



Full wwPDB EM Validation Report ⓘ

Dec 28, 2024 – 09:32 AM EST

PDB ID : 6VU3
EMDB ID : EMD-21386
Title : Cryo-EM structure of Escherichia coli transcription-translation complex A (TTC-A) containing mRNA with a 12 nt long spacer
Authors : Molodtsov, V.; Wang, C.; Su, M.; Ebright, R.
Deposited on : 2020-02-14
Resolution : 3.70 Å(reported)

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.dev113
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.40

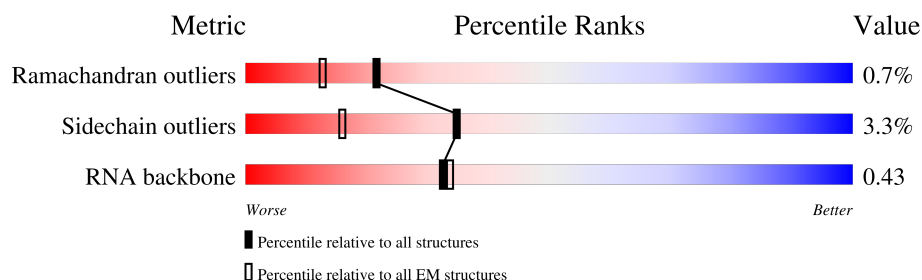
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.70 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.



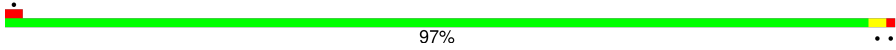




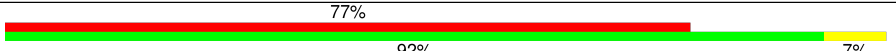
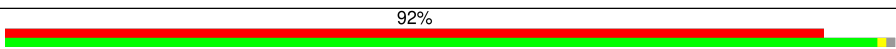

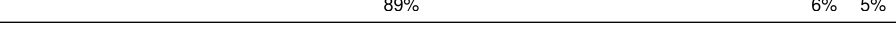
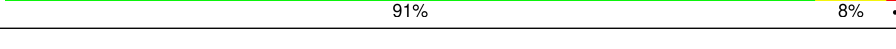

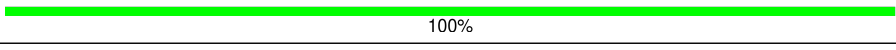
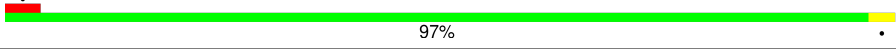
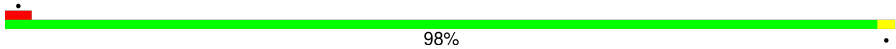

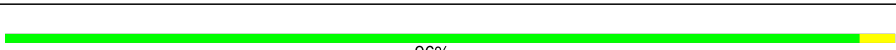

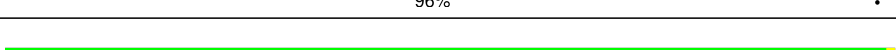
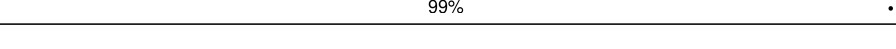
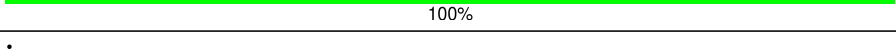
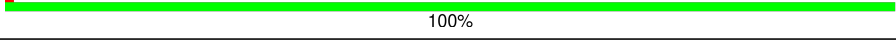
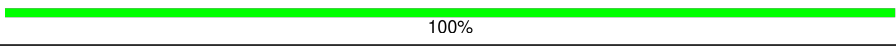
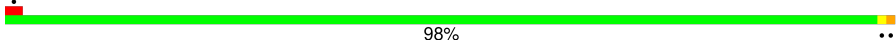

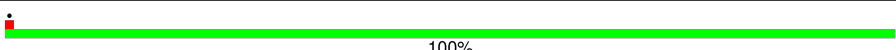
Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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	103	
2	1	110	
3	2	94	
4	3	103	
5	4	94	
6	5	36	
7	6	27	
8	7	29	

