



## wwPDB EM Validation Summary Report ⓘ

Apr 16, 2024 – 11:12 am BST

PDB ID : 8CMJ  
EMDB ID : EMD-16729  
Title : Translocation intermediate 4 (TI-4\*) of 80S *S. cerevisiae* ribosome with eEF2  
in the absence of sordarin  
Authors : Milicevic, N.; Jenner, L.; Myasnikov, A.; Yusupov, M.; Yusupova, G.  
Deposited on : 2023-02-20  
Resolution : 3.79 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](mailto: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>.

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

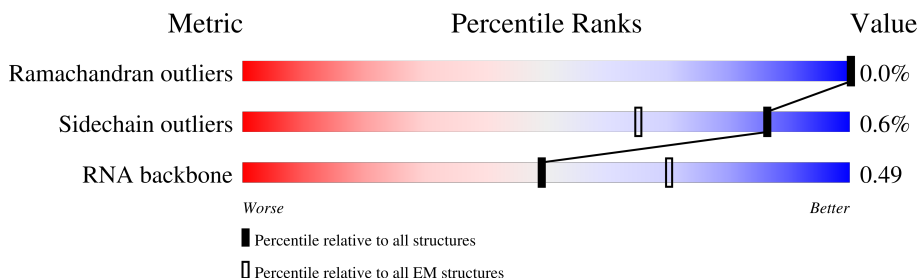
EMDB validation analysis : 0.0.1.dev92  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : **FAILED**  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal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

# 1 Overall quality at a glance i

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

The reported resolution of this entry is 3.79 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	0	135	99% ..
2	1	108	64% . 35%
3	2	119	82% 18%
4	3	82	99% .
5	4	67	93% . 6%
6	5	56	86% . 12%
7	6	63	75% 10% 16%
8	7	319	99% .
9	8	152	24% 76%

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Mol	Chain	Length	Quality of chain
10	A	199	98% ..
11	AA	3396	74% 19% 6%
12	Aa	842	96% .
13	B	184	83% . 16%
14	BB	121	83% 17%
15	C	186	99% ..
16	CC	158	82% 18%
17	D	189	93% . 7%
18	DD	312	63% 37%
19	E	172	100%
20	EE	254	99% .
21	Ee	165	96% .
22	F	160	99% ..
23	FF	387	99%
24	G	121	80% 20%
25	GG	362	99% .
26	H	137	94% 6%
27	HH	297	100%
28	I	155	40% . 59%
29	II	176	88% 12%
30	J	142	84% . 15%
31	JJ	244	90% . 9%
32	K	127	98% ..
33	KK	256	91% 9%
34	L	136	99% ..



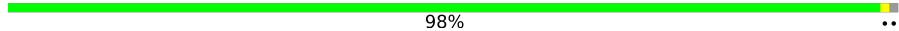


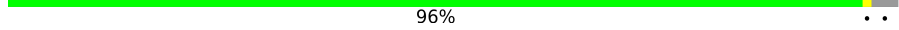
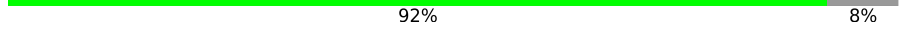
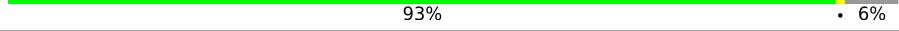

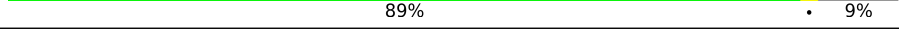
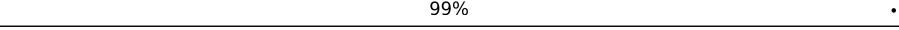
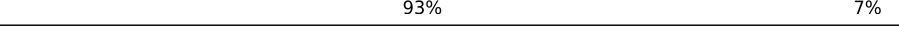

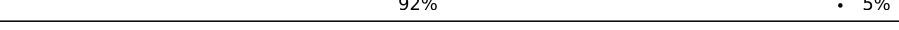

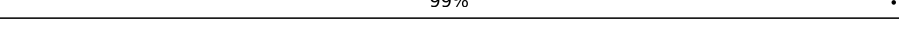
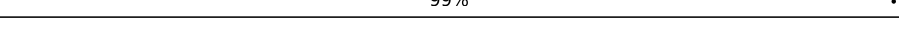

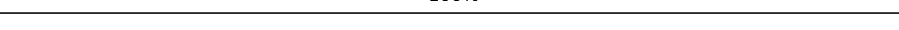


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Mol	Chain	Length	Quality of chain
35	LL	191	100%
36	M	149	99%
37	MM	221	97%
38	N	59	98%
39	NN	174	97%
40	O	105	92% 8%
41	OO	199	96%
42	P	113	96%
43	PP	138	99%
44	Q	130	97%
45	QQ	204	100%
46	R	107	99%
47	S	121	90% 10%
48	T	120	98%
49	U	100	99%
50	V	88	92% 5%
51	W	78	99%
52	X	51	98%
53	Y	128	38% 59%
54	Z	25	100%
55	a	106	95%
56	b	92	98%
57	c	1800	61% 26% 11%
58	d	252	82% 18%
59	e	255	82% 17%

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Mol	Chain	Length	Quality of chain
60	f	254	 85% 15%
61	g	240	 75% 24%
62	h	261	 98% ..
63	i	225	 88% 12%
64	j	236	 89% 7%
65	k	190	 96% ..
66	l	200	 92% 8%
67	m	197	 93% 6%
68	n	105	 31% 69%
69	o	156	 89% 9%
70	p	151	 99% .
71	q	137	 93% 7%
72	r	142	 63% 36%
73	s	143	 92% 5%
74	t	136	 88% 11%
75	u	146	 99% ..
76	v	144	 99% .
77	w	121	 81% 17%
78	x	87	 100%
79	y	130	 98% ..
80	z	145	 98% ..

## 2 Entry composition [i](#)

There are 85 unique types of molecules in this entry. The entry contains 202630 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 protein called 40S ribosomal protein S24-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
1	0	134	1073	676	208	189	0	0

- Molecule 2 is a protein called 40S ribosomal protein S25-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	1	70	563	360	104	99	0	0

- Molecule 3 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	2	97	769	475	160	129	5	0	0

- Molecule 4 is a protein called 40S ribosomal protein S27-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	3	81	610	382	110	113	5	0	0

- Molecule 5 is a protein called 40S ribosomal protein S28-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	4	63	497	306	99	91	1	0	0

- Molecule 6 is a protein called HLJ1\_G0030400.mRNA.1.CDS.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	5	49	404	249	86	65	4	0	0

- Molecule 7 is a protein called 40S ribosomal protein S30-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	6	53	427	269	88	69	1	0	0

- Molecule 8 is a protein called Guanine nucleotide-binding protein subunit beta-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	7	318	2436	1541	418	469	8	0	0

- Molecule 9 is a protein called Ubiquitin-40S ribosomal protein S31.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	8	36	276	173	54	45	4	0	0

- Molecule 10 is a protein called 60S ribosomal protein L16-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	A	197	1555	1003	289	262	1	0	0

- Molecule 11 is a RNA chain called 25S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
11	AA	3197	68429	30589	12334	22309	3197	0	0

- Molecule 12 is a protein called Elongation factor 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	Aa	816	6368	4051	1088	1198	31	0	0

- Molecule 13 is a protein called 60S ribosomal protein L17-A.

Mol	Chain	Residues	Atoms			AltConf	Trace	
			Total	C	N			O
13	B	154	1222	761	237	224	0	0

- Molecule 14 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
14	BB	121	2579	1152	461	845	121	0	0

- Molecule 15 is a protein called 60S ribosomal protein L18-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	C	185	1441	908	290	241	2	0	0

- Molecule 16 is a RNA chain called 5.8S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
16	CC	158	3353	1500	586	1109	158	0	0

- Molecule 17 is a protein called 60S ribosomal protein L19-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
17	D	176	1423	875	308	240	0	0

- Molecule 18 is a protein called 60S acidic ribosomal protein P0.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	DD	197	1531	980	266	281	4	0	0

- Molecule 19 is a protein called 60S ribosomal protein L20-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	E	172	1445	930	267	244	4	0	0

- Molecule 20 is a protein called 60S ribosomal protein L2-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	EE	252	1914	1191	388	334	1	0	0

- Molecule 21 is a protein called 60S ribosomal protein L12-A.



Mol	Chain	Residues	Atoms					AltConf	Trace
21	Ee	158	Total	C	N	O	S	0	0
			1196	750	216	228	2		

- Molecule 22 is a protein called 60S ribosomal protein L21-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	F	159	Total	C	N	O	S	0	0
			1276	805	246	221	4		

- Molecule 23 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	FF	386	Total	C	N	O	S	0	0
			3075	1950	584	533	8		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
24	G	97	Total	C	N	O	0	0
			770	499	126	145		

- Molecule 25 is a protein called 60S ribosomal protein L4-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	GG	361	Total	C	N	O	S	0	0
			2748	1729	522	494	3		

- Molecule 26 is a protein called 60S ribosomal protein L23-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	H	129	Total	C	N	O	S	0	0
			963	607	180	169	7		

- Molecule 27 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	HH	296	Total	C	N	O	S	0	0
			2375	1501	414	458	2		

- Molecule 28 is a protein called 60S ribosomal protein L24-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	I	63	Total	C	N	O	S	0	0
			521	336	102	82	1		

- Molecule 29 is a protein called 60S ribosomal protein L6-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	II	155	Total	C	N	O	S	0	0
			1230	795	221	213	1		

- Molecule 30 is a protein called 60S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	J	120	Total	C	N	O	S	0	0
			959	617	168	172	2		

- Molecule 31 is a protein called 60S ribosomal protein L7-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	JJ	222	Total	C	N	O	S	0	0
			1784	1151	324	308	1		

- Molecule 32 is a protein called 60S ribosomal protein L26-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	K	126	Total	C	N	O	0	0
			993	625	192	176		

- Molecule 33 is a protein called 60S ribosomal protein L8-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	KK	233	Total	C	N	O	S	0	0
			1804	1151	323	327	3		

- Molecule 34 is a protein called 60S ribosomal protein L27-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
34	L	135	Total	C	N	O	0	0
			1092	710	202	180		

