



wwPDB EM Map/Model Validation Report ⓘ

Jun 22, 2016 – 06:21 AM EDT

PDB ID : 5IMQ
EMDB ID: : EMD-6584
Title : Structure of ribosome bound to cofactor at 3.8 angstrom resolution
Authors : Kumar, V.; Ero, R.; Jian, G.K.; Ahmed, T.; Zhan, Y.; Bhushan, S.; Gao, Y.G.
Deposited on : 2016-03-06
Resolution : 3.80 Å(reported)
Based on PDB ID : 4W2E, 5AA0

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027790

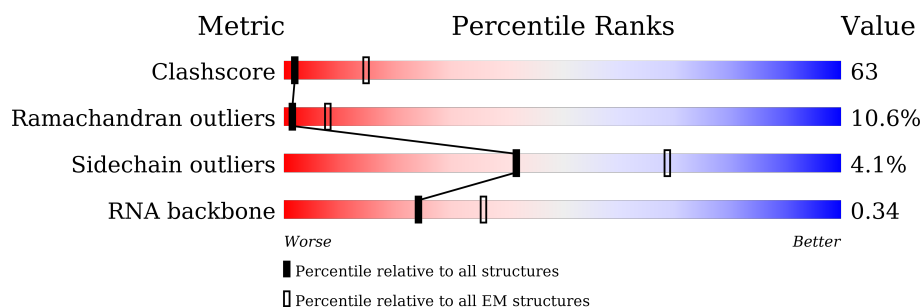
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.80 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.



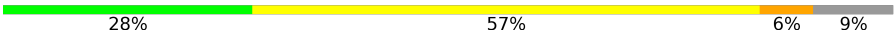


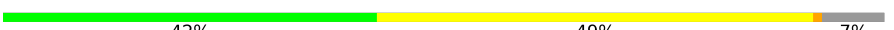
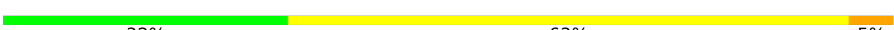
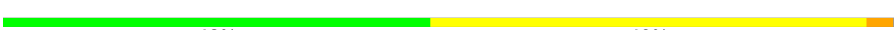




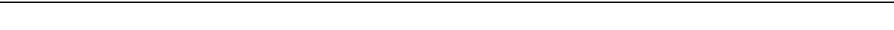

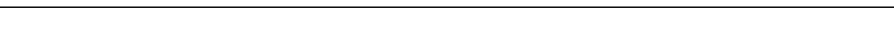
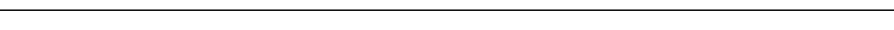



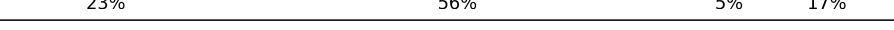







Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686
RNA backbone	3027	244

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	1	37	35% 49% 16%
2	2	173	58% 17% 25%
3	3	147	13% 55% 20% 9%
4	4	77	19% 52% 29%
5	5	76	11% 50% 36%
6	A	1522	11% 54% 33%
7	D	2893	9% 44% 39% 8%
8	E	123	12% 53% 34%

















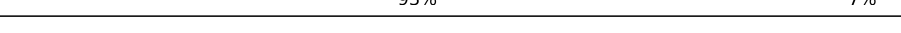
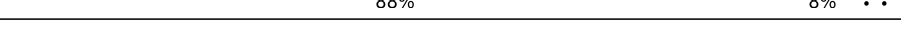





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Mol	Chain	Length	Quality of chain
9	F	256	
10	G	239	
11	H	209	
12	I	162	
13	J	101	
14	K	156	
15	L	138	
16	M	128	
17	N	105	
18	O	129	
19	P	132	
20	Q	126	
21	R	61	
22	S	89	
23	T	88	
24	U	105	
25	V	88	
26	W	93	
27	X	106	
28	Y	27	
29	Z	229	
30	a	276	
31	b	206	
32	c	210	
33	d	182	

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Mol	Chain	Length	Quality of chain
34	e	180	 83% 13% ..
35	f	140	 88% 11% ..
36	g	122	 85% 15%
37	h	150	 79% 16% ..
38	i	141	 84% 13% .
39	j	118	 93% 6% .
40	k	112	 88% 10% .
41	l	146	 66% 12% . 20%
42	m	118	 96% ..
43	n	101	 86% 14%
44	o	113	 89% 8% .
45	p	96	 91% 6% ..
46	q	110	 78% 22%
47	r	206	 77% 10% 13%
48	s	85	 91% . 7%
49	t	67	 93% 7%
50	u	60	 88% 8% ..
51	v	71	 77% 21% .
52	w	60	 77% 15% . 5%
53	x	54	 56% 33% . 9%
54	y	49	 88% 12%
55	z	65	 80% 14% 5% .
56	B	610	 8% 52% 32% 5% .

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	GCP	B	701	-	-	X	-

2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 153046 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 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	37	Total	C	N	O	S	0	0
			307	188	68	47	4		

- Molecule 2 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	2	130	Total	C	N	O	0	0
			641	381	130	130		

- Molecule 3 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	134	Total	C	N	O	S	0	0
			993	632	175	181	5		

- Molecule 4 is a RNA chain called P- site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	4	77	Total	C	N	O	P	0	0
			1640	732	297	535	76		

- Molecule 5 is a RNA chain called E site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	5	76	Total	C	N	O	P	0	0
			1623	723	290	534	76		

- Molecule 6 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	A	1515	Total	C	N	O	P	0	0
			32554	14490	6022	10527	1515		

- Molecule 7 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	D	2889	Total	C	N	O	P	0	0
			62218	27691	11629	20009	2889		

- Molecule 8 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	E	123	Total	C	N	O	P	0	0
			2641	1175	488	855	123		

- Molecule 9 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	F	234	Total	C	N	O	S	0	0
			1900	1213	341	341	5		

- Molecule 10 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	G	206	Total	C	N	O	S	0	0
			1612	1016	314	281	1		

- Molecule 11 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	H	208	Total	C	N	O	S	0	0
			1703	1066	339	291	7		

- Molecule 12 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	I	150	Total	C	N	O	S	0	0
			1146	724	217	201	4		

- Molecule 13 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	J	101	Total	C	N	O	S	0	0
			843	531	155	154	3		

- Molecule 14 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	K	155	Total	C	N	O	S	0	0
			1257	781	252	218	6		

- Molecule 15 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	L	138	Total	C	N	O	S	0	0
			1116	705	215	193	3		

- Molecule 16 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	M	127	Total	C	N	O	S	0	0
			1010	639	197	174			

- Molecule 17 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	N	98	Total	C	N	O	S	0	0
			794	499	156	138	1		

- Molecule 18 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	O	119	Total	C	N	O	S	0	0
			885	549	168	165	3		

- Molecule 19 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	P	124	Total	C	N	O	S	0	0
			970	611	195	163	1		

- Molecule 20 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	Q	114	Total	C	N	O	S	0	0
			914	565	189	158	2		

- Molecule 21 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	R	60	Total	C	N	O	S	0	0
			492	312	104	72	4		

- Molecule 22 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	S	88	Total	C	N	O	S	0	0
			734	459	147	126	2		

- Molecule 23 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	T	83	Total	C	N	O	S	0	0
			700	443	139	117	1		

- Molecule 24 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	U	104	Total	C	N	O	S	0	0
			857	547	161	147	2		

- Molecule 25 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	V	73	Total	C	N	O	0	0
			597	380	118	99		

- Molecule 26 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	W	80	Total	C	N	O	S	0	0
			647	414	119	112	2		

- Molecule 27 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	X	99	Total	C	N	O	S	0	0
			763	470	162	129	2		

- Molecule 28 is a protein called 30S ribosomal protein Thx.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	Y	24	Total	C	N	O	0	0
			208	128	50	30		

- Molecule 29 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Z	228	Total	C	N	O	S	0	0
			1742	1102	318	319	3		

- Molecule 30 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	a	272	Total	C	N	O	S	0	0
			2124	1339	424	358	3		

- Molecule 31 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	b	206	Total	C	N	O	S	0	0
			1578	997	302	273	6		

- Molecule 32 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	c	208	Total	C	N	O	S	0	0
			1625	1034	303	286	2		

- Molecule 33 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	d	182	Total	C	N	O	S	0	0
			1482	947	269	261	5		

- Molecule 34 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	e	174	Total	C	N	O	S	0	0
			1328	844	248	235	1		

- Molecule 35 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	f	139	Total	C	N	O	S	0	0
			1113	717	207	186	3		

- Molecule 36 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	g	122	Total	C	N	O	S	0	0
			932	587	171	170	4		

- Molecule 37 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	h	145	Total	C	N	O	S	0	0
			1106	688	226	190	2		

- Molecule 38 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	i	136	Total	C	N	O	S	0	0
			1080	688	204	183	5		

- Molecule 39 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms				AltConf	Trace
39	j	117	Total	C	N	O	0	0
			960	599	202	159		

- Molecule 40 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				AltConf	Trace
40	k	110	Total	C	N	O	0	0
			877	553	175	149		

- Molecule 41 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	l	117	Total	C	N	O	S	0	0
			976	614	197	164	1		

- Molecule 42 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	m	117	Total	C	N	O	S	0	0
			964	610	202	151	1		

- Molecule 43 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	n	101	Total	C	N	O	S	0	0
			779	501	142	135	1		

