



wwPDB EM Validation Summary Report ⓘ

Jun 21, 2026 – 12:52 pm BST

PDB ID : 9RPV / pdb_00009rpv
EMDB ID : EMD-54172
Title : Structure of the ZAK-bound human disome
Authors : Niu, S.; Beckmann, R.
Deposited on : 2025-06-25
Resolution : 2.35 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

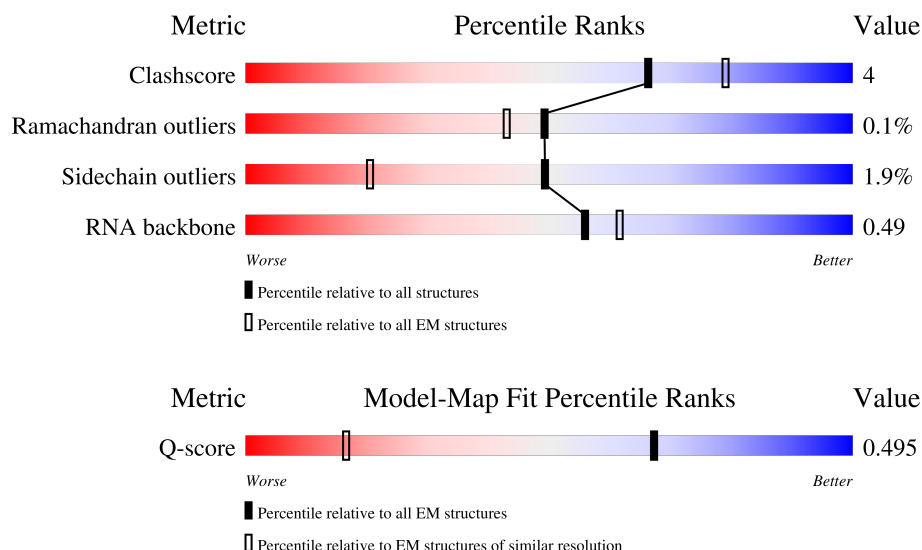
EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

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

The reported resolution of this entry is 2.35 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.



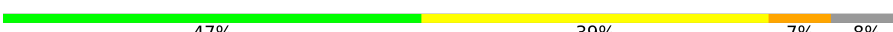
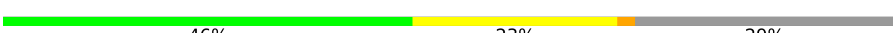
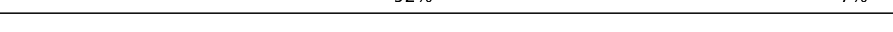
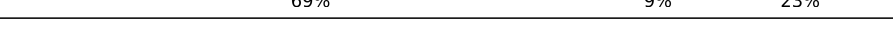
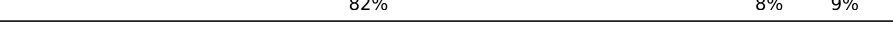
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	4607 (1.85 - 2.85)

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	A4	14	
2	A5	8	
3	B4	150	

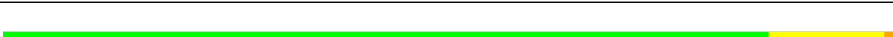
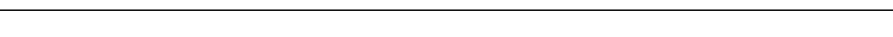
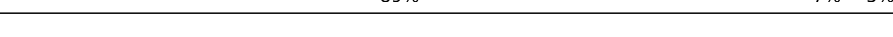
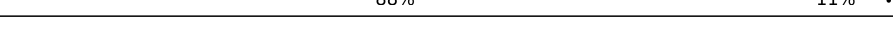
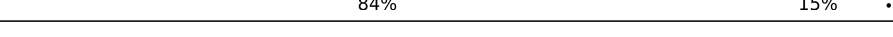
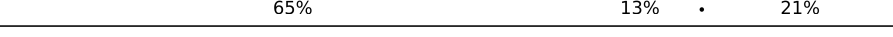
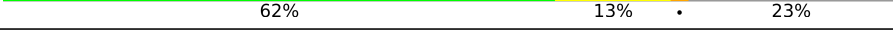
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Mol	Chain	Length	Quality of chain
4	B5	77	 78%19%.
5	D4	152	 22%22%.52%
6	E4	148	 65%14%21%
7	E5	75	 47%39%7%8%
8	L5	5070	 46%23%.29%
9	L7	120	 86%13%.
9	M7	120	 90%8%.
10	L8	156	 60%38%.
11	LA	257	 82%13%..
12	LB	403	 84%14%.
13	LC	427	 78%8%15%
13	MC	427	 81%5%14%
14	LD	297	 88%10%..
14	MD	297	 92%7%.
15	LE	288	 66%10%24%
15	ME	288	 69%9%23%
16	LF	248	 82%8%9%
16	MF	248	 85%5%9%
17	LG	266	 79%7%14%
17	MG	266	 85%6%9%
18	LH	192	 86%12%.
18	MH	192	 92%7%.
19	LI	214	 85%10%5%
20	LJ	178	 86%7%.6%
20	MJ	178	 84%12%.

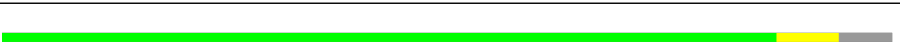
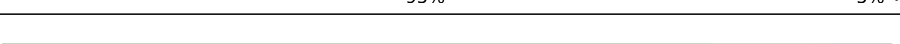
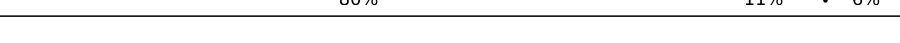
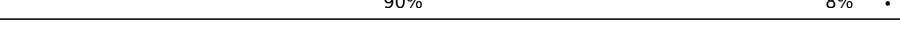
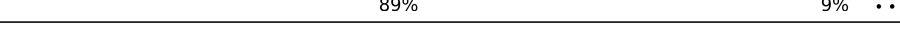
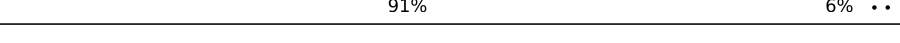
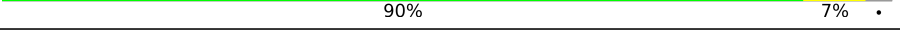
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Mol	Chain	Length	Quality of chain
21	LL	211	 91% 6% .
21	ML	211	 91% 6% .
22	LM	215	 55% 8% 37%
22	MM	215	 60% . 37%
23	LN	204	 80% 19%
23	MN	204	 90% 9%
24	LO	203	 88% 10% ..
24	MO	203	 91% 8%
25	LP	184	 74% 9% 17%
25	MP	184	 75% 8% 17%
26	LQ	188	 86% 13% ..
26	MQ	188	 95% 5% .
27	LR	196	 80% 8% . 11%
27	MR	196	 89% 7% 5%
28	LS	176	 88% 11% .
28	MS	176	 90% 9% .
29	LT	160	 84% 15% .
29	MT	160	 89% 9% ..
30	LU	128	 65% 13% . 21%
30	MU	128	 62% 13% . 23%
31	LV	140	 74% 19% 6%
31	MV	140	 83% 12% 5%
32	LW	157	 68% 5% 27%
32	MW	157	 66% 8% . 25%
33	LX	156	 65% 12% 23%

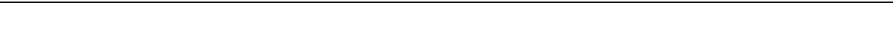
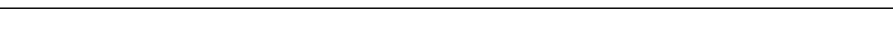
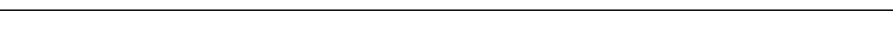
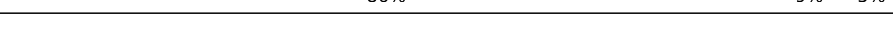
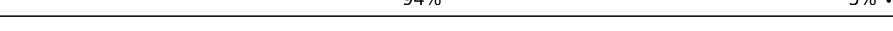
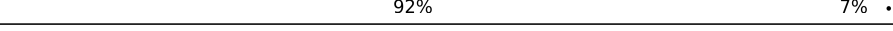
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Mol	Chain	Length	Quality of chain
33	MX	156	
34	LY	145	
34	MY	145	
35	LZ	136	
35	MZ	136	
36	La	148	
37	Lb	159	
38	Lc	115	
38	Mc	115	
39	Ld	125	
39	Md	125	
40	Le	135	
40	Me	135	
41	Lf	110	
41	Mf	110	
42	Lg	117	
42	Mg	117	
43	Lh	123	
43	Mh	123	
44	Li	105	
44	Mi	105	
45	Lj	97	
45	Mj	97	
46	Lk	70	
46	Mk	70	

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Mol	Chain	Length	Quality of chain
47	Ll	51	 92% 6% .
47	Ml	51	 92% 6% .
48	Lm	128	 35% . 61%
49	Ln	25	 92% . .
49	Mn	25	 80% 20%
50	Lo	106	 84% 8% 8%
51	Lp	92	 92% 7% .
51	Mp	92	 95% . .
52	Lr	137	 74% 18% 9%
53	M5	5069	 48% 19% . 30%
54	M8	156	 71% 27% .
55	MA	257	 88% 9% .
56	MB	403	 92% 8%
57	MI	214	 86% 9% 5%
58	Ma	148	 94% 5% .
59	Mb	159	 60% 9% 30%
60	Mm	128	 38% . 59%
61	Mo	106	 92% 7% .
62	Mr	137	 82% 9% 8%
63	Ms	217	 86% 14%
64	N1	800	 16% . 82%
64	N2	800	 14% . 86%
65	RA	295	 62% 14% 24%
66	RB	264	 78% 10% 11%
66	SB	264	 70% 10% . 19%

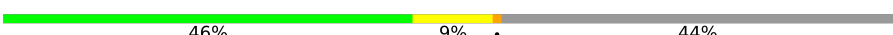
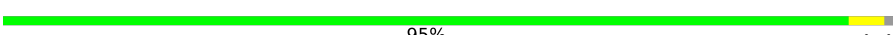
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Mol	Chain	Length	Quality of chain
67	RC	293	
67	SC	293	
68	RD	243	
68	SD	243	
69	RE	263	
69	SE	263	
70	RF	204	
70	SF	204	
71	RG	249	
71	SG	249	
72	RH	194	
72	SH	194	
73	RI	208	
73	SI	208	
74	RJ	194	
74	SJ	194	
75	RK	165	
75	SK	165	
76	RL	158	
76	SL	158	
77	RM	132	
77	Sf	132	
78	RN	151	
78	SN	151	
79	RO	151	

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Mol	Chain	Length	Quality of chain
79	SO	151	
80	RP	145	
80	SP	145	
81	RQ	146	
81	SQ	146	
82	RR	135	
82	SR	135	
83	RS	152	
83	SS	152	
84	RT	145	
84	ST	145	
85	RU	119	
85	SU	119	
86	RV	84	
87	RW	130	
87	SW	130	
88	RX	143	
88	SX	143	
89	RY	133	
89	SY	133	
90	RZ	125	
90	SZ	125	
91	Ra	115	
91	Sa	115	
92	Rb	84	

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Mol	Chain	Length	Quality of chain
92	Sb	84	 86% 13% .
93	Rc	69	 77% 17% 6%
93	Sc	69	 87% . 12%
94	Rd	56	 84% 14% .
94	Sd	56	 75% 18% 7%
95	Re	133	 34% . 62%
95	Se	133	 26% 7% 67%
96	Rf	156	 33% 6% . 60%
96	sh	156	 36% . 60%
97	Rg	317	 87% 12% .
97	Sg	317	 91% 9%
98	S2	1869	 54% 34% 5% 6%
99	S3	1869	 56% 30% . 11%
100	SA	295	 61% 11% 28%
101	SV	83	 93% 7%

2 Entry composition

There are 104 unique types of molecules in this entry. The entry contains 428966 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called mRNA of the collided 80S.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A4	14	Total	C	N	O	P	0	0
			287	129	38	106	14		

- Molecule 2 is a RNA chain called mRNA of the stalled 80S.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A5	7	Total	C	N	O	P	0	0
			150	67	27	49	7		

- Molecule 3 is a RNA chain called P/E tRNA on the collided 80S.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B4	75	Total	C	N	O	P	0	0
			1604	717	298	515	74		

- Molecule 4 is a RNA chain called P-site tRNA of the stalled 80S.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	B5	77	Total	C	N	O	P	S	0	0
			1645	734	298	535	77	1		

- Molecule 5 is a RNA chain called A/P tRNA on the collided 80S.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	D4	73	Total	C	N	O	P	0	0
			1559	696	283	508	72		

- Molecule 6 is a protein called Endothelial differentiation-related factor 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	E4	117	Total	C	N	O	0	0
			921	566	180	175		

- Molecule 7 is a RNA chain called E-site tRNA of the stalled 80S.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	E5	69	Total	C	N	O	P	0	0
			1467	655	262	481	69		

- Molecule 8 is a RNA chain called 28S rRNA of the collided 80S.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	L5	3583	Total	C	N	O	P	0	0
			76803	34202	14050	24969	3582		

- Molecule 9 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	L7	120	Total	C	N	O	P	0	0
			2558	1141	456	842	119		
9	M7	120	Total	C	N	O	P	0	0
			2558	1141	456	842	119		

- Molecule 10 is a RNA chain called 5.8S rRNA of the collided 80S.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L8	156	Total	C	N	O	P	0	0
			3314	1480	585	1094	155		

- Molecule 11 is a protein called 60S ribosomal protein L8.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	LA	248	Total	C	N	O	S	0	0
			1886	1183	386	311	6		

- Molecule 12 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	LB	393	Total	C	N	O	S	0	0
			3101	1979	583	525	14		

- Molecule 13 is a protein called 60S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	LC	365	Total	C	N	O	S	0	0
			2894	1819	578	482	15		

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Mol	Chain	Residues	Atoms					AltConf	Trace
13	MC	366	Total	C	N	O	S	0	0
			2914	1832	581	487	14		

- Molecule 14 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	LD	293	Total	C	N	O	S	0	0
			2287	1455	426	392	14		
14	MD	294	Total	C	N	O	S	0	0
			2391	1513	436	428	14		

- Molecule 15 is a protein called Large ribosomal subunit protein eL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	LE	220	Total	C	N	O	S	0	0
			1713	1104	326	279	4		
15	ME	223	Total	C	N	O	S	0	0
			1786	1150	339	293	4		

- Molecule 16 is a protein called Large ribosomal subunit protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	LF	225	Total	C	N	O	S	0	0
			1844	1189	355	291	9		
16	MF	225	Total	C	N	O	S	2	0
			1885	1212	364	300	9		

- Molecule 17 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	LG	229	Total	C	N	O	S	0	0
			1733	1106	335	288	4		
17	MG	241	Total	C	N	O	S	0	0
			1926	1228	371	323	4		

- Molecule 18 is a protein called 60S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	LH	189	Total	C	N	O	S	0	0
			1439	910	273	250	6		
18	MH	190	Total	C	N	O	S	0	0
			1518	956	284	272	6		

- Molecule 19 is a protein called Ribosomal protein uL16-like.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	LI	203	Total	C	N	O	S	0	0
			1582	1007	306	255	14		

- Molecule 20 is a protein called 60S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	LJ	167	Total	C	N	O	S	0	0
			1226	780	228	212	6		
20	MJ	170	Total	C	N	O	S	0	0
			1362	861	254	241	6		

- Molecule 21 is a protein called Large ribosomal subunit protein eL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	LL	204	Total	C	N	O	S	0	0
			1580	992	335	249	4		
21	ML	206	Total	C	N	O	S	1	0
			1672	1046	348	274	4		

- Molecule 22 is a protein called 60S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	LM	136	Total	C	N	O	S	0	0
			1097	705	211	174	7		
22	MM	136	Total	C	N	O	S	0	0
			1120	719	215	179	7		

- Molecule 23 is a protein called 60S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	LN	203	Total	C	N	O	S	0	0
			1693	1068	359	262	4		
23	MN	203	Total	C	N	O	S	0	0
			1700	1072	359	265	4		

- Molecule 24 is a protein called 60S ribosomal protein L13a.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	LO	201	Total	C	N	O	S	0	0
			1613	1042	318	248	5		

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Mol	Chain	Residues	Atoms					AltConf	Trace
24	MO	202	Total	C	N	O	S	0	0
			1654	1066	322	261	5		

- Molecule 25 is a protein called 60S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	LP	153	Total	C	N	O	S	0	0
			1203	754	238	202	9		
25	MP	153	Total	C	N	O	S	1	0
			1249	781	243	216	9		

- Molecule 26 is a protein called 60S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	LQ	187	Total	C	N	O	S	0	0
			1493	931	311	246	5		
26	MQ	187	Total	C	N	O	S	0	0
			1512	944	314	249	5		

- Molecule 27 is a protein called 60S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	LR	175	Total	C	N	O	S	0	0
			1412	874	312	218	8		
27	MR	187	Total	C	N	O	S	0	0
			1566	971	336	250	9		

- Molecule 28 is a protein called 60S ribosomal protein L18a.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	LS	175	Total	C	N	O	S	0	0
			1436	915	281	230	10		
28	MS	176	Total	C	N	O	S	0	0
			1460	930	284	235	11		

- Molecule 29 is a protein called 60S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	LT	159	Total	C	N	O	S	0	0
			1268	805	249	209	5		
29	MT	159	Total	C	N	O	S	2	0
			1311	833	256	216	6		

- Molecule 30 is a protein called 60S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	LU	101	Total	C	N	O	S	0	0
			768	497	136	133	2		
30	MU	99	Total	C	N	O	S	0	0
			808	518	141	147	2		

- Molecule 31 is a protein called 60S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	LV	131	Total	C	N	O	S	0	0
			954	604	180	165	5		
31	MV	133	Total	C	N	O	S	0	0
			988	623	186	174	5		

- Molecule 32 is a protein called 60S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	LW	115	Total	C	N	O	S	0	0
			784	493	154	135	2		
32	MW	118	Total	C	N	O	S	0	0
			950	595	192	159	4		

- Molecule 33 is a protein called 60S ribosomal protein L23a.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	LX	120	Total	C	N	O	S	0	0
			951	611	182	157	1		
33	MX	118	Total	C	N	O	S	0	0
			966	618	181	166	1		

- Molecule 34 is a protein called 60S ribosomal protein L26.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	LY	134	Total	C	N	O	S	0	0
			1084	681	220	180	3		
34	MY	134	Total	C	N	O	S	0	0
			1115	700	226	186	3		

- Molecule 35 is a protein called 60S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	LZ	135	Total	C	N	O	S	0	0
			1082	703	207	169	3		
35	MZ	135	Total	C	N	O	S	1	0
			1115	719	211	182	3		

- Molecule 36 is a protein called 60S ribosomal protein L27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	La	146	Total	C	N	O	S	0	0
			1145	726	233	183	3		

- Molecule 37 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	Lb	63	Total	C	N	O	S	0	0
			499	310	107	80	2		

- Molecule 38 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	Lc	93	Total	C	N	O	S	0	0
			716	456	125	129	6		
38	Mc	99	Total	C	N	O	S	0	0
			770	488	136	140	6		

- Molecule 39 is a protein called 60S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	Ld	107	Total	C	N	O	S	0	0
			856	546	168	140	2		
39	Md	107	Total	C	N	O	S	0	0
			888	560	171	155	2		

- Molecule 40 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	Le	127	Total	C	N	O	S	0	0
			1045	661	215	164	5		
40	Me	128	Total	C	N	O	S	1	0
			1061	672	219	165	5		

- Molecule 41 is a protein called 60S ribosomal protein L35a.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	Lf	109	Total	C	N	O	S	0	0
			865	547	173	142	3		
41	Mf	110	Total	C	N	O	S	0	0
			883	560	175	144	4		

- Molecule 42 is a protein called 60S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	Lg	110	Total	C	N	O	S	0	0
			851	531	175	139	6		
42	Mg	114	Total	C	N	O	S	0	0
			906	566	187	147	6		

- Molecule 43 is a protein called 60S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	Lh	121	Total	C	N	O	S	0	0
			975	617	200	157	1		
43	Mh	122	Total	C	N	O	S	0	0
			1014	641	205	167	1		

- Molecule 44 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	Li	101	Total	C	N	O	S	0	0
			797	500	170	122	5		
44	Mi	102	Total	C	N	O	S	0	0
			832	521	177	129	5		

- Molecule 45 is a protein called Large ribosomal subunit protein eL37.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	Lj	86	Total	C	N	O	S	0	0
			701	431	154	111	5		
45	Mj	86	Total	C	N	O	S	1	0
			712	439	157	111	5		

- Molecule 46 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	Lk	69	Total	C	N	O	S	0	0
			528	339	99	89	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
46	Mk	69	Total	C	N	O	S	0	0
			568	366	103	98	1		

- Molecule 47 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	Ll	50	Total	C	N	O	S	0	0
			440	278	97	64	1		
47	Ml	50	Total	C	N	O	S	0	0
			443	281	98	63	1		

- Molecule 48 is a protein called Ubiquitin-60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	Lm	50	Total	C	N	O	S	0	0
			393	244	82	61	6		

- Molecule 49 is a protein called 60S ribosomal protein L41.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	Ln	24	Total	C	N	O	S	0	0
			230	139	62	26	3		
49	Mn	25	Total	C	N	O	S	0	0
			239	145	64	27	3		

- Molecule 50 is a protein called 60S ribosomal protein L36a.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	Lo	98	Total	C	N	O	S	0	0
			774	488	159	121	6		

- Molecule 51 is a protein called 60S ribosomal protein L37a.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	Lp	91	Total	C	N	O	S	0	0
			690	436	132	115	7		
51	Mp	91	Total	C	N	O	S	1	0
			715	450	139	119	7		

- Molecule 52 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	Lr	125	Total	C	N	O	S	0	0
			982	609	205	164	4		

- Molecule 53 is a RNA chain called 28S rRNA of the stalled 80S.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	M5	3546	Total	C	N	O	P	0	0
			76094	33925	13918	24706	3545		

- Molecule 54 is a RNA chain called 5.8S rRNA of the stalled 80S.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	M8	156	Total	C	N	O	P	0	0
			3316	1482	585	1094	155		

- Molecule 55 is a protein called Large ribosomal subunit protein uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	MA	251	Total	C	N	O	S	1	0
			1930	1209	396	319	6		

- Molecule 56 is a protein called Large ribosomal subunit protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	MB	402	Total	C	N	O	S	0	0
			3239	2061	608	556	14		

- Molecule 57 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	MI	203	Total	C	N	O	S	0	0
			1645	1045	317	270	13		

- Molecule 58 is a protein called Large ribosomal subunit protein uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	Ma	147	Total	C	N	O	S	0	0
			1162	736	237	186	3		

- Molecule 59 is a protein called Large ribosomal subunit protein eL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	Mb	111	Total	C	N	O	S	0	0
			898	560	195	139	4		

- Molecule 60 is a protein called Ubiquitin-ribosomal protein eL40 fusion protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	Mm	52	Total	C	N	O	S	1	0
			436	272	91	67	6		

- Molecule 61 is a protein called Large ribosomal subunit protein eL42.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	Mo	105	Total	C	N	O	S	1	0
			870	548	177	139	6		

- Molecule 62 is a protein called Large ribosomal subunit protein eL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	Mr	126	Total	C	N	O	S	1	0
			1011	629	208	169	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Mr	1	ACE	-	acetylation	UNP P46779

- Molecule 63 is a protein called 60S ribosomal protein L10a.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	Ms	217	Total	C	N	O	S	0	0
			1744	1114	314	307	9		

- Molecule 64 is a protein called Mitogen-activated protein kinase kinase kinase 20.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	N1	141	Total	C	N	O	S	0	0
			1140	734	192	209	5		
64	N2	116	Total	C	N	O	S	0	0
			933	603	155	172	3		

- Molecule 65 is a protein called Small ribosomal subunit protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	RA	223	Total	C	N	O	S	0	0
			1750	1111	306	325	8		

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 66 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	RB	234	Total	C	N	O	S	0	0
			1892	1198	337	343	14		
66	SB	214	Total	C	N	O	S	0	0
			1627	1041	296	277	13		

- Molecule 67 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	RC	222	Total	C	N	O	S	0	0
			1725	1115	298	302	10		
67	SC	217	Total	C	N	O	S	0	0
			1590	1039	276	266	9		

- Molecule 68 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	RD	226	Total	C	N	O	S	0	0
			1756	1119	315	314	8		
68	SD	226	Total	C	N	O	S	0	0
			1756	1119	315	314	8		

- Molecule 69 is a protein called Small ribosomal subunit protein eS4, X isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	RE	262	Total	C	N	O	S	0	0
			2076	1324	386	358	8		
69	SE	257	Total	C	N	O	S	0	0
			1891	1218	358	307	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
70	RF	180	Total	C	N	O	S	0	0
			1426	894	266	259	7		
70	SF	180	Total	C	N	O	S	0	0
			1365	861	261	237	6		

- Molecule 71 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	RG	237	Total	C	N	O	S	0	0
			1923	1200	387	329	7		
71	SG	212	Total	C	N	O	S	0	0
			1544	968	312	258	6		

- Molecule 72 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	RH	189	Total	C	N	O	S	0	0
			1517	966	279	271	1		
72	SH	176	Total	C	N	O	S	0	0
			1342	871	249	221	1		

- Molecule 73 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	RI	206	Total	C	N	O	S	0	0
			1686	1058	332	291	5		
73	SI	206	Total	C	N	O	S	0	0
			1686	1058	332	291	5		

- Molecule 74 is a protein called 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	RJ	185	Total	C	N	O	S	0	0
			1525	969	306	248	2		
74	SJ	176	Total	C	N	O	S	0	0
			1407	899	280	226	2		

- Molecule 75 is a protein called 40S ribosomal protein S10.

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

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Mol	Chain	Residues	Atoms					AltConf	Trace
75	SK	95	Total	C	N	O	S	0	0
			736	482	131	119	4		

- Molecule 76 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	RL	146	Total	C	N	O	S	0	0
			1200	766	226	202	6		
76	SL	140	Total	C	N	O	S	0	0
			1139	725	214	194	6		

- Molecule 77 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	RM	122	Total	C	N	O	S	0	0
			950	596	168	177	9		
77	Sf	122	Total	C	N	O	S	0	0
			950	596	168	177	9		

- Molecule 78 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	RN	150	Total	C	N	O	S	1	0
			1214	778	231	204	1		
78	SN	150	Total	C	N	O	S	0	0
			1199	766	229	203	1		

- Molecule 79 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	RO	135	Total	C	N	O	S	0	0
			1009	618	198	187	6		
79	SO	135	Total	C	N	O	S	0	0
			1003	615	198	184	6		

- Molecule 80 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	RP	131	Total	C	N	O	S	0	0
			1078	684	204	183	7		
80	SP	127	Total	C	N	O	S	0	0
			1001	636	188	170	7		

- Molecule 81 is a protein called 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	RQ	141	Total	C	N	O	S	0	0
			1123	715	212	193	3		
81	SQ	141	Total	C	N	O	S	0	0
			1078	690	207	178	3		

- Molecule 82 is a protein called 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	RR	134	Total	C	N	O	S	0	0
			1082	680	201	197	4		
82	SR	125	Total	C	N	O	S	0	0
			879	551	166	159	3		

- Molecule 83 is a protein called 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	RS	148	Total	C	N	O	S	0	0
			1214	761	245	207	1		
83	SS	138	Total	C	N	O	S	0	0
			1080	684	220	175	1		

- Molecule 84 is a protein called 40S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
84	RT	142	Total	C	N	O	S	1	0
			1121	707	212	199	3		
84	ST	141	Total	C	N	O	S	0	0
			993	624	195	172	2		

- Molecule 85 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
85	RU	101	Total	C	N	O	S	0	0
			803	504	153	142	4		
85	SU	99	Total	C	N	O	S	0	0
			745	467	143	133	2		

- Molecule 86 is a protein called Small ribosomal subunit protein eS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
86	RV	84	Total	C	N	O	S	0	0
			639	395	117	122	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
RV	0	ACE	-	acetylation	UNP P63220

- Molecule 87 is a protein called 40S ribosomal protein S15a.

Mol	Chain	Residues	Atoms					AltConf	Trace
87	RW	129	Total	C	N	O	S	0	0
			1034	659	193	176	6		
87	SW	129	Total	C	N	O	S	0	0
			1027	655	192	174	6		

- Molecule 88 is a protein called 40S ribosomal protein S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
88	RX	140	Total	C	N	O	S	0	0
			1087	687	215	182	3		
88	SX	141	Total	C	N	O	S	0	0
			1048	663	206	176	3		

- Molecule 89 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
89	RY	131	Total	C	N	O	S	0	0
			1065	673	209	178	5		
89	SY	113	Total	C	N	O	S	0	0
			855	544	164	143	4		

- Molecule 90 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
90	RZ	84	Total	C	N	O	S	0	0
			674	433	126	114	1		
90	SZ	70	Total	C	N	O	S	0	0
			487	311	90	85	1		

- Molecule 91 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
91	Ra	99	Total	C	N	O	S	1	0
			800	497	168	130	5		
91	Sa	99	Total	C	N	O	S	0	0
			762	478	157	122	5		

- Molecule 92 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
92	Rb	83	Total	C	N	O	S	0	0
			651	408	121	115	7		
92	Sb	83	Total	C	N	O	S	0	0
			651	408	121	115	7		

- Molecule 93 is a protein called 40S ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
93	Rc	65	Total	C	N	O	S	0	0
			512	311	103	96	2		
93	Sc	61	Total	C	N	O	S	0	0
			430	267	83	78	2		

- Molecule 94 is a protein called 40S ribosomal protein S29.

