



Full wwPDB EM Validation Report ⓘ

Oct 6, 2022 – 11:02 PM EDT

PDB ID : 7SFR
EMDB ID : EMD-25100
Title : Unmethylated Mtb Ribosome 50S with SEQ-9
Authors : Xing, Z.; Cui, Z.; Zhang, J.; TB Structural Genomics Consortium (TBSGC)
Deposited on : 2021-10-04
Resolution : 2.60 Å(reported)
Based on initial model : 7KGB

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

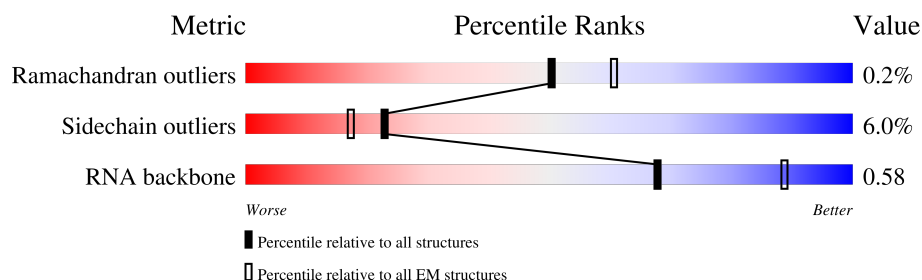
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

1 Overall quality at a glance

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

The reported resolution of this entry is 2.60 Å.

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



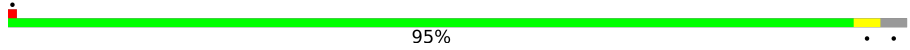
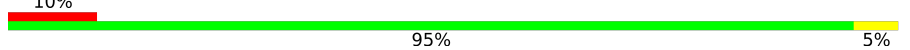
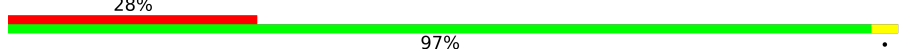

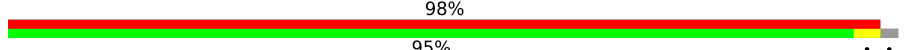

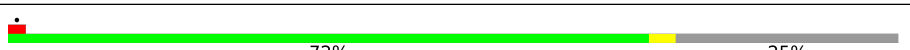
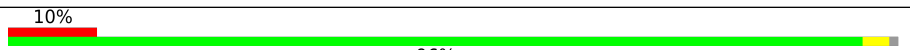
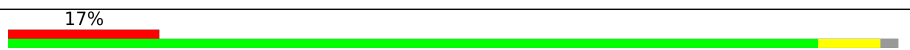
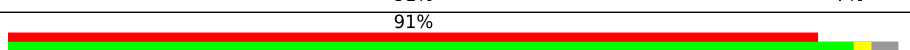
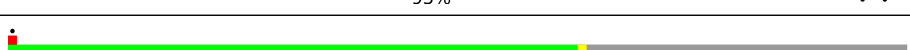

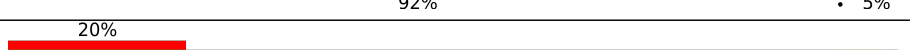
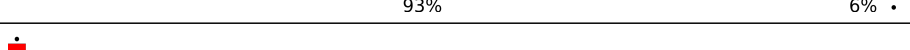
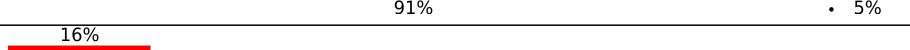
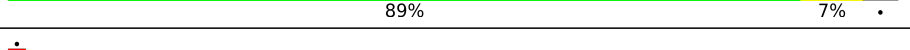

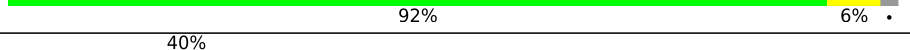



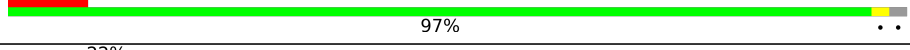
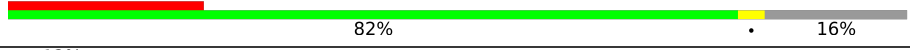


Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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

Mol	Chain	Length	Quality of chain
1	0	57	
2	1	55	
3	2	47	
4	3	64	
5	4	37	
6	6	80	
7	A	3138	
8	B	115	

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Mol	Chain	Length	Quality of chain
9	C	279	
10	D	213	
11	E	207	
12	F	178	
13	G	177	
14	H	152	
15	J	195	
16	K	122	
17	L	146	
18	M	138	
19	N	180	
20	O	122	
21	P	113	
22	Q	129	
23	R	104	
24	S	197	
25	T	100	
26	U	105	
27	V	215	
28	W	86	
29	X	64	
30	Y	77	
31	Z	65	
32	a	1537	
33	c	274	

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Mol	Chain	Length	Quality of chain
34	d	201	
35	e	220	
36	f	96	
37	g	156	
38	h	132	
39	i	151	
40	j	101	
41	k	139	
42	l	124	
43	m	124	
44	n	61	
45	o	89	
46	p	162	
47	q	135	
48	r	84	
49	s	93	
50	t	86	
51	v	22	

2 Entry composition

There are 54 unique types of molecules in this entry. The entry contains 143665 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 L32.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	0	54	Total	C	N	O	0	0
			429	266	94	69		

- Molecule 2 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	48	Total	C	N	O	S	0	0
			400	245	84	67	4		

- Molecule 3 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	42	Total	C	N	O	S	0	0
			358	212	94	51	1		

- Molecule 4 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	3	62	Total	C	N	O	0	0
			494	298	112	84		

- Molecule 5 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	4	37	Total	C	N	O	S	0	0
			299	182	66	47	4		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
4	1	VAL	MET	conflict	UNP A0A3E0V5U0

- Molecule 6 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	6	57	Total	C	N	O	S	0	0
			446	277	82	82	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	A	3118	Total	C	N	O	P	0	0
			66961	29850	12340	21653	3118		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	B	115	Total	C	N	O	P	0	0
			2458	1097	456	790	115		

- Molecule 9 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	C	272	Total	C	N	O	S	0	0
			2088	1277	437	369	5		

- Molecule 10 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	D	213	Total	C	N	O	S	0	0
			1590	985	307	292	6		

- Molecule 11 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	E	207	Total	C	N	O	S	0	0
			1552	958	303	289	2		

- Molecule 12 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	F	178	Total	C	N	O	S	0	0
			1408	885	267	251	5		

- Molecule 13 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	G	174	Total	C	N	O	S	0	0
			1330	836	249	244	1		

- Molecule 14 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	H	47	Total	C	N	O	S	0	0
			350	220	64	65	1		

- Molecule 15 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	J	146	Total	C	N	O	S	0	0
			1143	724	217	199	3		

- Molecule 16 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	K	121	Total	C	N	O	S	0	0
			934	585	179	168	2		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	1	VAL	MET	conflict	UNP A0A045HTP7

- Molecule 17 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	L	143	Total	C	N	O	S	0	0
			1068	662	216	188	2		

- Molecule 18 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	M	134	Total	C	N	O	S	0	0
			1072	679	215	177	1		

- Molecule 19 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	N	116	Total	C	N	O	S	0	0
			908	574	175	158	1		

- Molecule 20 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	O	116	Total	C	N	O		0	0
			886	541	188	157			

- Molecule 21 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	P	112	Total	C	N	O	S	0	0
			907	573	174	159	1		

- Molecule 22 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Q	122	Total	C	N	O		0	0
			980	608	205	167			

- Molecule 23 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	R	100	Total	C	N	O		0	0
			757	482	138	137			

- Molecule 24 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	S	113	Total	C	N	O		0	0
			860	533	178	149			

- Molecule 25 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	T	98	Total	C	N	O		0	0
			759	480	141	138			

- Molecule 26 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	U	90	Total	C	N	O	S	0	0
			699	430	138	129	2		

- Molecule 27 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	V	95	Total	C	N	O		0	0
			735	456	152	127			

- Molecule 28 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	W	71	Total	C	N	O		0	0
			526	325	108	93			

- Molecule 29 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	X	63	Total	C	N	O	S	0	0
			476	289	101	81	5		

- Molecule 30 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Y	65	Total	C	N	O	S	0	0
			541	331	106	103	1		

- Molecule 31 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Z	59	Total	C	N	O		0	0
			476	293	101	82			

- Molecule 32 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	a	1519	Total	C	N	O	P	0	0
			32621	14536	5961	10605	1519		

- Molecule 33 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	c	207	Total	C	N	O	S	0	0
			1654	1030	322	298	4		

- Molecule 34 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	d	200	Total	C	N	O	S	0	0
			1650	1036	316	296	2		

- Molecule 35 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	e	160	Total	C	N	O	S	0	0
			1149	726	214	206	3		

- Molecule 36 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	f	95	Total	C	N	O	S	0	0
			757	480	133	141	3		

- Molecule 37 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	g	152	Total	C	N	O	S	0	0
			1193	742	234	215	2		

- Molecule 38 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	h	130	Total	C	N	O	S	0	0
			999	627	187	184	1		

- Molecule 39 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	i	127	Total	C	N	O		0	0
			993	628	195	170			

- Molecule 40 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	j	99	Total	C	N	O	S	0	0
			789	496	146	144	3		

- Molecule 41 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	k	117	Total	C	N	O		0	0
			873	540	175	158			

- Molecule 42 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	l	122	Total	C	N	O	S	0	0
			959	594	197	166	2		

- Molecule 43 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	m	116	Total	C	N	O	S	0	0
			945	578	196	168	3		

- Molecule 44 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	n	60	Total	C	N	O	S	0	0
			468	294	96	73	5		

- Molecule 45 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	o	87	Total	C	N	O		0	0
			718	449	144	125			

- Molecule 46 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	p	91	Total	C	N	O		0	0
			728	462	140	126			

- Molecule 47 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	q	93	Total	C	N	O	S	0	0
			754	471	149	131	3		

- Molecule 48 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	r	63	Total	C	N	O	S	0	0
			497	309	96	89	3		

- Molecule 49 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	s	83	Total	C	N	O	S	0	0
			672	432	125	114	1		

- Molecule 50 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	t	82	Total	C	N	O		0	0
			631	381	137	113			

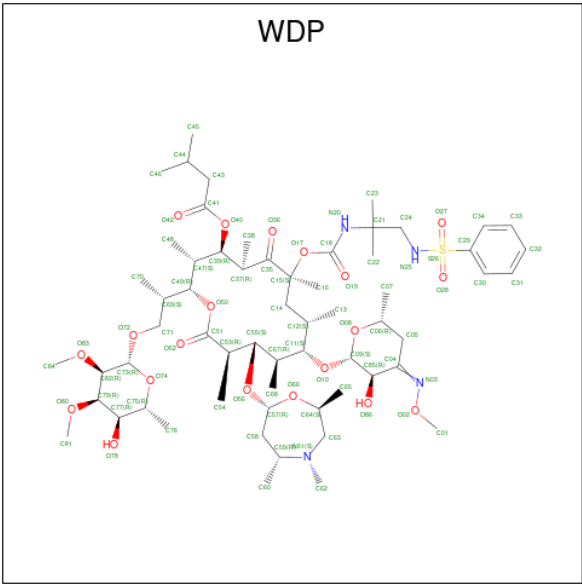
- Molecule 51 is a protein called peptide.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	v	22	Total	C	N	O		0	0
			186	111	47	28			

- Molecule 52 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
52	1	1	Total	Zn	0
			1	1	
52	4	1	Total	Zn	0
			1	1	
52	6	1	Total	Zn	0
			1	1	
52	X	1	Total	Zn	0
			1	1	
52	n	1	Total	Zn	0
			1	1	
52	r	1	Total	Zn	0
			1	1	

- Molecule 53 is Sequanamycin 9 (three-letter code: WDP) (formula: C₆₁H₁₀₂N₄O₂₀S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
53	A	1	Total	C	N	O	S	0
			86	61	4	20	1	

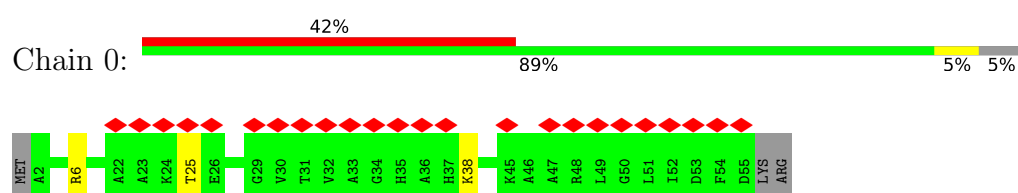
- Molecule 54 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
54	A	307	Total	Mg	0
			307	307	
54	B	7	Total	Mg	0
			7	7	
54	C	3	Total	Mg	0
			3	3	
54	D	1	Total	Mg	0
			1	1	
54	L	1	Total	Mg	0
			1	1	
54	M	1	Total	Mg	0
			1	1	
54	a	125	Total	Mg	0
			125	125	
54	e	1	Total	Mg	0
			1	1	
54	t	1	Total	Mg	0
			1	1	

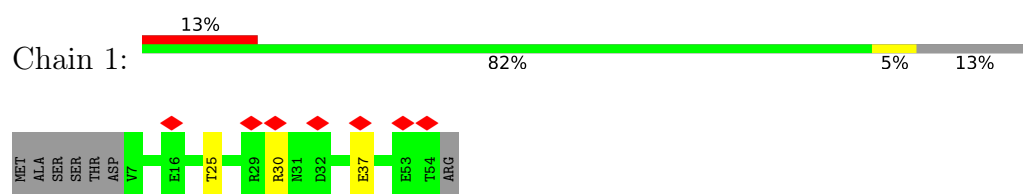
3 Residue-property plots [i](#)