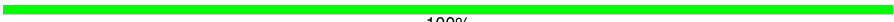













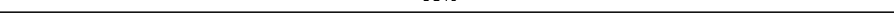
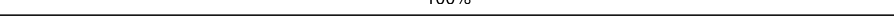
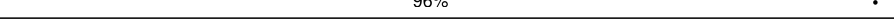
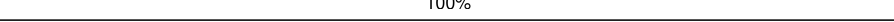
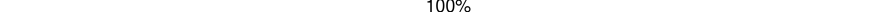
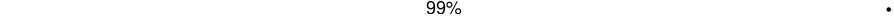

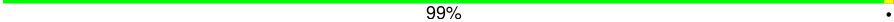
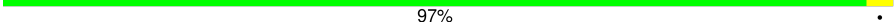
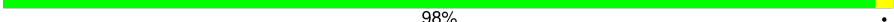

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Mol	Chain	Length	Quality of chain
9	9	148	
10	A	76	
10	B	76	
11	AA	1342	
12	AB	181	
13	AC	230	
13	AD	230	
14	AE	1407	
15	C	66	
16	D	1542	
17	E	86	
18	F	70	
19	G	225	
20	H	557	
21	I	208	
22	J	205	
23	K	156	
24	L	104	
25	M	151	
26	N	129	
27	O	127	
28	P	99	
29	Q	117	
30	R	124	
31	S	100	

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Mol	Chain	Length	Quality of chain
32	T	88	 100%
33	U	82	 99%
34	V	80	 99%
35	W	83	 100%
36	X	116	 99%
37	Y	141	 99%
38	Z	30	 100%
39	a	2904	 75% 22%
40	b	76	 5% 97%
41	c	77	 100%
42	d	120	 83% 17%
43	e	62	 100%
44	f	58	 100%
45	g	66	 6% 98%
46	h	271	 100%
47	i	56	 96%
48	j	209	 100%
49	k	52	 100%
50	l	201	 99%
51	m	46	 93% 7%
52	n	177	 99%
53	o	64	 97%
54	p	175	 98%
55	q	38	 95% 5%
56	r	149	 100%

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Mol	Chain	Length	Quality of chain
57	s	142	 100%
58	t	123	 100%
59	u	144	 100%
60	v	136	 99% .
61	w	119	 99% .
62	x	116	 100%
63	y	114	 99% .
64	z	117	 99% .

2 Entry composition

There are 66 unique types of molecules in this entry. The entry contains 300609 atoms, of which 124724 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 L21.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	0	103	Total	C	H	N	O	S	0	0
			1655	516	839	153	145	2		

- Molecule 2 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	1	110	Total	C	H	N	O	S	0	0
			1779	532	922	166	156	3		

- Molecule 3 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	2	94	Total	C	H	N	O	S	0	0
			1557	470	811	140	134	2		

- Molecule 4 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	103	Total	C	H	N	O	0	0
			1632	498	844	148	142		

- Molecule 5 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	4	94	Total	C	H	N	O	S	0	0
			1533	479	780	137	134	3		

- Molecule 6 is a DNA chain called NT DNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	5	23	Total	C	H	N	O	P	0	0
			732	225	260	87	137	23		

- Molecule 7 is a DNA chain called T DNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	6	27	Total	C	H	N	O	P	0	0
			848	259	306	89	167	27		

- Molecule 8 is a RNA chain called mRNA with 12 nt long spacer.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	7	29	Total	C	H	N	O	P	0	0
			709	273	97	94	216	29		

- Molecule 9 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	9	148	Total	C	N	O	S	0	0
			1117	705	196	209	7		

- Molecule 10 is a RNA chain called E-site and A-site tRNA (fMet).

Mol	Chain	Residues	Atoms						AltConf	Trace
10	A	76	Total	C	H	N	O	P	0	0
			2446	723	826	295	527	75		
10	B	76	Total	C	H	N	O	P	0	0
			2433	723	813	295	527	75		

- Molecule 11 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	AA	1322	Total	C	H	N	O	S	0	0
			20851	6539	10426	1817	2026	43		

- Molecule 12 is a protein called Transcription termination/antitermination protein NusG.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	AB	98	Total	C	H	N	O	S	0	0
			1573	505	783	139	140	6		

- Molecule 13 is a protein called DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	AC	230	Total	C	H	N	O	S	0	0
			3599	1112	1813	317	351	6		

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Mol	Chain	Residues	Atoms						AltConf	Trace
13	AD	228	Total	C	H	N	O	S	0	0
			3556	1100	1789	312	349	6		