Mol	Chain	Residues	Atoms					AltConf	Trace
94	Rd	55	Total	C	N	O	S	0	0
			458	286	94	73	5		
94	Sd	52	Total	C	N	O	S	0	0
			420	264	83	69	4		

- Molecule 95 is a protein called Ubiquitin-like FUBI-ribosomal protein eS30 fusion protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
95	Re	50	Total	C	N	O	S	0	0
			394	241	88	64	1		
95	Se	44	Total	C	N	O	S	0	0
			338	211	73	53	1		

- Molecule 96 is a protein called Ubiquitin.

Mol	Chain	Residues	Atoms					AltConf	Trace
96	Rf	63	Total	C	N	O	S	0	0
			515	324	98	86	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
96	sh	63	Total	C	N	O	S	0	0
			515	324	98	86	7		

- Molecule 97 is a protein called Receptor of activated protein C kinase 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
97	Rg	317	Total	C	N	O	S	0	0
			2467	1552	431	471	13		
97	Sg	317	Total	C	N	O	S	0	0
			2467	1552	431	471	13		

- Molecule 98 is a RNA chain called 18S rRNA of the collided 80S.

Mol	Chain	Residues	Atoms					AltConf	Trace
98	S2	1756	Total	C	N	O	P	0	0
			37129	16555	6634	12185	1755		

- Molecule 99 is a RNA chain called 18S rRNA of the stalled 80S.

Mol	Chain	Residues	Atoms					AltConf	Trace
99	S3	1672	Total	C	N	O	P	0	0
			35736	15981	6403	11681	1671		

- Molecule 100 is a protein called 40S ribosomal protein SA.

Mol	Chain	Residues	Atoms					AltConf	Trace
100	SA	212	Total	C	N	O	S	0	0
			1575	1016	285	266	8		

- Molecule 101 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
101	SV	83	Total	C	N	O	S	0	0
			590	369	111	105	5		

- Molecule 102 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
102	A4	1	Total	Mg	0
			1	1	
102	A5	1	Total	Mg	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
102	B5	2	Total 2	Mg 2	0
102	L5	92	Total 92	Mg 92	0
102	L7	2	Total 2	Mg 2	0
102	L8	5	Total 5	Mg 5	0
102	LQ	1	Total 1	Mg 1	0
102	LV	1	Total 1	Mg 1	0
102	Lj	1	Total 1	Mg 1	0
102	M5	454	Total 454	Mg 454	0
102	M7	13	Total 13	Mg 13	0
102	M8	15	Total 15	Mg 15	0
102	MC	1	Total 1	Mg 1	0
102	MD	2	Total 2	Mg 2	0
102	MF	1	Total 1	Mg 1	0
102	MI	3	Total 3	Mg 3	0
102	ML	2	Total 2	Mg 2	0
102	MN	4	Total 4	Mg 4	0
102	MO	3	Total 3	Mg 3	0
102	MP	3	Total 3	Mg 3	0
102	MQ	1	Total 1	Mg 1	0
102	MS	2	Total 2	Mg 2	0
102	MT	1	Total 1	Mg 1	0

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Mol	Chain	Residues	Atoms		AltConf
102	MV	1	Total 1	Mg 1	0
102	MY	1	Total 1	Mg 1	0
102	Ma	2	Total 2	Mg 2	0
102	Mc	1	Total 1	Mg 1	0
102	Me	1	Total 1	Mg 1	0
102	Mf	2	Total 2	Mg 2	0
102	Mg	2	Total 2	Mg 2	0
102	Mj	2	Total 2	Mg 2	0
102	Mo	1	Total 1	Mg 1	0
102	Mp	3	Total 3	Mg 3	0
102	Mr	3	Total 3	Mg 3	0
102	RE	1	Total 1	Mg 1	0
102	RG	1	Total 1	Mg 1	0
102	RN	1	Total 1	Mg 1	0
102	RO	1	Total 1	Mg 1	0
102	RS	1	Total 1	Mg 1	0
102	RT	1	Total 1	Mg 1	0
102	RU	1	Total 1	Mg 1	0
102	RX	1	Total 1	Mg 1	0
102	Rd	1	Total 1	Mg 1	0
102	S2	57	Total 57	Mg 57	0

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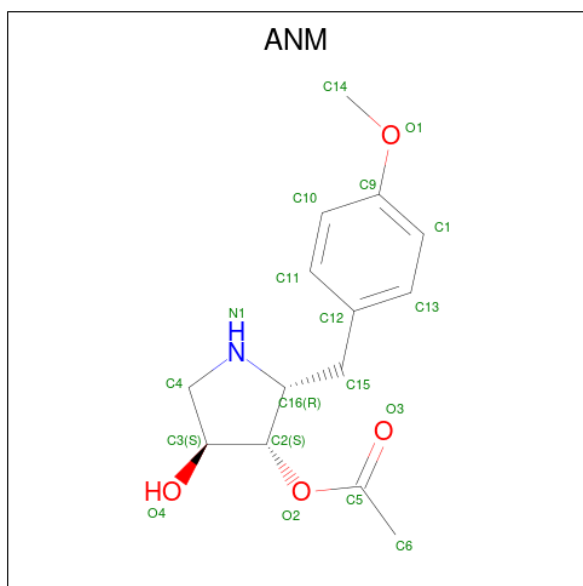
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Mol	Chain	Residues	Atoms		AltConf
102	S3	134	Total	Mg	0
			134	134	

- Molecule 103 is ZINC ION (CCD ID: ZN) (formula: Zn).

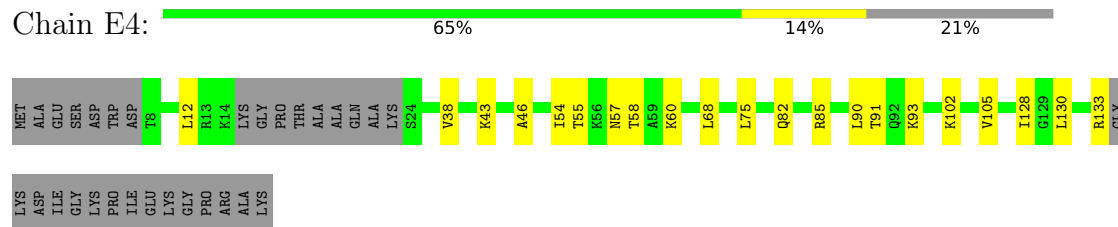
Mol	Chain	Residues	Atoms		AltConf
103	Lg	1	Total	Zn	0
			1	1	
103	Lj	1	Total	Zn	0
			1	1	
103	Lm	1	Total	Zn	0
			1	1	
103	Lo	1	Total	Zn	0
			1	1	
103	Lp	1	Total	Zn	0
			1	1	
103	Sa	1	Total	Zn	0
			1	1	
103	Sd	1	Total	Zn	0
			1	1	

- Molecule 104 is ANISOMYCIN (CCD ID: ANM) (formula: C₁₄H₁₉NO₄).

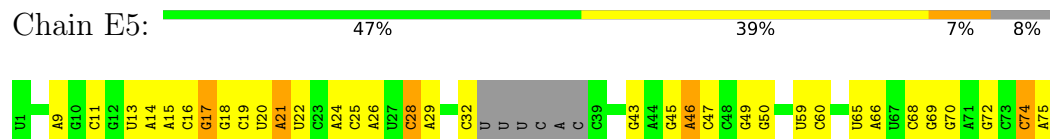


Mol	Chain	Residues	Atoms				AltConf
104	M5	1	Total	C	N	O	0
			19	14	1	4	

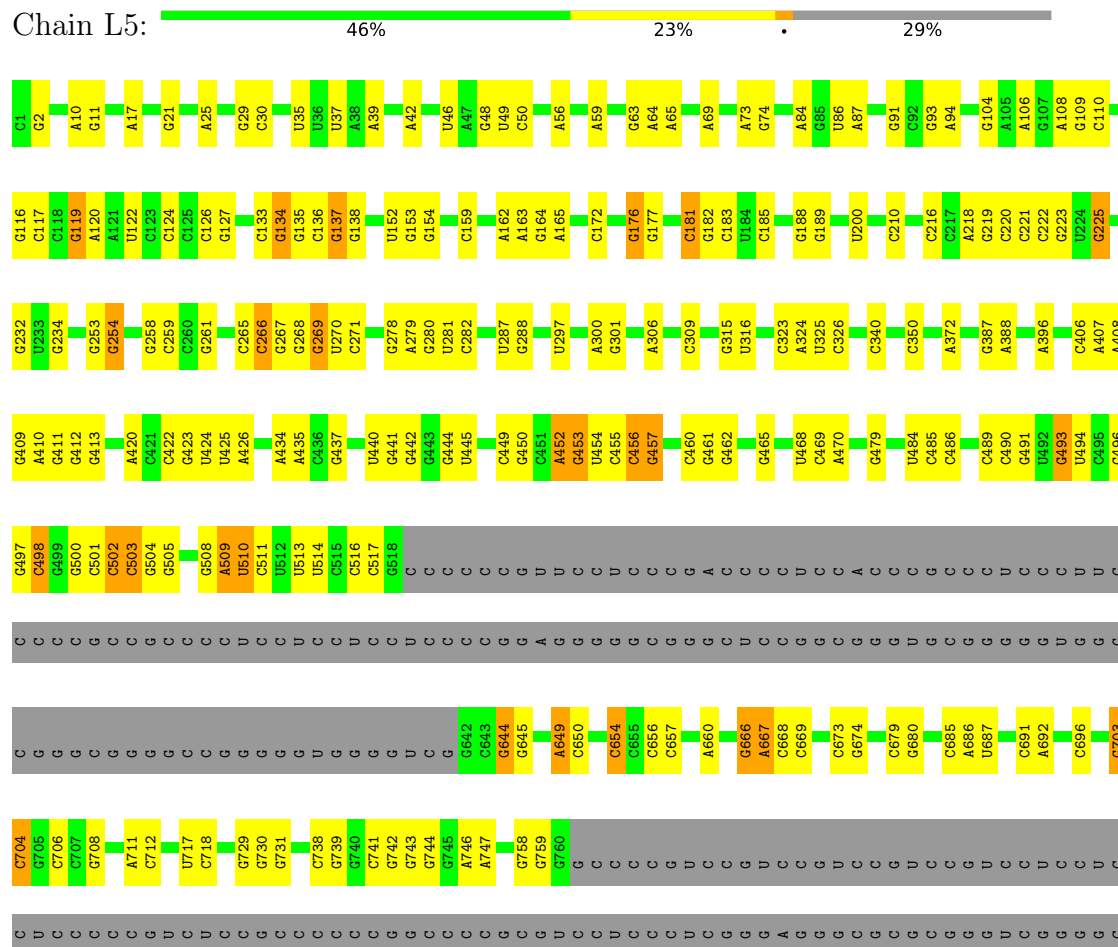
- Molecule 6: Endothelial differentiation-related factor 1



- Molecule 7: E-site tRNA of the stalled 80S



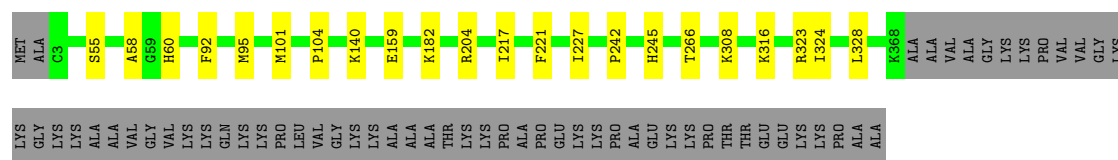
- Molecule 8: 28S rRNA of the collided 80S







Chain MC:  81% 5% 14%

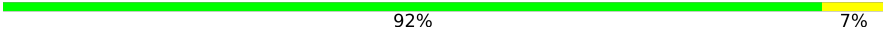


- Molecule 14: 60S ribosomal protein L5

Chain LD:  88% 10% ..



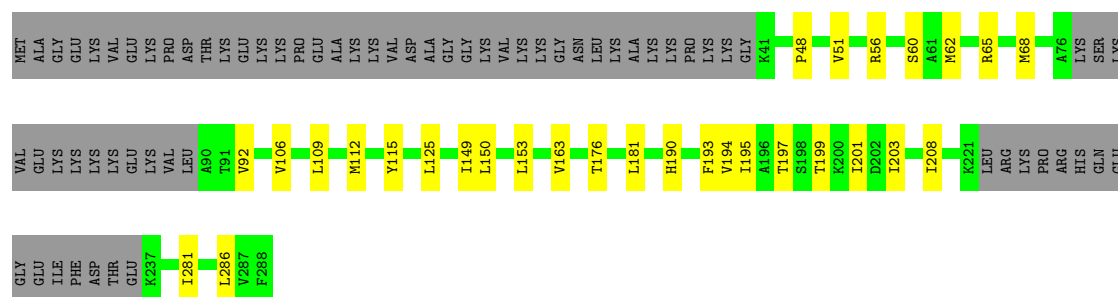
- Molecule 14: 60S ribosomal protein L5

Chain MD:  92% 7% .



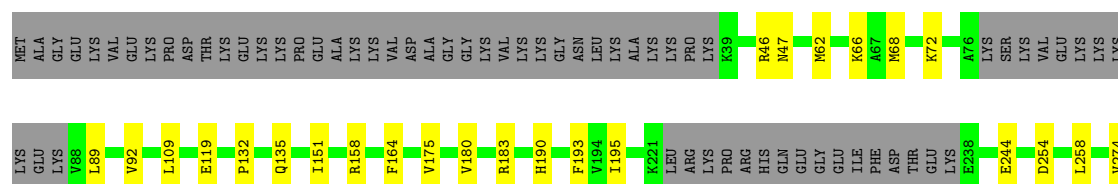
- Molecule 15: Large ribosomal subunit protein eL6

Chain LE:  66% 10% 24%



- Molecule 15: Large ribosomal subunit protein eL6

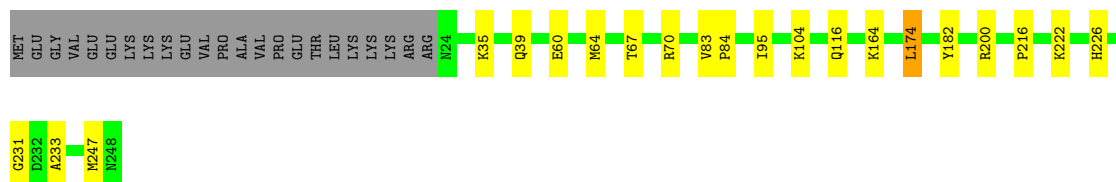
Chain ME:  69% 9% 23%





- Molecule 16: Large ribosomal subunit protein uL30

Chain LF: 82% 8% 9%



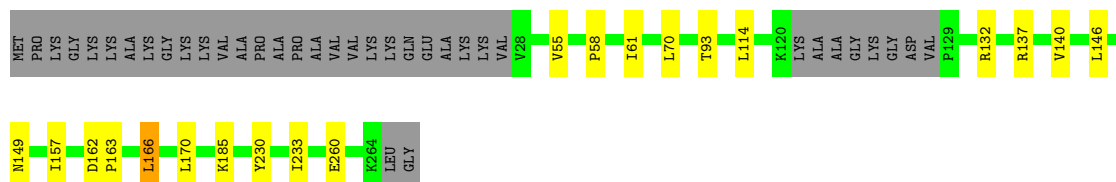
- Molecule 16: Large ribosomal subunit protein uL30

Chain MF: 85% 5% 9%



- Molecule 17: 60S ribosomal protein L7a

Chain LG: 79% 7% 14%



- Molecule 17: 60S ribosomal protein L7a

Chain MG: 85% 6% 9%



- Molecule 18: 60S ribosomal protein L9

Chain LH: 86% 12% 2%



- Molecule 18: 60S ribosomal protein L9

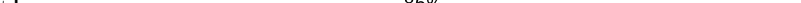
Chain MH: 92% 7% 1%

- Molecule 19: Ribosomal protein uL16-like

Chain LI:  85% 10% 5%

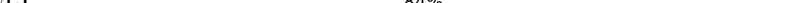


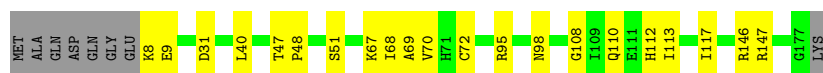
- Molecule 20: 60S ribosomal protein L11

Chain LJ:  86% 7% • 6%



- Molecule 20: 60S ribosomal protein L11

Chain MJ: 

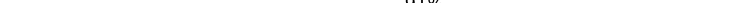


- Molecule 21: Large ribosomal subunit protein eL13

Chain LL: 91% 6%

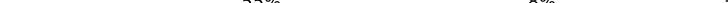


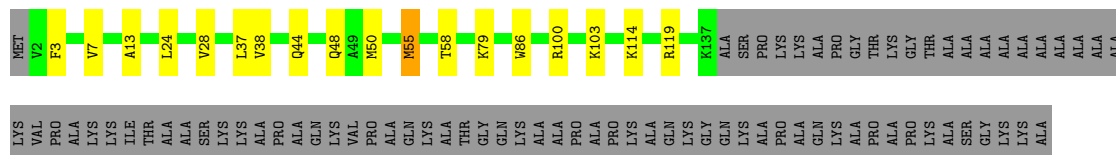
- Molecule 21: Large ribosomal subunit protein eL13

Chain ML:  91% 6%



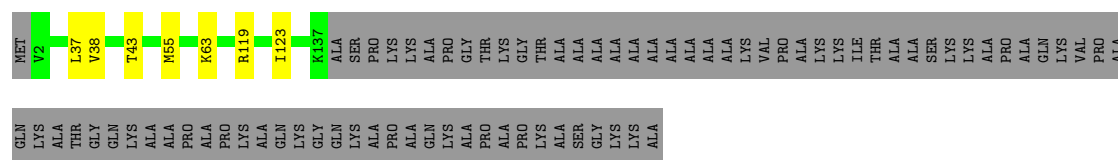
- Molecule 22: 60S ribosomal protein L14

Chain LM:  55% 8% 37%



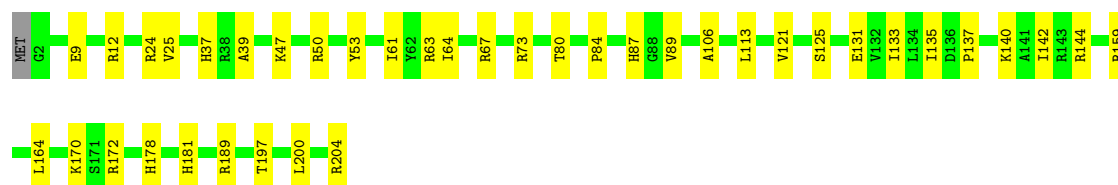
- Molecule 22: 60S ribosomal protein L14

Chain MM:  60% 37%



- Molecule 23: 60S ribosomal protein L15

Chain LN:  80% 19%



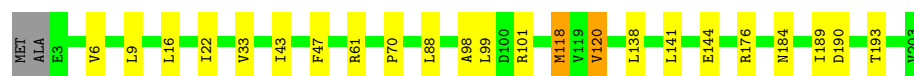
- Molecule 23: 60S ribosomal protein L15

Chain MN:  90% 9%



- Molecule 24: 60S ribosomal protein L13a

Chain LO:  88% 10% ..



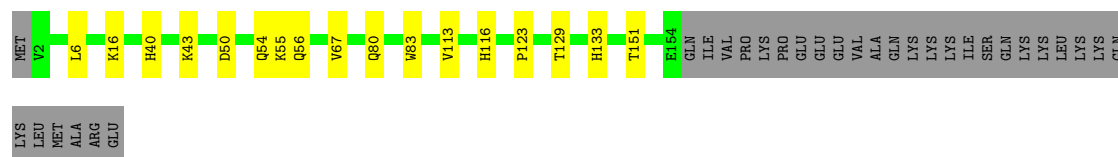
- Molecule 24: 60S ribosomal protein L13a

Chain MO:  91% 8%



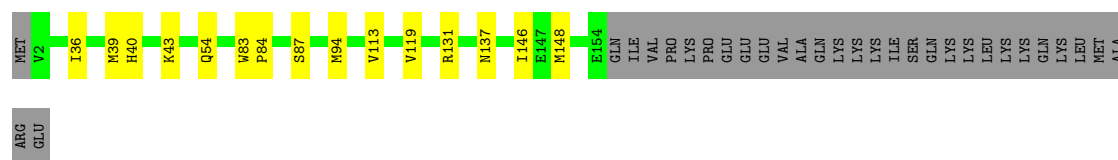
- Molecule 25: 60S ribosomal protein L17

Chain LP:  74% 9% 17%



- Molecule 25: 60S ribosomal protein L17

Chain MP:  75% 8% 17%

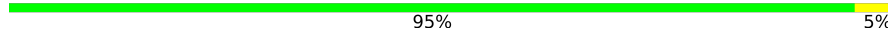


- Molecule 26: 60S ribosomal protein L18

Chain LQ:  86% 13% ..



- Molecule 26: 60S ribosomal protein L18

Chain MQ:  95% 5% .



- Molecule 27: 60S ribosomal protein L19

Chain LR:  80% 8% . 11%



- Molecule 27: 60S ribosomal protein L19

Chain MR:  89% 7% 5%



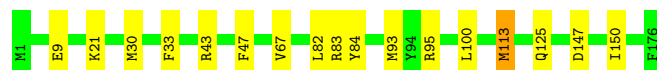
- Molecule 28: 60S ribosomal protein L18a

Chain LS:  88% 11% .



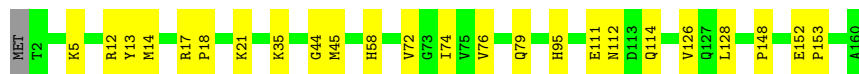
- Molecule 28: 60S ribosomal protein L18a

Chain MS:  90% 9% .



- Molecule 29: 60S ribosomal protein L21

Chain LT:  84% 15%



- Molecule 29: 60S ribosomal protein L21

Chain MT:  89% 9%



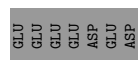
- Molecule 30: 60S ribosomal protein L22

Chain LU:  65% 13% 21%



- Molecule 30: 60S ribosomal protein L22

Chain MU:  62% 13% 23%



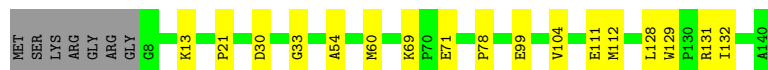
- Molecule 31: 60S ribosomal protein L23

Chain LV:  74% 19% 6%



- Molecule 31: 60S ribosomal protein L23

Chain MV:  83% 12% 5%



- | | | | | | | | | | | | | | | | | | | |
|----|----|-----|-----|-----|-----|-----|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| M1 | K2 | V44 | R45 | S46 | Q66 | K89 | K134 | TYR | LYS | GLU | GLU | THR | ILE | GLU | LYS | MET | GLN | GLU |
|----|----|-----|-----|-----|-----|-----|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

- Molecule 35: 60S ribosomal protein L27

Chain LZ:  85% 13% ..



- Molecule 35: 60S ribosomal protein L27

Chain MZ:  86% 13% .



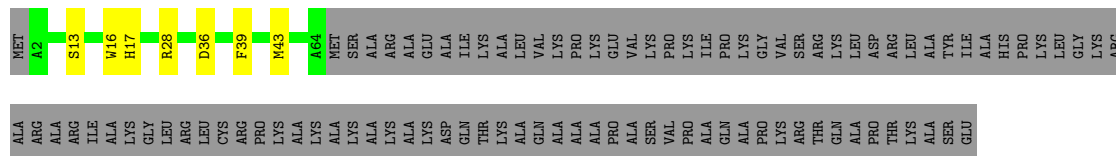
- Molecule 36: 60S ribosomal protein L27a

Chain La:  89% 10% .



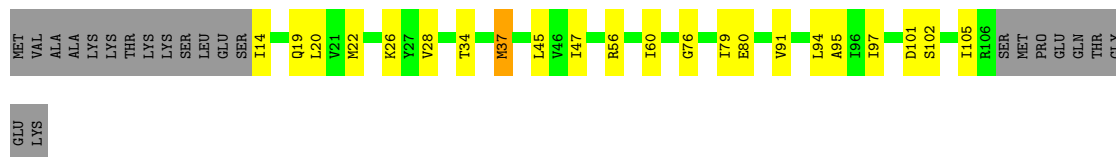
- Molecule 37: 60S ribosomal protein L29

Chain Lb:  35% 60%



- Molecule 38: 60S ribosomal protein L30

Chain Lc:  62% 18% 19%



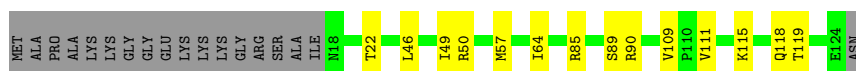
- Molecule 38: 60S ribosomal protein L30

Chain Mc:  70% 14% 14%

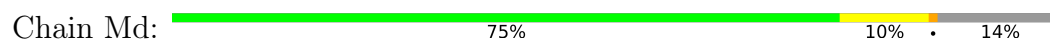


- Molecule 39: 60S ribosomal protein L31

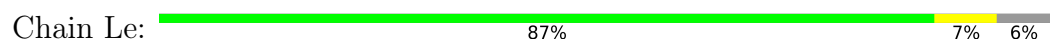
Chain Ld:  74% 11% 14%



- Molecule 39: 60S ribosomal protein L31



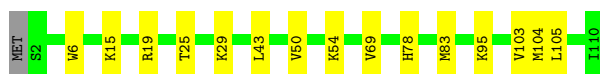
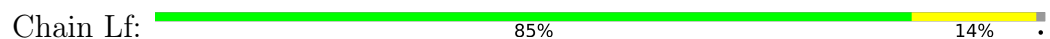
- Molecule 40: 60S ribosomal protein L32



- Molecule 40: 60S ribosomal protein L32



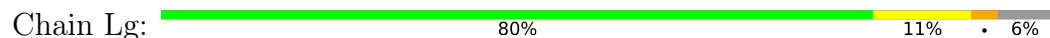
- Molecule 41: 60S ribosomal protein L35a



- Molecule 41: 60S ribosomal protein L35a



- Molecule 42: 60S ribosomal protein L34



- Molecule 42: 60S ribosomal protein L34





- Molecule 43: 60S ribosomal protein L35

Chain Lh: 89% 9% ..



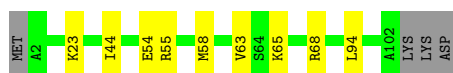
- Molecule 43: 60S ribosomal protein L35

Chain Mh: 91% 6% ..



- Molecule 44: 60S ribosomal protein L36

Chain Li: 88% 9% .



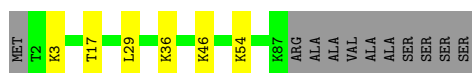
- Molecule 44: 60S ribosomal protein L36

Chain Mi: 90% 7% .



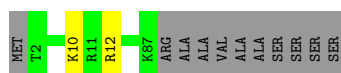
- Molecule 45: Large ribosomal subunit protein eL37

Chain Lj: 82% 6% 11%



- Molecule 45: Large ribosomal subunit protein eL37

Chain Mj: 87% . 11%



- Molecule 46: 60S ribosomal protein L38

Chain Lk: 90% 9% .



- Molecule 46: 60S ribosomal protein L38

Chain Mk: 80% 16% . .



- Molecule 47: 60S ribosomal protein L39

Chain Ll: 92% 6% .



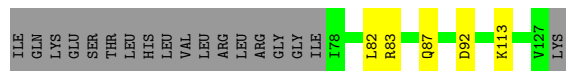
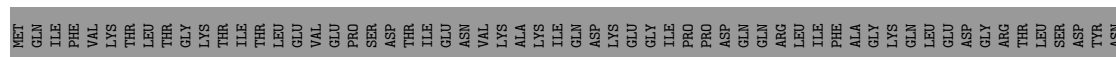
- Molecule 47: 60S ribosomal protein L39

Chain Ml: 92% 6% .



- Molecule 48: Ubiquitin-60S ribosomal protein L40

Chain Lm: 35% . 61%



- Molecule 49: 60S ribosomal protein L41

Chain Ln: 92% . .