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

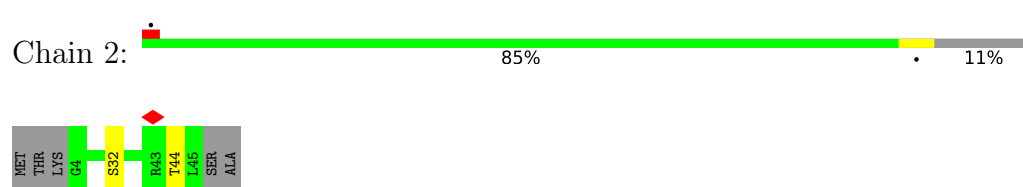
- Molecule 1: 50S ribosomal protein L32



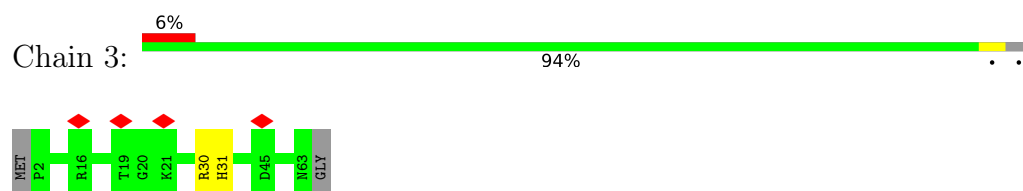
- Molecule 2: 50S ribosomal protein L33



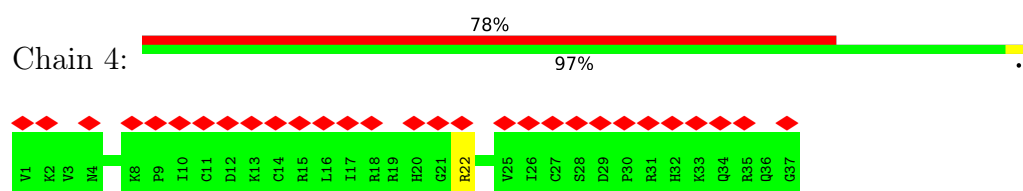
- Molecule 3: 50S ribosomal protein L34



- Molecule 4: 50S ribosomal protein L35

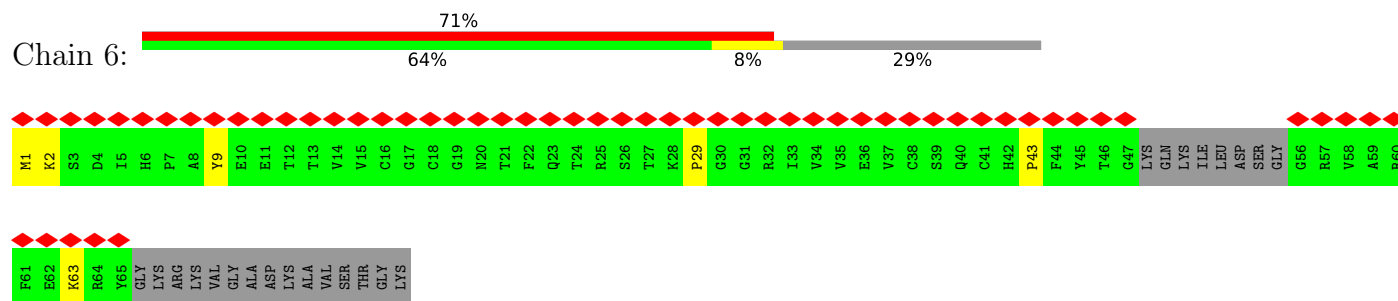


- Molecule 5: 50S ribosomal protein L36



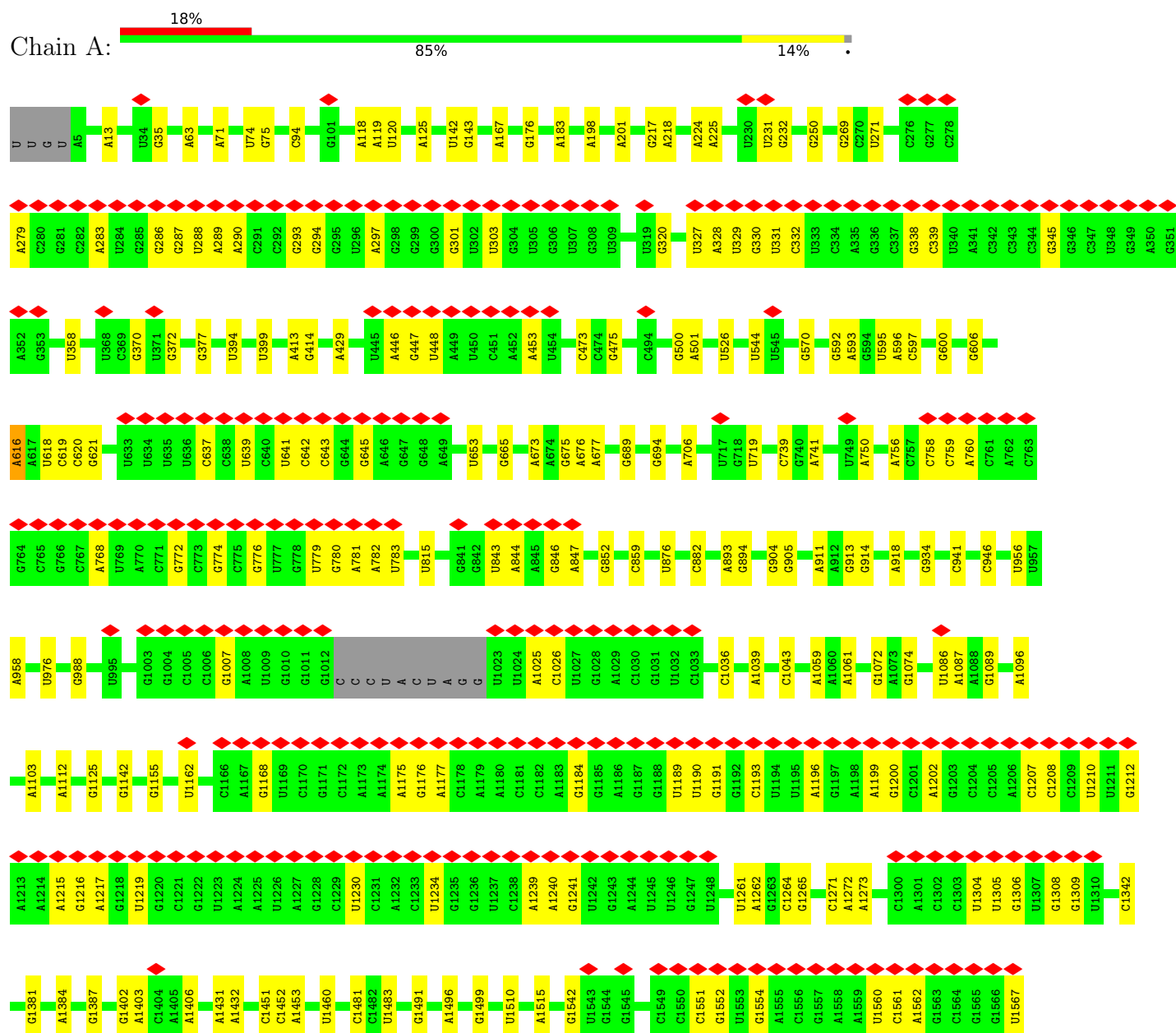
- Molecule 6: 50S ribosomal protein L31

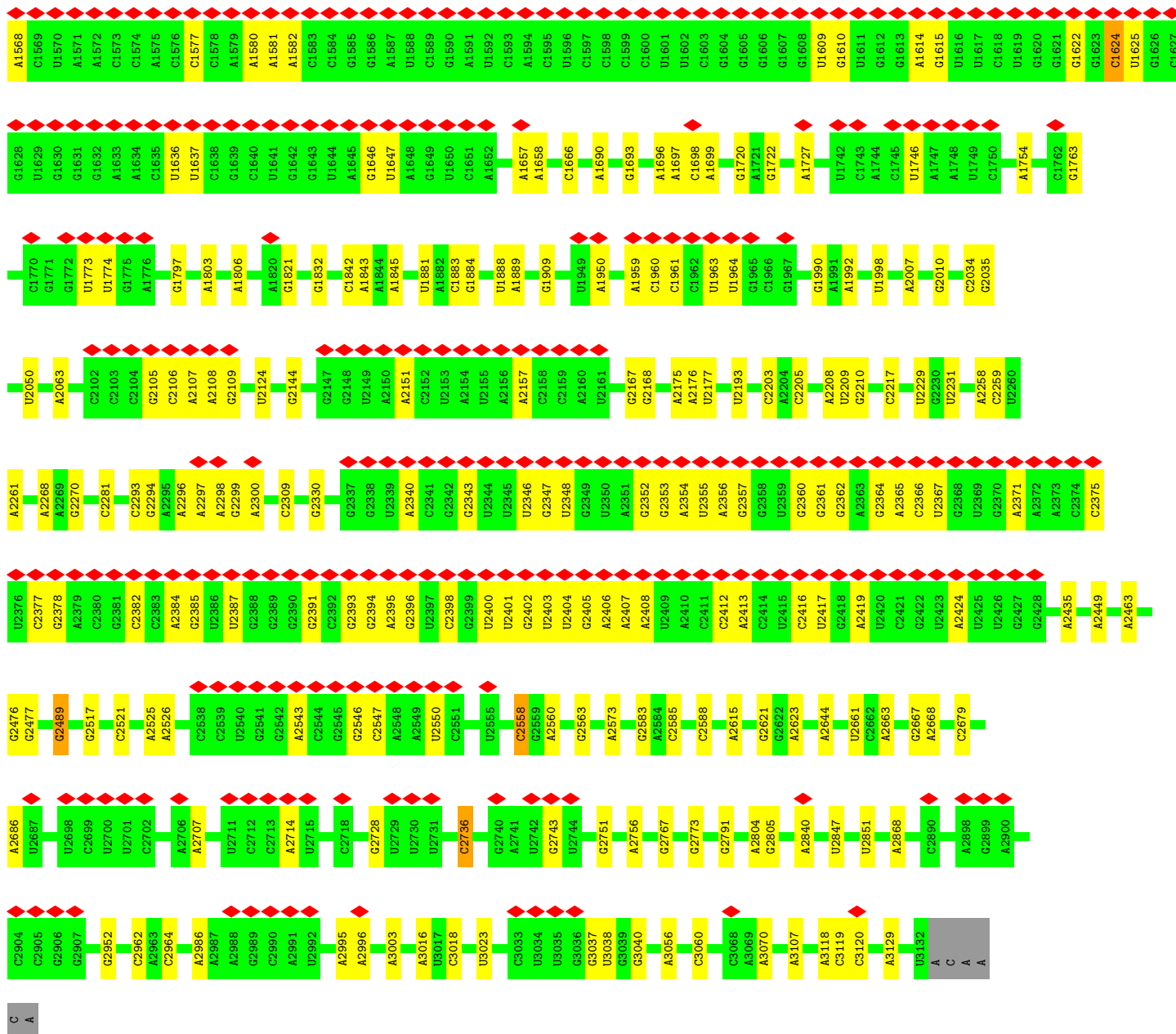
Chain 6:



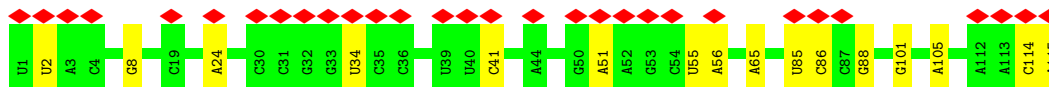
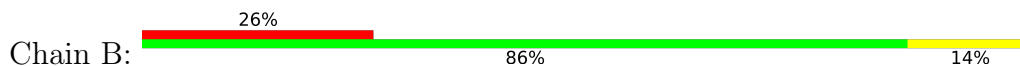
- Molecule 7: 23S rRNA

Chain A:





● Molecule 8: 5S rRNA



● Molecule 9: 50S ribosomal protein L2

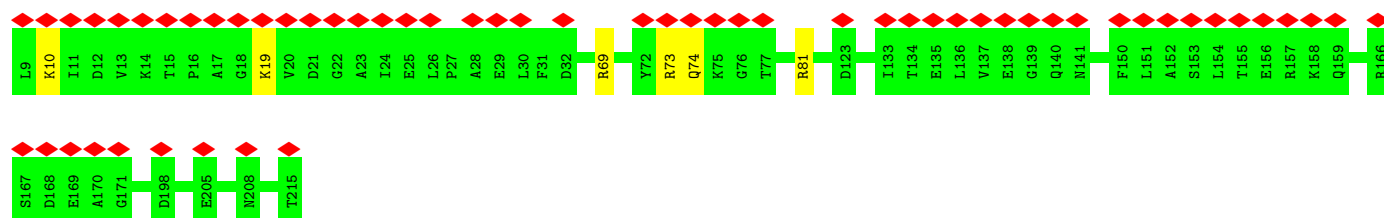




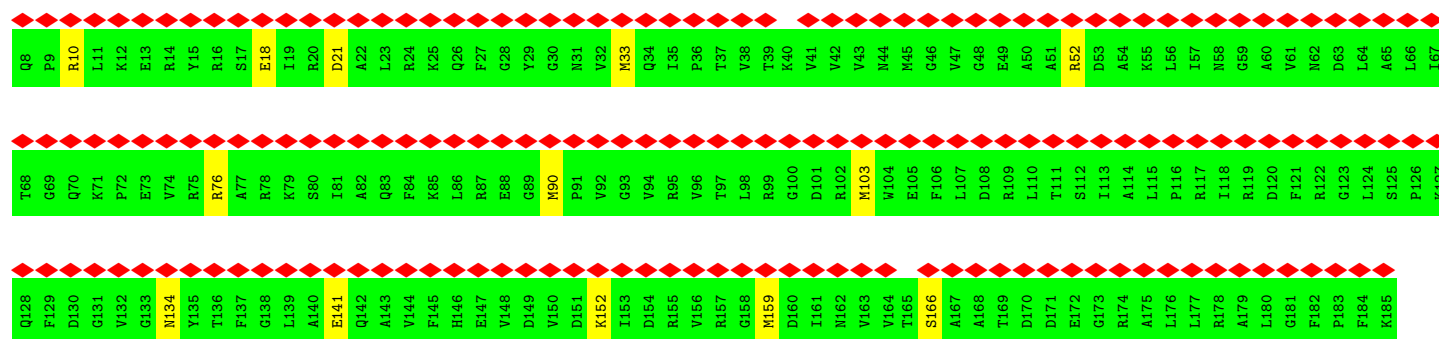
- Molecule 10: 50S ribosomal protein L3



- Molecule 11: 50S ribosomal protein L4

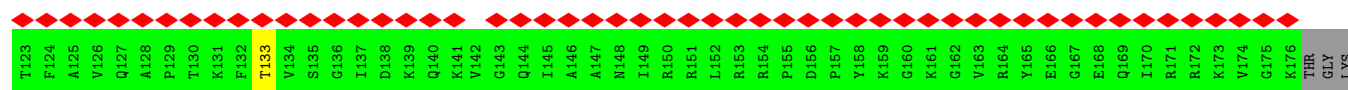


- Molecule 12: 50S ribosomal protein L5

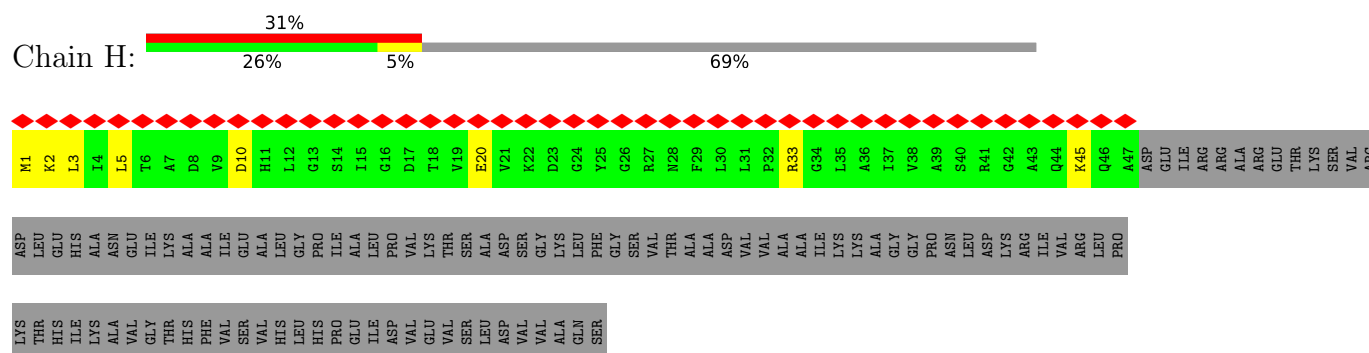


- Molecule 13: 50S ribosomal protein L6

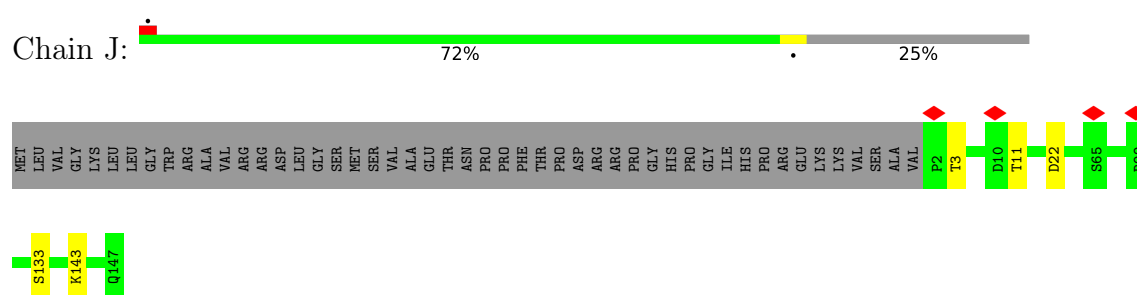




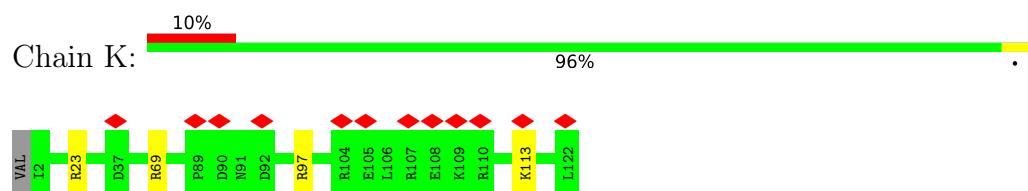
- Molecule 14: 50S ribosomal protein L9



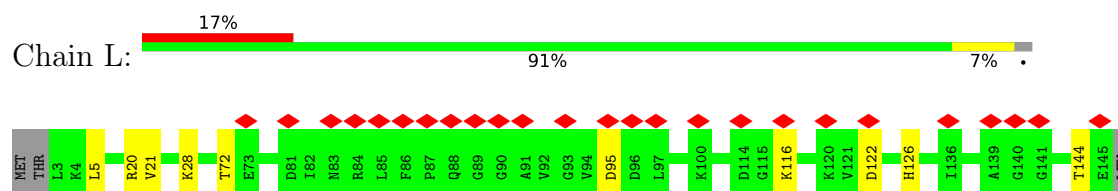
- Molecule 15: 50S ribosomal protein L13



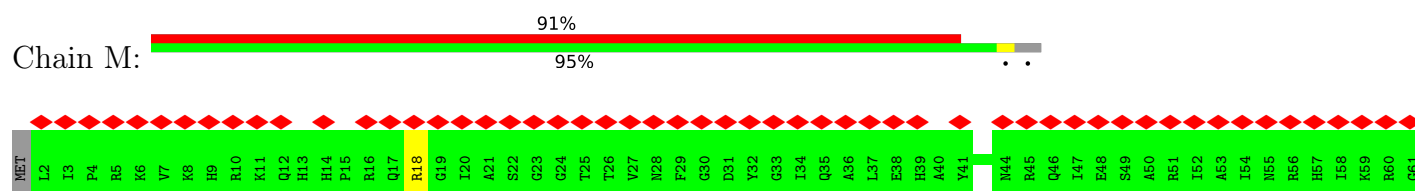
- Molecule 16: 50S ribosomal protein L14



- Molecule 17: 50S ribosomal protein L15

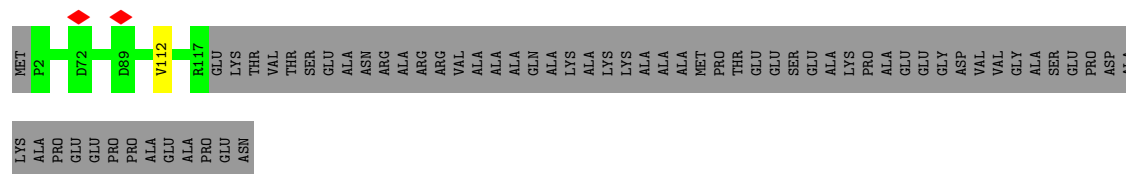


- Molecule 18: 50S ribosomal protein L16

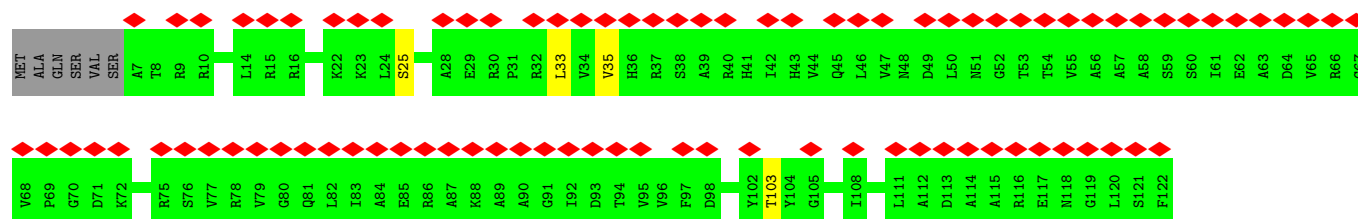
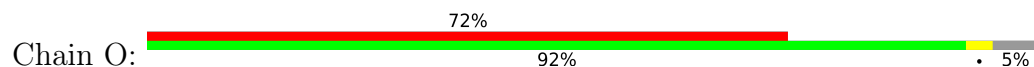




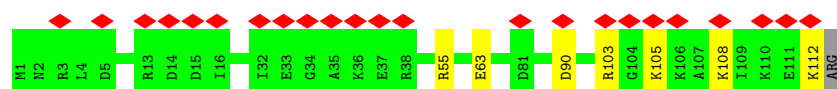
- Molecule 19: 50S ribosomal protein L17



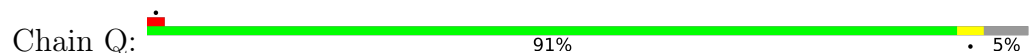
- Molecule 20: 50S ribosomal protein L18



- Molecule 21: 50S ribosomal protein L19

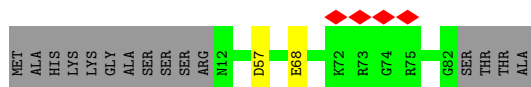
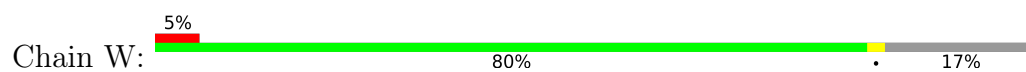


- Molecule 22: 50S ribosomal protein L20

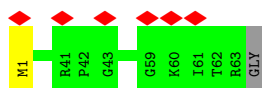


- Molecule 23: 50S ribosomal protein L21

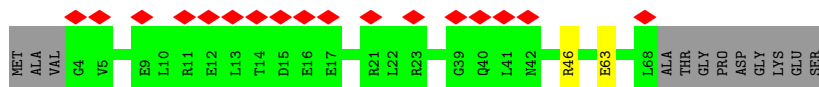
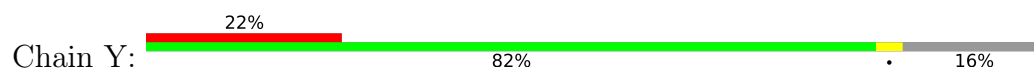




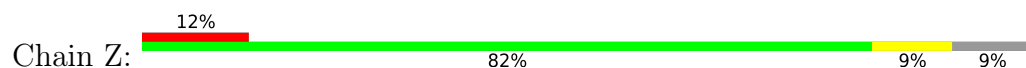
- Molecule 29: 50S ribosomal protein L28



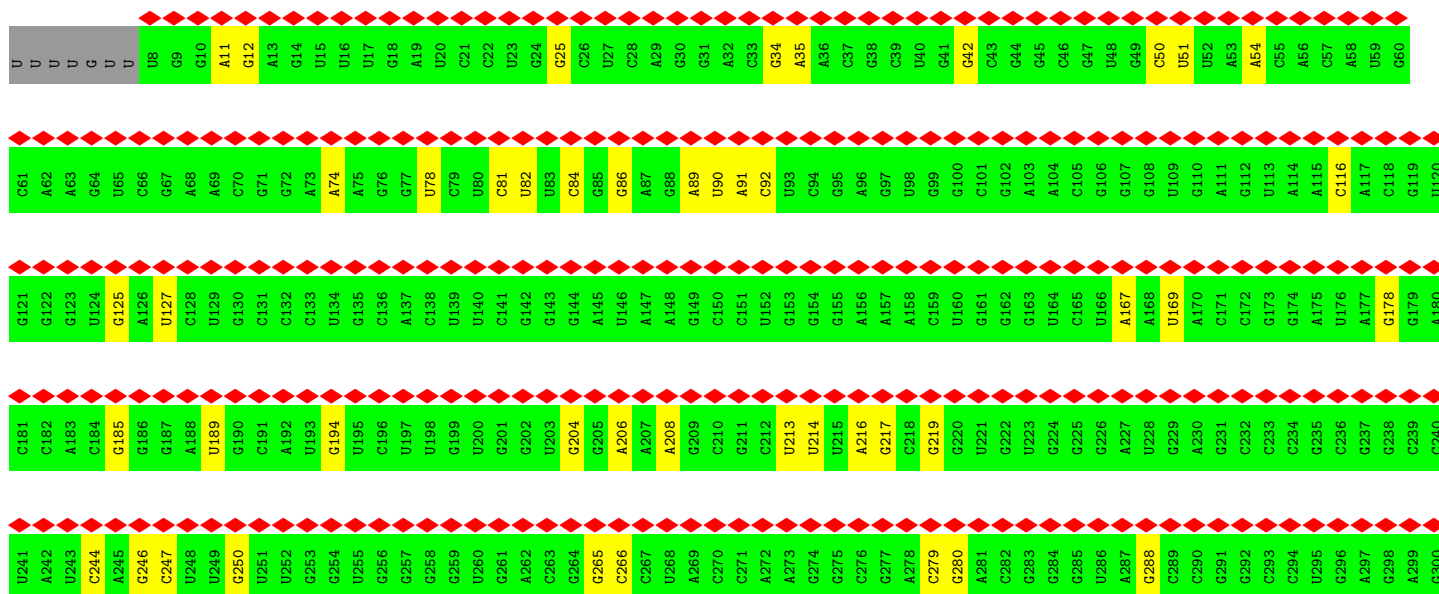
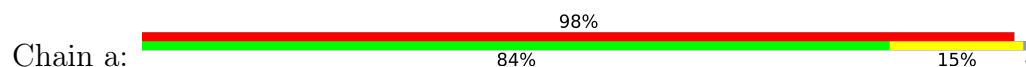
- Molecule 30: 50S ribosomal protein L29



