	Trace
25	AY	130	Total	C	H	N	O	S	0	0
			2236	676	1166	221	168	5		

- Molecule 26 is a protein called Large ribosomal subunit protein eL33.

Mol	Chain	Residues	Atoms						AltConf	Trace
26	AZ	109	Total	C	H	N	O	S	0	0
			1788	555	912	174	144	3		

- Molecule 27 is a protein called 60S ribosomal protein L34.

Mol	Chain	Residues	Atoms						AltConf	Trace
27	Aa	109	Total	C	H	N	O	S	0	0
			1827	544	959	179	139	6		

- Molecule 28 is a protein called 60S ribosomal protein L35.

Mol	Chain	Residues	Atoms						AltConf	Trace
28	Ab	122	Total	C	H	N	O	S	0	0
			2163	641	1148	205	168	1		

- Molecule 29 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms						AltConf	Trace
29	Ac	102	Total	C	H	N	O	S	0	0
			1749	521	917	177	129	5		

- Molecule 30 is a protein called Large ribosomal subunit protein eL37.

Mol	Chain	Residues	Atoms						AltConf	Trace
30	Ad	86	Total	C	H	N	O	S	2	0
			1466	440	750	159	112	5		

- Molecule 31 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms						AltConf	Trace
31	Ae	69	Total	C	H	N	O	S	0	0
			1206	366	637	103	99	1		

- Molecule 32 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms						AltConf	Trace
32	Af	50	Total	C	H	N	O	S	0	0
			927	281	483	98	64	1		

- Molecule 33 is a protein called Large ribosomal subunit protein eL40.

Mol	Chain	Residues	Atoms						AltConf	Trace
33	Ag	52	Total	C	H	N	O	S	0	0
			896	267	466	90	67	6		

- Molecule 34 is a protein called 60S ribosomal protein L36a.

Mol	Chain	Residues	Atoms						AltConf	Trace
34	Ah	103	Total	C	H	N	O	S	0	0
			1754	528	912	172	136	6		

- Molecule 35 is a protein called 60S ribosomal protein L37a.

Mol	Chain	Residues	Atoms						AltConf	Trace
35	Ai	91	Total	C	H	N	O	S	0	0
			1463	445	756	136	119	7		

- Molecule 36 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms						AltConf	Trace
36	Aj	125	Total	C	H	N	O	S	0	0
			2071	622	1069	207	168	5		

- Molecule 37 is a RNA chain called 28S rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
37	BA	3433	Total	C	H	N	O	P	0	0
			110574	32847	36901	13479	23915	3432		

- Molecule 38 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
38	BB	119	Total	C	H	N	O	P	0	0
			3823	1132	1285	454	834	118		

- Molecule 39 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
39	BC	156	Total	C	H	N	O	P	0	0
			4989	1481	1674	585	1094	155		

- Molecule 40 is a protein called Large ribosomal subunit protein uL2.

Mol	Chain	Residues	Atoms						AltConf	Trace
40	BD	246	Total	C	H	N	O	S	0	0
			3867	1183	1979	387	312	6		

- Molecule 41 is a protein called Large ribosomal subunit protein uL3.

Mol	Chain	Residues	Atoms						AltConf	Trace
41	CA	396	Total	C	H	N	O	S	0	0
			6538	2037	3340	601	546	14		

- Molecule 42 is a protein called 60S ribosomal protein L4.

Mol	Chain	Residues	Atoms						AltConf	Trace
42	CB	352	Total	C	H	N	O	S	0	0
			5812	1776	2992	564	467	13		

- Molecule 43 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms						AltConf	Trace
43	CC	293	Total	C	H	N	O	S	0	0
			4807	1510	2421	435	427	14		

- Molecule 44 is a protein called Large ribosomal subunit protein eL6.

Mol	Chain	Residues	Atoms						AltConf	Trace
44	CD	215	Total	C	H	N	O	S	0	0
			3603	1113	1875	327	284	4		

- Molecule 45 is a RNA chain called tRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
45	DA	77	Total	C	H	N	O	P	0	0
			2474	731	830	290	546	77		

- Molecule 46 is a protein called Elongation factor 2.

Mol	Chain	Residues	Atoms						AltConf	Trace
46	ER	820	Total	C	H	N	O	S	0	0
			12877	4067	6470	1101	1195	44		

- Molecule 47 is a protein called Plasminogen activator inhibitor 1 RNA-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	GF	40	Total	C	H	N	O	0	0
			595	188	275	67	65		

- Molecule 48 is a protein called 60S ribosomal protein L41.

Mol	Chain	Residues	Atoms					AltConf	Trace	
48	Hi	20	Total	C	H	N	O	S	0	0
			430	119	237	51	20	3		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
49	HA	1646	Total	C	H	N	O	P	7	0
			52994	15805	17647	6355	11535	1652		

- Molecule 50 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms						AltConf	Trace
50	HC	210	Total	C	H	N	O	S	0	0
			3492	1086	1781	306	305	14		

- Molecule 51 is a protein called Small ribosomal subunit protein eS4, X isoform.

Mol	Chain	Residues	Atoms						AltConf	Trace
51	HF	257	Total	C	H	N	O	S	0	0
			4184	1305	2143	379	349	8		

- Molecule 52 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms						AltConf	Trace
52	HI	184	Total	C	H	N	O	S	0	0
			3050	942	1573	271	263	1		

- Molecule 53 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms						AltConf	Trace
53	HJ	205	Total	C	H	N	O	S	0	0
			3451	1056	1769	331	290	5		

- Molecule 54 is a protein called Small ribosomal subunit protein uS17.

Mol	Chain	Residues	Atoms						AltConf	Trace
54	HM	141	Total	C	H	N	O	S	0	0
			2380	737	1223	217	197	6		

- Molecule 55 is a protein called 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms						AltConf	Trace
55	HS	131	Total	C	H	N	O	S	0	0
			2182	668	1118	198	194	4		

- Molecule 56 is a protein called Small ribosomal subunit protein eS21.

Mol	Chain	Residues	Atoms						AltConf	Trace
56	A	84	Total	C	H	N	O	S	0	0
			1268	395	629	117	122	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	ACE	-	acetylation	UNP P63220

- Molecule 57 is a protein called Small ribosomal subunit protein uS12.

Mol	Chain	Residues	Atoms						AltConf	Trace
57	HY	140	Total	C	H	N	O	S	0	0
			2235	687	1147	215	183	3		

- Molecule 58 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms						AltConf	Trace
58	Hb	99	Total	C	H	N	O	S	0	0
			1633	492	841	165	130	5		

- Molecule 59 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms						AltConf	Trace
59	HD	219	Total	C	H	N	O	S	1	0
			3506	1105	1798	295	298	10		

- Molecule 60 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms						AltConf	Trace
60	HH	227	Total	C	H	N	O	S	0	0
			3829	1149	1989	367	317	7		

- Molecule 61 is a protein called 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms						AltConf	Trace
61	HK	185	Total	C	H	N	O	S	0	0
			3165	969	1640	306	248	2		

- Molecule 62 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms						AltConf	Trace
62	HO	150	Total	C	H	N	O	S	0	0
			2501	773	1293	229	205	1		

- Molecule 63 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms						AltConf	Trace
63	HP	127	Total	C	H	N	O	S	0	0
			1934	585	977	189	177	6		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
HP	138	IAS	ASP	conflict	UNP P62263

- Molecule 64 is a protein called 40S ribosomal protein S15a.

Mol	Chain	Residues	Atoms						AltConf	Trace
64	HX	129	Total	C	H	N	O	S	0	0
			2114	659	1080	193	176	6		

- Molecule 65 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms						AltConf	Trace
65	HZ	122	Total	C	H	N	O	S	0	0
			2077	635	1075	196	166	5		

- Molecule 66 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms						AltConf	Trace
66	Hc	82	Total	C	H	N	O	S	0	0
			1305	402	665	118	113	7		

- Molecule 67 is a protein called Ubiquitin-like FUBI-ribosomal protein eS30 fusion protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
67	Hf	55	Total	C	H	N	O	S	0	0
			922	271	484	95	71	1		

- Molecule 68 is a protein called Small ribosomal subunit protein uS2.

Mol	Chain	Residues	Atoms						AltConf	Trace
68	B	207	Total	C	H	N	O	S	1	0
			3276	1042	1648	287	291	8		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	ACE	-	acetylation	UNP P08865

- Molecule 69 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms						AltConf	Trace
69	HE	224	Total	C	H	N	O	S	0	0
			3580	1112	1835	314	312	7		

- Molecule 70 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms						AltConf	Trace
70	HG	182	Total	C	H	N	O	S	0	0
			2940	906	1495	271	261	7		

- Molecule 71 is a protein called 40S ribosomal protein S10.

Mol	Chain	Residues	Atoms						AltConf	Trace
71	HL	97	Total	C	H	N	O	S	0	0
			1657	533	841	144	133	6		

- Molecule 72 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms						AltConf	Trace
72	HQ	123	Total	C	H	N	O	S	0	0
			2058	638	1053	188	172	7		

- Molecule 73 is a protein called 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms						AltConf	Trace
73	HR	139	Total	C	H	N	O	S	0	0
			2277	704	1172	207	191	3		

- Molecule 74 is a protein called 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms						AltConf	Trace
74	HT	143	Total	C	H	N	O	S	1	0
			2445	751	1253	240	200	1		

- Molecule 75 is a protein called 40S ribosomal protein S19.

Mol	Chain	Residues	Atoms						AltConf	Trace
75	HU	143	Total	C	H	N	O	S	0	0
			2259	697	1147	214	198	3		

- Molecule 76 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms						AltConf	Trace
76	HV	104	Total	C	H	N	O	S	0	0
			1704	514	883	155	148	4		

- Molecule 77 is a protein called 40S ribosomal protein S28.

Mol	Chain	Residues	Atoms						AltConf	Trace
77	Hd	59	Total	C	H	N	O	S	0	0
			952	281	488	93	88	2		

- Molecule 78 is a protein called 40S ribosomal protein S29.

Mol	Chain	Residues	Atoms						AltConf	Trace
78	He	55	Total	C	H	N	O	S	0	0
			907	286	448	94	74	5		

- Molecule 79 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms						AltConf	Trace
79	HN	104	Total	C	H	N	O	S	0	0
			1598	494	808	138	151	7		

- Molecule 80 is a protein called Small ribosomal subunit protein eS25.

Mol	Chain	Residues	Atoms						AltConf	Trace
80	Ha	72	Total	C	H	N	O	S	0	0
			1196	366	626	104	99	1		

- Molecule 81 is a protein called Ubiquitin.

Mol	Chain	Residues	Atoms						AltConf	Trace
81	Hg	64	Total	C	H	N	O	S	0	0
			1051	329	529	99	87	7		

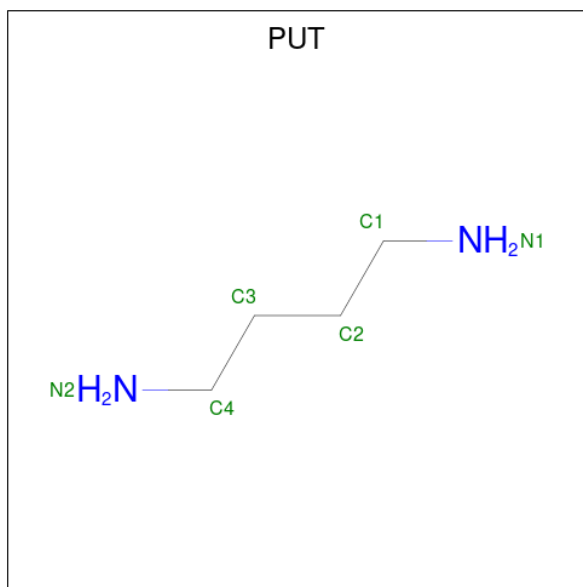
- Molecule 82 is a protein called Receptor of activated protein C kinase 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
82	Hh	312	Total	C	H	N	O	S	0	0
			4815	1531	2386	423	463	12		

- Molecule 83 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
83	AD	1	Total	Mg	0
			1	1	
83	AJ	1	Total	Mg	0
			1	1	
83	AP	1	Total	Mg	0
			1	1	
83	AY	1	Total	Mg	0
			1	1	
83	AZ	1	Total	Mg	0
			1	1	
83	Ad	1	Total	Mg	0
			1	1	
83	BA	168	Total	Mg	0
			168	168	
83	BB	2	Total	Mg	0
			2	2	
83	BC	3	Total	Mg	0
			3	3	
83	HA	72	Total	Mg	0
			72	72	
83	HH	1	Total	Mg	0
			1	1	

- Molecule 84 is 1,4-DIAMINOBTUTANE (CCD ID: PUT) (formula: C₄H₁₂N₂).



Mol	Chain	Residues	Atoms			AltConf
84	AH	1	Total	C	N	0
			6	4	2	
84	BA	1	Total	C	N	0
			6	4	2	
84	BA	1	Total	C	N	0
			6	4	2	
84	BB	1	Total	C	N	0
			6	4	2	

- Molecule 85 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
85	AM	1	Total	K	0
			1	1	
85	AN	1	Total	K	0
			1	1	
85	AP	1	Total	K	0
			1	1	
85	BA	38	Total	K	0
			38	38	
85	BC	1	Total	K	0
			1	1	
85	BD	2	Total	K	0
			2	2	
85	HA	66	Total	K	0
			66	66	
85	HF	1	Total	K	0
			1	1	

Continued on next page...

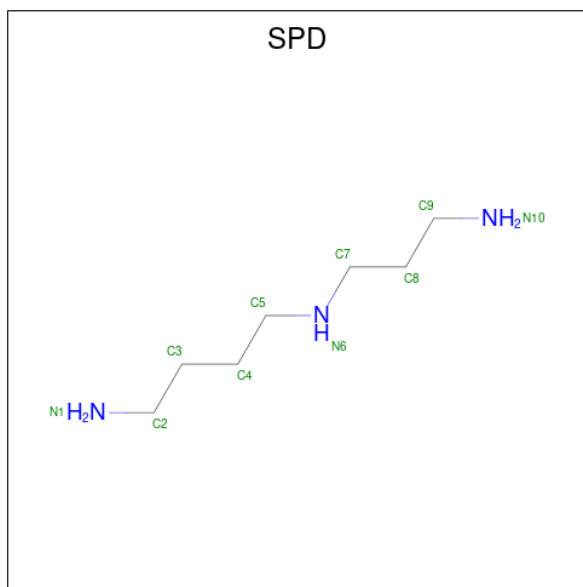
Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
85	HJ	1	Total K 1 1	0
85	HP	1	Total K 1 1	0
85	HT	2	Total K 2 2	0
85	HV	1	Total K 1 1	0
85	He	1	Total K 1 1	0

- Molecule 86 is ZINC ION (CCD ID: ZN) (formula: Zn).

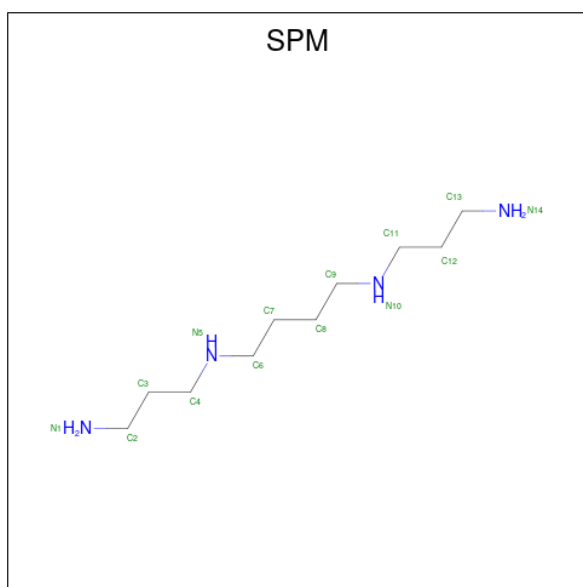
Mol	Chain	Residues	Atoms	AltConf
86	Aa	1	Total Zn 1 1	0
86	Ad	1	Total Zn 1 1	0
86	Ag	1	Total Zn 1 1	0
86	Ah	1	Total Zn 1 1	0
86	Ai	1	Total Zn 1 1	0
86	Hb	1	Total Zn 1 1	0
86	He	1	Total Zn 1 1	0
86	Hg	1	Total Zn 1 1	0

- Molecule 87 is SPERMIDINE (CCD ID: SPD) (formula: C₇H₁₉N₃).



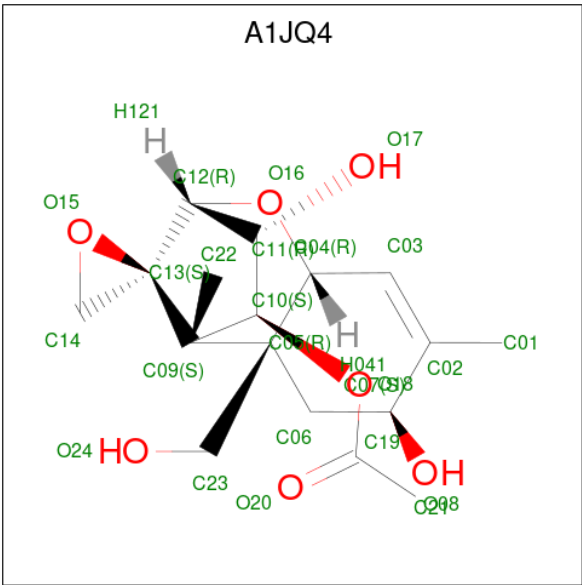
Mol	Chain	Residues	Atoms				AltConf
87	BA	1	Total	C	H	N	0
			12	7	2	3	
87	BA	1	Total	C	H	N	0
			12	7	2	3	
87	BA	1	Total	C	H	N	0
			12	7	2	3	
87	BA	1	Total	C	H	N	0
			12	7	2	3	
87	BA	1	Total	C	H	N	0
			12	7	2	3	
87	BA	1	Total	C	H	N	0
			12	7	2	3	

- Molecule 88 is SPERMINE (CCD ID: SPM) (formula: $C_{10}H_{26}N_4$).



Mol	Chain	Residues	Atoms				AltConf
88	BA	1	Total	C	H	N	0
			23	10	9	4	
88	BA	1	Total	C	H	N	0
			23	10	9	4	
88	BA	1	Total	C	H	N	0
			23	10	9	4	
88	BA	1	Total	C	H	N	0
			23	10	9	4	
88	BA	1	Total	C	H	N	0
			23	10	9	4	

- Molecule 89 is Toxin NT-2 (CCD ID: A1JQ4) (formula: C₁₇H₂₄O₇) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	H	O	
89	BA	1	48	17	24	7	0

- Molecule 90 is water.

Mol	Chain	Residues	Atoms		AltConf
90	AD	1	Total	O	0
			1	1	
90	AH	1	Total	O	0
			1	1	
90	AJ	1	Total	O	0
			1	1	
90	AP	3	Total	O	0
			3	3	
90	AU	4	Total	O	0
			4	4	
90	AY	2	Total	O	0
			2	2	
90	Ad	2	Total	O	0
			2	2	
90	BA	728	Total	O	0
			728	728	
90	BB	9	Total	O	0
			9	9	
90	BC	16	Total	O	0
			16	16	
90	BD	4	Total	O	0
			4	4	

Continued on next page...

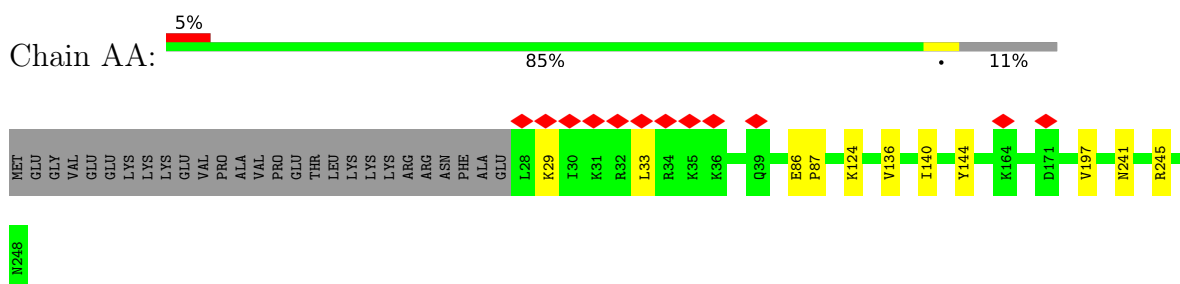
Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
90	DA	1	Total 1	O 1	0
90	HA	278	Total 278	O 278	0
90	HY	1	Total 1	O 1	0
90	HO	1	Total 1	O 1	0
90	HP	2	Total 2	O 2	0
90	HR	1	Total 1	O 1	0
90	HU	3	Total 3	O 3	0

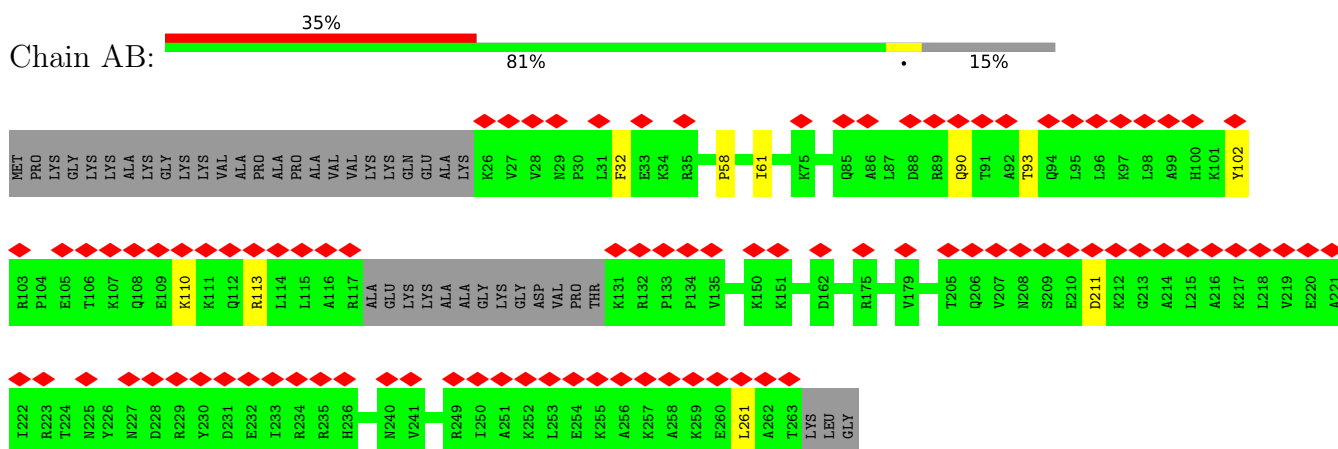
3 Residue-property plots [i](#)

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

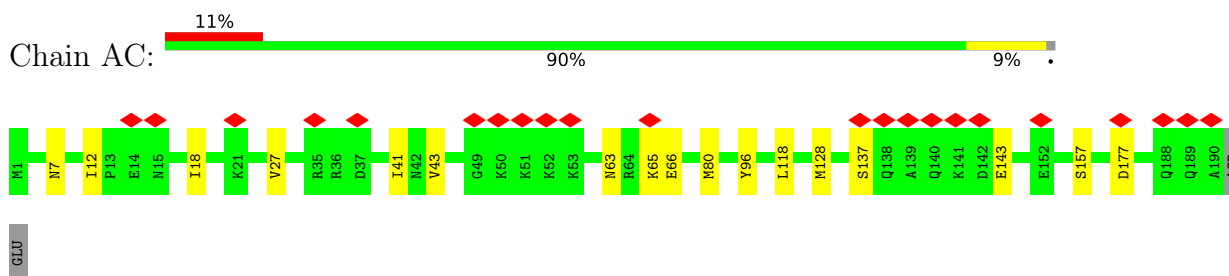
- Molecule 1: Large ribosomal subunit protein uL30



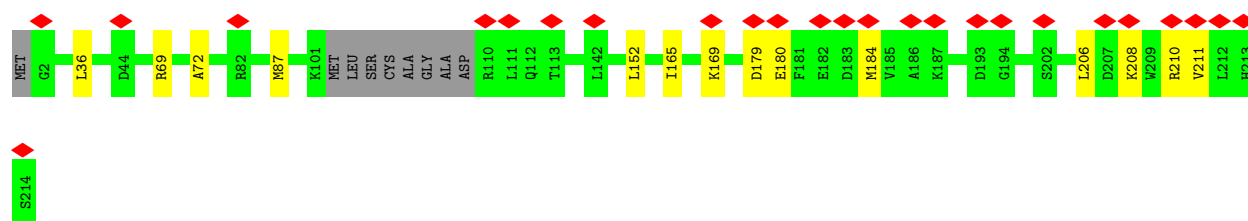
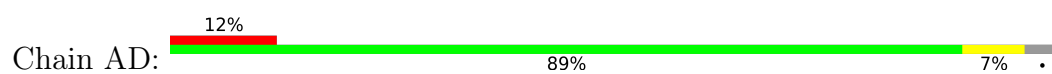
- Molecule 2: 60S ribosomal protein L7a



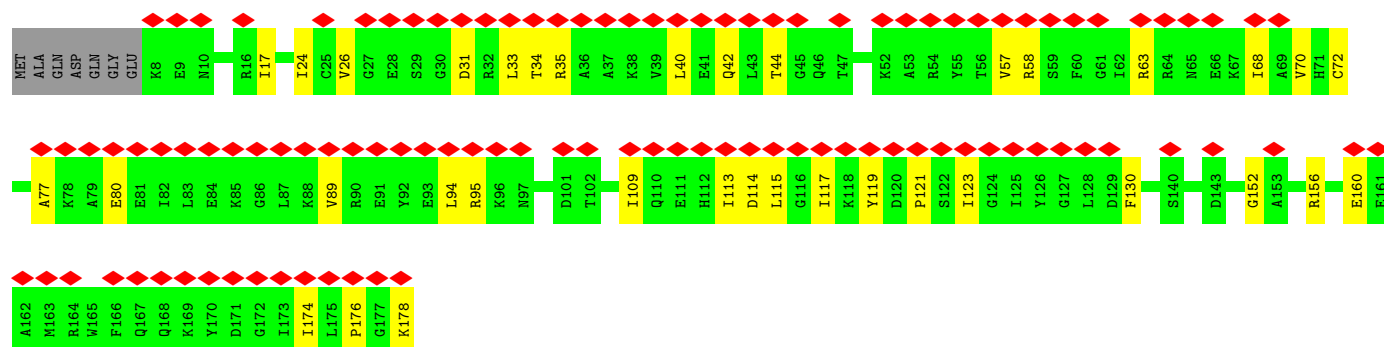
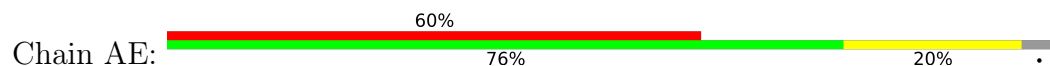
- Molecule 3: 60S ribosomal protein L9



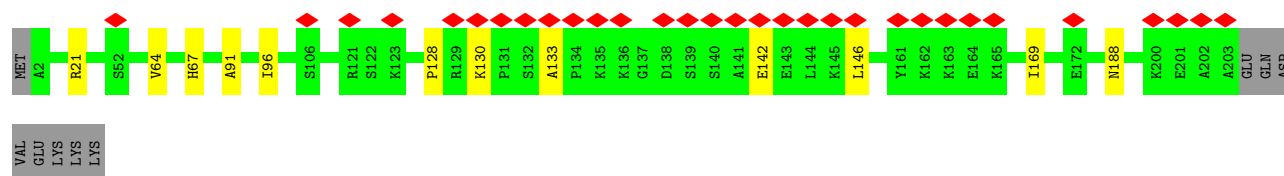
- Molecule 4: Ribosomal protein uL16-like



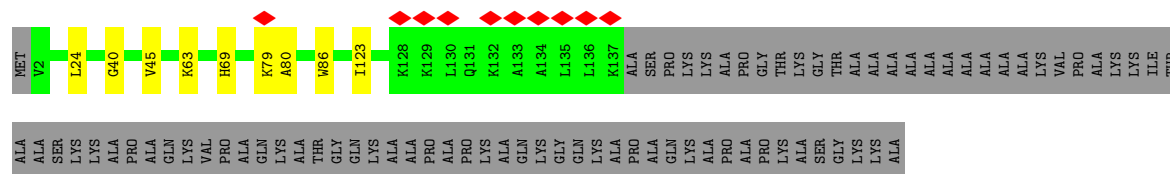
- Molecule 5: 60S ribosomal protein L11



- Molecule 6: 60S ribosomal protein L13

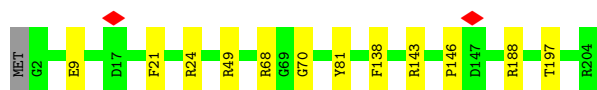


- Molecule 7: 60S ribosomal protein L14

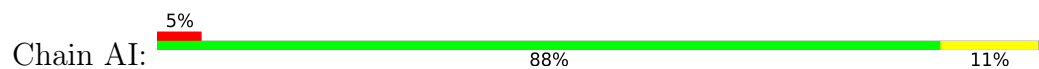


- Molecule 8: 60S ribosomal protein L15

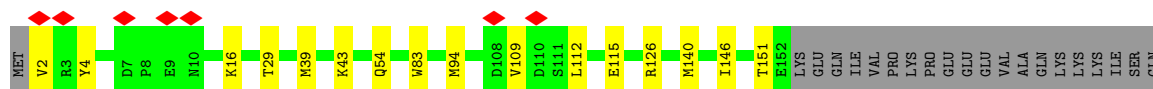
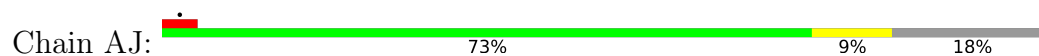