- Molecule 14 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	AE	1335	Total	C	H	N	O	S	0	0
			21000	6526	10612	1854	1958	50		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AE	1384	VAL	MET	conflict	UNP A0A4S1NBU2

- Molecule 15 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	C	66	Total	C	H	N	O	S	0	0
			1103	344	559	102	97	1		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
16	D	1524	Total	C	H	N	O	P	0	0
			49126	14585	16423	6003	10591	1524		

- Molecule 17 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	E	86	Total	C	H	N	O	S	0	0
			1388	414	719	138	114	3		

- Molecule 18 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	F	70	Total	C	H	N	O	S	0	0
			1218	366	629	125	97	1		

- Molecule 19 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms						AltConf	Trace
19	G	225	Total	C	H	N	O	S	0	0
			3545	1113	1785	316	323	8		

- Molecule 20 is a protein called 30S ribosomal protein S1.

Mol	Chain	Residues	Atoms						AltConf	Trace
20	H	259	Total	C	H	N	O	S	0	0
			3184	1073	1454	305	349	3		

- Molecule 21 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms						AltConf	Trace
21	I	208	Total	C	H	N	O	S	0	0
			3346	1036	1710	307	290	3		

- Molecule 22 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms						AltConf	Trace
22	J	205	Total	C	H	N	O	S	0	0
			3350	1026	1707	315	298	4		

- Molecule 23 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms						AltConf	Trace
23	K	156	Total	C	H	N	O	S	0	0
			2348	717	1196	217	212	6		

- Molecule 24 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms						AltConf	Trace
24	L	104	Total	C	H	N	O	S	0	0
			1694	536	846	153	152	7		

- Molecule 25 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms						AltConf	Trace
25	M	151	Total	C	H	N	O	S	0	0
			2416	735	1235	227	215	4		

- Molecule 26 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms						AltConf	Trace
26	N	129	Total	C	H	N	O	S	0	0
			2010	616	1031	173	184	6		

- Molecule 27 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms						AltConf	Trace
27	O	127	Total	C	H	N	O	S	0	0
			2092	634	1070	206	179	3		

- Molecule 28 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms						AltConf	Trace
28	P	99	Total	C	H	N	O	S	0	0
			1621	495	831	151	143	1		

- Molecule 29 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms						AltConf	Trace
29	Q	117	Total	C	H	N	O	S	0	0
			1764	540	887	174	160	3		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
30	R	121	Total	C	H	N	O	S	0	0
			1940	580	1001	194	161	4		

- Molecule 31 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms						AltConf	Trace
31	S	100	Total	C	H	N	O	S	0	0
			1649	499	844	164	139	3		

- Molecule 32 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms						AltConf	Trace
32	T	88	Total	C	H	N	O	S	0	0
			1448	439	734	144	130	1		

- Molecule 33 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms						AltConf	Trace
33	U	82	Total	C	H	N	O	S	0	0
			1315	406	666	128	114	1		

- Molecule 34 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms						AltConf	Trace
34	V	80	Total	C	H	N	O	S	0	0
			1339	411	691	121	113	3		

- Molecule 35 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms						AltConf	Trace
35	W	83	Total	C	H	N	O	S	0	0
			1351	424	688	126	111	2		

- Molecule 36 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms						AltConf	Trace
36	X	116	Total	C	H	N	O	S	0	0
			1864	558	964	181	158	3		

- Molecule 37 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	Y	141	Total	C	N	O	S	0	0
			1032	651	179	196	6		

- Molecule 38 is a protein called 50S ribosomal protein L7/L12.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	Z	30	Total	C	N	O	S	0	0
			227	144	33	47	3		

- Molecule 39 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
39	a	2880	Total	C	H	N	O	P	0	0
			92918	27587	31077	11398	19976	2880		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	887	A	U	conflict	GB 937521852

- Molecule 40 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms						AltConf	Trace
40	b	76	Total	C	H	N	O	S	0	0
			1181	360	599	117	104	1		

- Molecule 41 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms						AltConf	Trace
41	c	77	Total	C	H	N	O	S	0	0
			1277	388	652	129	106	2		

- Molecule 42 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
42	d	120	Total	C	H	N	O	P	0	0
			3870	1144	1301	468	837	120		