- Molecule 35 is a protein called RPL9A isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	LL	191	Total	C	N	O	S	0	0
			1518	963	274	277	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
36	M	148	Total	C	N	O	S	0	0
			1173	749	231	190	3		

- Molecule 37 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	MM	215	Total	C	N	O	S	0	0
			1743	1102	331	303	7		

- Molecule 38 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms				AltConf	Trace
38	N	58	Total	C	N	O	0	0
			462	289	100	73		

- Molecule 39 is a protein called 60S ribosomal protein L11-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	NN	169	Total	C	N	O	S	0	0
			1353	847	253	249	4		

- Molecule 40 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	O	97	Total	C	N	O	S	0	0
			742	479	124	138	1		

- Molecule 41 is a protein called 60S ribosomal protein L13-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
41	OO	193	Total	C	N	O	0	0
			1543	962	315	266		

- Molecule 42 is a protein called 60S ribosomal protein L31-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	P	109	Total	C	N	O	S	0	0
			883	559	167	156	1		

- Molecule 43 is a protein called 60S ribosomal protein L14-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	PP	136	Total	C	N	O	S	0	0
			1053	675	199	177	2		

- Molecule 44 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	Q	127	Total	C	N	O	S	0	0
			1020	647	205	167	1		

- Molecule 45 is a protein called 60S ribosomal protein L15-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	QQ	203	Total	C	N	O	S	0	0
			1720	1077	361	281	1		

- Molecule 46 is a protein called 60S ribosomal protein L33-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	R	106	Total	C	N	O	S	0	0
			850	540	165	144	1		

- Molecule 47 is a protein called 60S ribosomal protein L34-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	S	109	Total	C	N	O	S	0	0
			861	533	175	149	4		

- Molecule 48 is a protein called 60S ribosomal protein L35-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	T	119	Total	C	N	O	S	0	0
			969	615	186	167	1		

- Molecule 49 is a protein called 60S ribosomal protein L36-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	U	99	Total	C	N	O	S	0	0
			771	481	156	132	2		

- Molecule 50 is a protein called 60S ribosomal protein L37-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	V	84	Total	C	N	O	S	0	0
			665	405	145	110	5		

- Molecule 51 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms				AltConf	Trace
51	W	77	Total	C	N	O	0	0
			612	391	115	106		

- Molecule 52 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	X	50	Total	C	N	O	S	0	0
			436	272	97	65	2		

- Molecule 53 is a protein called Ubiquitin-60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	Y	52	Total	C	N	O	S	0	0
			417	259	86	67	5		

- Molecule 54 is a protein called 60S ribosomal protein L41.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	Z	25	Total	C	N	O	S	0	0
			233	142	63	27	1		

- Molecule 55 is a protein called 60S ribosomal protein L42-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	a	102	Total	C	N	O	S	0	0
			819	514	166	134	5		

- Molecule 56 is a protein called 60S ribosomal protein L43-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	b	91	Total	C	N	O	S	0	0
			694	429	138	121	6		

- Molecule 57 is a RNA chain called 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	c	1608	Total	C	N	O	P	0	0
			34321	15360	6093	11260	1608		

- Molecule 58 is a protein called 40S ribosomal protein S0-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	d	206	Total	C	N	O	S	0	0
			1583	1017	281	283	2		

- Molecule 59 is a protein called 40S ribosomal protein S1-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	e	212	Total	C	N	O	S	0	0
			1689	1073	303	309	4		

- Molecule 60 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	f	217	Total	C	N	O	S	0	0
			1635	1047	289	297	2		

- Molecule 61 is a protein called RPS3 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	g	183	Total	C	N	O	S	0	0
			1412	893	260	253	6		

- Molecule 62 is a protein called 40S ribosomal protein S4-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	h	258	Total	C	N	O	S	0	0
			2056	1308	387	358	3		

- Molecule 63 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	i	199	Total	C	N	O	S	0	0
			1572	987	290	292	3		

- Molecule 64 is a protein called 40S ribosomal protein S6-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	j	219	Total	C	N	O	S	0	0
			1766	1108	341	314	3		

- Molecule 65 is a protein called 40S ribosomal protein S7-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
65	k	184	Total	C	N	O	0	0
			1481	951	265	265		

- Molecule 66 is a protein called 40S ribosomal protein S8-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	l	184	Total	C	N	O	S	0	0
			1457	906	291	258	2		

- Molecule 67 is a protein called 40S ribosomal protein S9-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	m	185	Total	C	N	O	S	0	0
			1494	943	289	261	1		

- Molecule 68 is a protein called 40S ribosomal protein S10-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
68	n	33	Total	C	N	O	0	0
			300	199	46	55		

- Molecule 69 is a protein called 40S ribosomal protein S11-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	o	142	Total	C	N	O	S	0	0
			1146	735	217	191	3		

- Molecule 70 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	p	150	Total	C	N	O	S	0	0
			1192	759	224	207	2		

- Molecule 71 is a protein called 40S ribosomal protein S14-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	q	127	Total	C	N	O	S	0	0
			891	545	182	163	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
72	r	91	Total	C	N	O	S	0	0
			732	469	138	120	5		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
73	s	136	Total	C	N	O	0	0
			1069	686	195	188		

- Molecule 74 is a protein called 40S ribosomal protein S17-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	t	121	Total	C	N	O	S	0	0
			961	599	182	178	2		

- Molecule 75 is a protein called 40S ribosomal protein S18-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	u	145	Total	C	N	O	S	0	0
			1192	743	237	210	2		

- Molecule 76 is a protein called 40S ribosomal protein S19-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	v	143	Total	C	N	O	S	0	0
			1112	694	208	208	2		

- Molecule 77 is a protein called 40S ribosomal protein S20.



Mol	Chain	Residues	Atoms					AltConf	Trace
77	w	100	Total	C	N	O	S	0	0
			800	509	144	146	1		

- Molecule 78 is a protein called 40S ribosomal protein S21-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	x	87	Total	C	N	O	S	0	0
			684	420	125	137	2		

- Molecule 79 is a protein called 40S ribosomal protein S22-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	y	129	Total	C	N	O	S	0	0
			1021	650	188	180	3		

- Molecule 80 is a protein called 40S ribosomal protein S23-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	z	144	Total	C	N	O	S	0	0
			1121	708	220	191	2		

- Molecule 81 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
81	2	1	Total	Zn	0
			1	1	
81	5	1	Total	Zn	0
			1	1	
81	8	1	Total	Zn	0
			1	1	
81	S	1	Total	Zn	0
			1	1	
81	V	1	Total	Zn	0
			1	1	
81	Y	1	Total	Zn	0
			1	1	
81	a	1	Total	Zn	0
			1	1	
81	b	1	Total	Zn	0
			1	1	

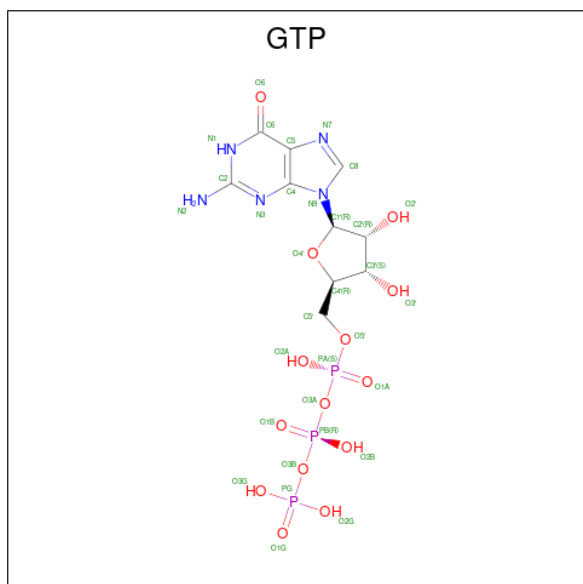
- Molecule 82 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
82	AA	119	Total	Mg	0
			119	119	
82	Aa	1	Total	Mg	0
			1	1	
82	BB	3	Total	Mg	0
			3	3	
82	CC	3	Total	Mg	0
			3	3	
82	H	1	Total	Mg	0
			1	1	
82	JJ	1	Total	Mg	0
			1	1	
82	c	25	Total	Mg	0
			25	25	

- Molecule 83 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
83	AA	9	Total	K	0
			9	9	
83	EE	1	Total	K	0
			1	1	

- Molecule 84 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>14</sub>P<sub>3</sub>).



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

- Molecule 85 is water.

Mol	Chain	Residues	Atoms		AltConf
85	AA	71	Total 71	O 71	0
85	B	1	Total 1	O 1	0
85	CC	8	Total 8	O 8	0
85	F	1	Total 1	O 1	0
85	JJ	1	Total 1	O 1	0
85	R	1	Total 1	O 1	0
85	V	1	Total 1	O 1	0
85	c	18	Total 18	O 18	0

### 3 Residue-property plots [i](#)

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

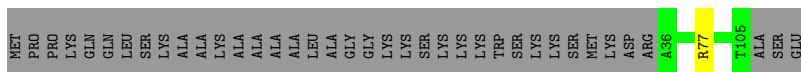
- Molecule 1: 40S ribosomal protein S24-A

Chain 0:  99%




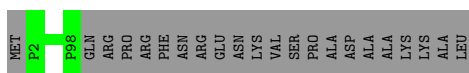
- Molecule 2: 40S ribosomal protein S25-A

Chain 1:  64% 35%



- Molecule 3: 40S ribosomal protein S26

Chain 2:  82% 18%



- Molecule 4: 40S ribosomal protein S27-A

Chain 3:  99%




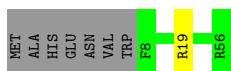
- Molecule 5: 40S ribosomal protein S28-A

Chain 4:  93% 6%

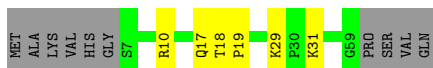


- Molecule 6: HLJ1\_G0030400.mRNA.1.CDS.1

Chain 5:  86% 12%



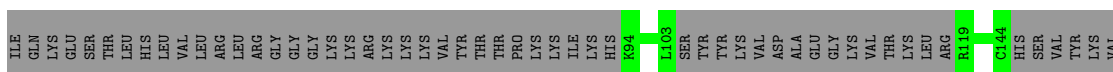
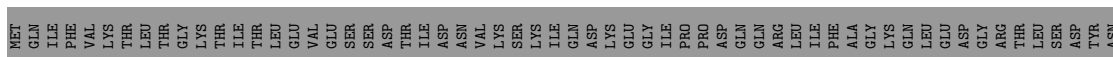
- Molecule 7: 40S ribosomal protein S30-A