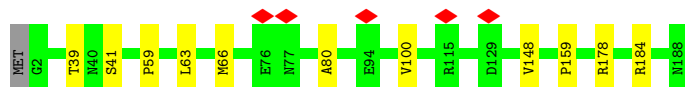
- Molecule 9: 60S ribosomal protein L13a



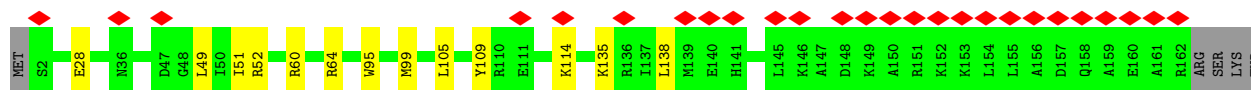
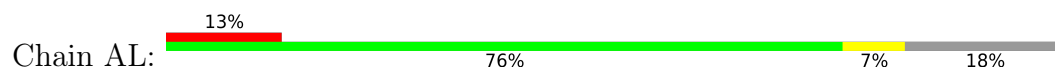
- Molecule 10: 60S ribosomal protein L17



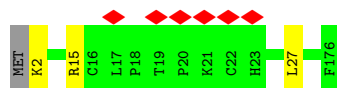
- Molecule 11: 60S ribosomal protein L18



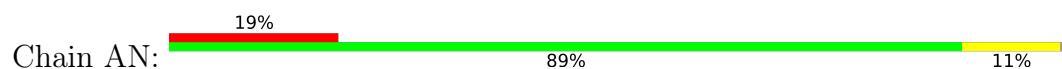
- Molecule 12: 60S ribosomal protein L19

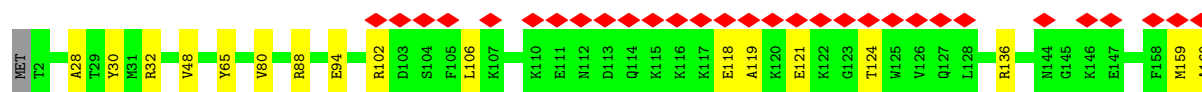


- Molecule 13: 60S ribosomal protein L18a

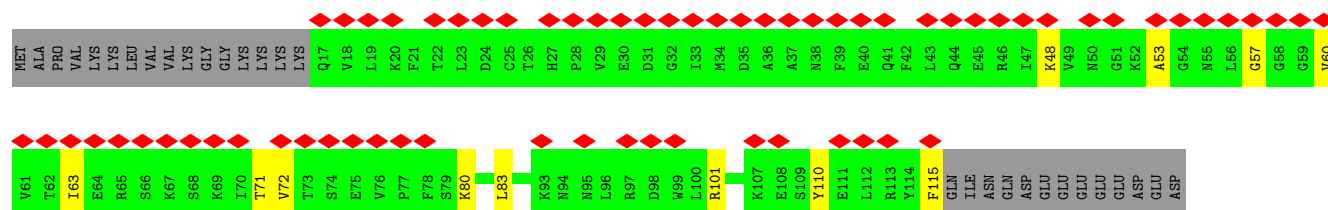
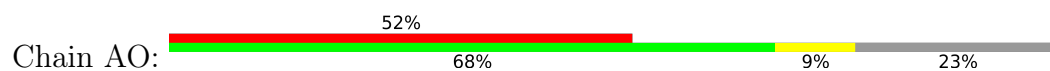


- Molecule 14: 60S ribosomal protein L21

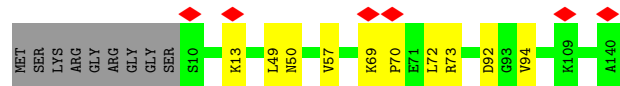
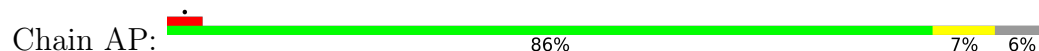




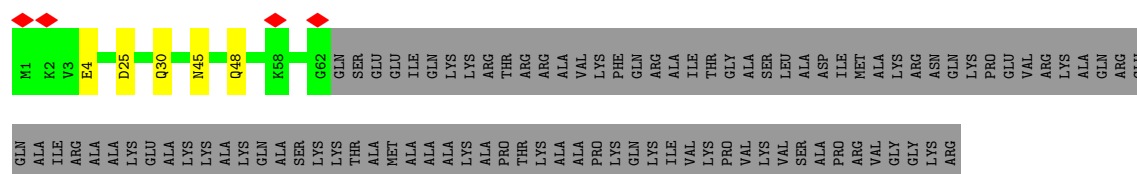
- Molecule 15: 60S ribosomal protein L22



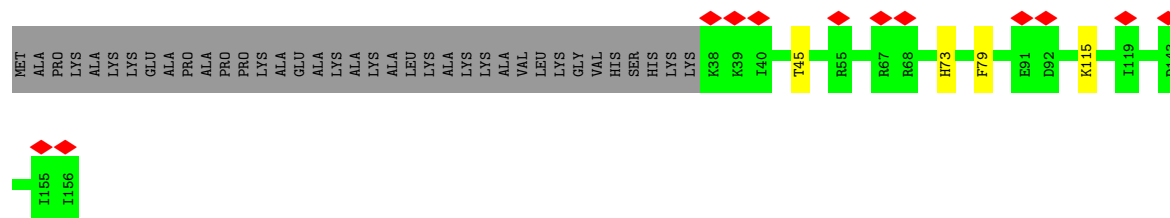
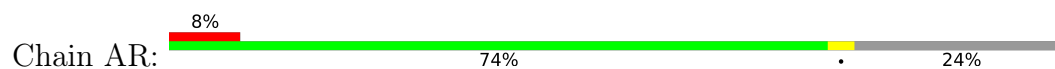
- Molecule 16: 60S ribosomal protein L23



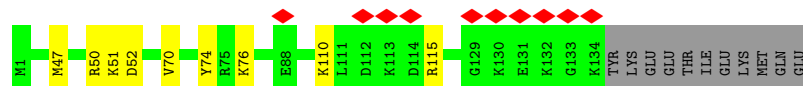
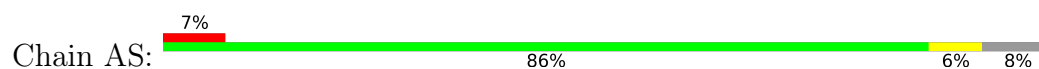
- Molecule 17: 60S ribosomal protein L24



- Molecule 18: 60S ribosomal protein L23a



- Molecule 19: 60S ribosomal protein L26



-

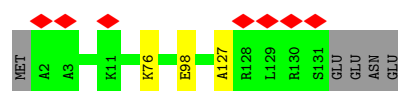
-
- | Category | Count |
|----------|-------|
| MET | 1 |
| P2 | 1 |
| V15 | 1 |
| A35 | 1 |
| V5139 | 1 |
| E84 | 1 |
| A90 | 1 |
| A91 | 1 |
| K92 | 1 |
| N93 | 1 |
| K94 | 1 |
| T95 | 1 |
| G96 | 1 |
| A97 | 1 |
| A98 | 1 |
| K119 | 1 |
| V122 | 1 |
| V140 | 1 |
| G141 | 1 |
| G142 | 1 |
| A148 | 1 |

- [illegible]

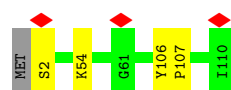
- [illegible]

- | MET | ALA | PRO | ALA | ALA | LYS | LYS | GLY | GLY | GLY | GLU | GLY | LYS | LYS | GLY | GLY | ARG | SER | | | | | | | | | | | | | |
|------|------|------|------|------|------|------|
| A16 | A16 | I17 | M18 | E19 | I29 | I33 | V36 | R44 | A45 | L46 | M54 | K55 | E56 | M57 | L68 | V72 | N93 | E94 | D95 | E96 | D97 | S98 | P99 | M100 | K101 | L102 | V106 | V122 | D123 | E124 |

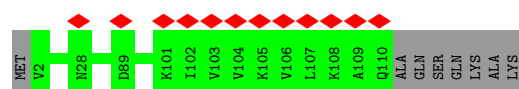
- Molecule 25: 60S ribosomal protein L32



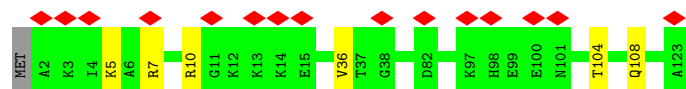
- Molecule 26: Large ribosomal subunit protein eL33



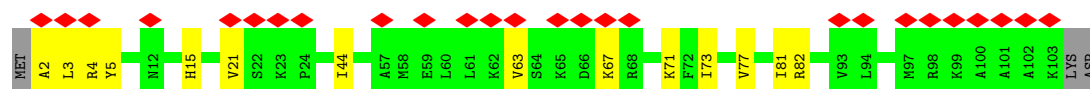
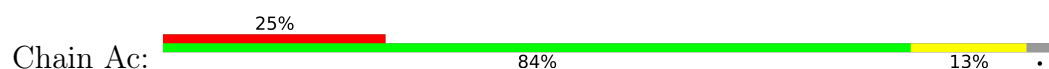
- Molecule 27: 60S ribosomal protein L34



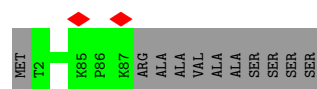
- Molecule 28: 60S ribosomal protein L35



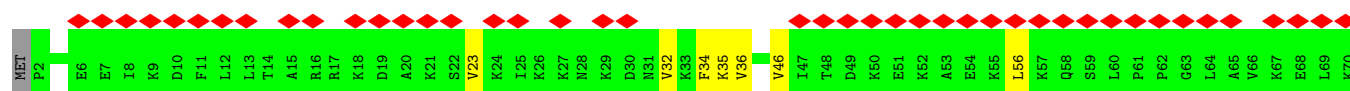
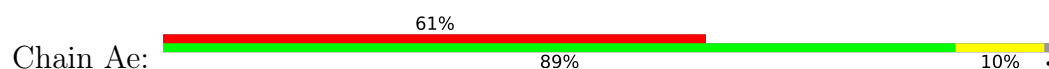
- Molecule 29: 60S ribosomal protein L36



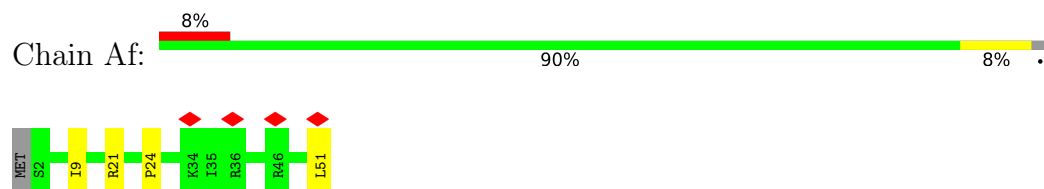
- Molecule 30: Large ribosomal subunit protein eL37



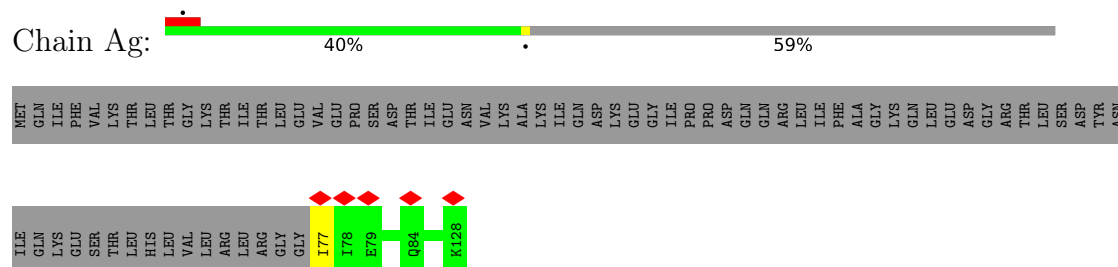
- Molecule 31: 60S ribosomal protein L38



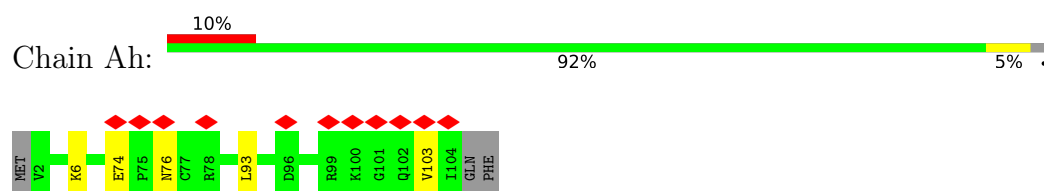
- Molecule 32: 60S ribosomal protein L39



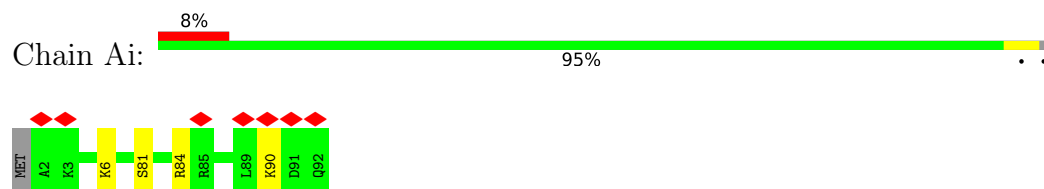
- Molecule 33: Large ribosomal subunit protein eL40



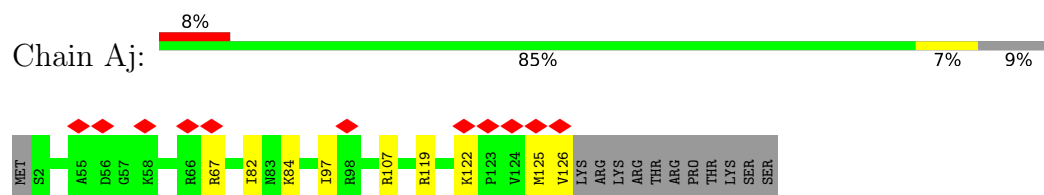
- Molecule 34: 60S ribosomal protein L36a



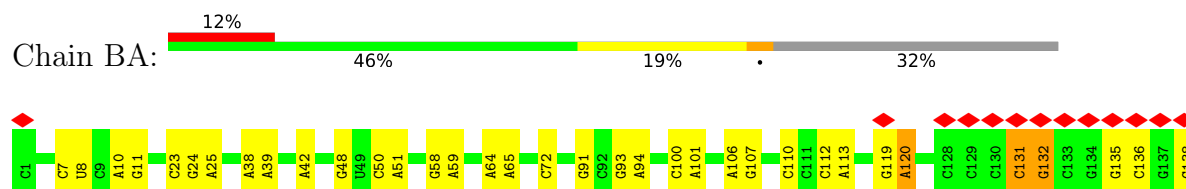
- Molecule 35: 60S ribosomal protein L37a



- Molecule 36: 60S ribosomal protein L28



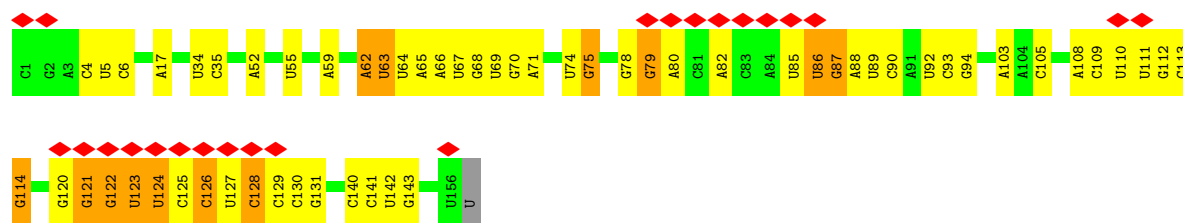
- Molecule 37: 28S rRNA



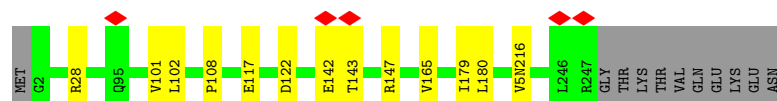




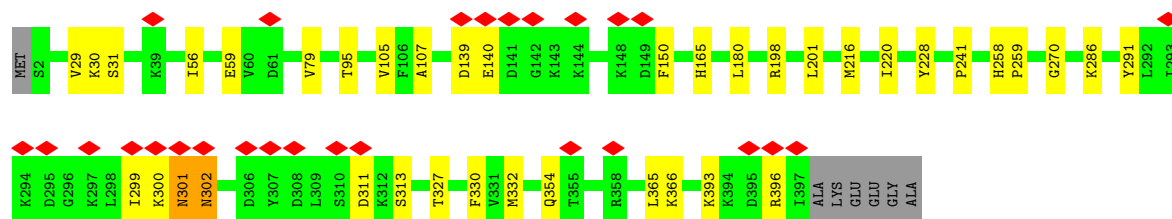
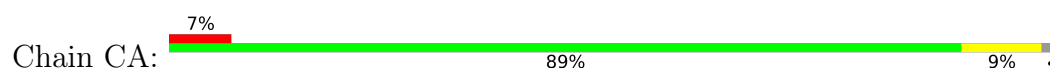




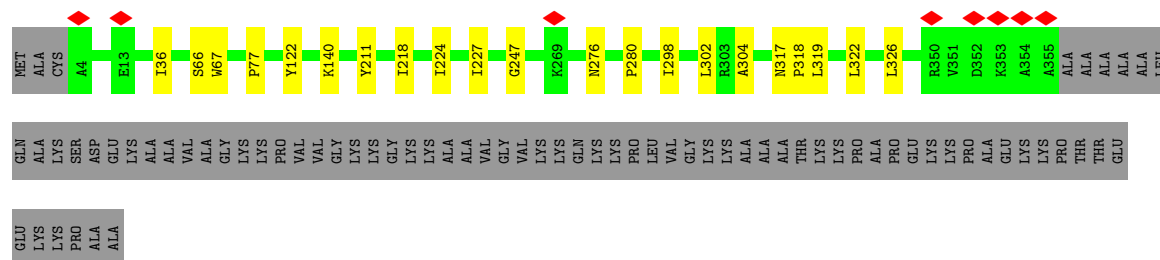
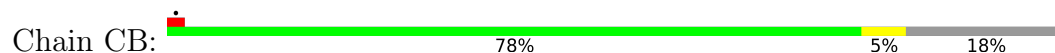
- Molecule 40: Large ribosomal subunit protein uL2



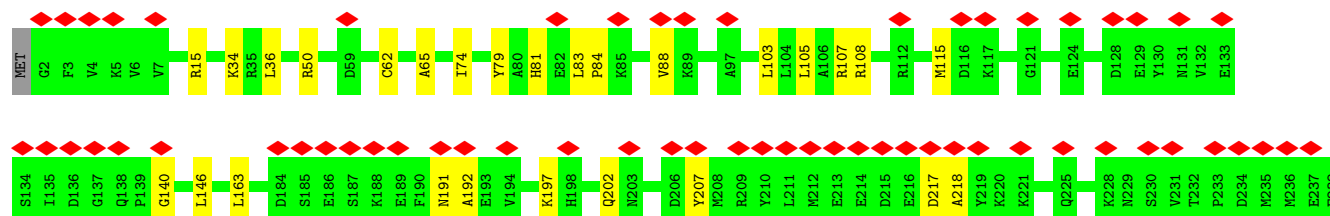
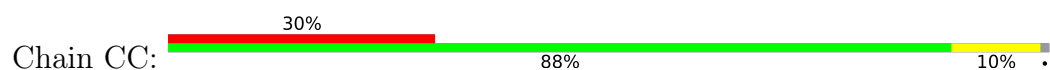
- Molecule 41: Large ribosomal subunit protein uL3

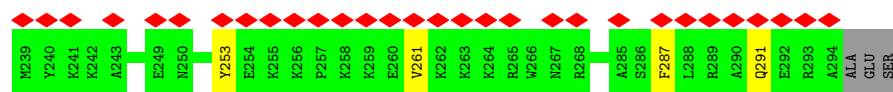


- Molecule 42: 60S ribosomal protein L4

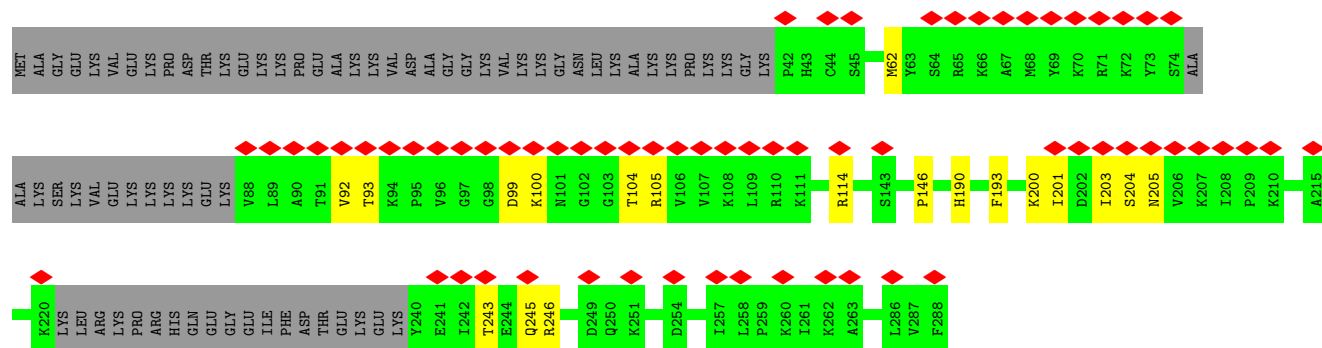


- Molecule 43: 60S ribosomal protein L5

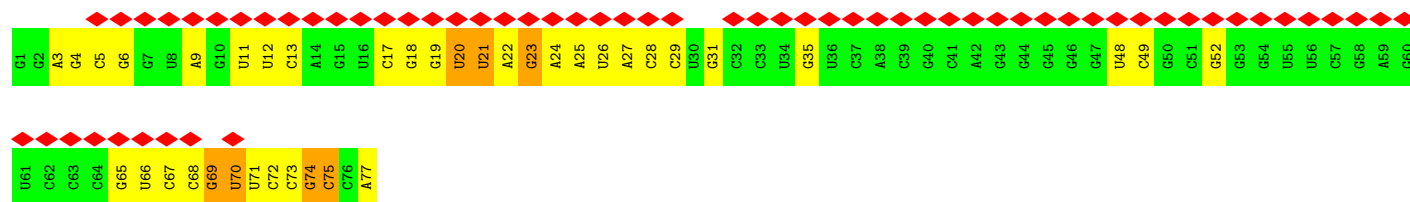
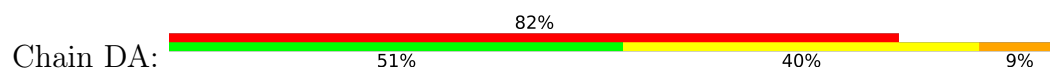




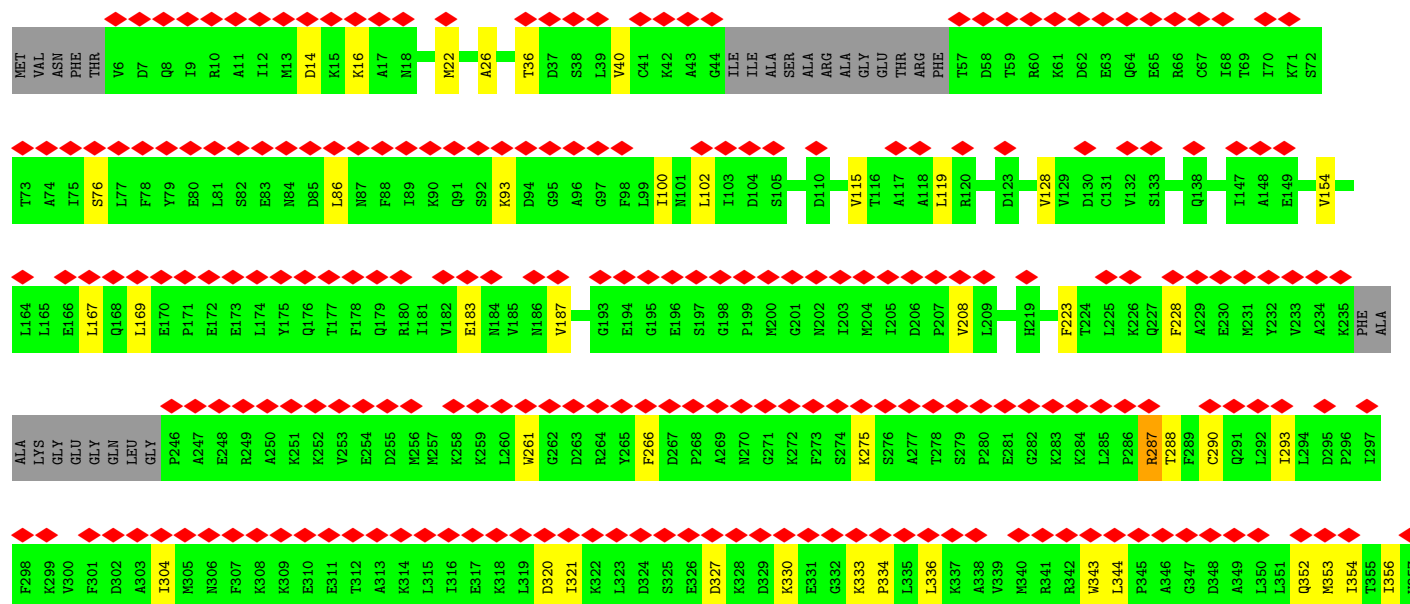
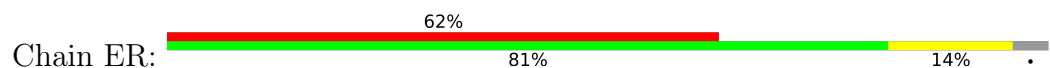
• Molecule 44: Large ribosomal subunit protein eL6