- Molecule 49: 60S ribosomal protein L41

Chain Mn: 80% 20%

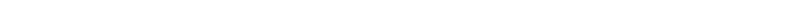


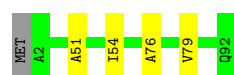
- Molecule 50: 60S ribosomal protein L36a

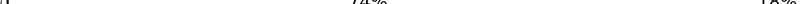
MET
V2
N3
V4
R8
C12
C15
Q36
G47
V67
C77
L93
R99
LYS
GLY
GLN
VAL
ILE
GLN
PHE

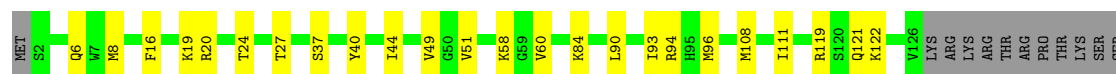
- Chain Lp: 92% 7%

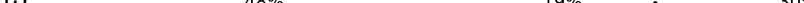


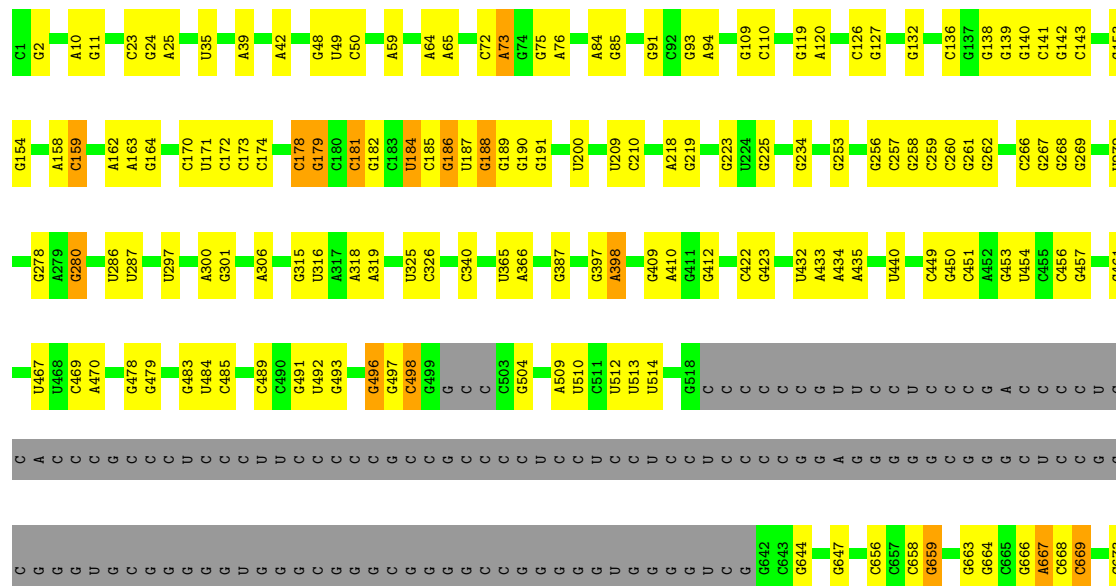
- Chain Mp:  95% .



- Chain Lr:  74% 18% 9%

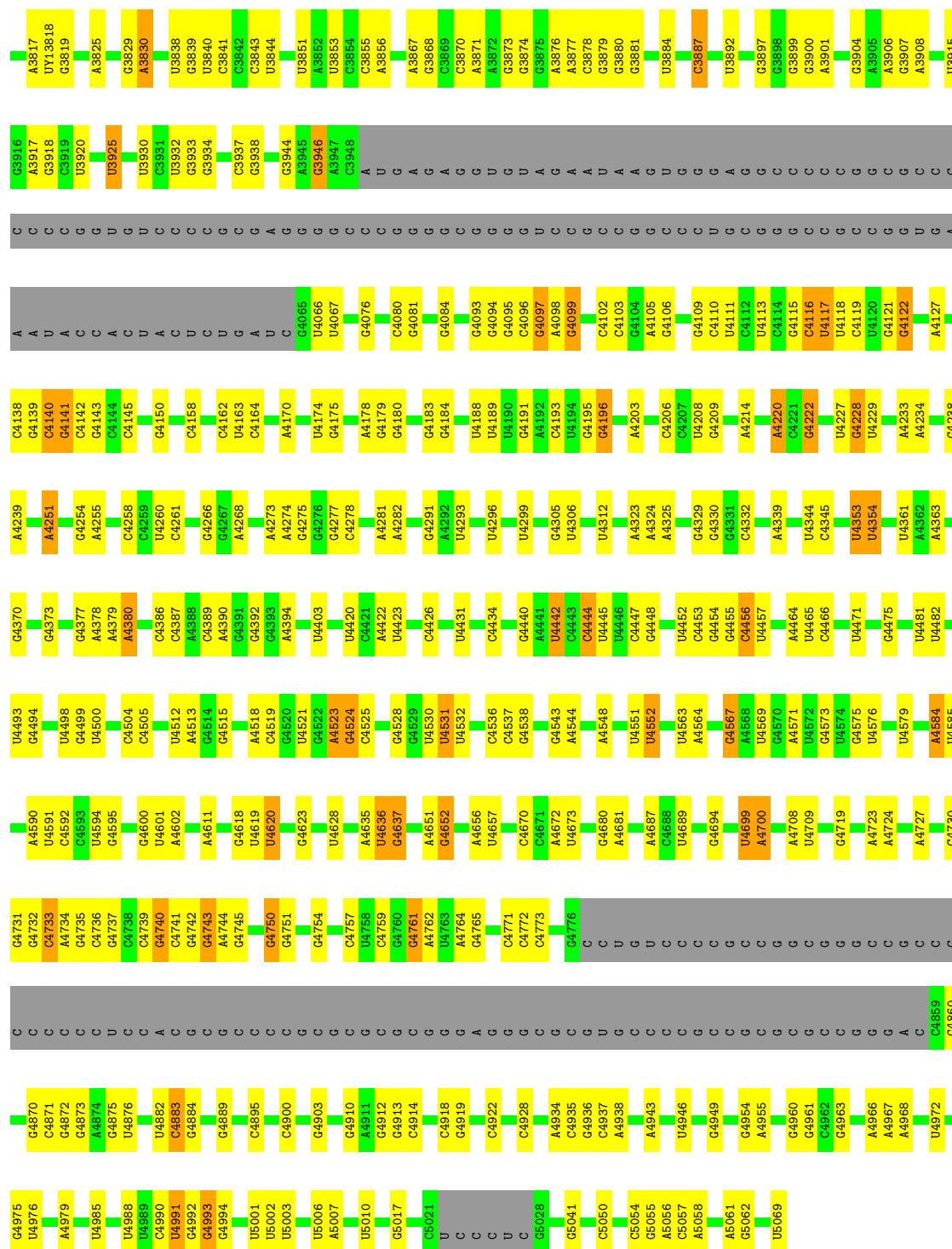


- Chain M5: 





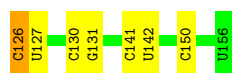




• Molecule 54: 5.8S rRNA of the stalled 80S

Chain M8: 71% 27% .





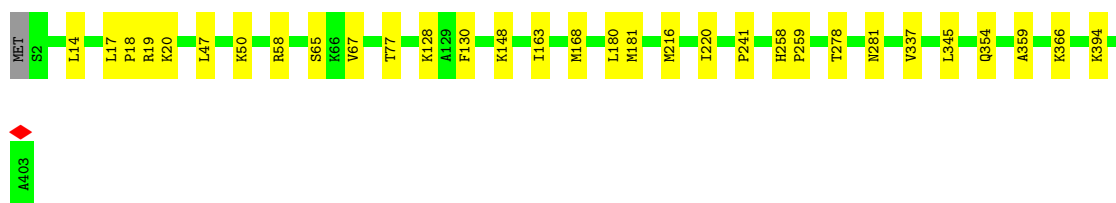
- Molecule 55: Large ribosomal subunit protein uL2

Chain MA: 88% 9%



- Molecule 56: Large ribosomal subunit protein uL3

Chain MB: 92% 8%



- Molecule 57: 60S ribosomal protein L10

Chain MI: 86% 9% 5%



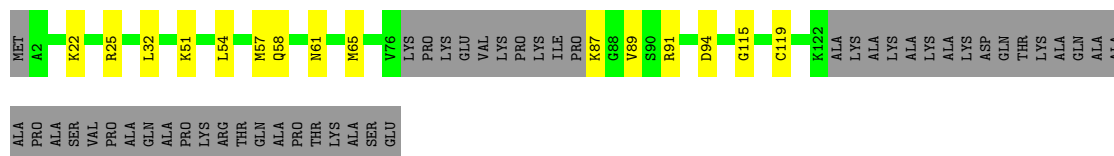
- Molecule 58: Large ribosomal subunit protein uL15

Chain Ma: 94% 5%



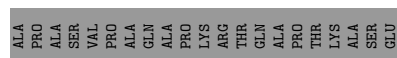
- Molecule 59: Large ribosomal subunit protein eL29

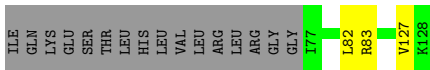
Chain Mb: 60% 9% 30%



- Molecule 60: Ubiquitin-ribosomal protein eL40 fusion protein

Chain Mm: 38% 59%

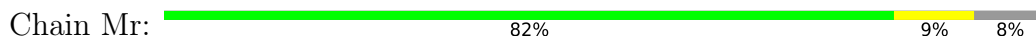




- Molecule 61: Large ribosomal subunit protein eL42



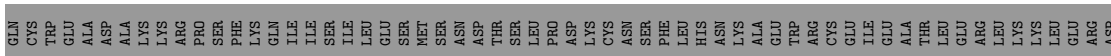
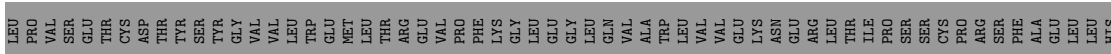
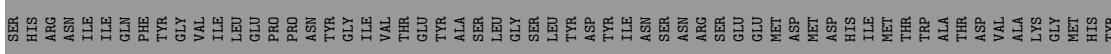
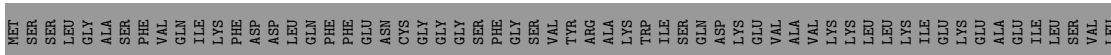
- Molecule 62: Large ribosomal subunit protein eL28

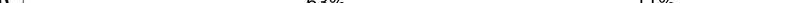


- Molecule 63: 60S ribosomal protein L10a

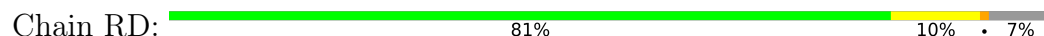


- Molecule 64: Mitogen-activated protein kinase kinase kinase 20

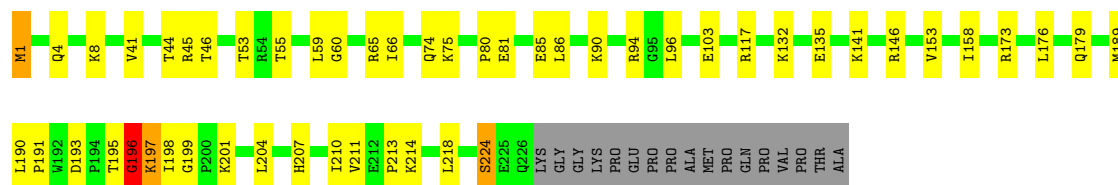


- Chain SC: 

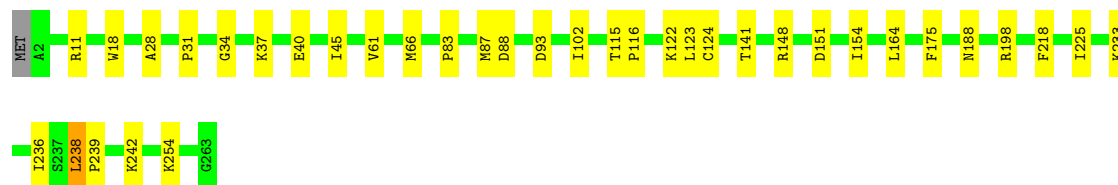
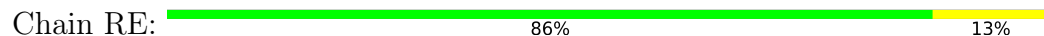
- Molecule 68: 40S ribosomal protein S3



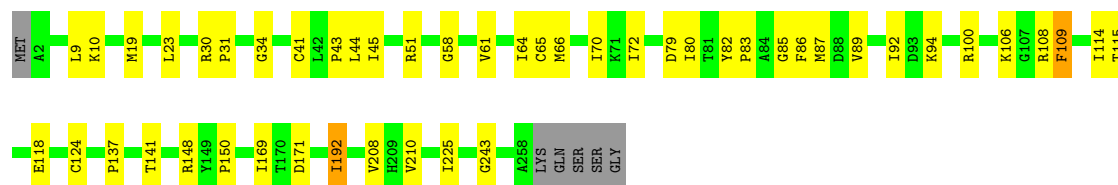
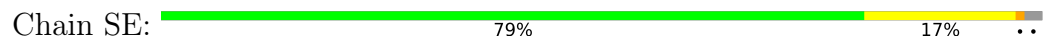
- Molecule 68: 40S ribosomal protein S3



- Molecule 69: Small ribosomal subunit protein eS4, X isoform



- Molecule 69: Small ribosomal subunit protein eS4, X isoform



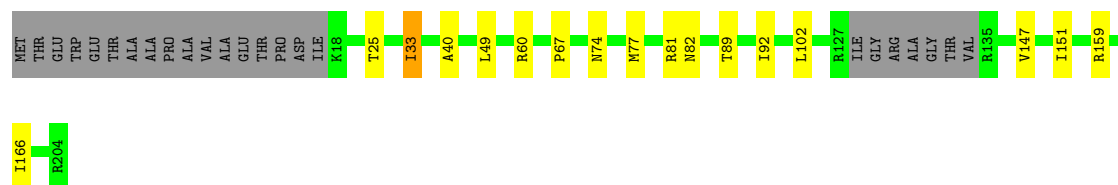
- Molecule 70: 40S ribosomal protein S5

Chain RF:  76% 11% 12%



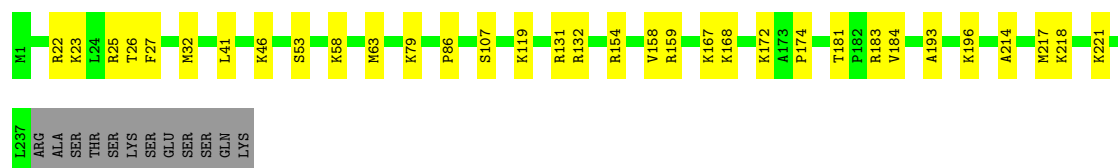
- Molecule 70: 40S ribosomal protein S5

Chain SF:  80% 8% 12%



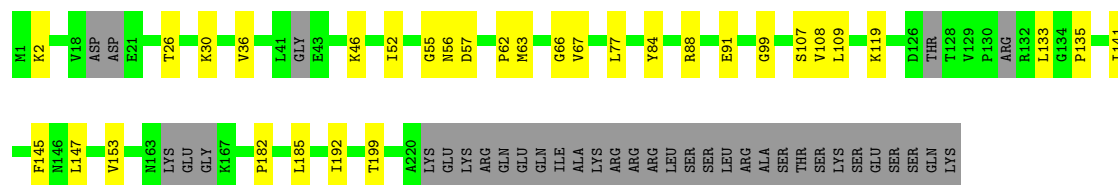
- Molecule 71: 40S ribosomal protein S6

Chain RG:  82% 13% 5%



- Molecule 71: 40S ribosomal protein S6

Chain SG:  72% 13% 15%



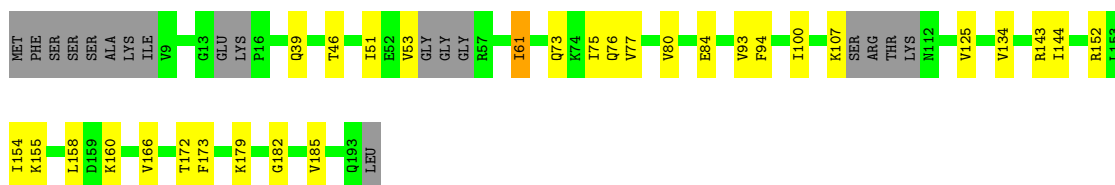
- Molecule 72: 40S ribosomal protein S7

Chain RH:  86% 11% 3%



- Molecule 72: 40S ribosomal protein S7

Chain SH:  75% 15% 9%



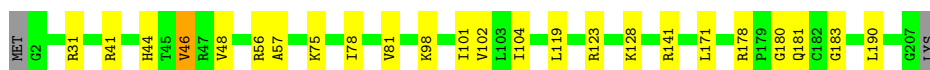
- Molecule 73: 40S ribosomal protein S8

Chain RI: 89% 10% .



- Molecule 73: 40S ribosomal protein S8

Chain SI: 88% 11% .



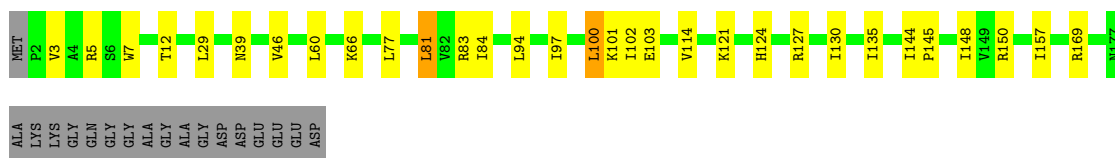
- Molecule 74: 40S ribosomal protein S9

Chain RJ: 84% 11% . 5%



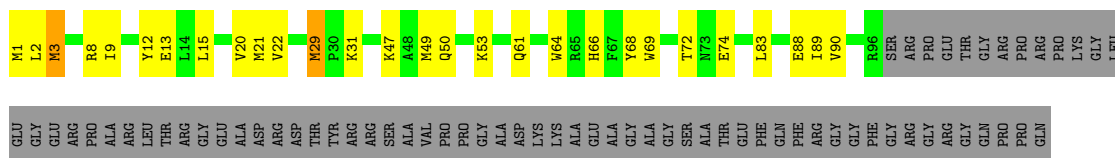
- Molecule 74: 40S ribosomal protein S9

Chain SJ: 75% 15% . 9%



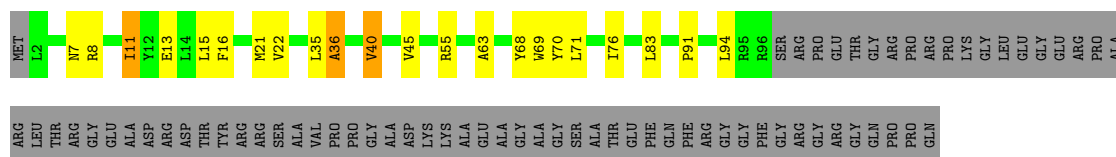
- Molecule 75: 40S ribosomal protein S10

Chain RK: 41% 16% . 42%



- Molecule 75: 40S ribosomal protein S10

Chain SK: 44% 12% . 42%



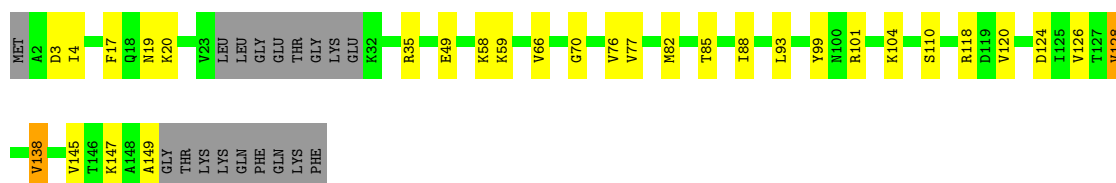
- Molecule 76: 40S ribosomal protein S11

Chain RL: 85% 7% 8%



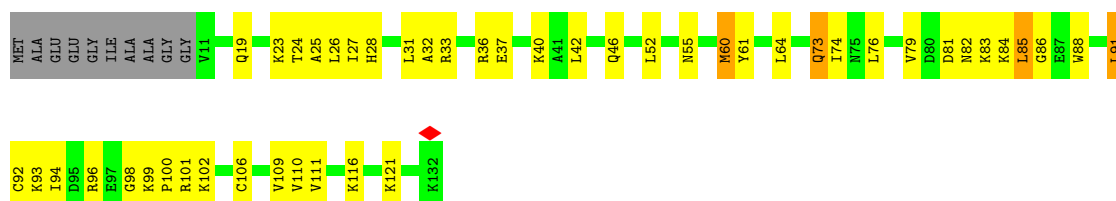
- Molecule 76: 40S ribosomal protein S11

Chain SL: 70% 18% 11%



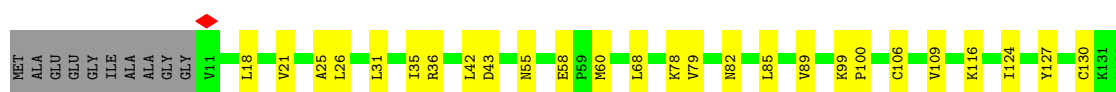
- Molecule 77: 40S ribosomal protein S12

Chain RM: 57% 33% 8%



- Molecule 77: 40S ribosomal protein S12

Chain Sf: 73% 20% 8%



- Molecule 78: 40S ribosomal protein S13

Chain RN: 94% 5%



- Molecule 78: 40S ribosomal protein S13

Chain SN:  91% 8%



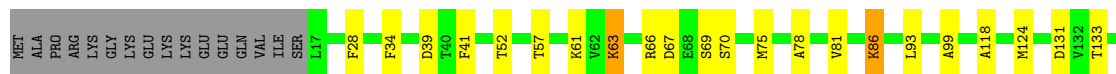
- Molecule 79: 40S ribosomal protein S14

Chain RO:  73% 15% 11%



- Molecule 79: 40S ribosomal protein S14

Chain SO:  75% 13% 11%



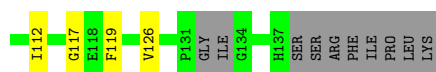
- Molecule 80: 40S ribosomal protein S15

Chain RP:  72% 17% 10%



- Molecule 80: 40S ribosomal protein S15

Chain SP:  66% 21% 12%

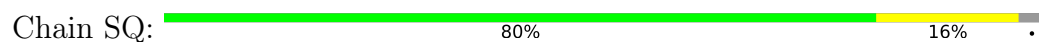


- Molecule 81: 40S ribosomal protein S16

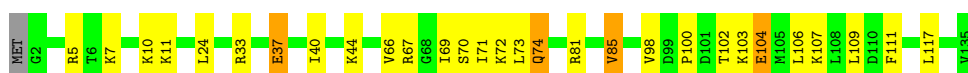
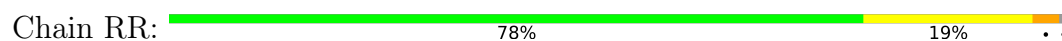
Chain RQ:  86% 11%



- Molecule 81: 40S ribosomal protein S16



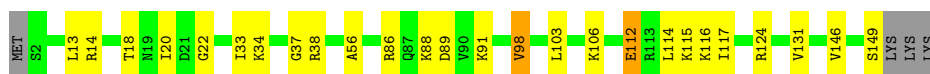
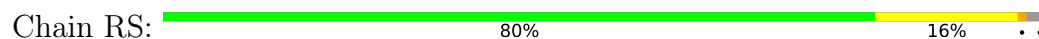
- Molecule 82: 40S ribosomal protein S17



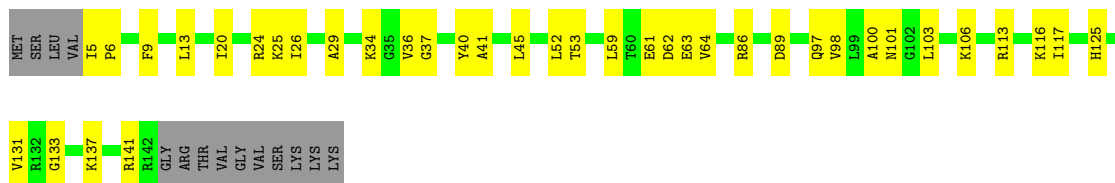
- Molecule 82: 40S ribosomal protein S17



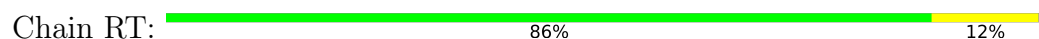
- Molecule 83: 40S ribosomal protein S18



- Molecule 83: 40S ribosomal protein S18

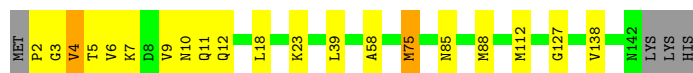


- Molecule 84: 40S ribosomal protein S19



- Molecule 84: 40S ribosomal protein S19

Chain ST:  83% 12% ..



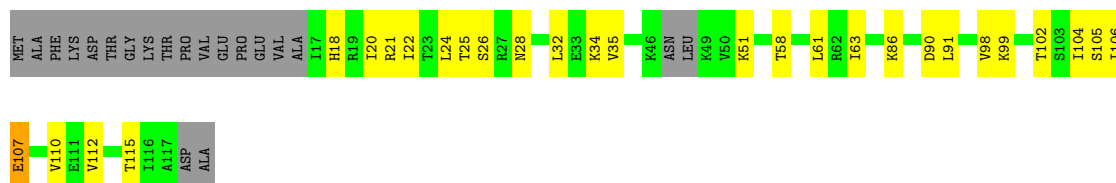
- Molecule 85: 40S ribosomal protein S20

Chain RU:  72% 13% 15%



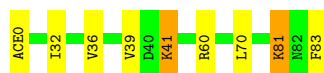
- Molecule 85: 40S ribosomal protein S20

Chain SU:  60% 23% 17%



- Molecule 86: Small ribosomal subunit protein eS21

Chain RV:  89% 8% .



- Molecule 87: 40S ribosomal protein S15a

Chain RW:  90% 9% .



- Molecule 87: 40S ribosomal protein S15a

Chain SW:  86% 12% ..



- Molecule 88: 40S ribosomal protein S23

Chain RX:  90% 8% .



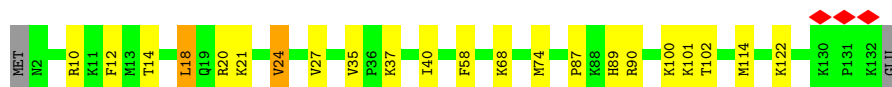
- Molecule 88: 40S ribosomal protein S23

Chain SX:  86% 12% ..



- Molecule 89: 40S ribosomal protein S24

Chain RY:  82% 15% ..