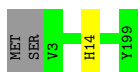
- Molecule 8: Guanine nucleotide-binding protein subunit beta-like protein



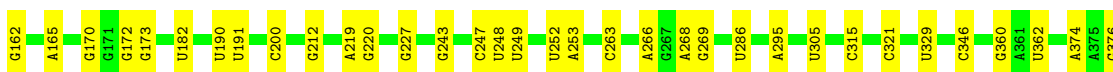
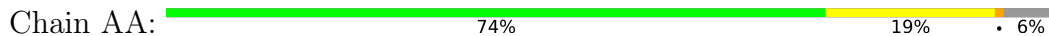
- Molecule 9: Ubiquitin-40S ribosomal protein S31



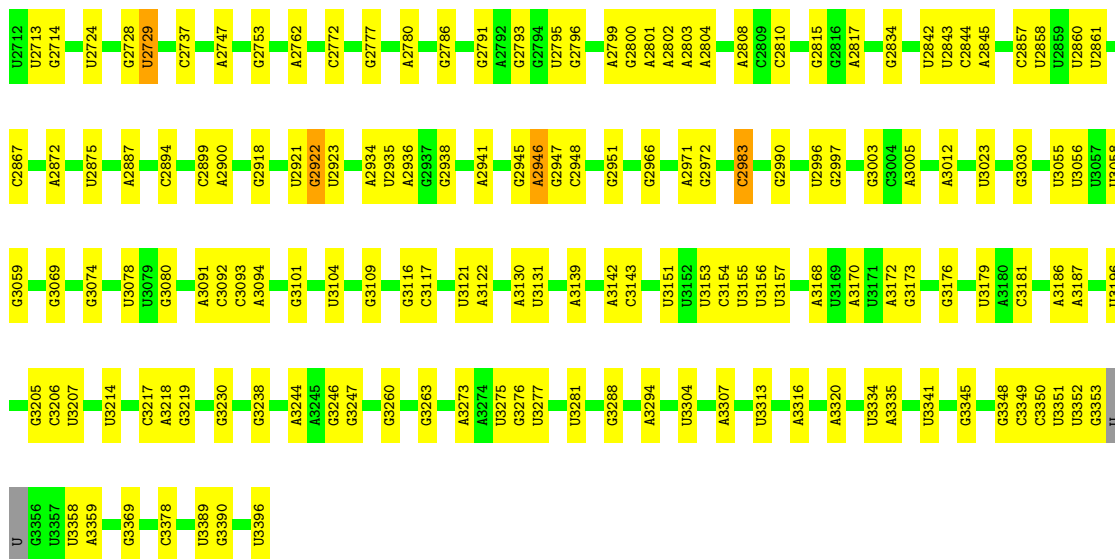
- Molecule 10: 60S ribosomal protein L16-A



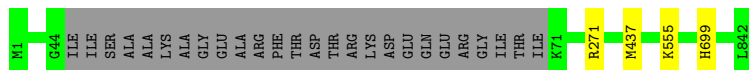
- Molecule 11: 25S ribosomal RNA



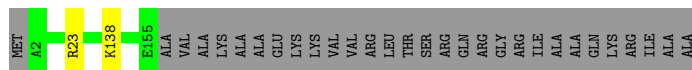
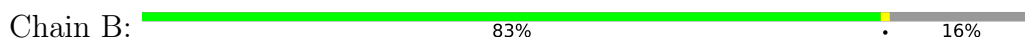
A9554	G2467	A2313	A2158	U1880	A1647	G1514	A1332	A1179	A1006	G867	C665	A
G2555	A2468	U2314	G2165	U1888	C1657	U1523	G1345	A1180	G1013	U874	A660	U
C2560	C2470	G2315	A2166	U1893	A1683	A1524	U1348	U1182	U1014	G875	G661	U
A2561	U2471	U2471	A2167	C1894	U1688	U1526	G1349	A1190	U1015	A876	U662	C
A2569	C2473	A	G2169	C1904	U1694	C1527	A1352	U1191	C1016	U879	C667	A
U2570	G2474	G	G2170	G1905	U1694	G1528	A1352	C1192	G1017	G880	A677	C
U2571	G2475	G	U1912	G1906	U1724	A1539	A1355	A1193	G1018	G890	A677	U
C2572	C2476	U	U1912	G1906	U1724	A1539	A1355	C1196	A1025	G890	G678	G
C2573	G2477	U	G1935	U1912	A1741	G1542	G1357	C1201	A1026	C890	U661	U
G2585	C2478	U	G1935	G1935	A1741	C1586	A1363	U1208	U1028	A896	A680	C
G2586	A2480	U	C1943	C1943	A1750	A1587	A1363	G1209	U1033	U899	A691	U
U2587	G2481	U	G1948	G1948	G1751	A1588	A1366	G1208	U1034	U899	A691	U
A2593	A2486	G	U1948	U1948	C1756	A1589	G1367	G1209	A1036	G907	A705	C
C2594	U2487	U	G1952	G1952	C1756	G1560	A1386	A1221	G1037	G908	U719	C
G2602	A2488	A	G1952	G1952	C1759	G1561	A1386	G1222	C1038	G909	U719	C
G2606	C2489	C	G	G	C1759	C1562	G1392	U1285	C1045	G910	U737	C
G2607	A2491	C	G	G	C1762	C1563	G1392	G1236	G1046	A914	A761	C
G2614	U2493	U	G	G	U1763	U1569	A1399	G1237	A1046	A915	G750	C
U2617	G2494	U	G	G	U1764	U1570	G1400	G1246	A1047	G916	U766	C
G2618	C2495	U	G	G	G1766	A1571	G1408	U1253	A1064	A917	C758	C
G2619	C2496	U	G	G	C1767	U1572	G1408	A1244	U1081	A921	A761	C
U2634	U2499	C	A	A	U1768	G1573	G1417	A1245	G1072	U922	A784	C
A2640	A2500	U	G	G	G1769	C1574	A1418	G1246	U1096	C923	U766	C
G2648	U2501	U	C	C	G1773	A1575	U1425	U1253	A1075	G924	U767	C
U2652	G2502	U	C	C	C1788	C1578	U1425	U1285	U1081	A925	A780	C
A2656	A2503	A	U	U	A1814	A1587	G1434	U1288	G1087	A926	A780	C
A2657	A2503	A	U	U	U1815	A1588	G1434	U1288	U1288	C937	G761	C
G2672	A2523	A	U	U	A1816	A1589	U1436	A1289	A1289	C937	A784	C
A2673	G2524	U	C	C	G1817	C1582	C1437	A1260	U1096	U939	G785	C
A2674	C2526	U	U	U	U1820	A1583	G1443	A1263	G1097	A925	A786	C
A2686	G2527	U	U	U	U1821	C1583	G1443	G1284	A1098	U943	U790	C
A2687	G2273	U	U	U	A1835	A1605	A1446	U1285	A1103	C944	A790	C
A2688	G2273	U	U	U	A1835	A1605	A1446	A1287	A1103	C953	G799	C
G2690	A2280	U	U	U	U1815	A1621	A1449	C1272	U1111	G959	G805	C
A2691	A2281	U	U	U	A1816	A1621	A1449	A1294	G1117	U960	A806	C
U2681	U2282	U	U	U	G1817	A1638	G1450	A1287	G1131	C361	A807	C
A2696	U2286	U	U	U	U1820	A1638	G1450	A1287	G1131	A962	A816	C
A2704	C2287	U	U	U	U1821	A1637	U1455	A1287	G1132	G974	A817	C
C2711	C2307	U	U	U	A1835	A1637	U1455	A1287	A1133	G978	G826	C
	A2309	U	U	U	A1835	A1637	U1455	A1287	A1133	U979	A850	C
	A2309	U	U	U	U1848	A1638	U1484	A1302	G1140	U981	A850	C
	A2309	U	U	U	C1849	A1638	U1484	A1302	G1140	U981	A850	C
	A2309	U	U	U	A1850	A1638	U1484	A1302	G1140	U981	A850	C
	A2309	U	U	U	C1854	A1638	U1484	A1302	G1140	U981	A850	C
	A2309	U	U	U	C1854	A1638	U1484	A1302	G1140	U981	A850	C
	A2309	U	U	U	C1866	A1642	U1495	U1325	A1159	U988	C849	C
	A2309	U	U	U	G1878	A1643	C1808	C1328	C1176	U988	C849	C
	A2309	U	U	U	A1879	C1644	A1509	U1329	G1177	C1000	G857	C
	A2309	U	U	U	A1879	G1646	G1510	U1331	G1178	C1000	C861	C



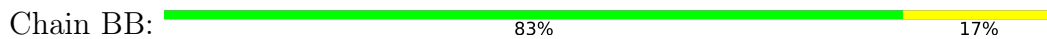
- Molecule 12: Elongation factor 2



- Molecule 13: 60S ribosomal protein L17-A



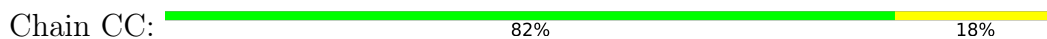
- Molecule 14: 5S ribosomal RNA



- Molecule 15: 60S ribosomal protein L18-A



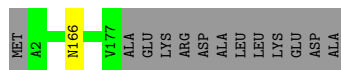
- Molecule 16: 5.8S ribosomal RNA





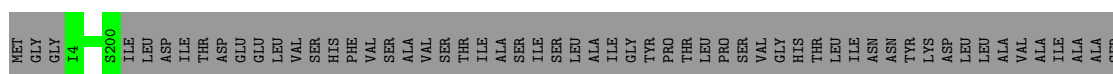
- Molecule 17: 60S ribosomal protein L19-A

Chain D: 93% 7%



- Molecule 18: 60S acidic ribosomal protein P0

Chain DD: 63% 37%



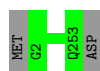
- Molecule 19: 60S ribosomal protein L20-A

Chain E: 100%

There are no outlier residues recorded for this chain.