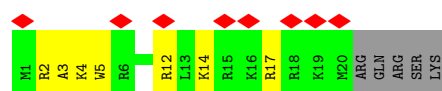


• Molecule 45: tRNA

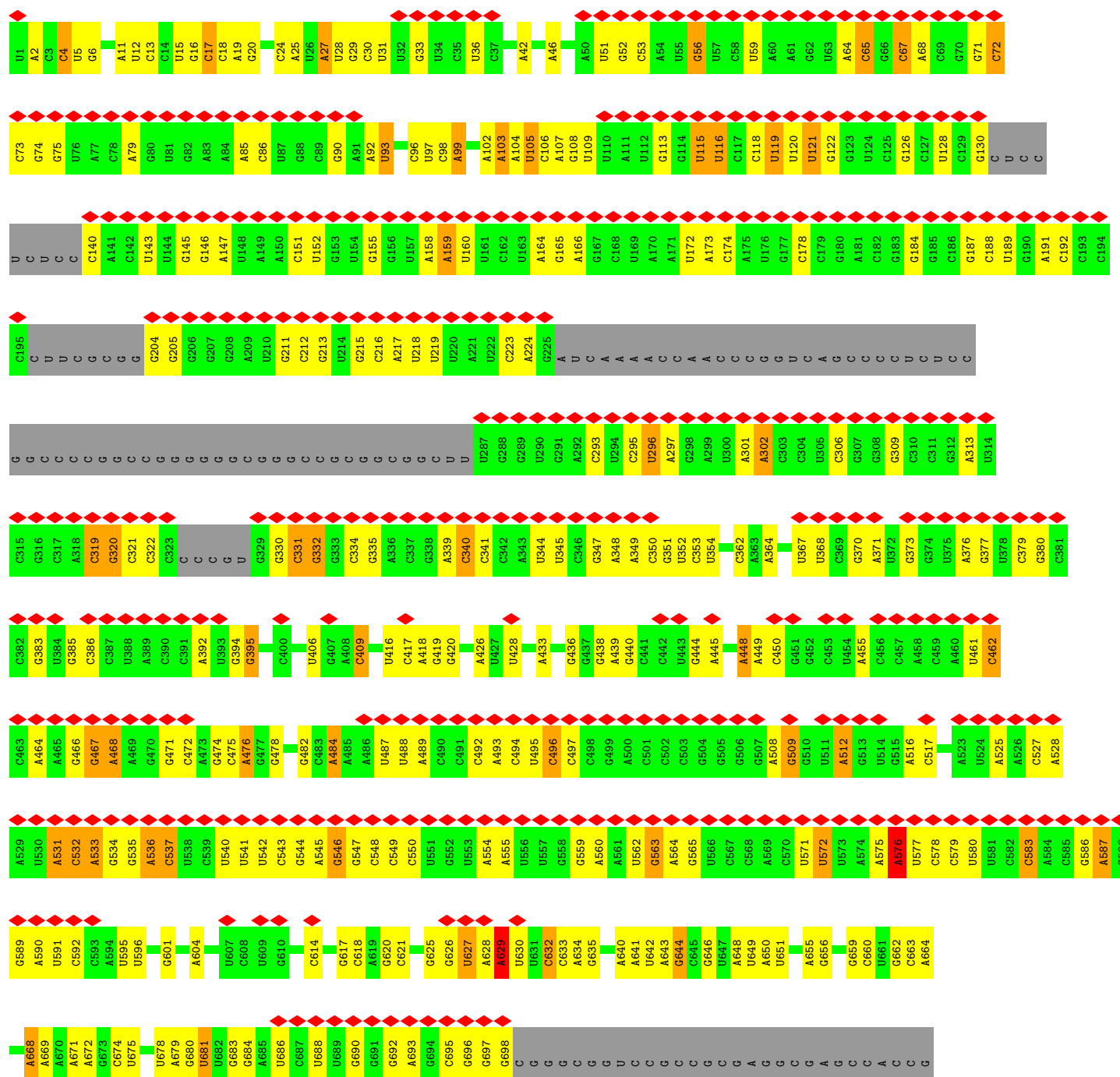


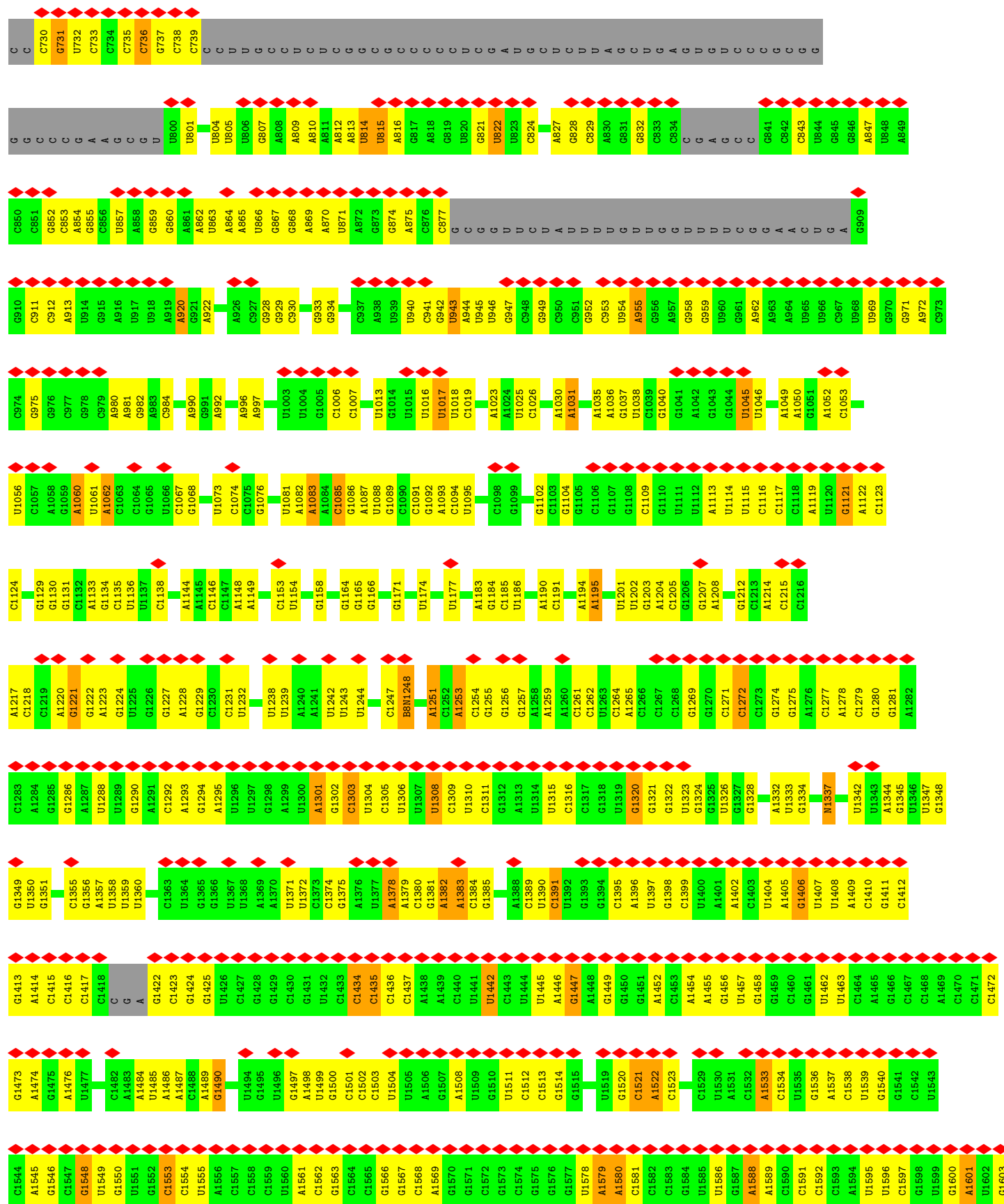
• Molecule 46: Elongation factor 2

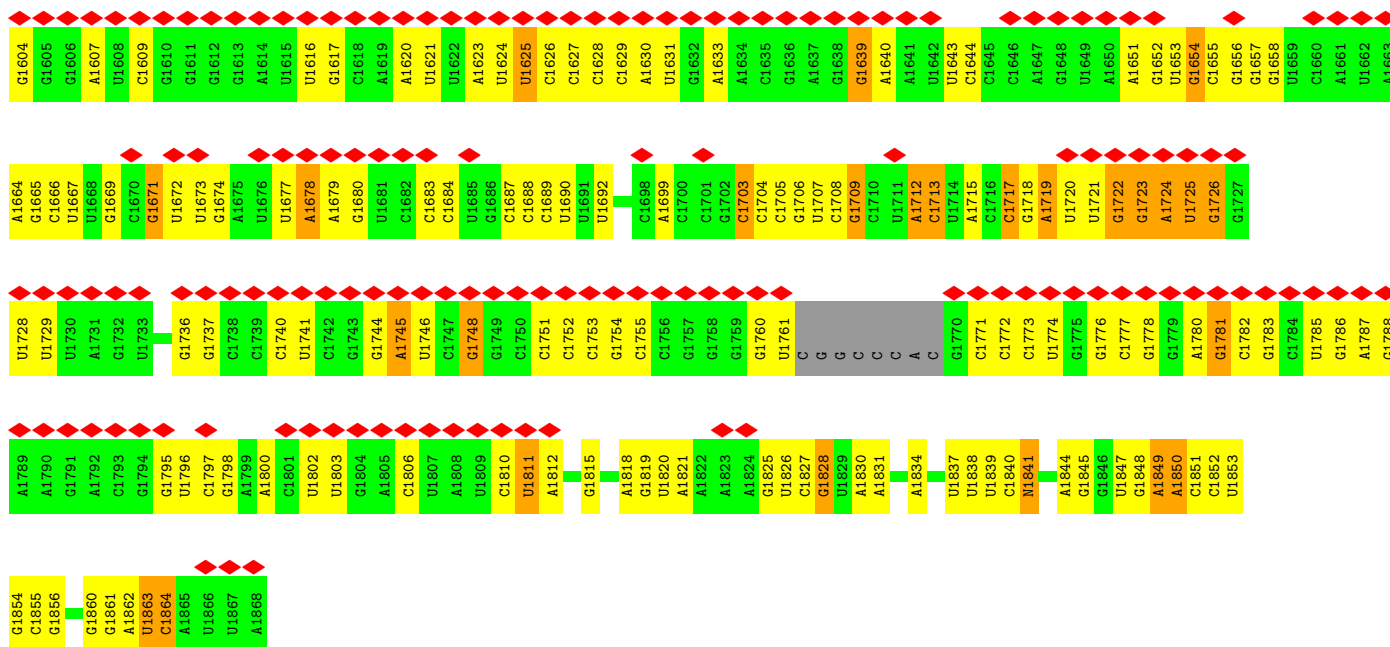




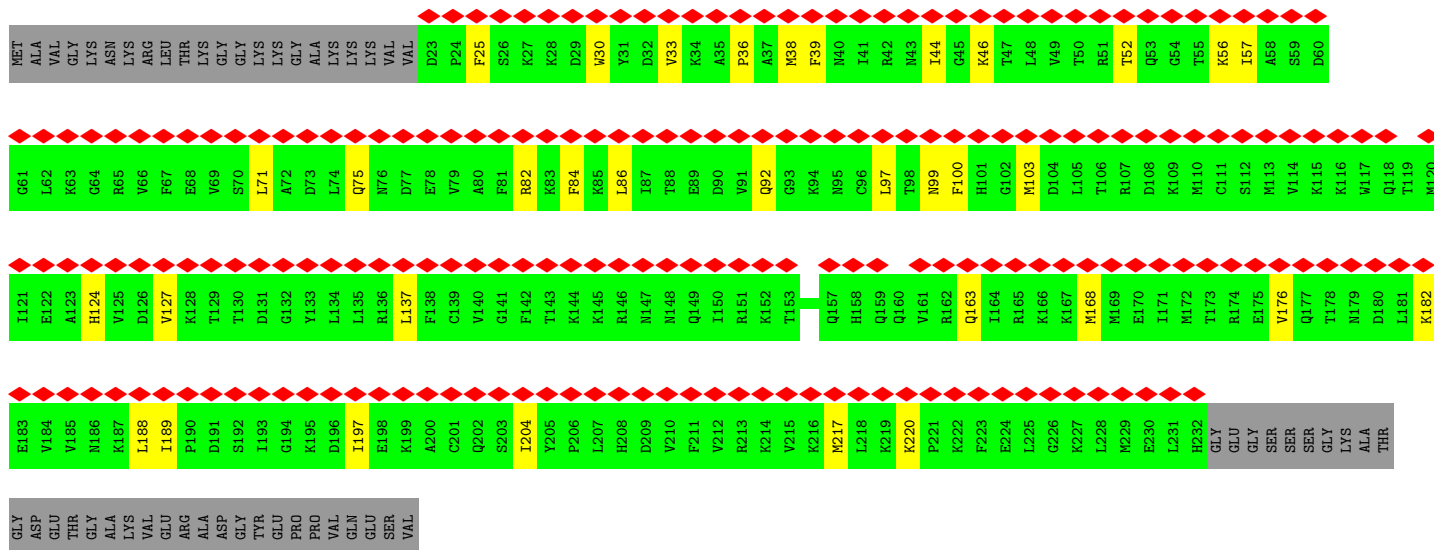
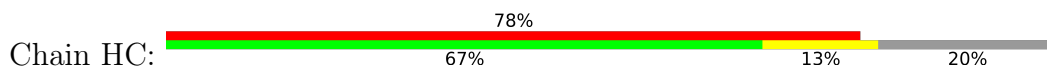
Chain HA:



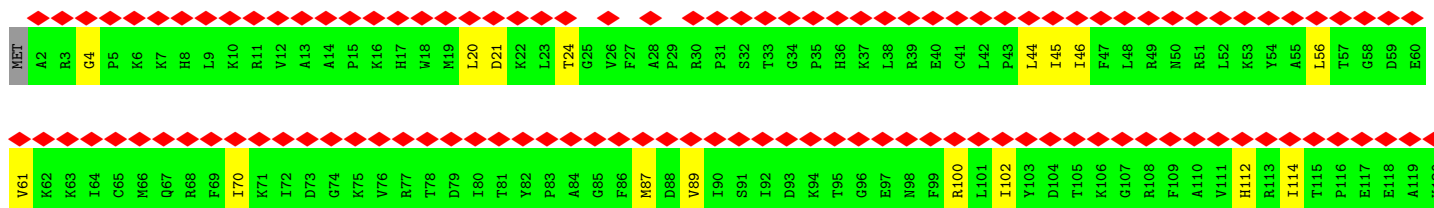
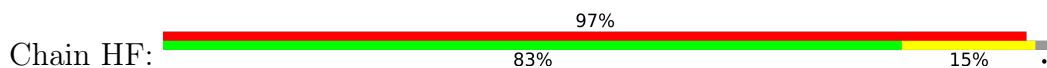




- Molecule 50: 40S ribosomal protein S3a

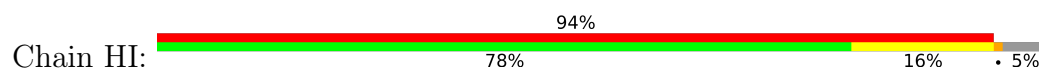


- Molecule 51: Small ribosomal subunit protein eS4, X isoform

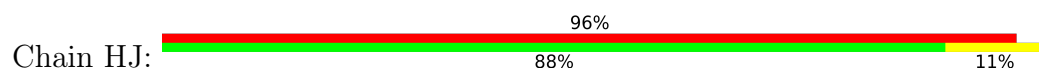




• Molecule 52: 40S ribosomal protein S7

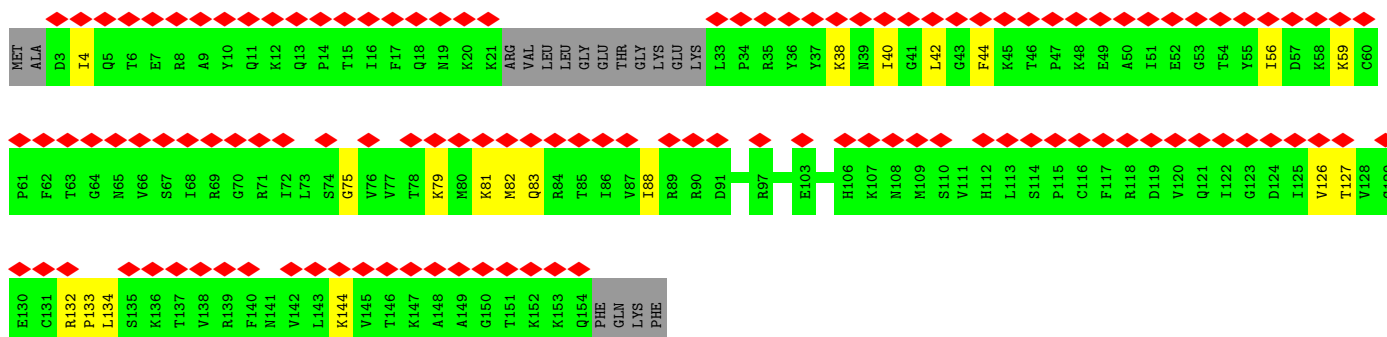


• Molecule 53: 40S ribosomal protein S8

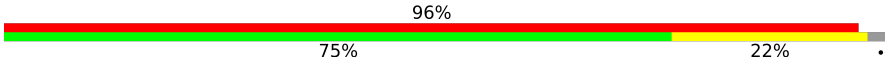


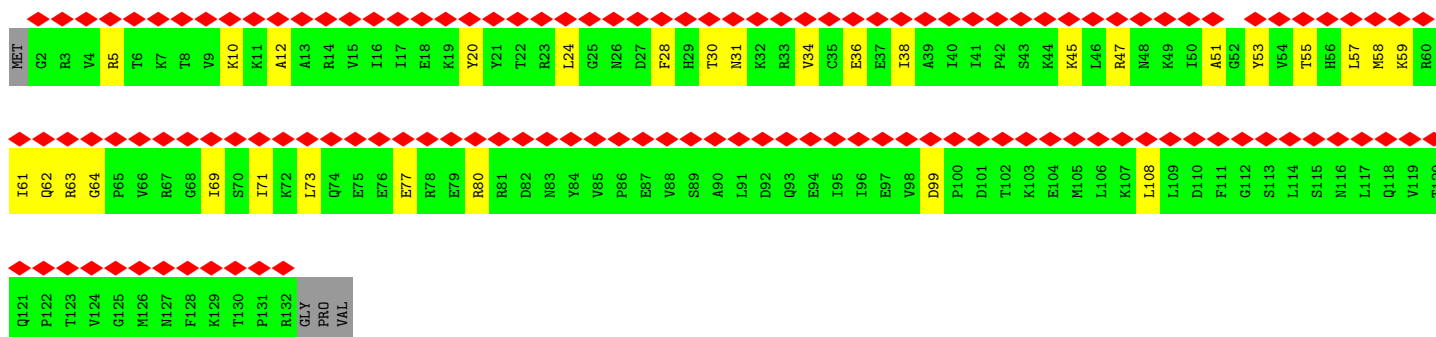
• Molecule 54: Small ribosomal subunit protein uS17

Chain HM: 

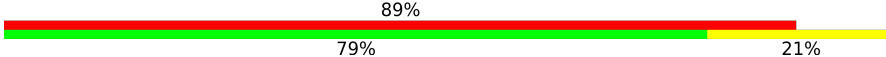


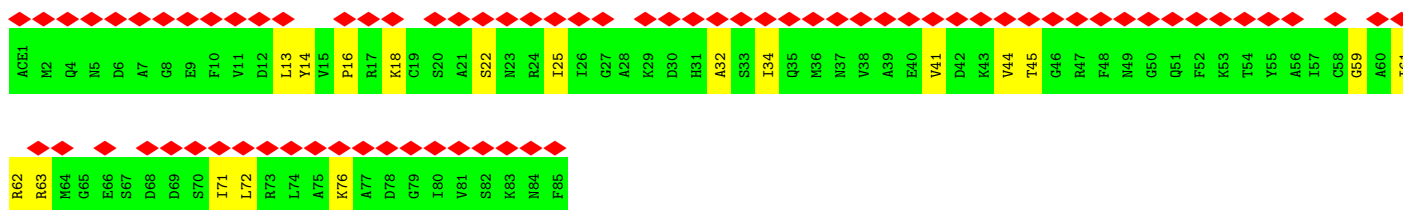
• Molecule 55: 40S ribosomal protein S17

Chain HS: 



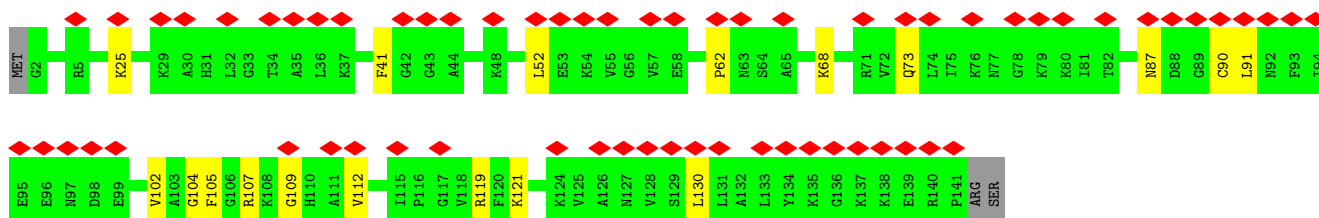
• Molecule 56: Small ribosomal subunit protein eS21

Chain A: 



• Molecule 57: Small ribosomal subunit protein uS12

Chain HY: 

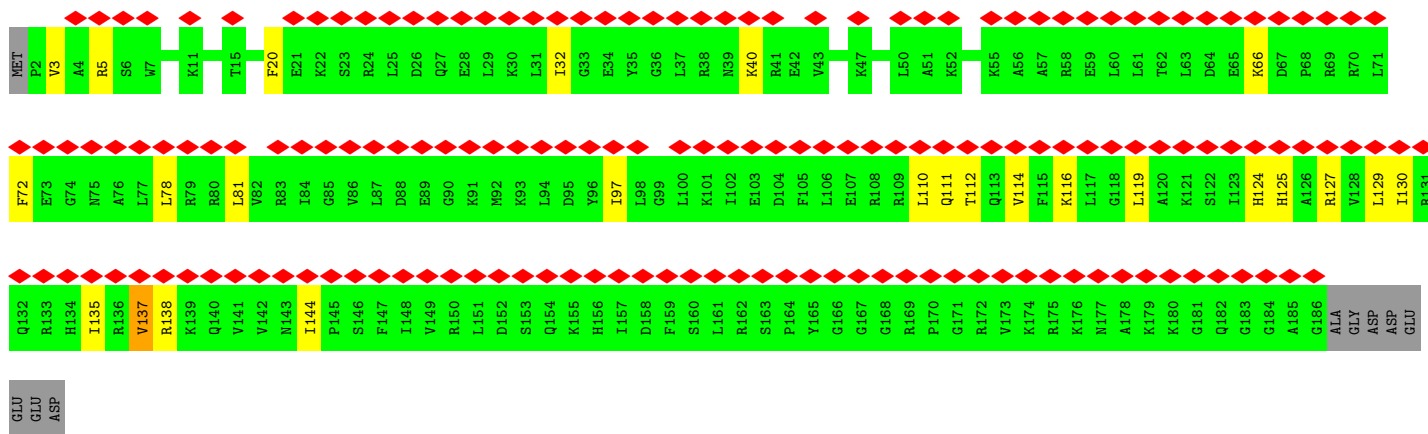


• Molecule 58: 40S ribosomal protein S26

THR
SER
LYS
SER
GLU
SER
SER
GLN
LYS

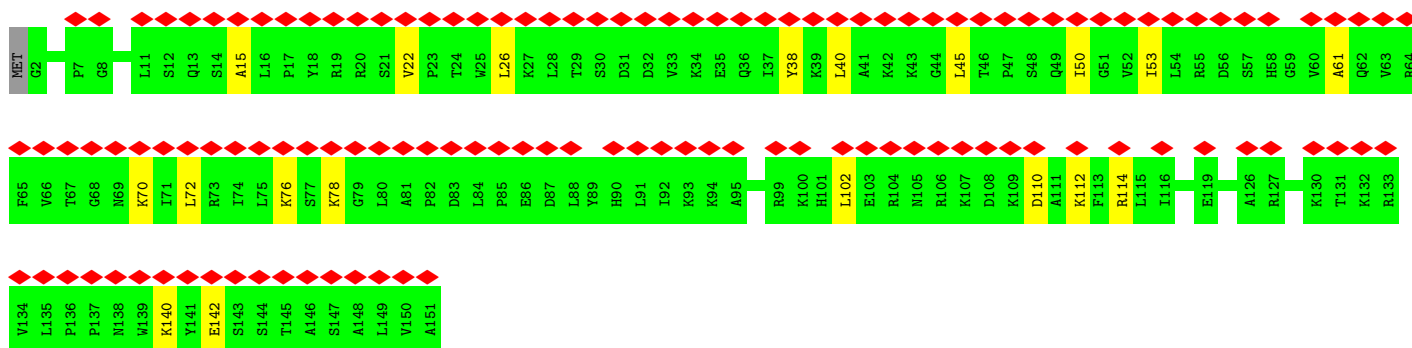
• Molecule 61: 40S ribosomal protein S9

Chain HK: 



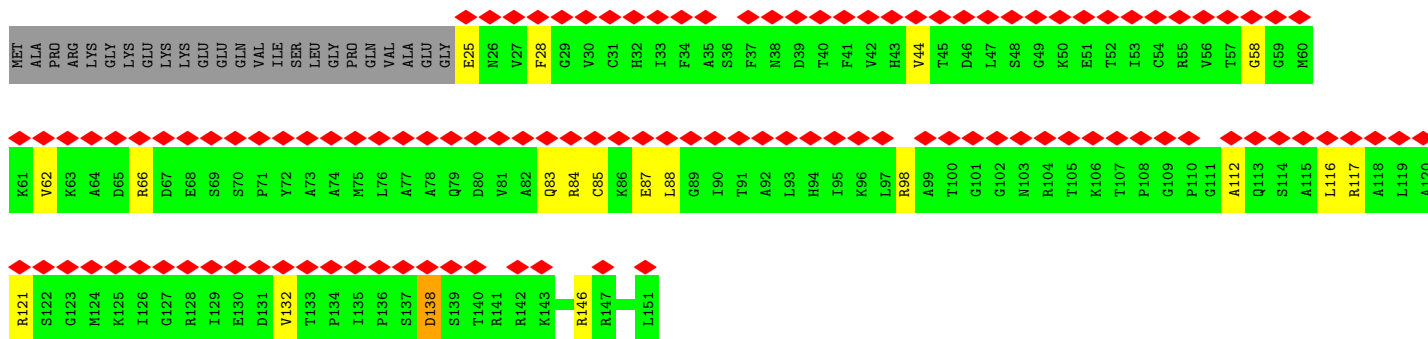
• Molecule 62: 40S ribosomal protein S13

Chain HO: 



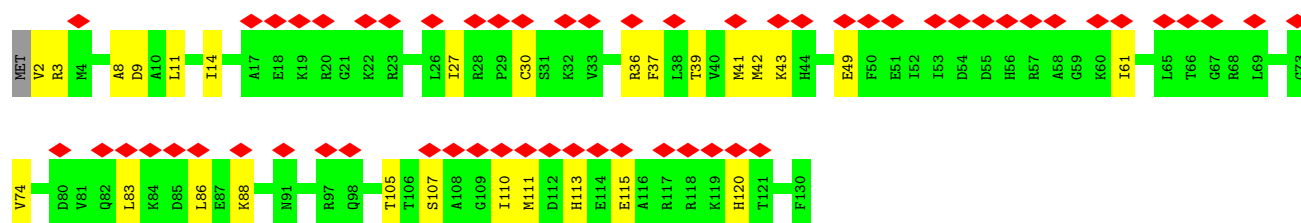
• Molecule 63: 40S ribosomal protein S14

Chain HP: 



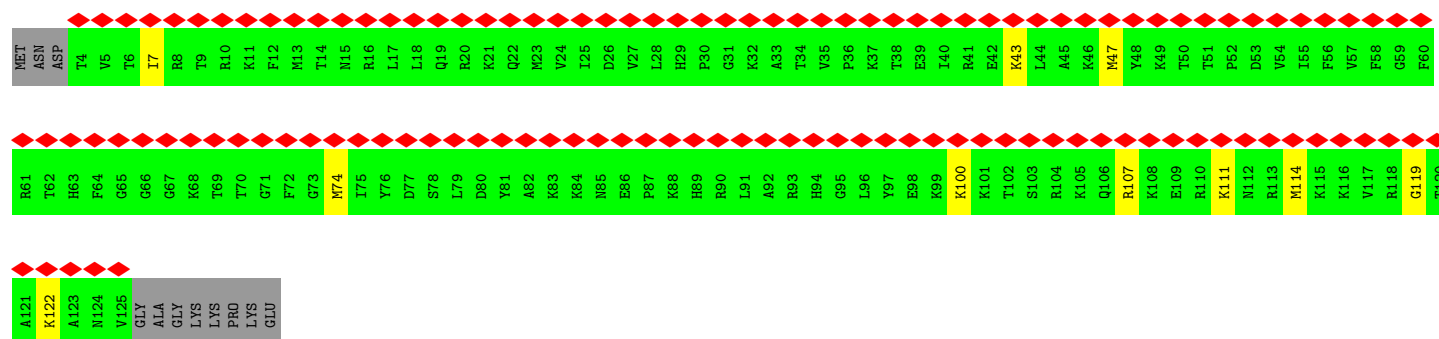
• Molecule 64: 40S ribosomal protein S15a

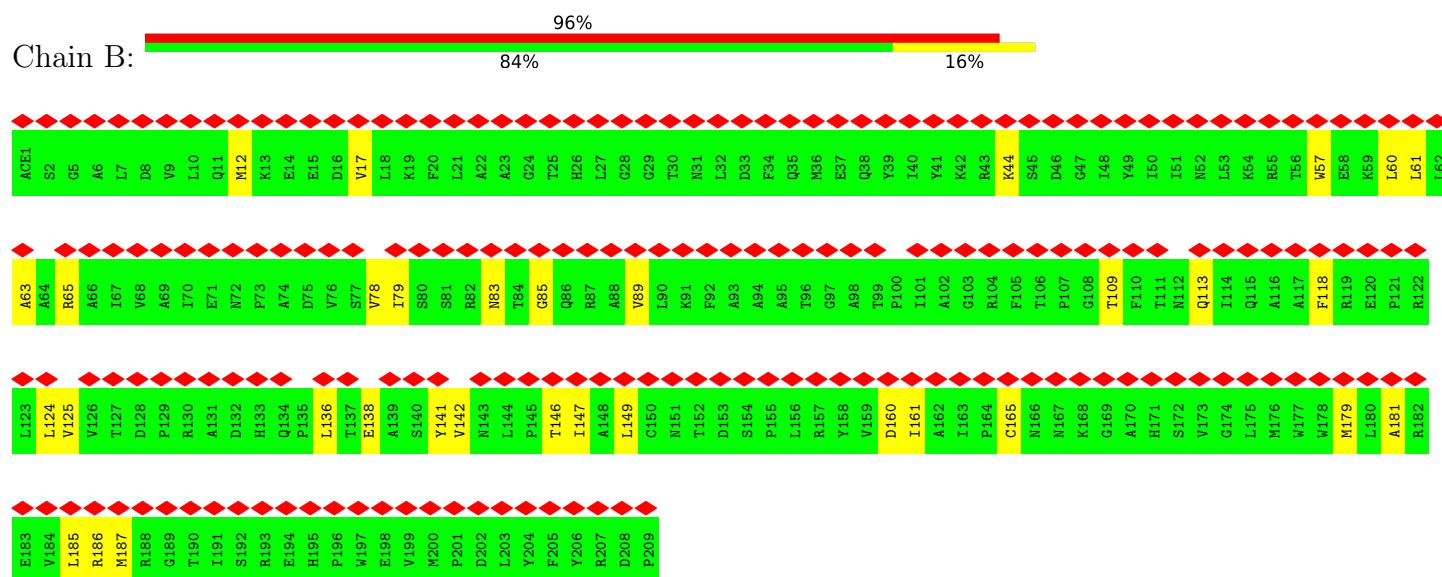
Chain HX: 