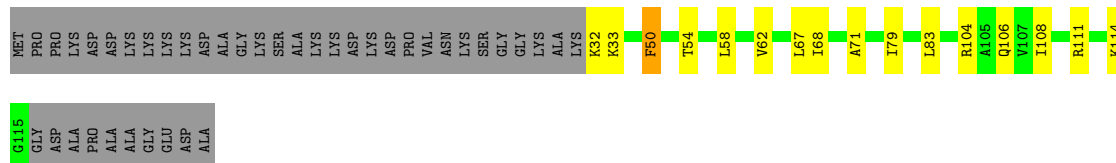
- Molecule 89: 40S ribosomal protein S24

Chain SY:  71% 14% 15%

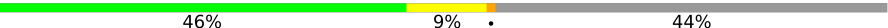


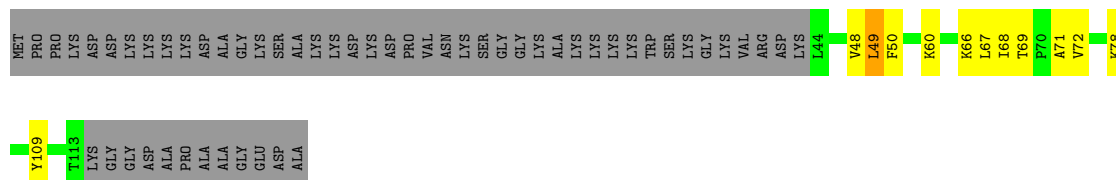
- Molecule 90: 40S ribosomal protein S25

Chain RZ:  54% 12% 33%



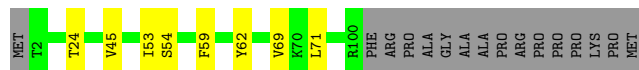
- Molecule 90: 40S ribosomal protein S25

Chain SZ:  46% 9% 44%



- Molecule 91: 40S ribosomal protein S26

Chain Ra:  79% 7% 14%

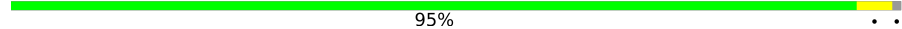


- Molecule 91: 40S ribosomal protein S26

Chain Sa:  77% 9% 14%



- Molecule 92: 40S ribosomal protein S27

Chain Rb:  95%



- Molecule 92: 40S ribosomal protein S27

Chain Sb:  86% 13%



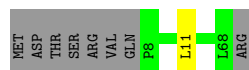
- Molecule 93: 40S ribosomal protein S28

Chain Rc:  77% 17% 6%



- Molecule 93: 40S ribosomal protein S28

Chain Sc:  87% 12%



- Molecule 94: 40S ribosomal protein S29

Chain Rd:  84% 14%



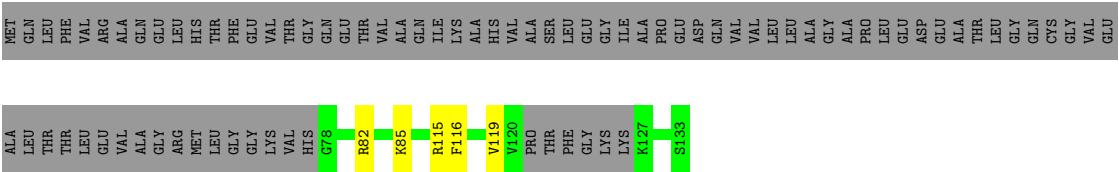
- Molecule 94: 40S ribosomal protein S29

Chain Sd:  75% 18% 7%



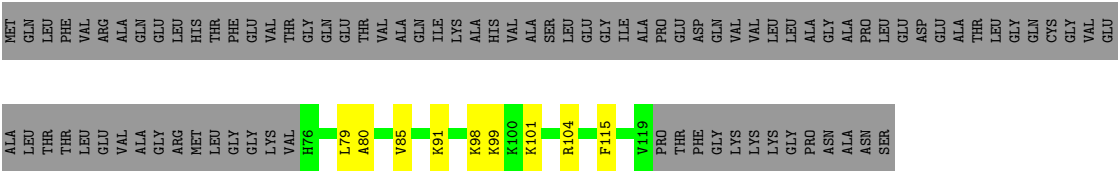
- Molecule 95: Ubiquitin-like FUBI-ribosomal protein eS30 fusion protein

Chain Re: 



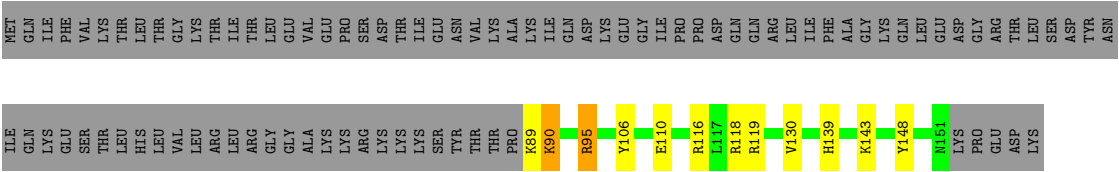
• Molecule 95: Ubiquitin-like FUBI-ribosomal protein eS30 fusion protein

Chain Se: 



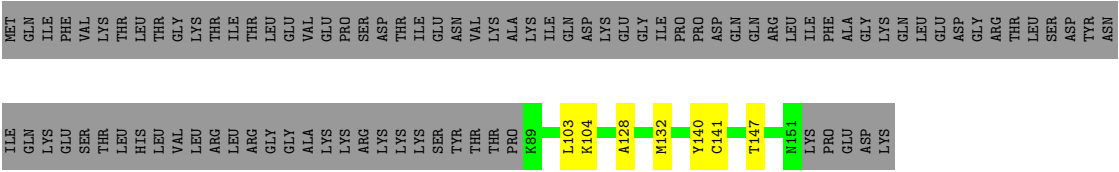
• Molecule 96: Ubiquitin

Chain Rf: 



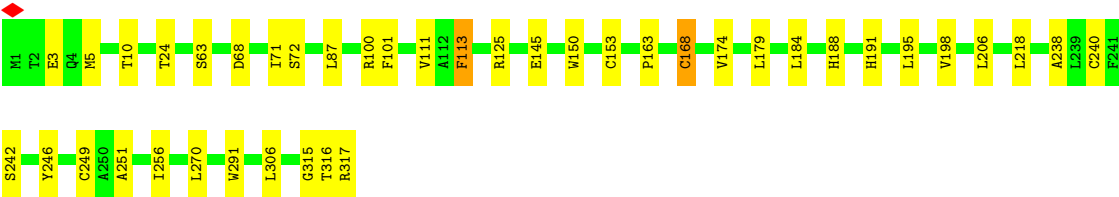
• Molecule 96: Ubiquitin

Chain sh: 



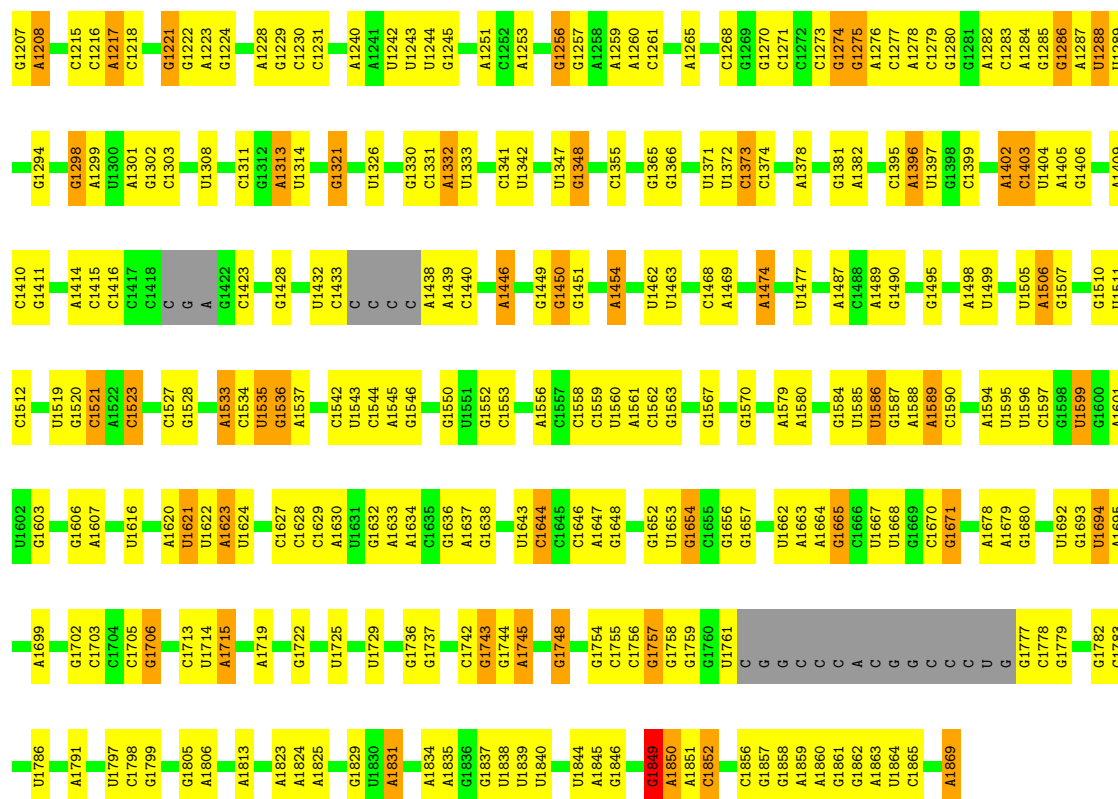
• Molecule 97: Receptor of activated protein C kinase 1

Chain Rg: 



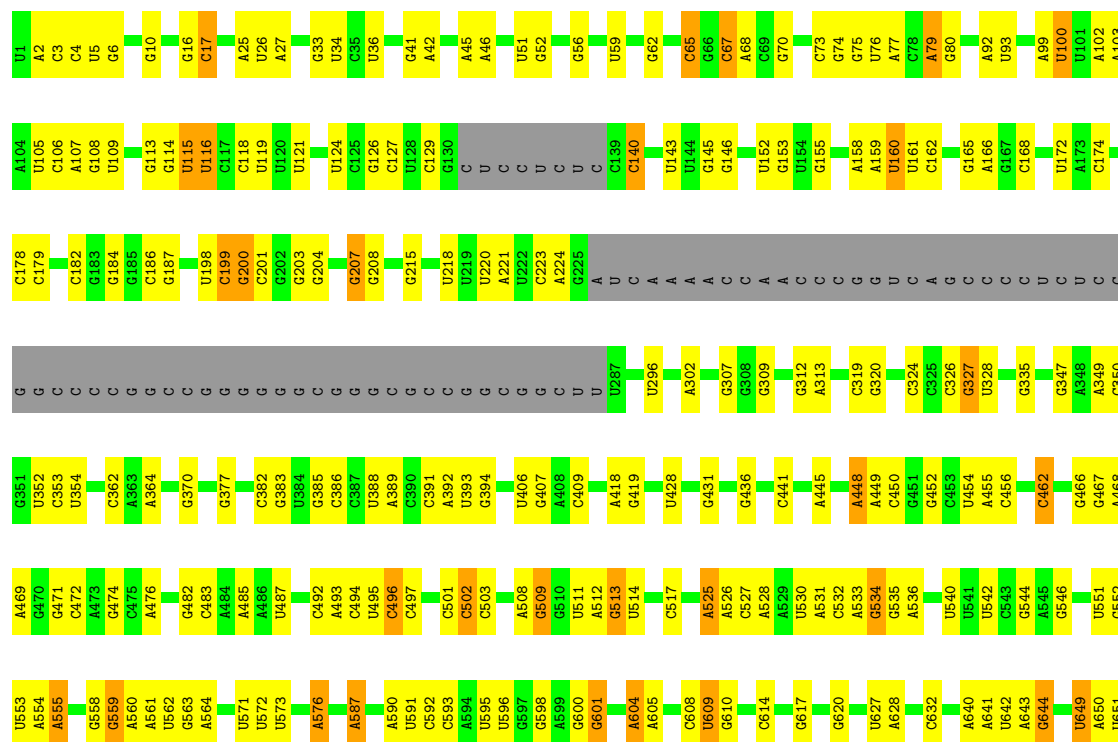
• Molecule 97: Receptor of activated protein C kinase 1

Chain Sg: 



• Molecule 99: 18S rRNA of the stalled 80S

Chain S3: 56% 30% 11%

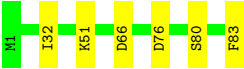




GLN
ALA
ALA
ALA
GLU
LYS
ALA
VAL
THR
GLN
LYS
GLU
GLU
PHE
GLN
GLY
GLU
THR
TRP
THR
ALA
PRO
ALA
ALA
PRO
PRO
GLU
PHE
THR
ALA
THR
GLN
PRO
GLU
VAL
ALA
ASP
TRP
SER
SER
GLU
GLY
VAL
GLN
VAL
PRO
SER
SER
VAL
PRO
THR
THR
GLN
PHE
GLN
THR
THR
GLU
ASP
SER
GLU

ASP
TRP
SER
ALA
ALA
PRO
THR
ALA
GLN
ALA
THR
GLU
TRP
VAL
GLY
ALA
THR
THR
ASP
TRP
SER

- Molecule 101: 40S ribosomal protein S21



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	139996	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 ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	3.537	Depositor
Minimum map value	-0.173	Depositor
Average map value	0.034	Depositor
Map value standard deviation	0.144	Depositor
Recommended contour level	0.15	Depositor
Map size (Å)	628.128, 628.128, 628.128	wwPDB
Map dimensions	432, 432, 432	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.454, 1.454, 1.454	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: OMU, OMC, A2M, OMG, ZN, G7M, 4SU, M3L, 1MA, UY1, ACE, ANM, 5MC, 4AC, B8N, UR3, MLZ, MG, 6MZ, V5N, HIC, MA6, PSU

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	A4	0.40	0/317	0.60	0/489
2	A5	0.37	0/167	0.59	1/258 (0.4%)
3	B4	0.21	0/1795	0.27	0/2798
4	B5	0.40	1/1743 (0.1%)	0.31	0/2713
5	D4	0.31	0/1741	0.49	0/2709
6	E4	0.29	0/927	0.74	0/1240
7	E5	0.18	0/1637	0.38	1/2546 (0.0%)
8	L5	0.33	1/85855 (0.0%)	0.39	10/133911 (0.0%)
9	L7	0.32	0/2858	0.34	0/4455
9	M7	0.35	0/2858	0.33	0/4455
10	L8	0.31	0/3701	0.38	0/5766
11	LA	0.33	0/1924	0.56	1/2581 (0.0%)
12	LB	0.30	0/3168	0.51	2/4253 (0.0%)
13	LC	0.30	0/2948	0.47	0/3960
13	MC	0.32	0/2968	0.41	0/3985
14	LD	0.29	0/2333	0.53	1/3139 (0.0%)
14	MD	0.28	0/2437	0.42	2/3263 (0.1%)
15	LE	0.26	0/1747	0.50	0/2354
15	ME	0.29	0/1820	0.45	1/2442 (0.0%)
16	LF	0.30	0/1879	0.54	0/2507
16	MF	0.32	0/1926	0.41	0/2567
17	LG	0.28	0/1765	0.60	3/2400 (0.1%)
17	MG	0.31	0/1959	0.52	0/2637
18	LH	0.30	0/1458	0.52	0/1973
18	MH	0.33	0/1537	0.53	0/2066
19	LI	0.29	0/1620	0.52	2/2170 (0.1%)
20	LJ	0.29	0/1249	0.51	0/1690
20	MJ	0.29	0/1385	0.55	0/1852
21	LL	0.28	0/1611	0.50	0/2167
21	ML	0.30	0/1706	0.44	0/2284
22	LM	0.32	0/1119	0.64	2/1501 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
22	MM	0.31	0/1142	0.49	0/1527
23	LN	0.30	0/1738	0.47	0/2328
23	MN	0.35	0/1745	0.42	0/2338
24	LO	0.34	0/1645	0.54	0/2205
24	MO	0.39	0/1686	0.65	2/2257 (0.1%)
25	LP	0.31	0/1229	0.48	0/1655
25	MP	0.34	0/1279	0.52	0/1716
26	LQ	0.32	0/1517	0.57	2/2030 (0.1%)
26	MQ	0.34	0/1536	0.46	0/2052
27	LR	0.31	0/1428	0.62	1/1897 (0.1%)
27	MR	0.33	0/1582	0.59	0/2091
28	LS	0.31	0/1476	0.50	0/1983
28	MS	0.37	0/1500	0.50	0/2013
29	LT	0.34	0/1296	0.60	0/1734
29	MT	0.35	0/1345	0.67	3/1795 (0.2%)
30	LU	0.31	0/782	0.67	0/1057
30	MU	0.33	0/822	0.72	0/1103
31	LV	0.33	0/968	0.61	0/1303
31	MV	0.36	0/1002	0.62	1/1345 (0.1%)
32	LW	0.30	0/798	0.47	0/1081
32	MW	0.35	0/964	0.63	1/1278 (0.1%)
33	LX	0.31	0/968	0.61	3/1304 (0.2%)
33	MX	0.34	0/983	0.57	0/1323
34	LY	0.30	0/1101	0.60	0/1469
34	MY	0.32	0/1132	0.56	2/1504 (0.1%)
35	LZ	0.28	0/1105	0.49	0/1475
35	MZ	0.34	0/1141	0.55	0/1521
36	La	0.29	0/1173	0.50	0/1568
37	Lb	0.34	0/509	0.57	1/675 (0.1%)
38	Lc	0.34	0/726	0.81	3/977 (0.3%)
38	Mc	0.32	0/780	0.58	2/1046 (0.2%)
39	Ld	0.31	0/871	0.51	0/1176
39	Md	0.36	0/903	0.57	1/1216 (0.1%)
40	Le	0.29	0/1063	0.44	0/1418
40	Me	0.34	0/1082	0.46	0/1443
41	Lf	0.29	0/884	0.54	1/1185 (0.1%)
41	Mf	0.39	0/902	0.48	0/1208
42	Lg	0.30	0/861	0.58	0/1153
42	Mg	0.32	0/916	0.51	0/1220
43	Lh	0.27	0/983	0.52	0/1304
43	Mh	0.32	0/1022	0.60	1/1351 (0.1%)
44	Li	0.29	0/808	0.56	1/1074 (0.1%)
44	Mi	0.29	0/843	0.57	0/1115

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
45	Lj	0.29	0/716	0.45	0/948
45	Mj	0.34	0/731	0.49	0/967
46	Lk	0.31	0/534	0.63	1/712 (0.1%)
46	Mk	0.38	0/574	0.71	0/761
47	Ll	0.29	0/450	0.55	0/595
47	Ml	0.37	0/453	0.46	0/599
48	Lm	0.35	0/399	0.73	3/532 (0.6%)
49	Ln	0.36	0/231	0.81	0/294
49	Mn	0.35	0/240	0.60	0/305
50	Lo	0.27	0/787	0.50	0/1042
51	Lp	0.30	0/700	0.55	0/931
51	Mp	0.34	0/728	0.46	0/967
52	Lr	0.27	0/997	0.49	0/1341
53	M5	0.38	2/82055 (0.0%)	0.37	0/128009
54	M8	0.37	0/3609	0.34	0/5623
55	MA	0.37	0/1958	0.52	0/2623
56	MB	0.37	0/3294	0.49	0/4406
57	MI	0.34	0/1683	0.57	1/2247 (0.0%)
58	Ma	0.32	0/1178	0.49	1/1573 (0.1%)
59	Mb	0.28	0/900	0.46	0/1187
60	Mm	0.34	0/433	0.61	0/575
61	Mo	0.36	0/877	0.54	0/1156
62	Mr	0.32	0/1027	0.41	0/1377
63	Ms	0.22	0/1772	0.56	2/2375 (0.1%)
64	N1	0.25	0/1165	0.54	0/1575
64	N2	0.25	0/955	0.57	1/1291 (0.1%)
65	RA	0.34	0/1785	0.60	1/2426 (0.0%)
66	RB	0.26	0/1920	0.47	2/2568 (0.1%)
66	SB	0.27	0/1654	0.55	0/2227
67	RC	0.31	0/1762	0.56	1/2381 (0.0%)
67	SC	0.27	0/1626	0.49	0/2211
68	RD	0.30	0/1784	0.67	3/2403 (0.1%)
68	SD	0.30	0/1784	0.67	7/2403 (0.3%)
69	RE	0.27	0/2118	0.49	0/2849
69	SE	0.26	0/1933	0.55	1/2623 (0.0%)
70	RF	0.31	0/1446	0.72	2/1944 (0.1%)
70	SF	0.25	0/1385	0.56	0/1870
71	RG	0.23	0/1946	0.52	0/2590
71	SG	0.23	0/1562	0.52	0/2099
72	RH	0.27	0/1540	0.58	0/2064
72	SH	0.27	0/1362	0.61	0/1831
73	RI	0.30	0/1715	0.56	3/2287 (0.1%)
73	SI	0.20	0/1715	0.41	0/2287

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
74	RJ	0.31	0/1550	0.61	0/2069
74	SJ	0.28	0/1432	0.68	0/1926
75	RK	0.36	0/834	0.96	3/1125 (0.3%)
75	SK	0.38	0/759	0.78	0/1036
76	RL	0.29	0/1221	0.47	0/1632
76	SL	0.31	0/1159	0.61	0/1555
77	RM	0.26	0/960	0.70	3/1286 (0.2%)
77	Sf	0.27	0/960	0.69	0/1286
78	RN	0.32	0/1242	0.55	2/1671 (0.1%)
78	SN	0.25	0/1223	0.48	0/1644
79	RO	0.34	0/1022	0.58	0/1372
79	SO	0.33	0/1016	0.68	2/1363 (0.1%)
80	RP	0.26	0/1100	0.66	1/1470 (0.1%)
80	SP	0.33	0/1020	0.78	0/1369
81	RQ	0.38	0/1141	0.75	1/1528 (0.1%)
81	SQ	0.31	0/1096	0.55	0/1473
82	RR	0.41	0/1097	0.88	4/1474 (0.3%)
82	SR	0.40	0/890	0.81	3/1207 (0.2%)
83	RS	0.30	0/1232	0.68	0/1651
83	SS	0.31	0/1098	0.67	0/1480
84	RT	0.31	0/1148	0.65	1/1540 (0.1%)
84	ST	0.29	0/1012	0.54	0/1371
85	RU	0.32	0/813	0.67	0/1092
85	SU	0.46	0/754	0.87	2/1018 (0.2%)
86	RV	0.44	1/644 (0.2%)	0.70	2/862 (0.2%)
87	RW	0.28	0/1051	0.50	0/1406
87	SW	0.38	0/1044	0.73	0/1398
88	RX	0.34	0/1105	0.61	1/1476 (0.1%)
88	SX	0.27	0/1066	0.58	0/1434
89	RY	0.27	0/1083	0.63	0/1438
89	SY	0.22	0/871	0.60	3/1169 (0.3%)
90	RZ	0.34	0/682	0.66	0/911
90	SZ	0.38	0/493	0.76	1/672 (0.1%)
91	Ra	0.41	0/816	0.63	0/1093
91	Sa	0.30	0/775	0.60	0/1042
92	Rb	0.31	0/665	0.59	0/891
92	Sb	0.31	0/665	0.67	0/891
93	Rc	0.31	0/514	0.75	0/688
93	Sc	0.30	0/432	0.65	0/582
94	Rd	0.33	0/469	0.63	0/623
94	Sd	0.32	0/430	0.57	0/573
95	Re	0.26	0/396	0.55	0/519
95	Se	0.29	0/341	0.77	2/449 (0.4%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
96	Rf	0.37	0/525	0.88	3/695 (0.4%)
96	sh	0.27	0/525	0.64	0/695
97	Rg	0.36	0/2524	0.52	1/3433 (0.0%)
97	Sg	0.29	0/2524	0.48	1/3433 (0.0%)
98	S2	0.31	0/41489	0.42	1/64620 (0.0%)
99	S3	0.34	0/37935	0.36	0/59125
100	SA	0.30	0/1612	0.58	0/2203
101	SV	0.30	0/597	0.58	0/800
All	All	0.33	5/454929 (0.0%)	0.46	117/668477 (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
17	LG	0	1
29	LT	0	1
41	Mf	0	1
56	MB	0	1
61	Mo	0	1
65	RA	0	1
68	SD	0	2
75	RK	0	2
84	ST	0	1
88	RX	0	1
All	All	0	12

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B5	21	U	C4-O4	8.36	1.40	1.23
86	RV	0	ACE	C-N	5.92	1.45	1.33
53	M5	3760	A2M	O3'-P	5.40	1.61	1.56
8	L5	1780	A	O3'-P	-5.06	1.53	1.61
53	M5	398	A2M	O3'-P	5.02	1.61	1.56

The worst 5 of 117 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	L5	509	A	P-O3'-C3'	-19.95	90.28	120.20
8	L5	509	A	O3'-P-O5'	-13.19	84.21	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	L5	649	A	P-O3'-C3'	12.82	139.44	120.20
8	L5	1780	A	P-O3'-C3'	10.52	135.98	120.20
68	SD	197	LYS	CA-CB-CG	9.46	133.01	114.10

There are no chirality outliers.

5 of 12 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
17	LG	162	ASP	Peptide
29	LT	126	VAL	Peptide
56	MB	19	ARG	Sidechain
41	Mf	1	MET	Peptide
61	Mo	99	ARG	Sidechain

5.2 Too-close contacts [i](#)

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	A4	287	0	145	0	0
2	A5	150	0	76	0	0
3	B4	1604	0	816	17	0
4	B5	1645	0	842	5	0
5	D4	1559	0	793	14	0
6	E4	921	0	967	13	0
7	E5	1467	0	748	18	0
8	L5	76803	0	38827	436	0
9	L7	2558	0	1296	3	0
9	M7	2558	0	1296	4	0
10	L8	3314	0	1683	21	0
11	LA	1886	0	1973	22	0
12	LB	3101	0	3177	34	0
13	LC	2894	0	3061	23	0
13	MC	2914	0	3087	13	0
14	LD	2287	0	2254	19	0
14	MD	2391	0	2426	15	0
15	LE	1713	0	1812	18	0
15	ME	1786	0	1945	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	LF	1844	0	1961	14	0
16	MF	1885	0	2022	8	0
17	LG	1733	0	1750	10	0
17	MG	1926	0	2074	10	0
18	LH	1439	0	1469	11	0
18	MH	1518	0	1601	10	0
19	LI	1582	0	1574	11	0
20	LJ	1226	0	1168	7	0
20	MJ	1362	0	1399	13	0
21	LL	1580	0	1646	7	0
21	ML	1672	0	1786	10	0
22	LM	1097	0	1142	10	0
22	MM	1120	0	1187	5	0
23	LN	1693	0	1741	23	0
23	MN	1700	0	1749	14	0
24	LO	1613	0	1737	11	0
24	MO	1654	0	1799	11	0
25	LP	1203	0	1210	10	0
25	MP	1249	0	1276	9	0
26	LQ	1493	0	1587	17	0
26	MQ	1512	0	1628	3	0
27	LR	1412	0	1513	15	0
27	MR	1566	0	1729	8	0
28	LS	1436	0	1457	10	0
28	MS	1460	0	1502	11	0
29	LT	1268	0	1309	13	0
29	MT	1311	0	1392	10	0
30	LU	768	0	762	8	0
30	MU	808	0	831	10	0
31	LV	954	0	994	14	0
31	MV	988	0	1047	9	0
32	LW	784	0	662	4	0
32	MW	950	0	999	10	0
33	LX	951	0	1010	9	0
33	MX	966	0	1040	4	0
34	LY	1084	0	1143	9	0
34	MY	1115	0	1205	3	0
35	LZ	1082	0	1152	9	0
35	MZ	1115	0	1195	10	0
36	La	1145	0	1178	9	0
37	Lb	499	0	506	3	0
38	Lc	716	0	740	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	Mc	770	0	809	11	0
39	Ld	856	0	890	7	0
39	Md	888	0	930	6	0
40	Le	1045	0	1133	7	0
40	Me	1061	0	1160	4	0
41	Lf	865	0	888	9	0
41	Mf	883	0	924	6	0
42	Lg	851	0	907	10	0
42	Mg	906	0	1002	10	0
43	Lh	975	0	1081	8	0
43	Mh	1014	0	1148	7	0
44	Li	797	0	859	7	0
44	Mi	832	0	917	4	0
45	Lj	701	0	726	4	0
45	Mj	712	0	748	2	0
46	Lk	528	0	554	3	0
46	Mk	568	0	637	7	0
47	Ll	440	0	472	1	0
47	MI	443	0	483	3	0
48	Lm	393	0	410	2	0
49	Ln	230	0	276	1	0
49	Mn	239	0	289	4	0
50	Lo	774	0	819	7	0
51	Lp	690	0	731	2	0
51	Mp	715	0	773	2	0
52	Lr	982	0	1026	19	0
53	M5	76094	0	38530	391	0
54	M8	3316	0	1687	17	0
55	MA	1930	0	2028	15	0
56	MB	3239	0	3377	22	0
57	MI	1645	0	1693	11	0
58	Ma	1162	0	1205	2	0
59	Mb	898	0	983	12	0
60	Mm	436	0	481	2	0
61	Mo	870	0	940	5	0
62	Mr	1011	0	1084	6	0
63	Ms	1744	0	1859	15	0
64	N1	1140	0	1136	12	0
64	N2	933	0	925	5	0
65	RA	1750	0	1755	24	0
66	RB	1892	0	1960	17	0
66	SB	1627	0	1616	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
67	RC	1725	0	1813	20	0
67	SC	1590	0	1606	17	0
68	RD	1756	0	1852	16	0
68	SD	1756	0	1852	32	0
69	RE	2076	0	2177	22	0
69	SE	1891	0	1867	31	0
70	RF	1426	0	1471	19	0
70	SF	1365	0	1367	11	0
71	RG	1923	0	2089	24	0
71	SG	1544	0	1503	18	0
72	RH	1517	0	1605	12	0
72	SH	1342	0	1382	19	0
73	RI	1686	0	1772	13	0
73	SI	1686	0	1772	17	0
74	RJ	1525	0	1640	15	0
74	SJ	1407	0	1450	25	0
75	RK	810	0	836	19	0
75	SK	736	0	691	14	0
76	RL	1200	0	1271	5	0
76	SL	1139	0	1185	19	0
77	RM	950	0	987	29	0
77	Sf	950	0	987	19	0
78	RN	1214	0	1301	4	0
78	SN	1199	0	1274	8	0
79	RO	1009	0	1034	12	0
79	SO	1003	0	1028	14	0
80	RP	1078	0	1121	21	0
80	SP	1001	0	1011	20	0
81	RQ	1123	0	1193	9	0
81	SQ	1078	0	1124	14	0
82	RR	1082	0	1137	19	0
82	SR	879	0	816	22	0
83	RS	1214	0	1275	20	0
83	SS	1080	0	1092	24	0
84	RT	1121	0	1151	11	0
84	ST	993	0	928	14	0
85	RU	803	0	873	10	0
85	SU	745	0	761	18	0
86	RV	639	0	638	6	0
87	RW	1034	0	1080	8	0
87	SW	1027	0	1067	14	0
88	RX	1087	0	1154	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
88	SX	1048	0	1065	11	0
89	RY	1065	0	1142	15	0
89	SY	855	0	831	16	0
90	RZ	674	0	748	8	0
90	SZ	487	0	453	8	0
91	Ra	800	0	858	4	0
91	Sa	762	0	799	5	0
92	Rb	651	0	672	3	0
92	Sb	651	0	672	6	0
93	Rc	512	0	541	7	0
93	Sc	430	0	425	1	0
94	Rd	458	0	452	8	0
94	Sd	420	0	397	7	0
95	Re	394	0	434	3	0
95	Se	338	0	365	6	0
96	Rf	515	0	525	9	0
96	sh	515	0	525	5	0
97	Rg	2467	0	2424	28	0
97	Sg	2467	0	2424	19	0
98	S2	37129	0	18705	329	0
99	S3	35736	0	18090	249	0
100	SA	1575	0	1533	22	0
101	SV	590	0	566	4	0
102	A4	1	0	0	0	0
102	A5	1	0	0	0	0
102	B5	2	0	0	0	0
102	L5	92	0	0	0	0
102	L7	2	0	0	0	0
102	L8	5	0	0	0	0
102	LQ	1	0	0	0	0
102	LV	1	0	0	0	0
102	Lj	1	0	0	0	0
102	M5	454	0	0	0	0
102	M7	13	0	0	0	0
102	M8	15	0	0	0	0
102	MC	1	0	0	0	0
102	MD	2	0	0	0	0
102	MF	1	0	0	0	0
102	MI	3	0	0	0	0
102	ML	2	0	0	0	0
102	MN	4	0	0	0	0
102	MO	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
102	MP	3	0	0	0	0
102	MQ	1	0	0	0	0
102	MS	2	0	0	0	0
102	MT	1	0	0	0	0
102	MV	1	0	0	0	0
102	MY	1	0	0	0	0
102	Ma	2	0	0	0	0
102	Mc	1	0	0	0	0
102	Me	1	0	0	0	0
102	Mf	2	0	0	0	0
102	Mg	2	0	0	0	0
102	Mj	2	0	0	0	0
102	Mo	1	0	0	0	0
102	Mp	3	0	0	0	0
102	Mr	3	0	0	0	0
102	RE	1	0	0	0	0
102	RG	1	0	0	0	0
102	RN	1	0	0	0	0
102	RO	1	0	0	0	0
102	RS	1	0	0	0	0
102	RT	1	0	0	0	0
102	RU	1	0	0	0	0
102	RX	1	0	0	0	0
102	Rd	1	0	0	0	0
102	S2	57	0	0	0	0
102	S3	134	0	0	0	0
103	Lg	1	0	0	0	0
103	Lj	1	0	0	0	0
103	Lm	1	0	0	0	0
103	Lo	1	0	0	0	0
103	Lp	1	0	0	0	0
103	Sa	1	0	0	0	0
103	Sd	1	0	0	0	0
104	M5	19	0	19	1	0
All	All	428966	0	314845	2901	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 4.