- Molecule 31: 50S ribosomal protein L30



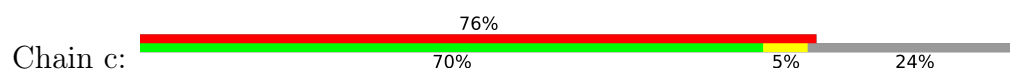
- Molecule 32: 16S rRNA



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U1023	C963	C903	U843	G783	C723	G663	U603	U543	C483	G423	A363	G303
G1024	G964	U904	C844	U784	G724	G664	C604	G544	A484	G424	U364	G304
U1025	C965	C905	C845	A785	G725	G665	A605	U545	C485	U425	A365	U305
G1026	G966	A906	G846	C786	G726	A666	C606	C546	A486	U426	U366	C306
U1027	A967	A907	U847	C787	G727	A667	G607	C547	A487	G427	U367	C307
C1028	A968	A908	G848	C788	C728	U668	G608	G548	C488	U428	U368	G308
G1029	G969	C909	C849	U789	U729	U669	G609	G549	A489	U429	G369	G309
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G1031	A971	A911	G851	G791	U731	C671	U611	A551	C491	A431	C371	C311
U1032	C972	A912	U852	U792	G732	U672	A612	U552	C492	C432	A372	A312
G1033	C973	U913	A853	C793	G733	G673	A613	U553	C493	C433	A373	C313
U1034	U974	U914	G854	G794	G734	G674	C614	A554	C494	U434	U374	A314
C1035	U975	G915	C855	U795	C735	U675	U615	C555	C495	C435	G375	C315
G1036	A976	A916	U856	C796	A736	G676	G616	U556	C496	U436	G376	U316
U1037	U977	C917	A857	C797	G737	U677	U617	U557	C497	U437	G377	U317
G1038	C978	G918	A858	U798	U738	A678	G618	G558	C498	U438	C378	G318
U1039	U979	C919	C859	C799	A739	G679	A619	G559	C499	C439	G379	G319
G1040	G980	G920	G860	G800	A740	C680	G620	C560	A500	A440	C380	A320
U1041	A981	G921	C861	C801	C741	G681	C621	G561	A501	C441	A381	C321
C1042	C982	C922	A862	C802	U742	G682	G622	U562	C502	C442	A382	U322
U1043	U983	C923	U863	G803	G743	U683	U623	A563	U503	A443	G383	A323
G1044	C984	C924	U864	U804	A744	G684	G624	A564	A504	U444	C384	A324
C1045	U985	C925	A865	A805	C745	G685	C625	A565	C505	C445	C385	G325
A1046	G986	G926	A866	A806	G746	A686	G626	G566	G506	G446	U386	A326
U1047	A987	C927	G867	A807	C747	A687	G627	U567	U507	A447	U387	U327
G1048	C988	A928	U868	C808	U748	G688	G628	G568	C508	C448	A388	A328
U1049	A989	C929	A869	G809	G749	U689	C629	C569	C509	G449	U389	G329
C1050	U990	A930	C870	G810	A750	C690	G630	U570	C510	A450	G390	G330
U1051	G991	C931	C871	U811	G751	G691	U631	C571	A511	A451	C391	G331
G1052	C992	C932	C872	G812	G752	C692	U632	G572	C512	G452	A392	C332
U1053	A993	C933	C873	G813	A753	A693	A633	U573	C513	G453	G393	C333
C1054	C994	G934	G874	U814	G754	G694	C634	A574	A514	U454	C394	C334
U1055	A995	G935	C875	U815	C755	A695	G635	G575	G515	C455	G395	A335
G1056	C996	C936	C876	A816	G756	U696	G636	G576	C516	C456	A396	G336
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A1058	A998	C938	G878	U818	U758	U698	C638	G578	C518	G458	G398	C338
G1059	U999	A939	C879	A819	A759	C699	A639	U579	C519	G459	C399	U339
C1060	G1000	C940	G880	G820	G760	U700	G640	U580	G520	U460	C400	C340
U1061	C1001	C941	G881	G821	C761	G701	A641	U581	G521	U461	C401	C341
C1062	G1002	A942	U882	U822	G762	G702	C642	U582	U522	C462	C402	U342
G1063	U1003	U943	C883	G823	U763	A703	U643	G583	A523	U463	C403	A343
U1064	C1004	C944	U884	U824	G764	G704	A644	U584	A524	C464	U404	C344
G1065	U1005	U945	A885	G825	C765	G705	G645	C585	U525	U465	C405	G345
U1066	A1006	G946	C886	G826	G766	A706	A646	G586	A526	C466	G406	G346
C1067	G1007	G947	G887	G827	U767	A707	G647	C587	C527	G467	C407	G347
U1068	A1008	A948	G888	U828	A768	C708	U648	G588	G528	C468	G408	A348
G1069	C1009	U949	C889	U829	G769	A709	A649	U589	U529	U469	C409	G349
U1070	A1010	U950	C890	U830	C770	C710	C650	U590	A530	U470	A410	G350
A1071	U1011	A951	G891	C831	G771	G712	U651	G591	G531	U471	C411	C351
G1072	A1012	A952	C892	C832	A772	G713	G652	U592	G532	G472	G412	A352
U1073	C1013	U953	U893	U833	C773	G714	C653	U593	G533	A473	C413	G353
G1074	U1014	U954	A894	U834	C774	U715	A654	G594	U534	C474	C414	C354
C1075	C1015	C955	G895	C835	A775	G716	G655	G595	G535	G475	G415	A355
U1076	G1016	G956	U896	C836	G776	G717	G656	U596	C536	G476	G416	G356
U1077	U1017	A957	C897	U837	G777	G718	G657	G597	G537	U477	C417	U357
G1078	U1018	U958	U898	U838	A778	G719	G658	A598	A538	A478	C418	G358
C1079	C1019	G959	A900	G839	U779	A719	A659	U599	G539	G479	C419	G359
U1080	C1020	C960		G840	U780	A720	G660	A600	C540	G480	U420	G360

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A1512	G1447	U1446	C1446	U1445	C1443	C1383	G1323	G1263	U1203	G1143	A1083
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G1514	A1449	U1448	U1386	U1386	C1387	U1386	G1326	A1266	U1206	G1146	G1086
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U1519	A1453	A1391	A1391	C1391	A1391	A1331	A1331	A1271	A1211	U1151	C1091
C1520	G1454	C1392	C1392	C1392	C1392	G1332	G1332	A1272	G1212	G1152	A1092
U1521	G1455	U1393	U1393	U1393	U1393	U1333	U1333	U1273	C1213	C1153	A1093
G1522	U1456	G1394	G1394	G1394	G1394	C1334	C1334	C1274	G1214	C1154	C1094
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U1525	C1459	C1397	C1397	C1397	C1397	U1337	U1337	U1277	G1217	G1157	G1097
C1526	G1460	G1398	G1398	U1399	U1399	A1338	A1338	A1278	C1218	G1158	C1098
A	A1461	U1399	U1399	C1400	C1400	G1339	G1339	A1279	A1219	U1159	G1099
C	A1462	C1400	C1400	C1401	C1401	U1340	U1340	A1280	C1220	C1160	C1100
C	G1463	A1401	A1401	A1341	A1341	A1341	A1341	A1281	A1221	A1161	C1101
U	G1464	C1402	C1402	A1342	A1342	A1342	A1342	G1282	C1222	A1162	A1102
U	U1465	G1403	G1403	U1343	U1343	U1343	U1343	C1283	A1223	C1163	C1103
C	G1466	U1404	U1404	C1344	C1344	C1344	C1344	C1284	U1224	U1164	C1104
U		C1405	C1405			G1345	G1345	G1285	G1225	C1165	C1105
U	A1469	A1406	A1406	C1346	C1346	G1346	G1346	G1286	C1226	G1166	U1106
C	U1470	U1407	U1407	A1347	A1347	U1287	U1287	U1287	U1227	G1167	U1107
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	G1472	A1409	A1409	A1349	A1349	U1289	U1289	U1289	C1229	G1169	U1109
	G1473	A1410	A1410	U1350	U1350	C1290	C1290	C1290	A1230	G1170	C1110
	C1474	A1411	A1411	C1351	C1351	A1291	A1291	A1291	A1231	A1171	C1111
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				G1353	G1353	U1293	U1293	U1293	G1233	G1173	A1113
				C1354	C1354	U1294	U1294	U1294	G1234	G1174	U1114
				A1355	A1355	C1295	C1295	C1295	C1235	U1175	G1115
				A1356	A1356	G1296	G1296	G1296	C1236	G1176	U1116
				C1357	C1357	G1297	G1297	G1297	G1237	G1177	U1117
				G1358	G1358	A1298	A1298	A1298	G1238	G1178	G1118
				C1359	C1359	U1299	U1299	U1299	U1239	G1179	C1119
				U1360	U1360	C1300	C1300	C1300	A1240	A1180	C1120
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				G1363	G1363	G1303	G1303	G1303	A1243	A1183	C1123
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				U1365	U1365	U1305	U1305	U1305	G1245	G1185	C1125
				G1366	G1366	C1306	C1306	C1306	G1246	U1186	G1126
				A1367	A1367	U1307	U1307	U1307	G1247	C1187	U1127
				A1368	A1368	G1308	G1308	G1308	C1248	A1188	A1128
				U1369	U1369	C1309	C1309	C1309	U1249	A1189	A1129
				A1370	A1370	A1310	A1310	A1310	G1250	G1190	U1130
				C1371	C1371	A1311	A1311	A1311	C1251	U1191	G1131
				G1372	G1372	C1312	C1312	C1312	G1252	C1192	G1132
				U1373	U1373	U1313	U1313	U1313	A1253	A1193	U1133
				U1374	U1374	C1314	C1314	C1314	U1254	U1194	G1134
				C1375	C1375	G1315	G1315	G1315	G1255	C1195	G1135
				U1376	U1376	A1316	A1316	A1316	C1256	A1196	G1136
				C1377	C1377	C1317	C1317	C1317	G1257	U1197	G1137
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				G1379	G1379	C1319	C1319	C1319	C1259	C1199	C1139
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• Molecule 33: 30S ribosomal protein S3

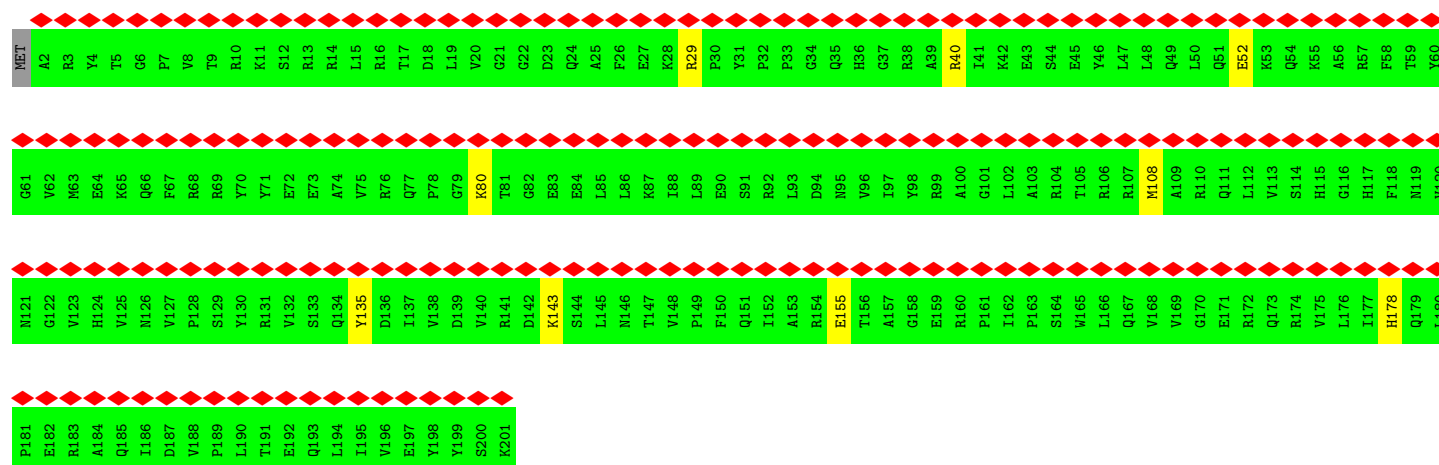


MET																																																													
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D61	R62	V63	R64	V65	D66	I67	H68	T69	A70	R71	P72	G73	I74	V75	I76	G77	R78	R79	G80	T81	E82	A83	D84	R85	I86	R87	A88	D89	L90	E91	K92	L93	T94	G95	K96	Q97	V98	Q99	L100	N101	I102	L103	E104	V105	K106	N107	P108	I109	E110	Q111	A112	Q113	L114	V115	I116	Q117	G118	V119	A120		
E121	Q122	L123	S124	N125	R126	V127	A128	F129	R130	R131	A132	M133	R134	K135	A136	I137	Q138	S139	A140	M141	R142	Q143	P144	N145	G146	K147	G148	I149	R150	V151	Q152	C153	S154	G155	R156	L157	G158	G159	A160	E161	M162	S163	R164	S165	E166	F167	V168	R169	E170	G171	R172	V173	P174	L175	H176	T177	G178	R179	A180		
D181	I182	D183	Y184	L185	L186	Y187	E188	A189	K190	T191	T192	F193	G194	R195	I196	G197	V198	K199	V200	W201	I202	Y203	K204	G205	D206	I207	G208	GLY	GLY	LYS	ARG	LEU	ALA	ALA	ALA	ALA	PRO	ALA	GLY	ALA	ALA	ASP	ARG	PRO	ARG	ARG	GLU	ARG	PRO	ARG	ARG	SER	GLY	THR	ARG	PRO	ARG	ARG	SER	GLY	ALA


SER
GLY
THR
THR
ALA
THR
GLY
THR
ASP
ALA
GLY
ARG
ALA
ALA
GLY
GLY
GLU
GLU
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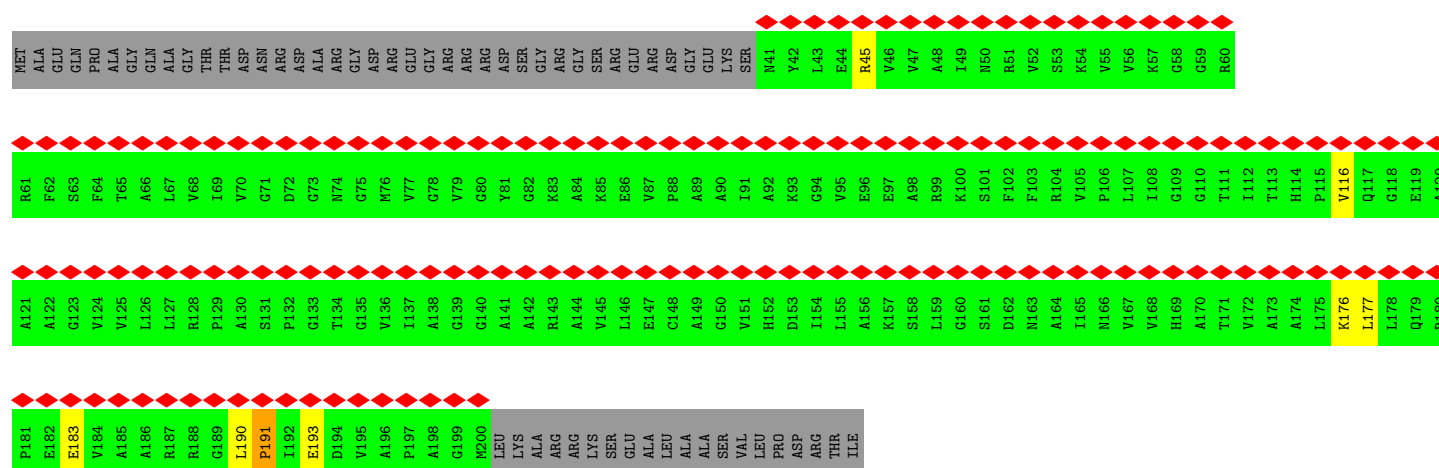
• Molecule 34: 30S ribosomal protein S4

Chain d: 

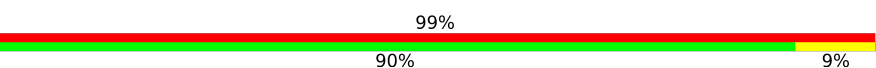


• Molecule 35: 30S ribosomal protein S5

Chain e: 

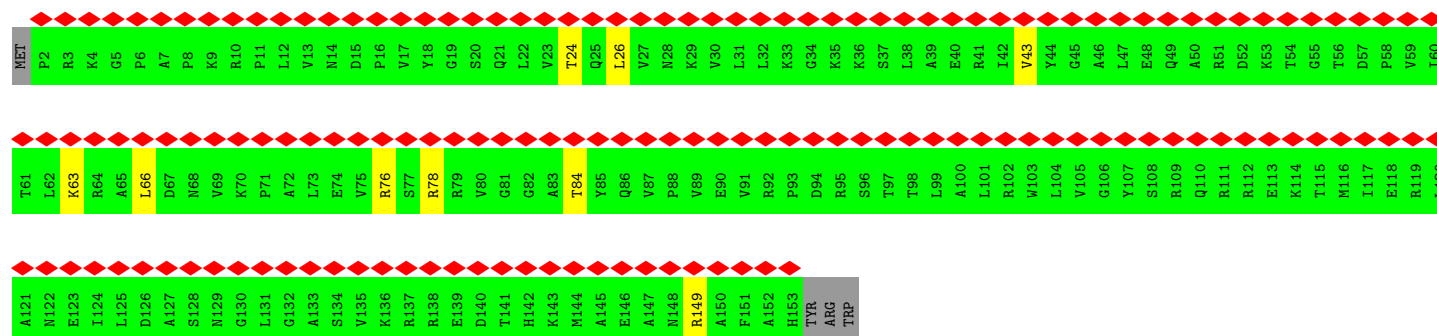
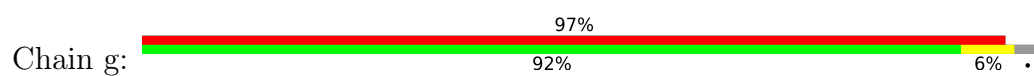


• Molecule 36: 30S ribosomal protein S6

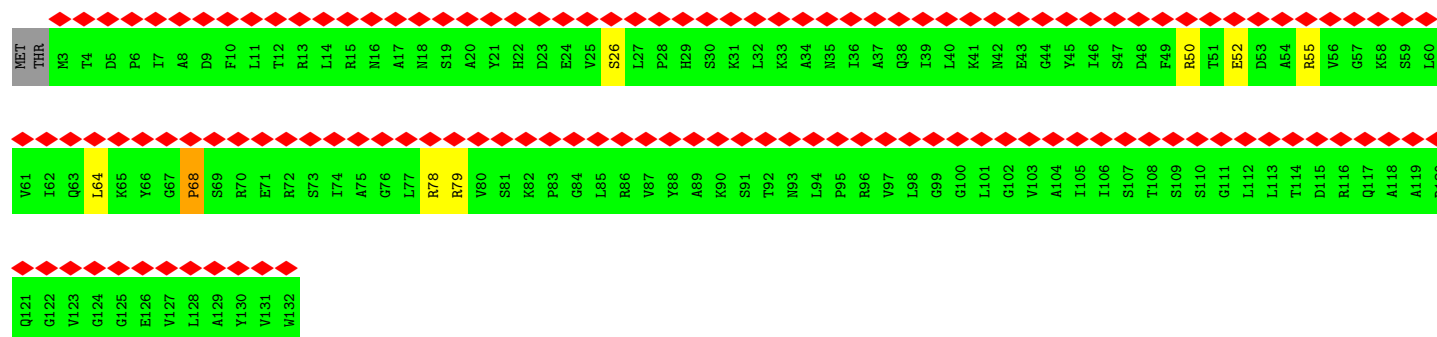
Chain f: 



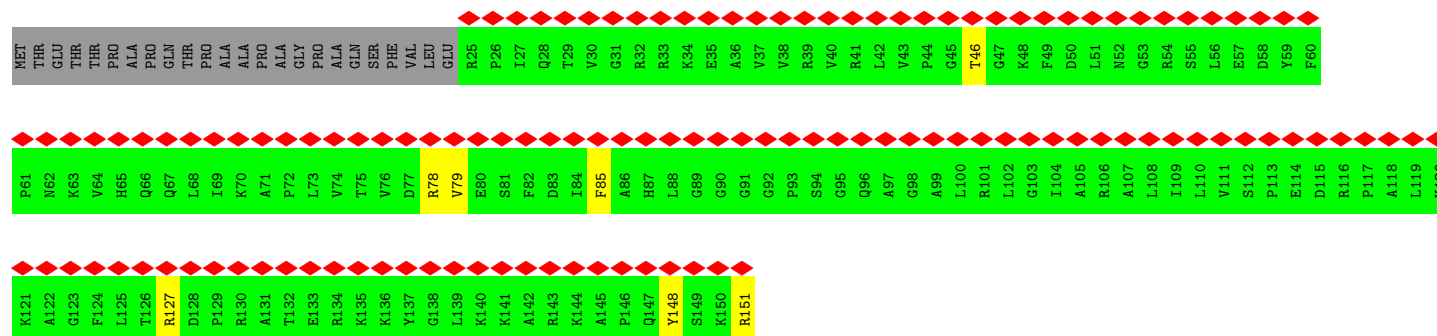
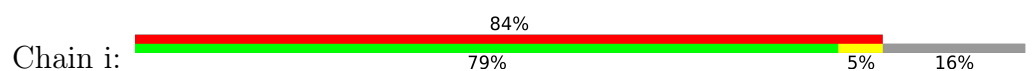
• Molecule 37: 30S ribosomal protein S7



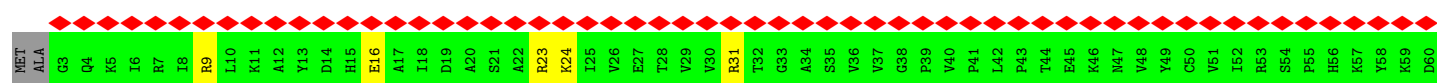
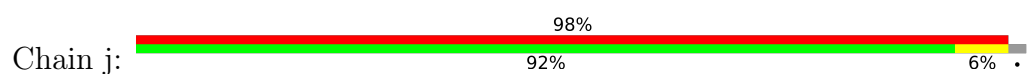
• Molecule 38: 30S ribosomal protein S8