- Molecule 43 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms						AltConf	Trace
43	e	62	Total	C	H	N	O	S	0	0
			1032	308	531	98	94	1		

- Molecule 44 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms						AltConf	Trace
44	f	58	Total	C	H	N	O	S	0	0
			936	281	488	87	78	2		

- Molecule 45 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms						AltConf	Trace
45	g	66	Total	C	H	N	O	S	0	0
			1042	323	520	99	94	6		

- Molecule 46 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms						AltConf	Trace
46	h	271	Total	C	H	N	O	S	0	0
			4236	1288	2154	423	364	7		

- Molecule 47 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms						AltConf	Trace
47	i	56	Total	C	H	N	O	S	0	0
			903	269	459	94	80	1		

- Molecule 48 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms						AltConf	Trace
48	j	209	Total	C	H	N	O	S	0	0
			3182	979	1617	288	294	4		

- Molecule 49 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms						AltConf	Trace
49	k	52	Total	C	H	N	O		0	0
			890	275	464	78	73			

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

Mol	Chain	Residues	Atoms						AltConf	Trace
50	l	201	Total	C	H	N	O	S	0	0
			3171	974	1619	283	290	5		

- Molecule 51 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms						AltConf	Trace
51	m	46	Total	C	H	N	O	S	0	0
			795	228	418	90	57	2		

- Molecule 52 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms						AltConf	Trace
52	n	177	Total	C	H	N	O	S	0	0
			2853	899	1443	249	256	6		

- Molecule 53 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms						AltConf	Trace
53	o	64	Total	C	H	N	O	S	0	0
			1076	323	572	105	74	2		

- Molecule 54 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms						AltConf	Trace
54	p	175	Total	C	H	N	O	S	0	0
			2671	826	1358	241	244	2		

- Molecule 55 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms						AltConf	Trace
55	q	38	Total	C	H	N	O	S	0	0
			645	185	343	65	48	4		

- Molecule 56 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms						AltConf	Trace
56	r	149	Total	C	H	N	O	S	0	0
			2259	699	1148	197	214	1		

- Molecule 57 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms						AltConf	Trace
57	s	142	Total	C	H	N	O	S	0	0
			2291	714	1162	212	199	4		

- Molecule 58 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms						AltConf	Trace
58	t	123	Total	C	H	N	O	S	0	0
			1969	593	1023	181	166	6		

- Molecule 59 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms						AltConf	Trace
59	u	144	Total	C	H	N	O	S	0	0
			2182	654	1129	207	190	2		

- Molecule 60 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms						AltConf	Trace
60	v	136	Total	C	H	N	O	S	0	0
			2231	686	1157	205	177	6		

- Molecule 61 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms						AltConf	Trace
61	w	119	Total	C	H	N	O	S	0	0
			1945	588	994	195	163	5		

- Molecule 62 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms						AltConf	Trace
62	x	116	Total	C	H	N	O		0	0
			1815	552	923	178	162			

- Molecule 63 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms						AltConf	Trace
63	y	114	Total	C	H	N	O	S	0	0
			1879	574	962	179	163	1		

- Molecule 64 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms						AltConf	Trace
64	z	117	Total	C	H	N	O		0	0
			1967	604	1020	192	151			

- Molecule 65 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
65	7	1	Total	Mg	0
			1	1	

- Molecule 66 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
66	AA	2	Total	Zn	0
			2	2	

3 Residue-property plots

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 L21

Chain 0:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: 50S ribosomal protein L22

Chain 1:  100%

There are no outlier residues recorded for this chain.

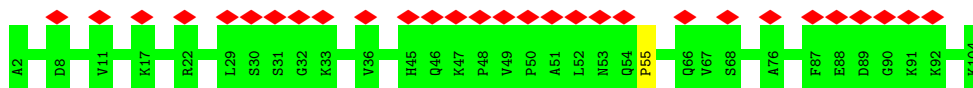
- Molecule 3: 50S ribosomal protein L23

Chain 2:  100%

There are no outlier residues recorded for this chain.