The worst 5 of 2901 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)
53:M5:664:G:H21	53:M5:667:A:N6	1.56	1.04
98:S2:1286:G:N2	98:S2:1313:A:N7	2.08	1.02
98:S2:1748:G:H1	98:S2:1786:U:H3	1.07	0.97
53:M5:664:G:N2	53:M5:667:A:H61	1.63	0.97
98:S2:1729:U:H3	98:S2:1805:G:H1	0.97	0.94

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	E4	113/148 (76%)	109 (96%)	4 (4%)	0	100	100
11	LA	246/257 (96%)	234 (95%)	12 (5%)	0	100	100
12	LB	389/403 (96%)	366 (94%)	23 (6%)	0	100	100
13	LC	363/427 (85%)	350 (96%)	13 (4%)	0	100	100
13	MC	364/427 (85%)	356 (98%)	8 (2%)	0	100	100
14	LD	291/297 (98%)	283 (97%)	8 (3%)	0	100	100
14	MD	292/297 (98%)	286 (98%)	6 (2%)	0	100	100
15	LE	214/288 (74%)	199 (93%)	15 (7%)	0	100	100
15	ME	217/288 (75%)	210 (97%)	7 (3%)	0	100	100
16	LF	223/248 (90%)	215 (96%)	8 (4%)	0	100	100
16	MF	225/248 (91%)	219 (97%)	6 (3%)	0	100	100
17	LG	225/266 (85%)	212 (94%)	13 (6%)	0	100	100
17	MG	239/266 (90%)	228 (95%)	11 (5%)	0	100	100
18	LH	187/192 (97%)	178 (95%)	9 (5%)	0	100	100
18	MH	188/192 (98%)	183 (97%)	5 (3%)	0	100	100
19	LI	199/214 (93%)	193 (97%)	6 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	LJ	165/178 (93%)	161 (98%)	4 (2%)	0	100	100
20	MJ	168/178 (94%)	165 (98%)	3 (2%)	0	100	100
21	LL	202/211 (96%)	193 (96%)	8 (4%)	1 (0%)	24	27
21	ML	205/211 (97%)	199 (97%)	6 (3%)	0	100	100
22	LM	134/215 (62%)	125 (93%)	9 (7%)	0	100	100
22	MM	134/215 (62%)	131 (98%)	3 (2%)	0	100	100
23	LN	201/204 (98%)	197 (98%)	4 (2%)	0	100	100
23	MN	201/204 (98%)	197 (98%)	4 (2%)	0	100	100
24	LO	199/203 (98%)	196 (98%)	3 (2%)	0	100	100
24	MO	200/203 (98%)	199 (100%)	1 (0%)	0	100	100
25	LP	151/184 (82%)	148 (98%)	3 (2%)	0	100	100
25	MP	152/184 (83%)	150 (99%)	2 (1%)	0	100	100
26	LQ	185/188 (98%)	179 (97%)	6 (3%)	0	100	100
26	MQ	185/188 (98%)	182 (98%)	3 (2%)	0	100	100
27	LR	173/196 (88%)	171 (99%)	2 (1%)	0	100	100
27	MR	185/196 (94%)	182 (98%)	3 (2%)	0	100	100
28	LS	173/176 (98%)	162 (94%)	11 (6%)	0	100	100
28	MS	174/176 (99%)	170 (98%)	4 (2%)	0	100	100
29	LT	157/160 (98%)	147 (94%)	10 (6%)	0	100	100
29	MT	159/160 (99%)	154 (97%)	5 (3%)	0	100	100
30	LU	99/128 (77%)	94 (95%)	5 (5%)	0	100	100
30	MU	97/128 (76%)	95 (98%)	1 (1%)	1 (1%)	12	12
31	LV	129/140 (92%)	120 (93%)	9 (7%)	0	100	100
31	MV	131/140 (94%)	129 (98%)	2 (2%)	0	100	100
32	LW	111/157 (71%)	105 (95%)	6 (5%)	0	100	100
32	MW	114/157 (73%)	110 (96%)	4 (4%)	0	100	100
33	LX	118/156 (76%)	111 (94%)	7 (6%)	0	100	100
33	MX	116/156 (74%)	113 (97%)	3 (3%)	0	100	100
34	LY	132/145 (91%)	125 (95%)	7 (5%)	0	100	100
34	MY	132/145 (91%)	129 (98%)	3 (2%)	0	100	100
35	LZ	133/136 (98%)	131 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
35	MZ	134/136 (98%)	131 (98%)	3 (2%)	0	100	100
36	La	142/148 (96%)	133 (94%)	9 (6%)	0	100	100
37	Lb	61/159 (38%)	57 (93%)	4 (7%)	0	100	100
38	Lc	91/115 (79%)	87 (96%)	4 (4%)	0	100	100
38	Mc	97/115 (84%)	96 (99%)	1 (1%)	0	100	100
39	Ld	105/125 (84%)	101 (96%)	4 (4%)	0	100	100
39	Md	105/125 (84%)	104 (99%)	1 (1%)	0	100	100
40	Le	125/135 (93%)	121 (97%)	4 (3%)	0	100	100
40	Me	127/135 (94%)	127 (100%)	0	0	100	100
41	Lf	107/110 (97%)	105 (98%)	2 (2%)	0	100	100
41	Mf	108/110 (98%)	107 (99%)	1 (1%)	0	100	100
42	Lg	108/117 (92%)	105 (97%)	3 (3%)	0	100	100
42	Mg	112/117 (96%)	111 (99%)	1 (1%)	0	100	100
43	Lh	119/123 (97%)	118 (99%)	1 (1%)	0	100	100
43	Mh	120/123 (98%)	118 (98%)	2 (2%)	0	100	100
44	Li	99/105 (94%)	98 (99%)	1 (1%)	0	100	100
44	Mi	100/105 (95%)	99 (99%)	1 (1%)	0	100	100
45	Lj	84/97 (87%)	82 (98%)	2 (2%)	0	100	100
45	Mj	85/97 (88%)	83 (98%)	2 (2%)	0	100	100
46	Lk	67/70 (96%)	65 (97%)	2 (3%)	0	100	100
46	Mk	67/70 (96%)	67 (100%)	0	0	100	100
47	Ll	48/51 (94%)	46 (96%)	2 (4%)	0	100	100
47	Ml	48/51 (94%)	47 (98%)	1 (2%)	0	100	100
48	Lm	48/128 (38%)	48 (100%)	0	0	100	100
49	Ln	22/25 (88%)	22 (100%)	0	0	100	100
49	Mn	23/25 (92%)	23 (100%)	0	0	100	100
50	Lo	96/106 (91%)	93 (97%)	3 (3%)	0	100	100
51	Lp	89/92 (97%)	86 (97%)	3 (3%)	0	100	100
51	Mp	90/92 (98%)	87 (97%)	3 (3%)	0	100	100
52	Lr	123/137 (90%)	118 (96%)	5 (4%)	0	100	100
55	MA	249/257 (97%)	240 (96%)	9 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
56	MB	399/403 (99%)	388 (97%)	11 (3%)	0	100	100
57	MI	199/214 (93%)	196 (98%)	3 (2%)	0	100	100
58	Ma	144/148 (97%)	138 (96%)	5 (4%)	1 (1%)	18	20
59	Mb	106/159 (67%)	102 (96%)	4 (4%)	0	100	100
60	Mm	50/128 (39%)	50 (100%)	0	0	100	100
61	Mo	103/106 (97%)	101 (98%)	2 (2%)	0	100	100
62	Mr	125/137 (91%)	125 (100%)	0	0	100	100
63	Ms	215/217 (99%)	204 (95%)	10 (5%)	1 (0%)	24	27
64	N1	133/800 (17%)	129 (97%)	4 (3%)	0	100	100
64	N2	110/800 (14%)	104 (94%)	6 (6%)	0	100	100
65	RA	221/295 (75%)	215 (97%)	5 (2%)	1 (0%)	24	27
66	RB	228/264 (86%)	226 (99%)	2 (1%)	0	100	100
66	SB	212/264 (80%)	205 (97%)	7 (3%)	0	100	100
67	RC	220/293 (75%)	214 (97%)	6 (3%)	0	100	100
67	SC	215/293 (73%)	213 (99%)	2 (1%)	0	100	100
68	RD	224/243 (92%)	212 (95%)	12 (5%)	0	100	100
68	SD	224/243 (92%)	213 (95%)	10 (4%)	1 (0%)	30	34
69	RE	260/263 (99%)	251 (96%)	9 (4%)	0	100	100
69	SE	255/263 (97%)	239 (94%)	16 (6%)	0	100	100
70	RF	176/204 (86%)	172 (98%)	3 (2%)	1 (1%)	21	24
70	SF	176/204 (86%)	170 (97%)	6 (3%)	0	100	100
71	RG	235/249 (94%)	229 (97%)	6 (3%)	0	100	100
71	SG	200/249 (80%)	189 (94%)	11 (6%)	0	100	100
72	RH	187/194 (96%)	180 (96%)	7 (4%)	0	100	100
72	SH	168/194 (87%)	162 (96%)	6 (4%)	0	100	100
73	RI	204/208 (98%)	195 (96%)	9 (4%)	0	100	100
73	SI	204/208 (98%)	194 (95%)	10 (5%)	0	100	100
74	RJ	183/194 (94%)	175 (96%)	8 (4%)	0	100	100
74	SJ	174/194 (90%)	167 (96%)	7 (4%)	0	100	100
75	RK	94/165 (57%)	91 (97%)	3 (3%)	0	100	100
75	SK	93/165 (56%)	84 (90%)	7 (8%)	2 (2%)	5	3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
76	RL	142/158 (90%)	136 (96%)	6 (4%)	0	100	100
76	SL	136/158 (86%)	124 (91%)	12 (9%)	0	100	100
77	RM	120/132 (91%)	113 (94%)	7 (6%)	0	100	100
77	Sf	120/132 (91%)	113 (94%)	7 (6%)	0	100	100
78	RN	149/151 (99%)	147 (99%)	2 (1%)	0	100	100
78	SN	148/151 (98%)	144 (97%)	4 (3%)	0	100	100
79	RO	133/151 (88%)	123 (92%)	9 (7%)	1 (1%)	16	17
79	SO	133/151 (88%)	127 (96%)	6 (4%)	0	100	100
80	RP	129/145 (89%)	125 (97%)	4 (3%)	0	100	100
80	SP	123/145 (85%)	117 (95%)	6 (5%)	0	100	100
81	RQ	139/146 (95%)	133 (96%)	6 (4%)	0	100	100
81	SQ	139/146 (95%)	130 (94%)	9 (6%)	0	100	100
82	RR	132/135 (98%)	123 (93%)	9 (7%)	0	100	100
82	SR	123/135 (91%)	113 (92%)	10 (8%)	0	100	100
83	RS	146/152 (96%)	142 (97%)	4 (3%)	0	100	100
83	SS	136/152 (90%)	124 (91%)	11 (8%)	1 (1%)	18	20
84	RT	142/145 (98%)	136 (96%)	6 (4%)	0	100	100
84	ST	139/145 (96%)	136 (98%)	2 (1%)	1 (1%)	18	20
85	RU	99/119 (83%)	96 (97%)	3 (3%)	0	100	100
85	SU	95/119 (80%)	86 (90%)	7 (7%)	2 (2%)	5	4
86	RV	82/84 (98%)	79 (96%)	3 (4%)	0	100	100
87	RW	127/130 (98%)	123 (97%)	4 (3%)	0	100	100
87	SW	127/130 (98%)	119 (94%)	8 (6%)	0	100	100
88	RX	138/143 (96%)	133 (96%)	5 (4%)	0	100	100
88	SX	139/143 (97%)	127 (91%)	12 (9%)	0	100	100
89	RY	129/133 (97%)	126 (98%)	3 (2%)	0	100	100
89	SY	111/133 (84%)	108 (97%)	3 (3%)	0	100	100
90	RZ	82/125 (66%)	74 (90%)	7 (8%)	1 (1%)	10	9
90	SZ	68/125 (54%)	66 (97%)	2 (3%)	0	100	100
91	Ra	98/115 (85%)	96 (98%)	2 (2%)	0	100	100
91	Sa	97/115 (84%)	91 (94%)	6 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
92	Rb	81/84 (96%)	76 (94%)	5 (6%)	0	100	100
92	Sb	81/84 (96%)	76 (94%)	5 (6%)	0	100	100
93	Rc	63/69 (91%)	60 (95%)	3 (5%)	0	100	100
93	Sc	59/69 (86%)	58 (98%)	1 (2%)	0	100	100
94	Rd	53/56 (95%)	52 (98%)	1 (2%)	0	100	100
94	Sd	50/56 (89%)	50 (100%)	0	0	100	100
95	Re	46/133 (35%)	44 (96%)	1 (2%)	1 (2%)	5	3
95	Se	42/133 (32%)	40 (95%)	2 (5%)	0	100	100
96	Rf	61/156 (39%)	55 (90%)	6 (10%)	0	100	100
96	sh	61/156 (39%)	56 (92%)	5 (8%)	0	100	100
97	Rg	315/317 (99%)	297 (94%)	18 (6%)	0	100	100
97	Sg	315/317 (99%)	303 (96%)	12 (4%)	0	100	100
100	SA	210/295 (71%)	201 (96%)	9 (4%)	0	100	100
101	SV	81/83 (98%)	79 (98%)	2 (2%)	0	100	100
All	All	22865/27490 (83%)	22026 (96%)	823 (4%)	16 (0%)	49	59

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
21	LL	47	ALA
79	RO	138	ASP
58	Ma	15	VAL
63	Ms	197	ASN
75	SK	36	ALA

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	
6	E4	99/121 (82%)	98 (99%)	1 (1%)	68	81
11	LA	187/199 (94%)	182 (97%)	5 (3%)	39	52

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	LB	324/349 (93%)	316 (98%)	8 (2%)	42	55
13	LC	301/348 (86%)	298 (99%)	3 (1%)	68	81
13	MC	305/348 (88%)	304 (100%)	1 (0%)	86	92
14	LD	218/250 (87%)	210 (96%)	8 (4%)	30	40
14	MD	247/250 (99%)	247 (100%)	0	100	100
15	LE	179/252 (71%)	175 (98%)	4 (2%)	45	59
15	ME	196/252 (78%)	195 (100%)	1 (0%)	81	89
16	LF	187/215 (87%)	186 (100%)	1 (0%)	81	89
16	MF	196/215 (91%)	196 (100%)	0	100	100
17	LG	167/223 (75%)	164 (98%)	3 (2%)	51	66
17	MG	203/223 (91%)	202 (100%)	1 (0%)	81	89
18	LH	150/171 (88%)	145 (97%)	5 (3%)	33	44
18	MH	169/171 (99%)	169 (100%)	0	100	100
19	LI	156/181 (86%)	154 (99%)	2 (1%)	61	76
20	LJ	113/149 (76%)	108 (96%)	5 (4%)	25	33
20	MJ	143/149 (96%)	141 (99%)	2 (1%)	59	73
21	LL	152/177 (86%)	149 (98%)	3 (2%)	48	63
21	ML	173/177 (98%)	170 (98%)	3 (2%)	53	68
22	LM	110/161 (68%)	105 (96%)	5 (4%)	24	32
22	MM	116/161 (72%)	115 (99%)	1 (1%)	70	82
23	LN	169/172 (98%)	167 (99%)	2 (1%)	63	77
23	MN	171/172 (99%)	170 (99%)	1 (1%)	78	87
24	LO	163/174 (94%)	158 (97%)	5 (3%)	35	47
24	MO	173/174 (99%)	172 (99%)	1 (1%)	78	87
25	LP	124/163 (76%)	121 (98%)	3 (2%)	43	57
25	MP	135/163 (83%)	135 (100%)	0	100	100
26	LQ	159/165 (96%)	157 (99%)	2 (1%)	61	76
26	MQ	164/165 (99%)	161 (98%)	3 (2%)	51	66
27	LR	141/175 (81%)	139 (99%)	2 (1%)	59	73
27	MR	166/175 (95%)	165 (99%)	1 (1%)	78	87
28	LS	151/157 (96%)	145 (96%)	6 (4%)	28	37

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
28	MS	157/157 (100%)	156 (99%)	1 (1%)	78	87
29	LT	130/140 (93%)	128 (98%)	2 (2%)	57	72
29	MT	141/140 (101%)	138 (98%)	3 (2%)	47	61
30	LU	77/115 (67%)	71 (92%)	6 (8%)	11	12
30	MU	89/115 (77%)	87 (98%)	2 (2%)	45	59
31	LV	94/107 (88%)	89 (95%)	5 (5%)	20	25
31	MV	102/107 (95%)	102 (100%)	0	100	100
32	LW	54/126 (43%)	52 (96%)	2 (4%)	30	40
32	MW	95/126 (75%)	94 (99%)	1 (1%)	65	79
33	LX	98/133 (74%)	95 (97%)	3 (3%)	35	47
33	MX	106/133 (80%)	105 (99%)	1 (1%)	70	82
34	LY	116/135 (86%)	113 (97%)	3 (3%)	40	54
34	MY	124/135 (92%)	122 (98%)	2 (2%)	55	70
35	LZ	109/118 (92%)	104 (95%)	5 (5%)	24	31
35	MZ	118/118 (100%)	115 (98%)	3 (2%)	42	55
36	La	116/121 (96%)	112 (97%)	4 (3%)	32	43
37	Lb	49/126 (39%)	48 (98%)	1 (2%)	48	63
38	Lc	76/97 (78%)	71 (93%)	5 (7%)	15	17
38	Mc	84/97 (87%)	82 (98%)	2 (2%)	43	57
39	Ld	88/110 (80%)	85 (97%)	3 (3%)	32	43
39	Md	98/110 (89%)	95 (97%)	3 (3%)	35	47
40	Le	113/121 (93%)	112 (99%)	1 (1%)	70	82
40	Me	115/121 (95%)	114 (99%)	1 (1%)	70	82
41	Lf	85/89 (96%)	83 (98%)	2 (2%)	43	57
41	Mf	89/89 (100%)	88 (99%)	1 (1%)	65	79
42	Lg	88/100 (88%)	80 (91%)	8 (9%)	9	9
42	Mg	98/100 (98%)	97 (99%)	1 (1%)	68	81
43	Lh	100/110 (91%)	99 (99%)	1 (1%)	68	81
43	Mh	109/110 (99%)	107 (98%)	2 (2%)	51	66
44	Li	79/89 (89%)	79 (100%)	0	100	100
44	Mi	86/89 (97%)	83 (96%)	3 (4%)	32	42

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
45	Lj	72/80 (90%)	72 (100%)	0	100	100
45	Mj	74/80 (92%)	74 (100%)	0	100	100
46	Lk	52/65 (80%)	51 (98%)	1 (2%)	50	65
46	Mk	64/65 (98%)	62 (97%)	2 (3%)	35	47
47	Ll	46/48 (96%)	45 (98%)	1 (2%)	45	59
47	Ml	47/48 (98%)	47 (100%)	0	100	100
48	Lm	42/116 (36%)	42 (100%)	0	100	100
49	Ln	23/24 (96%)	23 (100%)	0	100	100
49	Mn	24/24 (100%)	24 (100%)	0	100	100
50	Lo	79/94 (84%)	77 (98%)	2 (2%)	42	55
51	Lp	70/75 (93%)	68 (97%)	2 (3%)	37	49
51	Mp	75/75 (100%)	75 (100%)	0	100	100
52	Lr	103/121 (85%)	101 (98%)	2 (2%)	50	65
55	MA	193/198 (98%)	193 (100%)	0	100	100
56	MB	347/348 (100%)	347 (100%)	0	100	100
57	MI	173/181 (96%)	170 (98%)	3 (2%)	53	68
58	Ma	119/120 (99%)	117 (98%)	2 (2%)	53	68
59	Mb	90/125 (72%)	89 (99%)	1 (1%)	65	79
60	Mm	48/115 (42%)	47 (98%)	1 (2%)	47	61
61	Mo	93/93 (100%)	93 (100%)	0	100	100
62	Mr	110/120 (92%)	108 (98%)	2 (2%)	51	66
63	Ms	196/196 (100%)	194 (99%)	2 (1%)	68	81
64	N1	125/718 (17%)	124 (99%)	1 (1%)	73	84
64	N2	102/718 (14%)	102 (100%)	0	100	100
65	RA	184/242 (76%)	180 (98%)	4 (2%)	45	59
66	RB	212/231 (92%)	206 (97%)	6 (3%)	38	51
66	SB	162/231 (70%)	158 (98%)	4 (2%)	42	55
67	RC	188/225 (84%)	185 (98%)	3 (2%)	55	70
67	SC	155/225 (69%)	150 (97%)	5 (3%)	34	46
68	RD	189/202 (94%)	185 (98%)	4 (2%)	47	61
68	SD	189/202 (94%)	186 (98%)	3 (2%)	55	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
69	RE	224/225 (100%)	221 (99%)	3 (1%)	61	76
69	SE	176/225 (78%)	170 (97%)	6 (3%)	32	43
70	RF	153/170 (90%)	147 (96%)	6 (4%)	28	39
70	SF	133/170 (78%)	130 (98%)	3 (2%)	44	58
71	RG	207/218 (95%)	207 (100%)	0	100	100
71	SG	136/218 (62%)	135 (99%)	1 (1%)	76	86
72	RH	168/174 (97%)	163 (97%)	5 (3%)	36	48
72	SH	134/174 (77%)	131 (98%)	3 (2%)	45	59
73	RI	178/180 (99%)	176 (99%)	2 (1%)	65	79
73	SI	178/180 (99%)	176 (99%)	2 (1%)	65	79
74	RJ	161/168 (96%)	158 (98%)	3 (2%)	50	65
74	SJ	140/168 (83%)	137 (98%)	3 (2%)	47	61
75	RK	87/136 (64%)	85 (98%)	2 (2%)	44	58
75	SK	68/136 (50%)	64 (94%)	4 (6%)	18	22
76	RL	132/142 (93%)	129 (98%)	3 (2%)	44	58
76	SL	124/142 (87%)	117 (94%)	7 (6%)	19	23
77	RM	104/108 (96%)	98 (94%)	6 (6%)	18	22
77	Sf	104/108 (96%)	104 (100%)	0	100	100
78	RN	131/131 (100%)	129 (98%)	2 (2%)	57	72
78	SN	127/131 (97%)	125 (98%)	2 (2%)	55	70
79	RO	105/119 (88%)	99 (94%)	6 (6%)	18	23
79	SO	103/119 (87%)	101 (98%)	2 (2%)	50	65
80	RP	117/130 (90%)	116 (99%)	1 (1%)	70	82
80	SP	103/130 (79%)	98 (95%)	5 (5%)	22	28
81	RQ	117/121 (97%)	115 (98%)	2 (2%)	53	68
81	SQ	105/121 (87%)	102 (97%)	3 (3%)	37	49
82	RR	121/122 (99%)	118 (98%)	3 (2%)	42	55
82	SR	77/122 (63%)	73 (95%)	4 (5%)	21	25
83	RS	128/132 (97%)	125 (98%)	3 (2%)	44	58
83	SS	103/132 (78%)	101 (98%)	2 (2%)	50	65
84	RT	114/115 (99%)	113 (99%)	1 (1%)	70	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
84	ST	82/115 (71%)	79 (96%)	3 (4%)	30	40
85	RU	93/107 (87%)	91 (98%)	2 (2%)	45	59
85	SU	78/107 (73%)	72 (92%)	6 (8%)	12	13
86	RV	67/67 (100%)	66 (98%)	1 (2%)	57	72
87	RW	112/113 (99%)	111 (99%)	1 (1%)	70	82
87	SW	110/113 (97%)	107 (97%)	3 (3%)	39	52
88	RX	112/115 (97%)	109 (97%)	3 (3%)	39	52
88	SX	101/115 (88%)	97 (96%)	4 (4%)	28	37
89	RY	113/115 (98%)	110 (97%)	3 (3%)	39	52
89	SY	79/115 (69%)	78 (99%)	1 (1%)	61	76
90	RZ	74/103 (72%)	71 (96%)	3 (4%)	27	36
90	SZ	40/103 (39%)	37 (92%)	3 (8%)	12	13
91	Ra	87/98 (89%)	85 (98%)	2 (2%)	44	58
91	Sa	79/98 (81%)	74 (94%)	5 (6%)	16	19
92	Rb	75/76 (99%)	74 (99%)	1 (1%)	61	76
92	Sb	75/76 (99%)	74 (99%)	1 (1%)	61	76
93	Rc	58/62 (94%)	56 (97%)	2 (3%)	32	43
93	Sc	41/62 (66%)	41 (100%)	0	100	100
94	Rd	48/49 (98%)	47 (98%)	1 (2%)	47	61
94	Sd	42/49 (86%)	41 (98%)	1 (2%)	43	57
95	Re	40/104 (38%)	40 (100%)	0	100	100
95	Se	32/104 (31%)	32 (100%)	0	100	100
96	Rf	56/140 (40%)	56 (100%)	0	100	100
96	sh	56/140 (40%)	56 (100%)	0	100	100
97	Rg	275/275 (100%)	274 (100%)	1 (0%)	84	91
97	Sg	275/275 (100%)	274 (100%)	1 (0%)	84	91
100	SA	147/243 (60%)	144 (98%)	3 (2%)	48	63
101	SV	53/67 (79%)	52 (98%)	1 (2%)	50	65
All	All	19094/23459 (81%)	18731 (98%)	363 (2%)	49	65

5 of 363 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
77	RM	91	LEU
68	SD	224	SER
79	RO	105	THR
89	RY	24	VAL
73	SI	46	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 192 such sidechains are listed below:

Mol	Chain	Res	Type
68	RD	22	ASN
100	SA	110	ASN
69	RE	224	ASN
80	RP	54	HIS
70	SF	95	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A4	13/14 (92%)	3 (23%)	0
10	L8	155/156 (99%)	37 (23%)	2 (1%)
2	A5	6/8 (75%)	2 (33%)	0
3	B4	74/150 (49%)	15 (20%)	0
4	B5	76/77 (98%)	8 (10%)	0
5	D4	70/152 (46%)	26 (37%)	1 (1%)
53	M5	3531/5069 (69%)	588 (16%)	6 (0%)
54	M8	155/156 (99%)	26 (16%)	0
7	E5	67/75 (89%)	15 (22%)	1 (1%)
8	L5	3564/5070 (70%)	766 (21%)	14 (0%)
9	L7	119/120 (99%)	15 (12%)	0
9	M7	119/120 (99%)	8 (6%)	0
98	S2	1717/1869 (91%)	442 (25%)	14 (0%)
99	S3	1667/1869 (89%)	298 (17%)	5 (0%)
All	All	11333/14905 (76%)	2249 (19%)	43 (0%)