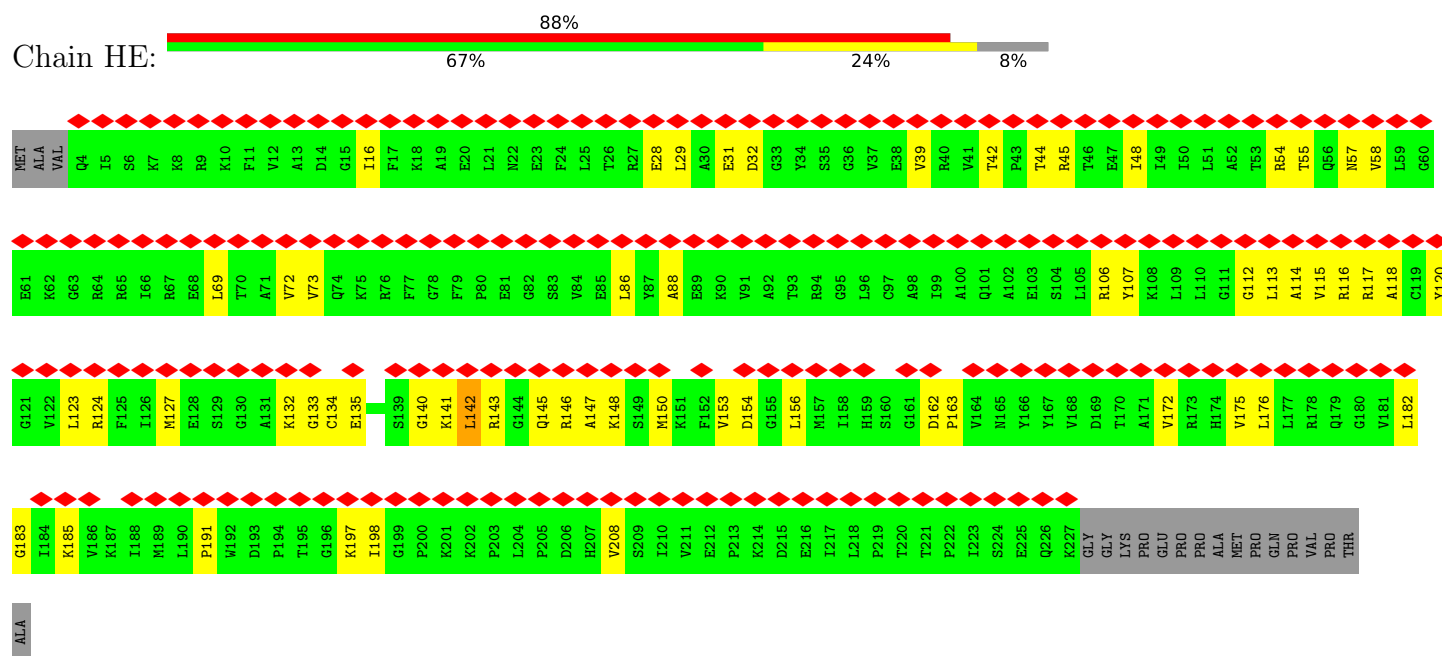
- Molecule 65: 40S ribosomal protein S24

Chain HZ: 

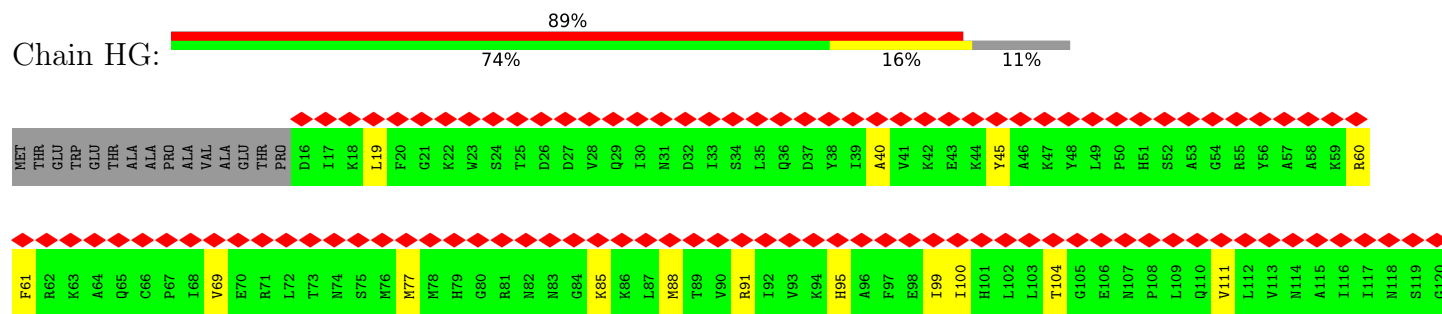


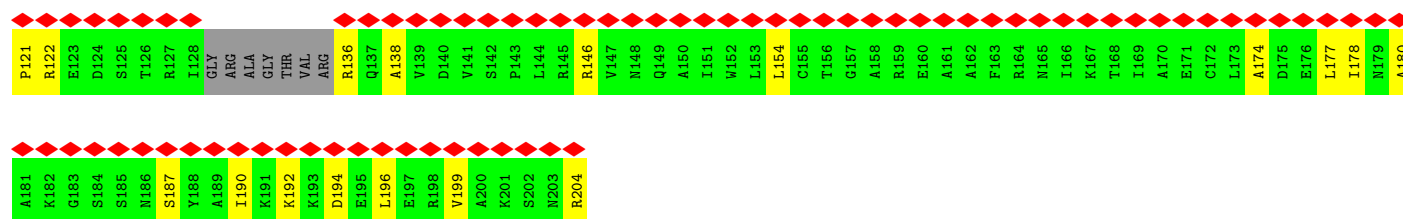


• Molecule 69: 40S ribosomal protein S3

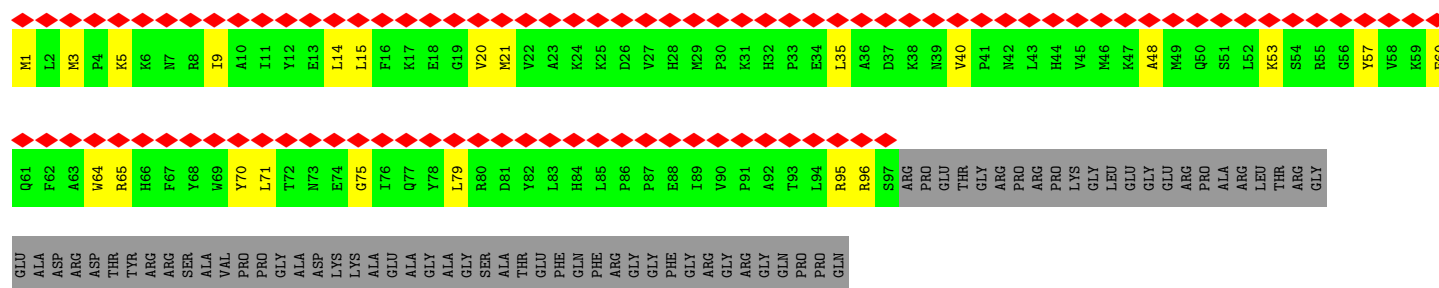


• Molecule 70: 40S ribosomal protein S5

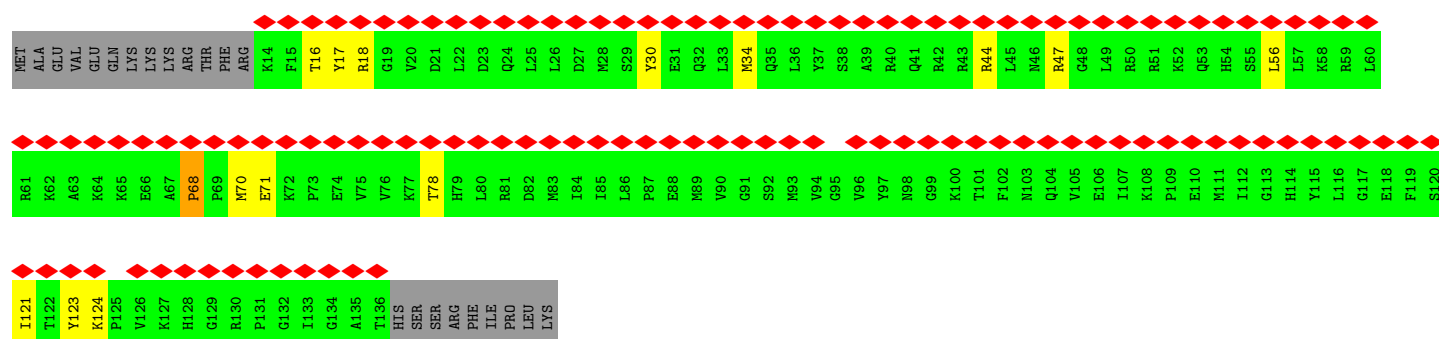
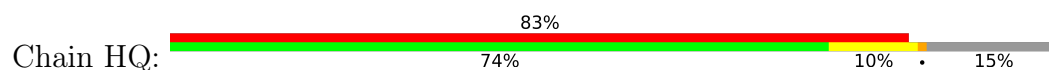




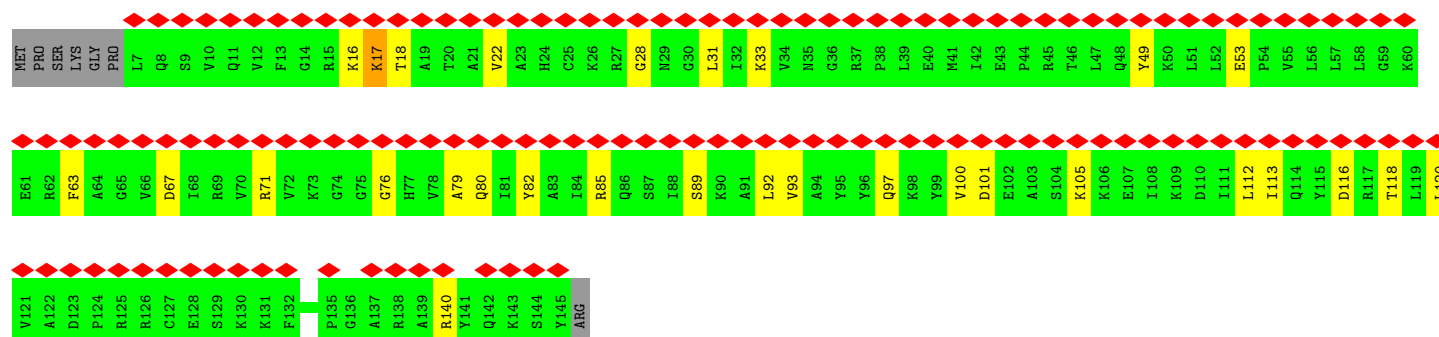
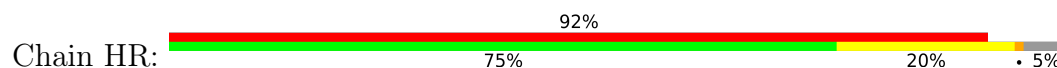
• Molecule 71: 40S ribosomal protein S10



• Molecule 72: 40S ribosomal protein S15

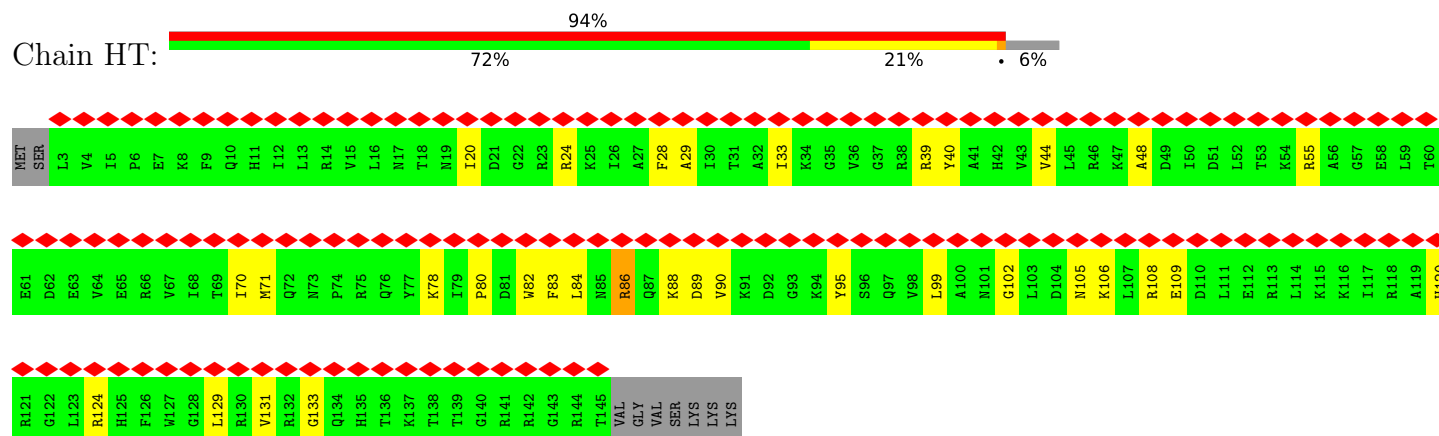


• Molecule 73: 40S ribosomal protein S16



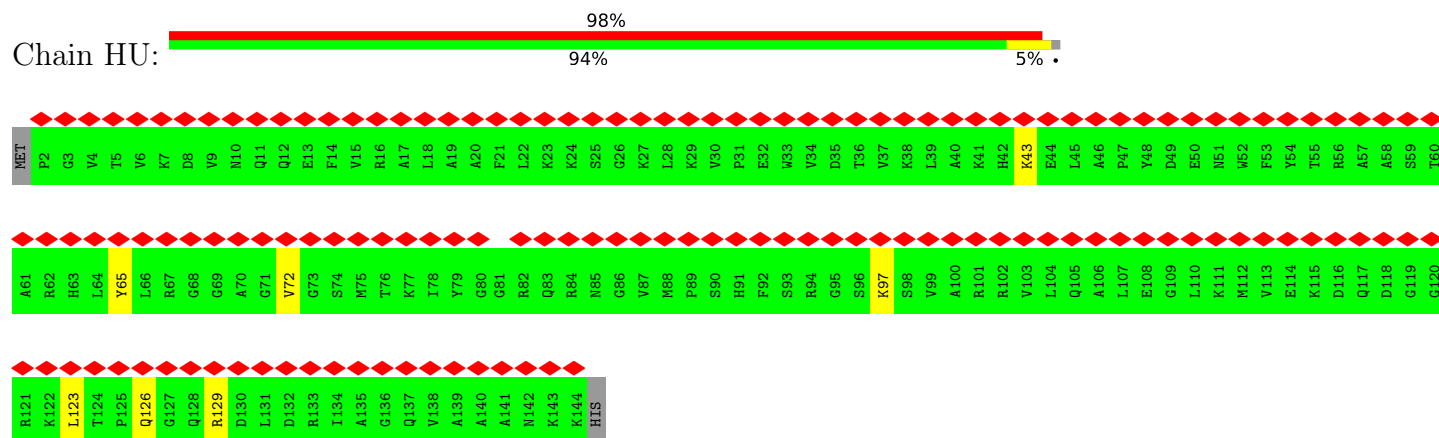
- Molecule 74: 40S ribosomal protein S18

Chain HT:



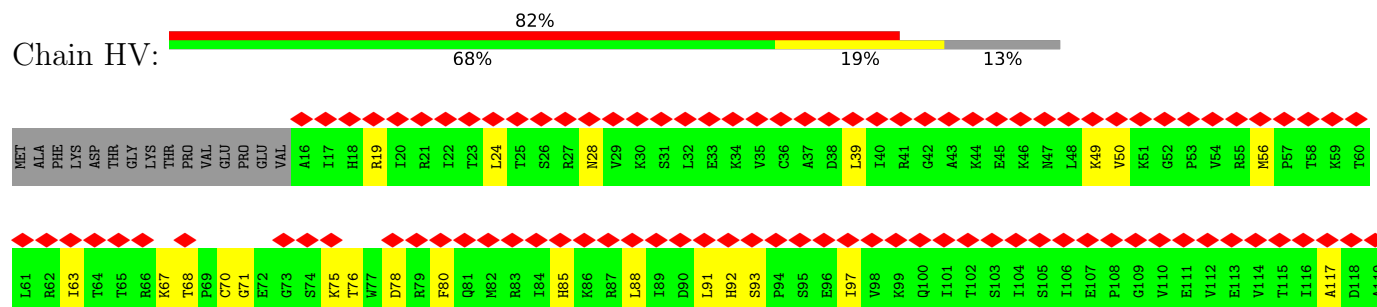
- Molecule 75: 40S ribosomal protein S19

Chain HU:



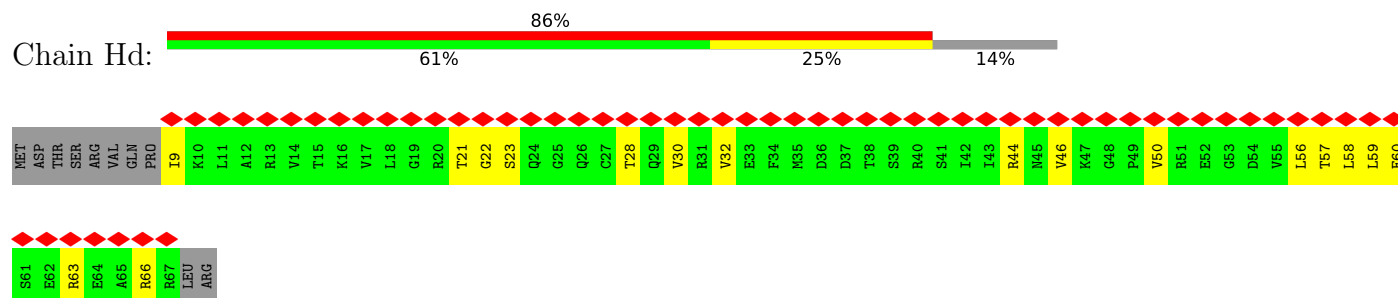
- Molecule 76: 40S ribosomal protein S20

Chain HV:

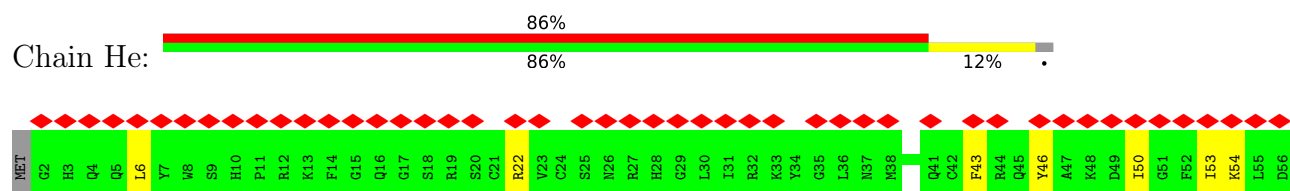


- Molecule 77: 40S ribosomal protein S28

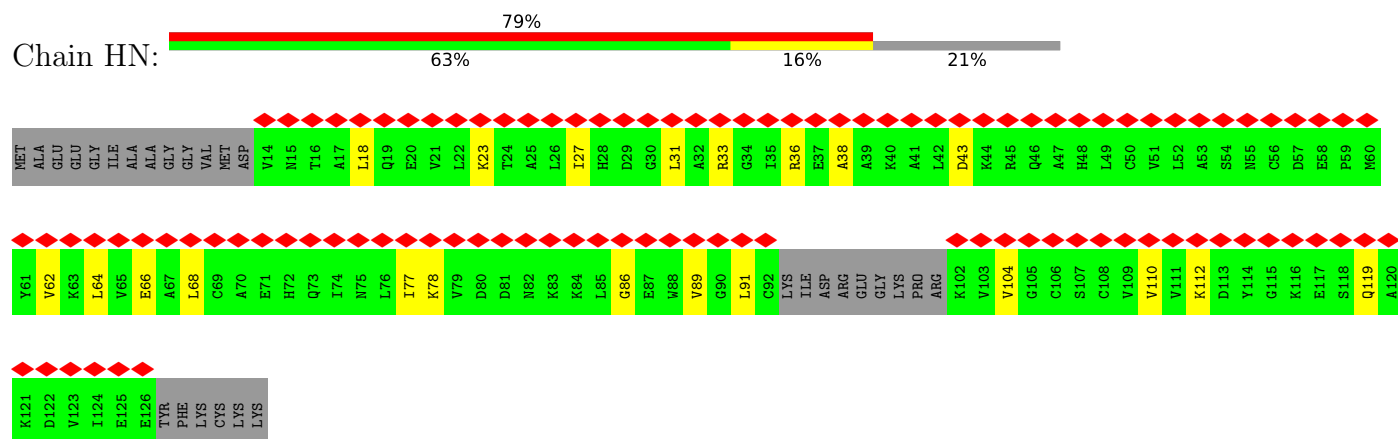
Chain Hd:



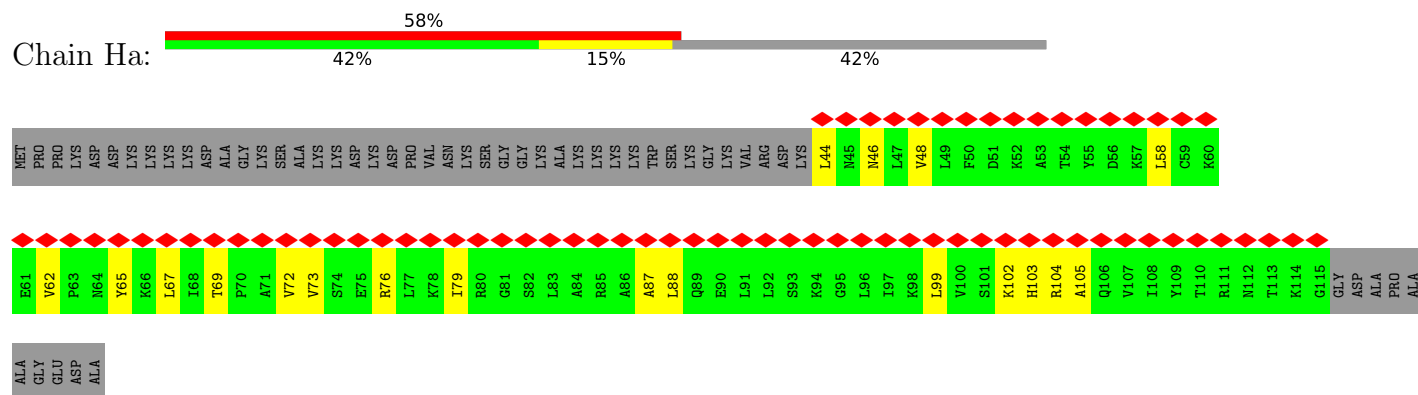
- Molecule 78: 40S ribosomal protein S29



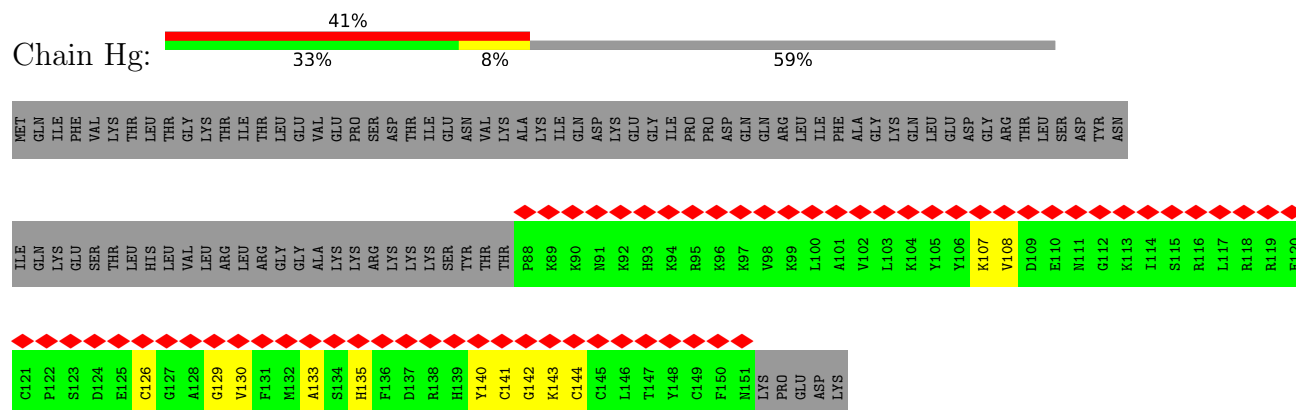
- Molecule 79: 40S ribosomal protein S12



- Molecule 80: Small ribosomal subunit protein eS25

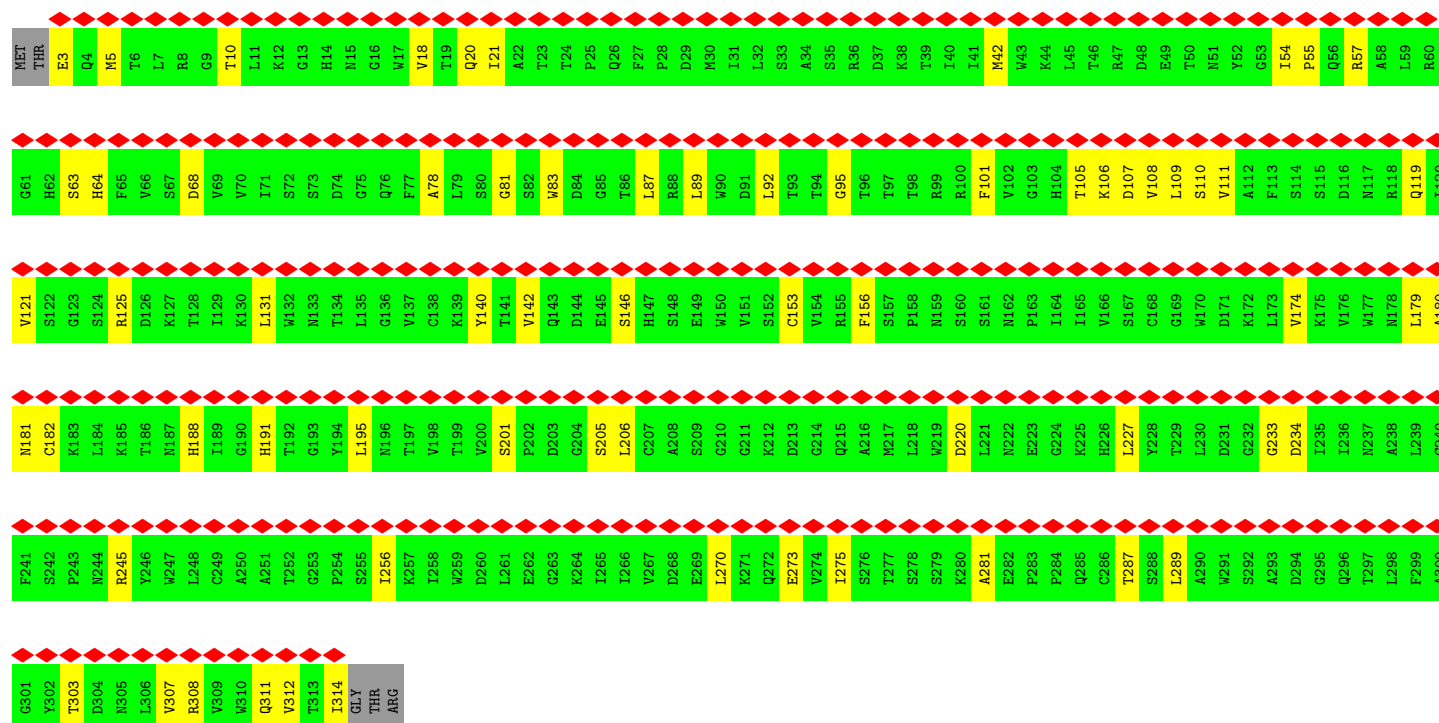


- Molecule 81: Ubiquitin



- Molecule 82: Receptor of activated protein C kinase 1

Response	Percentage
Yes	98%
No	2%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	202290	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.158	Depositor
Minimum map value	-0.553	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.029	Depositor
Recommended contour level	0.115	Depositor
Map size (Å)	414.72, 414.72, 414.72	wwPDB
Map dimensions	640, 640, 640	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.648, 0.648, 0.648	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 5MC, 1MA, G7M, MA6, K, SPD, ZN, A1JQ4, PUT, HY3, PSU, MG, B8T, OMU, UR3, OMC, 6MZ, ACE, MLZ, 4AC, UY1, SPM, B8N, V5N, IAS, OMG, A2M, HIC