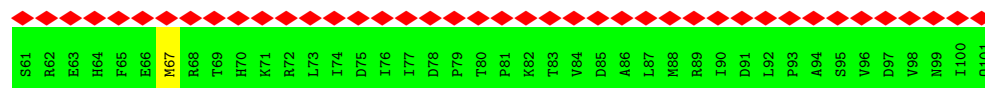


• Molecule 39: 30S ribosomal protein S9

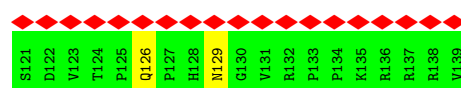
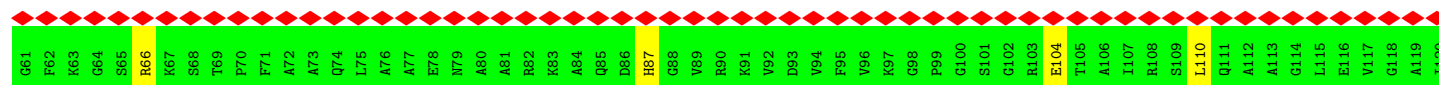
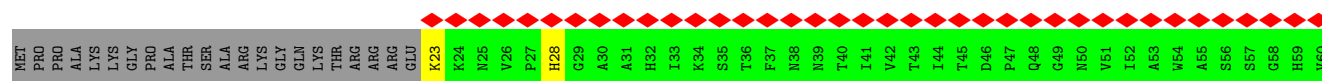
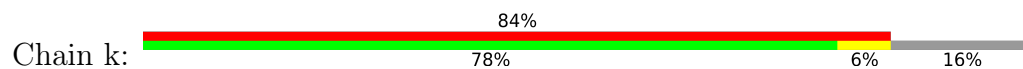


• Molecule 40: 30S ribosomal protein S10

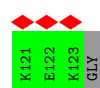
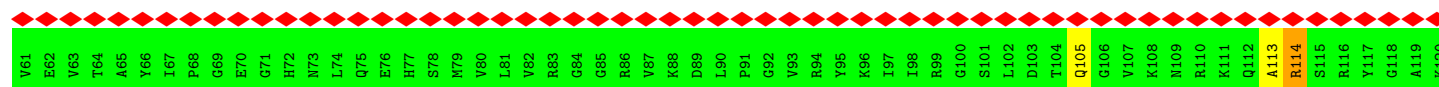
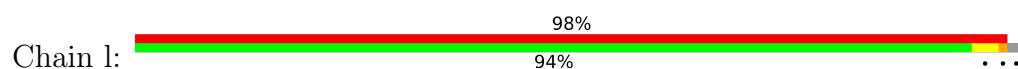




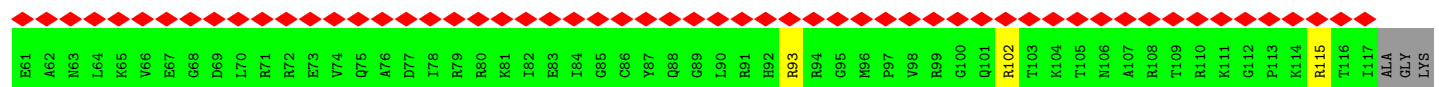
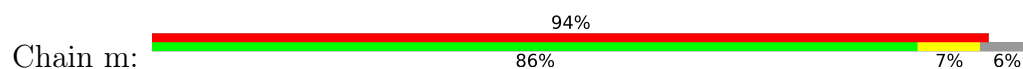
• Molecule 41: 30S ribosomal protein S11



• Molecule 42: 30S ribosomal protein S12

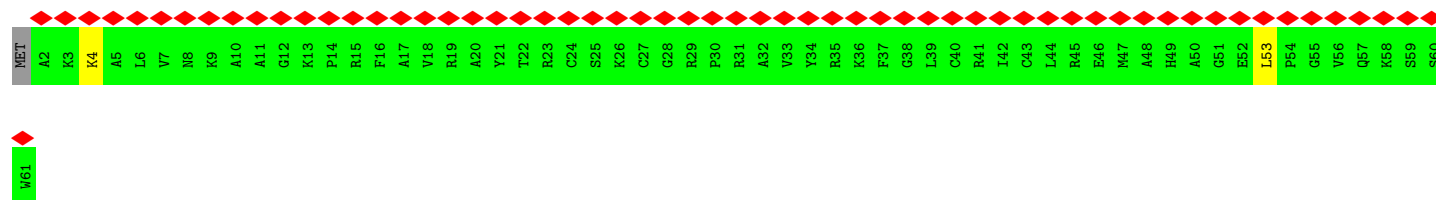


• Molecule 43: 30S ribosomal protein S13

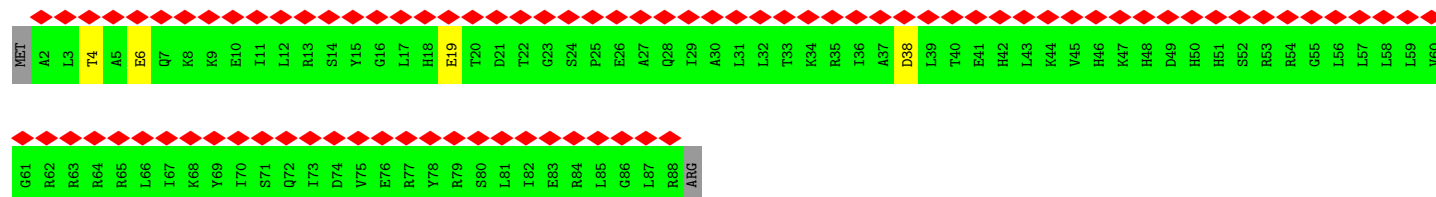


• Molecule 44: 30S ribosomal protein S14 type Z

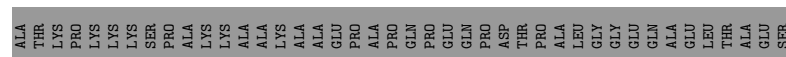
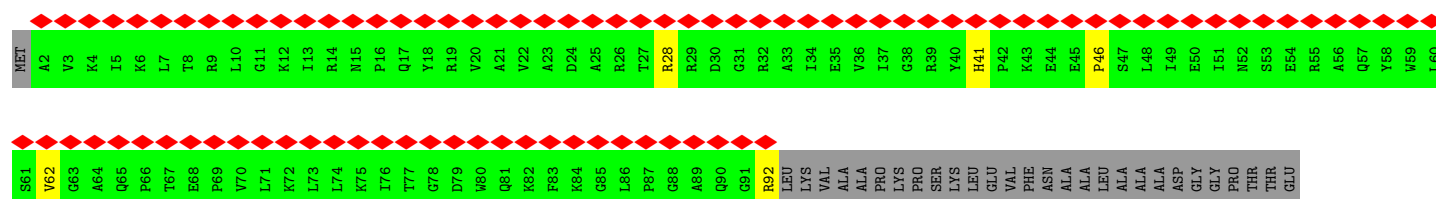




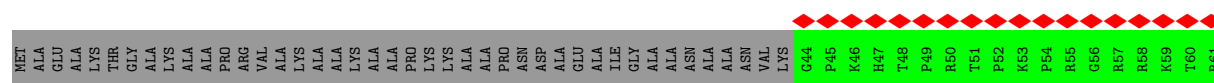
- Molecule 45: 30S ribosomal protein S15



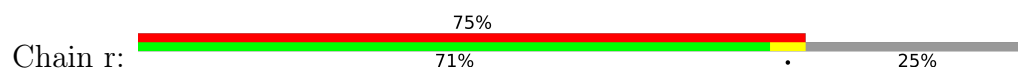
- Molecule 46: 30S ribosomal protein S16

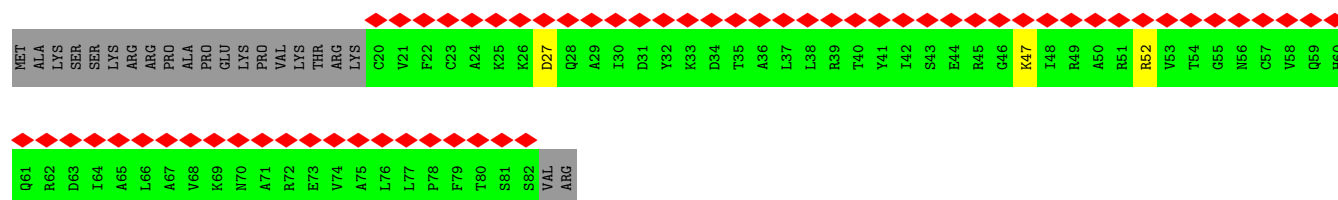


- Molecule 47: 30S ribosomal protein S17

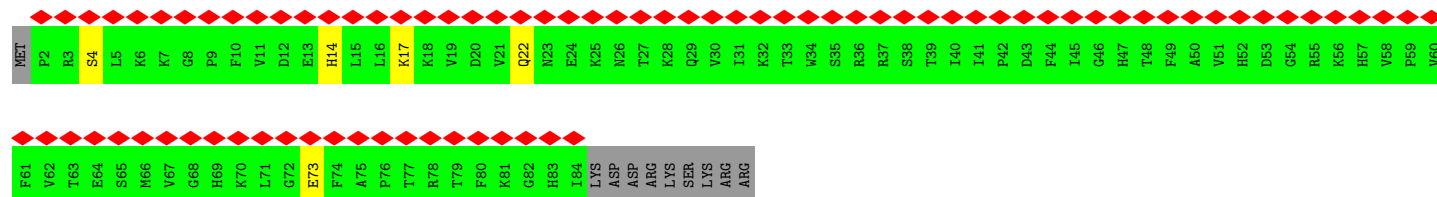
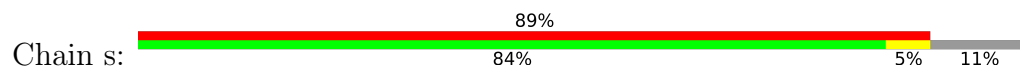


- Molecule 48: 30S ribosomal protein S18

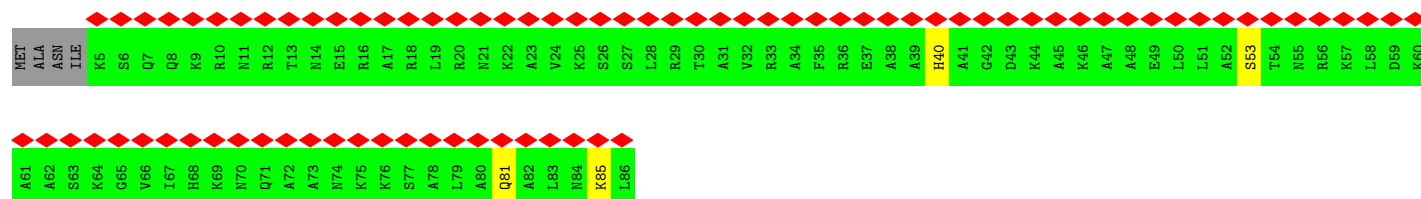
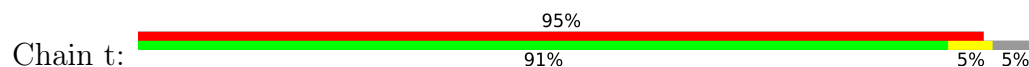




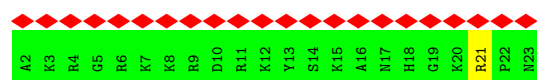
• Molecule 49: 30S ribosomal protein S19



• Molecule 50: 30S ribosomal protein S20



• Molecule 51: peptide



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	719250	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	42	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.618	Depositor
Minimum map value	-0.335	Depositor
Average map value	0.018	Depositor
Map value standard deviation	0.082	Depositor
Recommended contour level	0.4	Depositor
Map size (\AA)	348.6, 348.6, 348.6	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.83000004, 0.83000004, 0.83000004	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 4OC, G7M, ZN, 2MG, OMC, WDP, MG, 5MC, MA6, UR3, OMG, 6MZ, 5MU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	0	0.27	0/435	0.58	0/581
2	1	0.30	0/407	0.57	0/543
3	2	0.39	0/361	0.75	0/473
4	3	0.28	0/499	0.61	0/664
5	4	0.27	0/303	0.60	0/402
6	6	0.53	1/455 (0.2%)	0.81	3/611 (0.5%)
7	A	0.68	4/74851 (0.0%)	0.81	28/116786 (0.0%)
8	B	0.36	0/2749	0.76	0/4284
9	C	0.37	0/2129	0.59	0/2861
10	D	0.38	0/1613	0.59	0/2174
11	E	0.36	0/1575	0.59	0/2129
12	F	0.27	0/1429	0.59	0/1921
13	G	0.28	0/1351	0.57	0/1824
14	H	0.25	0/353	0.55	0/474
15	J	0.40	0/1170	0.55	0/1584
16	K	0.37	0/944	0.60	0/1268
17	L	0.33	0/1081	0.62	0/1443
18	M	0.27	0/1098	0.54	0/1481
19	N	0.38	0/925	0.54	0/1242
20	O	0.27	0/895	0.64	0/1202
21	P	0.38	0/922	0.59	0/1236
22	Q	0.41	0/992	0.63	1/1329 (0.1%)
23	R	0.39	0/766	0.59	0/1030
24	S	0.37	0/874	0.60	0/1186
25	T	0.35	0/770	0.57	0/1038
26	U	0.33	0/705	0.67	2/941 (0.2%)
27	V	0.26	0/747	0.60	0/1010
28	W	0.34	0/531	0.59	0/707
29	X	0.37	0/484	0.62	0/648
30	Y	0.32	0/544	0.59	0/727
31	Z	0.34	0/480	0.66	0/645
32	a	0.22	0/36305	0.76	6/56645 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	c	0.24	0/1678	0.55	0/2254
34	d	0.24	0/1683	0.54	0/2269
35	e	0.50	2/1165 (0.2%)	0.79	4/1578 (0.3%)
36	f	0.25	0/767	0.55	0/1036
37	g	0.24	0/1210	0.58	2/1631 (0.1%)
38	h	0.28	0/1014	0.63	1/1369 (0.1%)
39	i	0.25	0/1011	0.59	0/1356
40	j	0.22	0/803	0.52	0/1086
41	k	0.26	0/891	0.55	0/1204
42	l	0.24	0/970	0.58	0/1295
43	m	0.24	0/953	0.64	0/1274
44	n	0.25	0/477	0.55	0/634
45	o	0.23	0/727	0.55	0/973
46	p	0.25	0/742	0.55	0/1000
47	q	0.25	0/766	0.62	0/1024
48	r	0.26	0/502	0.52	0/674
49	s	0.25	0/690	0.54	0/928
50	t	0.26	0/633	0.60	0/838
51	v	0.24	0/188	0.64	0/243
All	All	0.51	7/155613 (0.0%)	0.75	47/233755 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
17	L	0	2
23	R	0	1
26	U	0	2
42	l	0	1
All	All	0	6

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	2296	A	C6-N6	15.53	1.46	1.33
35	e	191	PRO	CG-CD	-13.69	1.05	1.50
6	6	43	PRO	CG-CD	-8.61	1.22	1.50
7	A	2296	A	N7-C5	-7.68	1.34	1.39
7	A	2296	A	N9-C8	-6.59	1.32	1.37
35	e	191	PRO	N-CD	5.38	1.55	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	616	A	N9-C4	-5.31	1.34	1.37

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	2296	A	C2-N3-C4	18.90	120.05	110.60
35	e	191	PRO	N-CD-CG	-15.42	80.07	103.20
7	A	2296	A	N1-C2-N3	-13.61	122.50	129.30
7	A	2296	A	N3-C4-C5	-10.82	119.22	126.80
6	6	43	PRO	N-CD-CG	-10.72	87.12	103.20
35	e	191	PRO	CA-N-CD	-10.28	97.11	111.50
38	h	68	PRO	CA-N-CD	-9.24	98.56	111.50
35	e	191	PRO	CA-CB-CG	-8.46	87.93	104.00
7	A	2296	A	N3-C4-N9	8.31	134.04	127.40
7	A	2296	A	C5-N7-C8	8.23	108.02	103.90
7	A	2296	A	N7-C8-N9	-8.16	109.72	113.80
32	a	92	C	N3-C2-O2	-7.66	116.53	121.90
6	6	43	PRO	CA-N-CD	-7.45	101.07	111.50
7	A	600	G	O4'-C1'-N9	7.39	114.11	108.20
7	A	2296	A	C4-C5-N7	-6.96	107.22	110.70
7	A	2309	C	C2-N1-C1'	6.26	125.69	118.80
7	A	2296	A	C8-N9-C4	6.26	108.31	105.80
7	A	946	C	N3-C2-O2	-6.25	117.52	121.90
32	a	430	A	N1-C6-N6	-6.21	114.87	118.60
7	A	1624	C	N1-C2-O2	6.16	122.59	118.90
7	A	3060	C	N3-C2-O2	-6.08	117.64	121.90
7	A	3060	C	C2-N1-C1'	6.04	125.44	118.80
22	Q	73	ASP	CB-CG-OD2	6.01	123.71	118.30
7	A	1624	C	C2-N1-C1'	5.95	125.34	118.80
7	A	946	C	C2-N1-C1'	5.88	125.27	118.80
32	a	92	C	N1-C2-O2	5.81	122.39	118.90
7	A	976	U	C2-N1-C1'	5.76	124.62	117.70
32	a	455	C	N1-C2-O2	5.66	122.30	118.90
26	U	89	GLU	C-N-CA	5.62	135.75	121.70
7	A	2217	C	C2-N1-C1'	5.61	124.97	118.80
35	e	177	LEU	CA-CB-CG	5.61	128.19	115.30
7	A	2558	C	N1-C2-O2	5.56	122.23	118.90
7	A	882	C	N3-C2-O2	-5.51	118.04	121.90
7	A	1072	G	C4-N9-C1'	5.33	133.43	126.50
7	A	616	A	C2-N3-C4	-5.28	107.96	110.60
7	A	1272	A	O4'-C1'-N9	5.25	112.40	108.20
37	g	66	LEU	CA-CB-CG	5.24	127.36	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	3060	C	N1-C2-O2	5.24	122.04	118.90
37	g	26	LEU	CA-CB-CG	5.18	127.22	115.30
7	A	739	C	C2-N1-C1'	5.15	124.47	118.80
26	U	90	GLU	N-CA-C	5.14	124.89	111.00
32	a	517	C	O4'-C1'-N1	5.09	112.27	108.20
7	A	2309	C	N3-C2-O2	-5.08	118.34	121.90
32	a	430	A	C5-C6-N6	5.05	127.74	123.70
6	6	43	PRO	CA-CB-CG	-5.04	94.42	104.00
7	A	882	C	C2-N1-C1'	5.04	124.34	118.80
7	A	2217	C	N3-C2-O2	-5.03	118.38	121.90

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
17	L	20	ARG	Peptide
17	L	28	LYS	Peptide
23	R	50	THR	Peptide
26	U	90	GLU	Peptide
26	U	91	THR	Peptide
42	l	113	ALA	Peptide