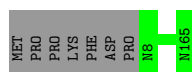
- Molecule 20: 60S ribosomal protein L2-A

Chain EE: 99%



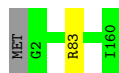
- Molecule 21: 60S ribosomal protein L12-A

Chain Ee: 96%



- Molecule 22: 60S ribosomal protein L21-A

Chain F: 99%




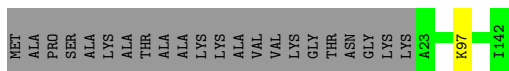
- Molecule 23: 60S ribosomal protein L3

Chain FF: 99%



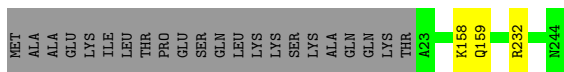


Chain J:  84% 15%



- Molecule 31: 60S ribosomal protein L7-A

Chain JJ:  90% 9%



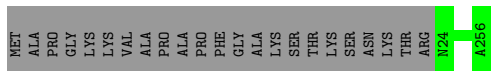
- Molecule 32: 60S ribosomal protein L26-A

Chain K:  98% ..



- Molecule 33: 60S ribosomal protein L8-A

Chain KK:  91% 9%



- Molecule 34: 60S ribosomal protein L27-A

Chain L:  99% ..



- Molecule 35: RPL9A isoform 1

Chain LL:  100%

There are no outlier residues recorded for this chain.

- Molecule 36: 60S ribosomal protein L28

Chain M:  99%



- Molecule 37: 60S ribosomal protein L10

Chain MM:  97%



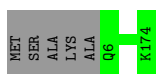
- Molecule 38: 60S ribosomal protein L29

Chain N: 98%



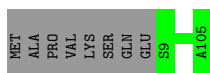
- Molecule 39: 60S ribosomal protein L11-A

Chain NN: 97%



- Molecule 40: 60S ribosomal protein L30

Chain O: 92% 8%



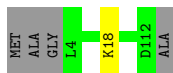
- Molecule 41: 60S ribosomal protein L13-A

Chain OO: 96%



- Molecule 42: 60S ribosomal protein L31-A

Chain P: 96%



- Molecule 43: 60S ribosomal protein L14-A

Chain PP: 99%



- Molecule 44: 60S ribosomal protein L32

Chain Q: 97%



- Molecule 45: 60S ribosomal protein L15-A

Chain QQ: 100%



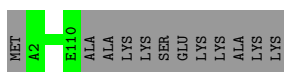
- Molecule 46: 60S ribosomal protein L33-A

Chain R: 99%



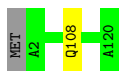
- Molecule 47: 60S ribosomal protein L34-A

Chain S: 90% 10%



- Molecule 48: 60S ribosomal protein L35-A

Chain T: 98%



- Molecule 49: 60S ribosomal protein L36-A

Chain U: 99%



- Molecule 50: 60S ribosomal protein L37-A

Chain V: 92% 5%



- Molecule 51: 60S ribosomal protein L38

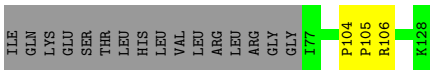
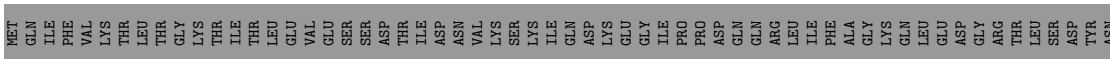
Chain W: 99%



- Molecule 52: 60S ribosomal protein L39



- Molecule 53: Ubiquitin-60S ribosomal protein L40

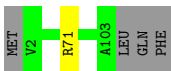


- Molecule 54: 60S ribosomal protein L41

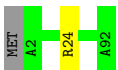


There are no outlier residues recorded for this chain.

- Molecule 55: 60S ribosomal protein L42-A

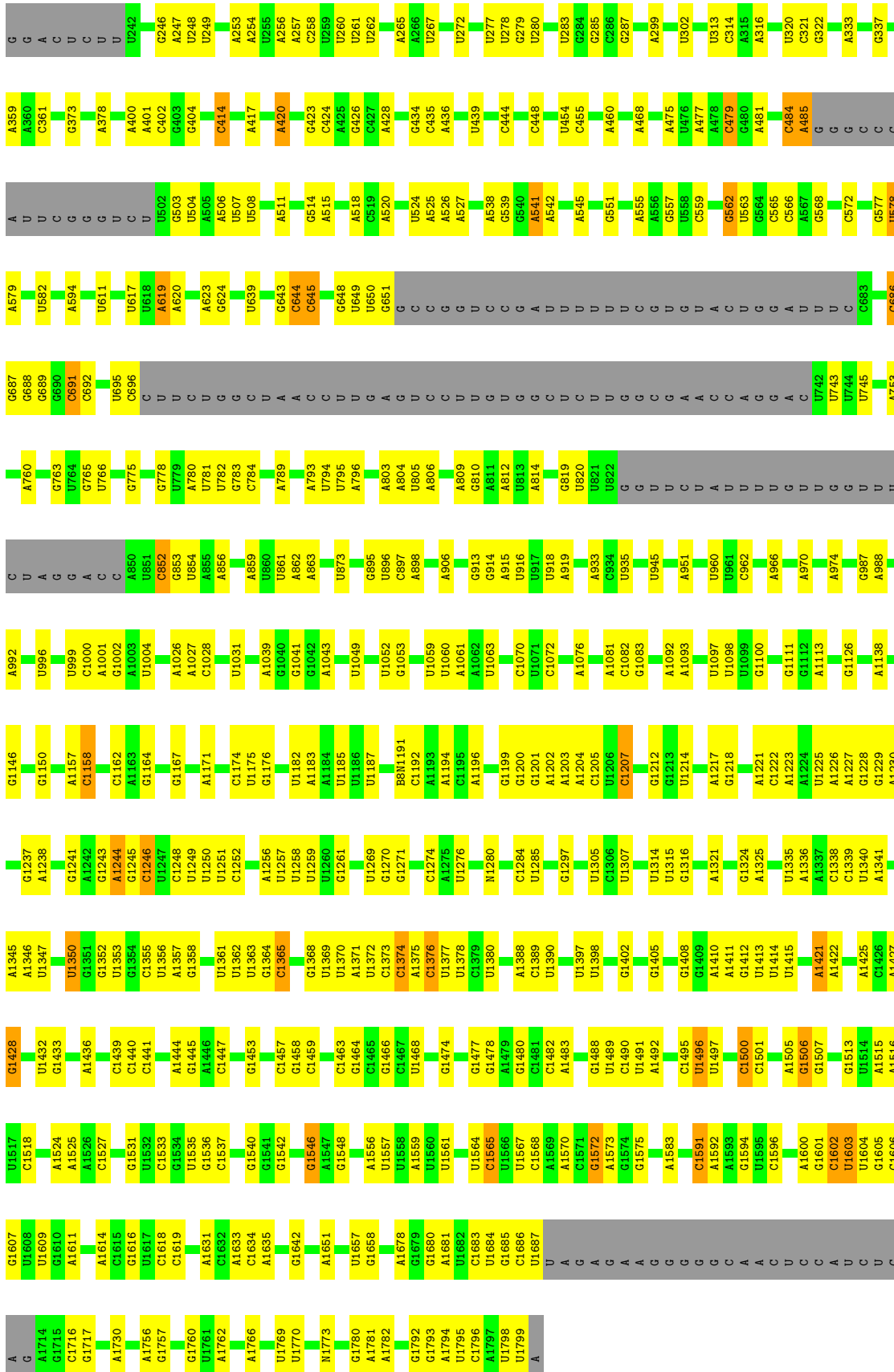


- Molecule 56: 60S ribosomal protein L43-A

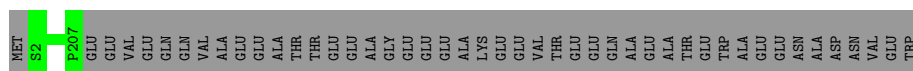
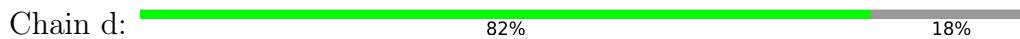


- Molecule 57: 18S ribosomal RNA

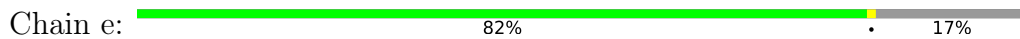




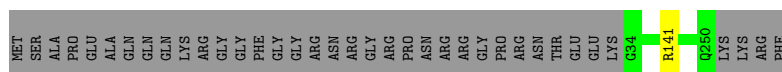
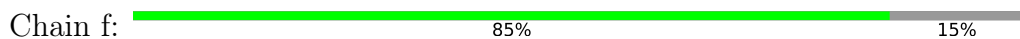
• Molecule 58: 40S ribosomal protein S0-A



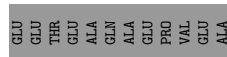
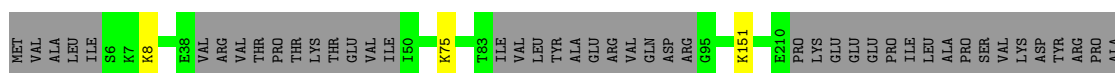
• Molecule 59: 40S ribosomal protein S1-A



• Molecule 60: 40S ribosomal protein S2



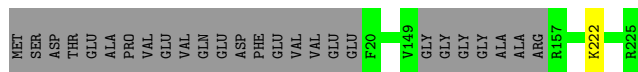
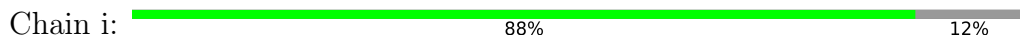
• Molecule 61: RPS3 isoform 1



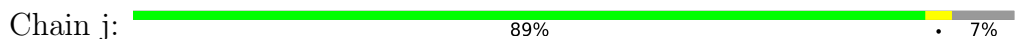
• Molecule 62: 40S ribosomal protein S4-A



• Molecule 63: 40S ribosomal protein S5



• Molecule 64: 40S ribosomal protein S6-A



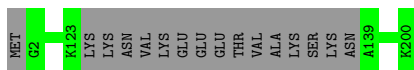
- Molecule 65: 40S ribosomal protein S7-A

Chain k:  96%



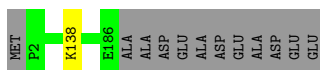
- Molecule 66: 40S ribosomal protein S8-B

