



wwPDB/EMDatabank EM Map/Model Validation Summary Report ⓘ

Mar 2, 2017 – 12:57 pm GMT

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/EMDatabank EM Map/Model Validation Summary Report
for a publicly released PDB/EMDB entry.

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

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : recalc29047

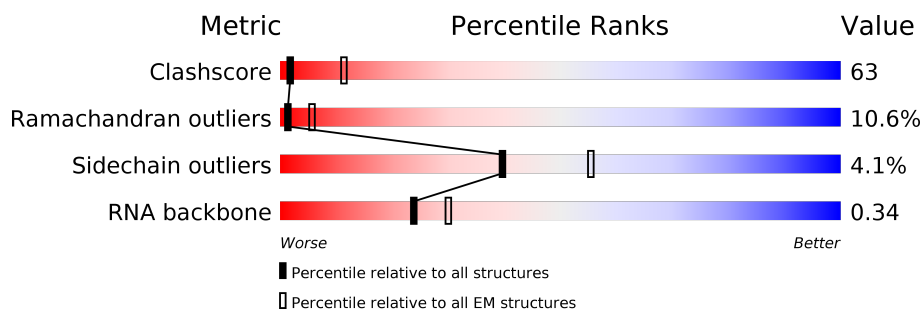
1 Overall quality at a glance

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	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026
RNA backbone	3398	335

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% 51% 34%
6	A	1522	11% 56% 31%
7	D	2893	9% 45% 38% 7%
8	E	123	12% 54% 33%

















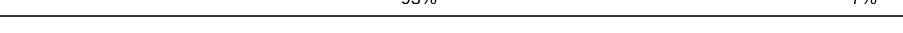
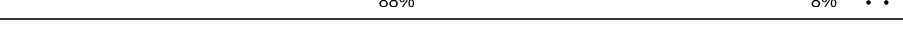

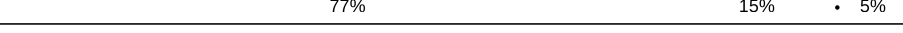



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Mol	Chain	Length	Quality of chain
9	F	256	
10	G	239	
11	H	209	
12	I	162	
13	J	101	
14	K	156	
15	L	138	
16	M	128	
17	N	105	
18	O	129	
19	P	132	
20	Q	126	
21	R	61	
22	S	89	
23	T	88	
24	U	105	
25	V	88	
26	W	93	
27	X	106	
28	Y	27	
29	Z	229	
30	a	276	
31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

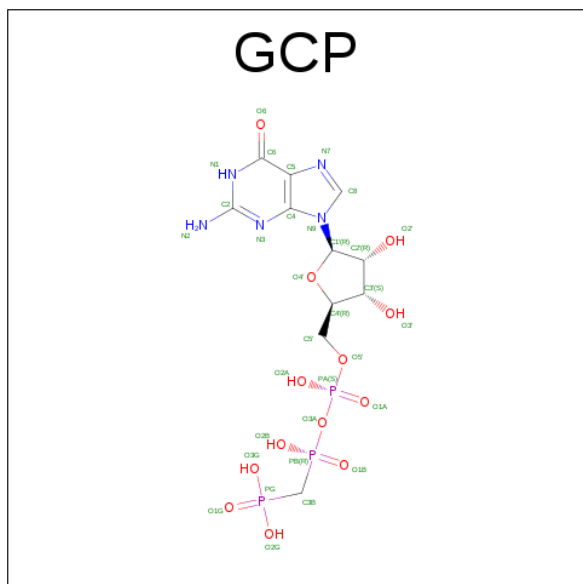
- Molecule 55 is a protein called 50S ribosomal protein L35.

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: $C_{11}H_{18}N_5O_{13}P_3$).



3 Residue-property plots

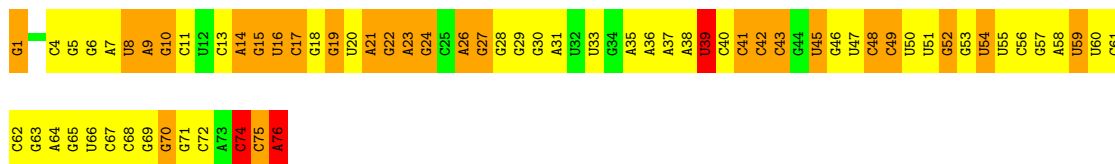
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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: 50S ribosomal protein L36

Chain 1: 