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	52/57 (91%)	52 (100%)	0	0	100	100
2	1	46/55 (84%)	45 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	2	40/47 (85%)	39 (98%)	1 (2%)	0	100	100
4	3	60/64 (94%)	60 (100%)	0	0	100	100
5	4	35/37 (95%)	35 (100%)	0	0	100	100
6	6	53/80 (66%)	46 (87%)	7 (13%)	0	100	100
9	C	270/279 (97%)	259 (96%)	11 (4%)	0	100	100
10	D	211/213 (99%)	198 (94%)	13 (6%)	0	100	100
11	E	205/207 (99%)	201 (98%)	4 (2%)	0	100	100
12	F	176/178 (99%)	162 (92%)	14 (8%)	0	100	100
13	G	172/177 (97%)	167 (97%)	5 (3%)	0	100	100
14	H	45/152 (30%)	38 (84%)	7 (16%)	0	100	100
15	J	144/195 (74%)	141 (98%)	3 (2%)	0	100	100
16	K	119/122 (98%)	117 (98%)	2 (2%)	0	100	100
17	L	141/146 (97%)	128 (91%)	12 (8%)	1 (1%)	22	43
18	M	132/138 (96%)	122 (92%)	10 (8%)	0	100	100
19	N	114/180 (63%)	110 (96%)	4 (4%)	0	100	100
20	O	114/122 (93%)	107 (94%)	7 (6%)	0	100	100
21	P	110/113 (97%)	105 (96%)	5 (4%)	0	100	100
22	Q	120/129 (93%)	117 (98%)	3 (2%)	0	100	100
23	R	98/104 (94%)	88 (90%)	9 (9%)	1 (1%)	15	32
24	S	111/197 (56%)	108 (97%)	3 (3%)	0	100	100
25	T	96/100 (96%)	88 (92%)	8 (8%)	0	100	100
26	U	86/105 (82%)	73 (85%)	12 (14%)	1 (1%)	13	27
27	V	93/215 (43%)	90 (97%)	3 (3%)	0	100	100
28	W	69/86 (80%)	64 (93%)	5 (7%)	0	100	100
29	X	61/64 (95%)	58 (95%)	3 (5%)	0	100	100
30	Y	63/77 (82%)	60 (95%)	3 (5%)	0	100	100
31	Z	57/65 (88%)	56 (98%)	1 (2%)	0	100	100
33	c	205/274 (75%)	191 (93%)	14 (7%)	0	100	100
34	d	198/201 (98%)	188 (95%)	10 (5%)	0	100	100
35	e	158/220 (72%)	145 (92%)	12 (8%)	1 (1%)	25	47
36	f	93/96 (97%)	90 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	g	150/156 (96%)	146 (97%)	4 (3%)	0	100	100
38	h	128/132 (97%)	123 (96%)	4 (3%)	1 (1%)	19	39
39	i	125/151 (83%)	107 (86%)	18 (14%)	0	100	100
40	j	97/101 (96%)	86 (89%)	11 (11%)	0	100	100
41	k	115/139 (83%)	108 (94%)	7 (6%)	0	100	100
42	l	120/124 (97%)	95 (79%)	24 (20%)	1 (1%)	19	39
43	m	114/124 (92%)	105 (92%)	9 (8%)	0	100	100
44	n	58/61 (95%)	55 (95%)	3 (5%)	0	100	100
45	o	85/89 (96%)	79 (93%)	5 (6%)	1 (1%)	13	27
46	p	89/162 (55%)	81 (91%)	7 (8%)	1 (1%)	14	30
47	q	91/135 (67%)	82 (90%)	9 (10%)	0	100	100
48	r	61/84 (73%)	58 (95%)	3 (5%)	0	100	100
49	s	81/93 (87%)	70 (86%)	11 (14%)	0	100	100
50	t	80/86 (93%)	80 (100%)	0	0	100	100
51	v	20/22 (91%)	20 (100%)	0	0	100	100
All	All	5161/6154 (84%)	4843 (94%)	310 (6%)	8 (0%)	50	71

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
23	R	51	THR
42	l	114	ARG
17	L	5	LEU
45	o	19	GLU
26	U	91	THR
46	p	46	PRO
35	e	191	PRO
38	h	68	PRO

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	0	44/47 (94%)	41 (93%)	3 (7%)	16	32
2	1	45/51 (88%)	42 (93%)	3 (7%)	16	33
3	2	36/40 (90%)	34 (94%)	2 (6%)	21	42
4	3	53/54 (98%)	51 (96%)	2 (4%)	33	59
5	4	35/35 (100%)	34 (97%)	1 (3%)	42	68
6	6	49/66 (74%)	44 (90%)	5 (10%)	7	14
9	C	212/218 (97%)	205 (97%)	7 (3%)	38	64
10	D	163/163 (100%)	153 (94%)	10 (6%)	18	38
11	E	159/159 (100%)	153 (96%)	6 (4%)	33	59
12	F	147/147 (100%)	134 (91%)	13 (9%)	10	19
13	G	143/145 (99%)	137 (96%)	6 (4%)	30	55
14	H	36/121 (30%)	28 (78%)	8 (22%)	1	1
15	J	120/161 (74%)	115 (96%)	5 (4%)	30	55
16	K	100/101 (99%)	96 (96%)	4 (4%)	31	57
17	L	107/110 (97%)	100 (94%)	7 (6%)	17	34
18	M	110/114 (96%)	107 (97%)	3 (3%)	44	71
19	N	94/139 (68%)	93 (99%)	1 (1%)	73	88
20	O	88/93 (95%)	84 (96%)	4 (4%)	27	52
21	P	98/99 (99%)	91 (93%)	7 (7%)	14	29
22	Q	95/99 (96%)	92 (97%)	3 (3%)	39	65
23	R	81/83 (98%)	76 (94%)	5 (6%)	18	37
24	S	87/140 (62%)	84 (97%)	3 (3%)	37	63
25	T	82/83 (99%)	76 (93%)	6 (7%)	14	28
26	U	77/88 (88%)	69 (90%)	8 (10%)	7	13
27	V	75/164 (46%)	68 (91%)	7 (9%)	9	17
28	W	51/62 (82%)	49 (96%)	2 (4%)	32	58
29	X	52/52 (100%)	51 (98%)	1 (2%)	57	79
30	Y	58/66 (88%)	56 (97%)	2 (3%)	37	63
31	Z	51/55 (93%)	45 (88%)	6 (12%)	5	9
33	c	170/210 (81%)	155 (91%)	15 (9%)	10	19
34	d	176/177 (99%)	167 (95%)	9 (5%)	24	46
35	e	114/159 (72%)	108 (95%)	6 (5%)	22	45

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	f	84/85 (99%)	75 (89%)	9 (11%)	6	12
37	g	127/131 (97%)	120 (94%)	7 (6%)	21	43
38	h	106/108 (98%)	99 (93%)	7 (7%)	16	33
39	i	102/120 (85%)	95 (93%)	7 (7%)	15	31
40	j	89/90 (99%)	83 (93%)	6 (7%)	16	33
41	k	90/107 (84%)	82 (91%)	8 (9%)	9	19
42	l	104/105 (99%)	100 (96%)	4 (4%)	33	59
43	m	99/104 (95%)	90 (91%)	9 (9%)	9	18
44	n	46/47 (98%)	44 (96%)	2 (4%)	29	54
45	o	77/79 (98%)	74 (96%)	3 (4%)	32	58
46	p	75/125 (60%)	71 (95%)	4 (5%)	22	45
47	q	83/105 (79%)	76 (92%)	7 (8%)	11	21
48	r	53/72 (74%)	50 (94%)	3 (6%)	20	41
49	s	75/85 (88%)	70 (93%)	5 (7%)	16	33
50	t	62/65 (95%)	58 (94%)	4 (6%)	17	34
51	v	18/18 (100%)	17 (94%)	1 (6%)	21	42
All	All	4298/4947 (87%)	4042 (94%)	256 (6%)	23	39

All (256) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	6	ARG
1	0	25	THR
1	0	38	LYS
2	1	25	THR
2	1	30	ARG
2	1	37	GLU
3	2	32	SER
3	2	44	THR
4	3	30	ARG
4	3	31	HIS
5	4	22	ARG
6	6	1	MET
6	6	2	LYS
6	6	9	TYR
6	6	29	PRO

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Mol	Chain	Res	Type
6	6	63	LYS
9	C	25	THR
9	C	27	SER
9	C	40	ARG
9	C	96	HIS
9	C	99	ASP
9	C	124	ASP
9	C	273	ARG
10	D	19	GLU
10	D	43	GLU
10	D	45	ASP
10	D	51	GLN
10	D	56	GLU
10	D	113	ASP
10	D	115	THR
10	D	135	GLN
10	D	185	VAL
10	D	212	ILE
11	E	10	LYS
11	E	19	LYS
11	E	69	ARG
11	E	73	ARG
11	E	74	GLN
11	E	81	ARG
12	F	10	ARG
12	F	18	GLU
12	F	21	ASP
12	F	33	MET
12	F	52	ARG
12	F	76	ARG
12	F	90	MET
12	F	103	MET
12	F	134	ASN
12	F	141	GLU
12	F	152	LYS
12	F	159	MET
12	F	166	SER
13	G	46	ASN
13	G	55	ARG
13	G	60	ARG
13	G	61	ARG
13	G	102	SER

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Mol	Chain	Res	Type
13	G	133	THR
14	H	1	MET
14	H	2	LYS
14	H	3	LEU
14	H	5	LEU
14	H	10	ASP
14	H	20	GLU
14	H	33	ARG
14	H	45	LYS
15	J	3	THR
15	J	11	THR
15	J	22	ASP
15	J	133	SER
15	J	143	LYS
16	K	23	ARG
16	K	69	ARG
16	K	97	ARG
16	K	113	LYS
17	L	21	VAL
17	L	72	THR
17	L	95	ASP
17	L	116	LYS
17	L	122	ASP
17	L	126	HIS
17	L	144	THR
18	M	18	ARG
18	M	94	VAL
18	M	110	ASN
19	N	112	VAL
20	O	25	SER
20	O	33	LEU
20	O	35	VAL
20	O	103	THR
21	P	55	ARG
21	P	63	GLU
21	P	90	ASP
21	P	103	ARG
21	P	105	LYS
21	P	108	LYS
21	P	112	LYS
22	Q	53	ARG
22	Q	101	SER

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Mol	Chain	Res	Type
22	Q	119	GLU
23	R	23	VAL
23	R	32	GLN
23	R	37	SER
23	R	58	LYS
23	R	92	ARG
24	S	69	GLN
24	S	119	SER
24	S	120	ARG
25	T	3	THR
25	T	4	LEU
25	T	26	ASP
25	T	68	ARG
25	T	70	ARG
25	T	85	THR
26	U	22	LYS
26	U	40	ARG
26	U	45	THR
26	U	63	GLU
26	U	69	SER
26	U	72	MET
26	U	98	SER
26	U	103	LYS
27	V	10	ARG
27	V	51	ASP
27	V	61	THR
27	V	68	ASP
27	V	69	ILE
27	V	98	VAL
27	V	99	ARG
28	W	57	ASP
28	W	68	GLU
29	X	1	MET
30	Y	46	ARG
30	Y	63	GLU
31	Z	22	SER
31	Z	40	ASN
31	Z	44	ARG
31	Z	55	GLU
31	Z	56	VAL
31	Z	57	GLU
33	c	21	ARG

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Mol	Chain	Res	Type
33	c	40	ARG
33	c	48	ARG
33	c	60	ARG
33	c	61	ASP
33	c	71	ARG
33	c	85	ARG
33	c	92	LYS
33	c	104	GLU
33	c	117	GLN
33	c	130	ARG
33	c	141	MET
33	c	162	MET
33	c	179	ARG
33	c	195	ARG
34	d	29	ARG
34	d	40	ARG
34	d	52	GLU
34	d	80	LYS
34	d	108	MET
34	d	135	TYR
34	d	143	LYS
34	d	155	GLU
34	d	178	HIS
35	e	45	ARG
35	e	116	VAL
35	e	176	LYS
35	e	183	GLU
35	e	190	LEU
35	e	193	GLU
36	f	1	MET
36	f	7	MET
36	f	23	LEU
36	f	36	LYS
36	f	39	LYS
36	f	47	ARG
36	f	84	SER
36	f	93	THR
36	f	95	LYS
37	g	24	THR
37	g	43	VAL
37	g	63	LYS
37	g	76	ARG

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Mol	Chain	Res	Type
37	g	78	ARG
37	g	84	THR
37	g	149	ARG
38	h	26	SER
38	h	50	ARG
38	h	52	GLU
38	h	55	ARG
38	h	64	LEU
38	h	78	ARG
38	h	79	ARG
39	i	46	THR
39	i	78	ARG
39	i	79	VAL
39	i	85	PHE
39	i	127	ARG
39	i	148	TYR
39	i	151	ARG
40	j	9	ARG
40	j	16	GLU
40	j	23	ARG
40	j	24	LYS
40	j	31	ARG
40	j	67	MET
41	k	23	LYS
41	k	28	HIS
41	k	66	ARG
41	k	87	HIS
41	k	104	GLU
41	k	110	LEU
41	k	126	GLN
41	k	129	ASN
42	l	30	ARG
42	l	43	LYS
42	l	105	GLN
42	l	114	ARG
43	m	3	ARG
43	m	11	ARG
43	m	15	MET
43	m	51	GLU
43	m	57	ARG
43	m	59	TYR
43	m	93	ARG

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Mol	Chain	Res	Type
43	m	102	ARG
43	m	115	ARG
44	n	4	LYS
44	n	53	LEU
45	o	4	THR
45	o	6	GLU
45	o	38	ASP
46	p	28	ARG
46	p	41	HIS
46	p	62	VAL
46	p	92	ARG
47	q	70	MET
47	q	82	MET
47	q	92	ARG
47	q	93	THR
47	q	105	VAL
47	q	115	MET
47	q	116	GLU
48	r	27	ASP
48	r	47	LYS
48	r	52	ARG
49	s	4	SER
49	s	14	HIS
49	s	17	LYS
49	s	22	GLN
49	s	73	GLU
50	t	40	HIS
50	t	53	SER
50	t	81	GLN
50	t	85	LYS
51	v	21	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	37	HIS
11	E	127	ASN
12	F	62	ASN
18	M	110	ASN
27	V	38	HIS
27	V	74	GLN
27	V	91	GLN

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Mol	Chain	Res	Type
34	d	24	GLN
34	d	167	GLN
43	m	55	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
32	a	1515/1537 (98%)	224 (14%)	0
7	A	3115/3138 (99%)	423 (13%)	2 (0%)
8	B	114/115 (99%)	16 (14%)	0
All	All	4744/4790 (99%)	663 (13%)	2 (0%)

All (663) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
7	A	13	A
7	A	35	G
7	A	63	A
7	A	71	A
7	A	74	U
7	A	75	G
7	A	94	C
7	A	118	A
7	A	119	A
7	A	120	U
7	A	125	A
7	A	142	U
7	A	143	G
7	A	167	A
7	A	176	G
7	A	183	A
7	A	198	A
7	A	201	A
7	A	217	G
7	A	218	A
7	A	224	A
7	A	225	A
7	A	231	U
7	A	232	G
7	A	250	G
7	A	269	G

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Mol	Chain	Res	Type
7	A	271	U
7	A	279	A
7	A	283	A
7	A	286	G
7	A	287	G
7	A	288	U
7	A	289	A
7	A	290	A
7	A	293	G
7	A	294	G
7	A	297	A
7	A	301	G
7	A	303	U
7	A	320	G
7	A	327	U
7	A	328	A
7	A	329	U
7	A	330	G
7	A	331	U
7	A	332	C
7	A	339	C
7	A	345	G
7	A	358	U
7	A	370	G
7	A	372	G
7	A	377	G
7	A	394	U
7	A	399	U
7	A	413	A
7	A	414	G
7	A	429	A
7	A	446	A
7	A	447	G
7	A	448	U
7	A	453	A
7	A	473	C
7	A	475	G
7	A	500	G
7	A	501	A
7	A	526	U
7	A	544	U
7	A	570	G

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Mol	Chain	Res	Type
7	A	592	G
7	A	593	A
7	A	595	U
7	A	596	A
7	A	597	C
7	A	606	G
7	A	616	A
7	A	618	U
7	A	619	C
7	A	620	C
7	A	621	G
7	A	637	C
7	A	639	U
7	A	641	U
7	A	642	C
7	A	643	C
7	A	645	G
7	A	653	U
7	A	665	G
7	A	673	A
7	A	675	G
7	A	676	A
7	A	677	A
7	A	689	G
7	A	694	G
7	A	706	A
7	A	719	U
7	A	741	A
7	A	750	A
7	A	756	A
7	A	758	C
7	A	759	C
7	A	760	A
7	A	768	A
7	A	772	G
7	A	774	G
7	A	776	G
7	A	779	U
7	A	780	G
7	A	781	A
7	A	782	A
7	A	783	U

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Mol	Chain	Res	Type
7	A	815	U
7	A	843	U
7	A	844	A
7	A	846	G
7	A	847	A
7	A	852	G
7	A	859	C
7	A	876	U
7	A	893	A
7	A	894	G
7	A	904	G
7	A	905	G
7	A	911	A
7	A	913	G
7	A	914	G
7	A	918	A
7	A	934	G
7	A	941	C
7	A	956	U
7	A	958	A
7	A	988	G
7	A	1007	G
7	A	1025	A
7	A	1026	C
7	A	1036	C
7	A	1039	A
7	A	1043	C
7	A	1059	A
7	A	1061	A
7	A	1074	G
7	A	1086	U
7	A	1087	A
7	A	1089	G
7	A	1096	A
7	A	1103	A
7	A	1112	A
7	A	1125	G
7	A	1142	G
7	A	1155	G
7	A	1162	U
7	A	1168	G
7	A	1175	A

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Mol	Chain	Res	Type
7	A	1176	G
7	A	1177	A
7	A	1184	G
7	A	1189	U
7	A	1190	U
7	A	1191	G
7	A	1193	C
7	A	1196	A
7	A	1199	A
7	A	1200	G
7	A	1202	A
7	A	1207	C
7	A	1208	C
7	A	1210	U
7	A	1212	G
7	A	1215	A
7	A	1216	G
7	A	1217	A
7	A	1219	U
7	A	1230	U
7	A	1234	U
7	A	1239	A
7	A	1240	A
7	A	1241	G
7	A	1261	U
7	A	1262	A
7	A	1264	C
7	A	1265	G
7	A	1271	C
7	A	1273	A
7	A	1304	U
7	A	1305	U
7	A	1306	G
7	A	1308	G
7	A	1309	G
7	A	1342	C
7	A	1381	G
7	A	1384	A
7	A	1387	G
7	A	1402	G
7	A	1403	A
7	A	1406	A

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Mol	Chain	Res	Type
7	A	1431	A
7	A	1432	A
7	A	1451	C
7	A	1452	C
7	A	1453	A
7	A	1460	U
7	A	1481	C
7	A	1483	U
7	A	1491	G
7	A	1496	A
7	A	1499	G
7	A	1510	U
7	A	1515	A
7	A	1542	G
7	A	1551	C
7	A	1552	G
7	A	1554	G
7	A	1560	U
7	A	1561	C
7	A	1562	A
7	A	1567	U
7	A	1568	A
7	A	1577	C
7	A	1580	A
7	A	1581	A
7	A	1582	A
7	A	1609	U
7	A	1610	G
7	A	1614	A
7	A	1615	G
7	A	1622	G
7	A	1624	C
7	A	1625	U
7	A	1636	U
7	A	1637	U
7	A	1646	G
7	A	1647	U
7	A	1657	A
7	A	1658	A
7	A	1666	C
7	A	1690	A
7	A	1693	G

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Mol	Chain	Res	Type
7	A	1696	A
7	A	1697	A
7	A	1698	C
7	A	1699	A
7	A	1720	G
7	A	1722	G
7	A	1727	A
7	A	1746	U
7	A	1754	A
7	A	1763	G
7	A	1773	U
7	A	1774	U
7	A	1797	G
7	A	1803	A
7	A	1806	A
7	A	1821	G
7	A	1832	G
7	A	1842	C
7	A	1843	A
7	A	1845	A
7	A	1881	U
7	A	1883	C
7	A	1884	G
7	A	1888	U
7	A	1889	A
7	A	1909	G
7	A	1950	A
7	A	1959	A
7	A	1960	C
7	A	1961	C
7	A	1963	U
7	A	1964	U
7	A	1990	G
7	A	1992	A
7	A	1998	U
7	A	2007	A
7	A	2010	G
7	A	2034	C
7	A	2035	G
7	A	2050	U
7	A	2063	A
7	A	2105	G

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Mol	Chain	Res	Type
7	A	2106	C
7	A	2107	A
7	A	2108	A
7	A	2109	G
7	A	2124	U
7	A	2144	G
7	A	2151	A
7	A	2157	A
7	A	2167	G
7	A	2168	G
7	A	2175	A
7	A	2176	A
7	A	2193	U
7	A	2203	C
7	A	2205	C
7	A	2208	A
7	A	2209	U
7	A	2210	G
7	A	2229	U
7	A	2231	U
7	A	2258	A
7	A	2259	C
7	A	2261	A
7	A	2270	G
7	A	2281	C
7	A	2293	C
7	A	2294	G
7	A	2297	A
7	A	2298	A
7	A	2299	G
7	A	2300	A
7	A	2330	G
7	A	2340	A
7	A	2343	G
7	A	2346	U
7	A	2347	G
7	A	2348	U
7	A	2352	G
7	A	2353	G
7	A	2354	A
7	A	2355	U
7	A	2356	A

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Mol	Chain	Res	Type
7	A	2357	G
7	A	2360	G
7	A	2361	G
7	A	2362	G
7	A	2364	G
7	A	2365	A
7	A	2366	C
7	A	2367	U
7	A	2371	A
7	A	2375	C
7	A	2377	C
7	A	2378	G
7	A	2382	C
7	A	2384	A
7	A	2385	G
7	A	2387	U
7	A	2391	G
7	A	2393	G
7	A	2394	G
7	A	2395	A
7	A	2396	G
7	A	2398	C
7	A	2400	U
7	A	2401	U
7	A	2402	G
7	A	2403	U
7	A	2404	U
7	A	2405	G
7	A	2406	A
7	A	2407	A
7	A	2408	A
7	A	2412	C
7	A	2413	A
7	A	2416	C
7	A	2417	U
7	A	2419	A
7	A	2424	A
7	A	2435	A
7	A	2449	A
7	A	2463	A
7	A	2476	G
7	A	2477	G