Chain l:  92%



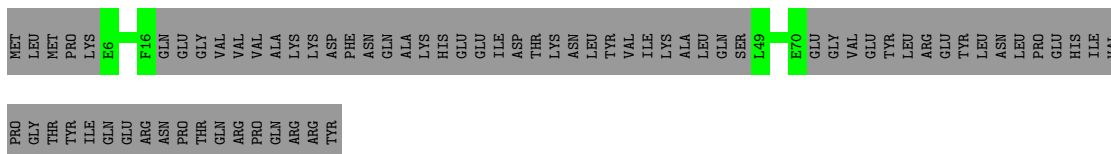
- Molecule 67: 40S ribosomal protein S9-A

Chain m:  93%




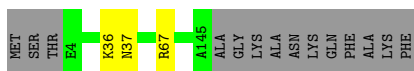
- Molecule 68: 40S ribosomal protein S10-A

Chain n:  31%



- Molecule 69: 40S ribosomal protein S11-A

Chain o:  89%



- Molecule 70: 40S ribosomal protein S13

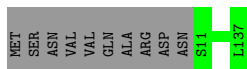
Chain p:  99%



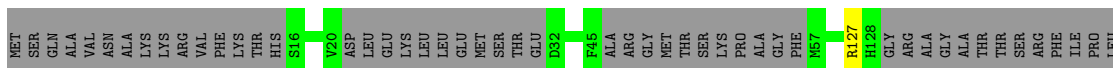
- Molecule 71: 40S ribosomal protein S14-A

Chain q:  93%

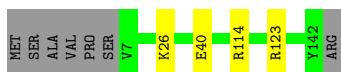
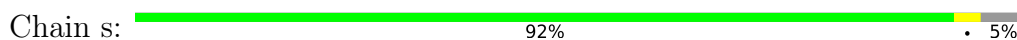




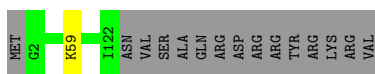
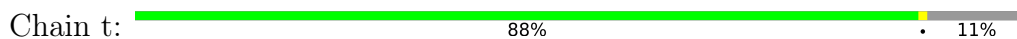
- Molecule 72: 40S ribosomal protein S15



- Molecule 73: 40S ribosomal protein S16-A



- Molecule 74: 40S ribosomal protein S17-A



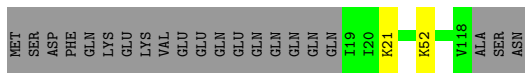
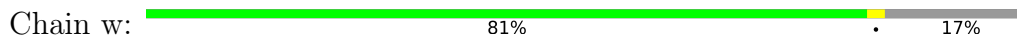
- Molecule 75: 40S ribosomal protein S18-A



- Molecule 76: 40S ribosomal protein S19-A



- Molecule 77: 40S ribosomal protein S20



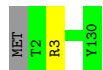
- Molecule 78: 40S ribosomal protein S21-A

Chain x:  100%

There are no outlier residues recorded for this chain.

- Molecule 79: 40S ribosomal protein S22-A

Chain y:  98%



- Molecule 80: 40S ribosomal protein S23-A

Chain z:  98%



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	38558	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	40	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	1000	Depositor
Magnification	165000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor

## 5 Model quality i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: OMG, A2M, ZN, 4AC, UR3, MG, GTP, G7M, 5MC, K, B8N, MA6, OMU, DDE, 1MA, OMC

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	0	0.28	0/1087	0.60	0/1449
2	1	0.26	0/571	0.66	0/768
3	2	0.31	0/782	0.64	0/1047
4	3	0.29	0/620	0.61	0/838
5	4	0.28	0/499	0.62	0/670
6	5	0.29	0/412	0.60	0/544
7	6	0.57	1/433 (0.2%)	1.05	5/575 (0.9%)
8	7	0.40	1/2489 (0.0%)	0.73	4/3389 (0.1%)
9	8	0.26	0/279	0.60	0/369
10	A	0.33	0/1585	0.54	0/2128
11	AA	0.40	0/75545	0.83	29/117782 (0.0%)
12	Aa	0.28	0/6470	0.55	0/8759
13	B	0.33	0/1245	0.59	0/1676
14	BB	0.38	0/2883	0.80	1/4491 (0.0%)
15	C	0.29	0/1465	0.58	1/1965 (0.1%)
16	CC	0.41	0/3746	0.81	0/5832
17	D	0.29	0/1440	0.58	0/1921
18	DD	0.27	0/1558	0.53	0/2107
19	E	0.34	0/1481	0.61	0/1990
20	EE	0.31	0/1948	0.60	0/2617
21	Ee	0.28	0/1210	0.55	0/1627
22	F	0.30	0/1300	0.55	0/1743
23	FF	0.30	0/3146	0.55	0/4228
24	G	0.30	0/786	0.53	0/1065
25	GG	0.30	0/2800	0.53	0/3790
26	H	0.31	0/978	0.58	0/1316
27	HH	0.30	0/2425	0.53	0/3271
28	I	0.34	0/533	0.57	0/707
29	II	0.30	0/1251	0.56	0/1682
30	J	0.29	0/974	0.55	0/1314
31	JJ	0.35	0/1821	0.54	0/2451
32	K	0.29	0/1004	0.56	0/1341

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
33	KK	0.27	0/1836	0.48	0/2481
34	L	0.31	0/1118	0.52	0/1497
35	LL	0.32	0/1539	0.56	0/2073
36	M	0.27	0/1204	0.56	0/1612
37	MM	0.30	0/1779	0.55	0/2386
38	N	0.26	0/473	0.54	0/629
39	NN	0.28	0/1374	0.60	0/1842
40	O	0.32	0/750	0.57	0/1008
41	OO	0.29	0/1568	0.59	0/2106
42	P	0.30	0/897	0.59	0/1205
43	PP	0.28	0/1068	0.55	0/1438
44	Q	0.29	0/1041	0.54	0/1394
45	QQ	0.29	0/1757	0.59	0/2354
46	R	0.35	0/868	0.60	0/1168
47	S	0.30	0/871	0.58	0/1164
48	T	0.28	0/978	0.55	0/1301
49	U	0.27	0/778	0.59	0/1034
50	V	0.31	0/680	0.64	0/901
51	W	0.29	0/618	0.59	0/826
52	X	0.30	0/443	0.67	0/588
53	Y	0.29	0/423	0.62	0/562
54	Z	0.29	0/234	0.88	0/300
55	a	0.29	0/831	0.61	0/1097
56	b	0.30	0/701	0.63	0/934
57	c	0.37	0/37760	0.94	120/58811 (0.2%)
58	d	0.28	0/1623	0.54	0/2222
59	e	0.29	0/1714	0.58	0/2308
60	f	0.29	0/1665	0.56	0/2263
61	g	0.29	0/1429	0.59	0/1913
62	h	0.31	0/2097	0.61	1/2823 (0.0%)
63	i	0.28	0/1591	0.61	0/2151
64	j	0.28	0/1790	0.62	1/2393 (0.0%)
65	k	0.28	0/1506	0.57	0/2028
66	l	0.31	0/1482	0.63	0/1980
67	m	0.28	0/1519	0.59	0/2035
68	n	0.29	0/309	0.49	0/416
69	o	0.30	0/1172	0.61	0/1580
70	p	0.31	0/1215	0.57	0/1638
71	q	0.29	0/901	0.62	0/1217
72	r	0.31	0/747	0.64	0/1002
73	s	0.27	0/1088	0.59	0/1459
74	t	0.27	0/971	0.59	0/1303
75	u	0.27	0/1211	0.60	0/1628

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
76	v	0.26	0/1130	0.56	0/1517
77	w	0.26	0/810	0.57	0/1095
78	x	0.31	0/693	0.60	0/935
79	y	0.31	0/1038	0.57	0/1395
80	z	0.29	0/1139	0.60	0/1518
All	All	0.35	2/215195 (0.0%)	0.76	162/314982 (0.1%)

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
7	6	0	1
31	JJ	0	2
34	L	0	1
50	V	0	1
53	Y	0	1
64	j	0	1
65	k	0	1
69	o	0	1
73	s	0	1
All	All	0	10

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	7	287	PRO	CG-CD	-13.52	1.06	1.50
7	6	19	PRO	CG-CD	-8.23	1.23	1.50

The worst 5 of 162 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	7	287	PRO	N-CD-CG	-18.44	75.55	103.20
57	c	94	U	C2-N3-C4	14.86	135.92	127.00
57	c	1501	C	N1-C2-O2	14.09	127.35	118.90
8	7	287	PRO	CA-CB-CG	-12.15	80.92	104.00
57	c	1602	C	OP1-P-O3'	-11.57	79.74	105.20

There are no chirality outliers.

5 of 10 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	6	17	GLN	Mainchain
31	JJ	158	LYS	Peptide
31	JJ	232	ARG	Peptide
34	L	102	GLU	Peptide
50	V	64	MET	Peptide