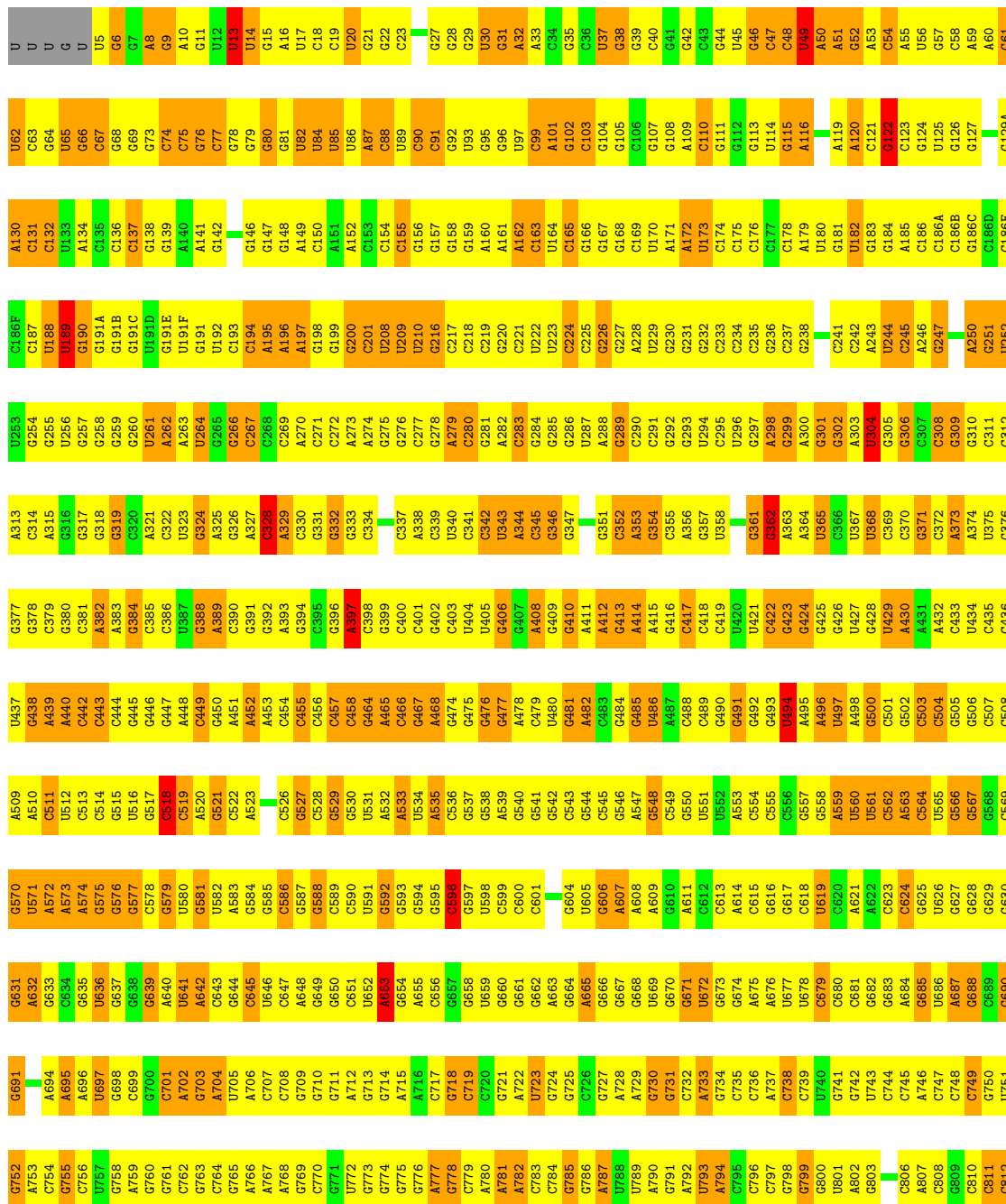


Chain 5: 11% 51% 34%



• Molecule 6: 16S ribosomal RNA

Chain A: 11% 56% 31%



- Molecule 7: 23S ribosomal RNA

Chain D: 9% 45% 38% 7%

A126	A127	A128	A129	C130	G131	C132	C133	A134	A135	A136	A137	A138	A139	A140	A141	A142	A143	A144	A145	A146	A147	A148	A149	A150	A151	A152	A153	A154	A155	A156	A157	A158	A159	A160	A161	A162	A163	A164	A165	A166	A167	A168	A169	A170	A171	A172	A173	A174	A175	A176	A177	A178	A179	A180	A181	A182	A183	A184	A185	A186	A187	A188	A189	A190	A191	A192	A193	A194	A195	A196	A197	A198	A199	A200	A201	A202	A203	A204	A205	A206	A207	A208	A209	A210	A211	A212	A213	A214	A215	A216	A217	A218	A219	A220	A221	A222	A223	A224	A225	A226	A227	A228	A229	A230	A231	A232	A233	A234	A235	A236	A237	A238	A239	A240	A241	A242	A243	A244	A245	A246	A247	A248	A249	A250	A251	A252	A253	A254	A255	A256	A257	A258	A259	A260	A261	A262	A263	A264	A265	A266	A267	A268	A269	A270	A271	A272	A273	A274	A275	A276	A277	A278	A279	A280	A281	A282	A283	A284	A285	A286	A287	A288	A289	A290	A291	A292	A293	A294	A295	A296	A297	A298	A299	A300	A301	A302	A303	A304	A305	A306	A307	A308	A309	A310	A311	A312	A313	A314	A315	A316	A317	A318	A319	A320	A321	A322	A323	A324	A325	A326	A327	A328	A329	A330	A331	A332	A333	A334	A335	A336	A337	A338	A339	A340	A341	A342	A343	A344	A345	A346	A347	A348	A349	A350	A351	A352	A353	A354	A355	A356	A357	A358	A359	A360	A361	A362	A363	A364	A365	A366	A367	A368	A369	A370	A371	A372	A373	A374	A375	A376	A377	A378	A379	A380	A381	A382	A383	A384	A385	A386	A387	A388	A389	A390	A391	A392	A393	A394	A395	A396	A397	A398	A399	A400	A401	A402	A403	A404	A405	A406	A407	A408	A409	A410	A411	A412	A413	A414	A415	A416	A417	A418	A419	A420	A421	A422	A423	A424	A425	A426	A427	A428	A429	A430	A431	A432	A433	A434	A435	A436	A437	A438	A439	A440	A441	A442	A443	A444	A445	A446	A447	A448	A449	A450	A451	A452	A453	A454	A455	A456	A457	A458	A459	A460	A461	A462	A463	A464	A465	A466	A467	A468	A469	A470	A471	A472	A473	A474	A475	A476	A477	A478	A479	A480	A481	A482	A483	A484	A485	A486	A487	A488	A489	A490	A491	A492	A493	A494	A495	A496	A497	A498	A499	A500	A501	A502	A503	A504	A505	A506	A507	A508	A509	A510	A511	A512	A513	A514	A515	A516	A517	A518	A519	A520	A521	A522	A523	A524	A525	A526	A527	A528	A529	A530	A531	A532	A533	A534	A535	A536	A537	A538	A539	A540	A541	A542	A543	A544	A545	A546	A547	A548	A549	A550	A551	A552	A553	A554	A555	A556	A557	A558	A559	A560	A561	A562	A563	A564	A565	A566	A567	A568	A569	A570	A571	A572	A573	A574	A575	A576	A577	A578	A579	A580	A581	A582	A583	A584	A585	A586	A587	A588	A589	A590	A591	A592	A593	A594	A595	A596	A597	A598	A599	A600	A601	A602	A603	A604	A605	A606	A607	A608	A609	A610	A611	A612	A613	A614	A615	A616	A617	A618	A619	A620	A621	A622	A623	A624	A625	A626	A627	A628	A629	A630	A631	A632	A633	A634	A635	A636	A637	A638	A639	A640	A641	A642	A643	A644	A645	A646	A647	A648	A649	A650	A651	A652	A653	A654	A655	A656	A657	A658	A659	A660	A661	A662	A663	A664	A665	A666	A667	A668	A669	A670	A671	A672	A673	A674	A675	A676	A677	A678	A679	A680	A681	A682	A683	A684	A685	A686	A687	A688	A689	A690	A691	A692	A693	A694	A695	A696	A697	A698	A699	A700	A701	A702	A703	A704	A705	A706	A707	A708	A709	A710	A711	A712	A713	A714	A715	A716	A717	A718	A719	A720	A721	A722	A723	A724	A725	A726	A727	A728	A729	A730	A731	A732	A733	A734	A735	A736	A737	A738	A739	A740	A741	A742	A743	A744	A745	A746	A747	A748	A749	A750	A751	