5 of 2249 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A4	52	U
1	A4	53	U
1	A4	54	U
2	A5	34	C

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Mol	Chain	Res	Type
2	A5	36	U

5 of 43 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
98	S2	732	U
98	S2	1664	A
98	S2	746	C
98	S2	1273	C
98	S2	1860	A

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

230 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	$\# Z > 2$
53	OMG	M5	1625	53	23,26,27	3.00	5 (21%)	33,38,41	1.80	10 (30%)
99	OMG	S3	436	99	23,26,27	2.97	5 (21%)	33,38,41	1.96	10 (30%)
99	MA6	S3	1851	102,99	23,26,27	1.34	3 (13%)	34,38,41	2.35	9 (26%)
99	OMG	S3	601	99	23,26,27	2.97	4 (17%)	33,38,41	1.78	10 (30%)
99	A2M	S3	1383	99	22,25,26	0.17	0	31,36,39	0.46	0
53	OMG	M5	4637	53	23,26,27	2.97	5 (21%)	33,38,41	1.87	10 (30%)
53	A2M	M5	4571	53	22,25,26	0.17	0	31,36,39	0.46	0
56	HIC	MB	245	56	10,11,12	0.66	0	8,14,16	0.45	0
53	OMC	M5	2351	102,53	19,22,23	2.02	4 (21%)	26,31,34	1.63	4 (15%)
53	OMG	M5	2424	53	23,26,27	3.00	5 (21%)	33,38,41	1.79	8 (24%)
99	PSU	S3	1238	99	18,21,22	2.39	6 (33%)	22,30,33	1.83	4 (18%)
53	A2M	M5	1871	102,53	22,25,26	0.16	0	31,36,39	0.49	0
53	OMC	M5	2365	102,53	19,22,23	0.27	0	26,31,34	0.37	0
53	OMC	M5	3808	53	19,22,23	2.07	5 (26%)	26,31,34	1.05	1 (3%)
99	OMG	S3	867	99	23,26,27	2.99	4 (17%)	33,38,41	1.81	10 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
53	5MC	M5	3782	102,53	18,22,23	2.07	5 (27%)	26,32,35	1.21	2 (7%)
53	OMG	M5	3744	53	23,26,27	2.96	5 (21%)	33,38,41	1.79	10 (30%)
99	PSU	S3	863	99	18,21,22	2.38	5 (27%)	22,30,33	1.85	4 (18%)
53	A2M	M5	398	53	22,25,26	0.17	0	31,36,39	0.48	0
53	OMU	M5	4620	53	19,22,23	2.39	5 (26%)	26,31,34	1.82	5 (19%)
53	OMC	M5	3841	53	19,22,23	2.03	3 (15%)	26,31,34	0.98	2 (7%)
99	OMU	S3	172	99	19,22,23	2.34	5 (26%)	26,31,34	1.88	5 (19%)
53	PSU	M5	4312	102,53	18,21,22	2.39	6 (33%)	22,30,33	1.81	3 (13%)
99	PSU	S3	1347	99	18,21,22	2.41	6 (33%)	22,30,33	1.81	3 (13%)
53	PSU	M5	1677	53	18,21,22	2.34	7 (38%)	22,30,33	1.84	4 (18%)
53	OMC	M5	2422	102,53	19,22,23	1.98	3 (15%)	26,31,34	1.33	3 (11%)
53	A2M	M5	3785	53	22,25,26	0.21	0	31,36,39	0.40	0
99	OMC	S3	1391	99	19,22,23	1.98	3 (15%)	26,31,34	1.13	1 (3%)
53	PSU	M5	4442	53	18,21,22	2.45	6 (33%)	22,30,33	1.95	4 (18%)
53	A2M	M5	2815	102,53	22,25,26	0.18	0	31,36,39	0.36	0
53	PSU	M5	3851	53	18,21,22	2.36	6 (33%)	22,30,33	1.85	3 (13%)
99	PSU	S3	1136	99	18,21,22	2.39	6 (33%)	22,30,33	1.91	3 (13%)
53	OMG	M5	3792	53	23,26,27	2.95	5 (21%)	33,38,41	1.92	10 (30%)
99	PSU	S3	1056	99	18,21,22	2.38	6 (33%)	22,30,33	1.89	4 (18%)
53	A2M	M5	3724	53	22,25,26	0.18	0	31,36,39	0.36	0
99	OMC	S3	462	99	19,22,23	1.98	4 (21%)	26,31,34	1.04	1 (3%)
53	OMC	M5	2804	53	19,22,23	2.02	4 (21%)	26,31,34	0.96	2 (7%)
53	PSU	M5	4576	53	18,21,22	2.39	6 (33%)	22,30,33	1.81	3 (13%)
53	A2M	M5	400	53	22,25,26	0.16	0	31,36,39	0.39	0
53	UY1	M5	3818	53	19,22,23	1.95	5 (26%)	22,31,34	1.99	4 (18%)
4	G7M	B5	47	4	23,26,27	2.37	5 (21%)	35,39,42	1.76	7 (20%)
53	PSU	M5	3639	53	18,21,22	2.43	6 (33%)	22,30,33	1.82	4 (18%)
99	OMG	S3	1490	102,99	23,26,27	2.98	4 (17%)	33,38,41	1.76	9 (27%)
53	PSU	M5	4628	53	18,21,22	2.35	6 (33%)	22,30,33	1.81	3 (13%)
53	OMU	M5	4306	53	19,22,23	2.36	5 (26%)	26,31,34	1.86	6 (23%)
99	PSU	S3	649	99	18,21,22	2.44	6 (33%)	22,30,33	1.82	3 (13%)
53	PSU	M5	1781	53	18,21,22	2.38	6 (33%)	22,30,33	1.75	4 (18%)
99	PSU	S3	105	99	18,21,22	2.35	6 (33%)	22,30,33	1.81	3 (13%)
99	PSU	S3	1081	99	18,21,22	2.28	6 (33%)	22,30,33	1.84	5 (22%)
99	PSU	S3	573	99	18,21,22	2.37	6 (33%)	22,30,33	1.74	3 (13%)
99	OMU	S3	1288	99	19,22,23	2.26	5 (26%)	26,31,34	1.76	6 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
99	PSU	S3	1625	99	18,21,22	2.33	6 (33%)	22,30,33	1.81	4 (18%)
53	PSU	M5	1744	53	18,21,22	2.36	6 (33%)	22,30,33	1.74	4 (18%)
99	A2M	S3	166	99	22,25,26	0.16	0	31,36,39	0.42	0
99	PSU	S3	36	99	18,21,22	2.34	6 (33%)	22,30,33	1.82	3 (13%)
99	A2M	S3	27	102,99	22,25,26	0.17	0	31,36,39	0.45	0
53	OMU	M5	4227	53	19,22,23	2.35	5 (26%)	26,31,34	1.95	6 (23%)
99	PSU	S3	866	99	18,21,22	2.36	6 (33%)	22,30,33	1.88	4 (18%)
53	6MZ	M5	4220	53	22,25,26	2.35	4 (18%)	30,36,39	2.39	11 (36%)
99	4AC	S3	1337	99	21,24,25	2.08	7 (33%)	29,34,37	1.18	3 (10%)
53	PSU	M5	1683	53	18,21,22	2.46	6 (33%)	22,30,33	1.89	3 (13%)
53	PSU	M5	5010	53	18,21,22	2.37	6 (33%)	22,30,33	1.78	3 (13%)
53	OMG	M5	4618	53	23,26,27	2.98	5 (21%)	33,38,41	1.91	11 (33%)
99	OMC	S3	174	102,99	19,22,23	1.95	3 (15%)	26,31,34	1.06	1 (3%)
99	MA6	S3	1850	99	23,26,27	1.34	3 (13%)	34,38,41	2.26	9 (26%)
54	PSU	M8	55	54	18,21,22	2.38	6 (33%)	22,30,33	1.92	3 (13%)
53	PSU	M5	3715	53	18,21,22	2.40	6 (33%)	22,30,33	1.85	4 (18%)
53	OMG	M5	4196	102,53,4	23,26,27	2.98	4 (17%)	33,38,41	1.83	10 (30%)
99	PSU	S3	109	99	18,21,22	2.40	6 (33%)	22,30,33	1.90	4 (18%)
53	PSU	M5	3695	53	18,21,22	2.38	6 (33%)	22,30,33	1.88	3 (13%)
99	PSU	S3	822	99	18,21,22	2.33	6 (33%)	22,30,33	1.86	4 (18%)
53	OMG	M5	2876	53	23,26,27	2.96	5 (21%)	33,38,41	1.92	9 (27%)
53	PSU	M5	3920	102,53	18,21,22	2.46	6 (33%)	22,30,33	1.83	4 (18%)
99	PSU	S3	686	99	18,21,22	2.43	6 (33%)	22,30,33	1.91	3 (13%)
53	A2M	M5	3867	53	22,25,26	0.19	0	31,36,39	0.35	0
99	PSU	S3	801	99	18,21,22	2.35	6 (33%)	22,30,33	1.91	4 (18%)
59	MLZ	Mb	5	59	8,9,10	0.80	0	4,9,11	0.61	0
53	PSU	M5	3844	53	18,21,22	2.50	6 (33%)	22,30,33	1.68	4 (18%)
53	PSU	M5	4431	53	18,21,22	2.46	6 (33%)	22,30,33	1.92	3 (13%)
99	PSU	S3	1174	99	18,21,22	2.38	6 (33%)	22,30,33	1.87	4 (18%)
99	PSU	S3	1445	99	18,21,22	2.37	6 (33%)	22,30,33	1.87	5 (22%)
53	PSU	M5	1860	53	18,21,22	2.47	6 (33%)	22,30,33	1.75	3 (13%)
99	PSU	S3	1243	99	18,21,22	2.39	6 (33%)	22,30,33	1.84	4 (18%)
53	OMU	M5	2415	53	19,22,23	2.31	6 (31%)	26,31,34	1.96	6 (23%)
53	PSU	M5	1536	53	18,21,22	2.48	6 (33%)	22,30,33	1.90	4 (18%)
53	A2M	M5	2363	102,53	22,25,26	0.17	0	31,36,39	0.34	0
53	PSU	M5	3770	53	18,21,22	2.36	6 (33%)	22,30,33	1.89	3 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
99	OMG	S3	1447	99	23,26,27	2.99	5 (21%)	33,38,41	1.87	10 (30%)
53	A2M	M5	2401	102,53	22,25,26	0.17	0	31,36,39	0.40	0
53	OMG	M5	4499	53	23,26,27	2.95	4 (17%)	33,38,41	1.85	10 (30%)
99	PSU	S3	815	99	18,21,22	2.37	6 (33%)	22,30,33	1.86	4 (18%)
8	OMG	L5	3944	8	23,26,27	0.31	0	33,38,41	0.38	0
53	OMG	M5	2364	53	23,26,27	0.29	0	33,38,41	0.40	0
99	A2M	S3	99	102,99	22,25,26	0.16	0	31,36,39	0.39	0
99	PSU	S3	651	99	18,21,22	2.36	6 (33%)	22,30,33	1.85	3 (13%)
55	V5N	MA	216	55	9,11,12	0.94	0	9,14,16	1.09	1 (11%)
99	PSU	S3	93	99	18,21,22	2.32	6 (33%)	22,30,33	1.78	4 (18%)
99	A2M	S3	576	99	22,25,26	0.18	0	31,36,39	0.33	0
99	PSU	S3	1692	99	18,21,22	2.42	6 (33%)	22,30,33	1.83	4 (18%)
53	PSU	M5	4531	53	18,21,22	2.39	6 (33%)	22,30,33	1.87	4 (18%)
53	PSU	M5	4420	53	18,21,22	2.30	6 (33%)	22,30,33	1.80	5 (22%)
53	OMU	M5	4498	102,53	19,22,23	2.36	5 (26%)	26,31,34	1.89	5 (19%)
53	PSU	M5	4471	53	18,21,22	2.43	6 (33%)	22,30,33	1.75	3 (13%)
53	PSU	M5	3762	53	18,21,22	0.88	1 (5%)	22,30,33	0.57	0
53	PSU	M5	4579	53	18,21,22	2.38	6 (33%)	22,30,33	1.77	3 (13%)
53	PSU	M5	4361	53	18,21,22	2.42	6 (33%)	22,30,33	1.83	4 (18%)
53	A2M	M5	4523	102,53	22,25,26	0.16	0	31,36,39	0.57	0
53	OMC	M5	2824	53	19,22,23	2.02	4 (21%)	26,31,34	1.04	1 (3%)
53	PSU	M5	3768	53	18,21,22	2.39	6 (33%)	22,30,33	1.81	4 (18%)
53	A2M	M5	3723	53	22,25,26	0.16	0	31,36,39	0.34	0
99	PSU	S3	966	99	18,21,22	2.43	6 (33%)	22,30,33	1.86	4 (18%)
99	OMC	S3	1703	102,99	19,22,23	1.99	3 (15%)	26,31,34	0.99	1 (3%)
53	PSU	M5	4569	53	18,21,22	2.46	6 (33%)	22,30,33	1.81	4 (18%)
99	OMU	S3	428	99	19,22,23	2.33	5 (26%)	26,31,34	1.87	5 (19%)
99	A2M	S3	668	102,99	22,25,26	0.23	0	31,36,39	0.47	0
53	OMU	M5	3925	53	19,22,23	2.37	5 (26%)	26,31,34	1.92	6 (23%)
99	OMU	S3	627	99	19,22,23	2.33	5 (26%)	26,31,34	1.87	5 (19%)
99	A2M	S3	512	99	22,25,26	0.16	0	31,36,39	0.46	0
99	PSU	S3	681	99	18,21,22	2.44	6 (33%)	22,30,33	1.80	3 (13%)
53	A2M	M5	3718	53	22,25,26	0.18	0	31,36,39	0.55	0
53	PSU	M5	3637	53	18,21,22	2.43	6 (33%)	22,30,33	1.78	3 (13%)
53	PSU	M5	4552	53	18,21,22	2.46	6 (33%)	22,30,33	1.81	3 (13%)
54	OMU	M8	14	53,54	19,22,23	2.42	6 (31%)	26,31,34	1.97	7 (26%)
99	PSU	S3	1244	99	18,21,22	2.34	6 (33%)	22,30,33	1.83	4 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
53	PSU	M5	4500	53	18,21,22	2.41	6 (33%)	22,30,33	1.88	3 (13%)
99	6MZ	S3	1832	102,99	22,25,26	2.52	3 (13%)	30,36,39	2.41	11 (36%)
53	OMG	M5	3627	53	23,26,27	2.94	5 (21%)	33,38,41	1.97	11 (33%)
53	PSU	M5	4972	53	18,21,22	2.42	6 (33%)	22,30,33	1.89	4 (18%)
99	PSU	S3	1367	99	18,21,22	2.40	6 (33%)	22,30,33	1.81	4 (18%)
53	PSU	M5	4403	53	18,21,22	2.40	6 (33%)	22,30,33	1.90	5 (22%)
53	A2M	M5	1534	102,53	22,25,26	0.22	0	31,36,39	0.53	0
99	OMG	S3	509	102,99	23,26,27	2.97	4 (17%)	33,38,41	1.81	8 (24%)
53	PSU	M5	4353	53	18,21,22	2.40	6 (33%)	22,30,33	1.88	3 (13%)
99	A2M	S3	159	99	22,25,26	0.18	0	31,36,39	0.40	0
99	PSU	S3	1177	99	18,21,22	2.36	6 (33%)	22,30,33	1.92	3 (13%)
99	PSU	S3	1232	99	18,21,22	2.40	6 (33%)	22,30,33	1.88	4 (18%)
99	OMU	S3	1442	102,99	19,22,23	2.36	6 (31%)	26,31,34	1.92	6 (23%)
53	PSU	M5	4493	53	18,21,22	2.44	6 (33%)	22,30,33	1.86	3 (13%)
53	OMC	M5	1881	102,53	19,22,23	2.07	5 (26%)	26,31,34	1.07	1 (3%)
53	5MC	M5	4447	53	18,22,23	2.15	6 (33%)	26,32,35	1.37	2 (7%)
53	OMG	M5	4392	53	23,26,27	2.89	5 (21%)	33,38,41	1.87	10 (30%)
53	OMG	M5	4228	53	23,26,27	2.97	6 (26%)	33,38,41	1.89	11 (33%)
53	PSU	M5	4293	53	18,21,22	2.43	6 (33%)	22,30,33	1.89	3 (13%)
53	PSU	M5	2632	53	18,21,22	2.33	6 (33%)	22,30,33	1.82	4 (18%)
53	PSU	M5	4673	53	18,21,22	2.44	6 (33%)	22,30,33	1.78	3 (13%)
53	PSU	M5	4636	102,53	18,21,22	2.37	6 (33%)	22,30,33	1.84	4 (18%)
99	PSU	S3	814	99	18,21,22	2.32	6 (33%)	22,30,33	1.82	3 (13%)
53	PSU	M5	2843	53	18,21,22	2.39	6 (33%)	22,30,33	1.92	4 (18%)
99	OMU	S3	116	99	19,22,23	2.34	5 (26%)	26,31,34	1.82	5 (19%)
53	OMC	M5	1340	53	19,22,23	2.03	5 (26%)	26,31,34	1.02	2 (7%)
53	PSU	M5	2508	53	18,21,22	2.37	6 (33%)	22,30,33	1.77	4 (18%)
53	PSU	M5	3729	53	18,21,22	2.38	5 (27%)	22,30,33	2.03	4 (18%)
54	OMG	M8	75	54	23,26,27	2.98	5 (21%)	33,38,41	1.85	10 (30%)
8	PSU	L5	1779	8	18,21,22	0.88	1 (5%)	22,30,33	0.72	1 (4%)
53	PSU	M5	3764	53	18,21,22	2.33	6 (33%)	22,30,33	1.77	3 (13%)
99	PSU	S3	119	99	18,21,22	2.30	6 (33%)	22,30,33	1.86	4 (18%)
53	A2M	M5	4590	53	22,25,26	0.18	0	31,36,39	0.43	0
53	A2M	M5	3760	53,99	22,25,26	0.23	0	31,36,39	0.53	0
53	UR3	M5	4530	53	19,22,23	3.08	7 (36%)	26,32,35	1.23	2 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
99	PSU	S3	609	99	18,21,22	2.40	6 (33%)	22,30,33	1.82	3 (13%)
53	PSU	M5	2839	53	18,21,22	2.36	6 (33%)	22,30,33	1.80	5 (22%)
99	A2M	S3	1031	99	22,25,26	0.17	0	31,36,39	0.43	0
53	PSU	M5	1582	53	18,21,22	2.45	6 (33%)	22,30,33	1.83	3 (13%)
99	A2M	S3	468	99	22,25,26	0.16	0	31,36,39	0.42	0
99	PSU	S3	918	99	18,21,22	2.40	6 (33%)	22,30,33	1.90	4 (18%)
53	OMG	M5	3899	102,53	23,26,27	2.96	5 (21%)	33,38,41	1.87	10 (30%)
99	OMC	S3	517	99	19,22,23	1.98	3 (15%)	26,31,34	1.13	1 (3%)
54	PSU	M8	69	102,54	18,21,22	2.35	6 (33%)	22,30,33	1.84	5 (22%)
99	PSU	S3	34	99	18,21,22	2.33	6 (33%)	22,30,33	1.79	3 (13%)
99	PSU	S3	406	99	18,21,22	2.45	6 (33%)	22,30,33	1.86	4 (18%)
53	PSU	M5	1792	53	18,21,22	2.26	6 (33%)	22,30,33	1.88	4 (18%)
53	A2M	M5	3830	53	22,25,26	0.19	0	31,36,39	0.40	0
53	OMC	M5	4456	53	19,22,23	2.12	4 (21%)	26,31,34	1.17	2 (7%)
53	PSU	M5	4532	53	18,21,22	2.44	6 (33%)	22,30,33	1.86	4 (18%)
53	OMC	M5	3887	102,53	19,22,23	2.01	4 (21%)	26,31,34	1.13	1 (3%)
99	OMU	S3	354	99	19,22,23	2.34	5 (26%)	26,31,34	1.90	6 (23%)
99	PSU	S3	572	99	18,21,22	2.35	6 (33%)	22,30,33	1.83	4 (18%)
4	4SU	B5	8	4	18,21,22	3.52	6 (33%)	26,30,33	1.95	5 (19%)
53	A2M	M5	2787	102,53	22,25,26	0.23	0	31,36,39	0.59	0
99	PSU	S3	296	99	18,21,22	2.33	6 (33%)	22,30,33	1.82	3 (13%)
53	A2M	M5	1326	53	22,25,26	0.18	0	31,36,39	0.41	0
53	PSU	M5	4689	53	18,21,22	2.49	6 (33%)	22,30,33	1.70	5 (22%)
53	OMC	M5	2861	53	19,22,23	2.01	3 (15%)	26,31,34	1.07	1 (3%)
53	PSU	M5	5001	102,53	18,21,22	2.40	6 (33%)	22,30,33	1.83	3 (13%)
53	A2M	M5	3825	53	22,25,26	0.18	0	31,36,39	0.38	0
99	4AC	S3	1842	99	21,24,25	2.17	7 (33%)	29,34,37	1.24	5 (17%)
99	A2M	S3	484	99	22,25,26	0.17	0	31,36,39	0.37	0
53	OMU	M5	2837	53	19,22,23	2.32	5 (26%)	26,31,34	1.88	6 (23%)
53	PSU	M5	1782	53	18,21,22	2.40	6 (33%)	22,30,33	1.86	4 (18%)
53	OMG	M5	1316	53	23,26,27	3.00	5 (21%)	33,38,41	1.77	9 (27%)
53	PSU	M5	4457	53	18,21,22	2.40	6 (33%)	22,30,33	1.86	4 (18%)
99	A2M	S3	1678	99	22,25,26	0.18	0	31,36,39	0.32	0
60	M3L	Mm	98	60	10,11,12	0.50	0	9,14,16	0.36	0
99	G7M	S3	1639	4,99	23,26,27	2.44	5 (21%)	35,39,42	1.68	7 (20%)
99	B8N	S3	1248	99	24,29,30	2.35	8 (33%)	29,42,45	1.78	6 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
53	PSU	M5	3884	53	18,21,22	2.52	7 (38%)	22,30,33	1.74	4 (18%)
53	PSU	M5	4296	53	18,21,22	2.34	6 (33%)	22,30,33	1.92	4 (18%)
53	PSU	M5	4423	53	18,21,22	2.35	6 (33%)	22,30,33	1.83	3 (13%)
99	PSU	S3	1004	99	18,21,22	2.45	6 (33%)	22,30,33	1.76	3 (13%)
53	OMG	M5	4623	53	23,26,27	2.95	5 (21%)	33,38,41	1.89	10 (30%)
53	PSU	M5	3758	53	18,21,22	0.91	1 (5%)	22,30,33	0.69	1 (4%)
99	OMU	S3	121	99	19,22,23	2.32	5 (26%)	26,31,34	1.83	5 (19%)
99	UY1	S3	1326	102,99	19,22,23	1.85	5 (26%)	22,31,34	2.04	4 (18%)
99	PSU	S3	1239	99	18,21,22	2.38	6 (33%)	22,30,33	1.80	3 (13%)
4	OMC	B5	33	4	19,22,23	1.92	4 (21%)	26,31,34	1.29	3 (11%)
53	OMG	M5	4494	102,53	23,26,27	2.98	5 (21%)	33,38,41	1.78	10 (30%)
99	PSU	S3	1643	102,99	18,21,22	2.36	6 (33%)	22,30,33	1.77	4 (18%)
53	OMG	M5	1522	53	23,26,27	2.96	5 (21%)	33,38,41	1.94	10 (30%)
53	PSU	M5	1862	53	18,21,22	2.35	6 (33%)	22,30,33	1.94	4 (18%)
53	PSU	M5	3734	53	18,21,22	2.35	6 (33%)	22,30,33	1.81	3 (13%)
53	OMC	M5	3869	53	19,22,23	0.26	0	26,31,34	0.43	0
99	OMG	S3	1328	99	23,26,27	2.97	4 (17%)	33,38,41	1.81	10 (30%)
53	OMG	M5	3944	53	23,26,27	2.98	4 (17%)	33,38,41	1.93	10 (30%)
53	OMC	M5	4536	53	19,22,23	2.00	4 (21%)	26,31,34	1.14	2 (7%)
58	V5N	Ma	39	58	9,11,12	1.12	1 (11%)	9,14,16	1.48	2 (22%)
4	PSU	B5	56	4	18,21,22	2.35	6 (33%)	22,30,33	1.80	4 (18%)
53	PSU	M5	4299	53	18,21,22	2.49	6 (33%)	22,30,33	1.77	3 (13%)
99	A2M	S3	590	99	22,25,26	0.20	0	31,36,39	0.48	0
99	OMG	S3	683	99	23,26,27	2.97	4 (17%)	33,38,41	1.87	10 (30%)
99	OMG	S3	644	99	23,26,27	2.96	4 (17%)	33,38,41	1.90	10 (30%)
99	OMU	S3	1804	99	19,22,23	2.32	5 (26%)	26,31,34	1.87	6 (23%)
53	1MA	M5	1322	102,53	21,25,26	1.70	3 (14%)	31,37,40	1.84	7 (22%)
53	PSU	M5	4521	102,53	18,21,22	2.43	7 (38%)	22,30,33	1.90	4 (18%)
61	MLZ	Mo	53	61	8,9,10	0.80	0	4,9,11	0.64	0
53	A2M	M5	1524	53	22,25,26	0.26	0	31,36,39	0.61	1 (3%)
99	PSU	S3	218	99	18,21,22	2.36	6 (33%)	22,30,33	1.83	3 (13%)
53	OMG	M5	4370	53	23,26,27	2.97	5 (21%)	33,38,41	1.88	10 (30%)
53	PSU	M5	1779	53	18,21,22	2.39	6 (33%)	22,30,33	1.87	3 (13%)
53	OMC	M5	3701	53	19,22,23	2.02	3 (15%)	26,31,34	0.89	1 (3%)
53	PSU	M5	3853	102,53	18,21,22	2.40	6 (33%)	22,30,33	1.84	4 (18%)