- Molecule 44 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	o	110	Total	C	N	O	S	0	0
			876	552	171	151	2		

- Molecule 45 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms				AltConf	Trace
45	p	94	Total	C	N	O	0	0
			742	483	133	126		

- Molecule 46 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	q	110	Total	C	N	O	S	0	0
			844	539	158	141	6		

- Molecule 47 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	r	180	Total	C	N	O	S	0	0
			1435	916	256	260	3		

- Molecule 48 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	s	79	Total	C	N	O	S	0	0
			625	387	131	106	1		

- Molecule 49 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	t	67	Total	C	N	O	S	0	0
			567	350	116	99	2		

- Molecule 50 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	u	59	Total	C	N	O		0	0
			469	298	90	81			

- Molecule 51 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	v	71	Total	C	N	O	S	0	0
			581	364	108	104	5		

- Molecule 52 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	w	57	Total	C	N	O	S	0	0
			445	279	87	74	5		

- Molecule 53 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	x	49	Total	C	N	O	S	0	0
			426	265	87	70	4		

- Molecule 54 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	y	49	Total	C	N	O	S	0	0
			430	263	108	57	2		

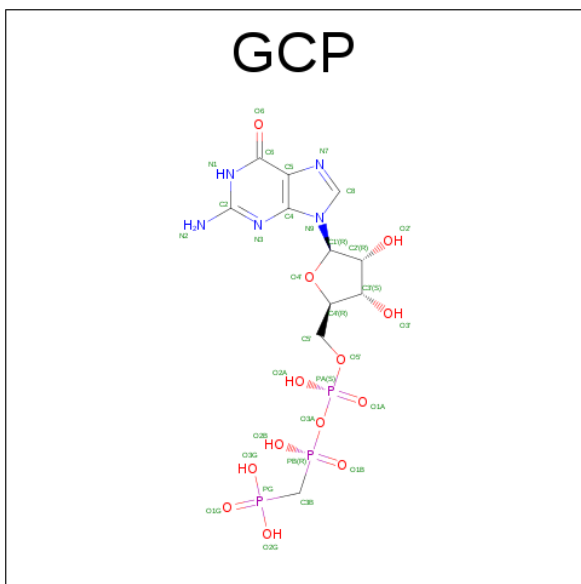
- Molecule 55 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	z	64	Total	C	N	O	S	0	0
			515	331	102	79	3		

- Molecule 56 is a protein called Elongation factor 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	B	591	Total	C	N	O	S	0	0
			4628	2968	794	857	9		

- Molecule 57 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (three-letter code: GCP) (formula: $C_{11}H_{18}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					AltConf
57	B	1	Total	C	N	O	P	0
			32	11	5	13	3	

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

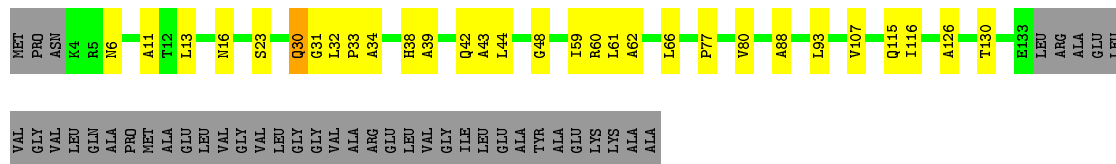
- Molecule 1: 50S ribosomal protein L36

Chain 1: 

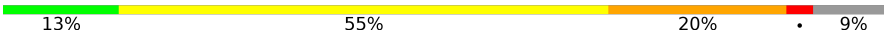


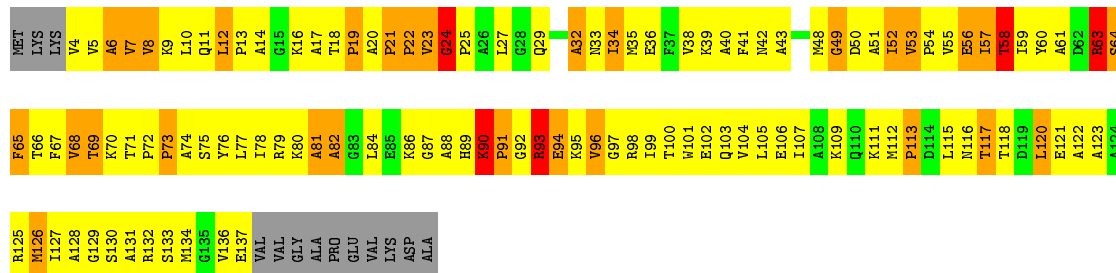
- Molecule 2: 50S ribosomal protein L10

Chain 2: 




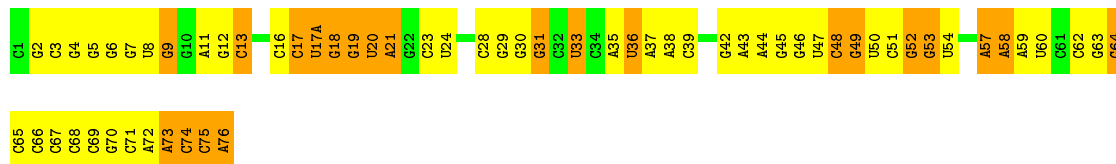
- Molecule 3: 50S ribosomal protein L11

Chain 3: 

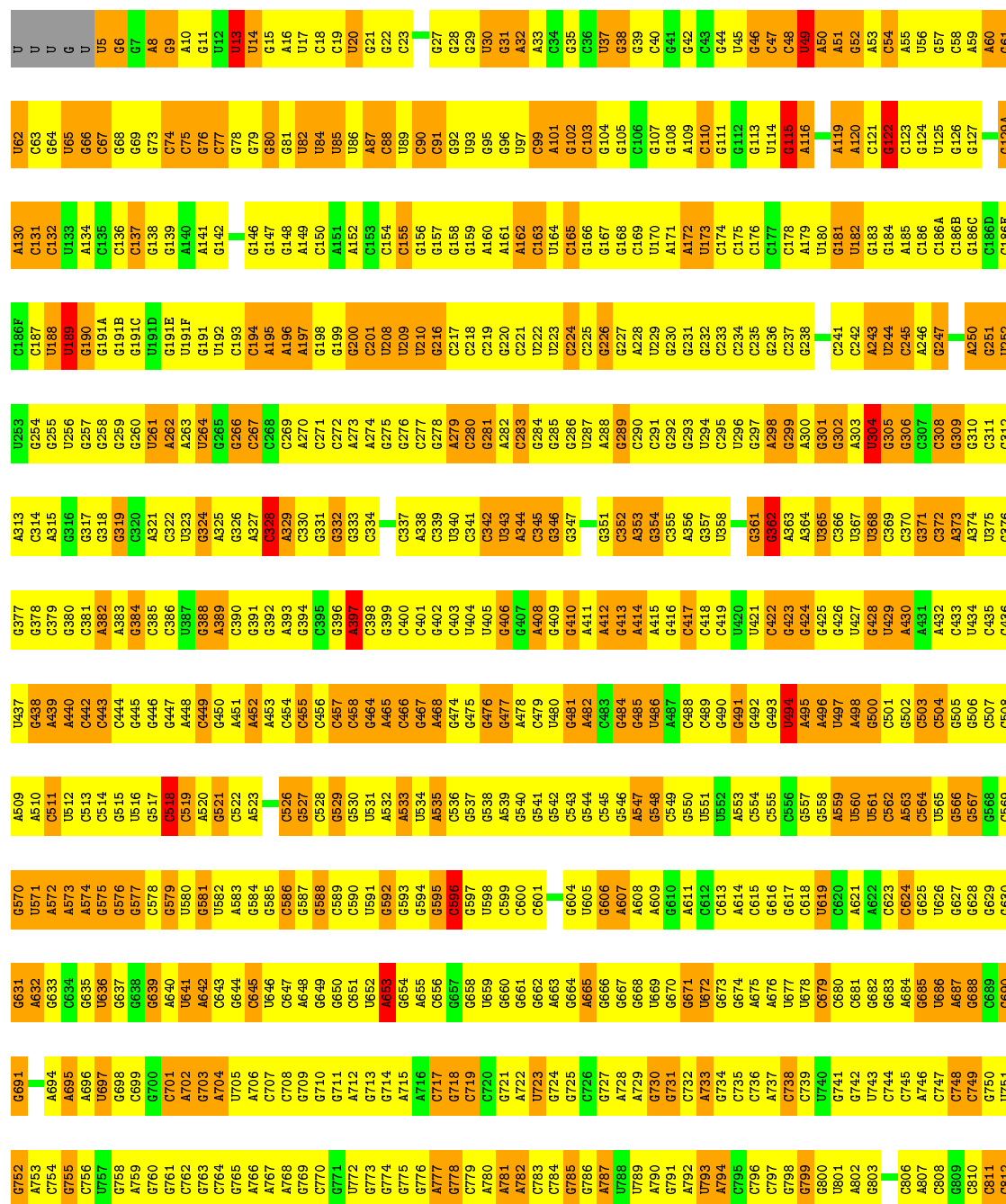


- Molecule 4: P- site tRNA

Chain 4: 