A752	A753	A754	A755	A756	A757	A758	A759	A760	A761	A762	A763	A764	A765	A766	A767	A768	A769	A770	A771	A772	A773	A774	A775	A776	A777	A778	A779	A780	A781	A782	A783	A784	A785	A786	A787	A788	A789	A790	A791	A792	A793	A794	A795	A796	A797	A798	A799	A800	A801	A802	A803	A804	A805	A806	A807	A808	A809	A810	A811	A812	A813	A814	A815	A816	A817	A818	A819	A820	A821	A822	A823	A824	A825	A826	A827	A828	A829	A830	A831	A832	A833	A834	A835	A836	A837	A838	A839	A840	A841	A842	A843	A844	A845	A846	A847	A848	A849	A850	A851	A852	A853	A854	A855	A856	A857	A858	A859	A860	A861	A862	A863	A864	A865	A866	A867	A868	A869	A870	A871	A872	A873	A874	A875	A876	A877	A878	A879	A880	A881	A882	A883	A884	A885	A886	A887	A888	A889	A890	A891	A892	A893	A894	A895	A896	A897	A898	A899	A900	A901	A902	A903	A904	A905	A906	A907	A908	A909	A910	A911	A912	A913	A914	A915	A916	A917	A918	A919	A920	A921	A922	A923	A924	A925	A926	A927	A928	A929	A930	A931	A932	A933	A934	A935	A936	A937	A938	A939	A940	A941	A942	A943	A944	A945	A946	A947	A948	A949	A950	A951	A952	A953	A954	A955	A956	A957	A958	A959	A960	A961	A962	A963	A964	A965	A966	A967	A968	A969	A970	A971	A972	A973	A974	A975	A976	A977	A978	A979	A980	A981	A982	A983	A984	A985	A986	A987	A988	A989	A990	A991	A992	A993	A994	A995	A996	A997	A998	A999	A1000
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A586	C587	U588	C589	A590	C591	U592	C593	U594	C595	C596	U597	C598	U599	C600	C601	C602	A603	C604	C605	U606	U607	C608	A609	C610	C611	C612	C613	C614	C615	C616	A617	C618	C619	C620	A621	C622	C623	C624	C625	U626	C627	U628	C629	C630	C631		C634	C635	C636	C637	C638	C639	C640	C641	A643								
U524	U525	A526	C527	A528	A529	C530	C531	A532	C533	U534	C535	A536	C537	C539	C540	C541	C542	C543	C544	C545	C546	A547	A548	C549	C550	C551	C552	C553	C554	C555	C556	C557	C558	C559	C560	C561	C562	C563	C564	C565	C566	A567	U568	U569	C570	A571	C572	C573	C574	C575	C576	C577	C578	C579	C580	C581	C582	C583	C584	C585			
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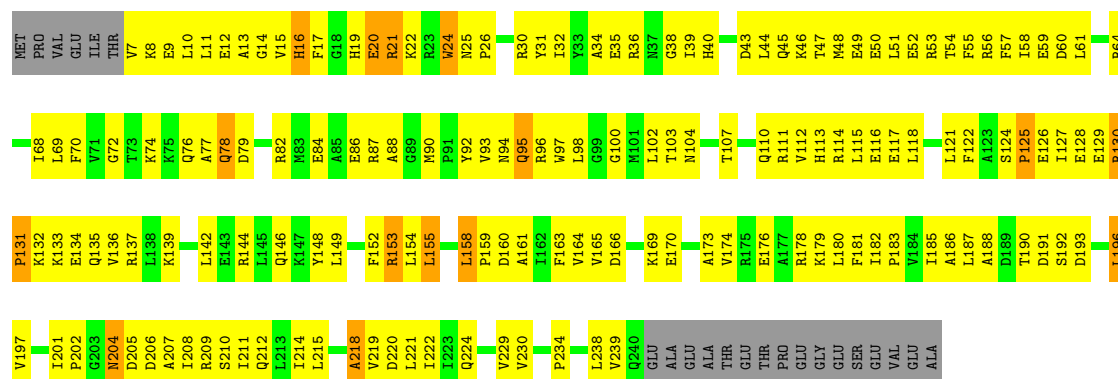
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G2010	G1949	G1886	U1818	G1758	G1682	G1622	G1560	C1501	G1441	A1378	A1317	C1257	A1194	G1134
U2011	G1950	A1889	A1819	A1759	C1683	G1623	A1561	C1502	G1442	A1379	C1318	G1258	G1195	G1135
G2012	A1890	A1880	A1820	A1760	C1684	G1624	A1562	U1503	G1443	G1380	G1319	G1259	G1196	G1136
A2013	A1951	G1891	A1821	C1761	C1685	G1625	G1564	C1504	G1444	G1381	C1320	G1260	G1197	G1137
A2014	A1953	C1892	G1822	A1762	C1686	G1626	G1565	C1505	A1444A	G1382	A1321	C1261	G1138	G1138
A2015	G1954	G1893	G1823	G1763	G1687	G1627	G1566	C1506	A1445	G1383	A1322	A1262	G1200	G1139
U2016	U1955	G1896	G1824	G1764	U1688	G1628	A1567	A1507	C1446	A1384	U1323	A1263	G1201	G1140
U1956	A1825	C1765	A1689	C1765	A1689	G1629	A1567	A1508	G1447	G1385	G1324	U1263	C1202	U1141
G2018	G1826	U1766	A1690	U1766	G1630	G1630	G1568	C1509	G1448	G1386	G1325	A1265	G1203	U1142
A2019	U1897	C1767	A1691	C1767	C1630A	G1630A	A1569	A1510	G1449	C1387	G1326	G1266	A1204	A1142A
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G2023	G1831	G1695	G1695	C1771	G1695	A1634	G1573	U1514	U1454	A1395	A1331	G1271	G1209	C1147
G2024	C1832	G1696	G1696	G1772	G1696	G1635	C1574	C1515	A1454	A1396	G1332	A1272	A1210	A1148
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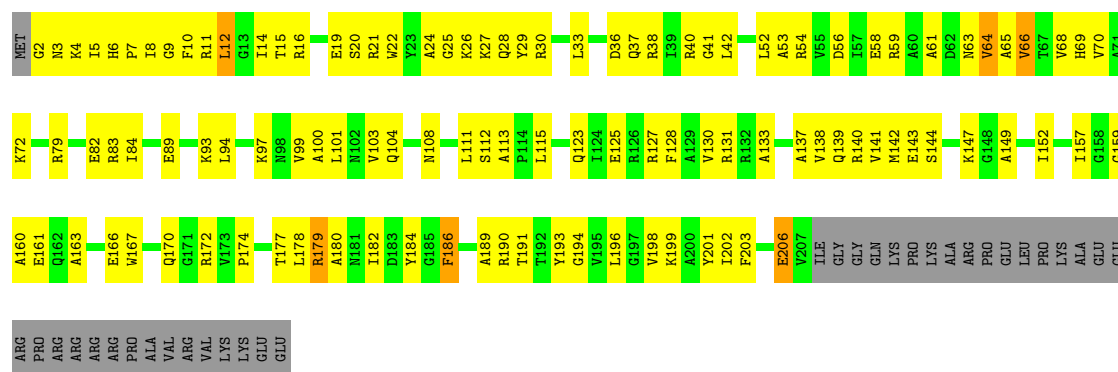
• Molecule 9: 30S ribosomal protein S2