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
53	OMG	M5	1625	53	-	1/9/27/28	0/3/3/3
99	OMG	S3	436	99	-	0/9/27/28	0/3/3/3
99	MA6	S3	1851	102,99	-	3/11/29/30	0/3/3/3
99	OMG	S3	601	99	-	0/9/27/28	0/3/3/3
99	A2M	S3	1383	99	-	4/9/27/28	0/3/3/3
53	OMG	M5	4637	53	-	3/9/27/28	0/3/3/3
53	A2M	M5	4571	53	-	1/9/27/28	0/3/3/3
56	HIC	MB	245	56	-	0/5/6/8	0/1/1/1
53	OMC	M5	2351	102,53	-	4/9/27/28	0/2/2/2
53	OMG	M5	2424	53	-	0/9/27/28	0/3/3/3
99	PSU	S3	1238	99	-	0/7/25/26	0/2/2/2
53	A2M	M5	1871	102,53	-	0/9/27/28	0/3/3/3
53	OMC	M5	2365	102,53	-	1/9/27/28	0/2/2/2
53	OMC	M5	3808	53	-	0/9/27/28	0/2/2/2
99	OMG	S3	867	99	-	1/9/27/28	0/3/3/3
53	5MC	M5	3782	102,53	-	2/7/25/26	0/2/2/2
53	OMG	M5	3744	53	-	0/9/27/28	0/3/3/3
99	PSU	S3	863	99	-	0/7/25/26	0/2/2/2
53	A2M	M5	398	53	-	0/9/27/28	0/3/3/3
53	OMU	M5	4620	53	-	0/9/27/28	0/2/2/2
53	OMC	M5	3841	53	-	0/9/27/28	0/2/2/2
99	OMU	S3	172	99	-	0/9/27/28	0/2/2/2
53	PSU	M5	4312	102,53	-	0/7/25/26	0/2/2/2
99	PSU	S3	1347	99	-	0/7/25/26	0/2/2/2
53	PSU	M5	1677	53	-	3/7/25/26	0/2/2/2
53	OMC	M5	2422	102,53	-	2/9/27/28	0/2/2/2
53	A2M	M5	3785	53	-	4/9/27/28	0/3/3/3
99	OMC	S3	1391	99	-	0/9/27/28	0/2/2/2
53	PSU	M5	4442	53	-	0/7/25/26	0/2/2/2
53	A2M	M5	2815	102,53	-	4/9/27/28	0/3/3/3
53	PSU	M5	3851	53	-	2/7/25/26	0/2/2/2
99	PSU	S3	1136	99	-	0/7/25/26	0/2/2/2
53	OMG	M5	3792	53	-	0/9/27/28	0/3/3/3
99	PSU	S3	1056	99	-	0/7/25/26	0/2/2/2
53	A2M	M5	3724	53	-	1/9/27/28	0/3/3/3
99	OMC	S3	462	99	-	0/9/27/28	0/2/2/2
53	OMC	M5	2804	53	-	0/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
53	PSU	M5	4576	53	-	0/7/25/26	0/2/2/2
53	A2M	M5	400	53	-	0/9/27/28	0/3/3/3
53	UY1	M5	3818	53	-	2/9/27/28	0/2/2/2
4	G7M	B5	47	4	-	0/7/25/26	0/3/3/3
53	PSU	M5	3639	53	-	0/7/25/26	0/2/2/2
99	OMG	S3	1490	102,99	-	2/9/27/28	0/3/3/3
53	PSU	M5	4628	53	-	0/7/25/26	0/2/2/2
53	OMU	M5	4306	53	-	0/9/27/28	0/2/2/2
99	PSU	S3	649	99	-	0/7/25/26	0/2/2/2
53	PSU	M5	1781	53	-	2/7/25/26	0/2/2/2
99	PSU	S3	105	99	-	0/7/25/26	0/2/2/2
99	PSU	S3	1081	99	-	1/7/25/26	0/2/2/2
99	PSU	S3	573	99	-	0/7/25/26	0/2/2/2
99	OMU	S3	1288	99	-	0/9/27/28	0/2/2/2
99	PSU	S3	1625	99	-	0/7/25/26	0/2/2/2
53	PSU	M5	1744	53	-	0/7/25/26	0/2/2/2
99	A2M	S3	166	99	-	1/9/27/28	0/3/3/3
99	PSU	S3	36	99	-	0/7/25/26	0/2/2/2
99	A2M	S3	27	102,99	-	0/9/27/28	0/3/3/3
53	OMU	M5	4227	53	-	0/9/27/28	0/2/2/2
99	PSU	S3	866	99	-	0/7/25/26	0/2/2/2
53	6MZ	M5	4220	53	-	0/9/27/28	0/3/3/3
99	4AC	S3	1337	99	-	2/11/29/30	0/2/2/2
53	PSU	M5	1683	53	-	0/7/25/26	0/2/2/2
53	PSU	M5	5010	53	-	0/7/25/26	0/2/2/2
53	OMG	M5	4618	53	-	1/9/27/28	0/3/3/3
99	OMC	S3	174	102,99	-	0/9/27/28	0/2/2/2
99	MA6	S3	1850	99	-	0/11/29/30	0/3/3/3
54	PSU	M8	55	54	-	0/7/25/26	0/2/2/2
53	PSU	M5	3715	53	-	0/7/25/26	0/2/2/2
53	OMG	M5	4196	102,53,4	-	1/9/27/28	0/3/3/3
99	PSU	S3	109	99	-	0/7/25/26	0/2/2/2
53	PSU	M5	3695	53	-	0/7/25/26	0/2/2/2
99	PSU	S3	822	99	-	0/7/25/26	0/2/2/2
53	OMG	M5	2876	53	-	0/9/27/28	0/3/3/3
53	PSU	M5	3920	102,53	-	0/7/25/26	0/2/2/2
99	PSU	S3	686	99	-	0/7/25/26	0/2/2/2
53	A2M	M5	3867	53	-	2/9/27/28	0/3/3/3
99	PSU	S3	801	99	-	0/7/25/26	0/2/2/2
59	MLZ	Mb	5	59	-	3/7/8/10	-
53	PSU	M5	3844	53	-	1/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
53	PSU	M5	4431	53	-	0/7/25/26	0/2/2/2
99	PSU	S3	1174	99	-	0/7/25/26	0/2/2/2
99	PSU	S3	1445	99	-	0/7/25/26	0/2/2/2
53	PSU	M5	1860	53	-	0/7/25/26	0/2/2/2
99	PSU	S3	1243	99	-	2/7/25/26	0/2/2/2
53	OMU	M5	2415	53	-	0/9/27/28	0/2/2/2
53	PSU	M5	1536	53	-	0/7/25/26	0/2/2/2
53	A2M	M5	2363	102,53	-	0/9/27/28	0/3/3/3
53	PSU	M5	3770	53	-	0/7/25/26	0/2/2/2
99	OMG	S3	1447	99	-	2/9/27/28	0/3/3/3
53	A2M	M5	2401	102,53	-	1/9/27/28	0/3/3/3
53	OMG	M5	4499	53	-	0/9/27/28	0/3/3/3
99	PSU	S3	815	99	-	0/7/25/26	0/2/2/2
8	OMG	L5	3944	8	-	2/9/27/28	0/3/3/3
53	OMG	M5	2364	53	-	1/9/27/28	0/3/3/3
99	A2M	S3	99	102,99	-	2/9/27/28	0/3/3/3
99	PSU	S3	651	99	-	0/7/25/26	0/2/2/2
55	V5N	MA	216	55	-	1/9/10/12	0/1/1/1
99	PSU	S3	93	99	-	0/7/25/26	0/2/2/2
99	A2M	S3	576	99	-	3/9/27/28	0/3/3/3
99	PSU	S3	1692	99	-	0/7/25/26	0/2/2/2
53	PSU	M5	4531	53	-	0/7/25/26	0/2/2/2
53	PSU	M5	4420	53	-	0/7/25/26	0/2/2/2
53	OMU	M5	4498	102,53	-	0/9/27/28	0/2/2/2
53	PSU	M5	4471	53	-	0/7/25/26	0/2/2/2
53	PSU	M5	3762	53	-	0/7/25/26	0/2/2/2
53	PSU	M5	4579	53	-	0/7/25/26	0/2/2/2
53	PSU	M5	4361	53	-	0/7/25/26	0/2/2/2
53	A2M	M5	4523	102,53	-	2/9/27/28	0/3/3/3
53	OMC	M5	2824	53	-	0/9/27/28	0/2/2/2
53	PSU	M5	3768	53	-	0/7/25/26	0/2/2/2
53	A2M	M5	3723	53	-	1/9/27/28	0/3/3/3
99	PSU	S3	966	99	-	0/7/25/26	0/2/2/2
99	OMC	S3	1703	102,99	-	1/9/27/28	0/2/2/2
53	PSU	M5	4569	53	-	0/7/25/26	0/2/2/2
99	OMU	S3	428	99	-	6/9/27/28	0/2/2/2
99	A2M	S3	668	102,99	-	4/9/27/28	0/3/3/3
53	OMU	M5	3925	53	-	0/9/27/28	0/2/2/2
99	OMU	S3	627	99	-	0/9/27/28	0/2/2/2
99	A2M	S3	512	99	-	2/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
99	PSU	S3	681	99	-	0/7/25/26	0/2/2/2
53	A2M	M5	3718	53	-	1/9/27/28	0/3/3/3
53	PSU	M5	3637	53	-	0/7/25/26	0/2/2/2
53	PSU	M5	4552	53	-	0/7/25/26	0/2/2/2
54	OMU	M8	14	53,54	-	1/9/27/28	0/2/2/2
99	PSU	S3	1244	99	-	0/7/25/26	0/2/2/2
53	PSU	M5	4500	53	-	1/7/25/26	0/2/2/2
99	6MZ	S3	1832	102,99	-	2/9/27/28	0/3/3/3
53	OMG	M5	3627	53	-	0/9/27/28	0/3/3/3
53	PSU	M5	4972	53	-	0/7/25/26	0/2/2/2
99	PSU	S3	1367	99	-	0/7/25/26	0/2/2/2
53	PSU	M5	4403	53	-	0/7/25/26	0/2/2/2
53	A2M	M5	1534	102,53	-	2/9/27/28	0/3/3/3
99	OMG	S3	509	102,99	-	1/9/27/28	0/3/3/3
53	PSU	M5	4353	53	-	0/7/25/26	0/2/2/2
99	A2M	S3	159	99	-	0/9/27/28	0/3/3/3
99	PSU	S3	1177	99	-	0/7/25/26	0/2/2/2
99	PSU	S3	1232	99	-	0/7/25/26	0/2/2/2
99	OMU	S3	1442	102,99	-	3/9/27/28	0/2/2/2
53	PSU	M5	4493	53	-	0/7/25/26	0/2/2/2
53	OMC	M5	1881	102,53	-	0/9/27/28	0/2/2/2
53	5MC	M5	4447	53	-	4/7/25/26	0/2/2/2
53	OMG	M5	4392	53	-	0/9/27/28	0/3/3/3
53	OMG	M5	4228	53	-	2/9/27/28	0/3/3/3
53	PSU	M5	4293	53	-	0/7/25/26	0/2/2/2
53	PSU	M5	2632	53	-	0/7/25/26	0/2/2/2
53	PSU	M5	4673	53	-	0/7/25/26	0/2/2/2
53	PSU	M5	4636	102,53	-	4/7/25/26	0/2/2/2
99	PSU	S3	814	99	-	0/7/25/26	0/2/2/2
53	PSU	M5	2843	53	-	0/7/25/26	0/2/2/2
99	OMU	S3	116	99	-	0/9/27/28	0/2/2/2
53	OMC	M5	1340	53	-	0/9/27/28	0/2/2/2
53	PSU	M5	2508	53	-	0/7/25/26	0/2/2/2
53	PSU	M5	3729	53	-	2/7/25/26	0/2/2/2
54	OMG	M8	75	54	-	1/9/27/28	0/3/3/3
8	PSU	L5	1779	8	-	0/7/25/26	0/2/2/2
53	PSU	M5	3764	53	-	0/7/25/26	0/2/2/2
99	PSU	S3	119	99	-	0/7/25/26	0/2/2/2
53	A2M	M5	4590	53	-	1/9/27/28	0/3/3/3
53	A2M	M5	3760	53,99	-	6/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
53	UR3	M5	4530	53	-	0/7/25/26	0/2/2/2
99	PSU	S3	609	99	-	0/7/25/26	0/2/2/2
53	PSU	M5	2839	53	-	0/7/25/26	0/2/2/2
99	A2M	S3	1031	99	-	3/9/27/28	0/3/3/3
53	PSU	M5	1582	53	-	0/7/25/26	0/2/2/2
99	A2M	S3	468	99	-	1/9/27/28	0/3/3/3
99	PSU	S3	918	99	-	2/7/25/26	0/2/2/2
53	OMG	M5	3899	102,53	-	0/9/27/28	0/3/3/3
99	OMC	S3	517	99	-	0/9/27/28	0/2/2/2
54	PSU	M8	69	102,54	-	0/7/25/26	0/2/2/2
99	PSU	S3	34	99	-	0/7/25/26	0/2/2/2
99	PSU	S3	406	99	-	0/7/25/26	0/2/2/2
53	PSU	M5	1792	53	-	0/7/25/26	0/2/2/2
53	A2M	M5	3830	53	-	3/9/27/28	0/3/3/3
53	OMC	M5	4456	53	-	0/9/27/28	0/2/2/2
53	PSU	M5	4532	53	-	0/7/25/26	0/2/2/2
53	OMC	M5	3887	102,53	-	1/9/27/28	0/2/2/2
99	OMU	S3	354	99	-	0/9/27/28	0/2/2/2
99	PSU	S3	572	99	-	0/7/25/26	0/2/2/2
4	4SU	B5	8	4	-	0/7/25/26	0/2/2/2
53	A2M	M5	2787	102,53	-	4/9/27/28	0/3/3/3
99	PSU	S3	296	99	-	0/7/25/26	0/2/2/2
53	A2M	M5	1326	53	-	1/9/27/28	0/3/3/3
53	PSU	M5	4689	53	-	0/7/25/26	0/2/2/2
53	OMC	M5	2861	53	-	0/9/27/28	0/2/2/2
53	PSU	M5	5001	102,53	-	0/7/25/26	0/2/2/2
53	A2M	M5	3825	53	-	0/9/27/28	0/3/3/3
99	4AC	S3	1842	99	-	0/11/29/30	0/2/2/2
99	A2M	S3	484	99	-	0/9/27/28	0/3/3/3
53	OMU	M5	2837	53	-	0/9/27/28	0/2/2/2
53	PSU	M5	1782	53	-	0/7/25/26	0/2/2/2
53	OMG	M5	1316	53	-	0/9/27/28	0/3/3/3
53	PSU	M5	4457	53	-	0/7/25/26	0/2/2/2
99	A2M	S3	1678	99	-	1/9/27/28	0/3/3/3
60	M3L	Mm	98	60	-	0/9/10/12	-
99	G7M	S3	1639	4,99	-	0/7/25/26	0/3/3/3
99	B8N	S3	1248	99	-	5/16/34/35	0/2/2/2
53	PSU	M5	3884	53	-	0/7/25/26	0/2/2/2
53	PSU	M5	4296	53	-	0/7/25/26	0/2/2/2
53	PSU	M5	4423	53	-	0/7/25/26	0/2/2/2
99	PSU	S3	1004	99	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
53	OMG	M5	4623	53	-	0/9/27/28	0/3/3/3
53	PSU	M5	3758	53	-	0/7/25/26	0/2/2/2
99	OMU	S3	121	99	-	0/9/27/28	0/2/2/2
99	UY1	S3	1326	102,99	-	2/9/27/28	0/2/2/2
99	PSU	S3	1239	99	-	0/7/25/26	0/2/2/2
4	OMC	B5	33	4	-	0/9/27/28	0/2/2/2
53	OMG	M5	4494	102,53	-	2/9/27/28	0/3/3/3
99	PSU	S3	1643	102,99	-	0/7/25/26	0/2/2/2
53	OMG	M5	1522	53	-	0/9/27/28	0/3/3/3
53	PSU	M5	1862	53	-	0/7/25/26	0/2/2/2
53	PSU	M5	3734	53	-	0/7/25/26	0/2/2/2
53	OMC	M5	3869	53	-	0/9/27/28	0/2/2/2
99	OMG	S3	1328	99	-	0/9/27/28	0/3/3/3
53	OMG	M5	3944	53	-	1/9/27/28	0/3/3/3
53	OMC	M5	4536	53	-	0/9/27/28	0/2/2/2
58	V5N	Ma	39	58	-	2/9/10/12	0/1/1/1
4	PSU	B5	56	4	-	0/7/25/26	0/2/2/2
53	PSU	M5	4299	53	-	0/7/25/26	0/2/2/2
99	A2M	S3	590	99	-	5/9/27/28	0/3/3/3
99	OMG	S3	683	99	-	2/9/27/28	0/3/3/3
99	OMG	S3	644	99	-	3/9/27/28	0/3/3/3
99	OMU	S3	1804	99	-	0/9/27/28	0/2/2/2
53	1MA	M5	1322	102,53	-	0/7/25/26	0/3/3/3
53	PSU	M5	4521	102,53	-	1/7/25/26	0/2/2/2
61	MLZ	Mo	53	61	-	1/7/8/10	-
53	A2M	M5	1524	53	-	1/9/27/28	0/3/3/3
99	PSU	S3	218	99	-	0/7/25/26	0/2/2/2
53	OMG	M5	4370	53	-	0/9/27/28	0/3/3/3
53	PSU	M5	1779	53	-	0/7/25/26	0/2/2/2
53	OMC	M5	3701	53	-	4/9/27/28	0/2/2/2
53	PSU	M5	3853	102,53	-	0/7/25/26	0/2/2/2

The worst 5 of 994 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	M5	3944	OMG	O6-C6	10.91	1.44	1.23
99	S3	867	OMG	O6-C6	10.91	1.44	1.23
53	M5	1625	OMG	O6-C6	10.89	1.44	1.23
99	S3	509	OMG	O6-C6	10.86	1.44	1.23
53	M5	2424	OMG	O6-C6	10.82	1.44	1.23

The worst 5 of 884 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
99	S3	1832	6MZ	C5-C4-N3	-6.20	118.66	126.75
53	M5	4227	OMU	N3-C2-N1	6.20	123.12	114.89
53	M5	4220	6MZ	C9-N6-C6	-6.17	117.56	122.87
99	S3	1326	UY1	N1-C2-N3	6.05	121.98	115.13
53	M5	4442	PSU	N1-C2-N3	6.00	121.93	115.13

There are no chirality outliers.

5 of 160 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
55	MA	216	V5N	O-C-CA-CB
59	Mb	5	MLZ	N-CA-CB-CG
59	Mb	5	MLZ	C-CA-CB-CG
8	L5	3944	OMG	O4'-C4'-C5'-O5'
8	L5	3944	OMG	C3'-C4'-C5'-O5'

There are no ring outliers.

69 monomers are involved in 107 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
99	S3	601	OMG	1	0
99	S3	1383	A2M	4	0
53	M5	4637	OMG	1	0
53	M5	4571	A2M	1	0
53	M5	2351	OMC	2	0
53	M5	1871	A2M	2	0
53	M5	2365	OMC	1	0
99	S3	867	OMG	1	0
53	M5	3782	5MC	1	0
53	M5	3744	OMG	1	0
53	M5	398	A2M	2	0
53	M5	4620	OMU	1	0
53	M5	1677	PSU	1	0
53	M5	4442	PSU	1	0
53	M5	2815	A2M	2	0
53	M5	3724	A2M	1	0
99	S3	462	OMC	1	0
99	S3	649	PSU	2	0
99	S3	166	A2M	1	0
99	S3	27	A2M	2	0
53	M5	4220	6MZ	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
99	S3	1337	4AC	1	0
53	M5	1683	PSU	1	0
99	S3	1850	MA6	1	0
53	M5	4196	OMG	1	0
53	M5	3867	A2M	3	0
99	S3	801	PSU	1	0
53	M5	2415	OMU	2	0
53	M5	1536	PSU	1	0
53	M5	2363	A2M	3	0
8	L5	3944	OMG	1	0
53	M5	2364	OMG	1	0
99	S3	99	A2M	2	0
99	S3	576	A2M	2	0
99	S3	1692	PSU	1	0
53	M5	4531	PSU	1	0
53	M5	4523	A2M	1	0
53	M5	2824	OMC	1	0
53	M5	3723	A2M	2	0
99	S3	1703	OMC	1	0
53	M5	3925	OMU	1	0
99	S3	512	A2M	5	0
99	S3	681	PSU	1	0
53	M5	3718	A2M	4	0
53	M5	4552	PSU	1	0
54	M8	14	OMU	1	0
53	M5	1534	A2M	2	0
99	S3	509	OMG	1	0
53	M5	4353	PSU	1	0
99	S3	159	A2M	4	0
99	S3	1442	OMU	1	0
99	S3	116	OMU	1	0
53	M5	1340	OMC	1	0
53	M5	3764	PSU	1	0
53	M5	3760	A2M	4	0
99	S3	609	PSU	1	0
99	S3	1031	A2M	2	0
99	S3	468	A2M	2	0
53	M5	3830	A2M	3	0
53	M5	4456	OMC	1	0
53	M5	3887	OMC	2	0
53	M5	1326	A2M	3	0
53	M5	3825	A2M	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
99	S3	1842	4AC	1	0
99	S3	1678	A2M	1	0
99	S3	1639	G7M	1	0
99	S3	1804	OMU	1	0
61	Mo	53	MLZ	1	0
53	M5	1524	A2M	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 838 ligands modelled in this entry, 837 are monoatomic - leaving 1 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	$\# Z > 2$
104	ANM	M5	5481	-	20,20,20	0.40	0	22,27,27	0.76	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
104	ANM	M5	5481	-	-	2/10/23/23	0/2/2/2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

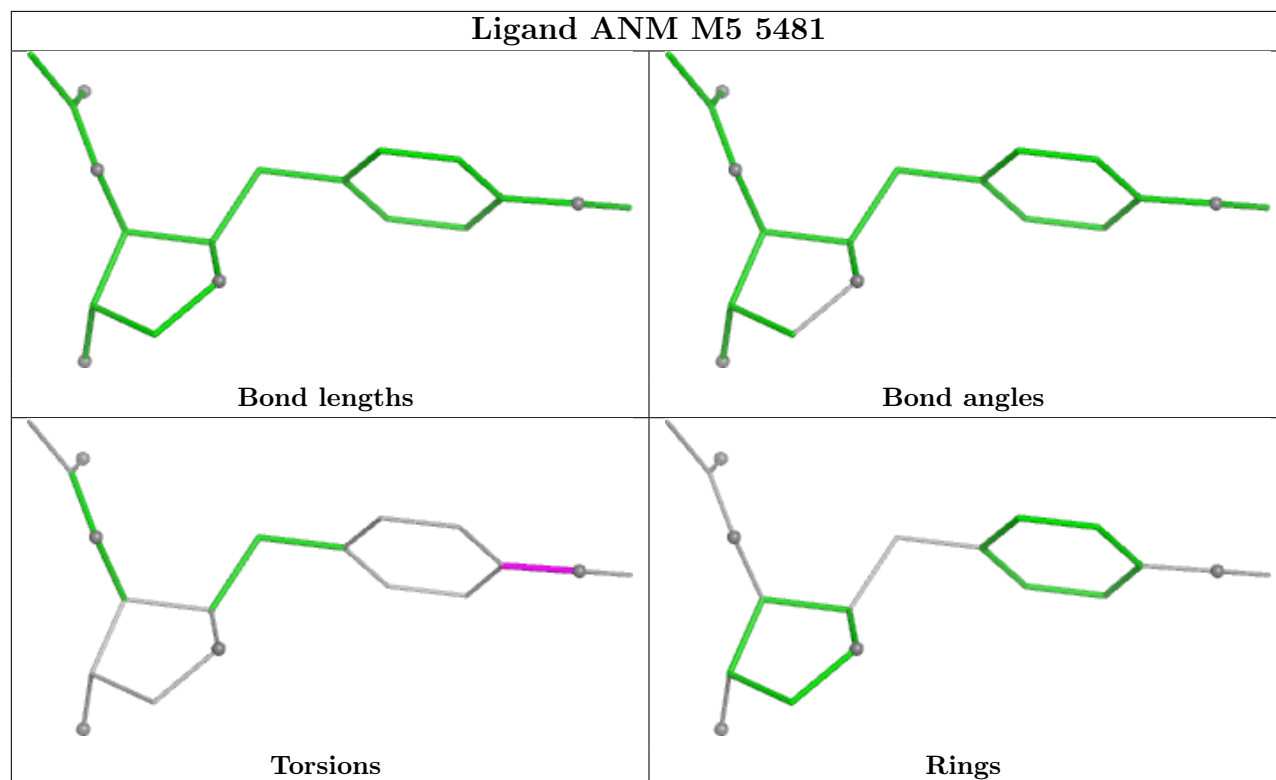
Mol	Chain	Res	Type	Atoms
104	M5	5481	ANM	C10-C9-O1-C14
104	M5	5481	ANM	C1-C9-O1-C14

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
104	M5	5481	ANM	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.

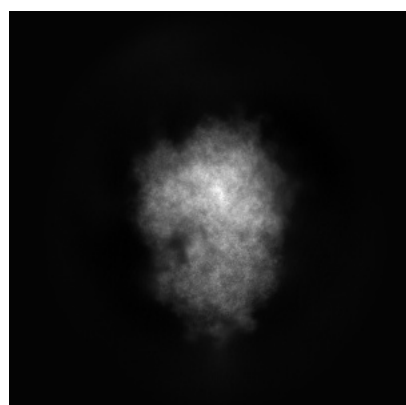
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-54172. These allow visual inspection of the internal detail of the map and identification of artifacts.

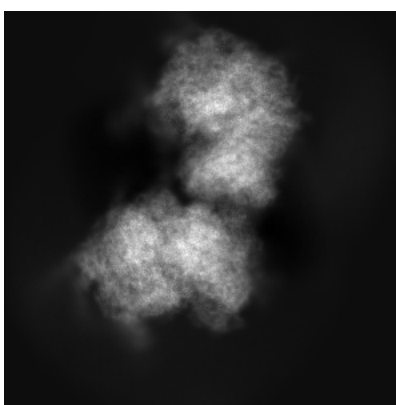
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

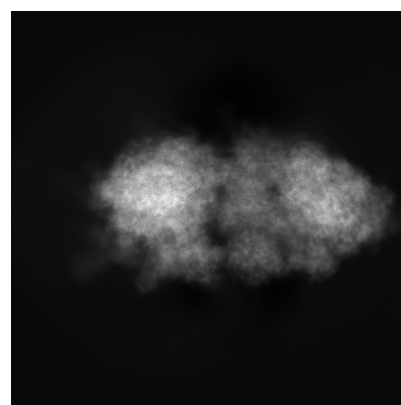
6.1.1 Primary map



X



Y

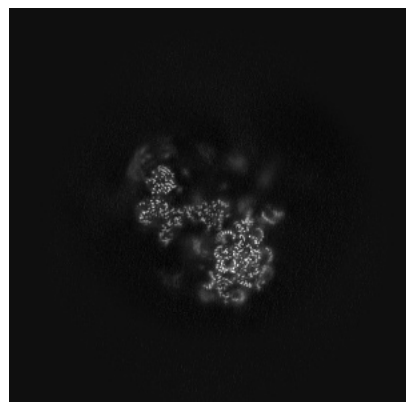


Z

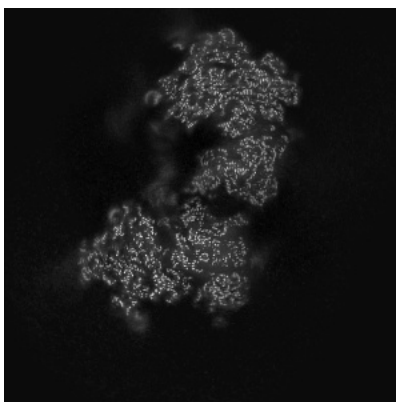
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

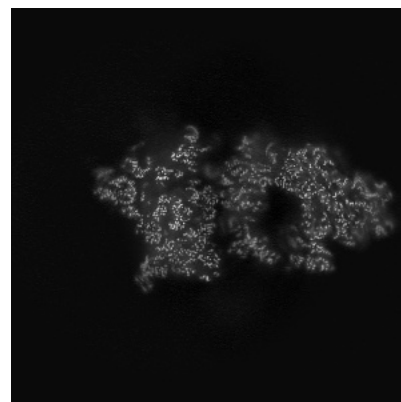
6.2.1 Primary map



X Index: 216



Y Index: 216

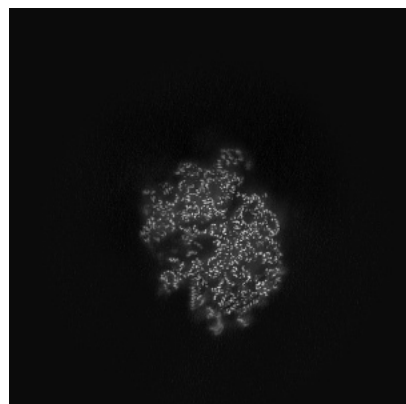


Z Index: 216

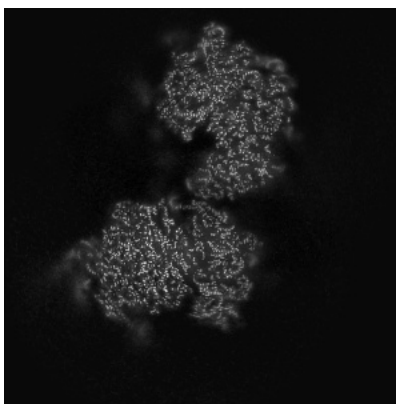
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

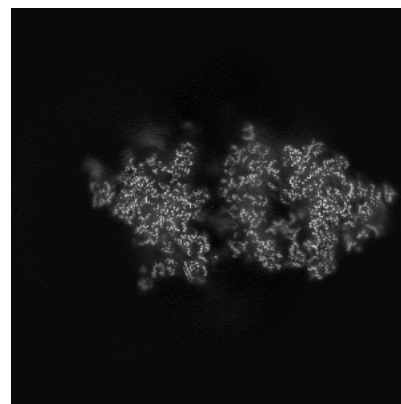
6.3.1 Primary map



X Index: 178



Y Index: 229

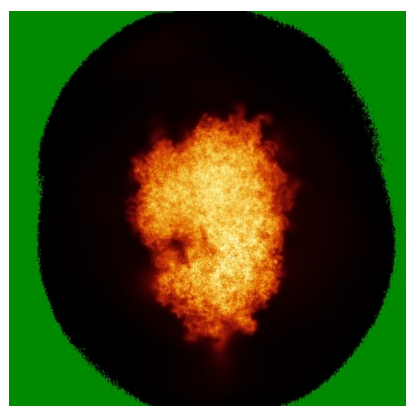


Z Index: 228

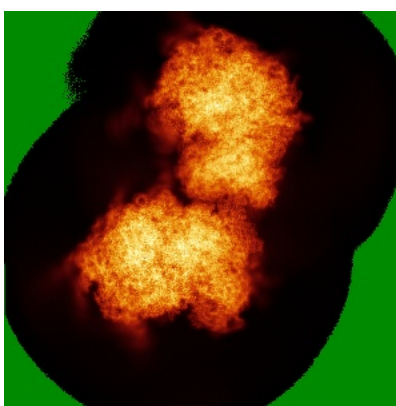
The images above show the largest variance slices of the map in three orthogonal directions.