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	AA	0.17	0/1882	0.36	0/2507
2	AB	0.17	0/1853	0.37	0/2495
3	AC	0.14	0/1537	0.36	0/2066
4	AD	0.16	0/1718	0.36	0/2292
5	AE	0.21	0/1394	0.47	0/1863
6	AF	0.15	0/1662	0.34	0/2225
7	AG	0.15	0/1142	0.40	0/1527
8	AH	0.13	0/1746	0.36	0/2338
9	AI	0.16	0/1682	0.37	0/2250
10	AJ	0.15	0/1250	0.39	0/1678
11	AK	0.20	1/1537 (0.1%)	0.36	1/2052 (0.0%)
12	AL	0.16	0/1357	0.37	0/1797
13	AM	0.17	0/1493	0.33	0/2003
14	AN	0.18	0/1335	0.39	0/1781
15	AO	0.15	0/822	0.37	0/1103
16	AP	0.27	0/993	0.43	0/1332
17	AQ	0.16	0/532	0.37	0/708
18	AR	0.13	0/993	0.31	0/1334
19	AS	0.20	0/1132	0.38	0/1504
20	AT	0.17	0/1130	0.35	0/1507
21	AU	0.14	0/1179	0.32	0/1573
22	AV	0.18	0/811	0.39	0/1069
23	AW	0.23	0/774	0.41	0/1038
24	AX	0.16	0/916	0.35	0/1234
25	AY	0.13	0/1088	0.32	0/1451
26	AZ	0.14	0/895	0.34	0/1198
27	Aa	0.15	0/878	0.31	0/1170
28	Ab	0.15	0/1023	0.34	0/1351
29	Ac	0.17	0/843	0.39	0/1115
30	Ad	0.13	0/742	0.35	0/980
31	Ae	0.26	0/575	0.43	0/761

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	Af	0.16	0/454	0.38	0/599
33	Ag	0.11	0/425	0.30	0/561
34	Ah	0.13	0/855	0.31	0/1128
35	Ai	0.18	0/717	0.39	0/953
36	Aj	0.16	0/1017	0.36	0/1364
37	BA	0.15	12/79666 (0.0%)	0.30	0/124273
38	BB	0.11	0/2836	0.27	0/4421
39	BC	0.11	0/3631	0.27	0/5657
40	BD	0.18	0/1913	0.41	0/2563
41	CA	0.18	0/3253	0.42	2/4352 (0.0%)
42	CB	0.16	0/2874	0.35	0/3859
43	CC	0.18	0/2432	0.39	0/3256
44	CD	0.15	0/1762	0.36	0/2366
45	DA	0.17	0/1835	0.37	0/2858
46	ER	0.18	1/6530 (0.0%)	0.36	0/8816
47	GF	0.74	0/325	0.95	1/427 (0.2%)
48	Hi	0.57	0/194	0.90	0/246
49	HA	0.19	10/37770 (0.0%)	0.35	3/58857 (0.0%)
50	HC	0.19	0/1738	0.42	0/2325
51	HF	0.33	1/2083 (0.0%)	0.39	0/2805
52	HI	0.25	0/1498	0.56	0/2005
53	HJ	0.17	0/1711	0.40	0/2282
54	HM	0.20	0/1177	0.42	0/1574
55	HS	0.20	0/1078	0.45	0/1447
56	A	0.24	0/644	0.45	0/862
57	HY	0.25	0/1096	0.47	0/1461
58	Hb	0.23	0/805	0.43	0/1079
59	HD	0.22	0/1748	0.46	0/2361
60	HH	0.16	0/1863	0.39	0/2481
61	HK	0.18	0/1550	0.42	0/2069
62	HO	0.25	0/1232	0.45	0/1656
63	HP	0.19	0/960	0.43	0/1284
64	HX	0.19	0/1051	0.45	0/1406
65	HZ	0.17	0/1019	0.42	0/1354
66	Hc	0.18	0/653	0.41	0/876
67	Hf	0.15	0/443	0.41	0/582
68	B	0.17	0/1666	0.39	0/2264
69	HE	0.27	0/1773	0.56	0/2387
70	HG	0.21	0/1465	0.49	0/1969
71	HL	0.22	0/840	0.53	0/1133
72	HQ	0.35	1/1024 (0.1%)	0.50	1/1369 (0.1%)
73	HR	0.20	0/1122	0.48	0/1503
74	HT	0.22	0/1214	0.44	0/1626

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
75	HU	0.16	0/1131	0.39	0/1515
76	HV	0.17	0/831	0.42	0/1115
77	Hd	0.21	0/465	0.48	0/621
78	He	0.17	0/470	0.40	0/623
79	HN	0.21	0/796	0.48	0/1072
80	Ha	0.19	0/576	0.47	0/774
81	Hg	0.17	0/533	0.44	0/706
82	Hh	0.23	0/2486	0.54	0/3384
All	All	0.18	26/224144 (0.0%)	0.36	8/327828 (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
40	BD	0	1
41	CA	0	1
44	CD	0	1
46	ER	0	1
48	Hi	0	1
60	HH	0	1
61	HK	0	1
69	HE	0	2
73	HR	0	1
74	HT	0	2
82	Hh	0	1
All	All	0	13

The worst 5 of 26 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	HF	149	TYR	C-O	-12.65	1.18	1.23
72	HQ	68	PRO	CA-C	-8.80	1.47	1.51
46	ER	722	ILE	CA-CB	-5.94	1.51	1.54
49	HA	590	A2M	O3'-P	5.71	1.61	1.56
49	HA	576	A2M	O3'-P	5.69	1.61	1.56

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	GF	223	ASN	N-CA-C	-6.89	98.96	109.85

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
72	HQ	68	PRO	O-C-N	-6.70	118.23	121.31
41	CA	301	ASN	N-CA-C	-6.58	99.52	109.79
49	HA	1709	G	N9-C1'-C2'	5.74	120.61	112.00
49	HA	1709	G	O4'-C1'-N9	5.58	116.88	108.50

There are no chirality outliers.

5 of 13 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
40	BD	28	ARG	Sidechain
41	CA	198	ARG	Sidechain
44	CD	105	ARG	Sidechain
46	ER	287	ARG	Sidechain
48	Hi	12	ARG	Sidechain

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	AA	1845	1983	1983	7	0
2	AB	1822	1962	1962	8	0
3	AC	1518	1601	1601	10	0
4	AD	1670	1715	1701	8	0
5	AE	1371	1412	1412	25	0
6	AF	1631	1746	1746	9	0
7	AG	1120	1187	1187	6	0
8	AH	1701	1749	1749	11	0
9	AI	1650	1795	1794	19	0
10	AJ	1224	1250	1250	10	0
11	AK	1513	1629	1628	7	0
12	AL	1341	1475	1475	9	0
13	AM	1453	1490	1490	2	0
14	AN	1304	1380	1379	11	0
15	AO	808	831	831	8	0
16	AP	979	1039	1039	8	0
17	AQ	519	533	533	4	0
18	AR	976	1053	1053	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	AS	1115	1205	1205	10	0
20	AT	1107	1182	1182	10	0
21	AU	1163	1210	1206	6	0
22	AV	798	862	862	3	0
23	AW	764	804	804	13	0
24	AX	901	947	946	8	0
25	AY	1070	1166	1165	3	0
26	AZ	876	912	912	3	0
27	Aa	868	959	959	0	0
28	Ab	1015	1148	1148	6	0
29	Ac	832	917	917	10	0
30	Ad	716	750	736	0	0
31	Ae	569	637	637	5	0
32	Af	444	483	483	4	0
33	Ag	430	466	466	1	0
34	Ah	842	912	912	3	0
35	Ai	707	756	755	3	0
36	Aj	1002	1069	1068	5	0
37	BA	73673	36901	37291	521	0
38	BB	2538	1285	1286	12	0
39	BC	3315	1674	1685	42	0
40	BD	1888	1979	1976	9	0
41	CA	3198	3340	3339	24	0
42	CB	2820	2992	2992	16	0
43	CC	2386	2421	2421	21	0
44	CD	1728	1875	1875	13	0
45	DA	1644	830	831	36	0
46	ER	6407	6470	6475	80	0
47	GF	320	275	285	24	0
48	Hi	193	237	237	9	0
49	HA	35347	17647	17898	552	0
50	HC	1711	1781	1782	26	0
51	HF	2041	2143	2143	35	0
52	HI	1477	1573	1573	24	0
53	HJ	1682	1769	1768	17	0
54	HM	1157	1223	1222	16	0
55	HS	1064	1118	1118	26	0
56	A	639	629	638	15	0
57	HY	1088	1147	1149	13	0
58	Hb	792	841	841	9	0
59	HD	1708	1798	1797	40	0
60	HH	1840	1989	1989	19	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	HK	1525	1640	1640	18	0
62	HO	1208	1293	1293	14	0
63	HP	957	977	981	14	0
64	HX	1034	1080	1080	18	0
65	HZ	1002	1075	1075	8	0
66	Hc	640	665	665	5	0
67	Hf	438	484	484	5	0
68	B	1628	1648	1649	27	0
69	HE	1745	1835	1837	58	0
70	HG	1445	1495	1495	28	0
71	HL	816	841	841	15	0
72	HQ	1005	1053	1053	14	0
73	HR	1105	1172	1172	22	0
74	HT	1192	1253	1253	29	0
75	HU	1112	1147	1146	6	0
76	HV	821	883	882	18	0
77	Hd	464	488	488	17	0
78	He	459	448	448	8	0
79	HN	790	808	808	16	0
80	Ha	570	626	626	16	0
81	Hg	522	529	529	9	0
82	Hh	2429	2386	2386	43	0
83	AD	1	0	0	0	0
83	AJ	1	0	0	0	0
83	AP	1	0	0	0	0
83	AY	1	0	0	0	0
83	AZ	1	0	0	0	0
83	Ad	1	0	0	0	0
83	BA	168	0	0	0	0
83	BB	2	0	0	0	0
83	BC	3	0	0	0	0
83	HA	72	0	0	0	0
83	HH	1	0	0	0	0
84	AH	6	0	0	0	0
84	BA	12	0	24	7	0
84	BB	6	0	12	4	0
85	AM	1	0	0	0	0
85	AN	1	0	0	0	0
85	AP	1	0	0	0	0
85	BA	38	0	0	0	0
85	BC	1	0	0	0	0
85	BD	2	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
85	HA	66	0	0	0	0
85	HF	1	0	0	0	0
85	HJ	1	0	0	0	0
85	HP	1	0	0	0	0
85	HT	2	0	0	0	0
85	HV	1	0	0	0	0
85	He	1	0	0	0	0
86	Aa	1	0	0	0	0
86	Ad	1	0	0	0	0
86	Ag	1	0	0	0	0
86	Ah	1	0	0	0	0
86	Ai	1	0	0	0	0
86	Hb	1	0	0	0	0
86	He	1	0	0	0	0
86	Hg	1	0	0	0	0
87	BA	60	12	114	20	0
88	BA	70	45	130	8	0
89	BA	24	24	0	0	0
90	AD	1	0	0	0	0
90	AH	1	0	0	0	0
90	AJ	1	0	0	0	0
90	AP	3	0	0	0	0
90	AU	4	0	0	0	0
90	AY	2	0	0	0	0
90	Ad	2	0	0	0	0
90	BA	728	0	0	1	0
90	BB	9	0	0	0	0
90	BC	16	0	0	0	0
90	BD	4	0	0	0	0
90	DA	1	0	0	0	0
90	HA	278	0	0	0	0
90	HO	1	0	0	0	0
90	HP	2	0	0	0	0
90	HR	1	0	0	0	0
90	HU	3	0	0	0	0
90	HY	1	0	0	0	0
All	All	214840	160059	160898	2051	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 2051 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)
37:BA:1534:A2M:C1'	37:BA:1534:A2M:O4'	1.63	1.20
37:BA:3760:A:H2	49:HA:1709:G:H1'	1.26	0.99
46:ER:409:ARG:HH22	49:HA:478:G:H5''	1.42	0.84
51:HF:87:MET:HE3	51:HF:123:LEU:HB2	1.60	0.83
48:Hi:4:LYS:HZ1	49:HA:1841:4AC:HM72	1.44	0.81

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AA	220/248 (89%)	216 (98%)	4 (2%)	0	100	100
2	AB	221/266 (83%)	216 (98%)	5 (2%)	0	100	100
3	AC	188/192 (98%)	185 (98%)	3 (2%)	0	100	100
4	AD	203/214 (95%)	202 (100%)	1 (0%)	0	100	100
5	AE	169/178 (95%)	161 (95%)	8 (5%)	0	100	100
6	AF	200/211 (95%)	192 (96%)	8 (4%)	0	100	100
7	AG	134/215 (62%)	131 (98%)	3 (2%)	0	100	100
8	AH	201/204 (98%)	196 (98%)	5 (2%)	0	100	100
9	AI	199/203 (98%)	198 (100%)	1 (0%)	0	100	100
10	AJ	149/184 (81%)	145 (97%)	4 (3%)	0	100	100
11	AK	185/188 (98%)	182 (98%)	3 (2%)	0	100	100
12	AL	159/196 (81%)	158 (99%)	1 (1%)	0	100	100
13	AM	173/176 (98%)	171 (99%)	2 (1%)	0	100	100
14	AN	158/160 (99%)	153 (97%)	5 (3%)	0	100	100
15	AO	97/128 (76%)	91 (94%)	6 (6%)	0	100	100
16	AP	129/140 (92%)	127 (98%)	2 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	AQ	60/157 (38%)	59 (98%)	1 (2%)	0	100	100
18	AR	117/156 (75%)	114 (97%)	3 (3%)	0	100	100
19	AS	132/145 (91%)	130 (98%)	2 (2%)	0	100	100
20	AT	133/136 (98%)	128 (96%)	5 (4%)	0	100	100
21	AU	144/148 (97%)	140 (97%)	3 (2%)	1 (1%)	18	14
22	AV	94/159 (59%)	90 (96%)	4 (4%)	0	100	100
23	AW	96/115 (84%)	94 (98%)	2 (2%)	0	100	100
24	AX	107/125 (86%)	104 (97%)	3 (3%)	0	100	100
25	AY	128/135 (95%)	127 (99%)	1 (1%)	0	100	100
26	AZ	107/110 (97%)	107 (100%)	0	0	100	100
27	Aa	107/117 (92%)	107 (100%)	0	0	100	100
28	Ab	120/123 (98%)	115 (96%)	5 (4%)	0	100	100
29	Ac	100/105 (95%)	97 (97%)	3 (3%)	0	100	100
30	Ad	86/97 (89%)	86 (100%)	0	0	100	100
31	Ae	67/70 (96%)	67 (100%)	0	0	100	100
32	Af	48/51 (94%)	45 (94%)	3 (6%)	0	100	100
33	Ag	49/128 (38%)	49 (100%)	0	0	100	100
34	Ah	101/106 (95%)	98 (97%)	3 (3%)	0	100	100
35	Ai	89/92 (97%)	86 (97%)	3 (3%)	0	100	100
36	Aj	123/137 (90%)	121 (98%)	2 (2%)	0	100	100
40	BD	243/257 (95%)	231 (95%)	12 (5%)	0	100	100
41	CA	393/403 (98%)	382 (97%)	11 (3%)	0	100	100
42	CB	350/427 (82%)	346 (99%)	4 (1%)	0	100	100
43	CC	291/297 (98%)	283 (97%)	8 (3%)	0	100	100
44	CD	209/288 (73%)	204 (98%)	5 (2%)	0	100	100
46	ER	810/858 (94%)	794 (98%)	16 (2%)	0	100	100
47	GF	36/408 (9%)	36 (100%)	0	0	100	100
48	Hi	18/25 (72%)	18 (100%)	0	0	100	100
50	HC	208/264 (79%)	204 (98%)	4 (2%)	0	100	100
51	HF	255/263 (97%)	253 (99%)	2 (1%)	0	100	100
52	HI	180/194 (93%)	160 (89%)	19 (11%)	1 (1%)	21	17

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
53	HJ	203/208 (98%)	200 (98%)	3 (2%)	0	100	100
54	HM	137/158 (87%)	131 (96%)	6 (4%)	0	100	100
55	HS	129/135 (96%)	127 (98%)	2 (2%)	0	100	100
56	A	82/84 (98%)	82 (100%)	0	0	100	100
57	HY	137/143 (96%)	133 (97%)	4 (3%)	0	100	100
58	Hb	97/115 (84%)	96 (99%)	1 (1%)	0	100	100
59	HD	218/293 (74%)	214 (98%)	4 (2%)	0	100	100
60	HH	225/249 (90%)	219 (97%)	6 (3%)	0	100	100
61	HK	183/194 (94%)	176 (96%)	7 (4%)	0	100	100
62	HO	148/151 (98%)	147 (99%)	1 (1%)	0	100	100
63	HP	123/151 (82%)	120 (98%)	3 (2%)	0	100	100
64	HX	127/130 (98%)	125 (98%)	2 (2%)	0	100	100
65	HZ	120/133 (90%)	120 (100%)	0	0	100	100
66	Hc	80/84 (95%)	78 (98%)	2 (2%)	0	100	100
67	Hf	53/133 (40%)	50 (94%)	3 (6%)	0	100	100
68	B	206/207 (100%)	202 (98%)	4 (2%)	0	100	100
69	HE	222/243 (91%)	221 (100%)	1 (0%)	0	100	100
70	HG	178/204 (87%)	171 (96%)	7 (4%)	0	100	100
71	HL	95/165 (58%)	88 (93%)	7 (7%)	0	100	100
72	HQ	121/145 (83%)	117 (97%)	4 (3%)	0	100	100
73	HR	137/146 (94%)	132 (96%)	5 (4%)	0	100	100
74	HT	142/152 (93%)	139 (98%)	3 (2%)	0	100	100
75	HU	141/145 (97%)	140 (99%)	1 (1%)	0	100	100
76	HV	102/119 (86%)	96 (94%)	6 (6%)	0	100	100
77	Hd	57/69 (83%)	54 (95%)	3 (5%)	0	100	100
78	He	53/56 (95%)	53 (100%)	0	0	100	100
79	HN	100/132 (76%)	97 (97%)	3 (3%)	0	100	100
80	Ha	70/125 (56%)	66 (94%)	4 (6%)	0	100	100
81	Hg	62/156 (40%)	58 (94%)	4 (6%)	0	100	100
82	Hh	310/317 (98%)	297 (96%)	13 (4%)	0	100	100
All	All	11844/13941 (85%)	11548 (98%)	294 (2%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
52	HI	19	PHE
21	AU	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	
1	AA	192/215 (89%)	192 (100%)	0	100	100
2	AB	195/223 (87%)	195 (100%)	0	100	100
3	AC	169/171 (99%)	169 (100%)	0	100	100
4	AD	177/181 (98%)	175 (99%)	2 (1%)	65	73
5	AE	144/149 (97%)	144 (100%)	0	100	100
6	AF	168/177 (95%)	168 (100%)	0	100	100
7	AG	116/161 (72%)	116 (100%)	0	100	100
8	AH	171/172 (99%)	171 (100%)	0	100	100
9	AI	173/174 (99%)	173 (100%)	0	100	100
10	AJ	132/163 (81%)	132 (100%)	0	100	100
11	AK	164/165 (99%)	164 (100%)	0	100	100
12	AL	142/175 (81%)	142 (100%)	0	100	100
13	AM	156/157 (99%)	156 (100%)	0	100	100
14	AN	140/140 (100%)	140 (100%)	0	100	100
15	AO	89/115 (77%)	89 (100%)	0	100	100
16	AP	101/107 (94%)	101 (100%)	0	100	100
17	AQ	54/126 (43%)	54 (100%)	0	100	100
18	AR	107/133 (80%)	107 (100%)	0	100	100
19	AS	124/135 (92%)	124 (100%)	0	100	100
20	AT	117/118 (99%)	117 (100%)	0	100	100
21	AU	119/120 (99%)	119 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
22	AV	81/126 (64%)	81 (100%)	0	100	100
23	AW	83/97 (86%)	83 (100%)	0	100	100
24	AX	99/110 (90%)	99 (100%)	0	100	100
25	AY	116/121 (96%)	116 (100%)	0	100	100
26	AZ	88/89 (99%)	88 (100%)	0	100	100
27	Aa	94/100 (94%)	94 (100%)	0	100	100
28	Ab	109/110 (99%)	109 (100%)	0	100	100
29	Ac	86/89 (97%)	86 (100%)	0	100	100
30	Ad	75/80 (94%)	75 (100%)	0	100	100
31	Ae	64/65 (98%)	64 (100%)	0	100	100
32	Af	47/48 (98%)	47 (100%)	0	100	100
33	Ag	47/115 (41%)	47 (100%)	0	100	100
34	Ah	91/94 (97%)	91 (100%)	0	100	100
35	Ai	74/75 (99%)	74 (100%)	0	100	100
36	Aj	109/121 (90%)	109 (100%)	0	100	100
40	BD	188/198 (95%)	188 (100%)	0	100	100
41	CA	344/348 (99%)	344 (100%)	0	100	100
42	CB	297/348 (85%)	297 (100%)	0	100	100
43	CC	247/250 (99%)	247 (100%)	0	100	100
44	CD	191/252 (76%)	191 (100%)	0	100	100
46	ER	704/730 (96%)	704 (100%)	0	100	100
47	GF	33/328 (10%)	33 (100%)	0	100	100
48	Hi	19/24 (79%)	19 (100%)	0	100	100
50	HC	192/231 (83%)	192 (100%)	0	100	100
51	HF	220/225 (98%)	220 (100%)	0	100	100
52	HI	164/174 (94%)	164 (100%)	0	100	100
53	HJ	178/180 (99%)	178 (100%)	0	100	100
54	HM	128/142 (90%)	128 (100%)	0	100	100
55	HS	119/122 (98%)	119 (100%)	0	100	100
56	A	67/67 (100%)	67 (100%)	0	100	100
57	HY	111/114 (97%)	111 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
58	Hb	86/98 (88%)	86 (100%)	0	100	100
59	HD	186/225 (83%)	186 (100%)	0	100	100
60	HH	198/218 (91%)	198 (100%)	0	100	100
61	HK	161/168 (96%)	161 (100%)	0	100	100
62	HO	130/131 (99%)	130 (100%)	0	100	100
63	HP	99/118 (84%)	99 (100%)	0	100	100
64	HX	112/113 (99%)	112 (100%)	0	100	100
65	HZ	107/115 (93%)	107 (100%)	0	100	100
66	Hc	74/76 (97%)	74 (100%)	0	100	100
67	Hf	45/104 (43%)	45 (100%)	0	100	100
68	B	173/172 (101%)	172 (99%)	1 (1%)	78	85
69	HE	188/202 (93%)	188 (100%)	0	100	100
70	HG	155/170 (91%)	155 (100%)	0	100	100
71	HL	88/136 (65%)	88 (100%)	0	100	100
72	HQ	109/130 (84%)	109 (100%)	0	100	100
73	HR	115/121 (95%)	115 (100%)	0	100	100
74	HT	125/132 (95%)	125 (100%)	0	100	100
75	HU	113/115 (98%)	113 (100%)	0	100	100
76	HV	94/107 (88%)	94 (100%)	0	100	100
77	Hd	52/62 (84%)	52 (100%)	0	100	100
78	He	48/49 (98%)	48 (100%)	0	100	100
79	HN	86/108 (80%)	86 (100%)	0	100	100
80	Ha	63/103 (61%)	63 (100%)	0	100	100
81	Hg	57/140 (41%)	57 (100%)	0	100	100
82	Hh	271/275 (98%)	271 (100%)	0	100	100
All	All	10350/11838 (87%)	10347 (100%)	3 (0%)	100	100

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	AD	169[A]	LYS
4	AD	169[B]	LYS
68	B	186	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 100 such sidechains are listed below:

Mol	Chain	Res	Type
43	CC	282	GLN
54	HM	94	HIS
82	Hh	76	GLN
46	ER	357	HIS
51	HF	8	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
37	BA	3416/5069 (67%)	518 (15%)	12 (0%)
38	BB	118/120 (98%)	7 (5%)	0
39	BC	155/157 (98%)	27 (17%)	0
45	DA	76/77 (98%)	16 (21%)	2 (2%)
49	HA	1628/1868 (87%)	269 (16%)	4 (0%)
All	All	5393/7291 (73%)	837 (15%)	18 (0%)

5 of 837 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
37	BA	39	A
37	BA	42	A
37	BA	48	G
37	BA	58	G
37	BA	59	A

5 of 18 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
49	HA	331	C
49	HA	1434	C
49	HA	629	A
37	BA	3760	A
45	DA	74	G