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Mol	Chain	Res	Type
7	A	2489	OMG
7	A	2517	G
7	A	2521	C
7	A	2525	A
7	A	2526	A
7	A	2543	A
7	A	2546	G
7	A	2547	C
7	A	2550	U
7	A	2558	C
7	A	2560	A
7	A	2563	G
7	A	2573	A
7	A	2583	G
7	A	2585	C
7	A	2588	C
7	A	2615	A
7	A	2621	G
7	A	2623	A
7	A	2644	A
7	A	2661	U
7	A	2663	A
7	A	2667	G
7	A	2668	A
7	A	2679	C
7	A	2686	A
7	A	2707	A
7	A	2714	A
7	A	2728	G
7	A	2736	OMC
7	A	2743	G
7	A	2751	G
7	A	2756	A
7	A	2767	G
7	A	2773	G
7	A	2804	A
7	A	2805	G
7	A	2840	A
7	A	2847	U
7	A	2851	U
7	A	2868	A
7	A	2952	G

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Mol	Chain	Res	Type
7	A	2962	C
7	A	2964	C
7	A	2986	A
7	A	2995	A
7	A	2996	A
7	A	3003	A
7	A	3016	A
7	A	3018	C
7	A	3023	U
7	A	3037	G
7	A	3038	U
7	A	3040	G
7	A	3056	A
7	A	3070	A
7	A	3107	A
7	A	3118	A
7	A	3119	C
7	A	3120	C
7	A	3129	A
8	B	2	U
8	B	8	G
8	B	24	A
8	B	34	U
8	B	41	C
8	B	51	A
8	B	55	U
8	B	56	A
8	B	65	A
8	B	85	U
8	B	86	C
8	B	88	G
8	B	101	G
8	B	105	A
8	B	114	C
8	B	115	A
32	a	11	A
32	a	12	G
32	a	25	G
32	a	34	G
32	a	35	A
32	a	42	G
32	a	50	C

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Mol	Chain	Res	Type
32	a	51	U
32	a	54	A
32	a	74	A
32	a	78	U
32	a	81	C
32	a	82	U
32	a	84	C
32	a	86	G
32	a	89	A
32	a	90	U
32	a	91	A
32	a	116	C
32	a	125	G
32	a	127	U
32	a	167	A
32	a	169	U
32	a	178	G
32	a	185	G
32	a	189	U
32	a	194	G
32	a	204	G
32	a	206	A
32	a	208	A
32	a	213	U
32	a	214	U
32	a	216	A
32	a	217	G
32	a	219	G
32	a	244	C
32	a	246	G
32	a	247	C
32	a	250	G
32	a	265	G
32	a	266	C
32	a	279	C
32	a	280	G
32	a	288	G
32	a	327	U
32	a	328	A
32	a	346	G
32	a	350	G
32	a	351	C

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Mol	Chain	Res	Type
32	a	353	G
32	a	366	U
32	a	368	G
32	a	371	C
32	a	381	A
32	a	391	C
32	a	397	C
32	a	405	G
32	a	408	G
32	a	409	G
32	a	410	A
32	a	411	U
32	a	412	G
32	a	413	A
32	a	414	C
32	a	420	U
32	a	421	C
32	a	428	U
32	a	437	U
32	a	439	C
32	a	451	A
32	a	452	G
32	a	453	G
32	a	455	C
32	a	457	G
32	a	459	G
32	a	460	U
32	a	461	U
32	a	463	U
32	a	465	U
32	a	473	A
32	a	476	G
32	a	485	G
32	a	486	A
32	a	487	A
32	a	488	G
32	a	490	A
32	a	500	A
32	a	501	A
32	a	502	C
32	a	508	G
32	a	509	C

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Mol	Chain	Res	Type
32	a	512	G
32	a	517	C
32	a	518	G7M
32	a	523	A
32	a	538	A
32	a	550	A
32	a	551	A
32	a	553	U
32	a	563	A
32	a	564	A
32	a	565	A
32	a	566	G
32	a	567	A
32	a	568	G
32	a	606	C
32	a	610	U
32	a	623	U
32	a	624	G
32	a	633	A
32	a	640	G
32	a	644	A
32	a	656	G
32	a	677	U
32	a	678	A
32	a	686	A
32	a	694	G
32	a	709	A
32	a	712	G
32	a	740	A
32	a	746	G
32	a	768	A
32	a	784	U
32	a	785	A
32	a	806	A
32	a	808	C
32	a	827	G
32	a	830	U
32	a	833	U
32	a	835	C
32	a	836	C
32	a	837	U
32	a	838	U

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Mol	Chain	Res	Type
32	a	865	A
32	a	866	A
32	a	883	G
32	a	895	G
32	a	900	A
32	a	919	G
32	a	927	C
32	a	951	A
32	a	953	U
32	a	954	U
32	a	962	A
32	a	968	A
32	a	969	G
32	a	970	A
32	a	985	U
32	a	986	G
32	a	987	A
32	a	993	A
32	a	997	G
32	a	1008	A
32	a	1010	A
32	a	1012	A
32	a	1019	C
32	a	1020	C
32	a	1021	C
32	a	1022	U
32	a	1023	U
32	a	1024	G
32	a	1033	G
32	a	1035	G
32	a	1044	G
32	a	1056	U
32	a	1085	G
32	a	1086	U
32	a	1092	A
32	a	1099	G
32	a	1116	U
32	a	1126	G
32	a	1129	A
32	a	1131	G
32	a	1137	G
32	a	1138	A

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Mol	Chain	Res	Type
32	a	1150	C
32	a	1151	U
32	a	1160	C
32	a	1161	A
32	a	1174	G
32	a	1175	U
32	a	1176	G
32	a	1188	A
32	a	1189	A
32	a	1199	C
32	a	1204	U
32	a	1205	A
32	a	1206	U
32	a	1218	C
32	a	1219	A
32	a	1228	A
32	a	1230	A
32	a	1232	U
32	a	1233	G
32	a	1249	U
32	a	1250	G
32	a	1252	G
32	a	1254	U
32	a	1270	G
32	a	1272	A
32	a	1277	U
32	a	1279	A
32	a	1292	G
32	a	1297	G
32	a	1312	C
32	a	1314	C
32	a	1328	C
32	a	1349	A
32	a	1356	A
32	a	1357	C
32	a	1369	U
32	a	1371	C
32	a	1419	A
32	a	1435	G
32	a	1439	A
32	a	1444	U
32	a	1485	A

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Mol	Chain	Res	Type
32	a	1486	A
32	a	1492	A
32	a	1496	A
32	a	1510	G
32	a	1513	G
32	a	1522	G
32	a	1523	G

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
7	A	338	G
7	A	913	G

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

13 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
7	OMG	A	2791	7	18,26,27	2.68	6 (33%)	19,38,41	1.49	4 (21%)
32	5MC	a	960	32	18,22,23	1.89	6 (33%)	26,32,35	1.17	1 (3%)
32	UR3	a	1491	32	19,22,23	2.78	4 (21%)	26,32,35	1.21	2 (7%)
32	2MG	a	1509	32	18,26,27	2.96	4 (22%)	16,38,41	1.17	2 (12%)
32	2MG	a	959	32	18,26,27	2.96	4 (22%)	16,38,41	1.25	2 (12%)
7	OMC	A	2736	7,54	19,22,23	1.62	2 (10%)	26,31,34	1.05	1 (3%)
32	MA6	a	1511	32	19,26,27	0.79	0	18,38,41	1.51	2 (11%)
32	G7M	a	518	32	20,26,27	2.58	4 (20%)	17,39,42	0.82	1 (5%)
32	MA6	a	1512	32	19,26,27	0.77	0	18,38,41	1.51	2 (11%)
7	OMG	A	2489	7	18,26,27	2.67	5 (27%)	19,38,41	1.46	4 (21%)
7	6MZ	A	2268	7	18,25,26	1.70	1 (5%)	16,36,39	2.54	3 (18%)
32	4OC	a	1395	32	20,23,24	2.56	4 (20%)	26,32,35	0.90	1 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	5MU	A	2177	7	19,22,23	2.28	8 (42%)	28,32,35	2.40	6 (21%)

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
7	OMG	A	2791	7	-	0/5/27/28	0/3/3/3
32	5MC	a	960	32	-	0/7/25/26	0/2/2/2
32	UR3	a	1491	32	-	1/7/25/26	0/2/2/2
32	2MG	a	1509	32	-	0/5/27/28	0/3/3/3
32	2MG	a	959	32	-	3/5/27/28	0/3/3/3
7	OMC	A	2736	7,54	-	0/9/27/28	0/2/2/2
32	MA6	a	1511	32	-	0/7/29/30	0/3/3/3
32	G7M	a	518	32	-	0/3/25/26	0/3/3/3
32	MA6	a	1512	32	-	2/7/29/30	0/3/3/3
7	OMG	A	2489	7	-	3/5/27/28	0/3/3/3
7	6MZ	A	2268	7	-	2/5/27/28	0/3/3/3
32	4OC	a	1395	32	-	0/9/29/30	0/2/2/2
7	5MU	A	2177	7	-	0/7/25/26	0/2/2/2

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	a	1491	UR3	O4-C4	10.14	1.45	1.23
32	a	518	G7M	O6-C6	9.96	1.43	1.23
32	a	959	2MG	O6-C6	9.16	1.41	1.23
32	a	1509	2MG	O6-C6	9.03	1.41	1.23
32	a	1395	4OC	O2-C2	9.00	1.40	1.23
7	A	2489	OMG	O6-C6	8.36	1.40	1.23
7	A	2791	OMG	O6-C6	8.31	1.40	1.23
32	a	959	2MG	C2-N2	6.86	1.48	1.33
32	a	1509	2MG	C2-N2	6.76	1.48	1.33
7	A	2268	6MZ	C6-N6	6.38	1.45	1.35
7	A	2736	OMC	C4-N4	5.58	1.47	1.33
32	a	1395	4OC	C4-N4	4.72	1.45	1.35
7	A	2791	OMG	C2-N2	4.70	1.45	1.34
7	A	2489	OMG	C2-N2	4.65	1.45	1.34
7	A	2177	5MU	C2-N1	-4.42	1.31	1.38
32	a	960	5MC	C4-N4	4.39	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	a	1491	UR3	C2-N1	-3.97	1.32	1.38
7	A	2177	5MU	C4-N3	-3.88	1.31	1.38
7	A	2177	5MU	C4-C5	-3.78	1.38	1.44
7	A	2177	5MU	C2-N3	-3.68	1.31	1.38
32	a	518	G7M	C2-N2	3.64	1.42	1.34
7	A	2177	5MU	C6-N1	-3.62	1.31	1.38
32	a	1395	4OC	C2-N1	-3.58	1.32	1.40
7	A	2489	OMG	C6-N1	-3.56	1.32	1.37
32	a	960	5MC	C2-N1	-3.54	1.32	1.40
7	A	2791	OMG	C6-N1	-3.48	1.32	1.37
7	A	2791	OMG	C5-C6	-3.31	1.40	1.47
32	a	960	5MC	C6-N1	-3.22	1.32	1.38
7	A	2489	OMG	C5-C6	-3.21	1.40	1.47
32	a	1509	2MG	C6-N1	-3.20	1.33	1.37
32	a	1491	UR3	C2-N3	-2.98	1.33	1.39
32	a	518	G7M	C6-N1	-2.96	1.33	1.37
32	a	1491	UR3	C4-N3	-2.96	1.34	1.40
32	a	959	2MG	C6-N1	-2.96	1.33	1.37
7	A	2177	5MU	O4-C4	-2.77	1.18	1.23
32	a	960	5MC	C6-C5	2.71	1.39	1.34
7	A	2177	5MU	O2-C2	-2.71	1.18	1.23
32	a	960	5MC	O2-C2	-2.64	1.18	1.23
7	A	2177	5MU	C6-C5	2.47	1.38	1.34
32	a	1509	2MG	C5-C6	-2.40	1.42	1.47
7	A	2736	OMC	C2-N1	-2.37	1.34	1.40
32	a	959	2MG	C5-C6	-2.33	1.42	1.47
32	a	518	G7M	C2-N1	-2.29	1.32	1.37
32	a	1395	4OC	C6-N1	-2.24	1.32	1.38
7	A	2791	OMG	C2-N1	-2.10	1.32	1.37
7	A	2791	OMG	C5-C4	-2.05	1.37	1.43
7	A	2489	OMG	C2-N1	-2.05	1.32	1.37
32	a	960	5MC	C2-N3	-2.02	1.32	1.36

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	2268	6MZ	C9-N6-C6	-7.06	116.79	122.87
7	A	2177	5MU	C5-C6-N1	-5.86	117.31	123.34
7	A	2177	5MU	C4-N3-C2	-5.85	119.78	127.35
7	A	2177	5MU	N3-C2-N1	5.46	122.14	114.89
7	A	2268	6MZ	C2-N1-C6	5.10	120.97	116.59
7	A	2177	5MU	C5-C4-N3	5.03	119.60	115.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	a	1511	MA6	N3-C2-N1	-4.83	121.13	128.68
32	a	1512	MA6	N3-C2-N1	-4.79	121.19	128.68
32	a	960	5MC	C5-C6-N1	-4.46	118.75	123.34
7	A	2268	6MZ	N3-C2-N1	-4.33	121.91	128.68
32	a	1491	UR3	C4-N3-C2	-3.92	120.88	124.56
7	A	2177	5MU	O4-C4-C5	-3.86	120.43	124.90
7	A	2791	OMG	C5-C6-N1	3.76	120.60	113.95
7	A	2489	OMG	C5-C6-N1	3.70	120.48	113.95
32	a	1512	MA6	C4-C5-N7	-3.26	106.00	109.40
32	a	1511	MA6	C4-C5-N7	-3.20	106.07	109.40
7	A	2791	OMG	C8-N7-C5	2.97	108.65	102.99
7	A	2177	5MU	O2-C2-N1	-2.95	118.87	122.79
32	a	1509	2MG	C8-N7-C5	2.94	108.59	102.99
32	a	959	2MG	C8-N7-C5	2.93	108.57	102.99
7	A	2489	OMG	C8-N7-C5	2.90	108.52	102.99
7	A	2489	OMG	C2-N1-C6	-2.84	119.86	125.10
7	A	2791	OMG	C2-N1-C6	-2.82	119.90	125.10
7	A	2736	OMC	O2-C2-N3	-2.65	118.02	122.33
7	A	2791	OMG	O6-C6-C5	-2.47	119.55	124.37
32	a	518	G7M	C2-N1-C6	-2.36	120.75	125.10
7	A	2489	OMG	O6-C6-C5	-2.34	119.80	124.37
32	a	1509	2MG	CM2-N2-C2	-2.09	119.24	123.86
32	a	1395	4OC	C5-C4-N3	-2.08	119.24	122.59
32	a	1491	UR3	C5-C6-N1	-2.07	118.34	121.81
32	a	959	2MG	C5-C6-N1	2.03	117.53	113.95

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	2489	OMG	O4'-C4'-C5'-O5'
7	A	2489	OMG	C1'-C2'-O2'-CM2
32	a	959	2MG	N1-C2-N2-CM2
32	a	959	2MG	N3-C2-N2-CM2
7	A	2268	6MZ	O4'-C4'-C5'-O5'
7	A	2268	6MZ	C3'-C4'-C5'-O5'
7	A	2489	OMG	C3'-C4'-C5'-O5'
32	a	1512	MA6	O4'-C4'-C5'-O5'
32	a	1491	UR3	O4'-C4'-C5'-O5'
32	a	959	2MG	C4'-C5'-O5'-P
32	a	1512	MA6	C3'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 454 ligands modelled in this entry, 453 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
53	WDP	A	3201	-	83,90,90	2.45	21 (25%)	102,132,132	2.26	18 (17%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
53	WDP	A	3201	-	-	37/103/158/158	1/4/5/5

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	A	3201	WDP	C18-N20	8.92	1.50	1.35
53	A	3201	WDP	S26-N25	7.37	1.73	1.61
53	A	3201	WDP	C62-N61	-6.42	1.33	1.46
53	A	3201	WDP	O17-C18	5.99	1.46	1.34
53	A	3201	WDP	O50-C51	5.82	1.47	1.34
53	A	3201	WDP	C04-N03	-5.33	1.22	1.27
53	A	3201	WDP	C14-C15	5.05	1.62	1.53
53	A	3201	WDP	O40-C41	4.66	1.47	1.34
53	A	3201	WDP	C43-C41	4.51	1.59	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	A	3201	WDP	C29-S26	4.29	1.83	1.76
53	A	3201	WDP	C59-N61	-4.03	1.35	1.48
53	A	3201	WDP	O17-C15	-4.00	1.41	1.46
53	A	3201	WDP	C24-C21	3.19	1.57	1.53
53	A	3201	WDP	O74-C73	2.84	1.49	1.41
53	A	3201	WDP	C24-N25	2.81	1.50	1.47
53	A	3201	WDP	C82-C79	-2.65	1.46	1.52
53	A	3201	WDP	O27-S26	2.38	1.46	1.43
53	A	3201	WDP	C53-C51	2.35	1.56	1.51
53	A	3201	WDP	O19-C18	-2.14	1.17	1.21
53	A	3201	WDP	C60-C59	2.13	1.59	1.52
53	A	3201	WDP	O02-C01	-2.02	1.40	1.43

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	A	3201	WDP	O28-S26-O27	-14.94	101.18	119.55
53	A	3201	WDP	O17-C18-N20	7.55	119.98	109.92
53	A	3201	WDP	C05-C04-N03	-5.83	120.13	126.93
53	A	3201	WDP	O02-N03-C04	5.35	119.95	110.97
53	A	3201	WDP	O40-C41-C43	4.61	119.94	111.46
53	A	3201	WDP	O50-C51-C53	3.96	120.25	111.56
53	A	3201	WDP	O19-C18-N20	-3.31	119.98	124.95
53	A	3201	WDP	O17-C18-O19	-3.06	120.04	125.62
53	A	3201	WDP	O28-S26-N25	2.72	111.29	107.04
53	A	3201	WDP	O28-S26-C29	2.72	111.32	107.97
53	A	3201	WDP	O27-S26-N25	2.72	111.29	107.04
53	A	3201	WDP	O27-S26-C29	2.66	111.24	107.97
53	A	3201	WDP	C49-O50-C51	-2.41	113.64	117.78
53	A	3201	WDP	C76-C75-C77	-2.30	108.82	113.07
53	A	3201	WDP	C07-C06-C05	-2.28	108.78	113.22
53	A	3201	WDP	O50-C51-O52	-2.18	119.86	123.94
53	A	3201	WDP	O42-C41-C43	-2.13	120.03	124.73
53	A	3201	WDP	O10-C11-C67	2.01	110.65	108.22

There are no chirality outliers.

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
53	A	3201	WDP	C22-C21-C24-N25
53	A	3201	WDP	C23-C21-C24-N25
53	A	3201	WDP	N20-C21-C24-N25

Continued on next page...