- Molecule 4: 50S ribosomal protein L24

Chain 3:  28% 99%



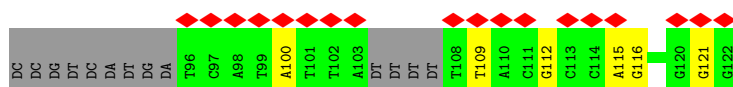
- Molecule 5: 50S ribosomal protein L25

Chain 4:  100%

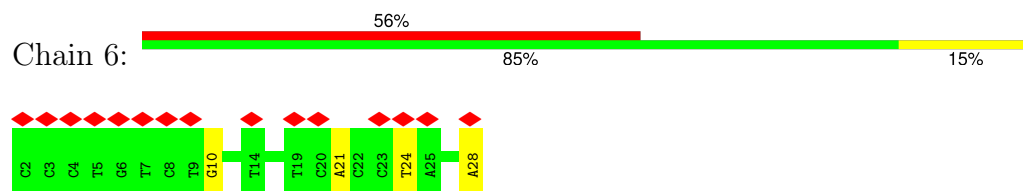
There are no outlier residues recorded for this chain.

- Molecule 6: NT DNA

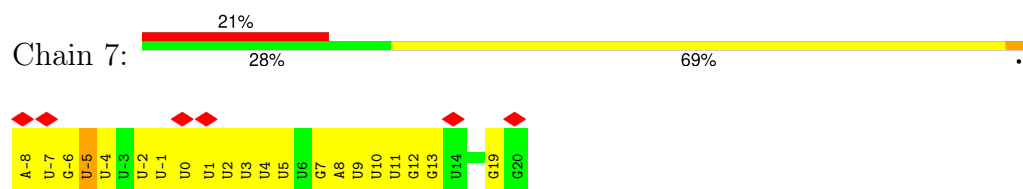
Chain 5:  50% 47% 17% 36%



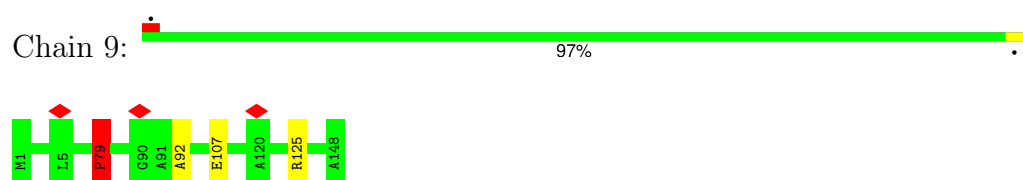
- Molecule 7: T DNA



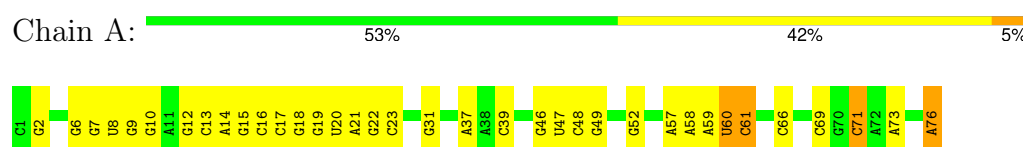
- Molecule 8: mRNA with 12 nt long spacer



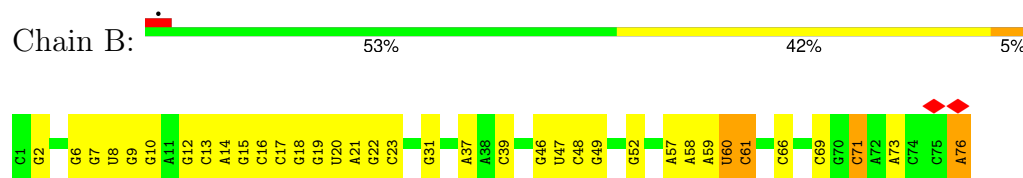
- Molecule 9: 50S ribosomal protein L10



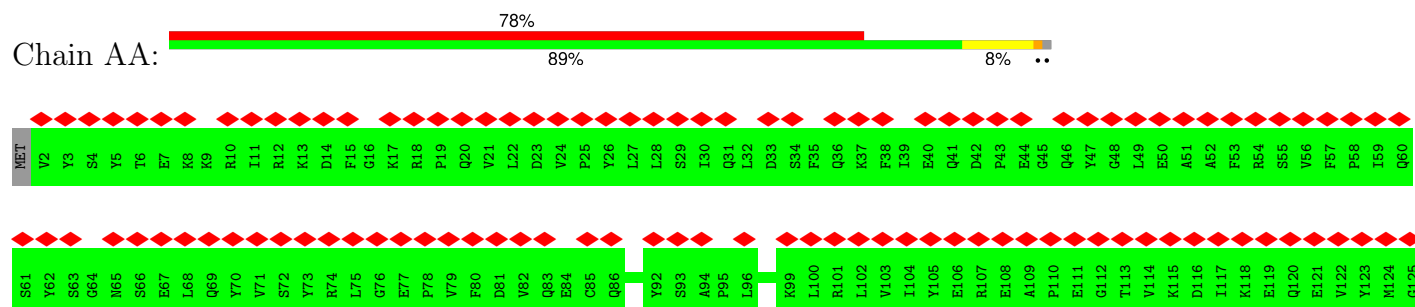
- Molecule 10: E-site and A-site tRNA (fMet)