## 5.2 Too-close contacts [i](#)

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

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	132/135 (98%)	126 (96%)	6 (4%)	0	100	100
2	1	68/108 (63%)	61 (90%)	7 (10%)	0	100	100
3	2	95/119 (80%)	90 (95%)	5 (5%)	0	100	100
4	3	79/82 (96%)	73 (92%)	6 (8%)	0	100	100
5	4	61/67 (91%)	59 (97%)	2 (3%)	0	100	100
6	5	47/56 (84%)	45 (96%)	2 (4%)	0	100	100
7	6	51/63 (81%)	48 (94%)	3 (6%)	0	100	100
8	7	316/319 (99%)	298 (94%)	18 (6%)	0	100	100
9	8	32/152 (21%)	19 (59%)	13 (41%)	0	100	100
10	A	195/199 (98%)	193 (99%)	2 (1%)	0	100	100
12	Aa	811/842 (96%)	794 (98%)	17 (2%)	0	100	100
13	B	152/184 (83%)	152 (100%)	0	0	100	100
15	C	183/186 (98%)	182 (100%)	1 (0%)	0	100	100
17	D	174/189 (92%)	170 (98%)	4 (2%)	0	100	100
18	DD	195/312 (62%)	192 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	E	170/172 (99%)	166 (98%)	4 (2%)	0	100	100
20	EE	250/254 (98%)	248 (99%)	2 (1%)	0	100	100
21	Ee	156/165 (94%)	148 (95%)	8 (5%)	0	100	100
22	F	157/160 (98%)	155 (99%)	2 (1%)	0	100	100
23	FF	384/387 (99%)	373 (97%)	11 (3%)	0	100	100
24	G	95/121 (78%)	95 (100%)	0	0	100	100
25	GG	359/362 (99%)	350 (98%)	9 (2%)	0	100	100
26	H	127/137 (93%)	127 (100%)	0	0	100	100
27	HH	294/297 (99%)	285 (97%)	9 (3%)	0	100	100
28	I	61/155 (39%)	61 (100%)	0	0	100	100
29	II	151/176 (86%)	150 (99%)	1 (1%)	0	100	100
30	J	118/142 (83%)	114 (97%)	4 (3%)	0	100	100
31	JJ	220/244 (90%)	212 (96%)	7 (3%)	1 (0%)	29	66
32	K	124/127 (98%)	123 (99%)	1 (1%)	0	100	100
33	KK	231/256 (90%)	226 (98%)	5 (2%)	0	100	100
34	L	133/136 (98%)	129 (97%)	3 (2%)	1 (1%)	19	57
35	LL	189/191 (99%)	184 (97%)	5 (3%)	0	100	100
36	M	146/149 (98%)	141 (97%)	5 (3%)	0	100	100
37	MM	213/221 (96%)	207 (97%)	6 (3%)	0	100	100
38	N	56/59 (95%)	54 (96%)	2 (4%)	0	100	100
39	NN	167/174 (96%)	159 (95%)	8 (5%)	0	100	100
40	O	95/105 (90%)	95 (100%)	0	0	100	100
41	OO	191/199 (96%)	180 (94%)	10 (5%)	1 (0%)	29	66
42	P	107/113 (95%)	105 (98%)	2 (2%)	0	100	100
43	PP	134/138 (97%)	131 (98%)	3 (2%)	0	100	100
44	Q	125/130 (96%)	123 (98%)	2 (2%)	0	100	100
45	QQ	201/204 (98%)	196 (98%)	5 (2%)	0	100	100
46	R	104/107 (97%)	103 (99%)	1 (1%)	0	100	100
47	S	107/121 (88%)	107 (100%)	0	0	100	100
48	T	117/120 (98%)	115 (98%)	2 (2%)	0	100	100
49	U	97/100 (97%)	91 (94%)	6 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
50	V	82/88 (93%)	79 (96%)	2 (2%)	1 (1%)	13	50
51	W	75/78 (96%)	72 (96%)	3 (4%)	0	100	100
52	X	48/51 (94%)	47 (98%)	1 (2%)	0	100	100
53	Y	50/128 (39%)	47 (94%)	2 (4%)	1 (2%)	7	41
54	Z	23/25 (92%)	23 (100%)	0	0	100	100
55	a	100/106 (94%)	97 (97%)	3 (3%)	0	100	100
56	b	89/92 (97%)	88 (99%)	1 (1%)	0	100	100
58	d	204/252 (81%)	193 (95%)	11 (5%)	0	100	100
59	e	210/255 (82%)	196 (93%)	14 (7%)	0	100	100
60	f	215/254 (85%)	201 (94%)	14 (6%)	0	100	100
61	g	177/240 (74%)	170 (96%)	7 (4%)	0	100	100
62	h	256/261 (98%)	244 (95%)	12 (5%)	0	100	100
63	i	195/225 (87%)	186 (95%)	9 (5%)	0	100	100
64	j	217/236 (92%)	217 (100%)	0	0	100	100
65	k	182/190 (96%)	172 (94%)	10 (6%)	0	100	100
66	l	180/200 (90%)	169 (94%)	11 (6%)	0	100	100
67	m	183/197 (93%)	175 (96%)	8 (4%)	0	100	100
68	n	29/105 (28%)	29 (100%)	0	0	100	100
69	o	140/156 (90%)	133 (95%)	7 (5%)	0	100	100
70	p	148/151 (98%)	145 (98%)	3 (2%)	0	100	100
71	q	125/137 (91%)	119 (95%)	6 (5%)	0	100	100
72	r	85/142 (60%)	80 (94%)	5 (6%)	0	100	100
73	s	134/143 (94%)	126 (94%)	8 (6%)	0	100	100
74	t	119/136 (88%)	114 (96%)	5 (4%)	0	100	100
75	u	143/146 (98%)	134 (94%)	9 (6%)	0	100	100
76	v	141/144 (98%)	137 (97%)	4 (3%)	0	100	100
77	w	98/121 (81%)	98 (100%)	0	0	100	100
78	x	85/87 (98%)	81 (95%)	4 (5%)	0	100	100
79	y	127/130 (98%)	125 (98%)	2 (2%)	0	100	100
80	z	142/145 (98%)	132 (93%)	10 (7%)	0	100	100
All	All	11672/13056 (89%)	11284 (97%)	383 (3%)	5 (0%)	100	100

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
31	JJ	159	GLN
50	V	65	ARG
34	L	102	GLU
53	Y	105	PRO
41	OO	63	VAL

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	112/113 (99%)	111 (99%)	1 (1%)	78	88
2	1	61/89 (68%)	60 (98%)	1 (2%)	62	79
3	2	83/101 (82%)	83 (100%)	0	100	100
4	3	70/71 (99%)	70 (100%)	0	100	100
5	4	56/60 (93%)	55 (98%)	1 (2%)	59	77
6	5	43/49 (88%)	42 (98%)	1 (2%)	50	72
7	6	46/54 (85%)	43 (94%)	3 (6%)	17	48
8	7	259/262 (99%)	258 (100%)	1 (0%)	91	95
9	8	30/135 (22%)	30 (100%)	0	100	100
10	A	160/162 (99%)	159 (99%)	1 (1%)	86	92
12	Aa	694/714 (97%)	691 (100%)	3 (0%)	91	95
13	B	125/146 (86%)	123 (98%)	2 (2%)	62	79
15	C	150/151 (99%)	150 (100%)	0	100	100
17	D	143/154 (93%)	142 (99%)	1 (1%)	84	91
18	DD	167/254 (66%)	167 (100%)	0	100	100
19	E	156/156 (100%)	156 (100%)	0	100	100
20	EE	193/196 (98%)	193 (100%)	0	100	100
21	Ee	129/136 (95%)	129 (100%)	0	100	100
22	F	136/137 (99%)	135 (99%)	1 (1%)	84	91

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	FF	320/323 (99%)	319 (100%)	1 (0%)	92	96
24	G	84/107 (78%)	84 (100%)	0	100	100
25	GG	288/289 (100%)	285 (99%)	3 (1%)	76	86
26	H	101/105 (96%)	101 (100%)	0	100	100
27	HH	244/245 (100%)	244 (100%)	0	100	100
28	I	55/129 (43%)	54 (98%)	1 (2%)	59	77
29	II	133/153 (87%)	133 (100%)	0	100	100
30	J	104/118 (88%)	103 (99%)	1 (1%)	76	86
31	JJ	186/205 (91%)	186 (100%)	0	100	100
32	K	109/110 (99%)	108 (99%)	1 (1%)	78	88
33	KK	187/208 (90%)	187 (100%)	0	100	100
34	L	115/116 (99%)	115 (100%)	0	100	100
35	LL	171/171 (100%)	171 (100%)	0	100	100
36	M	118/119 (99%)	118 (100%)	0	100	100
37	MM	184/187 (98%)	183 (100%)	1 (0%)	88	94
38	N	46/47 (98%)	46 (100%)	0	100	100
39	NN	147/150 (98%)	147 (100%)	0	100	100
40	O	81/88 (92%)	81 (100%)	0	100	100
41	OO	154/159 (97%)	153 (99%)	1 (1%)	86	92
42	P	94/97 (97%)	93 (99%)	1 (1%)	73	85
43	PP	107/109 (98%)	107 (100%)	0	100	100
44	Q	109/111 (98%)	108 (99%)	1 (1%)	78	88
45	QQ	175/176 (99%)	175 (100%)	0	100	100
46	R	90/91 (99%)	90 (100%)	0	100	100
47	S	94/103 (91%)	94 (100%)	0	100	100
48	T	104/105 (99%)	103 (99%)	1 (1%)	76	86
49	U	81/82 (99%)	81 (100%)	0	100	100
50	V	69/71 (97%)	67 (97%)	2 (3%)	42	67
51	W	68/69 (99%)	68 (100%)	0	100	100
52	X	45/46 (98%)	45 (100%)	0	100	100
53	Y	47/116 (40%)	46 (98%)	1 (2%)	53	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
54	Z	23/23 (100%)	23 (100%)	0	100	100
55	a	87/91 (96%)	86 (99%)	1 (1%)	73	85
56	b	71/72 (99%)	70 (99%)	1 (1%)	67	81
58	d	165/210 (79%)	165 (100%)	0	100	100
59	e	189/224 (84%)	187 (99%)	2 (1%)	73	85
60	f	176/205 (86%)	175 (99%)	1 (1%)	86	92
61	g	145/195 (74%)	142 (98%)	3 (2%)	53	74
62	h	220/222 (99%)	219 (100%)	1 (0%)	88	94
63	i	172/191 (90%)	171 (99%)	1 (1%)	86	92
64	j	188/201 (94%)	182 (97%)	6 (3%)	39	65
65	k	165/170 (97%)	164 (99%)	1 (1%)	86	92
66	l	146/161 (91%)	146 (100%)	0	100	100
67	m	158/166 (95%)	157 (99%)	1 (1%)	86	92
68	n	32/98 (33%)	32 (100%)	0	100	100
69	o	127/137 (93%)	125 (98%)	2 (2%)	62	79
70	p	127/128 (99%)	127 (100%)	0	100	100
71	q	81/105 (77%)	81 (100%)	0	100	100
72	r	77/118 (65%)	76 (99%)	1 (1%)	69	82
73	s	113/119 (95%)	110 (97%)	3 (3%)	44	69
74	t	105/124 (85%)	104 (99%)	1 (1%)	76	86
75	u	128/129 (99%)	127 (99%)	1 (1%)	81	89
76	v	115/116 (99%)	115 (100%)	0	100	100
77	w	94/114 (82%)	92 (98%)	2 (2%)	53	74
78	x	74/74 (100%)	74 (100%)	0	100	100
79	y	110/111 (99%)	109 (99%)	1 (1%)	78	88
80	z	119/120 (99%)	117 (98%)	2 (2%)	60	78
All	All	9930/10969 (90%)	9868 (99%)	62 (1%)	86	92