Chain F: 28% 57% 6% 9%



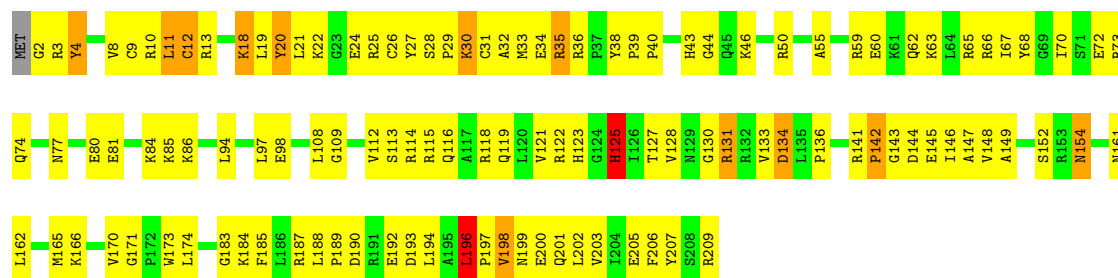
• Molecule 10: 30S ribosomal protein S3

Chain G: 39% 44% 14%



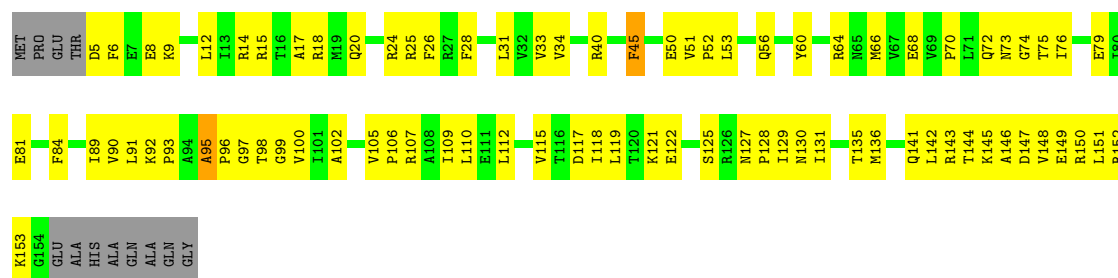
• Molecule 11: 30S ribosomal protein S4

Chain H: 44% 49% 6%



• Molecule 12: 30S ribosomal protein S5

Chain I: 42% 49% 7%



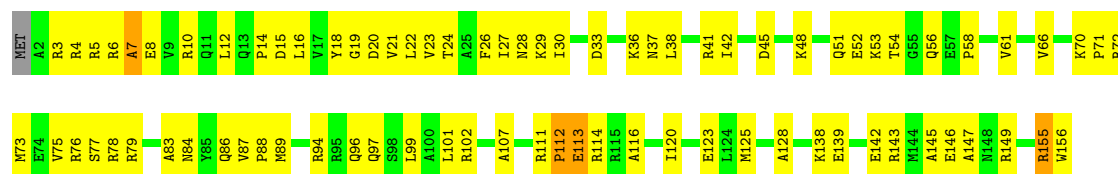
• Molecule 13: 30S ribosomal protein S6

Chain J: 32% 63% 5%



• Molecule 14: 30S ribosomal protein S7

Chain K: 48% 49% ..