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

197 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$
49	A2M	HA	484	49	22,25,26	3.36	9 (40%)	31,36,39	2.66	12 (38%)
37	PSU	BA	2839	37	18,21,22	1.18	1 (5%)	22,30,33	1.37	3 (13%)
37	OMG	BA	4392	37	23,26,27	2.49	7 (30%)	33,38,41	1.89	10 (30%)
37	PSU	BA	4423	37	18,21,22	1.18	1 (5%)	22,30,33	1.45	3 (13%)
37	PSU	BA	4532	37	18,21,22	1.18	1 (5%)	22,30,33	1.41	3 (13%)
49	OMC	HA	1391	49	19,22,23	3.16	8 (42%)	26,31,34	0.70	0
49	PSU	HA	1056	49	18,21,22	1.18	1 (5%)	22,30,33	1.28	3 (13%)
49	A2M	HA	468	49	22,25,26	3.36	9 (40%)	31,36,39	2.73	13 (41%)
37	PSU	BA	4500	37	18,21,22	1.17	1 (5%)	22,30,33	1.38	3 (13%)
37	OMC	BA	1881	37,83	19,22,23	3.16	8 (42%)	26,31,34	0.79	0
37	OMC	BA	3841	37	19,22,23	3.14	8 (42%)	26,31,34	0.64	0
37	OMC	BA	3808	37	19,22,23	3.14	8 (42%)	26,31,34	0.72	0
37	PSU	BA	1677	37	18,21,22	1.30	3 (16%)	22,30,33	1.43	3 (13%)
49	PSU	HA	681	49	18,21,22	1.13	1 (5%)	22,30,33	1.33	3 (13%)
37	OMG	BA	4228	37	23,26,27	2.48	8 (34%)	33,38,41	1.98	10 (30%)
49	PSU	HA	1046	49	18,21,22	1.25	3 (16%)	22,30,33	1.19	3 (13%)
49	G7M	HA	1639	49	23,26,27	4.16	9 (39%)	35,39,42	1.54	7 (20%)
49	4AC	HA	1337	49	21,24,25	3.87	10 (47%)	29,34,37	1.40	5 (17%)
37	OMG	BA	4618	37	23,26,27	2.49	7 (30%)	33,38,41	1.89	9 (27%)
37	OMU	BA	4620	37	19,22,23	0.65	0	26,31,34	1.17	3 (11%)
37	OMU	BA	2415	37	19,22,23	0.76	1 (5%)	26,31,34	1.09	3 (11%)
37	OMC	BA	2824	37	19,22,23	3.16	8 (42%)	26,31,34	0.75	0
37	OMC	BA	2351	37,83	19,22,23	3.11	8 (42%)	26,31,34	0.90	2 (7%)
49	PSU	HA	1177	49	18,21,22	1.31	3 (16%)	22,30,33	1.35	3 (13%)
49	PSU	HA	1232	49	18,21,22	1.18	1 (5%)	22,30,33	1.34	3 (13%)
39	OMG	BC	75	39	23,26,27	2.51	7 (30%)	33,38,41	1.91	10 (30%)
49	PSU	HA	296	49	18,21,22	1.19	2 (11%)	22,30,33	1.35	3 (13%)
49	PSU	HA	1081	49	18,21,22	1.25	2 (11%)	22,30,33	1.49	4 (18%)
49	6MZ	HA	1831	49,83,85	22,25,26	3.83	9 (40%)	30,36,39	2.44	12 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
49	OMU	HA	1288	49	19,22,23	0.69	0	26,31,34	1.16	2 (7%)
49	PSU	HA	572	49	18,21,22	1.22	1 (5%)	22,30,33	1.44	3 (13%)
37	A2M	BA	2401	37	22,25,26	3.37	9 (40%)	31,36,39	2.67	13 (41%)
37	OMU	BA	4306	37	19,22,23	0.67	0	26,31,34	1.21	4 (15%)
49	PSU	HA	1347	49	18,21,22	1.29	2 (11%)	22,30,33	1.47	3 (13%)
37	OMG	BA	4623	37	23,26,27	2.50	7 (30%)	33,38,41	1.92	10 (30%)
49	4AC	HA	1841	49	21,24,25	3.84	10 (47%)	29,34,37	1.48	6 (20%)
37	OMG	BA	3669	37	23,26,27	2.52	7 (30%)	33,38,41	1.96	11 (33%)
37	PSU	BA	2508	37	18,21,22	1.16	1 (5%)	22,30,33	1.42	3 (13%)
37	PSU	BA	1683	37,85	18,21,22	1.18	1 (5%)	22,30,33	1.39	3 (13%)
49	B8N	HA	1248	49	24,29,30	3.31	7 (29%)	29,42,45	1.95	6 (20%)
49	A2M	HA	99	49,83	22,25,26	3.34	9 (40%)	31,36,39	2.70	12 (38%)
37	A2M	BA	2787	37	22,25,26	3.38	9 (40%)	31,36,39	2.49	10 (32%)
37	OMG	BA	4494	37	23,26,27	2.52	7 (30%)	33,38,41	1.87	9 (27%)
37	OMC	BA	2804	37	19,22,23	3.14	8 (42%)	26,31,34	0.68	0
37	PSU	BA	4431	37	18,21,22	1.17	1 (5%)	22,30,33	1.44	3 (13%)
49	PSU	HA	1625	49	18,21,22	1.18	1 (5%)	22,30,33	1.29	3 (13%)
37	PSU	BA	1860	37	18,21,22	1.14	1 (5%)	22,30,33	1.57	4 (18%)
37	OMU	BA	4227	37	19,22,23	0.69	0	26,31,34	1.22	4 (15%)
49	OMU	HA	354	49	19,22,23	0.75	1 (5%)	26,31,34	1.16	2 (7%)
37	UY1	BA	3818	37,85	19,22,23	4.31	5 (26%)	22,31,34	1.99	6 (27%)
49	A2M	HA	668	49,83	22,25,26	3.42	8 (36%)	31,36,39	2.50	10 (32%)
49	OMU	HA	116	49	19,22,23	0.69	1 (5%)	26,31,34	1.16	2 (7%)
63	IAS	HP	138	63	6,7,8	1.17	0	6,8,10	1.55	1 (16%)
37	A2M	BA	2363	37,83	22,25,26	3.33	9 (40%)	31,36,39	2.70	13 (41%)
37	OMC	BA	1340	37	19,22,23	3.12	8 (42%)	26,31,34	0.72	0
37	PSU	BA	1536	37	18,21,22	1.13	1 (5%)	22,30,33	1.44	3 (13%)
49	OMC	HA	174	49,83	19,22,23	3.20	8 (42%)	26,31,34	0.73	0
37	A2M	BA	1534	37,83	22,25,26	3.54	9 (40%)	31,36,39	2.61	11 (35%)
37	OMC	BA	4456	37	19,22,23	3.15	8 (42%)	26,31,34	0.79	0
37	5MC	BA	4447	37,85	18,22,23	3.53	7 (38%)	26,32,35	1.12	2 (7%)
37	PSU	BA	4552	37	18,21,22	1.17	1 (5%)	22,30,33	1.43	3 (13%)
49	A2M	HA	1678	49	22,25,26	3.42	9 (40%)	31,36,39	2.65	12 (38%)
49	OMC	HA	1272	49	19,22,23	3.17	8 (42%)	26,31,34	0.85	1 (3%)
37	A2M	BA	4571	37	22,25,26	3.33	9 (40%)	31,36,39	2.82	18 (58%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
37	A2M	BA	2815	37,83	22,25,26	3.34	9 (40%)	31,36,39	2.74	14 (45%)
37	1MA	BA	1322	37,83	21,25,26	2.91	5 (23%)	31,37,40	2.11	8 (25%)
49	OMU	HA	1326	49,83	19,22,23	0.77	0	26,31,34	1.25	4 (15%)
37	OMG	BA	1522	37	23,26,27	2.51	7 (30%)	33,38,41	1.91	10 (30%)
37	OMU	BA	4498	37	19,22,23	0.70	0	26,31,34	1.14	4 (15%)
37	A2M	BA	398	37	22,25,26	3.36	9 (40%)	31,36,39	2.84	15 (48%)
49	PSU	HA	863	49	18,21,22	1.20	1 (5%)	22,30,33	1.40	3 (13%)
37	OMG	BA	2876	37	23,26,27	2.54	7 (30%)	33,38,41	1.94	10 (30%)
49	A2M	HA	27	49,83	22,25,26	3.36	9 (40%)	31,36,39	2.67	11 (35%)
37	OMG	BA	3627	37	23,26,27	2.50	7 (30%)	33,38,41	1.94	10 (30%)
37	OMU	BA	2837	37	19,22,23	0.68	0	26,31,34	1.30	4 (15%)
37	A2M	BA	3867	37	22,25,26	3.39	9 (40%)	31,36,39	2.80	13 (41%)
37	PSU	BA	4521	37,83	18,21,22	1.18	1 (5%)	22,30,33	1.46	4 (18%)
49	A2M	HA	590	49	22,25,26	3.37	9 (40%)	31,36,39	2.84	12 (38%)
49	OMG	HA	683	49	23,26,27	2.56	7 (30%)	33,38,41	2.02	11 (33%)
37	6MZ	BA	4220	37	22,25,26	3.78	9 (40%)	30,36,39	2.37	11 (36%)
37	PSU	BA	4471	37	18,21,22	1.18	1 (5%)	22,30,33	1.38	3 (13%)
37	OMG	BA	3899	37,83	23,26,27	2.50	7 (30%)	33,38,41	1.89	10 (30%)
49	PSU	HA	649	49	18,21,22	1.17	1 (5%)	22,30,33	1.40	3 (13%)
49	A2M	HA	512	49	22,25,26	3.38	9 (40%)	31,36,39	2.69	13 (41%)
37	OMG	BA	3792	37	23,26,27	2.53	7 (30%)	33,38,41	1.91	7 (21%)
49	OMG	HA	644	49	23,26,27	2.53	7 (30%)	33,38,41	1.93	10 (30%)
21	V5N	AU	39	21	9,11,12	1.60	2 (22%)	9,14,16	2.04	3 (33%)
37	OMG	BA	1625	37	23,26,27	2.52	7 (30%)	33,38,41	1.85	8 (24%)
49	OMU	HA	172	49	19,22,23	0.81	1 (5%)	26,31,34	1.30	4 (15%)
49	OMC	HA	1703	49	19,22,23	3.19	8 (42%)	26,31,34	0.74	0
49	A2M	HA	166	49	22,25,26	3.41	9 (40%)	31,36,39	2.70	13 (41%)
37	OMG	BA	4370	37	23,26,27	2.52	7 (30%)	33,38,41	1.88	9 (27%)
37	OMG	BA	2424	37	23,26,27	2.51	7 (30%)	33,38,41	1.89	10 (30%)
37	OMG	BA	4196	37	23,26,27	2.53	7 (30%)	33,38,41	1.90	8 (24%)
37	PSU	BA	3637	37,85	18,21,22	1.09	1 (5%)	22,30,33	1.42	4 (18%)
37	A2M	BA	400	37	22,25,26	3.37	9 (40%)	31,36,39	2.79	13 (41%)
37	PSU	BA	4493	37,85	18,21,22	1.18	1 (5%)	22,30,33	1.41	3 (13%)
37	OMC	BA	2365	37	19,22,23	3.14	8 (42%)	26,31,34	0.71	0
37	OMU	BA	3925	37	19,22,23	0.72	0	26,31,34	1.18	3 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
49	PSU	HA	1136	49	18,21,22	1.22	2 (11%)	22,30,33	1.36	3 (13%)
49	MA6	HA	1850	49	23,26,27	1.35	3 (13%)	34,38,41	3.77	13 (38%)
37	OMC	BA	4536	37	19,22,23	3.12	8 (42%)	26,31,34	0.75	0
37	PSU	BA	3639	37	18,21,22	1.15	1 (5%)	22,30,33	1.31	3 (13%)
37	PSU	BA	3822	37	18,21,22	1.18	2 (11%)	22,30,33	1.19	3 (13%)
37	A2M	BA	3718	37	22,25,26	3.39	9 (40%)	31,36,39	2.74	13 (41%)
49	OMG	HA	1328	49,85	23,26,27	2.51	8 (34%)	33,38,41	2.02	13 (39%)
49	PSU	HA	1445	49	18,21,22	1.18	1 (5%)	22,30,33	1.36	3 (13%)
37	PSU	BA	2632	37	18,21,22	1.23	2 (11%)	22,30,33	1.29	3 (13%)
37	PSU	BA	4312	37	18,21,22	1.16	1 (5%)	22,30,33	1.43	3 (13%)
37	UR3	BA	4530	37	19,22,23	3.07	8 (42%)	26,32,35	1.44	3 (11%)
49	PSU	HA	822	49	18,21,22	1.20	1 (5%)	22,30,33	1.40	4 (18%)
37	OMC	BA	3869	37	19,22,23	3.15	8 (42%)	26,31,34	0.72	0
37	PSU	BA	1779	37	18,21,22	1.17	1 (5%)	22,30,33	1.37	3 (13%)
37	PSU	BA	1781	37	18,21,22	1.16	1 (5%)	22,30,33	1.39	3 (13%)
49	PSU	HA	109	49,85	18,21,22	1.19	1 (5%)	22,30,33	1.28	3 (13%)
37	OMG	BA	4637	37	23,26,27	2.50	7 (30%)	33,38,41	1.92	10 (30%)
37	PSU	BA	4673	37,83	18,21,22	1.18	1 (5%)	22,30,33	1.32	3 (13%)
49	PSU	HA	815	49	18,21,22	1.16	1 (5%)	22,30,33	1.51	3 (13%)
49	PSU	HA	651	49	18,21,22	1.19	1 (5%)	22,30,33	1.50	3 (13%)
49	PSU	HA	814	49	18,21,22	1.12	3 (16%)	22,30,33	1.28	3 (13%)
37	PSU	BA	4296	37	18,21,22	1.20	1 (5%)	22,30,33	1.39	3 (13%)
37	PSU	BA	3884	37	18,21,22	1.11	1 (5%)	22,30,33	1.43	3 (13%)
37	PSU	BA	4576	37	18,21,22	1.18	1 (5%)	22,30,33	1.28	3 (13%)
37	PSU	BA	4972	37	18,21,22	1.20	1 (5%)	22,30,33	1.39	3 (13%)
49	MA6	HA	1849	49	23,26,27	1.39	3 (13%)	34,38,41	3.37	13 (38%)
39	PSU	BC	69	39	18,21,22	1.18	2 (11%)	22,30,33	1.13	2 (9%)
49	A2M	HA	576	49	22,25,26	3.33	9 (40%)	31,36,39	2.60	13 (41%)
37	PSU	BA	1782	37	18,21,22	1.17	1 (5%)	22,30,33	1.40	3 (13%)
37	PSU	BA	4293	37	18,21,22	1.16	1 (5%)	22,30,33	1.44	3 (13%)
37	PSU	BA	4403	37	18,21,22	1.15	1 (5%)	22,30,33	1.42	3 (13%)
37	PSU	BA	4628	37	18,21,22	1.17	1 (5%)	22,30,33	1.41	3 (13%)
49	PSU	HA	1643	49,83	18,21,22	1.27	3 (16%)	22,30,33	1.23	3 (13%)
37	PSU	BA	1792	37	18,21,22	1.16	1 (5%)	22,30,33	1.39	3 (13%)
49	PSU	HA	1692	49,85	18,21,22	1.24	2 (11%)	22,30,33	1.37	3 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
49	OMC	HA	462	49	19,22,23	3.17	8 (42%)	26,31,34	0.75	0
37	OMC	BA	2422	37,83	19,22,23	3.17	8 (42%)	26,31,34	0.70	0
37	PSU	BA	4420	37	18,21,22	1.18	2 (11%)	22,30,33	1.17	2 (9%)
37	PSU	BA	4361	37	18,21,22	1.16	1 (5%)	22,30,33	1.45	3 (13%)
37	PSU	BA	4442	37	18,21,22	1.16	1 (5%)	22,30,33	1.16	2 (9%)
37	A2M	BA	1524	37	22,25,26	3.36	8 (36%)	31,36,39	2.80	12 (38%)
40	V5N	BD	216	40	9,11,12	1.54	2 (22%)	9,14,16	1.91	3 (33%)
49	PSU	HA	1045	49	18,21,22	1.18	1 (5%)	22,30,33	1.39	3 (13%)
49	A2M	HA	1383	49	22,25,26	3.39	9 (40%)	31,36,39	2.84	14 (45%)
37	A2M	BA	1326	37	22,25,26	3.38	9 (40%)	31,36,39	2.78	14 (45%)
37	PSU	BA	3844	37	18,21,22	1.15	1 (5%)	22,30,33	1.33	3 (13%)
57	HY3	HY	62	57	6,8,9	1.05	0	5,10,12	1.22	1 (20%)
49	OMG	HA	509	49,83	23,26,27	2.54	7 (30%)	33,38,41	2.00	10 (30%)
49	OMG	HA	1447	49	23,26,27	2.55	7 (30%)	33,38,41	2.01	10 (30%)
33	MLZ	Ag	98	33	8,9,10	0.76	0	4,9,11	0.82	0
37	OMG	BA	1316	37	23,26,27	2.50	7 (30%)	33,38,41	1.89	10 (30%)
49	OMU	HA	121	49	19,22,23	0.64	0	26,31,34	1.14	3 (11%)
37	PSU	BA	224	37	18,21,22	1.19	2 (11%)	22,30,33	1.36	3 (13%)
37	PSU	BA	3695	37	18,21,22	1.19	1 (5%)	22,30,33	1.23	3 (13%)
39	PSU	BC	55	39	18,21,22	1.17	1 (5%)	22,30,33	1.46	3 (13%)
37	PSU	BA	1862	37	18,21,22	1.14	1 (5%)	22,30,33	1.44	3 (13%)
37	PSU	BA	3920	37,83	18,21,22	1.17	1 (5%)	22,30,33	1.31	3 (13%)
49	PSU	HA	1238	49	18,21,22	1.23	1 (5%)	22,30,33	1.45	3 (13%)
37	B8T	BA	1859	37	19,22,23	0.96	1 (5%)	26,31,34	0.77	1 (3%)
49	PSU	HA	406	49	18,21,22	1.16	1 (5%)	22,30,33	1.45	3 (13%)
37	5MC	BA	3782	37,83	18,22,23	3.56	7 (38%)	26,32,35	1.02	2 (7%)
37	PSU	BA	4457	37	18,21,22	1.16	1 (5%)	22,30,33	1.25	3 (13%)
37	PSU	BA	4353	37	18,21,22	1.14	1 (5%)	22,30,33	1.48	3 (13%)
37	A2M	BA	1871	37,83	22,25,26	3.41	9 (40%)	31,36,39	2.72	12 (38%)
37	OMG	BA	2364	37,83	23,26,27	2.50	7 (30%)	33,38,41	1.87	9 (27%)
49	A2M	HA	159	49	22,25,26	3.40	9 (40%)	31,36,39	2.69	12 (38%)
49	OMU	HA	428	49	19,22,23	0.84	2 (10%)	26,31,34	1.25	4 (15%)
37	A2M	BA	1323	37	22,25,26	3.36	9 (40%)	31,36,39	2.77	14 (45%)
49	PSU	HA	1174	49,85	18,21,22	1.29	3 (16%)	22,30,33	1.43	3 (13%)
37	OMG	BA	4499	37	23,26,27	2.52	6 (26%)	33,38,41	1.96	10 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
37	OMC	BA	3887	37	19,22,23	3.15	8 (42%)	26,31,34	0.70	0
49	A2M	HA	1031	49	22,25,26	3.40	9 (40%)	31,36,39	2.78	13 (41%)
49	PSU	HA	119	49	18,21,22	1.17	2 (11%)	22,30,33	1.21	3 (13%)
37	A2M	BA	3825	37	22,25,26	3.40	9 (40%)	31,36,39	2.76	14 (45%)
37	PSU	BA	5001	37	18,21,22	1.20	2 (11%)	22,30,33	1.31	3 (13%)
37	PSU	BA	4689	37	18,21,22	1.11	1 (5%)	22,30,33	1.35	3 (13%)
37	OMC	BA	2861	37	19,22,23	3.18	8 (42%)	26,31,34	0.69	0
49	PSU	HA	36	49	18,21,22	1.29	3 (16%)	22,30,33	1.21	3 (13%)
49	PSU	HA	93	49	18,21,22	1.16	1 (5%)	22,30,33	1.50	3 (13%)
37	PSU	BA	3851	37	18,21,22	1.19	1 (5%)	22,30,33	1.34	3 (13%)
49	PSU	HA	105	49,85	18,21,22	1.25	1 (5%)	22,30,33	1.36	3 (13%)
49	OMG	HA	601	49	23,26,27	2.54	7 (30%)	33,38,41	1.94	10 (30%)
41	HIC	CA	245	41	10,11,12	0.50	0	8,14,16	0.51	0
37	PSU	BA	4579	37	18,21,22	1.14	1 (5%)	22,30,33	1.32	3 (13%)
49	OMG	HA	436	49	23,26,27	2.55	7 (30%)	33,38,41	2.00	11 (33%)
37	A2M	BA	4523	37,83	22,25,26	3.39	9 (40%)	31,36,39	2.82	13 (41%)
37	A2M	BA	3830	37	22,25,26	3.36	9 (40%)	31,36,39	2.69	12 (38%)
37	PSU	BA	1744	37	18,21,22	1.20	1 (5%)	22,30,33	1.44	3 (13%)
49	PSU	HA	686	49	18,21,22	1.23	3 (16%)	22,30,33	1.53	3 (13%)
49	OMG	HA	1490	49,83	23,26,27	2.58	7 (30%)	33,38,41	1.78	10 (30%)
37	OMG	BA	3744	37	23,26,27	2.50	7 (30%)	33,38,41	1.87	10 (30%)
49	PSU	HA	1244	49	18,21,22	1.22	1 (5%)	22,30,33	1.45	3 (13%)
37	PSU	BA	4299	37	18,21,22	1.15	1 (5%)	22,30,33	1.40	3 (13%)
37	A2M	BA	3785	37	22,25,26	3.42	9 (40%)	31,36,39	2.66	11 (35%)
49	OMU	HA	1442	49,83	19,22,23	0.83	1 (5%)	26,31,34	1.09	4 (15%)
49	OMC	HA	517	49	19,22,23	3.14	8 (42%)	26,31,34	0.71	0
37	OMC	BA	3701	37,85	19,22,23	3.10	8 (42%)	26,31,34	0.75	0
37	PSU	BA	3715	37	18,21,22	1.15	2 (11%)	22,30,33	1.36	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
49	A2M	HA	484	49	-	1/9/27/28	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	PSU	BA	2839	37	-	0/7/25/26	0/2/2/2
37	OMG	BA	4392	37	-	0/9/27/28	0/3/3/3
37	PSU	BA	4423	37	-	0/7/25/26	0/2/2/2
37	PSU	BA	4532	37	-	0/7/25/26	0/2/2/2
49	OMC	HA	1391	49	-	0/9/27/28	0/2/2/2
49	PSU	HA	1056	49	-	0/7/25/26	0/2/2/2
49	A2M	HA	468	49	-	1/9/27/28	0/3/3/3
37	PSU	BA	4500	37	-	3/7/25/26	0/2/2/2
37	OMC	BA	1881	37,83	-	0/9/27/28	0/2/2/2
37	OMC	BA	3841	37	-	0/9/27/28	0/2/2/2
37	OMC	BA	3808	37	-	0/9/27/28	0/2/2/2
37	PSU	BA	1677	37	-	0/7/25/26	0/2/2/2
49	PSU	HA	681	49	-	0/7/25/26	0/2/2/2
37	OMG	BA	4228	37	-	0/9/27/28	0/3/3/3
49	PSU	HA	1046	49	-	0/7/25/26	0/2/2/2
49	G7M	HA	1639	49	-	0/7/25/26	0/3/3/3
49	4AC	HA	1337	49	-	2/11/29/30	0/2/2/2
37	OMG	BA	4618	37	-	0/9/27/28	0/3/3/3
37	OMU	BA	4620	37	-	0/9/27/28	0/2/2/2
37	OMU	BA	2415	37	-	0/9/27/28	0/2/2/2
37	OMC	BA	2824	37	-	0/9/27/28	0/2/2/2
37	OMC	BA	2351	37,83	-	3/9/27/28	0/2/2/2
49	PSU	HA	1177	49	-	0/7/25/26	0/2/2/2
49	PSU	HA	1232	49	-	0/7/25/26	0/2/2/2
39	OMG	BC	75	39	-	0/9/27/28	0/3/3/3
49	PSU	HA	296	49	-	0/7/25/26	0/2/2/2
49	PSU	HA	1081	49	-	1/7/25/26	0/2/2/2
49	6MZ	HA	1831	49,83,85	-	1/9/27/28	0/3/3/3
49	OMU	HA	1288	49	-	0/9/27/28	0/2/2/2
49	PSU	HA	572	49	-	0/7/25/26	0/2/2/2
37	A2M	BA	2401	37	-	2/9/27/28	0/3/3/3
37	OMU	BA	4306	37	-	0/9/27/28	0/2/2/2
49	PSU	HA	1347	49	-	0/7/25/26	0/2/2/2
37	OMG	BA	4623	37	-	0/9/27/28	0/3/3/3
49	4AC	HA	1841	49	-	2/11/29/30	0/2/2/2
37	OMG	BA	3669	37	-	2/9/27/28	0/3/3/3
37	PSU	BA	2508	37	-	0/7/25/26	0/2/2/2
37	PSU	BA	1683	37,85	-	0/7/25/26	0/2/2/2
49	B8N	HA	1248	49	-	7/16/34/35	0/2/2/2
49	A2M	HA	99	49,83	-	1/9/27/28	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	A2M	BA	2787	37	-	3/9/27/28	0/3/3/3
37	OMG	BA	4494	37	-	2/9/27/28	0/3/3/3
37	OMC	BA	2804	37	-	0/9/27/28	0/2/2/2
37	PSU	BA	4431	37	-	0/7/25/26	0/2/2/2
49	PSU	HA	1625	49	-	0/7/25/26	0/2/2/2
37	PSU	BA	1860	37	-	0/7/25/26	0/2/2/2
37	OMU	BA	4227	37	-	0/9/27/28	0/2/2/2
49	OMU	HA	354	49	-	0/9/27/28	0/2/2/2
37	UY1	BA	3818	37,85	-	1/9/27/28	0/2/2/2
49	A2M	HA	668	49,83	-	3/9/27/28	0/3/3/3
49	OMU	HA	116	49	-	0/9/27/28	0/2/2/2
63	IAS	HP	138	63	-	1/7/7/8	-
37	A2M	BA	2363	37,83	-	0/9/27/28	0/3/3/3
37	OMC	BA	1340	37	-	0/9/27/28	0/2/2/2
37	PSU	BA	1536	37	-	0/7/25/26	0/2/2/2
49	OMC	HA	174	49,83	-	0/9/27/28	0/2/2/2
37	A2M	BA	1534	37,83	-	3/9/27/28	0/3/3/3
37	OMC	BA	4456	37	-	1/9/27/28	0/2/2/2
37	5MC	BA	4447	37,85	-	4/7/25/26	0/2/2/2
37	PSU	BA	4552	37	-	0/7/25/26	0/2/2/2
49	A2M	HA	1678	49	-	1/9/27/28	0/3/3/3
49	OMC	HA	1272	49	-	0/9/27/28	0/2/2/2
37	A2M	BA	4571	37	-	2/9/27/28	0/3/3/3
37	A2M	BA	2815	37,83	-	1/9/27/28	0/3/3/3
37	1MA	BA	1322	37,83	-	1/7/25/26	0/3/3/3
49	OMU	HA	1326	49,83	-	0/9/27/28	0/2/2/2
37	OMG	BA	1522	37	-	0/9/27/28	0/3/3/3
37	OMU	BA	4498	37	-	2/9/27/28	0/2/2/2
37	A2M	BA	398	37	-	1/9/27/28	0/3/3/3
49	PSU	HA	863	49	-	0/7/25/26	0/2/2/2
37	OMG	BA	2876	37	-	1/9/27/28	0/3/3/3
49	A2M	HA	27	49,83	-	1/9/27/28	0/3/3/3
37	OMG	BA	3627	37	-	0/9/27/28	0/3/3/3
37	OMU	BA	2837	37	-	0/9/27/28	0/2/2/2
37	A2M	BA	3867	37	-	3/9/27/28	0/3/3/3
37	PSU	BA	4521	37,83	-	1/7/25/26	0/2/2/2
49	A2M	HA	590	49	-	1/9/27/28	0/3/3/3
49	OMG	HA	683	49	-	0/9/27/28	0/3/3/3
37	6MZ	BA	4220	37	-	0/9/27/28	0/3/3/3
37	PSU	BA	4471	37	-	0/7/25/26	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	OMG	BA	3899	37,83	-	0/9/27/28	0/3/3/3
49	PSU	HA	649	49	-	0/7/25/26	0/2/2/2
49	A2M	HA	512	49	-	2/9/27/28	0/3/3/3
37	OMG	BA	3792	37	-	2/9/27/28	0/3/3/3
49	OMG	HA	644	49	-	1/9/27/28	0/3/3/3
21	V5N	AU	39	21	-	2/9/10/12	0/1/1/1
37	OMG	BA	1625	37	-	0/9/27/28	0/3/3/3
49	OMU	HA	172	49	-	1/9/27/28	0/2/2/2
49	OMC	HA	1703	49	-	0/9/27/28	0/2/2/2
49	A2M	HA	166	49	-	0/9/27/28	0/3/3/3
37	OMG	BA	4370	37	-	1/9/27/28	0/3/3/3
37	OMG	BA	2424	37	-	1/9/27/28	0/3/3/3
37	OMG	BA	4196	37	-	1/9/27/28	0/3/3/3
37	PSU	BA	3637	37,85	-	0/7/25/26	0/2/2/2
37	A2M	BA	400	37	-	1/9/27/28	0/3/3/3
37	PSU	BA	4493	37,85	-	0/7/25/26	0/2/2/2
37	OMC	BA	2365	37	-	0/9/27/28	0/2/2/2
37	OMU	BA	3925	37	-	0/9/27/28	0/2/2/2
49	PSU	HA	1136	49	-	0/7/25/26	0/2/2/2
49	MA6	HA	1850	49	-	6/11/29/30	0/3/3/3
37	OMC	BA	4536	37	-	0/9/27/28	0/2/2/2
37	PSU	BA	3639	37	-	0/7/25/26	0/2/2/2
37	PSU	BA	3822	37	-	0/7/25/26	0/2/2/2
37	A2M	BA	3718	37	-	1/9/27/28	0/3/3/3
49	OMG	HA	1328	49,85	-	0/9/27/28	0/3/3/3
49	PSU	HA	1445	49	-	1/7/25/26	0/2/2/2
37	PSU	BA	2632	37	-	0/7/25/26	0/2/2/2
37	PSU	BA	4312	37	-	0/7/25/26	0/2/2/2
37	UR3	BA	4530	37	-	2/7/25/26	0/2/2/2
49	PSU	HA	822	49	-	0/7/25/26	0/2/2/2
37	OMC	BA	3869	37	-	0/9/27/28	0/2/2/2
37	PSU	BA	1779	37	-	0/7/25/26	0/2/2/2
37	PSU	BA	1781	37	-	1/7/25/26	0/2/2/2
49	PSU	HA	109	49,85	-	0/7/25/26	0/2/2/2
37	OMG	BA	4637	37	-	1/9/27/28	0/3/3/3
37	PSU	BA	4673	37,83	-	0/7/25/26	0/2/2/2
49	PSU	HA	815	49	-	0/7/25/26	0/2/2/2
49	PSU	HA	651	49	-	0/7/25/26	0/2/2/2
49	PSU	HA	814	49	-	1/7/25/26	0/2/2/2
37	PSU	BA	4296	37	-	0/7/25/26	0/2/2/2
37	PSU	BA	3884	37	-	0/7/25/26	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	PSU	BA	4576	37	-	0/7/25/26	0/2/2/2
37	PSU	BA	4972	37	-	0/7/25/26	0/2/2/2
49	MA6	HA	1849	49	-	3/11/29/30	0/3/3/3
39	PSU	BC	69	39	-	0/7/25/26	0/2/2/2
49	A2M	HA	576	49	-	2/9/27/28	0/3/3/3
37	PSU	BA	1782	37	-	0/7/25/26	0/2/2/2
37	PSU	BA	4293	37	-	0/7/25/26	0/2/2/2
37	PSU	BA	4403	37	-	0/7/25/26	0/2/2/2
37	PSU	BA	4628	37	-	0/7/25/26	0/2/2/2
49	PSU	HA	1643	49,83	-	0/7/25/26	0/2/2/2
37	PSU	BA	1792	37	-	0/7/25/26	0/2/2/2
49	PSU	HA	1692	49,85	-	0/7/25/26	0/2/2/2
49	OMC	HA	462	49	-	0/9/27/28	0/2/2/2
37	OMC	BA	2422	37,83	-	2/9/27/28	0/2/2/2
37	PSU	BA	4420	37	-	3/7/25/26	0/2/2/2
37	PSU	BA	4361	37	-	0/7/25/26	0/2/2/2
37	PSU	BA	4442	37	-	0/7/25/26	0/2/2/2
37	A2M	BA	1524	37	-	0/9/27/28	0/3/3/3
40	V5N	BD	216	40	-	1/9/10/12	0/1/1/1
49	PSU	HA	1045	49	-	0/7/25/26	0/2/2/2
49	A2M	HA	1383	49	-	1/9/27/28	0/3/3/3
37	A2M	BA	1326	37	-	1/9/27/28	0/3/3/3
37	PSU	BA	3844	37	-	1/7/25/26	0/2/2/2
57	HY3	HY	62	57	-	1/1/12/14	0/1/1/1
49	OMG	HA	509	49,83	-	0/9/27/28	0/3/3/3
49	OMG	HA	1447	49	-	2/9/27/28	0/3/3/3
33	MLZ	Ag	98	33	-	2/7/8/10	-
37	OMG	BA	1316	37	-	0/9/27/28	0/3/3/3
49	OMU	HA	121	49	-	0/9/27/28	0/2/2/2
37	PSU	BA	224	37	-	2/7/25/26	0/2/2/2
37	PSU	BA	3695	37	-	0/7/25/26	0/2/2/2
39	PSU	BC	55	39	-	0/7/25/26	0/2/2/2
37	PSU	BA	1862	37	-	0/7/25/26	0/2/2/2
37	PSU	BA	3920	37,83	-	0/7/25/26	0/2/2/2
49	PSU	HA	1238	49	-	0/7/25/26	0/2/2/2
37	B8T	BA	1859	37	-	1/7/27/28	0/2/2/2
49	PSU	HA	406	49	-	0/7/25/26	0/2/2/2
37	5MC	BA	3782	37,83	-	0/7/25/26	0/2/2/2
37	PSU	BA	4457	37	-	0/7/25/26	0/2/2/2
37	PSU	BA	4353	37	-	0/7/25/26	0/2/2/2
37	A2M	BA	1871	37,83	-	0/9/27/28	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	OMG	BA	2364	37,83	-	0/9/27/28	0/3/3/3
49	A2M	HA	159	49	-	0/9/27/28	0/3/3/3
49	OMU	HA	428	49	-	4/9/27/28	0/2/2/2
37	A2M	BA	1323	37	-	2/9/27/28	0/3/3/3
49	PSU	HA	1174	49,85	-	0/7/25/26	0/2/2/2
37	OMG	BA	4499	37	-	0/9/27/28	0/3/3/3
37	OMC	BA	3887	37	-	0/9/27/28	0/2/2/2
49	A2M	HA	1031	49	-	1/9/27/28	0/3/3/3
49	PSU	HA	119	49	-	1/7/25/26	0/2/2/2
37	A2M	BA	3825	37	-	1/9/27/28	0/3/3/3
37	PSU	BA	5001	37	-	0/7/25/26	0/2/2/2
37	PSU	BA	4689	37	-	0/7/25/26	0/2/2/2
37	OMC	BA	2861	37	-	0/9/27/28	0/2/2/2
49	PSU	HA	36	49	-	0/7/25/26	0/2/2/2
49	PSU	HA	93	49	-	0/7/25/26	0/2/2/2
37	PSU	BA	3851	37	-	1/7/25/26	0/2/2/2
49	PSU	HA	105	49,85	-	0/7/25/26	0/2/2/2
49	OMG	HA	601	49	-	0/9/27/28	0/3/3/3
41	HIC	CA	245	41	-	0/5/6/8	0/1/1/1
37	PSU	BA	4579	37	-	0/7/25/26	0/2/2/2
49	OMG	HA	436	49	-	0/9/27/28	0/3/3/3
37	A2M	BA	4523	37,83	-	1/9/27/28	0/3/3/3
37	A2M	BA	3830	37	-	1/9/27/28	0/3/3/3
37	PSU	BA	1744	37	-	0/7/25/26	0/2/2/2
49	PSU	HA	686	49	-	0/7/25/26	0/2/2/2
49	OMG	HA	1490	49,83	-	1/9/27/28	0/3/3/3
37	OMG	BA	3744	37	-	0/9/27/28	0/3/3/3
49	PSU	HA	1244	49	-	0/7/25/26	0/2/2/2
37	PSU	BA	4299	37	-	0/7/25/26	0/2/2/2
37	A2M	BA	3785	37	-	2/9/27/28	0/3/3/3
49	OMU	HA	1442	49,83	-	0/9/27/28	0/2/2/2
49	OMC	HA	517	49	-	0/9/27/28	0/2/2/2
37	OMC	BA	3701	37,85	-	4/9/27/28	0/2/2/2
37	PSU	BA	3715	37	-	0/7/25/26	0/2/2/2