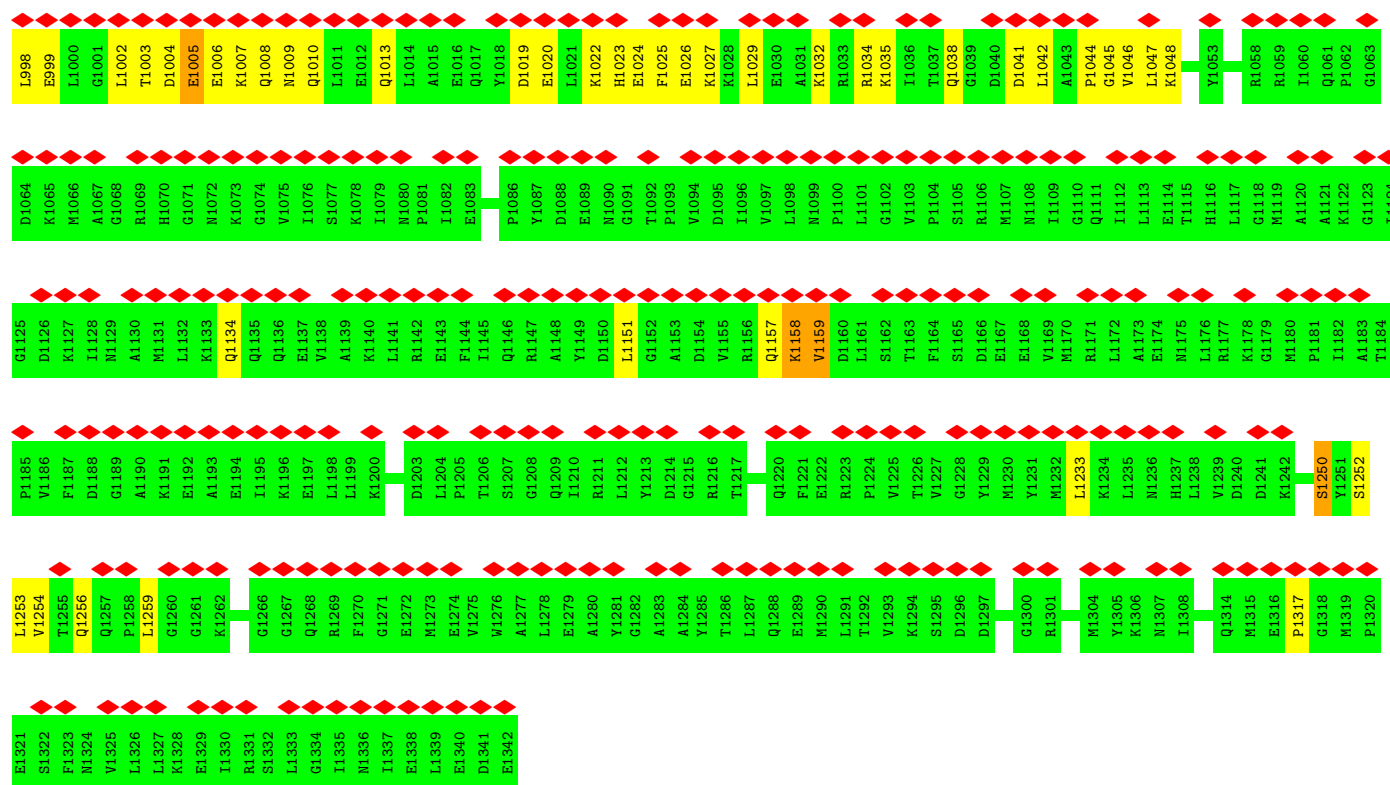
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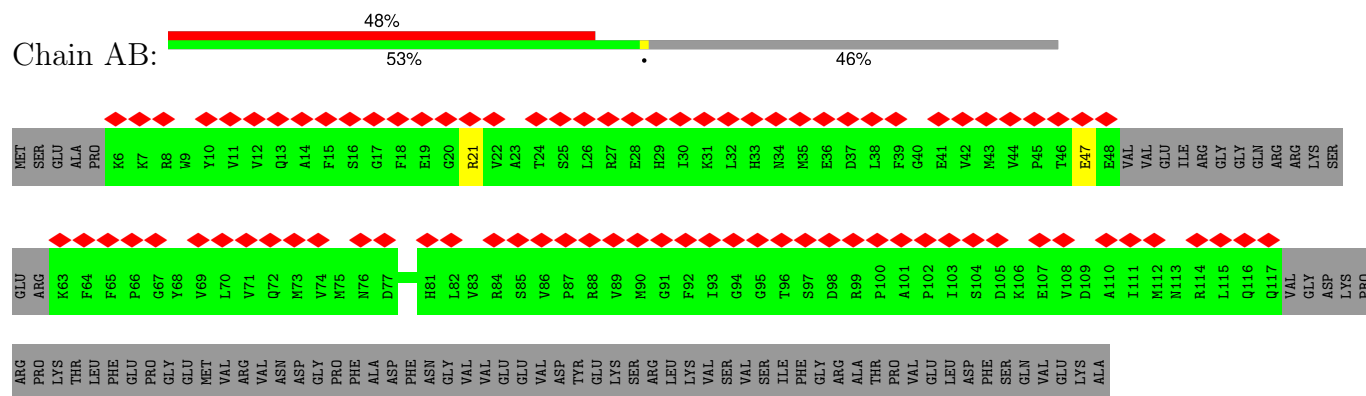
- Molecule 11: DNA-directed RNA polymerase subunit beta