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Mol	Chain	Res	Type	Atoms
53	A	3201	WDP	C22-C21-N20-C18
53	A	3201	WDP	C24-C21-N20-C18
53	A	3201	WDP	C21-C24-N25-S26
53	A	3201	WDP	C05-C04-N03-O02
53	A	3201	WDP	C85-C04-N03-O02
53	A	3201	WDP	C12-C11-C67-C55
53	A	3201	WDP	O17-C18-N20-C21
53	A	3201	WDP	O19-C18-N20-C21
53	A	3201	WDP	N20-C18-O17-C15
53	A	3201	WDP	O19-C18-O17-C15
53	A	3201	WDP	C15-C35-C37-C38
53	A	3201	WDP	O36-C35-C37-C38
53	A	3201	WDP	C37-C39-O40-C41
53	A	3201	WDP	C47-C39-O40-C41
53	A	3201	WDP	C43-C41-O40-C39
53	A	3201	WDP	C49-C69-C71-O72
53	A	3201	WDP	C70-C69-C71-O72
53	A	3201	WDP	C04-N03-O02-C01
53	A	3201	WDP	O42-C41-O40-C39
53	A	3201	WDP	O08-C09-O10-C11
53	A	3201	WDP	C24-N25-S26-O28
53	A	3201	WDP	O10-C11-C67-C55
53	A	3201	WDP	C23-C21-N20-C18
53	A	3201	WDP	C12-C11-C67-C68
53	A	3201	WDP	C24-N25-S26-O27
53	A	3201	WDP	C24-N25-S26-C29
53	A	3201	WDP	C41-C43-C44-C45
53	A	3201	WDP	C82-C73-O72-C71
53	A	3201	WDP	O10-C11-C67-C68
53	A	3201	WDP	C37-C39-C47-C49
53	A	3201	WDP	C16-C15-O17-C18
53	A	3201	WDP	C41-C43-C44-C46
53	A	3201	WDP	C82-C79-O80-C81
53	A	3201	WDP	C38-C37-C39-O40

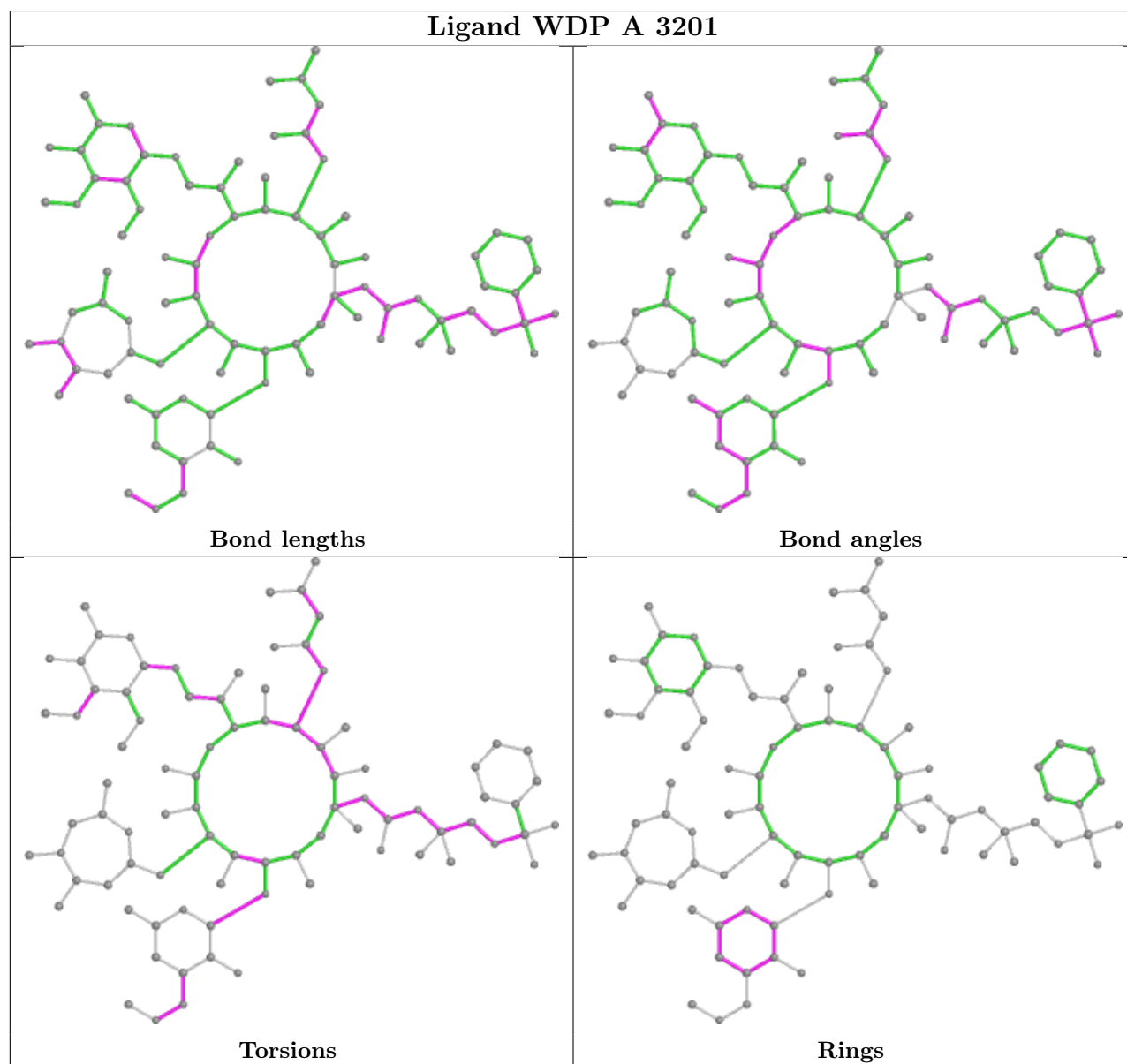
All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
53	A	3201	WDP	C04-C05-C06-C09-C85-O08

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

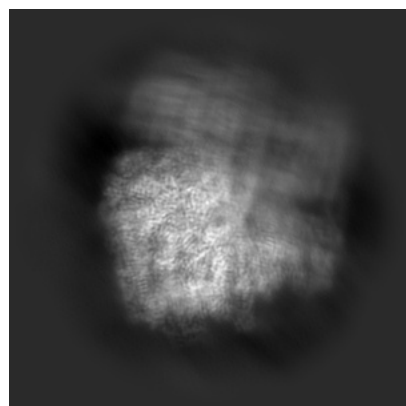
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-25100. These allow visual inspection of the internal detail of the map and identification of artifacts.

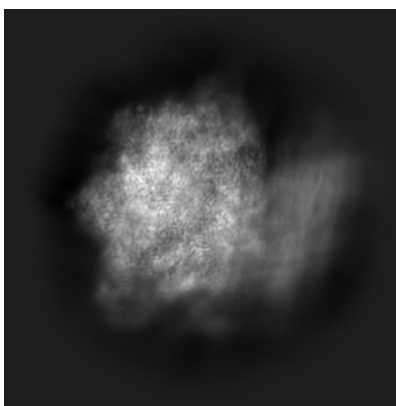
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

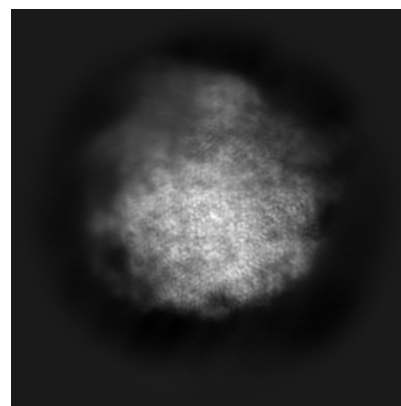
6.1.1 Primary map



X

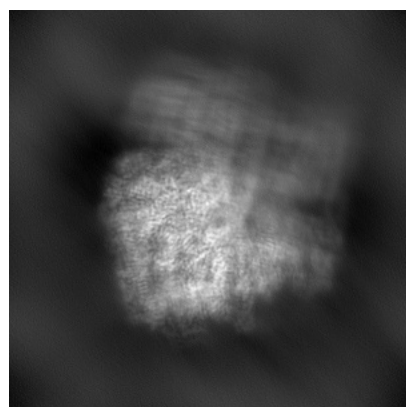


Y

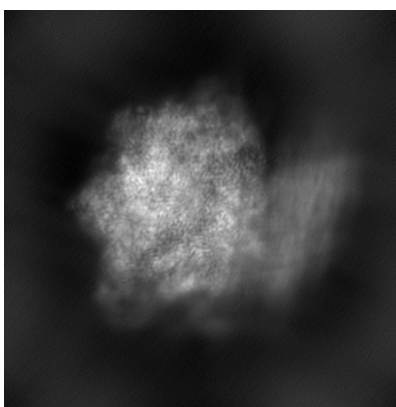


Z

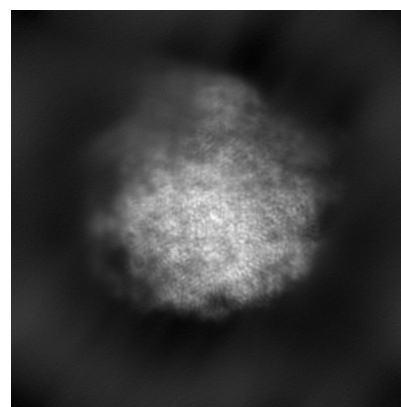
6.1.2 Raw map



X



Y

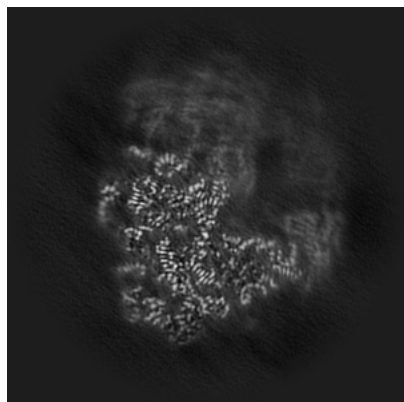


Z

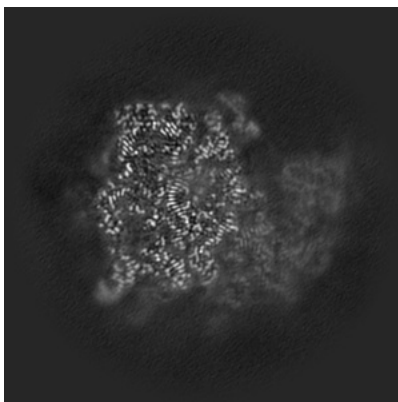
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

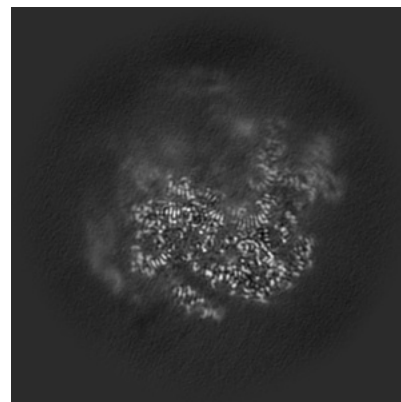
6.2.1 Primary map



X Index: 210

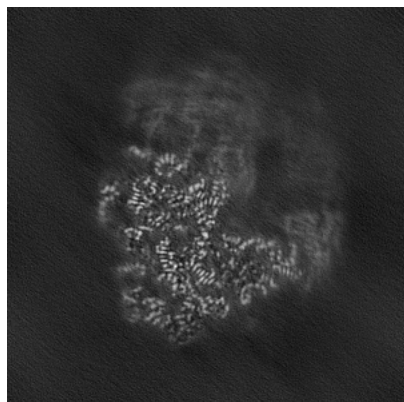


Y Index: 210

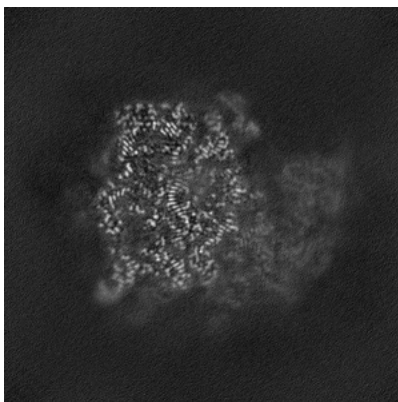


Z Index: 210

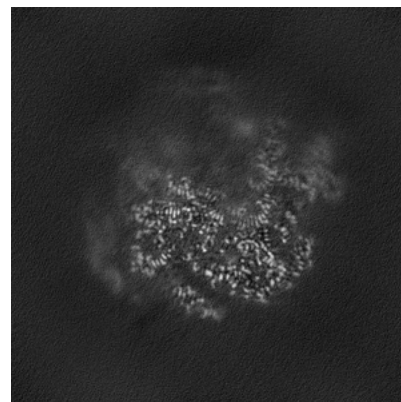
6.2.2 Raw map



X Index: 210



Y Index: 210

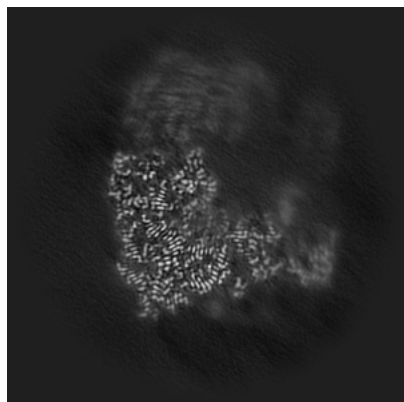


Z Index: 210

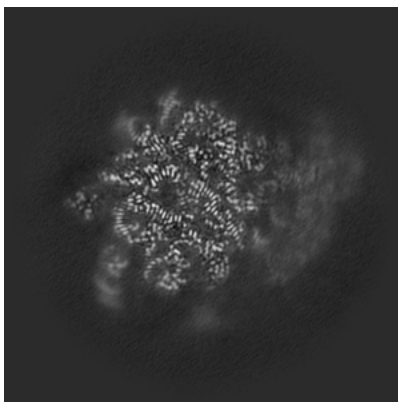
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

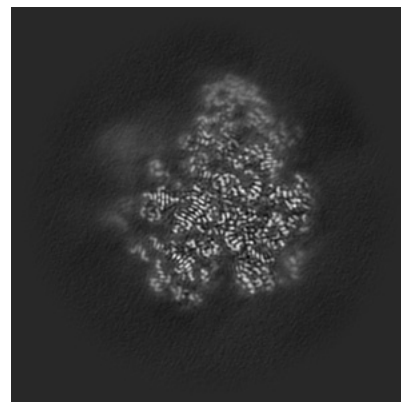
6.3.1 Primary map



X Index: 244

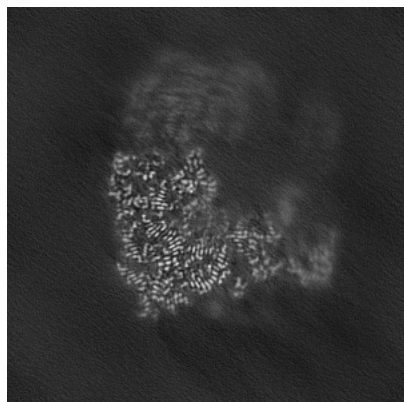


Y Index: 172

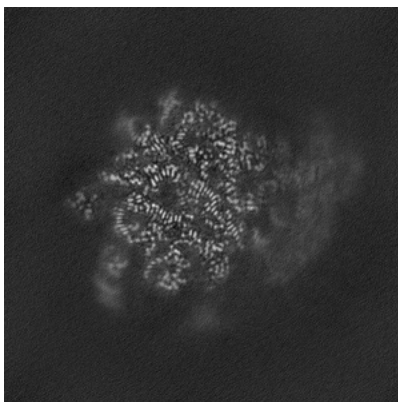


Z Index: 158

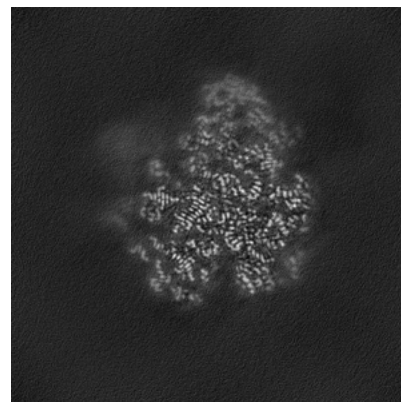
6.3.2 Raw map



X Index: 244



Y Index: 172



Z Index: 158

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

6.4 Orthogonal surface views [i](#)

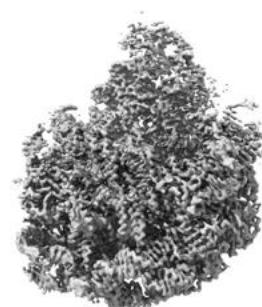
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.4. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

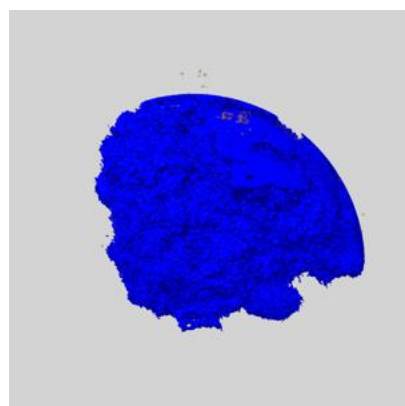
6.5 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

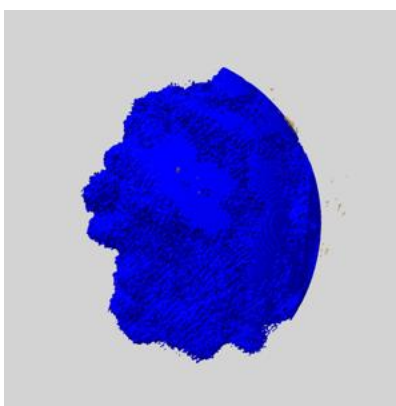
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

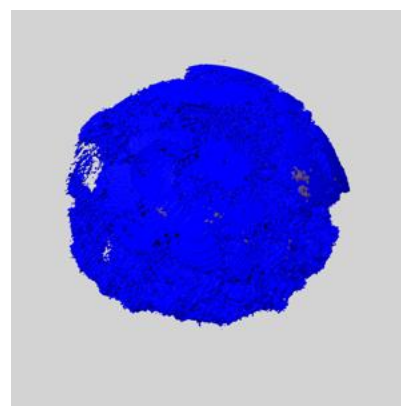
6.5.1 emd_25100_msk_1.map [i](#)



X



Y

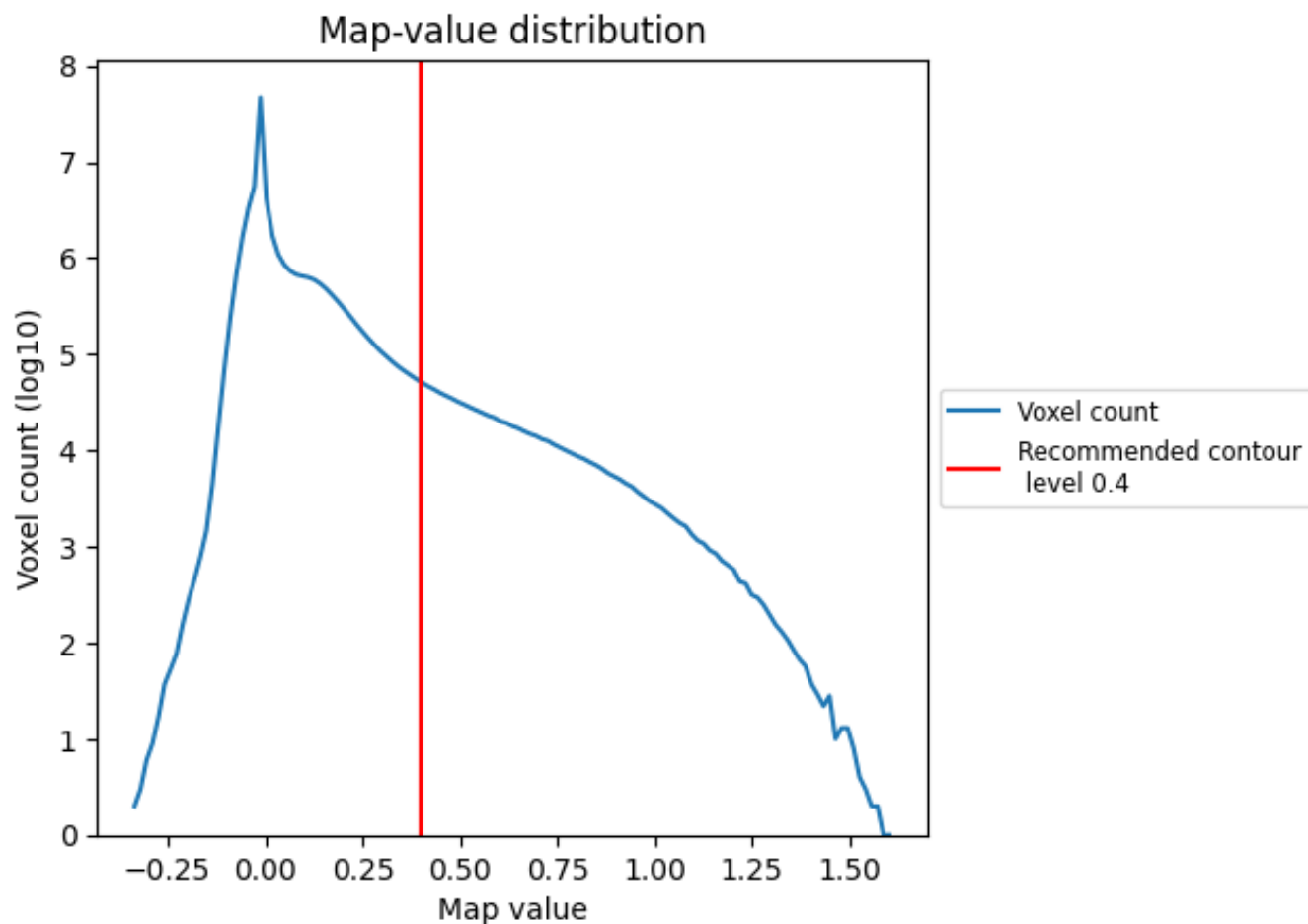


Z

7 Map analysis [i](#)

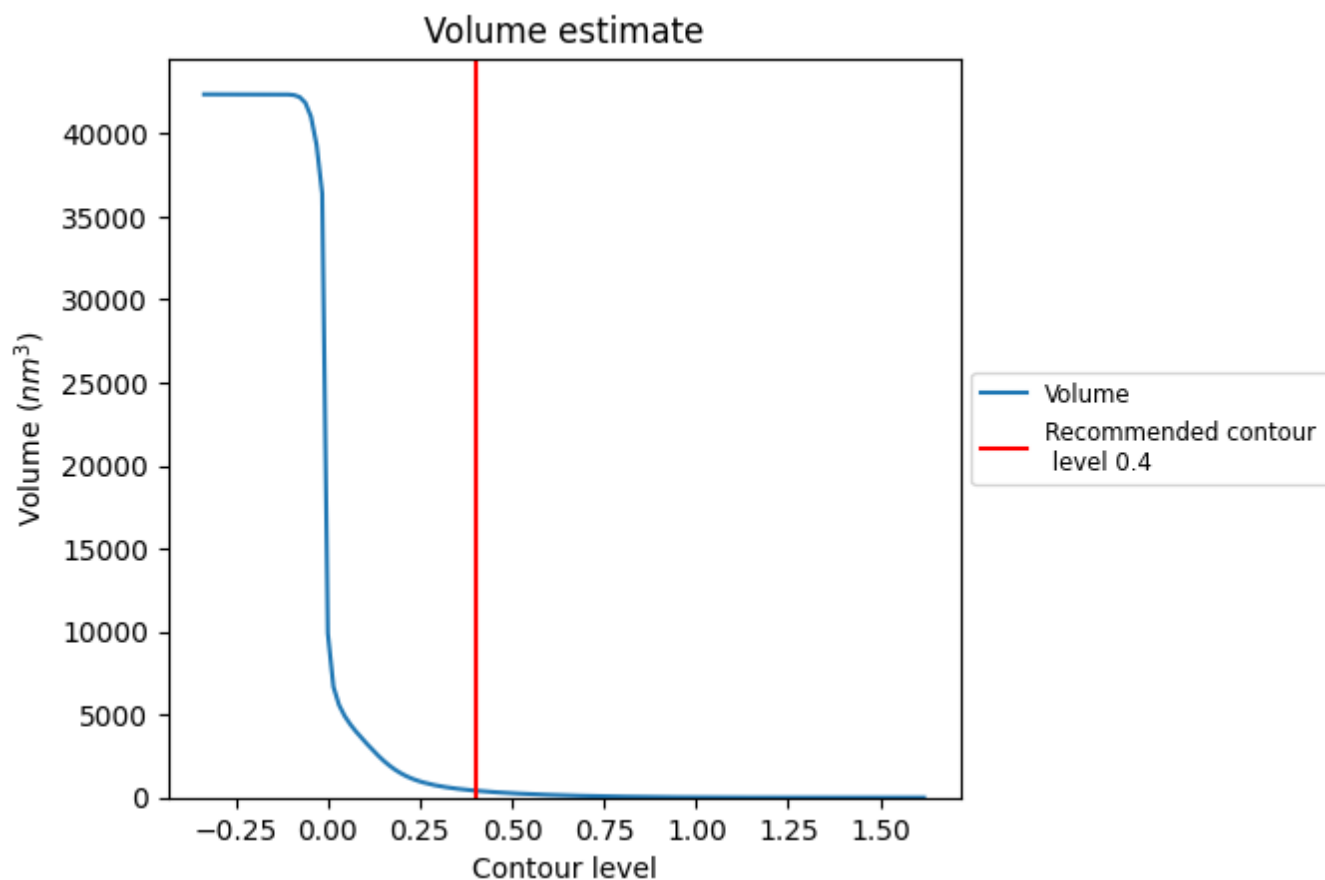
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