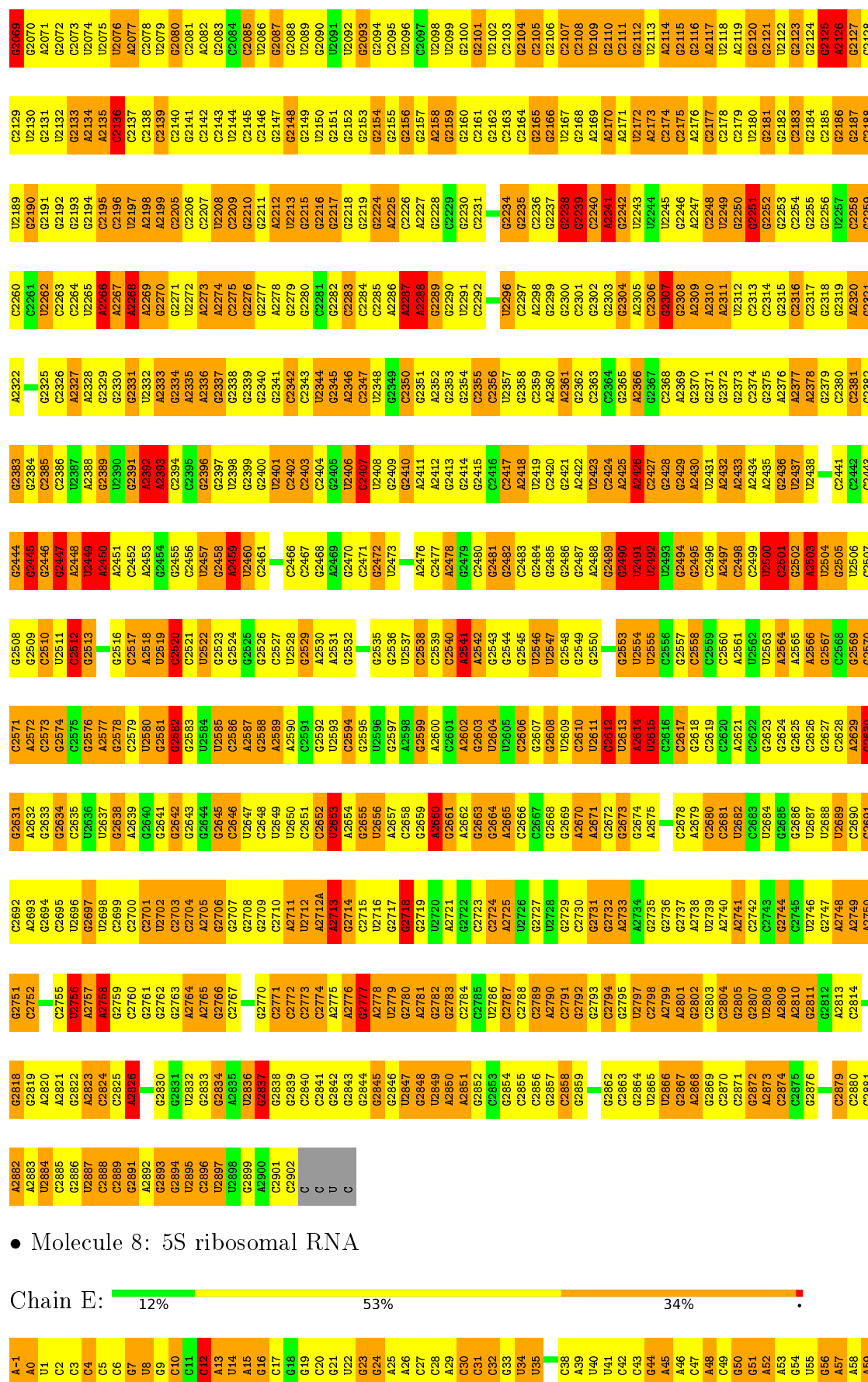
- Molecule 5: E site tRNA



A126	A127	C128	G129	G130	G131	G132	G133	G134	G135	G136	G137	G138	G139	G140	G141	G142	G143	G144	G145	G146	G147	G148	G149	G150	G151	G152	G153	G154	G155	G156	G157	G158	G159	G160	G161	G162	G163	G164	G165	G166	G167	G168	G169	G170	G171	G172	G173	G174	G175	G176	G177	G178	G179	G180	G181	G182	G183	G184	G185	G186	G187	G188	G189	G190	G191	G192	G193	G194	G195	G196	G197	G198	G199	G200	G201	G202	G203	G204	G205	G206	G207	G208	G209	G210	G211	G212	G213	G214	G215	G216	G217	G218	G219	G220	G221	G222	G223	G224	G225	G226	G227	G228	G229	G230	G231	G232	G233	G234	G235	G236	G237	G238	G239	G240	G241	G242	G243	G244	G245	G246	G247	G248	G249	G250	G251	G252	G253	G254	G255	G256	G257	G258	G259	G260	G261	G262	G263	G264	G265	G266	G267	G268	G269	G270	G271	G272	G273	G274	G275	G276	G277	G278	G279	G280	G281	G282	G283	G284	G285	G286	G287	G288	G289	G290	G291	G292	G293	G294	G295	G296	G297	G298	G299	G300	G301	G302	G303	G304	G305	G306	G307	G308	G309	G310	G311	G312	G313	G314	G315	G316	G317	G318	G319	G320	G321	G322	G323	G324	G325	G326	G327	G328	G329	G330	G331	G332	G333	G334	G335	G336	G337	G338	G339	G340	G341	G342	G343	G344	G345	G346	G347	G348	G349	G350	G351	G352	G353	G354	G355	G356	G357	G358	G359	G360	G361	G362	G363	G364	G365	G366	G367	G368	G369	G370	G371	G372	G373	G374	G375	G376	G377	G378	G379	G380	G381	G382	G383	G384	G385	G386	G387	G388	G389	G390	G391	G392	G393	G394	G395	G396	G397	G398	G399	G400	G401	G402	G403	G404	G405	G406	G407	G408	G409	G410	G411	G412	G413	G414	G415	G416	G417	G418	G419	G420	G421	G422	G423	G424	G425	G426	G427	G428	G429	G430	G431	G432	G433	G434	G435	G436	G437	G438	G439	G440	G441	G442	G443	G444	G445	G446	G447	G448	G449	G450	G451	G452	G453	G454	G455	G456	G457	G458	G459	G460	G461	G462	G463	G464	G465	G466	G467	G468	G469	G470	G471	G472	G473	G474	G475	G476	G477	G478	G479	G480	G481	G482	G483	G484	G485	G486	G487	G488	G489	G490	G491	G492	G493	G494	G495	G496	G497	G498	G499	G500	G501	G502	G503	G504	G505	G506	G507	G508	G509	G510	G511	G512	G513	G514	G515	G516	G517	G518	G519	G520	G521	G522	G523	G524	G525	G526	G527	G528	G529	G530	G531	G532	G533	G534	G535	G536	G537	G538	G539	G540	G541	G542	G543	G544	G545	G546	G547	G548	G549	G550	G551	G552	G553	G554	G555	G556	G557	G558	G559	G560	G561	G562	G563	G564	G565	G566	G567	G568	G569	G570	G571	G572	G573	G574	G575	G576	G577	G578	G579	G580	G581	G582	G583	G584	G585	G586	G587	G588	G589	G590	G591	G592	G593	G594	G595	G596	G597	G598	G599	G600	G601	G602	G603	G604	G605	G606	G607	G608	G609	G610	G611	G612	G613	G614	G615	G616	G617	G618	G619	G620	G621	G622	G623	G624	G625	G626	G627	G628	G629	G630	G631	G632	G633	G634	G635	G636	G637	G638	G639	G640	G641	G642	G643	G644	G645	G646	G647	G648	G649	G650	G651	G652	G653	G654	G655	G656	G657	G658	G659	G660	G661	G662	G663	G664	G665	G666	G667	G668	G669	G670	G671	G672	G673	G674	G675	G676	G677	G678	G679	G680	G681	G682	G683	G684	G685	G686	G687	G688	G689	G690	G691	G692	G693	G694	G695	G696	G697	G698	G699	G700	G701	G702	G703	G704	G705	G706	G707	G708	G709	G710	G711	G712	G713	G714	G715	G716	G717	G718	G719	G720	G721	G722	G723	G724	G725	G726	G727	G728	G729	G730	G731	G732	G733	G734	G735	G736	G737	G738	G739	G740	G741	G742	G743	G744	G745	G746	G747	G748	G749	G750	G751	G752	G753	G754	G755	G756	G757	G758	G759	G760	G761	G762	G763	G764	G765	G766	G767	G768	G769	G770	G771	G772	G773	G774	G775	G776	G777	G778	G779	G780	G781	G782	G783	G784	G785	G786	G787	G788	G789	G790	G791	G792	G793	G794	G795	G796	G797	G798	G799	G800	G801	G802	G803	G804	G805	G806	G807	G808	G809	G810	G811	G812	G813	G814	G815	G816	G817	G818	G819	G820	G821	G822	G823	G824	G825	G826	G827	G828	G829	G830	G831	G832	G833	G834	G835	G836	G837	G838	G839	G840	G841	G842	G843	G844	G845	G846	G847	G848	G849	G850	G851	G852	G853	G854	G855	G856	G857	G858	G859	G860	G861	G862	G863	G864	G865	G866	G867	G868	G869	G870	G871	G872	G873	G874	G875	G876	G877	G878	G879	G880	G881	G882	G883	G884	G885	G886	G887	G888	G889	G890	G891	G892	G893	G894	G895	G896	G897	G898	G899	G900	G901	G902	G903	G904	G905	G906	G907	G908	G909	G910	G911	G912	G913	G914	G915	G916	G917	G918	G919	G920	G921	G922	G923	G924	G925	G926	G927	G928	G929	G930	G931	G932	G933	G934	G935	G936	G937	G938	G939	G940	G941	G942	G943	G944	G945	G946	G947	G948	G949	G950	G951	G952	G953	G954	G955	G956	G957	G958	G959	G960	G961	G962	G963	G964	G965	G966	G967	G968	G969	G970	G971	G972	G973	G974	G975	G976	G977	G978	G979	G980	G981	G982	G983	G984	G985	G986	G987	G988	G989	G990	G991	G992	G993	G994	G995	G996	G997	G998	G999	G1000	G1001	G1002	G1003	G1004	G1005	G1006	G1007	G1008	G1009	G1010	G1011	G1012	G1013	G1014	G1015	G1016	G1017	G1018	G1019	G1020	G1021	G1022	G1023	G1024	G1025	G1026	G1027	G1028	G1029	G1030	G1031	G1032	G1033	G1034	G1035	G1036	G1037	G1038	G1039	G1040	G1041	G1042	G1043	G1044	G1045	G1046	G1047	G1048	G1049	G1050	G1051	G1052	G1053	G1054	G1055	G1056	G1057	G1058	G1059	G1060	G1061	G1062	G1063	G1064	G1065	G1066	G1067	G1068	G1069	G1070	G1071	G1072	G1073	G1074	G1075	G1076	G1077	G1078	G1079	G1080	G1081	G1082	G1083	G1084	G1085	G1086	G1087	G1088	G1089	G1090	G1091	G1092	G1093	G1094	G1095	G1096	G1097	G1098	G1099	G1100	G1101	G1102	G1103	G1104	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A1073	U1012	C951	C888	U828	C766	A706	A644	A586	U524	C462	A401	G342	G281	A256	A195
G1074	C1013	G952	C889	A829	U767	G707	A644	C587	U525	C463	A402	C343	A282	A196	
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A1076	G1015		G892	G841	G769	U709	G647	C589	C527	G465	C404	A345	U284	G259	C198
A1077	G1016	G856	C893	G832	G770	G711	G648	A590	A528	G466	U405	A346	C285	G260	A199
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C1079	U1019	U958	U895	C834	G772	G712	G650	G592	C531	G468	G407	G348	C287	A262	C201
A1080	A1020	A959	A896	A835	G773	G713	G651	G593	C530	C469	G408	G349	C288	A263	U202
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C1082	G1022	C961	C988	C837	G776	G715	A653	C595	G533	A471	G410	G351	A290	A265	A204
U1083	U1023	G962	A899	C838	G776	A716	A654	G596	U534	A472	G411	G352	C291	G266	G205
A1084	G1024	U963	A900	U839	A777	G717	A655	U597	C535	G473	A412	G353	C292	C267	U206
U1085	G1025	C964	A901	U840	G778	A718	G656	G598	A536	G474	C413	G354	U293	C268	A207
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A1088	U1028	C967	C904	G843	A781	C721	G659	C601	G540	A477	C416	A357	G296	A270A	C210
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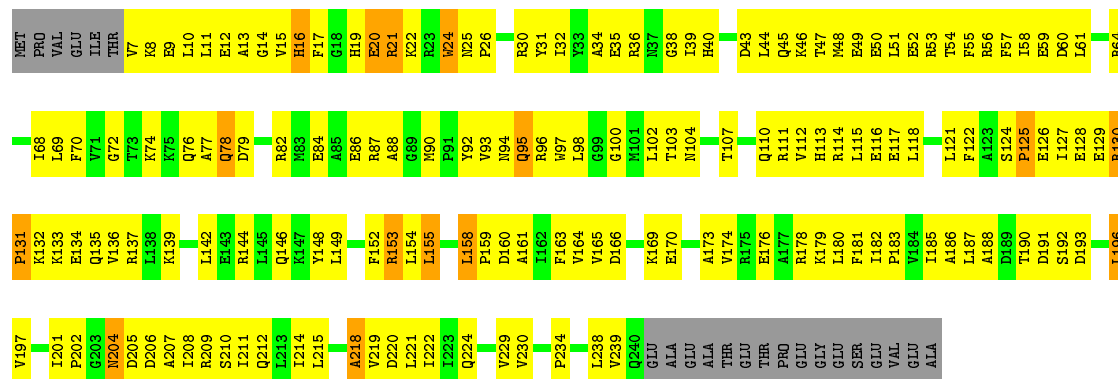
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U2016	U1955	G1824	G1824	G1764	U1688	G1628	A1566	A1508	C1446	A1384	U1323	U1263	C1200	C1200
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G2023	G1957	G1826	G1826	U1766	A1690	G1630	G1568	C1509	G1448	G1386	G1325	A1265	G1202	U1141
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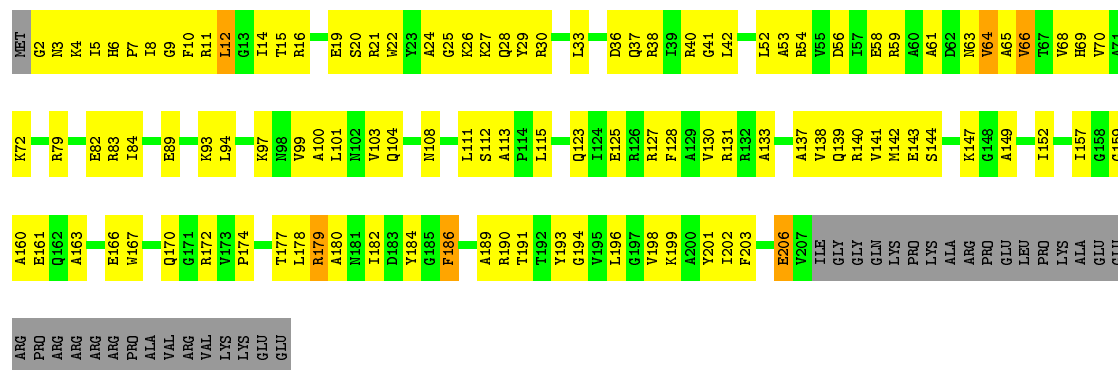
• Molecule 9: 30S ribosomal protein S2