The worst 5 of 863 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	HA	1639	G7M	C8-N7	12.55	1.55	1.33
37	BA	3818	UY1	C6-C5	12.11	1.49	1.35
49	HA	1831	6MZ	C6-N6	11.84	1.47	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	BA	4220	6MZ	C6-N6	11.76	1.46	1.34
37	BA	3818	UY1	C2-N1	9.84	1.50	1.36

The worst 5 of 1081 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	HA	1850	MA6	N1-C6-N6	-15.63	99.99	117.08
49	HA	1849	MA6	N1-C6-N6	-12.92	102.96	117.08
49	HA	1850	MA6	C5-C6-N6	8.54	140.17	125.30
49	HA	1849	MA6	C5-C6-N6	7.09	137.66	125.30
49	HA	590	A2M	N6-C6-N1	-6.68	103.71	118.35

There are no chirality outliers.

5 of 125 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
33	Ag	98	MLZ	O-C-CA-CB
40	BD	216	V5N	O-C-CA-CB
57	HY	62	HY3	O-C-CA-C3
37	BA	224	PSU	C2'-C1'-C5-C4
37	BA	398	A2M	C1'-C2'-O2'-CM'

There are no ring outliers.

71 monomers are involved in 117 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
49	HA	484	A2M	2	0
49	HA	1391	OMC	1	0
49	HA	468	A2M	2	0
37	BA	4500	PSU	1	0
37	BA	3808	OMC	1	0
49	HA	681	PSU	2	0
49	HA	1337	4AC	3	0
37	BA	4620	OMU	1	0
37	BA	2415	OMU	1	0
37	BA	2351	OMC	1	0
39	BC	75	OMG	1	0
49	HA	296	PSU	2	0
49	HA	572	PSU	1	0
37	BA	4306	OMU	1	0
49	HA	1841	4AC	5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
49	HA	99	A2M	1	0
49	HA	1625	PSU	3	0
37	BA	1860	PSU	1	0
49	HA	116	OMU	2	0
63	HP	138	IAS	1	0
37	BA	1340	OMC	3	0
37	BA	1534	A2M	1	0
37	BA	4456	OMC	3	0
37	BA	4447	5MC	1	0
37	BA	4552	PSU	1	0
49	HA	1678	A2M	2	0
49	HA	1272	OMC	2	0
37	BA	2815	A2M	2	0
37	BA	4498	OMU	4	0
49	HA	27	A2M	1	0
37	BA	3867	A2M	2	0
49	HA	512	A2M	3	0
37	BA	3792	OMG	1	0
49	HA	644	OMG	1	0
37	BA	1625	OMG	2	0
49	HA	1703	OMC	1	0
37	BA	2424	OMG	2	0
37	BA	4196	OMG	1	0
37	BA	3925	OMU	1	0
37	BA	4536	OMC	4	0
37	BA	3718	A2M	4	0
37	BA	3869	OMC	1	0
37	BA	4637	OMG	1	0
37	BA	4673	PSU	1	0
49	HA	815	PSU	2	0
49	HA	814	PSU	2	0
49	HA	1849	MA6	2	0
49	HA	576	A2M	3	0
49	HA	462	OMC	1	0
37	BA	1524	A2M	1	0
49	HA	1045	PSU	1	0
49	HA	1383	A2M	5	0
37	BA	1326	A2M	1	0
49	HA	509	OMG	3	0
49	HA	1447	OMG	2	0
49	HA	121	OMU	1	0
37	BA	1859	B8T	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
37	BA	1871	A2M	1	0
49	HA	159	A2M	2	0
37	BA	1323	A2M	1	0
37	BA	4499	OMG	2	0
49	HA	1031	A2M	2	0
49	HA	119	PSU	1	0
37	BA	3825	A2M	2	0
49	HA	93	PSU	1	0
49	HA	105	PSU	1	0
37	BA	4579	PSU	2	0
37	BA	3744	OMG	1	0
37	BA	3785	A2M	2	0
49	HA	1442	OMU	1	0
37	BA	3715	PSU	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 393 ligands modelled in this entry, 377 are monoatomic - leaving 16 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	$\# Z > 2$
88	SPM	BA	5109	-	13,13,13	0.60	0	12,12,12	0.93	0
87	SPD	BA	5104	-	9,9,9	0.84	0	8,8,8	1.51	1 (12%)
87	SPD	BA	5107	-	9,9,9	0.62	0	8,8,8	1.43	1 (12%)
89	A1JQ4	BA	5320	85	27,27,27	2.80	9 (33%)	37,46,46	3.25	16 (43%)
87	SPD	BA	5105	-	9,9,9	0.67	0	8,8,8	1.49	1 (12%)
84	PUT	AH	10000	-	5,5,5	0.34	0	4,4,4	0.28	0
88	SPM	BA	5111	-	13,13,13	0.67	0	12,12,12	0.90	0
88	SPM	BA	5113	-	13,13,13	0.54	0	12,12,12	0.92	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	SPD	BA	5108	-	9,9,9	0.38	0	8,8,8	1.34	1 (12%)
88	SPM	BA	5110	-	13,13,13	0.46	0	12,12,12	1.06	0
87	SPD	BA	5103	-	9,9,9	0.42	0	8,8,8	1.22	1 (12%)
88	SPM	BA	5112	-	13,13,13	0.52	0	12,12,12	1.08	0
87	SPD	BA	5106	-	9,9,9	0.57	0	8,8,8	1.61	1 (12%)
84	PUT	BA	5101	-	5,5,5	0.17	0	4,4,4	0.39	0
84	PUT	BB	201	-	5,5,5	0.31	0	4,4,4	0.31	0
84	PUT	BA	5102	-	5,5,5	0.31	0	4,4,4	0.28	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
88	SPM	BA	5109	-	-	1/11/11/11	-
87	SPD	BA	5104	-	-	3/7/7/7	-
87	SPD	BA	5107	-	-	4/7/7/7	-
89	A1JQ4	BA	5320	85	-	6/7/72/72	0/5/4/4
87	SPD	BA	5105	-	-	3/7/7/7	-
84	PUT	AH	10000	-	-	1/3/3/3	-
88	SPM	BA	5111	-	-	7/11/11/11	-
88	SPM	BA	5113	-	-	7/11/11/11	-
87	SPD	BA	5108	-	-	6/7/7/7	-
88	SPM	BA	5110	-	-	3/11/11/11	-
87	SPD	BA	5103	-	-	4/7/7/7	-
88	SPM	BA	5112	-	-	7/11/11/11	-
87	SPD	BA	5106	-	-	6/7/7/7	-
84	PUT	BA	5101	-	-	1/3/3/3	-
84	PUT	BB	201	-	-	1/3/3/3	-
84	PUT	BA	5102	-	-	1/3/3/3	-

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
89	BA	5320	A1JQ4	C09-C10	11.02	1.70	1.55
89	BA	5320	A1JQ4	C07-C02	3.88	1.54	1.51
89	BA	5320	A1JQ4	O16-C04	3.60	1.49	1.45
89	BA	5320	A1JQ4	C23-C05	3.52	1.59	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
89	BA	5320	A1JQ4	O18-C19	3.17	1.42	1.35

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
89	BA	5320	A1JQ4	O15-C13-C09	10.84	132.56	118.00
89	BA	5320	A1JQ4	O15-C13-C12	-7.35	101.64	115.59
89	BA	5320	A1JQ4	C13-C09-C05	5.71	110.31	106.90
89	BA	5320	A1JQ4	C01-C02-C07	5.51	119.76	115.93
89	BA	5320	A1JQ4	C14-C13-C09	5.50	137.53	127.57

There are no chirality outliers.

5 of 61 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
87	BA	5103	SPD	C8-C7-N6-C5
87	BA	5105	SPD	C8-C7-N6-C5
87	BA	5106	SPD	C4-C5-N6-C7
87	BA	5108	SPD	C4-C5-N6-C7
88	BA	5110	SPM	C3-C4-N5-C6

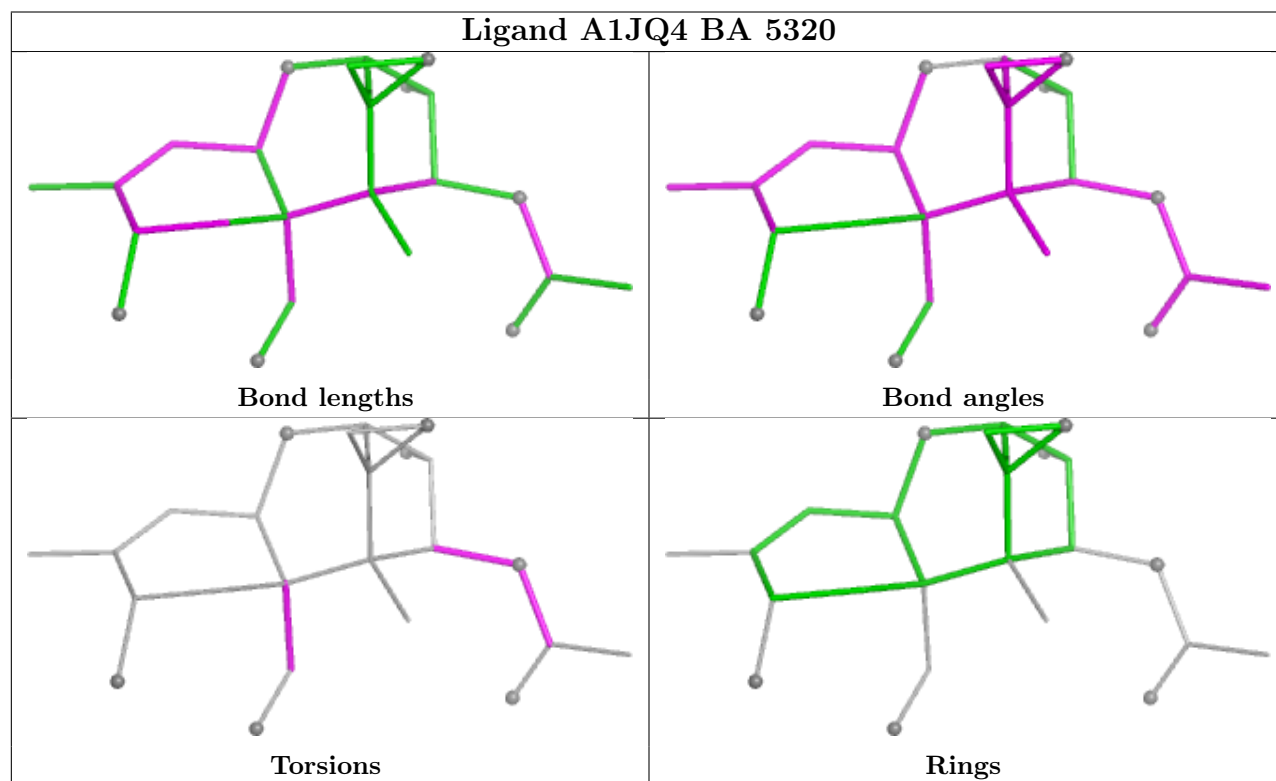
There are no ring outliers.

11 monomers are involved in 39 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
87	BA	5107	SPD	1	0
87	BA	5105	SPD	1	0
88	BA	5111	SPM	4	0
88	BA	5113	SPM	3	0
87	BA	5108	SPD	14	0
87	BA	5103	SPD	2	0
88	BA	5112	SPM	1	0
87	BA	5106	SPD	2	0
84	BA	5101	PUT	6	0
84	BB	201	PUT	4	0
84	BA	5102	PUT	1	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 [i](#)

There are no chain breaks in this entry.

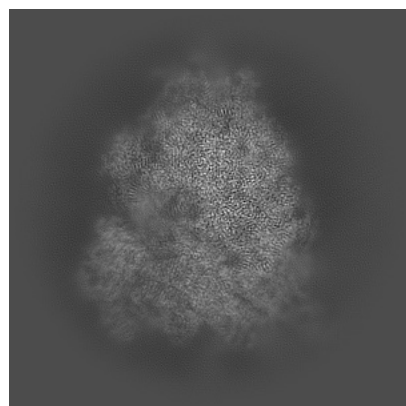
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-57204. These allow visual inspection of the internal detail of the map and identification of artifacts.

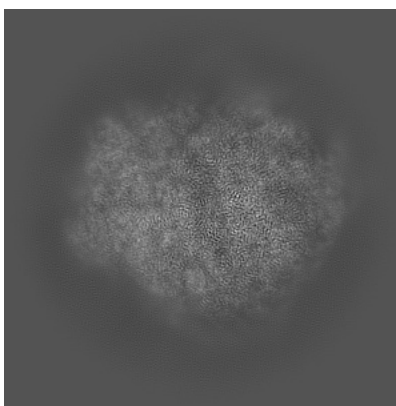
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

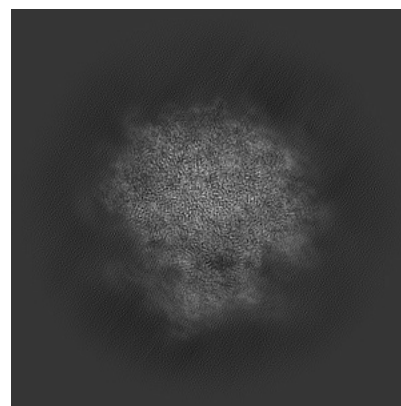
6.1.1 Primary map



X

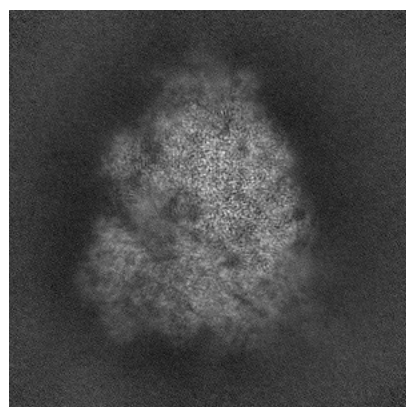


Y

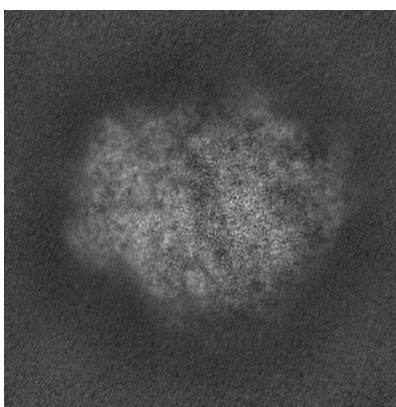


Z

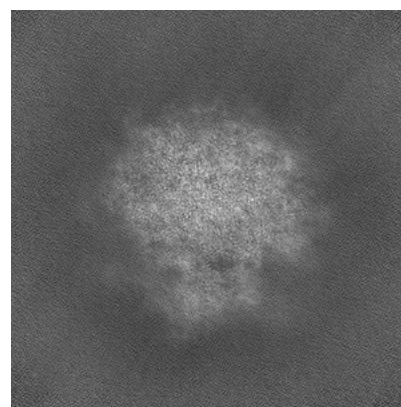
6.1.2 Raw map



X



Y

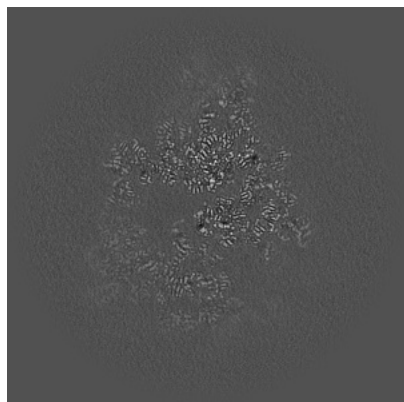


Z

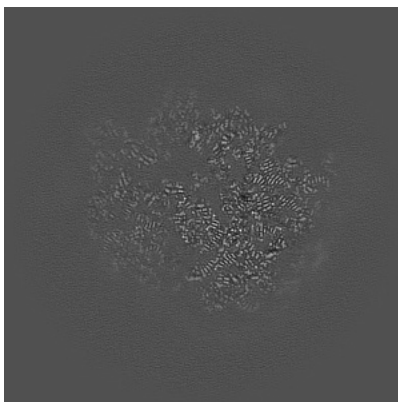
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

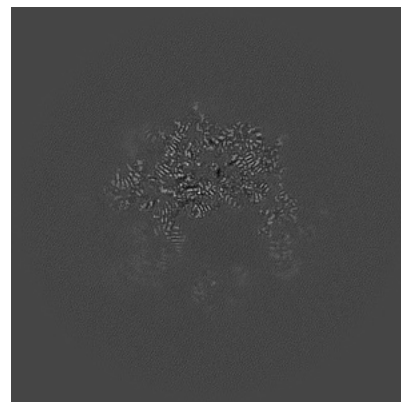
6.2.1 Primary map



X Index: 320

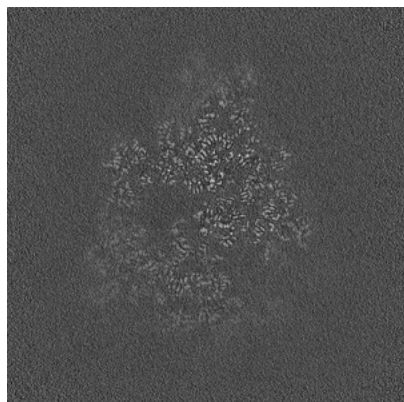


Y Index: 320

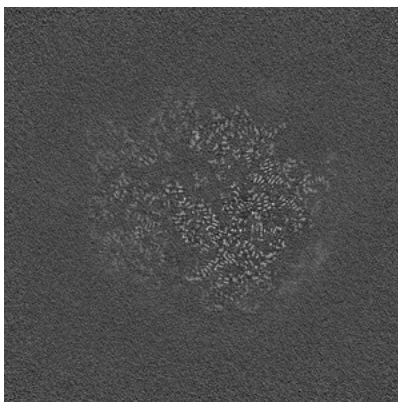


Z Index: 320

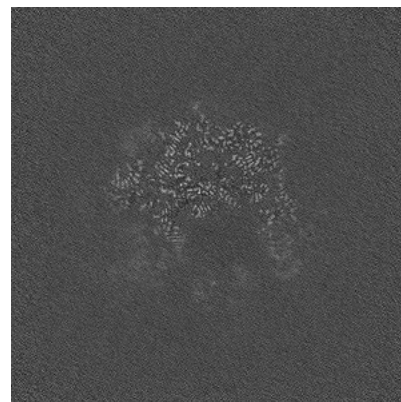
6.2.2 Raw map



X Index: 320



Y Index: 320

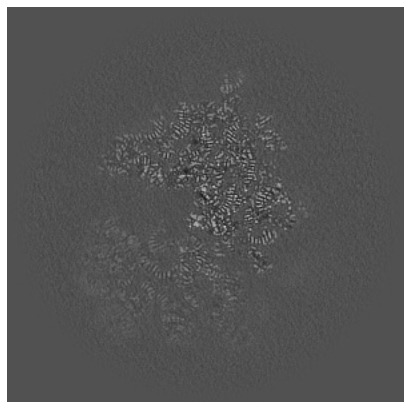


Z Index: 320

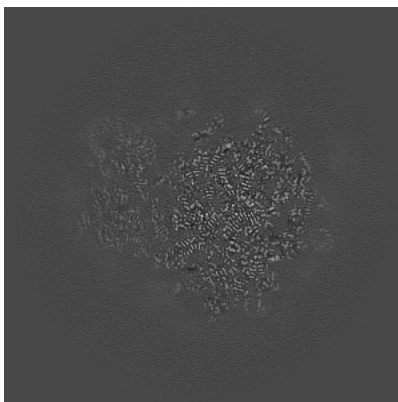
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

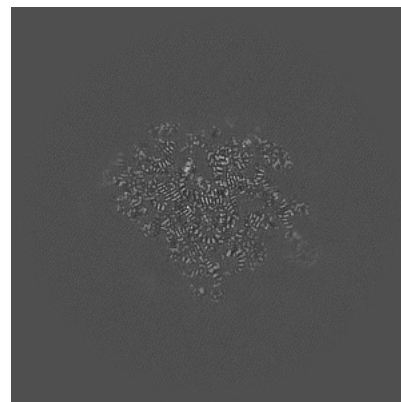
6.3.1 Primary map



X Index: 286

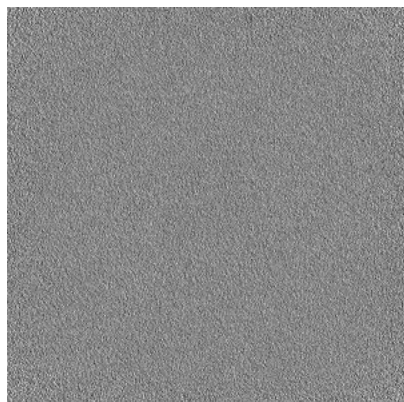


Y Index: 339

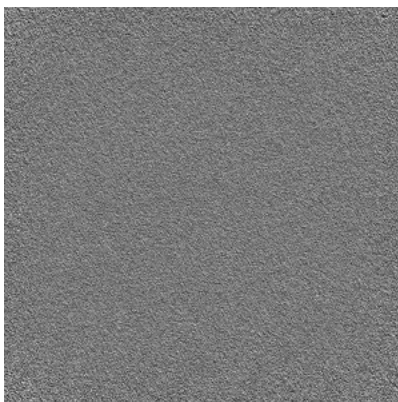


Z Index: 365

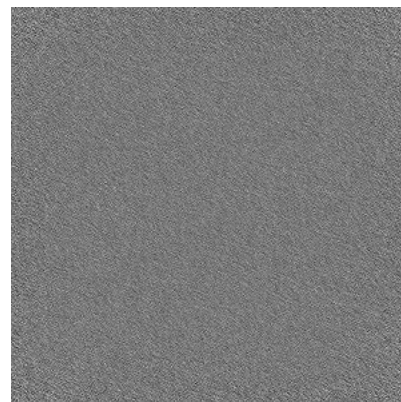
6.3.2 Raw map



X Index: 0



Y Index: 0

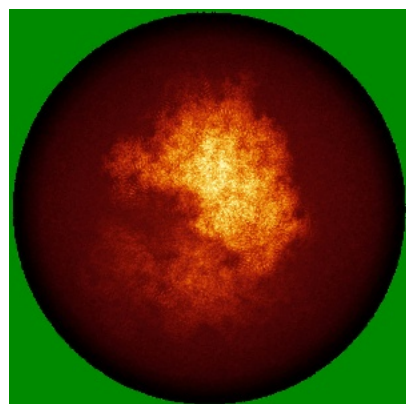


Z Index: 0

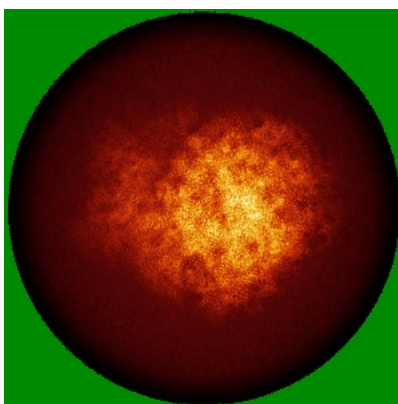
The images above show the largest variance slices of the map in three orthogonal directions.

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

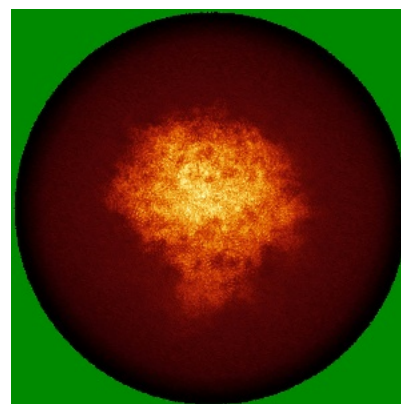
6.4.1 Primary map



X

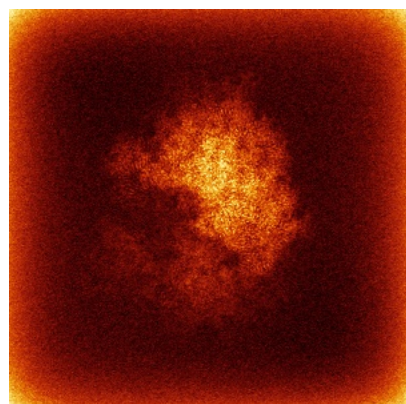


Y

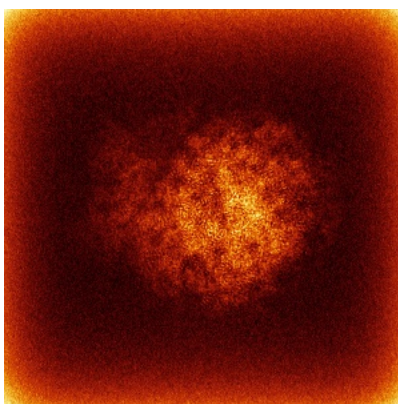


Z

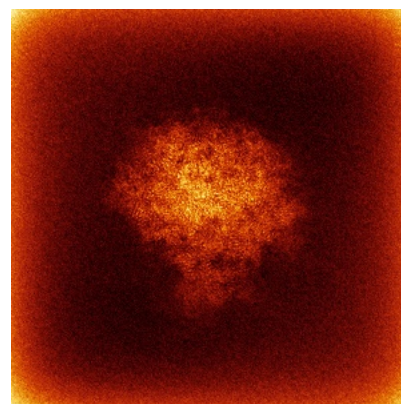
6.4.2 Raw map



X



Y

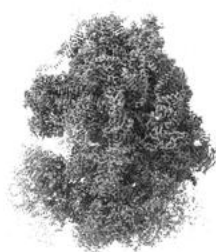


Z

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



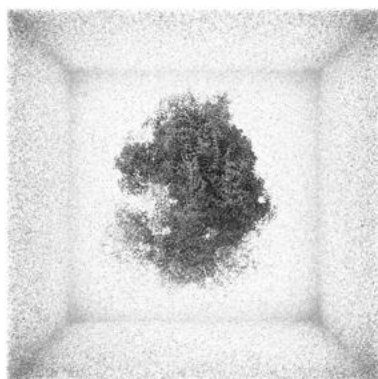
Y



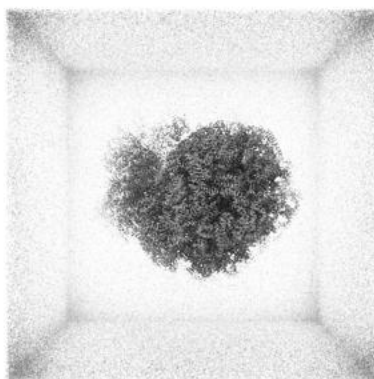
Z

The images above show the 3D surface view of the map at the recommended contour level 0.115. 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.