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

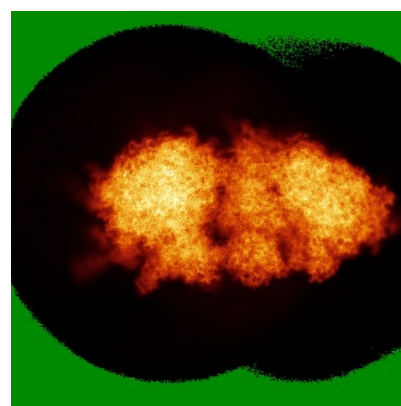
6.4.1 Primary map



X



Y

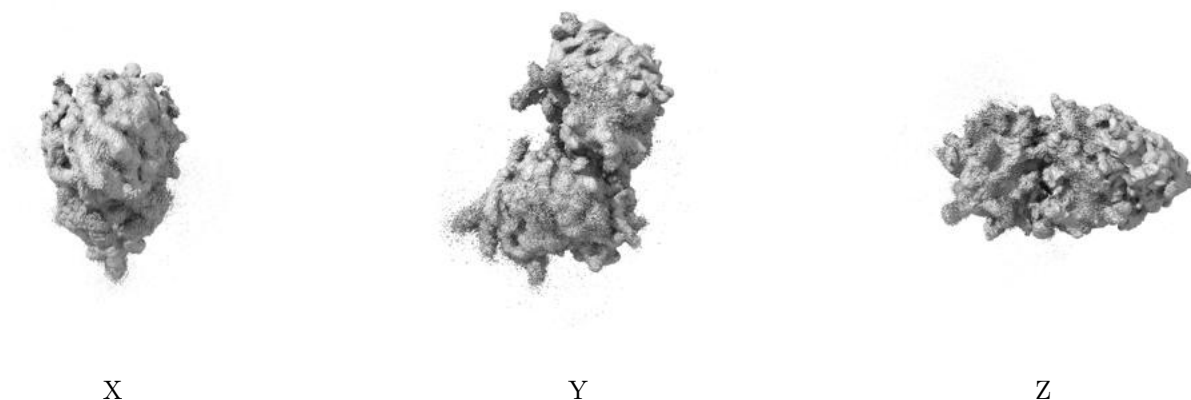


Z

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



The images above show the 3D surface view of the map at the recommended contour level 0.15. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

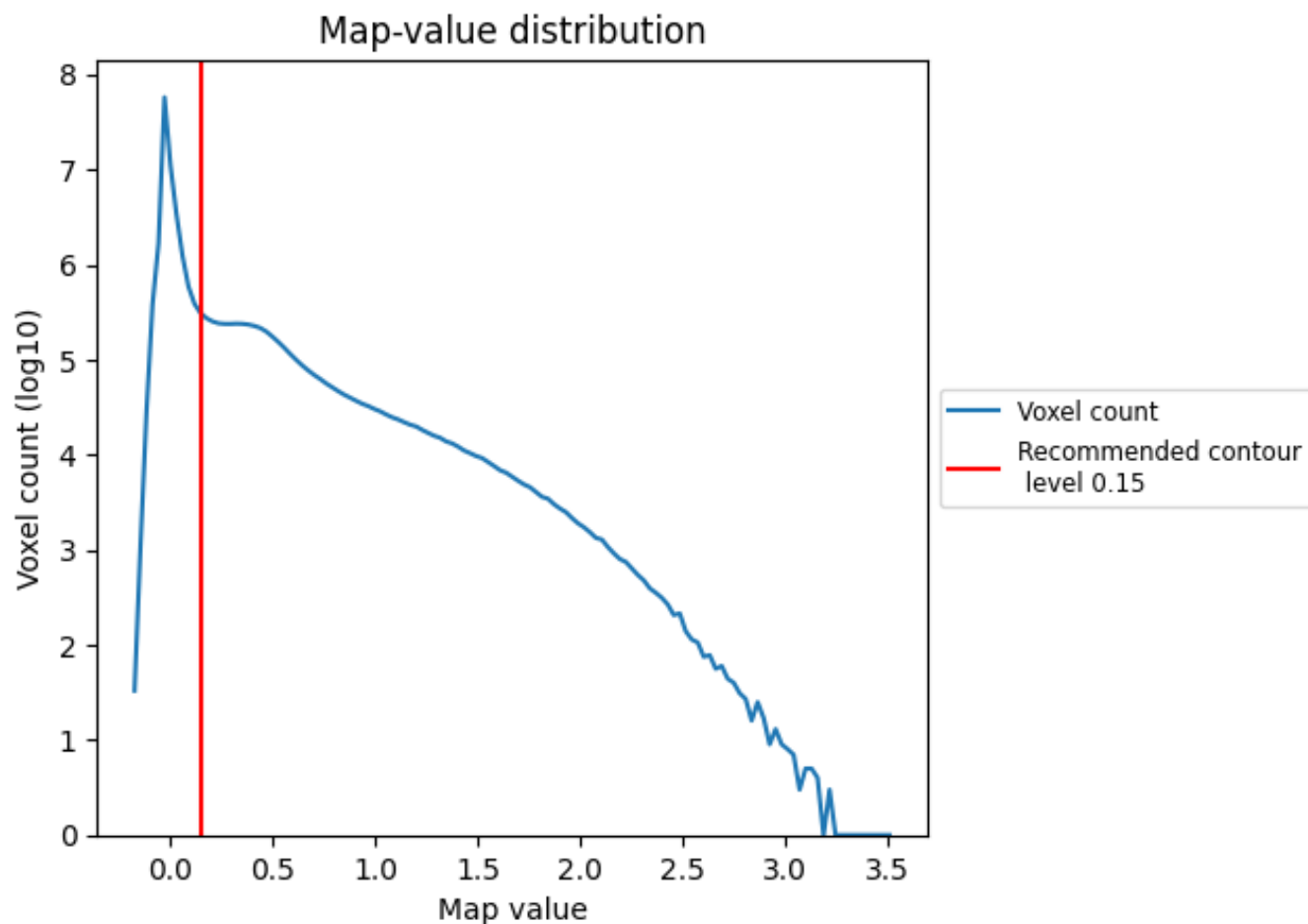
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

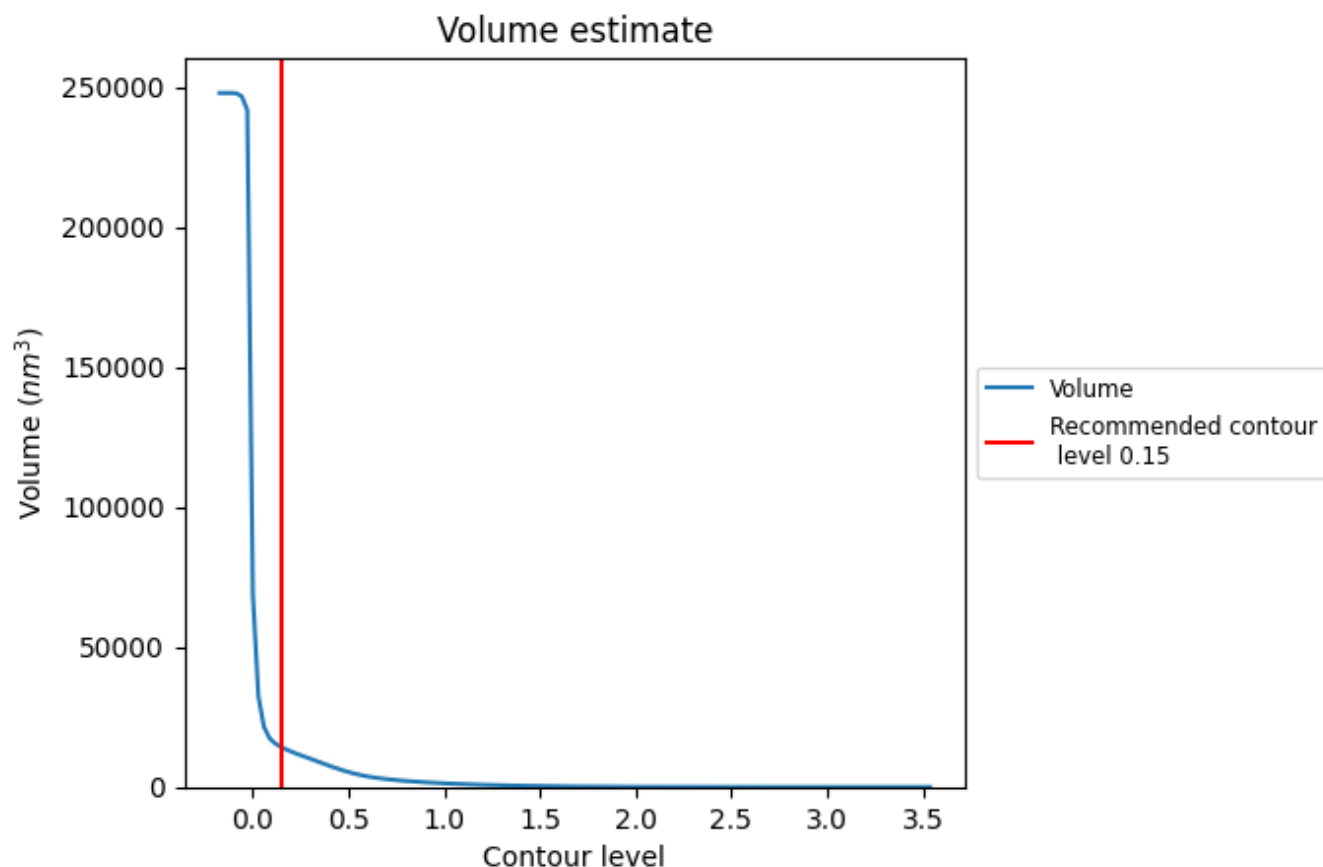
This section contains the results of statistical analysis of the map.

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.

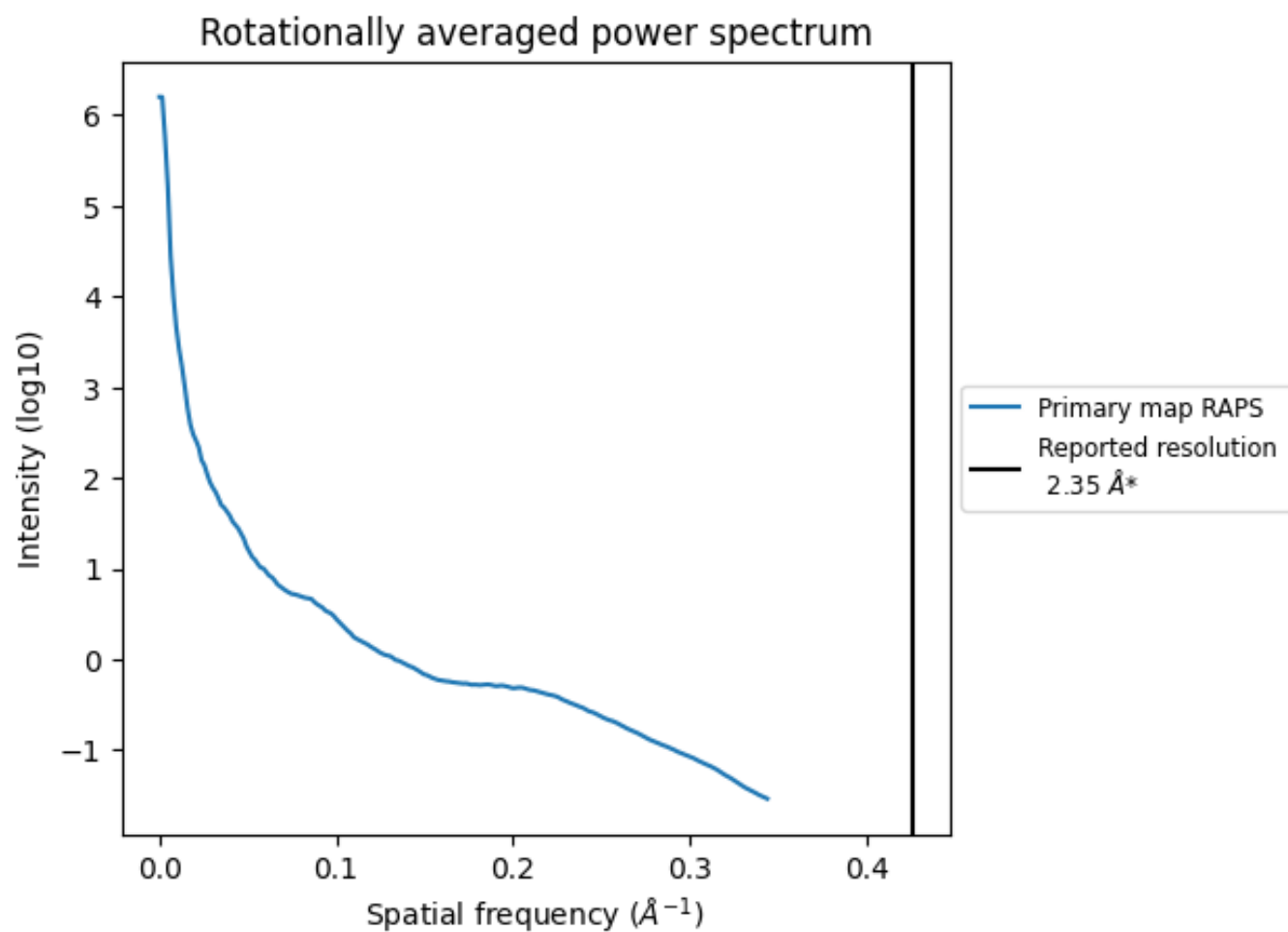
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 14216 nm^3 ; this corresponds to an approximate mass of 12841 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 0.426 Å⁻¹

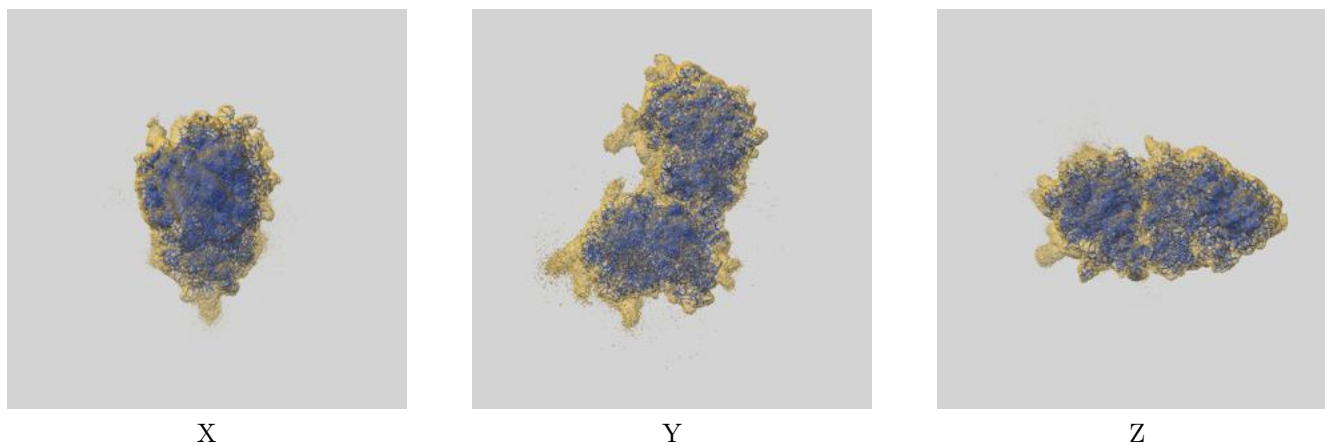
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

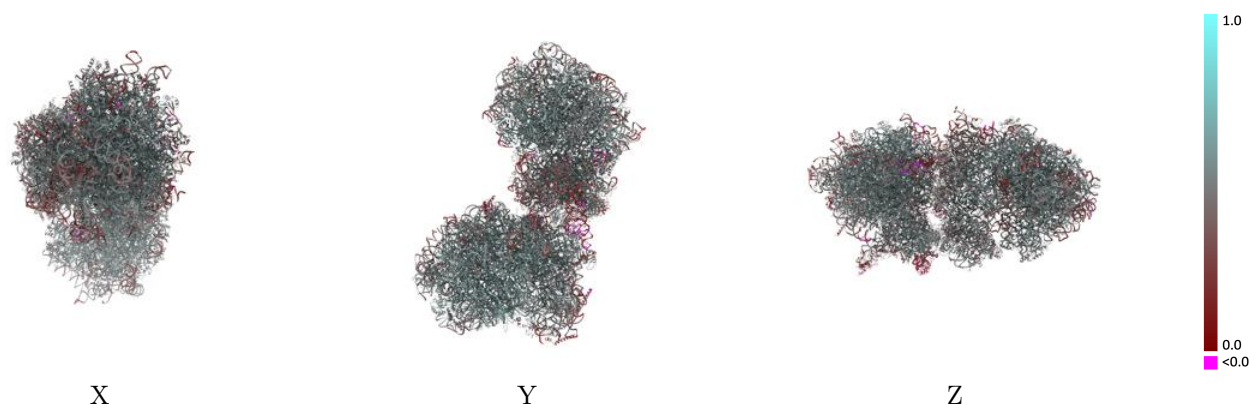
This section contains information regarding the fit between EMDB map EMD-54172 and PDB model 9RPV. Per-residue inclusion information can be found in section [3](#) on page [31](#).

9.1 Map-model overlay [i](#)



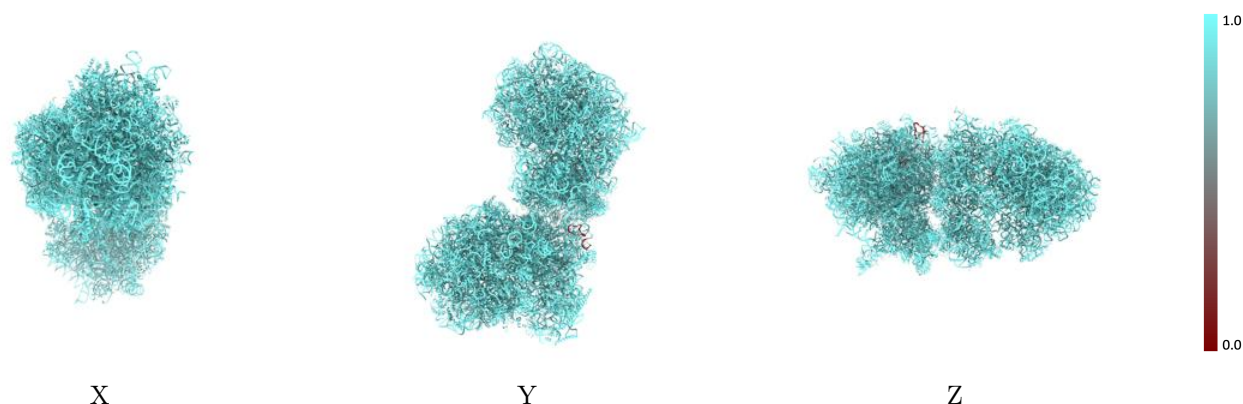
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



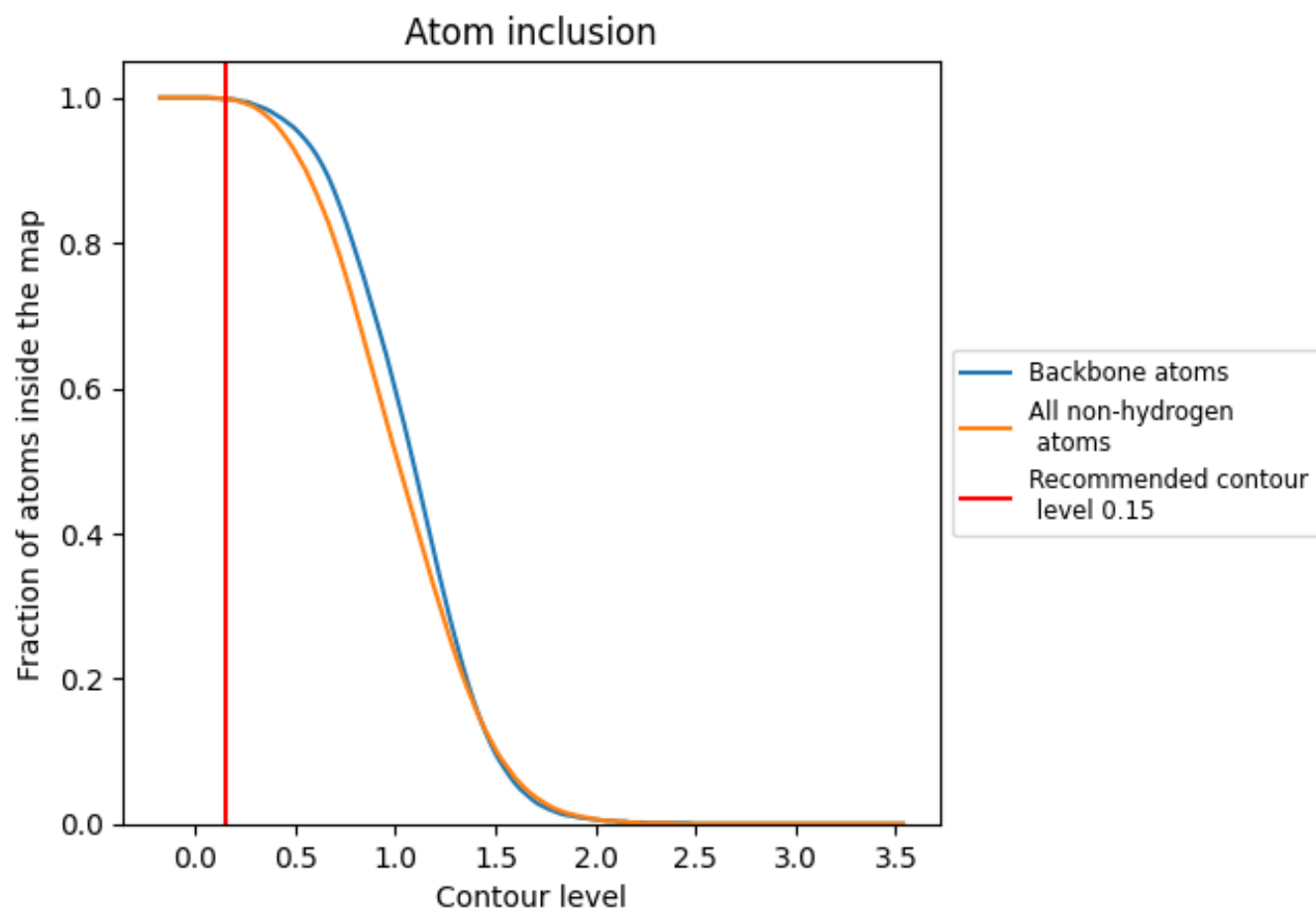
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.15).

9.4 Atom inclusion ⓘ



At the recommended contour level, 100% of all backbone atoms, 100% 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 (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9980	 0.4950
A4	 1.0000	 0.3680
A5	 1.0000	 0.5000
B4	 1.0000	 0.3960
B5	 0.9980	 0.4770
D4	 1.0000	 0.2990
E4	 0.9960	 0.3630
E5	 1.0000	 0.3130
L5	 1.0000	 0.4950
L7	 1.0000	 0.5240
L8	 1.0000	 0.5000
LA	 1.0000	 0.5340
LB	 1.0000	 0.5360
LC	 1.0000	 0.5160
LD	 1.0000	 0.4830
LE	 1.0000	 0.4940
LF	 1.0000	 0.5050
LG	 1.0000	 0.4770
LH	 1.0000	 0.5250
LI	 1.0000	 0.5300
LJ	 1.0000	 0.4910
LL	 1.0000	 0.5060
LM	 1.0000	 0.5060
LN	 1.0000	 0.5330
LO	 1.0000	 0.5290
LP	 1.0000	 0.5370
LQ	 1.0000	 0.5210
LR	 1.0000	 0.4980
LS	 1.0000	 0.5380
LT	 1.0000	 0.5040
LU	 1.0000	 0.4590
LV	 1.0000	 0.5610
LW	 1.0000	 0.4410
LX	 1.0000	 0.5030
LY	 1.0000	 0.5050



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Chain	Atom inclusion	Q-score
LZ	 1.0000	 0.5040
La	 1.0000	 0.5330
Lb	 1.0000	 0.4940
Lc	 1.0000	 0.4840
Ld	 1.0000	 0.5270
Le	 1.0000	 0.5360
Lf	 1.0000	 0.5500
Lg	 1.0000	 0.5200
Lh	 1.0000	 0.4980
Li	 1.0000	 0.4800
Lj	 1.0000	 0.5490
Lk	 1.0000	 0.4810
Ll	 1.0000	 0.5190
Lm	 1.0000	 0.5420
Ln	 1.0000	 0.5170
Lo	 1.0000	 0.5350
Lp	 1.0000	 0.5320
Lr	 1.0000	 0.5230
M5	 1.0000	 0.5300
M7	 1.0000	 0.5510
M8	 1.0000	 0.5410
MA	 1.0000	 0.5910
MB	 0.9990	 0.5700
MC	 1.0000	 0.5560
MD	 1.0000	 0.5040
ME	 1.0000	 0.5230
MF	 1.0000	 0.5510
MG	 0.9980	 0.5070
MH	 1.0000	 0.5370
MI	 1.0000	 0.5440
MJ	 1.0000	 0.4900
ML	 0.9980	 0.5240
MM	 1.0000	 0.5260
MN	 1.0000	 0.5900
MO	 1.0000	 0.5570
MP	 1.0000	 0.5700
MQ	 1.0000	 0.5700
MR	 1.0000	 0.5100
MS	 1.0000	 0.5670
MT	 1.0000	 0.5420
MU	 1.0000	 0.4610
MV	 1.0000	 0.5700

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Chain	Atom inclusion	Q-score
MW	 0.9990	 0.4260
MX	 1.0000	 0.5420
MY	 1.0000	 0.5330
MZ	 1.0000	 0.5380
Ma	 1.0000	 0.5710
Mb	 0.9950	 0.4680
Mc	 1.0000	 0.5400
Md	 1.0000	 0.5530
Me	 1.0000	 0.5720
Mf	 1.0000	 0.5760
Mg	 1.0000	 0.5400
Mh	 1.0000	 0.5240
Mi	 0.9990	 0.5230
Mj	 1.0000	 0.5740
Mk	 1.0000	 0.4800
MI	 1.0000	 0.5740
Mm	 1.0000	 0.5510
Mn	 1.0000	 0.5660
Mo	 1.0000	 0.5570
Mp	 1.0000	 0.5640
Mr	 1.0000	 0.5520
Ms	 0.9850	 0.1540
N1	 0.9630	 0.1960
N2	 0.9620	 0.2010
RA	 0.9840	 0.4790
RB	 0.9990	 0.5030
RC	 0.9990	 0.5070
RD	 0.9980	 0.4310
RE	 1.0000	 0.4780
RF	 1.0000	 0.4960
RG	 1.0000	 0.4120
RH	 1.0000	 0.4280
RI	 1.0000	 0.4940
RJ	 0.9970	 0.4500
RK	 1.0000	 0.3860
RL	 1.0000	 0.5150
RM	 0.9810	 0.2340
RN	 1.0000	 0.5260
RO	 0.9960	 0.5360
RP	 1.0000	 0.4120
RQ	 1.0000	 0.5050
RR	 0.9940	 0.4400

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Chain	Atom inclusion	Q-score
RS	 1.0000	 0.4380
RT	 1.0000	 0.4600
RU	 1.0000	 0.4550
RV	 1.0000	 0.5030
RW	 1.0000	 0.5200
RX	 1.0000	 0.5360
RY	 0.9710	 0.4100
RZ	 1.0000	 0.4130
Ra	 1.0000	 0.5440
Rb	 1.0000	 0.5020
Rc	 0.9880	 0.4880
Rd	 1.0000	 0.4850
Re	 1.0000	 0.4660
Rf	 0.9880	 0.2580
Rg	 0.9920	 0.4970
S2	 0.9910	 0.4530
S3	 1.0000	 0.5040
SA	 1.0000	 0.4860
SB	 1.0000	 0.4870
SC	 1.0000	 0.4950
SD	 1.0000	 0.4280
SE	 1.0000	 0.4460
SF	 1.0000	 0.4500
SG	 1.0000	 0.3990
SH	 1.0000	 0.4210
SI	 1.0000	 0.4060
SJ	 1.0000	 0.3910
SK	 1.0000	 0.4080
SL	 1.0000	 0.4620
SN	 1.0000	 0.4820
SO	 1.0000	 0.4610
SP	 1.0000	 0.4360
SQ	 1.0000	 0.4840
SR	 0.9990	 0.4360
SS	 1.0000	 0.4660
ST	 1.0000	 0.4800
SU	 1.0000	 0.4430
SV	 1.0000	 0.4970
SW	 1.0000	 0.4910
SX	 1.0000	 0.4920
SY	 1.0000	 0.4010
SZ	 1.0000	 0.4380

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Chain	Atom inclusion	Q-score
Sa	 1.0000	 0.4960
Sb	 1.0000	 0.4450
Sc	 1.0000	 0.4700
Sd	 1.0000	 0.4710
Se	 1.0000	 0.3890
Sf	 0.9810	 0.2530
Sg	 0.9890	 0.4750
sh	 1.0000	 0.3280