Chain F: 28% 57% 6% 9%



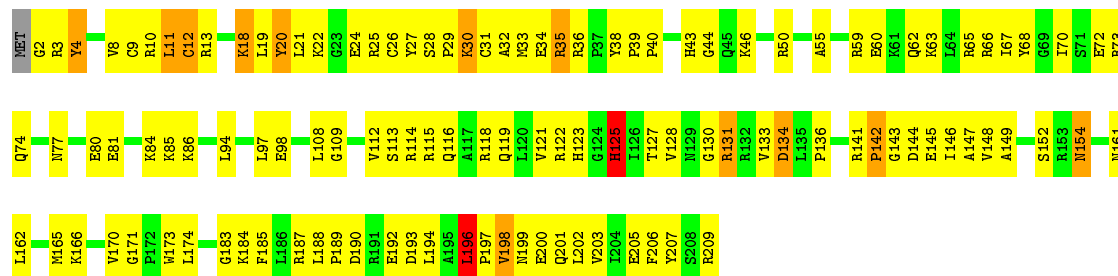
• Molecule 10: 30S ribosomal protein S3

Chain G: 39% 44% 14%



• Molecule 11: 30S ribosomal protein S4

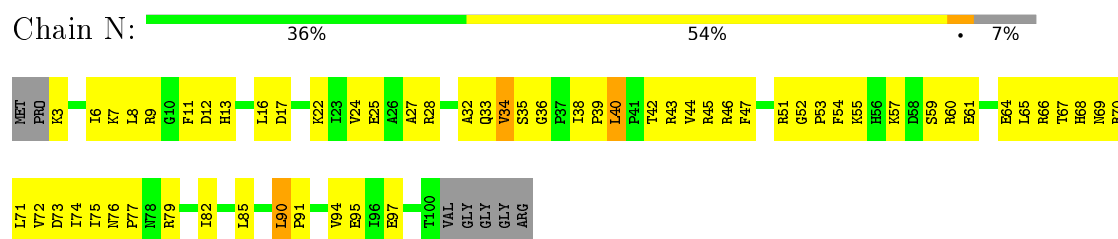
Chain H: 44% 49% 6%



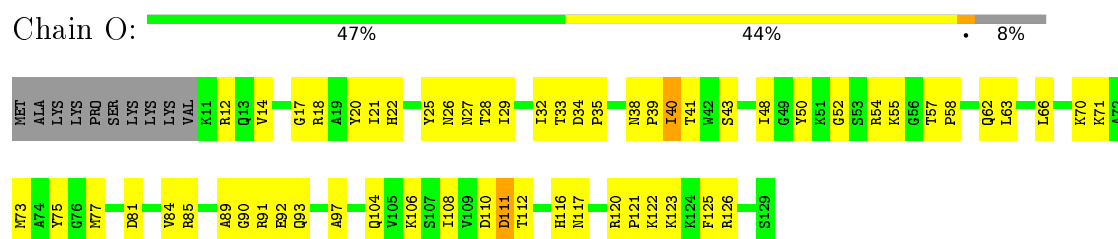
• Molecule 12: 30S ribosomal protein S5

Chain I: 42% 49% 7%

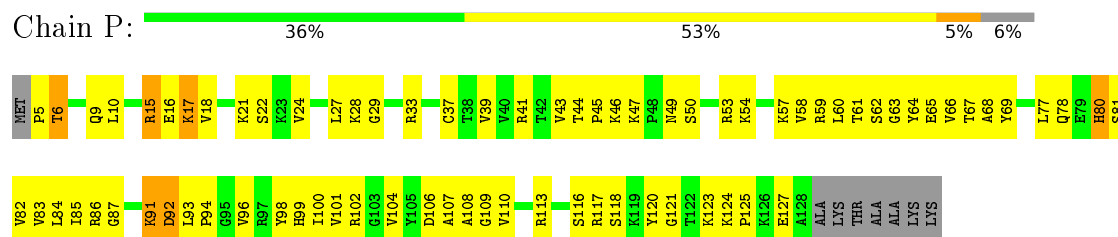
- Molecule 17: 30S ribosomal protein S10