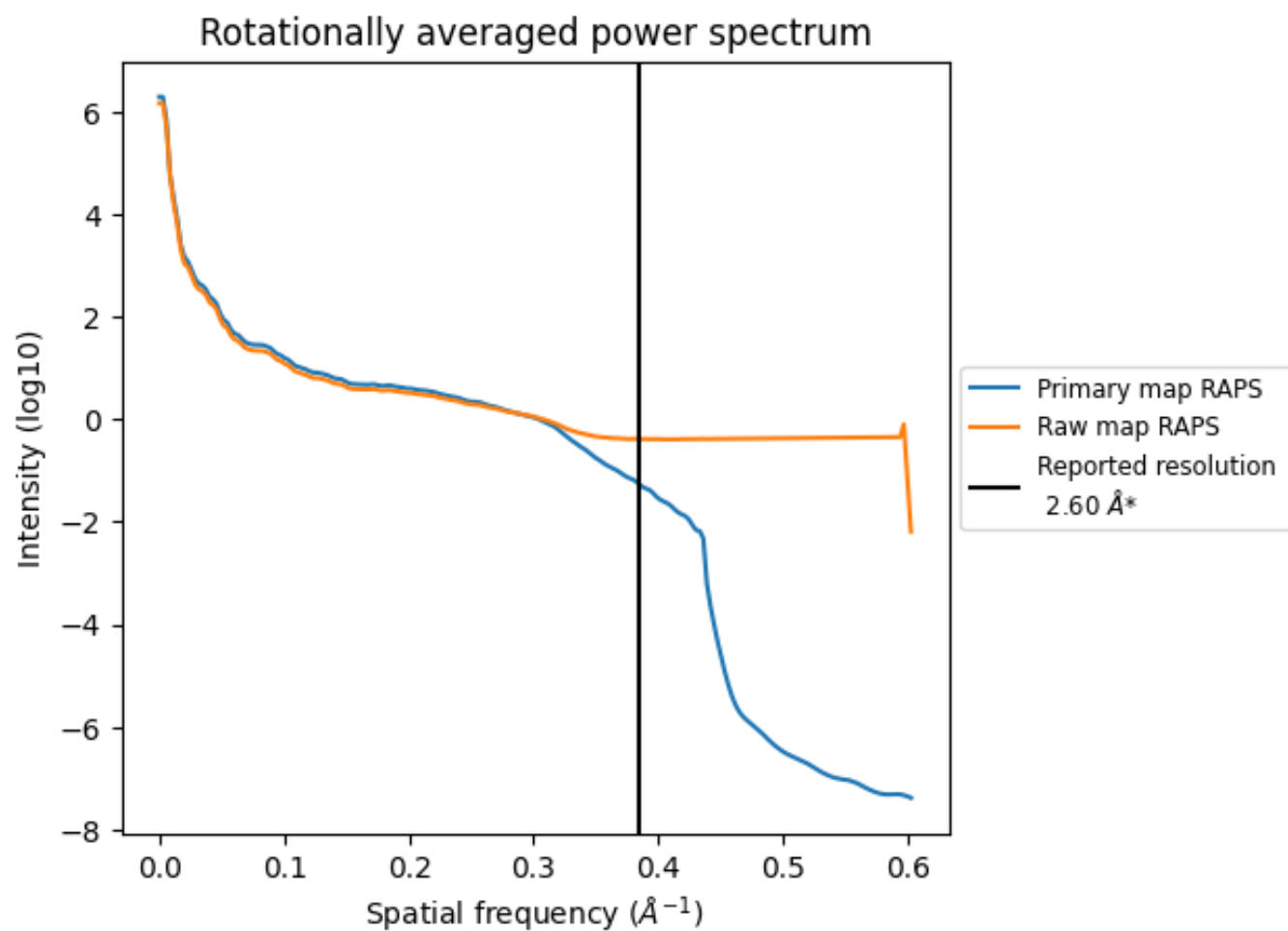
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 418 nm³; this corresponds to an approximate mass of 377 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

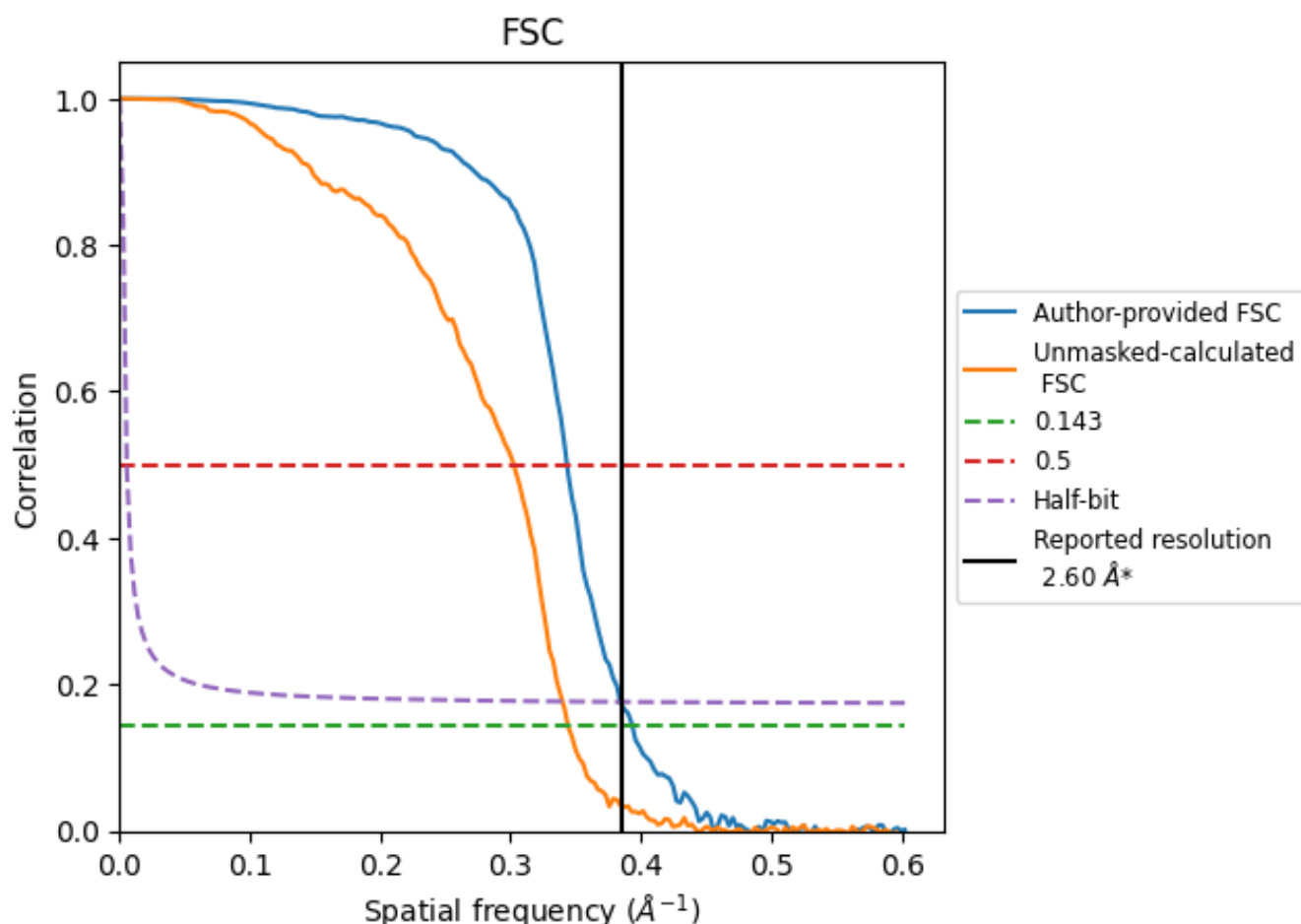


*Reported resolution corresponds to spatial frequency of 0.385 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.385 \AA^{-1}

8.2 Resolution estimates

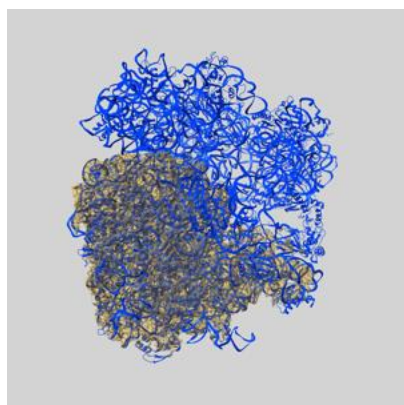
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.60	-	-
Author-provided FSC curve	2.54	2.91	2.60
Unmasked-calculated*	2.91	3.31	2.94

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.91 differs from the reported value 2.6 by more than 10 %

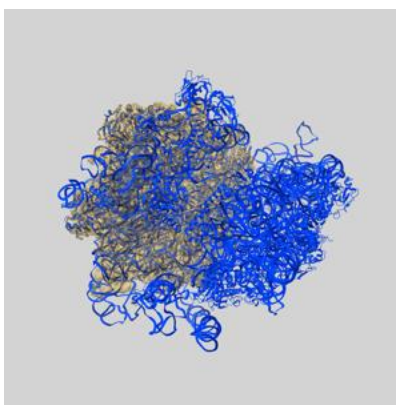
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-25100 and PDB model 7SFR. Per-residue inclusion information can be found in section [3](#) on page [14](#).

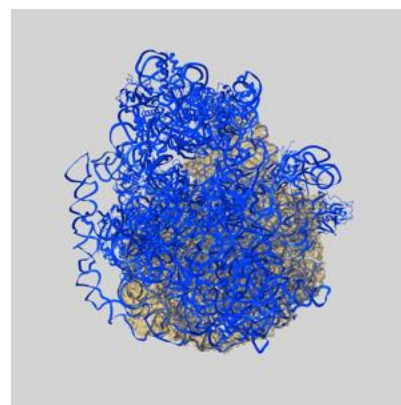
9.1 Map-model overlay [i](#)



X



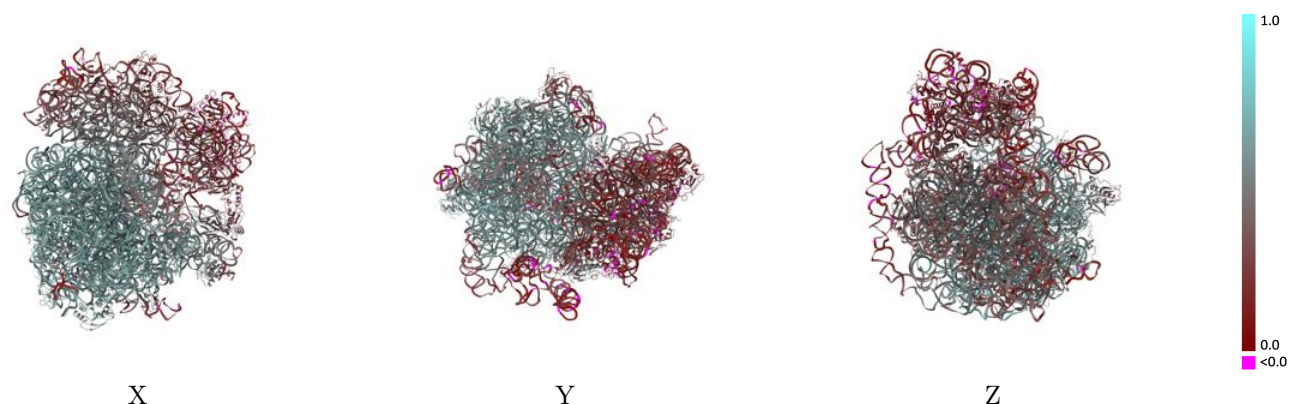
Y



Z

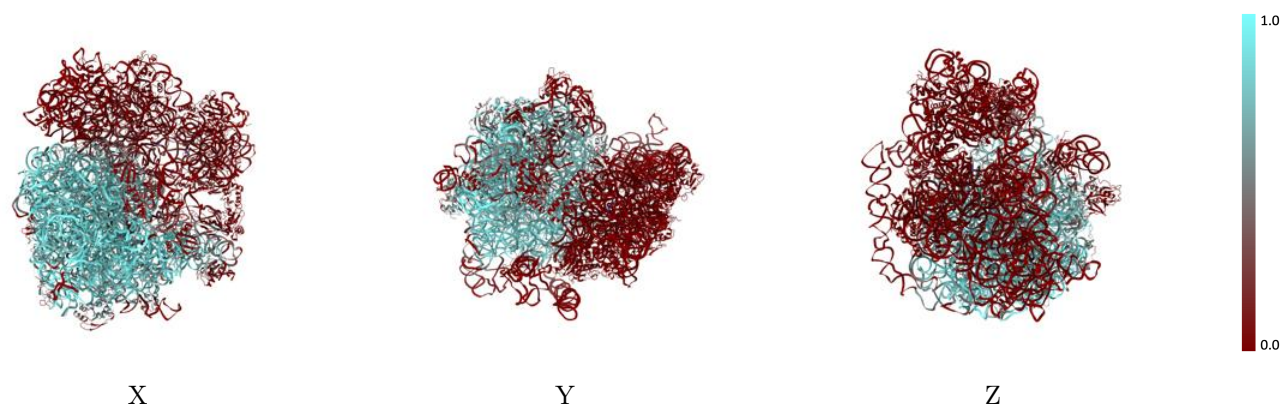
The images above show the 3D surface view of the map at the recommended contour level 0.4 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



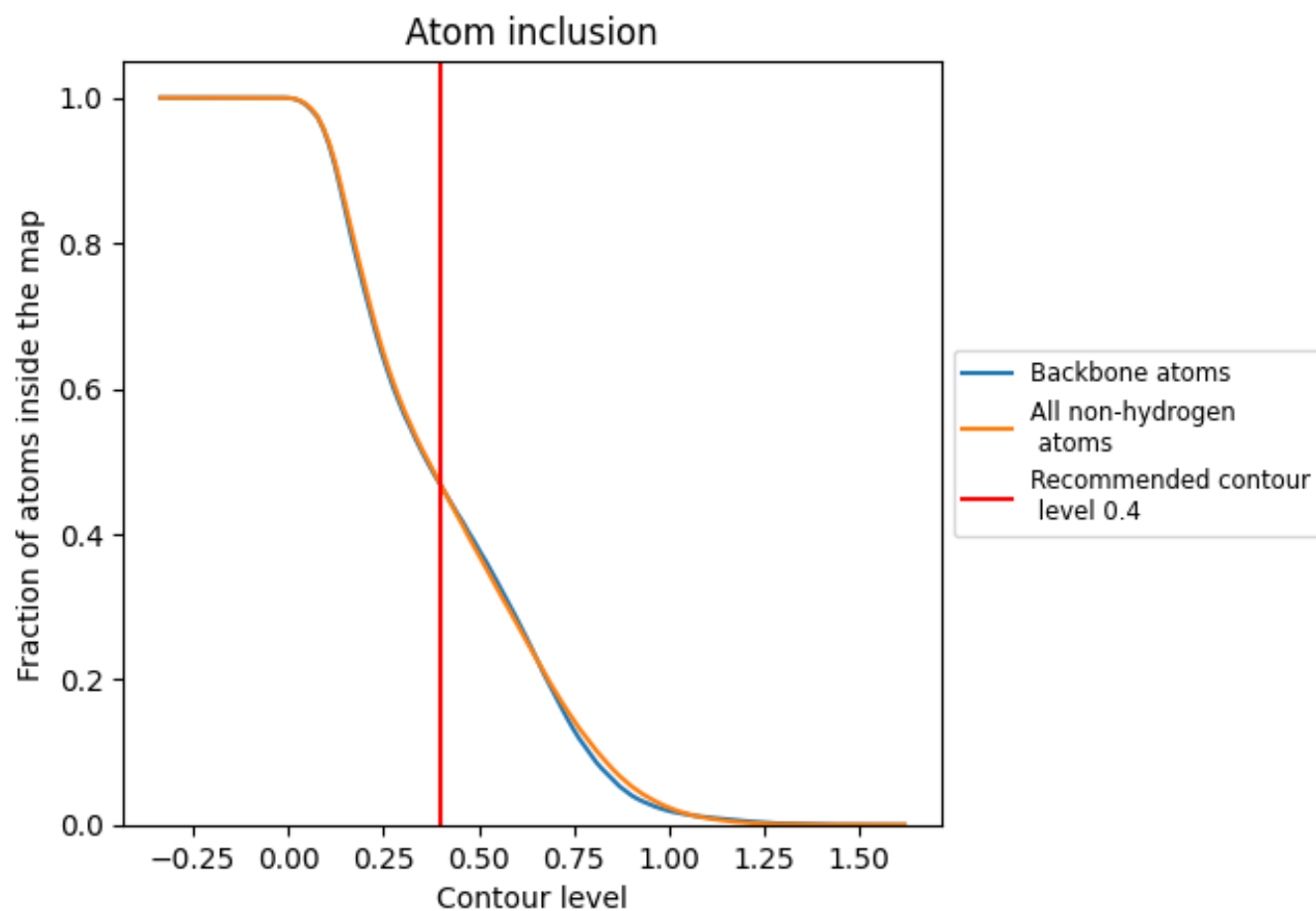
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.4).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 47% of all backbone atoms, 47% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ



































The table lists the average atom inclusion at the recommended contour level (0.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4681	 0.4680
0	 0.4537	 0.6090
1	 0.6701	 0.5810
2	 0.9573	 0.6490
3	 0.7055	 0.6210
4	 0.1910	 0.5570
6	 0.0000	 0.2530
A	 0.7685	 0.5450
B	 0.5465	 0.4700
C	 0.8569	 0.6210
D	 0.7294	 0.6040
E	 0.6066	 0.5910
F	 0.0140	 0.3610
G	 0.0402	 0.4250
H	 0.0262	 0.3940
J	 0.8133	 0.6090
K	 0.6925	 0.6030
L	 0.6590	 0.5850
M	 0.1205	 0.5530
N	 0.8348	 0.6250
O	 0.2182	 0.4590
P	 0.6230	 0.5890
Q	 0.8515	 0.6190
R	 0.6471	 0.6010
S	 0.8141	 0.6220
T	 0.6409	 0.5780
U	 0.4141	 0.5220
V	 0.0436	 0.4840
W	 0.7623	 0.5990
X	 0.7662	 0.6190
Y	 0.5869	 0.5510
Z	 0.6989	 0.5880
a	 0.0181	 0.3330
c	 0.0000	 0.2250
d	 0.0000	 0.2260



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Chain	Atom inclusion	Q-score
e	 0.0000	 0.3140
f	 0.0000	 0.4430
g	 0.0000	 0.2290
h	 0.0000	 0.3360
i	 0.0000	 0.1610
j	 0.0000	 0.1700
k	 0.0000	 0.4060
l	 0.0000	 0.3460
m	 0.0000	 0.2100
n	 0.0000	 0.2030
o	 0.0000	 0.4150
p	 0.0000	 0.3030
q	 0.0000	 0.3330
r	 0.0000	 0.4080
s	 0.0000	 0.1790
t	 0.0000	 0.3420
v	 0.0171	 0.5040