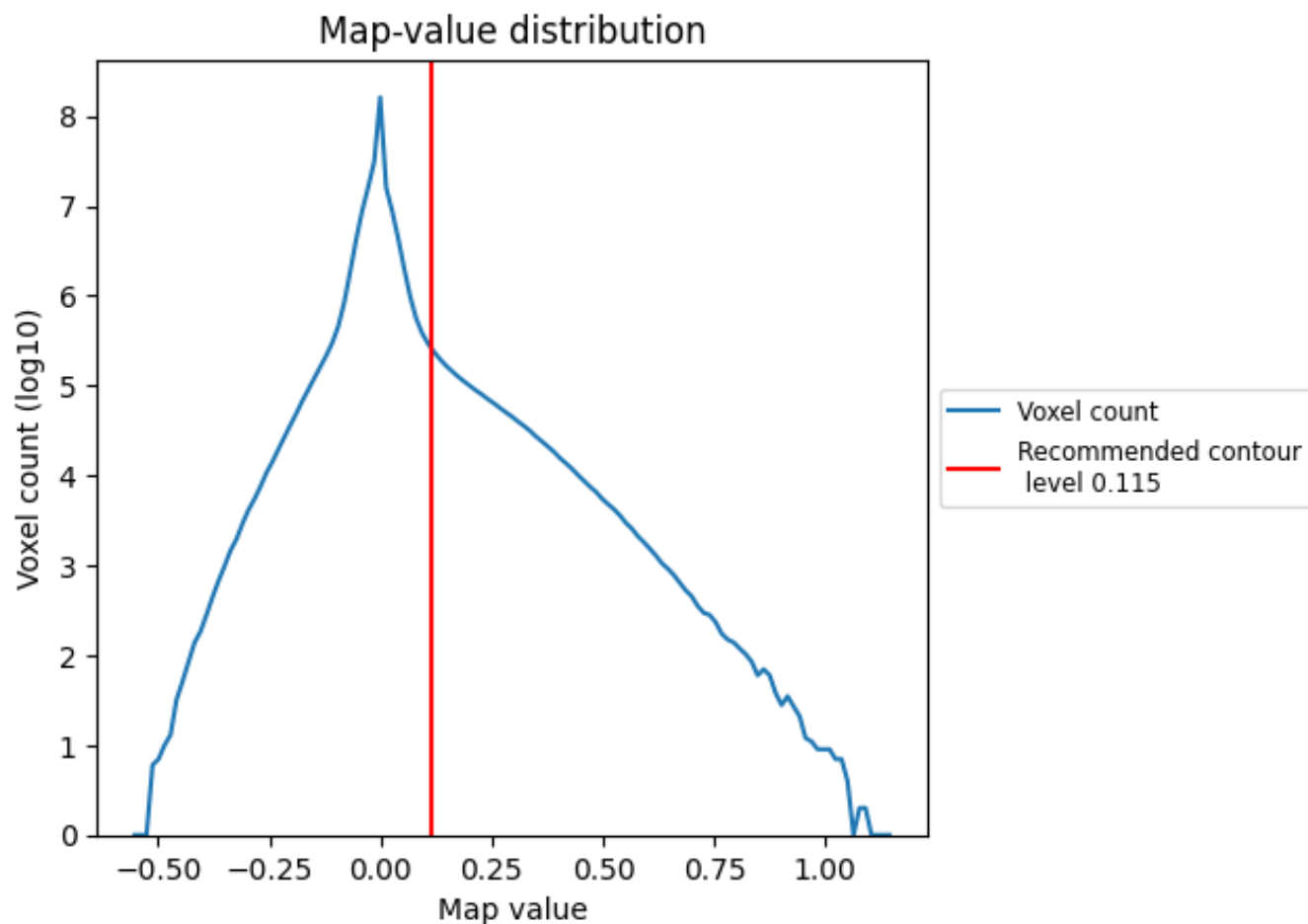
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

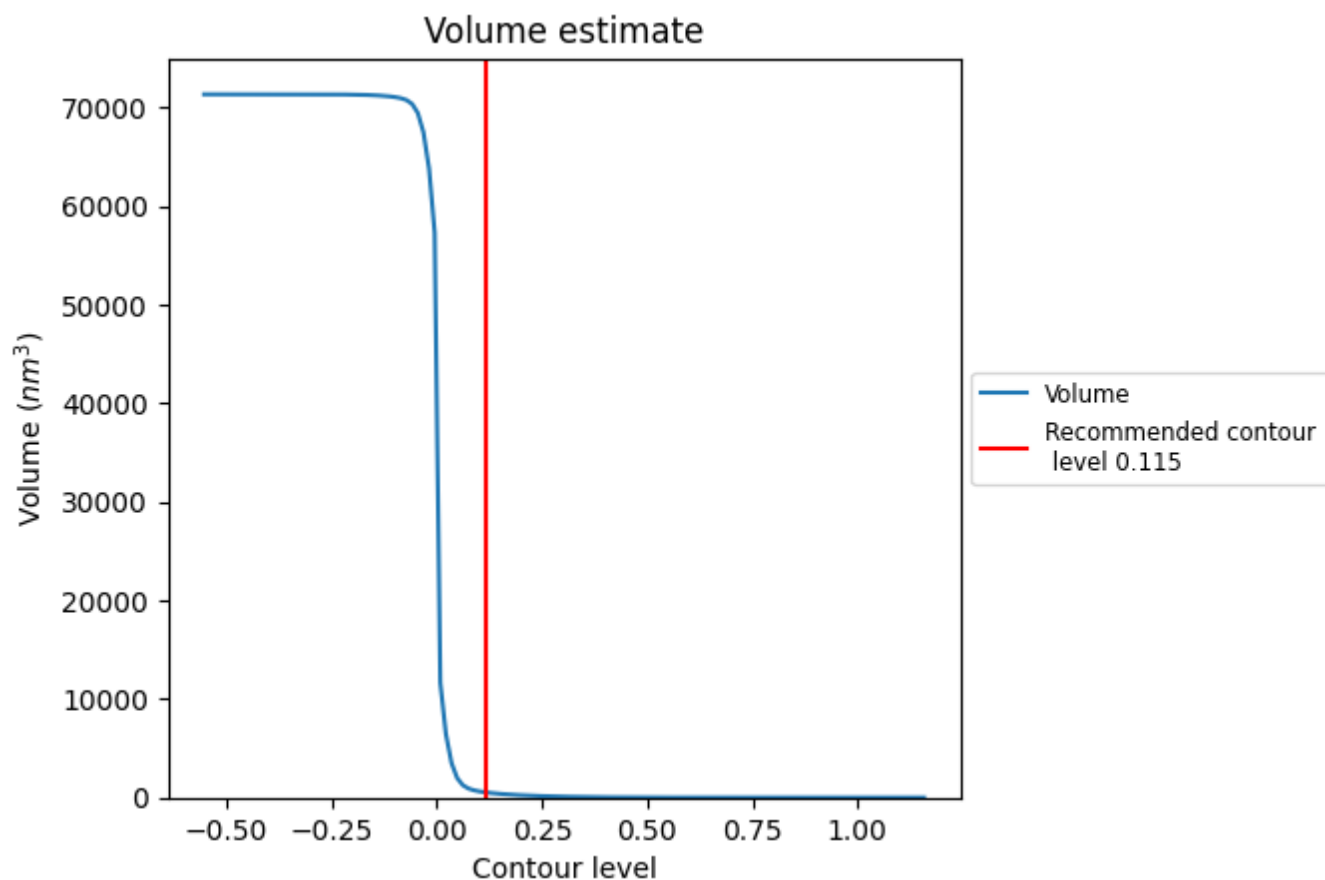
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

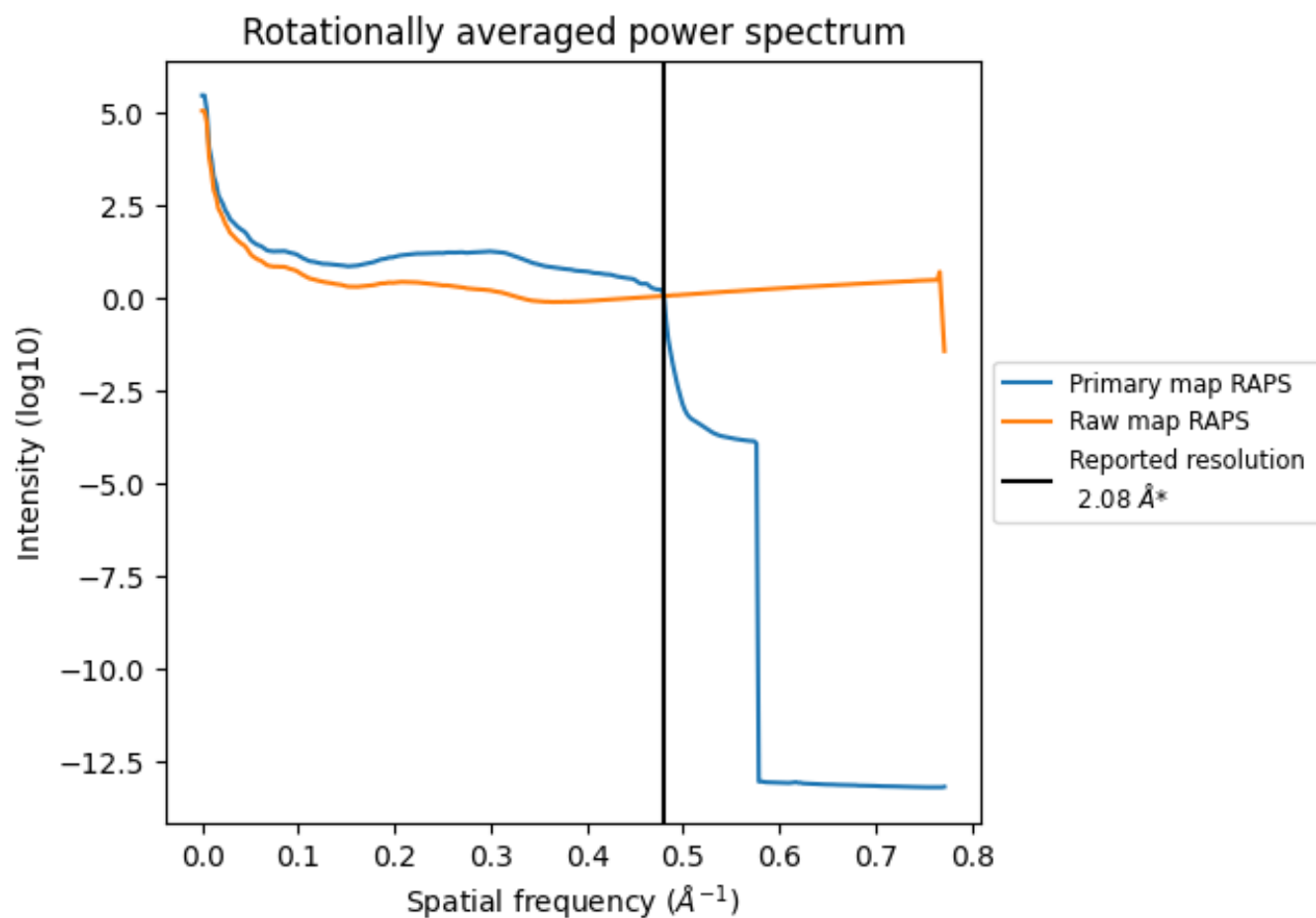
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 534 nm³; this corresponds to an approximate mass of 482 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 ⓘ

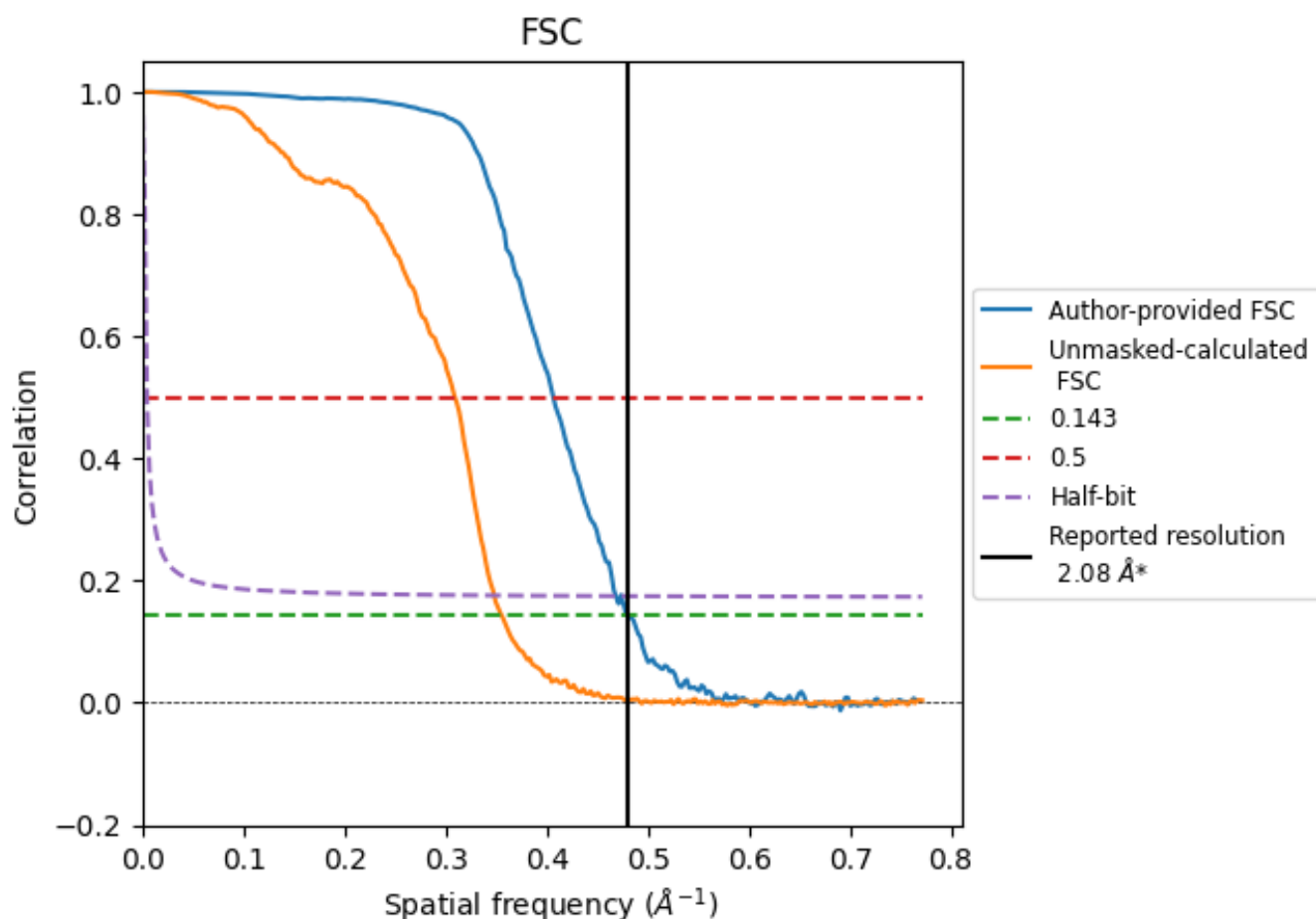


*Reported resolution corresponds to spatial frequency of 0.481 Å⁻¹

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 0.481 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

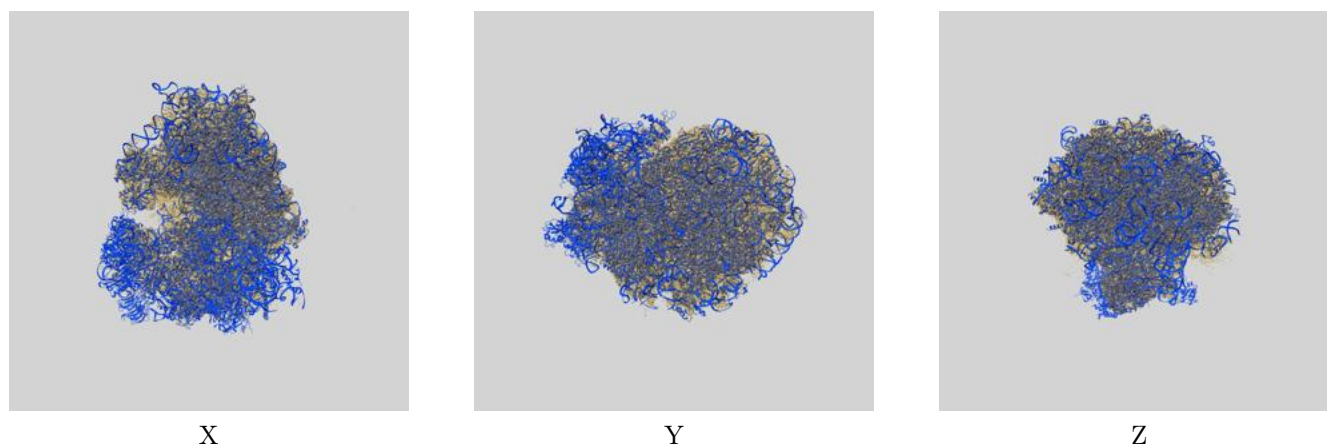
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.08	-	-
Author-provided FSC curve	2.08	2.46	2.13
Unmasked-calculated*	2.81	3.23	2.87

*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 2.81 differs from the reported value 2.08 by more than 10 %

9 Map-model fit [i](#)

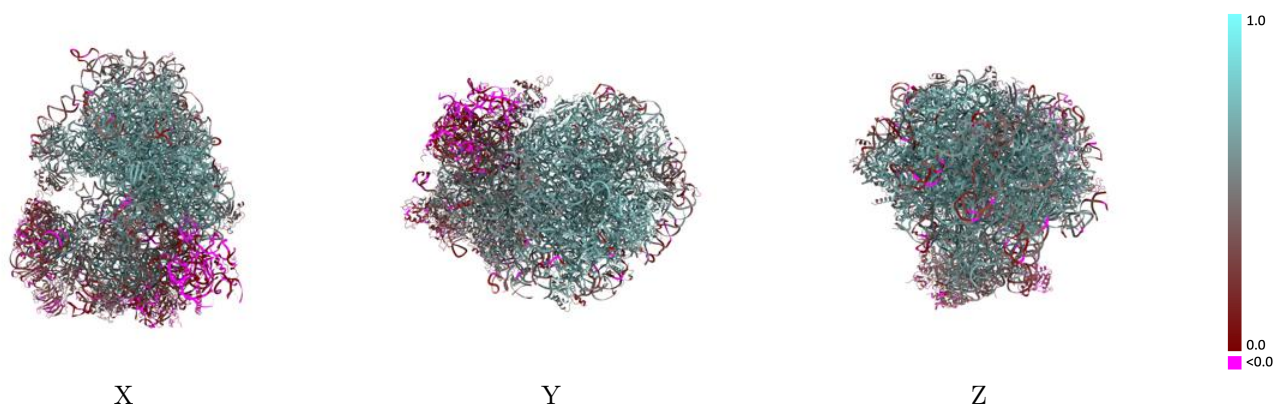
This section contains information regarding the fit between EMDB map EMD-57204 and PDB model 29IZ. Per-residue inclusion information can be found in section [3](#) on page [26](#).

9.1 Map-model overlay [i](#)



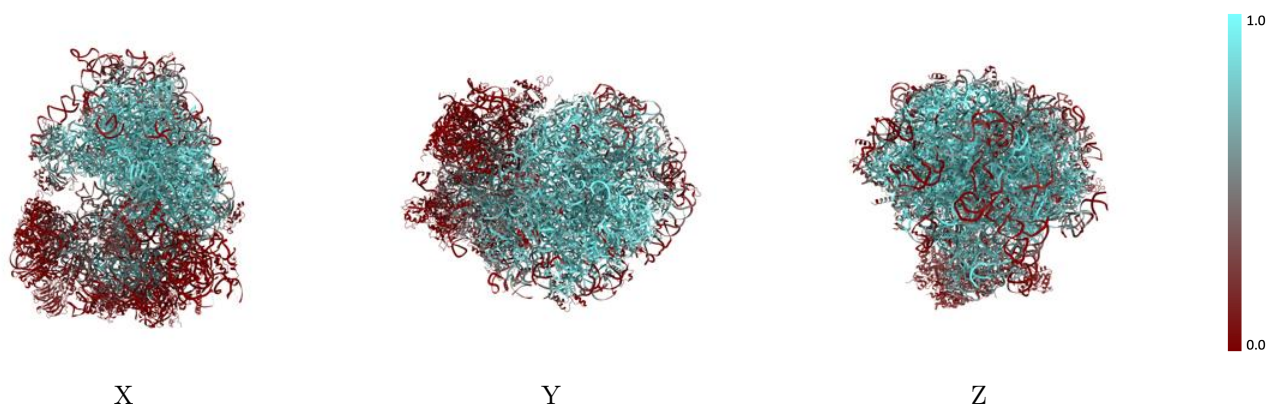
The images above show the 3D surface view of the map at the recommended contour level 0.115 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



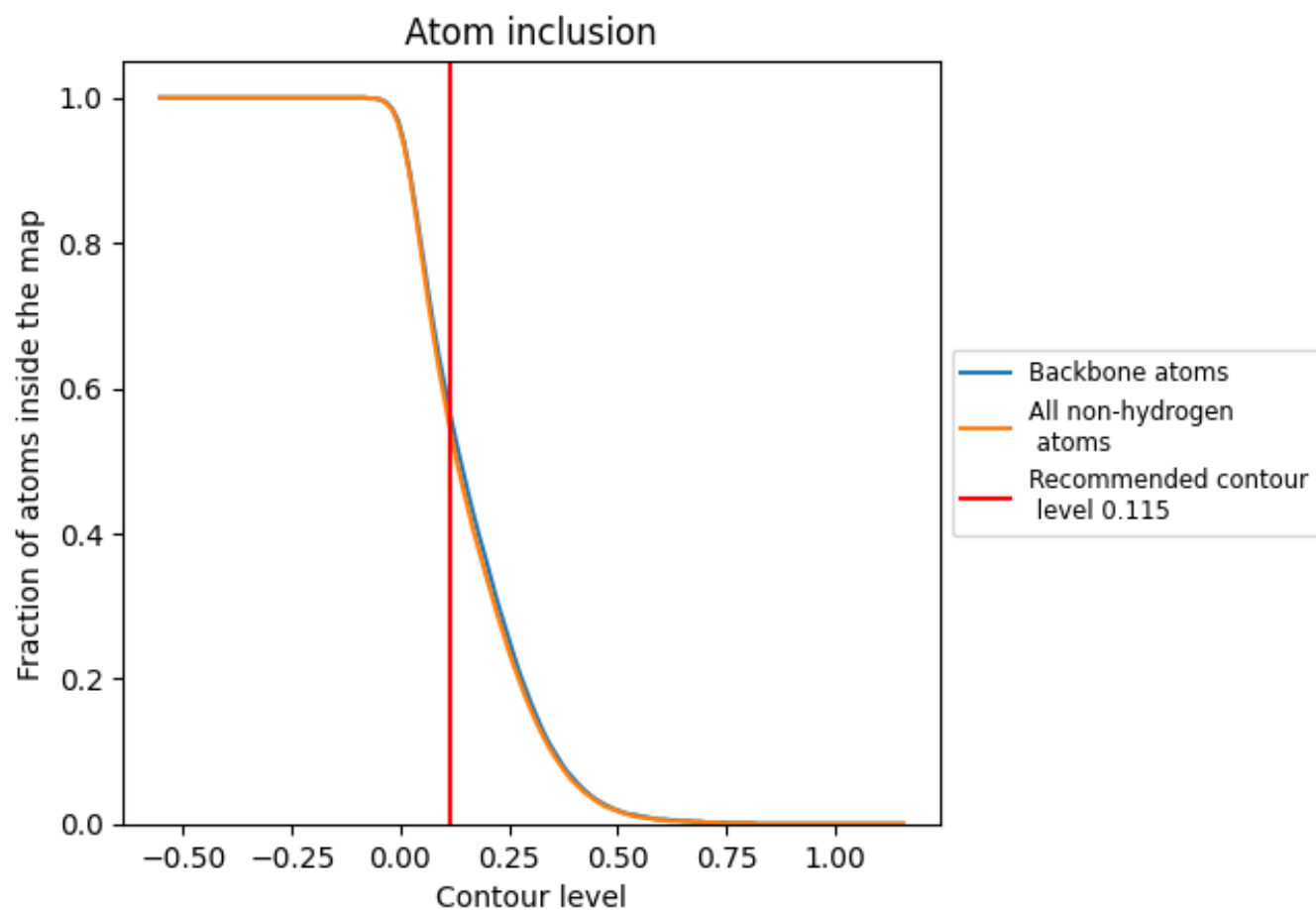
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.115).

9.4 Atom inclusion [i](#)



At the recommended contour level, 56% of all backbone atoms, 54% 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 (0.115) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5420	 0.5080
A	 0.1440	 0.3940
AA	 0.8690	 0.6750
AB	 0.5170	 0.5070
AC	 0.7450	 0.6320
AD	 0.7590	 0.6270
AE	 0.3420	 0.4010
AF	 0.7440	 0.6310
AG	 0.7540	 0.6090
AH	 0.9320	 0.7080
AI	 0.8590	 0.6780
AJ	 0.8800	 0.6970
AK	 0.8910	 0.6940
AL	 0.7380	 0.5770
AM	 0.8660	 0.6730
AN	 0.7310	 0.6150
AO	 0.3110	 0.4230
AP	 0.8510	 0.6840
AQ	 0.8040	 0.6430
AR	 0.7530	 0.6280
AS	 0.7760	 0.6390
AT	 0.5650	 0.5240
AU	 0.8700	 0.6820
AV	 0.5840	 0.5630
AW	 0.5770	 0.5020
AX	 0.7130	 0.5800
AY	 0.8650	 0.6850
AZ	 0.9160	 0.7020
Aa	 0.8000	 0.6220
Ab	 0.7150	 0.6230
Ac	 0.6070	 0.5530
Ad	 0.9180	 0.7100
Ae	 0.3380	 0.4330
Af	 0.8160	 0.6600
Ag	 0.7820	 0.6410



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
Ah	 0.8020	 0.6580
Ai	 0.7990	 0.6390
Aj	 0.8200	 0.6400
B	 0.0830	 0.3030
BA	 0.7710	 0.6100
BB	 0.8360	 0.6160
BC	 0.8040	 0.6000
BD	 0.9030	 0.6950
CA	 0.8360	 0.6670
CB	 0.8640	 0.6760
CC	 0.5830	 0.5140
CD	 0.6020	 0.5730
DA	 0.2480	 0.4000
ER	 0.3130	 0.4790
GF	 0.3140	 0.5200
HA	 0.3460	 0.3800
HC	 0.0780	 0.2000
HD	 0.3220	 0.4840
HE	 0.0800	 0.2900
HF	 0.0430	 0.2140
HG	 0.0160	 0.2720
HH	 0.0040	 -0.0080
HI	 0.0320	 0.2240
HJ	 0.0520	 0.1380
HK	 0.1680	 0.3660
HL	 0.0360	 0.2650
HM	 0.2070	 0.3390
HN	 0.0000	 0.0420
HO	 0.2040	 0.4410
HP	 0.1190	 0.2260
HQ	 0.0410	 0.2560
HR	 0.0620	 0.3610
HS	 0.0430	 0.2680
HT	 0.0330	 0.2520
HU	 0.0230	 0.2650
HV	 0.0920	 0.2790
HX	 0.4330	 0.5950
HY	 0.4390	 0.5140
HZ	 0.0030	 0.0560
Ha	 0.0020	 0.1550
Hb	 0.3260	 0.4130
Hc	 0.0810	 0.3370

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
Hd	 0.0200	 0.2030
He	 0.2030	 0.4620
Hf	 0.1300	 0.3380
Hg	 0.0000	 0.0870
Hh	 0.0010	 0.1560
Hi	 0.4490	 0.3600