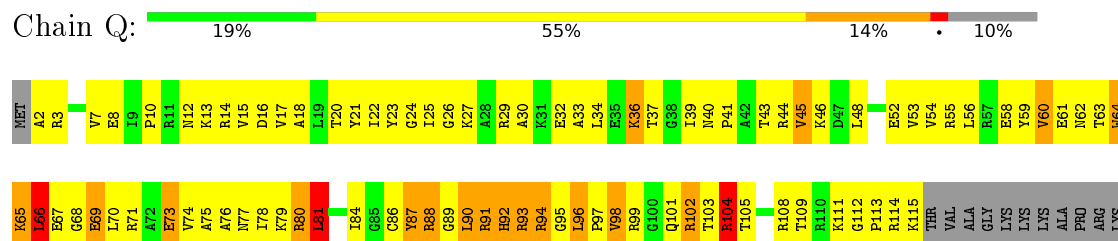
- Molecule 18: 30S ribosomal protein S11



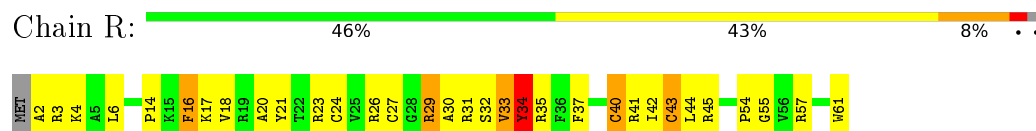
- Molecule 19: 30S ribosomal protein S12



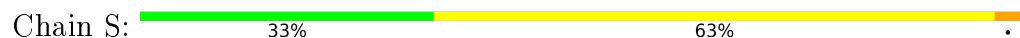
- Molecule 20: 30S ribosomal protein S13

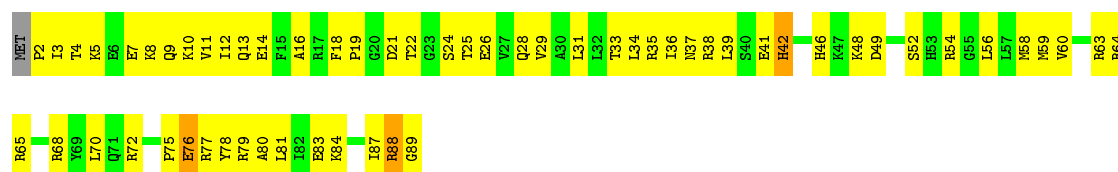


- Molecule 21: 30S ribosomal protein S14 type Z



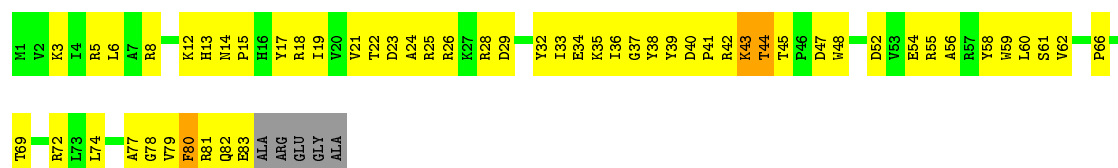
- Molecule 22: 30S ribosomal protein S15





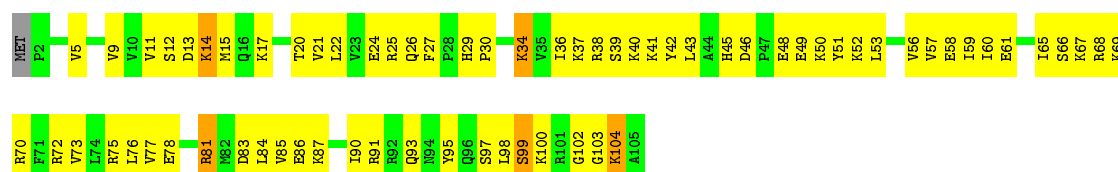
• Molecule 23: 30S ribosomal protein S16

Chain T: 32% 59% 6%



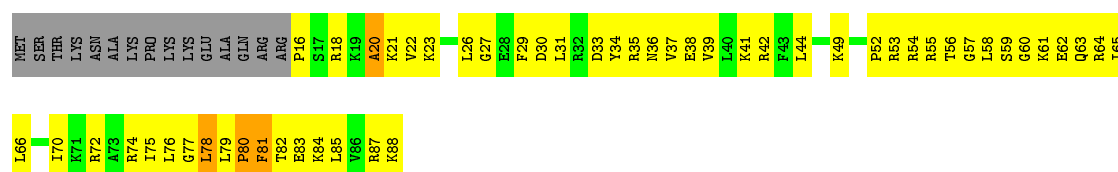
• Molecule 24: 30S ribosomal protein S17

Chain U: 33% 61% 5%



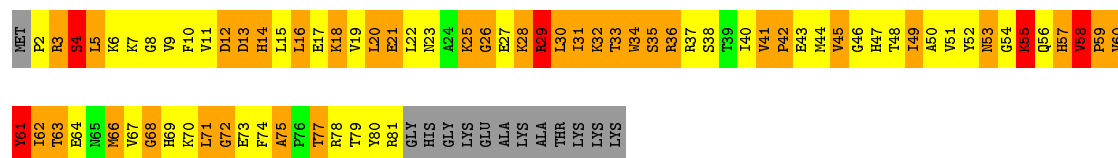
• Molecule 25: 30S ribosomal protein S18

Chain V: 23% 56% 5% 17%



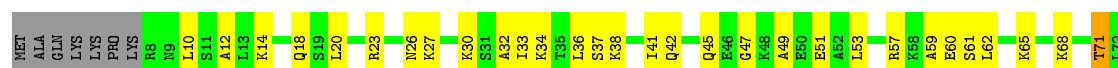
• Molecule 26: 30S ribosomal protein S19

Chain W: 39% 38% 5% 14%



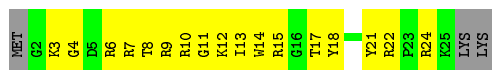
• Molecule 27: 30S ribosomal protein S20

Chain X: 44% 48% 7%

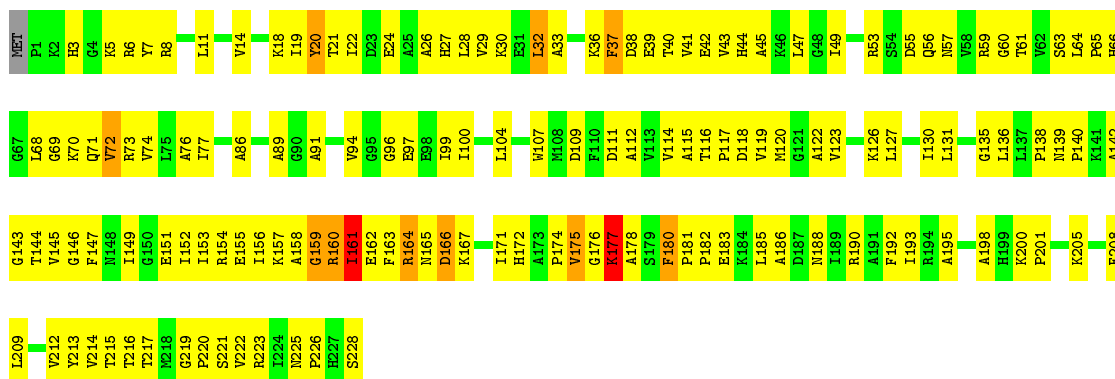
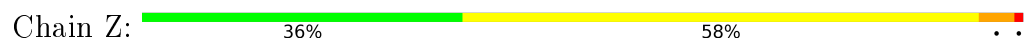




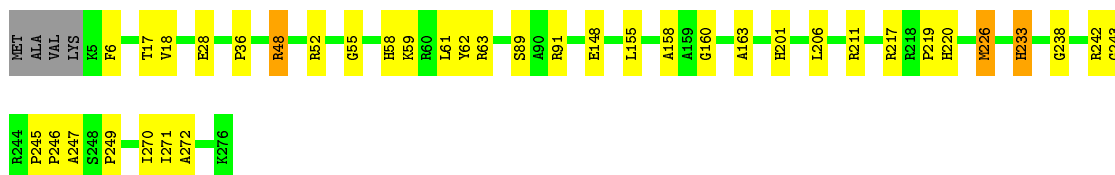
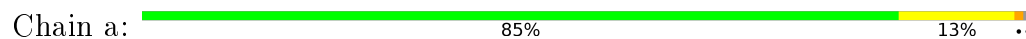
- Molecule 28: 30S ribosomal protein Thx



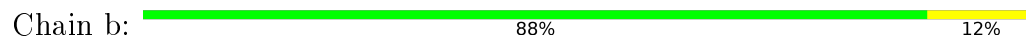
- Molecule 29: 50S ribosomal protein L1



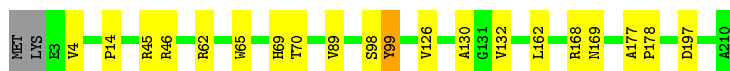
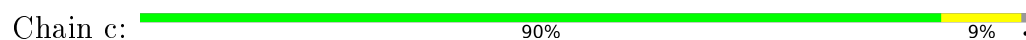
- Molecule 30: 50S ribosomal protein L2