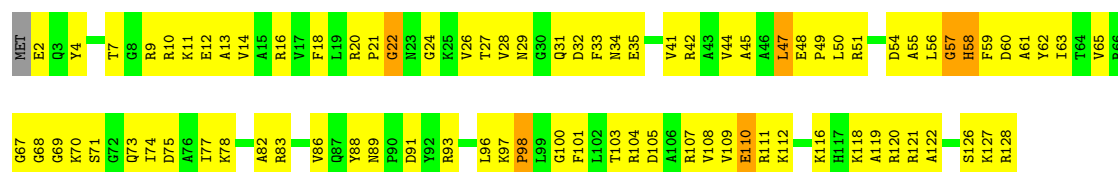
• Molecule 15: 30S ribosomal protein S8

Chain L: 33% 62% *

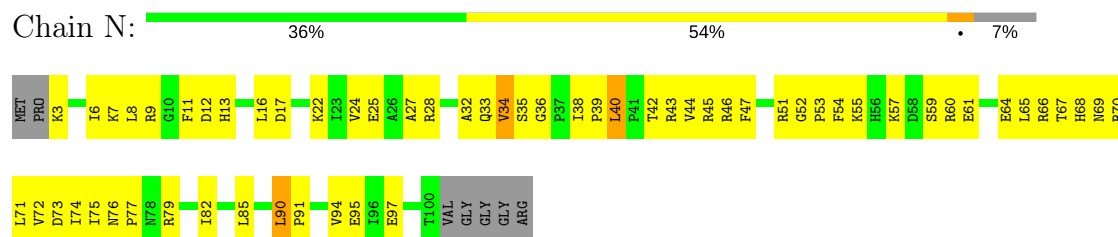


• Molecule 16: 30S ribosomal protein S9

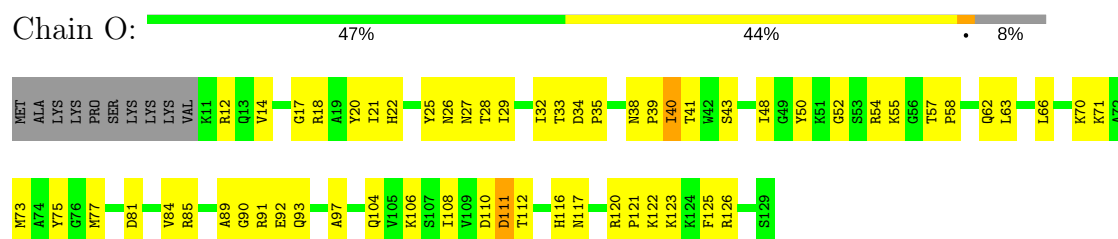
Chain M: 34% 61% 5% *



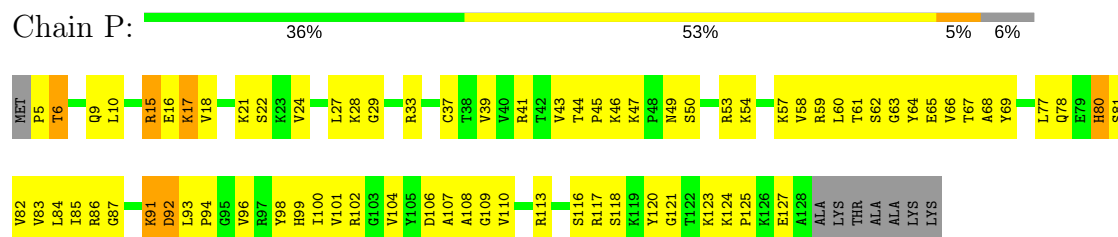
- Molecule 17: 30S ribosomal protein S10



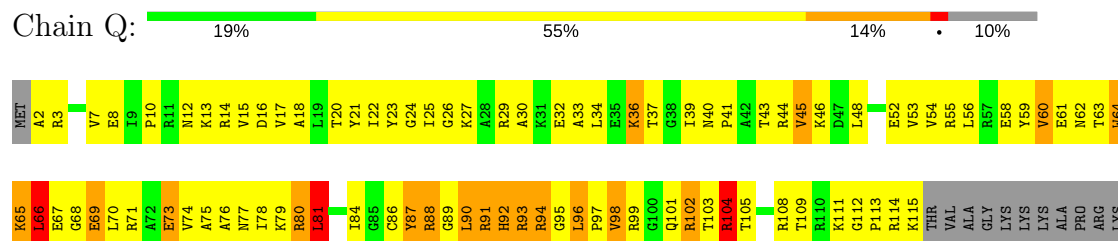
- Molecule 18: 30S ribosomal protein S11



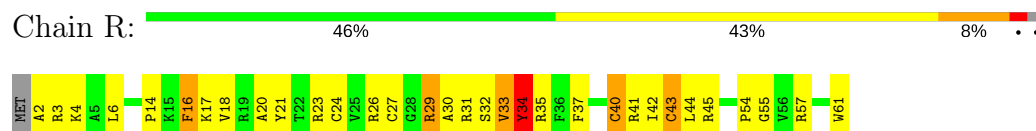
- Molecule 19: 30S ribosomal protein S12



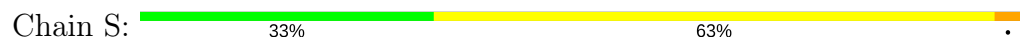
- Molecule 20: 30S ribosomal protein S13



- Molecule 21: 30S ribosomal protein S14 type Z

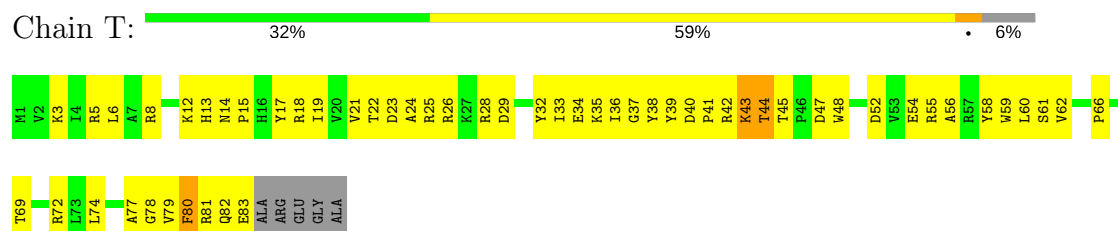


- Molecule 22: 30S ribosomal protein S15

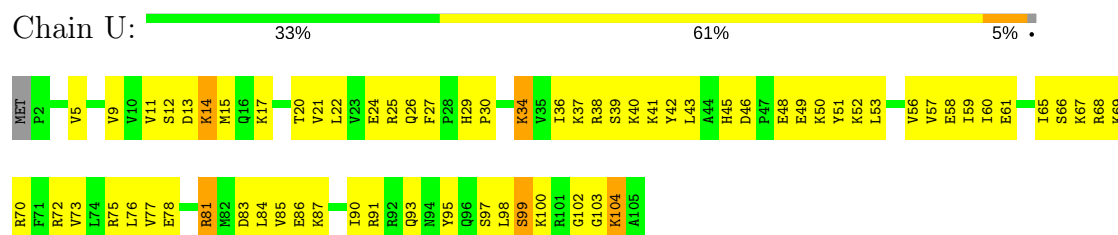




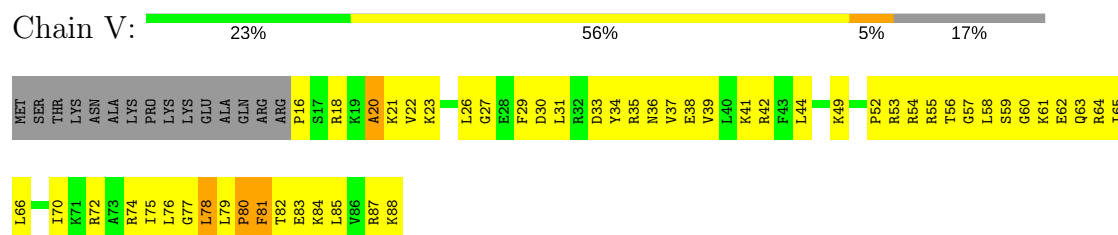
- Molecule 23: 30S ribosomal protein S16