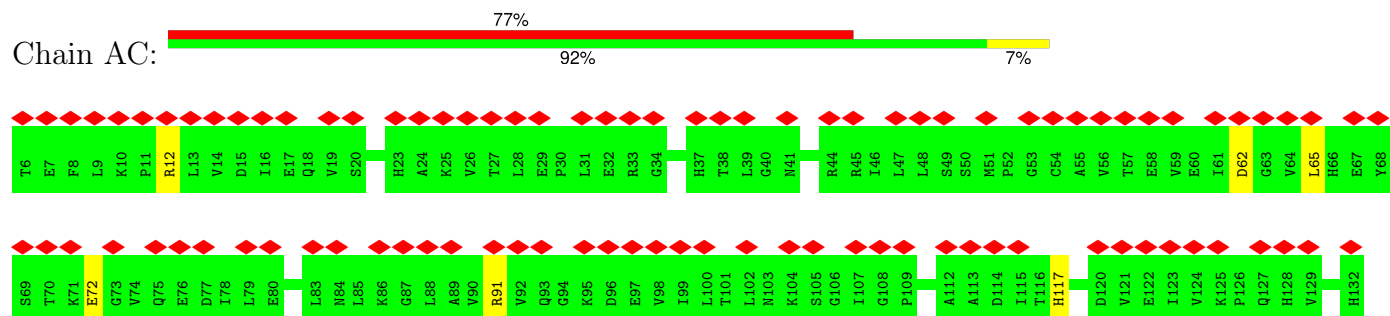
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D866	E867	S868	G869	I870	V871	W872	I873	G874	A875	E876	V877	L883	V884	G885	K886	P889	K890	G891	GLU	THR	GLN	LEU	THR	PRO	GLU	GLU	LYS	LEU	LEU	ARG	ALA	ALA	ILE	PHE	GLY	GLU	LYS	ALA	S911	D912	V913	K914	G846	P847	E848	E849	T850	T851	A852	D853	I854	P855	I856	W857	G858	E859	A860	V861	L862	S863	K864	T865																																						
I734	K735	V736	W737	E738	D739	E740	W741	V742	P743	G744	E745	A746	G747	I748	D749	W750	Y751	W752	L753	T754	S759	W760	Q761	W762	T763	C764	W765	I766	Q767	W768	P769	C770	C771	W771	S772	L773	G774	E775	P776	V777	E778	R779	G780	D781	V782	L783	A784	P885	I886	W887	G888	E889	V890	V891	V892	V893	V894	V895	V896	V897	V898	V899	V900	V901	V902	V903	V904	V905	V906	V907	V908	V909	V910	V911	V912	V913	V914	V915	V916	V917	V918	V919	V920	V921	V922	V923	V924	V925	V926	V927	V928	V929	V930	V931	V932	V933	V934	V935	V936	V937
H673	D674	D675	A676	R677	R678	A679	L680	G681	G682	A683	G684	G685	Q686	R687	Q688	V689	P691	T692	L693	R694	A695	D696	K697	P698	L699	V700	G701	T702	G703	W704	E705	S643	L644	F645	S646	R647	D648	Q649	V650	D651	V652	H653	D654	V655	S656	T657	V658	V659	T660	D601	E602	L603	H604	V605	L606	S607	A608	L609	E610	G664	A665	S666	L667	T668	P669	F670	L671	E672																																
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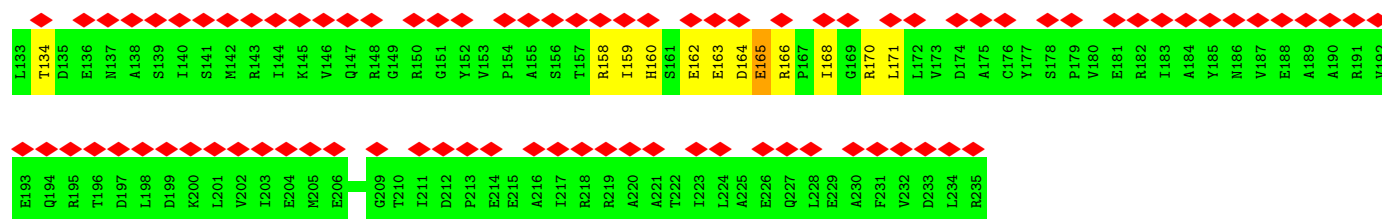