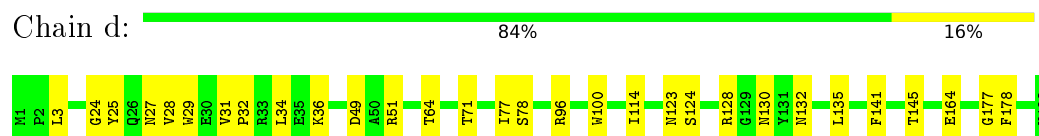
- Molecule 31: 50S ribosomal protein L3



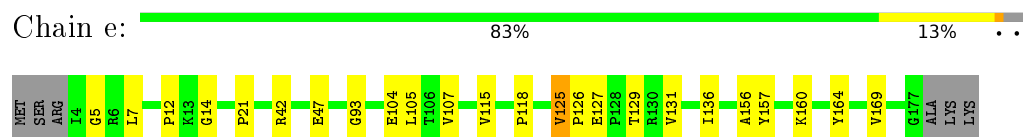
- Molecule 32: 50S ribosomal protein L4



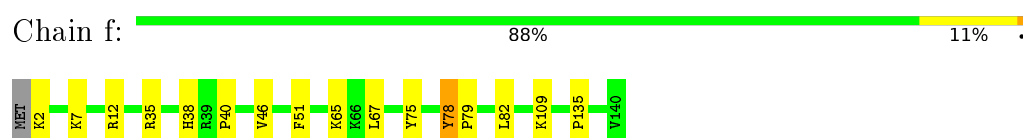
- Molecule 33: 50S ribosomal protein L5



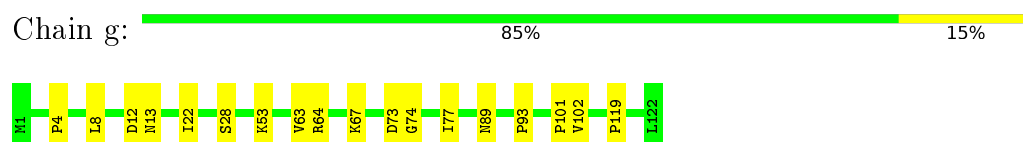
- Molecule 34: 50S ribosomal protein L6



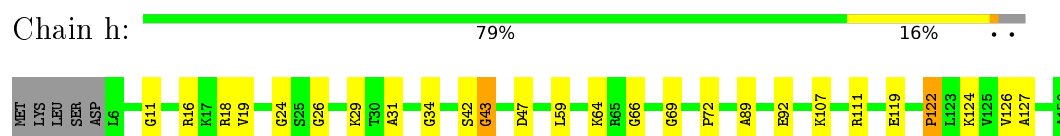
- Molecule 35: 50S ribosomal protein L13



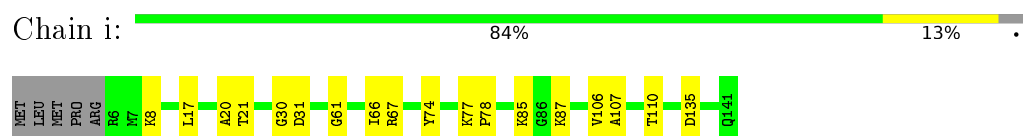
- Molecule 36: 50S ribosomal protein L14



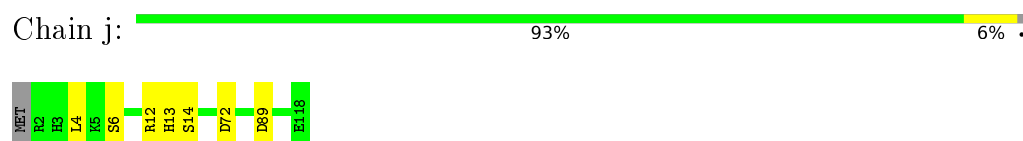
- Molecule 37: 50S ribosomal protein L15



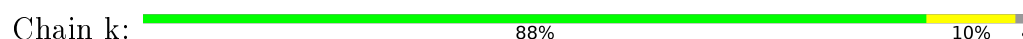
- Molecule 38: 50S ribosomal protein L16

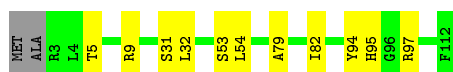


- Molecule 39: 50S ribosomal protein L17

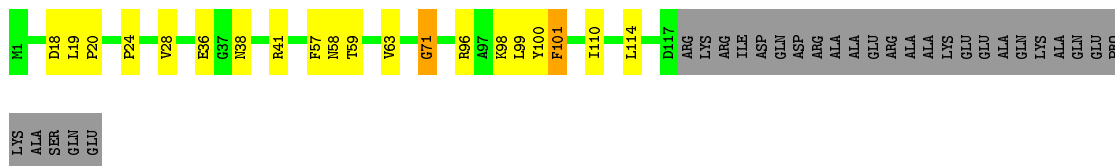


- Molecule 40: 50S ribosomal protein L18





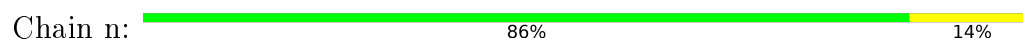
- Molecule 41: 50S ribosomal protein L19



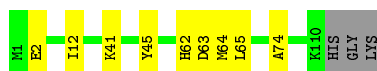
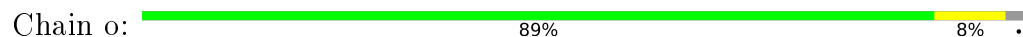
- Molecule 42: 50S ribosomal protein L20



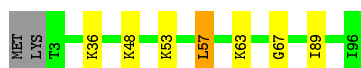
- Molecule 43: 50S ribosomal protein L21



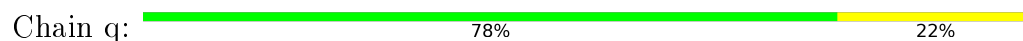
- Molecule 44: 50S ribosomal protein L22



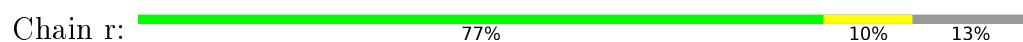
- Molecule 45: 50S ribosomal protein L23

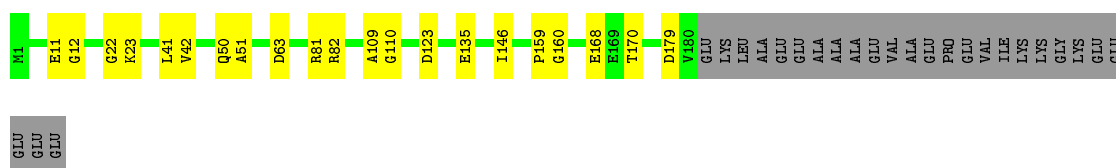


- Molecule 46: 50S ribosomal protein L24



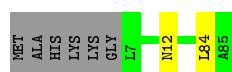
- Molecule 47: 50S ribosomal protein L25





- Molecule 48: 50S ribosomal protein L27

Chain s: 91% 7%



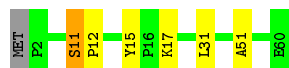
- Molecule 49: 50S ribosomal protein L29

Chain t: 93% 7%



- Molecule 50: 50S ribosomal protein L30

Chain u: 88% 8% . .



- Molecule 51: 50S ribosomal protein L31

Chain v: 77% 21% .



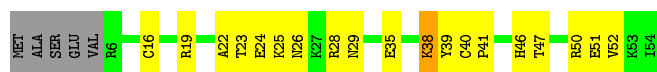
- Molecule 52: 50S ribosomal protein L32

Chain w: 77% 15% . 5%



- Molecule 53: 50S ribosomal protein L33

Chain x: 56% 33% . 9%



- Molecule 54: 50S ribosomal protein L34

Chain y: 88% 12%



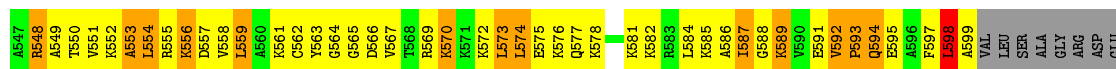
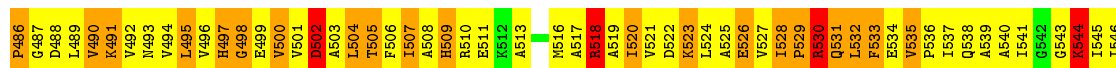
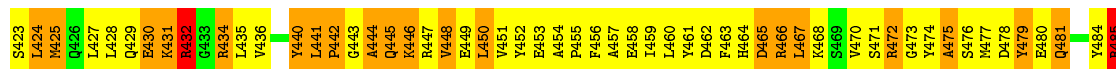
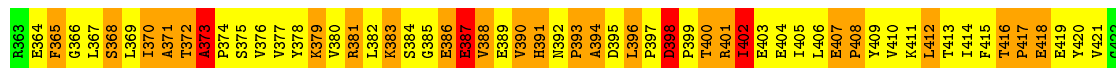
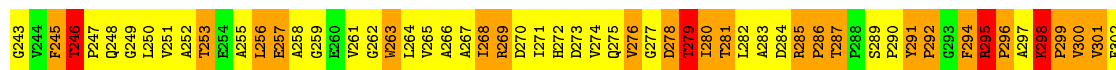
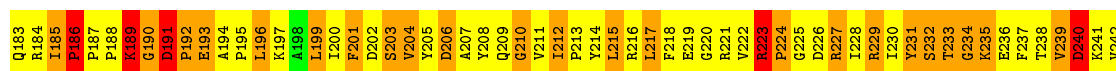
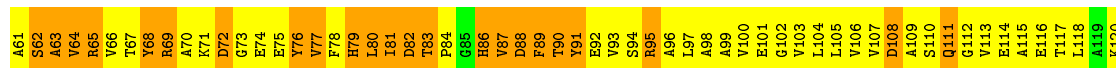
- Molecule 55: 50S ribosomal protein L35

Chain z: 80% 14% 5% .