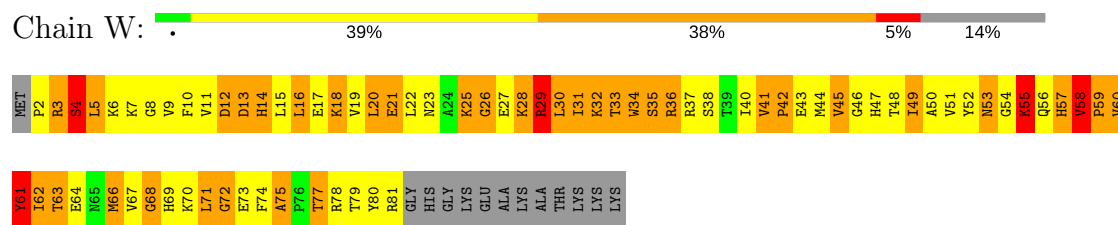
- Molecule 24: 30S ribosomal protein S17



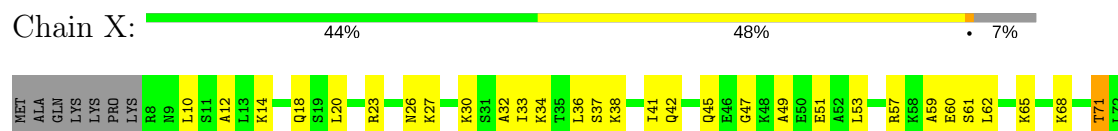
- Molecule 25: 30S ribosomal protein S18

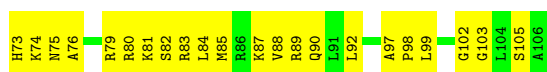


- Molecule 26: 30S ribosomal protein S19

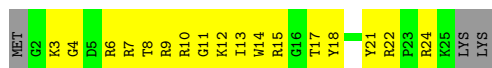


- Molecule 27: 30S ribosomal protein S20

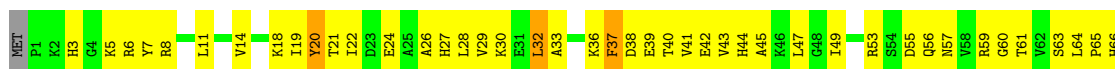




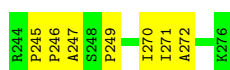
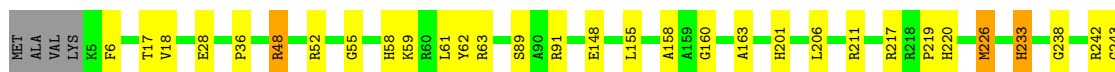
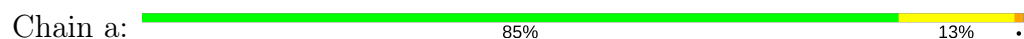
- Molecule 28: 30S ribosomal protein Thx



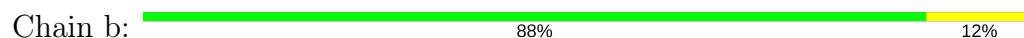
- Molecule 29: 50S ribosomal protein L1



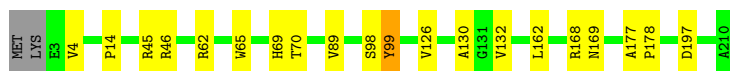
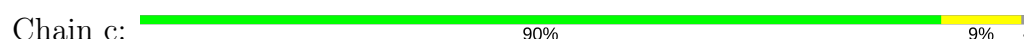
- Molecule 30: 50S ribosomal protein L2



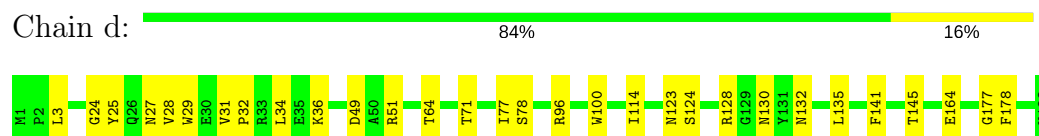
- Molecule 31: 50S ribosomal protein L3



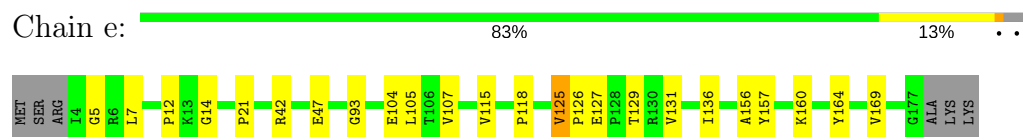
- Molecule 32: 50S ribosomal protein L4



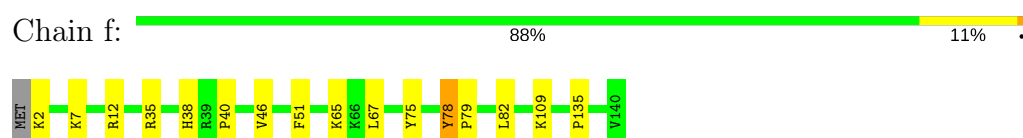
- Molecule 33: 50S ribosomal protein L5



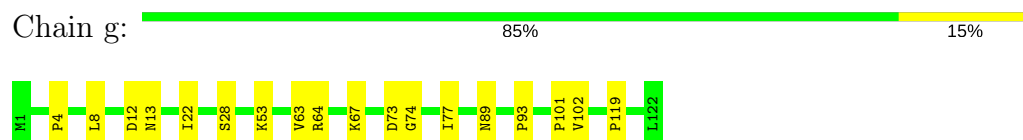
- Molecule 34: 50S ribosomal protein L6



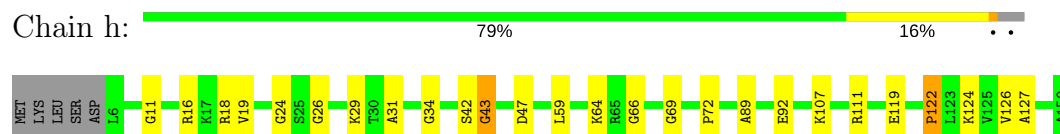
- Molecule 35: 50S ribosomal protein L13