5 of 62 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
50	V	57	HIS
74	t	59	LYS

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Mol	Chain	Res	Type
60	f	141	ARG
73	s	123	ARG
79	y	3	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 49 such sidechains are listed below:

Mol	Chain	Res	Type
47	S	108	GLN
63	i	128	ASN
49	U	12	ASN
61	g	74	GLN
64	j	199	GLN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
11	AA	3193/3396 (94%)	636 (19%)	21 (0%)
14	BB	120/121 (99%)	18 (15%)	1 (0%)
16	CC	157/158 (99%)	28 (17%)	1 (0%)
57	c	1593/1800 (88%)	468 (29%)	0
All	All	5063/5475 (92%)	1150 (22%)	23 (0%)

5 of 1150 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
11	AA	4	U
11	AA	6	A
11	AA	12	A
11	AA	14	U
11	AA	26	A

5 of 23 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
11	AA	2490	C
11	AA	2570	U
11	AA	2501	U
11	AA	2971	A
11	AA	1348	U

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

67 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$
11	OMG	AA	2791	11	18,26,27	1.19	2 (11%)	19,38,41	0.83	1 (5%)
57	OMG	c	1428	57	18,26,27	1.14	2 (11%)	19,38,41	0.82	1 (5%)
11	A2M	AA	1449	82,11	18,25,26	3.63	8 (44%)	18,36,39	3.42	4 (22%)
57	A2M	c	100	82,57	18,25,26	3.63	8 (44%)	18,36,39	3.31	3 (16%)
11	A2M	AA	2256	11	18,25,26	3.58	8 (44%)	18,36,39	3.57	5 (27%)
11	OMG	AA	2288	11	18,26,27	1.18	2 (11%)	19,38,41	0.79	1 (5%)
57	OMG	c	1572	57	18,26,27	1.17	2 (11%)	19,38,41	0.87	1 (5%)
57	4AC	c	1773	57	21,24,25	3.47	10 (47%)	29,34,37	1.61	5 (17%)
11	OMG	AA	1450	11	18,26,27	1.14	2 (11%)	19,38,41	0.80	1 (5%)
11	OMU	AA	1888	11	19,22,23	3.03	8 (42%)	26,31,34	1.72	5 (19%)
11	A2M	AA	2220	11	18,25,26	3.59	8 (44%)	18,36,39	3.45	4 (22%)
57	OMG	c	562	57	18,26,27	1.24	2 (11%)	19,38,41	0.80	0
11	UR3	AA	2634	11	19,22,23	2.76	7 (36%)	26,32,35	1.25	1 (3%)
57	OMC	c	414	57	19,22,23	0.62	0	26,31,34	1.08	2 (7%)
11	5MC	AA	2278	82,11	18,22,23	0.59	0	26,32,35	0.67	0
11	OMC	AA	1437	82,11	19,22,23	0.62	0	26,31,34	1.34	2 (7%)
11	OMU	AA	2347	11	19,22,23	3.00	8 (42%)	26,31,34	1.75	4 (15%)
11	OMC	AA	2948	11	19,22,23	0.61	0	26,31,34	1.03	2 (7%)
12	DDE	Aa	699	12	14,20,21	1.02	1 (7%)	14,28,30	1.17	2 (14%)
11	OMU	AA	898	11	19,22,23	3.04	8 (42%)	26,31,34	1.72	5 (19%)
11	OMG	AA	2922	11	18,26,27	1.15	2 (11%)	19,38,41	0.87	1 (5%)
11	OMC	AA	2337	11	19,22,23	0.60	0	26,31,34	0.80	1 (3%)
11	OMC	AA	2197	11,83	19,22,23	0.54	0	26,31,34	0.66	0
11	OMU	AA	2421	11	19,22,23	3.02	8 (42%)	26,31,34	1.70	5 (19%)
11	A2M	AA	2280	11	18,25,26	3.63	8 (44%)	18,36,39	3.34	4 (22%)
57	A2M	c	28	80,57	18,25,26	3.62	9 (50%)	18,36,39	3.36	4 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
11	A2M	AA	1133	82,11	18,25,26	3.64	8 (44%)	18,36,39	3.32	3 (16%)
57	4AC	c	1280	57	21,24,25	3.54	10 (47%)	29,34,37	1.77	7 (24%)
57	G7M	c	1575	57	20,26,27	2.46	7 (35%)	17,39,42	1.15	1 (5%)
11	A2M	AA	2640	11	18,25,26	3.58	8 (44%)	18,36,39	3.42	4 (22%)
11	OMU	AA	2724	11	19,22,23	3.02	8 (42%)	26,31,34	1.75	5 (19%)
11	OMC	AA	2959	11	19,22,23	0.55	0	26,31,34	0.68	0
11	1MA	AA	2142	82,11	16,25,26	0.95	2 (12%)	18,37,40	1.10	2 (11%)
11	OMG	AA	805	11	18,26,27	1.16	2 (11%)	19,38,41	0.83	1 (5%)
11	OMC	AA	650	11	19,22,23	0.55	0	26,31,34	0.80	1 (3%)
11	A2M	AA	2281	11	18,25,26	3.69	9 (50%)	18,36,39	3.41	4 (22%)
11	OMG	AA	2793	11	18,26,27	1.21	2 (11%)	19,38,41	0.76	1 (5%)
11	A2M	AA	876	11	18,25,26	3.62	9 (50%)	18,36,39	3.40	4 (22%)
11	OMC	AA	663	11	19,22,23	0.57	0	26,31,34	0.70	0
57	A2M	c	420	57	18,25,26	3.60	8 (44%)	18,36,39	3.41	3 (16%)
57	OMG	c	1271	57	18,26,27	1.14	2 (11%)	19,38,41	0.79	0
57	MA6	c	1782	57	18,26,27	1.03	2 (11%)	19,38,41	3.50	2 (10%)
57	OMG	c	1126	57	18,26,27	1.20	2 (11%)	19,38,41	0.77	1 (5%)
57	A2M	c	541	57	18,25,26	3.62	8 (44%)	18,36,39	3.29	4 (22%)
11	A2M	AA	807	11	18,25,26	3.61	8 (44%)	18,36,39	3.36	4 (22%)
57	MA6	c	1781	57	18,26,27	1.05	2 (11%)	19,38,41	3.46	2 (10%)
11	5MC	AA	2870	11,83	18,22,23	0.65	0	26,32,35	0.59	0
11	A2M	AA	649	11	18,25,26	3.62	8 (44%)	18,36,39	3.33	4 (22%)
11	A2M	AA	817	82,11	18,25,26	3.63	8 (44%)	18,36,39	3.55	4 (22%)
57	A2M	c	974	57	18,25,26	3.62	8 (44%)	18,36,39	3.43	4 (22%)
57	OMU	c	1269	57	19,22,23	3.12	8 (42%)	26,31,34	1.67	5 (19%)
57	OMC	c	1639	82,57	19,22,23	0.56	0	26,31,34	0.67	0
11	1MA	AA	645	82,11	16,25,26	0.92	2 (12%)	18,37,40	1.03	1 (5%)
57	A2M	c	619	82,57	18,25,26	3.69	9 (50%)	18,36,39	3.39	4 (22%)
11	OMG	AA	908	11	18,26,27	1.20	2 (11%)	19,38,41	0.83	1 (5%)
57	OMC	c	1007	57	19,22,23	0.55	0	26,31,34	0.70	0
57	B8N	c	1191	57	24,29,30	3.07	8 (33%)	29,42,45	1.72	5 (17%)
57	OMU	c	578	57	19,22,23	3.06	8 (42%)	26,31,34	1.69	5 (19%)
11	OMG	AA	867	11,83	18,26,27	1.16	2 (11%)	19,38,41	0.90	2 (10%)
11	OMU	AA	2729	11	19,22,23	3.01	8 (42%)	26,31,34	1.74	4 (15%)
57	A2M	c	436	57	18,25,26	3.61	8 (44%)	18,36,39	3.37	4 (22%)
11	OMU	AA	2417	11	19,22,23	2.99	8 (42%)	26,31,34	1.72	5 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
57	A2M	c	796	57	18,25,26	3.64	8 (44%)	18,36,39	3.39	3 (16%)
11	A2M	AA	2946	82,11	18,25,26	3.62	8 (44%)	18,36,39	3.31	4 (22%)
11	OMG	AA	2815	11	18,26,27	1.15	2 (11%)	19,38,41	0.88	1 (5%)
11	OMU	AA	2921	11	19,22,23	3.00	8 (42%)	26,31,34	1.71	5 (19%)
11	OMG	AA	2619	11	18,26,27	1.16	2 (11%)	19,38,41	0.82	1 (5%)