- Molecule 56: Elongation factor 4

Chain B: 8% 52% 32% 5% .



4 Experimental information

Property	Value	Source
Reconstruction method	Not provided	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images used	110981	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	Not provided	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	Not provided	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GCP

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	$\# Z > 2$	RMSZ	$\# Z > 2$
1	1	0.77	0/310	0.90	0/407
10	G	0.54	0/1636	0.67	0/2205
11	H	0.53	0/1733	0.76	3/2318 (0.1%)
12	I	0.69	0/1162	0.80	0/1564
13	J	0.48	0/856	0.70	1/1154 (0.1%)
14	K	0.47	0/1276	0.66	0/1709
15	L	0.59	0/1136	0.73	0/1527
16	M	0.46	0/1029	0.68	0/1379
17	N	0.49	0/807	0.69	0/1085
18	O	0.51	0/900	0.64	0/1213
19	P	0.67	0/986	0.79	0/1320
2	2	0.26	0/640	0.50	0/889
20	Q	0.39	0/924	0.66	1/1238 (0.1%)
21	R	0.64	0/501	0.76	1/664 (0.2%)
22	S	0.54	0/745	0.77	0/992
23	T	0.60	0/716	0.73	0/963
24	U	0.54	0/870	0.74	0/1159
25	V	0.44	0/603	0.71	0/799
26	W	0.39	0/661	0.50	2/890 (0.2%)
27	X	0.52	0/765	0.77	0/1007
28	Y	0.51	0/212	0.67	0/277
29	Z	0.37	0/1775	0.63	1/2393 (0.0%)
3	3	0.54	0/1012	0.82	6/1373 (0.4%)
30	a	0.81	0/2174	0.93	3/2927 (0.1%)
31	b	0.77	0/1611	0.94	1/2171 (0.0%)
32	c	0.77	0/1660	0.90	0/2247
33	d	0.55	0/1507	0.81	1/2027 (0.0%)
34	e	0.58	0/1354	0.78	1/1831 (0.1%)
35	f	0.75	0/1140	0.95	2/1537 (0.1%)
36	g	0.79	0/942	0.93	2/1268 (0.2%)
37	h	0.64	0/1123	1.03	3/1493 (0.2%)
38	i	0.75	0/1100	0.90	0/1470

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
39	j	0.74	0/974	0.91	0/1302
4	4	0.85	0/1832	1.03	0/2855
40	k	0.61	0/887	0.95	0/1180
41	l	0.70	0/990	0.93	2/1325 (0.2%)
42	m	0.91	0/982	0.96	0/1306
43	n	0.65	0/790	0.94	1/1057 (0.1%)
44	o	0.78	0/886	0.83	0/1189
45	p	0.71	0/756	0.85	1/1015 (0.1%)
46	q	0.51	0/857	0.84	0/1142
47	r	0.56	0/1467	0.75	0/1992
48	s	0.81	0/633	0.84	0/843
49	t	0.59	0/569	0.82	1/751 (0.1%)
5	5	0.62	2/1813 (0.1%)	1.14	7/2823 (0.2%)
50	u	0.69	0/474	0.93	1/635 (0.2%)
51	v	0.82	0/594	1.11	2/795 (0.3%)
52	w	0.80	0/459	0.99	1/621 (0.2%)
53	x	0.67	0/433	1.00	2/576 (0.3%)
54	y	0.83	0/438	0.98	1/575 (0.2%)
55	z	0.79	0/523	0.96	1/690 (0.1%)
56	B	0.41	0/4718	0.52	25/6392 (0.4%)
6	A	1.00	4/36438 (0.0%)	1.10	59/56869 (0.1%)
7	D	1.40	164/69685 (0.2%)	1.34	623/108786 (0.6%)
8	E	1.10	1/2954 (0.0%)	1.15	6/4606 (0.1%)
9	F	0.50	0/1935	0.74	0/2609
All	All	1.09	171/165953 (0.1%)	1.14	761/247430 (0.3%)

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	N	0	1
19	P	0	1
21	R	0	1
30	a	0	4
32	c	0	2
33	d	0	2
35	f	0	3
37	h	0	1
40	k	0	2
41	l	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
47	r	0	1
51	v	0	1
52	w	0	5
53	x	0	3
55	z	0	3
9	F	0	1
All	All	0	34

The worst 5 of 171 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	D	1786	A	N9-C4	12.42	1.45	1.37
5	5	1	G	OP3-P	-10.94	1.48	1.61
7	D	1	G	OP3-P	-10.91	1.48	1.61
8	E	-1	A	OP3-P	-10.79	1.48	1.61
7	D	363(F)	A	O3'-P	9.72	1.72	1.61

The worst 5 of 761 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	D	775	G	N3-C4-C5	-15.67	120.77	128.60
7	D	2491	U	C6-N1-C2	-13.29	113.03	121.00
7	D	1664	A	C8-N9-C4	-13.09	100.56	105.80
7	D	1779	U	C5-C4-O4	-12.85	118.19	125.90
7	D	775	G	C8-N9-C4	-12.80	101.28	106.40

There are no chirality outliers.

5 of 34 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
9	F	95	GLN	Peptide
17	N	33	GLN	Peptide
19	P	15	ARG	Peptide
21	R	34	TYR	Peptide
30	a	226	MET	Peptide

5.2 Too-close contacts

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

the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	307	0	335	38	0
2	2	641	0	309	20	0
3	3	993	0	1030	310	0
4	4	1640	0	837	65	0
5	5	1623	0	821	102	0
6	A	32554	0	16429	2728	0
7	D	62218	0	31354	5215	0
8	E	2641	0	1337	129	0
9	F	1900	0	1951	165	0
10	G	1612	0	1677	107	0
11	H	1703	0	1763	146	0
12	I	1146	0	1207	73	0
13	J	843	0	857	81	0
14	K	1257	0	1296	93	0
15	L	1116	0	1177	100	0
16	M	1010	0	1035	104	0
17	N	794	0	840	77	0
18	O	885	0	904	61	0
19	P	970	0	1057	116	0
20	Q	914	0	967	226	0
21	R	492	0	529	45	0
22	S	734	0	771	63	0
23	T	700	0	720	75	0
24	U	857	0	930	85	0
25	V	597	0	668	73	0
26	W	647	0	670	438	0
27	X	763	0	861	68	0
28	Y	208	0	221	25	0
29	Z	1742	0	1796	282	0
30	a	2124	0	2207	0	0
31	b	1578	0	1647	0	0
32	c	1625	0	1666	0	0
33	d	1482	0	1546	0	0
34	e	1328	0	1408	0	0
35	f	1113	0	1183	0	0
36	g	932	0	994	0	0
37	h	1106	0	1183	0	0
38	i	1080	0	1127	0	0
39	j	960	0	1021	0	0
40	k	877	0	938	0	0
41	l	976	0	1033	0	0
42	m	964	0	1022	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	n	779	0	852	0	0
44	o	876	0	941	0	0
45	p	742	0	800	0	0
46	q	844	0	930	0	0
47	r	1435	0	1463	0	0
48	s	625	0	647	0	0
49	t	567	0	621	0	0
50	u	469	0	518	0	0
51	v	581	0	577	0	0
52	w	445	0	459	0	0
53	x	426	0	452	0	0
54	y	430	0	480	0	0
55	z	515	0	587	0	0
56	B	4628	0	4707	2436	0
57	B	32	0	12	51	0
All	All	153046	0	105370	12757	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 63.