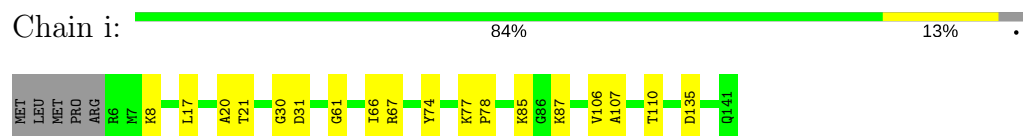
- Molecule 36: 50S ribosomal protein L14



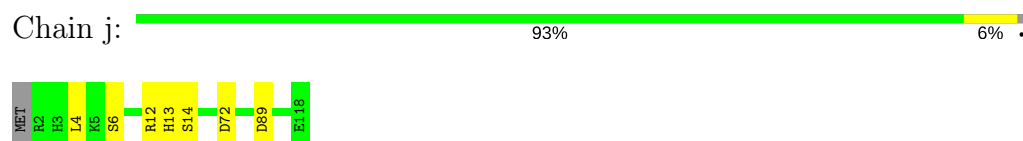
- Molecule 37: 50S ribosomal protein L15



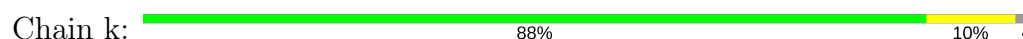
- Molecule 38: 50S ribosomal protein L16



- Molecule 39: 50S ribosomal protein L17



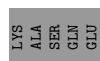
- Molecule 40: 50S ribosomal protein L18





- Molecule 41: 50S ribosomal protein L19

Chain l: 66% 12% 20%



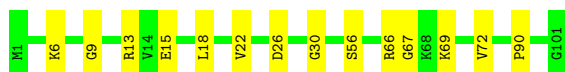
- Molecule 42: 50S ribosomal protein L20

Chain m: 96% ..



- Molecule 43: 50S ribosomal protein L21

Chain n: 86% 14%



- Molecule 44: 50S ribosomal protein L22

Chain o: 89% 8% .



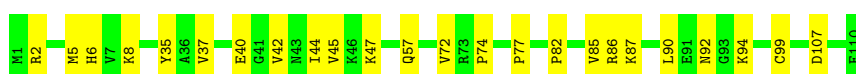
- Molecule 45: 50S ribosomal protein L23

Chain p: 91% 6% ..



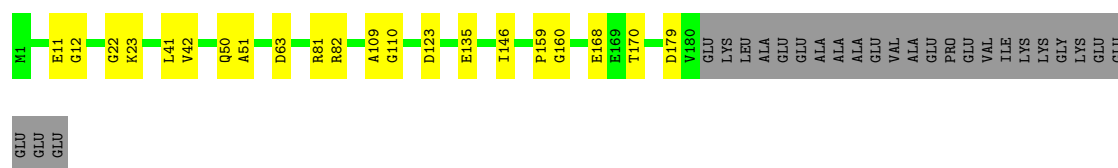
- Molecule 46: 50S ribosomal protein L24

Chain q: 78% 22%

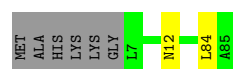
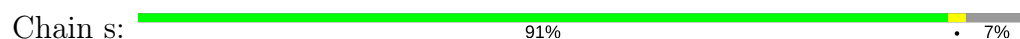


- Molecule 47: 50S ribosomal protein L25

Chain r: 77% 10% 13%



- Molecule 48: 50S ribosomal protein L27



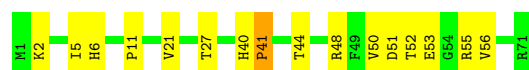
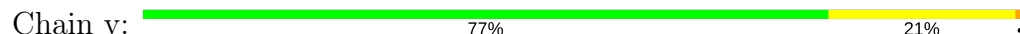
- Molecule 49: 50S ribosomal protein L29



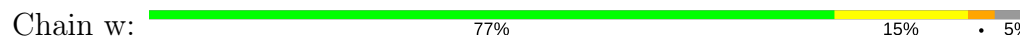
- Molecule 50: 50S ribosomal protein L30



- Molecule 51: 50S ribosomal protein L31



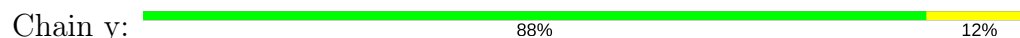
- Molecule 52: 50S ribosomal protein L32



- Molecule 53: 50S ribosomal protein L33



- Molecule 54: 50S ribosomal protein L34





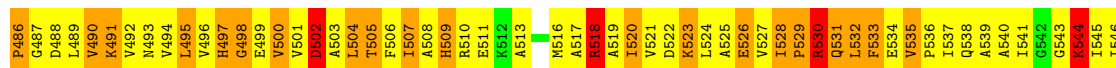
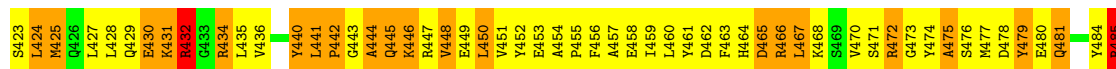
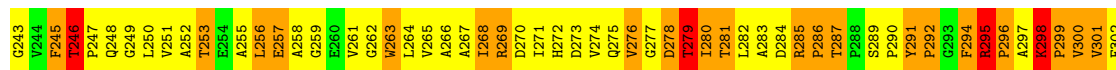
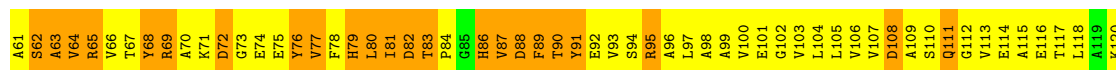
- Molecule 55: 50S ribosomal protein L35