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
11	OMG	AA	2791	11	-	0/5/27/28	0/3/3/3
57	OMG	c	1428	57	-	3/5/27/28	0/3/3/3
11	A2M	AA	1449	82,11	-	0/5/27/28	0/3/3/3
57	A2M	c	100	82,57	-	0/5/27/28	0/3/3/3
11	A2M	AA	2256	11	-	3/5/27/28	0/3/3/3
11	OMG	AA	2288	11	-	0/5/27/28	0/3/3/3
57	OMG	c	1572	57	-	3/5/27/28	0/3/3/3
57	4AC	c	1773	57	-	3/11/29/30	0/2/2/2
11	OMG	AA	1450	11	-	3/5/27/28	0/3/3/3
11	OMU	AA	1888	11	-	0/9/27/28	0/2/2/2
11	A2M	AA	2220	11	-	1/5/27/28	0/3/3/3
57	OMG	c	562	57	-	2/5/27/28	0/3/3/3
11	UR3	AA	2634	11	-	0/7/25/26	0/2/2/2
57	OMC	c	414	57	-	3/9/27/28	0/2/2/2
11	5MC	AA	2278	82,11	-	2/7/25/26	0/2/2/2
11	OMC	AA	1437	82,11	-	5/9/27/28	0/2/2/2
11	OMU	AA	2347	11	-	1/9/27/28	0/2/2/2
11	OMC	AA	2948	11	-	4/9/27/28	0/2/2/2
12	DDE	Aa	699	12	-	12/20/21/23	0/1/1/1
11	OMU	AA	898	11	-	2/9/27/28	0/2/2/2
11	OMG	AA	2922	11	-	2/5/27/28	0/3/3/3
11	OMC	AA	2337	11	-	3/9/27/28	0/2/2/2
11	OMC	AA	2197	11,83	-	2/9/27/28	0/2/2/2
11	OMU	AA	2421	11	-	1/9/27/28	0/2/2/2
11	A2M	AA	2280	11	-	2/5/27/28	0/3/3/3
57	A2M	c	28	80,57	-	3/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	A2M	AA	1133	82,11	-	0/5/27/28	0/3/3/3
57	4AC	c	1280	57	-	6/11/29/30	0/2/2/2
57	G7M	c	1575	57	-	2/3/25/26	0/3/3/3
11	A2M	AA	2640	11	-	1/5/27/28	0/3/3/3
11	OMU	AA	2724	11	-	1/9/27/28	0/2/2/2
11	OMC	AA	2959	11	-	1/9/27/28	0/2/2/2
11	1MA	AA	2142	82,11	-	0/3/25/26	0/3/3/3
11	OMG	AA	805	11	-	1/5/27/28	0/3/3/3
11	OMC	AA	650	11	-	1/9/27/28	0/2/2/2
11	A2M	AA	2281	11	-	3/5/27/28	0/3/3/3
11	OMG	AA	2793	11	-	1/5/27/28	0/3/3/3
11	A2M	AA	876	11	-	0/5/27/28	0/3/3/3
11	OMC	AA	663	11	-	1/9/27/28	0/2/2/2
57	A2M	c	420	57	-	3/5/27/28	0/3/3/3
57	OMG	c	1271	57	-	1/5/27/28	0/3/3/3
57	MA6	c	1782	57	-	1/7/29/30	0/3/3/3
57	OMG	c	1126	57	-	1/5/27/28	0/3/3/3
57	A2M	c	541	57	-	3/5/27/28	0/3/3/3
11	A2M	AA	807	11	-	4/5/27/28	0/3/3/3
57	MA6	c	1781	57	-	0/7/29/30	0/3/3/3
11	5MC	AA	2870	11,83	-	5/7/25/26	0/2/2/2
11	A2M	AA	649	11	-	1/5/27/28	0/3/3/3
11	A2M	AA	817	82,11	-	2/5/27/28	0/3/3/3
57	A2M	c	974	57	-	0/5/27/28	0/3/3/3
57	OMU	c	1269	57	-	5/9/27/28	0/2/2/2
57	OMC	c	1639	82,57	-	0/9/27/28	0/2/2/2
11	1MA	AA	645	82,11	-	2/3/25/26	0/3/3/3
57	A2M	c	619	82,57	-	2/5/27/28	0/3/3/3
11	OMG	AA	908	11	-	3/5/27/28	0/3/3/3
57	OMC	c	1007	57	-	0/9/27/28	0/2/2/2
57	B8N	c	1191	57	-	7/16/34/35	0/2/2/2
57	OMU	c	578	57	-	0/9/27/28	0/2/2/2
11	OMG	AA	867	11,83	-	0/5/27/28	0/3/3/3
11	OMU	AA	2729	11	-	1/9/27/28	0/2/2/2
57	A2M	c	436	57	-	0/5/27/28	0/3/3/3
11	OMU	AA	2417	11	-	0/9/27/28	0/2/2/2
57	A2M	c	796	57	-	1/5/27/28	0/3/3/3
11	A2M	AA	2946	82,11	-	3/5/27/28	0/3/3/3
11	OMG	AA	2815	11	-	1/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	OMU	AA	2921	11	-	1/9/27/28	0/2/2/2
11	OMG	AA	2619	11	-	0/5/27/28	0/3/3/3

The worst 5 of 325 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	c	28	A2M	C3'-C4'	-9.16	1.29	1.53
11	AA	1133	A2M	C3'-C4'	-8.99	1.30	1.53
11	AA	1449	A2M	C3'-C4'	-8.99	1.30	1.53
57	c	619	A2M	C3'-C4'	-8.95	1.30	1.53
57	c	974	A2M	C3'-C4'	-8.94	1.30	1.53

The worst 5 of 175 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	c	1782	MA6	N1-C6-N6	-14.09	102.23	117.06
57	c	1781	MA6	N1-C6-N6	-13.88	102.45	117.06
11	AA	817	A2M	C5-C6-N6	11.00	137.07	120.35
11	AA	2256	A2M	C5-C6-N6	10.75	136.68	120.35
11	AA	1449	A2M	C5-C6-N6	10.72	136.64	120.35

There are no chirality outliers.

5 of 125 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	AA	649	A2M	C1'-C2'-O2'-CM'
11	AA	663	OMC	C1'-C2'-O2'-CM2
11	AA	805	OMG	C1'-C2'-O2'-CM2
11	AA	807	A2M	C1'-C2'-O2'-CM'
11	AA	898	OMU	C1'-C2'-O2'-CM2

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry

Of 172 ligands modelled in this entry, 171 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
84	GTP	Aa	901	82	26,34,34	0.99	1 (3%)	32,54,54	1.59	5 (15%)

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
84	GTP	Aa	901	82	-	3/18/38/38	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
84	Aa	901	GTP	C6-N1	-2.97	1.33	1.37

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
84	Aa	901	GTP	PB-O3B-PG	-4.43	117.61	132.83
84	Aa	901	GTP	PA-O3A-PB	-4.25	118.25	132.83
84	Aa	901	GTP	C3'-C2'-C1'	3.25	105.86	100.98
84	Aa	901	GTP	C5-C6-N1	2.17	117.79	113.95
84	Aa	901	GTP	C8-N7-C5	2.09	106.97	102.99

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
84	Aa	901	GTP	O4'-C4'-C5'-O5'
84	Aa	901	GTP	C3'-C4'-C5'-O5'

*Continued on next page...*

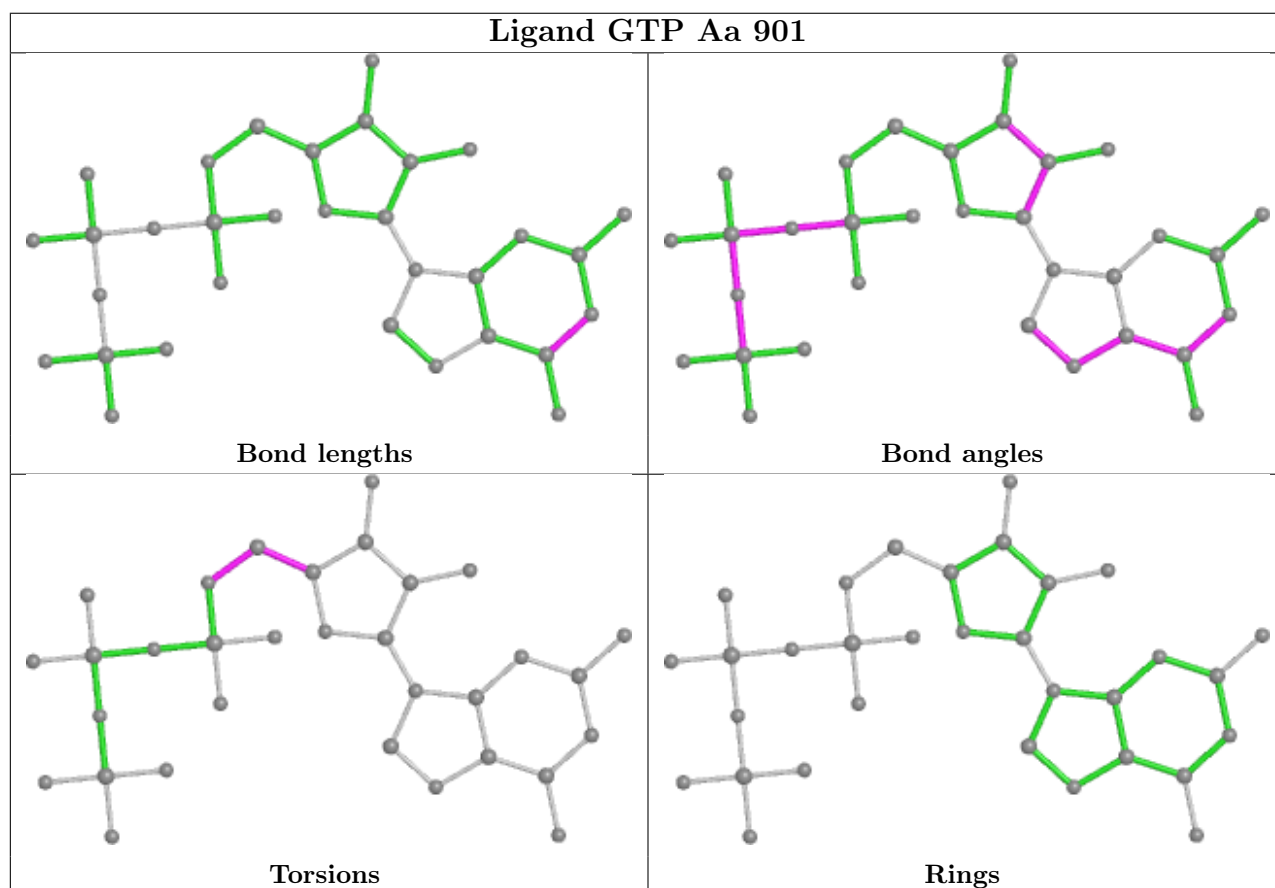
*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
84	Aa	901	GTP	C4'-C5'-O5'-PA

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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

This section contains visualisations of the EMDB entry EMD-16729. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

### 6.1 Orthogonal projections

This section was not generated.

### 6.2 Central slices

This section was not generated.

### 6.3 Largest variance slices

This section was not generated.

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

This section was not generated.

### 6.5 Orthogonal surface views

This section was not generated.

### 6.6 Mask visualisation

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

## 7 Map analysis

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

### 7.1 Map-value distribution

This section was not generated.

### 7.2 Volume estimate versus contour level

This section was not generated.

### 7.3 Rotationally averaged power spectrum

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

## 8 Fourier-Shell correlation

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



## 9 Map-model fit

This section was not generated.