The worst 5 of 12757 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)
56:B:79:HIS:CD2	56:B:261:VAL:HG23	1.16	1.68
7:D:884:C:C2	7:D:885:C:C5	1.74	1.66
56:B:382:LEU:HG	56:B:401:ARG:CD	1.24	1.66
3:3:10:LEU:HD11	3:3:57:ILE:CG1	1.22	1.64
3:3:6:ALA:HB3	3:3:59:ILE:CB	1.23	1.64

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	35/37 (95%)	23 (66%)	6 (17%)	6 (17%)	0	4
2	2	128/173 (74%)	96 (75%)	23 (18%)	9 (7%)	1	23
3	3	132/147 (90%)	68 (52%)	37 (28%)	27 (20%)	0	2
9	F	232/256 (91%)	179 (77%)	32 (14%)	21 (9%)	1	16
10	G	204/239 (85%)	170 (83%)	21 (10%)	13 (6%)	2	26
11	H	206/209 (99%)	172 (84%)	17 (8%)	17 (8%)	1	18
12	I	148/162 (91%)	125 (84%)	15 (10%)	8 (5%)	2	30
13	J	99/101 (98%)	85 (86%)	8 (8%)	6 (6%)	2	27
14	K	153/156 (98%)	138 (90%)	11 (7%)	4 (3%)	7	48
15	L	136/138 (99%)	112 (82%)	17 (12%)	7 (5%)	2	31
16	M	125/128 (98%)	90 (72%)	27 (22%)	8 (6%)	2	26
17	N	96/105 (91%)	80 (83%)	12 (12%)	4 (4%)	3	36
18	O	117/129 (91%)	104 (89%)	8 (7%)	5 (4%)	3	35
19	P	122/132 (92%)	91 (75%)	24 (20%)	7 (6%)	2	28
20	Q	112/126 (89%)	77 (69%)	23 (20%)	12 (11%)	0	11
21	R	58/61 (95%)	43 (74%)	9 (16%)	6 (10%)	1	12
22	S	86/89 (97%)	74 (86%)	10 (12%)	2 (2%)	8	51
23	T	81/88 (92%)	69 (85%)	8 (10%)	4 (5%)	3	32
24	U	102/105 (97%)	80 (78%)	16 (16%)	6 (6%)	2	27
25	V	71/88 (81%)	57 (80%)	10 (14%)	4 (6%)	2	29
26	W	78/93 (84%)	30 (38%)	25 (32%)	23 (30%)	0	0
27	X	97/106 (92%)	85 (88%)	8 (8%)	4 (4%)	3	37
28	Y	22/27 (82%)	19 (86%)	3 (14%)	0	100	100
29	Z	226/229 (99%)	187 (83%)	28 (12%)	11 (5%)	3	32
30	a	270/276 (98%)	201 (74%)	38 (14%)	31 (12%)	0	9
31	b	204/206 (99%)	150 (74%)	31 (15%)	23 (11%)	0	10
32	c	206/210 (98%)	165 (80%)	25 (12%)	16 (8%)	1	20
33	d	180/182 (99%)	115 (64%)	42 (23%)	23 (13%)	0	7
34	e	172/180 (96%)	125 (73%)	24 (14%)	23 (13%)	0	6
35	f	137/140 (98%)	107 (78%)	19 (14%)	11 (8%)	1	19
36	g	120/122 (98%)	81 (68%)	24 (20%)	15 (12%)	0	8
37	h	143/150 (95%)	93 (65%)	28 (20%)	22 (15%)	0	5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
38	i	134/141 (95%)	92 (69%)	25 (19%)	17 (13%)	0	7
39	j	115/118 (98%)	104 (90%)	6 (5%)	5 (4%)	3	35
40	k	108/112 (96%)	77 (71%)	22 (20%)	9 (8%)	1	18
41	l	115/146 (79%)	80 (70%)	19 (16%)	16 (14%)	0	6
42	m	115/118 (98%)	100 (87%)	11 (10%)	4 (4%)	4	42
43	n	99/101 (98%)	66 (67%)	20 (20%)	13 (13%)	0	7
44	o	108/113 (96%)	86 (80%)	14 (13%)	8 (7%)	1	21
45	p	92/96 (96%)	71 (77%)	14 (15%)	7 (8%)	1	20
46	q	108/110 (98%)	63 (58%)	21 (19%)	24 (22%)	0	1
47	r	178/206 (86%)	130 (73%)	28 (16%)	20 (11%)	0	10
48	s	77/85 (91%)	65 (84%)	10 (13%)	2 (3%)	7	48
49	t	65/67 (97%)	54 (83%)	7 (11%)	4 (6%)	2	26
50	u	57/60 (95%)	44 (77%)	8 (14%)	5 (9%)	1	16
51	v	69/71 (97%)	35 (51%)	21 (30%)	13 (19%)	0	3
52	w	55/60 (92%)	37 (67%)	11 (20%)	7 (13%)	0	7
53	x	47/54 (87%)	16 (34%)	16 (34%)	15 (32%)	0	0
54	y	47/49 (96%)	33 (70%)	9 (19%)	5 (11%)	0	11
55	z	62/65 (95%)	45 (73%)	8 (13%)	9 (14%)	0	6
56	B	587/610 (96%)	267 (46%)	188 (32%)	132 (22%)	0	1
All	All	6536/6972 (94%)	4756 (73%)	1087 (17%)	693 (11%)	1	11

5 of 693 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	4	ARG
1	1	33	LYS
2	2	77	PRO
2	2	93	LEU
2	2	107	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	34/34 (100%)	34 (100%)	0	100	100
3	3	101/111 (91%)	93 (92%)	8 (8%)	15	55
9	F	202/220 (92%)	201 (100%)	1 (0%)	92	97
10	G	160/188 (85%)	159 (99%)	1 (1%)	90	96
11	H	180/181 (99%)	179 (99%)	1 (1%)	90	96
12	I	115/123 (94%)	114 (99%)	1 (1%)	84	93
13	J	90/90 (100%)	90 (100%)	0	100	100
14	K	126/127 (99%)	126 (100%)	0	100	100
15	L	119/119 (100%)	119 (100%)	0	100	100
16	M	98/99 (99%)	98 (100%)	0	100	100
17	N	88/92 (96%)	88 (100%)	0	100	100
18	O	90/99 (91%)	90 (100%)	0	100	100
19	P	104/109 (95%)	103 (99%)	1 (1%)	82	92
20	Q	92/101 (91%)	78 (85%)	14 (15%)	3	25
21	R	49/50 (98%)	49 (100%)	0	100	100
22	S	79/80 (99%)	78 (99%)	1 (1%)	76	91
23	T	72/74 (97%)	72 (100%)	0	100	100
24	U	96/97 (99%)	96 (100%)	0	100	100
25	V	64/77 (83%)	64 (100%)	0	100	100
26	W	71/80 (89%)	47 (66%)	24 (34%)	0	2
27	X	76/82 (93%)	76 (100%)	0	100	100
28	Y	19/22 (86%)	19 (100%)	0	100	100
29	Z	180/181 (99%)	177 (98%)	3 (2%)	68	89
30	a	215/218 (99%)	212 (99%)	3 (1%)	74	90
31	b	166/166 (100%)	165 (99%)	1 (1%)	90	96
32	c	164/166 (99%)	161 (98%)	3 (2%)	66	88
33	d	156/156 (100%)	152 (97%)	4 (3%)	54	82
34	e	143/148 (97%)	142 (99%)	1 (1%)	88	95
35	f	118/119 (99%)	117 (99%)	1 (1%)	86	94
36	g	100/100 (100%)	99 (99%)	1 (1%)	82	92

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
37	h	111/116 (96%)	109 (98%)	2 (2%)	66	88
38	i	106/111 (96%)	105 (99%)	1 (1%)	84	93
39	j	100/101 (99%)	98 (98%)	2 (2%)	63	87
40	k	87/88 (99%)	87 (100%)	0	100	100
41	l	105/127 (83%)	104 (99%)	1 (1%)	82	92
42	m	93/94 (99%)	93 (100%)	0	100	100
43	n	82/82 (100%)	82 (100%)	0	100	100
44	o	90/92 (98%)	89 (99%)	1 (1%)	80	92
45	p	76/78 (97%)	76 (100%)	0	100	100
46	q	91/91 (100%)	91 (100%)	0	100	100
47	r	159/179 (89%)	159 (100%)	0	100	100
48	s	63/67 (94%)	63 (100%)	0	100	100
49	t	62/62 (100%)	62 (100%)	0	100	100
50	u	51/52 (98%)	50 (98%)	1 (2%)	63	87
51	v	63/63 (100%)	62 (98%)	1 (2%)	70	89
52	w	50/52 (96%)	50 (100%)	0	100	100
53	x	48/52 (92%)	48 (100%)	0	100	100
54	y	42/42 (100%)	42 (100%)	0	100	100
55	z	54/55 (98%)	52 (96%)	2 (4%)	41	76
56	B	490/505 (97%)	347 (71%)	143 (29%)	0	4
All	All	5390/5618 (96%)	5167 (96%)	223 (4%)	42	74

5 of 223 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
56	B	80	LEU
56	B	201	PHE
56	B	532	LEU
56	B	91	TYR
56	B	153	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 92 such sidechains are listed below:

Mol	Chain	Res	Type
30	a	115	GLN
34	e	158	HIS
56	B	248	GLN
30	a	116	GLN
31	b	129	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
4	4	76/77 (98%)	29 (38%)	0
5	5	75/76 (98%)	32 (42%)	3 (4%)
6	A	1515/1522 (99%)	529 (34%)	102 (6%)
7	D	2888/2893 (99%)	1316 (45%)	205 (7%)
8	E	122/123 (99%)	48 (39%)	4 (3%)
All	All	4676/4691 (99%)	1954 (41%)	314 (6%)

5 of 1954 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
4	4	5	G
4	4	8	U
4	4	9	G
4	4	13	C
4	4	17	C

5 of 314 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
7	D	481	G
7	D	899	A
7	D	2500	U
7	D	507	A
7	D	726	G

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

1 ligand is 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$
57	GCP	B	701	-	29,34,34	2.51	9 (31%)	31,54,54	1.21	3 (9%)

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
57	GCP	B	701	-	-	0/18/38/38	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	B	701	GCP	C4-N9	-10.27	1.34	1.47
57	B	701	GCP	C8-N9	-3.77	1.35	1.47
57	B	701	GCP	C5-C6	-2.44	1.48	1.53
57	B	701	GCP	C2-N1	-2.13	1.35	1.44
57	B	701	GCP	PB-O2B	2.09	1.61	1.56

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	B	701	GCP	C3'-C2'-C1'	2.41	106.27	101.44
57	B	701	GCP	C4-C5-N7	2.50	106.57	102.67
57	B	701	GCP	C8-N9-C4	3.21	108.44	104.78

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 51 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	B	701	GCP	51	0

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.