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	22
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	15
10	G	204/239 (85%)	170 (83%)	21 (10%)	13 (6%)	1	25
11	H	206/209 (99%)	172 (84%)	17 (8%)	17 (8%)	1	17
12	I	148/162 (91%)	125 (84%)	15 (10%)	8 (5%)	2	28
13	J	99/101 (98%)	85 (86%)	8 (8%)	6 (6%)	2	25
14	K	153/156 (98%)	138 (90%)	11 (7%)	4 (3%)	6	43
15	L	136/138 (99%)	112 (82%)	17 (12%)	7 (5%)	2	29
16	M	125/128 (98%)	90 (72%)	27 (22%)	8 (6%)	1	25
17	N	96/105 (91%)	80 (83%)	12 (12%)	4 (4%)	3	33
18	O	117/129 (91%)	104 (89%)	8 (7%)	5 (4%)	3	32
19	P	122/132 (92%)	91 (75%)	24 (20%)	7 (6%)	2	27
20	Q	112/126 (89%)	77 (69%)	23 (20%)	12 (11%)	0	10
21	R	58/61 (95%)	43 (74%)	9 (16%)	6 (10%)	0	11
22	S	86/89 (97%)	74 (86%)	10 (12%)	2 (2%)	7	46
23	T	81/88 (92%)	69 (85%)	8 (10%)	4 (5%)	2	30
24	U	102/105 (97%)	80 (78%)	16 (16%)	6 (6%)	2	26
25	V	71/88 (81%)	57 (80%)	10 (14%)	4 (6%)	2	27
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	34
28	Y	22/27 (82%)	19 (86%)	3 (14%)	0	100	100
29	Z	226/229 (99%)	187 (83%)	28 (12%)	11 (5%)	2	30
30	a	270/276 (98%)	201 (74%)	38 (14%)	31 (12%)	0	8
31	b	204/206 (99%)	150 (74%)	31 (15%)	23 (11%)	0	9
32	c	206/210 (98%)	165 (80%)	25 (12%)	16 (8%)	1	19
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	5
35	f	137/140 (98%)	107 (78%)	19 (14%)	11 (8%)	1	18
36	g	120/122 (98%)	81 (68%)	24 (20%)	15 (12%)	0	7
37	h	143/150 (95%)	93 (65%)	28 (20%)	22 (15%)	0	4

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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	32
40	k	108/112 (96%)	77 (71%)	22 (20%)	9 (8%)	1	17
41	l	115/146 (79%)	80 (70%)	19 (16%)	16 (14%)	0	5
42	m	115/118 (98%)	100 (87%)	11 (10%)	4 (4%)	4	38
43	n	99/101 (98%)	66 (67%)	20 (20%)	13 (13%)	0	6
44	o	108/113 (96%)	86 (80%)	14 (13%)	8 (7%)	1	20
45	p	92/96 (96%)	71 (77%)	14 (15%)	7 (8%)	1	19
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	9
48	s	77/85 (91%)	65 (84%)	10 (13%)	2 (3%)	6	43
49	t	65/67 (97%)	54 (83%)	7 (11%)	4 (6%)	2	25
50	u	57/60 (95%)	44 (77%)	8 (14%)	5 (9%)	1	15
51	v	69/71 (97%)	35 (51%)	21 (30%)	13 (19%)	0	2
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	10
55	z	62/65 (95%)	45 (73%)	8 (13%)	9 (14%)	0	5
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	10

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%)	14	51
9	F	202/220 (92%)	201 (100%)	1 (0%)	91	96
10	G	160/188 (85%)	159 (99%)	1 (1%)	89	95
11	H	180/181 (99%)	179 (99%)	1 (1%)	89	95
12	I	115/123 (94%)	114 (99%)	1 (1%)	82	92
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%)	80	90
20	Q	92/101 (91%)	78 (85%)	14 (15%)	3	22
21	R	49/50 (98%)	49 (100%)	0	100	100
22	S	79/80 (99%)	78 (99%)	1 (1%)	73	88
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	1
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%)	66	85
30	a	215/218 (99%)	212 (99%)	3 (1%)	71	87
31	b	166/166 (100%)	165 (99%)	1 (1%)	89	95
32	c	164/166 (99%)	161 (98%)	3 (2%)	64	85
33	d	156/156 (100%)	152 (97%)	4 (3%)	51	78
34	e	143/148 (97%)	142 (99%)	1 (1%)	87	94
35	f	118/119 (99%)	117 (99%)	1 (1%)	85	93
36	g	100/100 (100%)	99 (99%)	1 (1%)	80	90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
37	h	111/116 (96%)	109 (98%)	2 (2%)	64	85
38	i	106/111 (96%)	105 (99%)	1 (1%)	82	92
39	j	100/101 (99%)	98 (98%)	2 (2%)	60	83
40	k	87/88 (99%)	87 (100%)	0	100	100
41	l	105/127 (83%)	104 (99%)	1 (1%)	80	90
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%)	78	89
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%)	60	83
51	v	63/63 (100%)	62 (98%)	1 (2%)	68	86
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%)	39	71
56	B	490/505 (97%)	347 (71%)	143 (29%)	0	3
All	All	5390/5618 (96%)	5167 (96%)	223 (4%)	40	69

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%)	0
6	A	1514/1522 (99%)	529 (34%)	0
7	D	2888/2893 (99%)	1316 (45%)	0
8	E	122/123 (99%)	48 (39%)	0
All	All	4675/4691 (99%)	1954 (41%)	0

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

There are no RNA pucker outliers to report.

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	-	25,34,34	2.57	8 (32%)	28,54,54	1.22	2 (7%)

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 8 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	-3.84	1.35	1.46
57	B	701	GCP	C5-C6	-2.44	1.48	1.53
57	B	701	GCP	C2-N1	-2.18	1.35	1.44
57	B	701	GCP	PB-O2B	2.08	1.61	1.56

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	B	701	GCP	PA-O3A-PB	-3.71	120.45	132.39
57	B	701	GCP	C3'-C2'-C1'	2.52	106.27	101.43

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.