- Molecule 12: Transcription termination/antitermination protein NusG

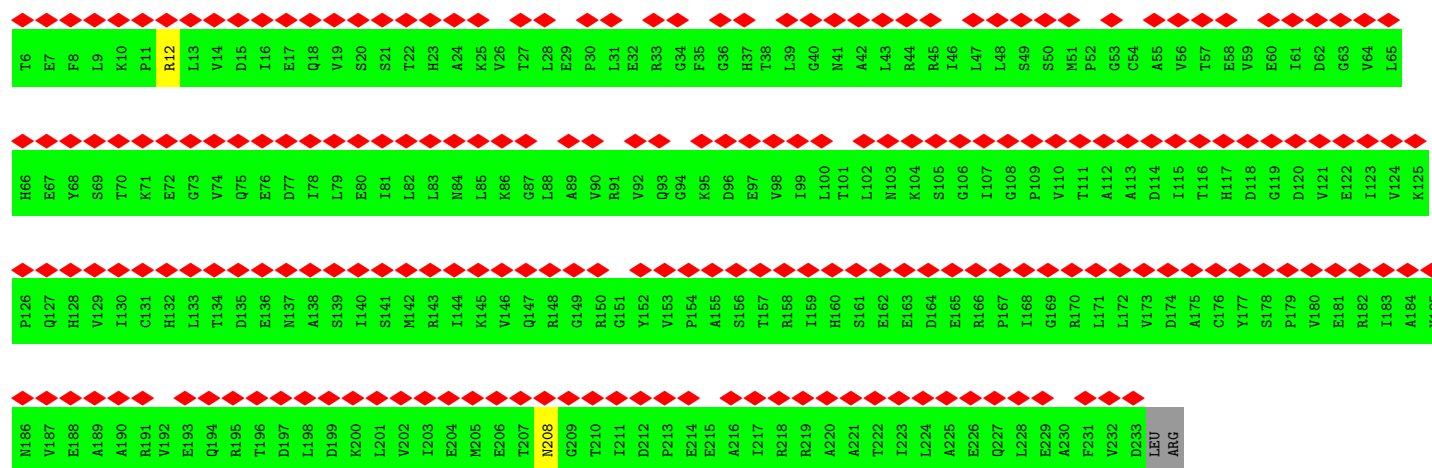


- Molecule 13: DNA-directed RNA polymerase subunit alpha

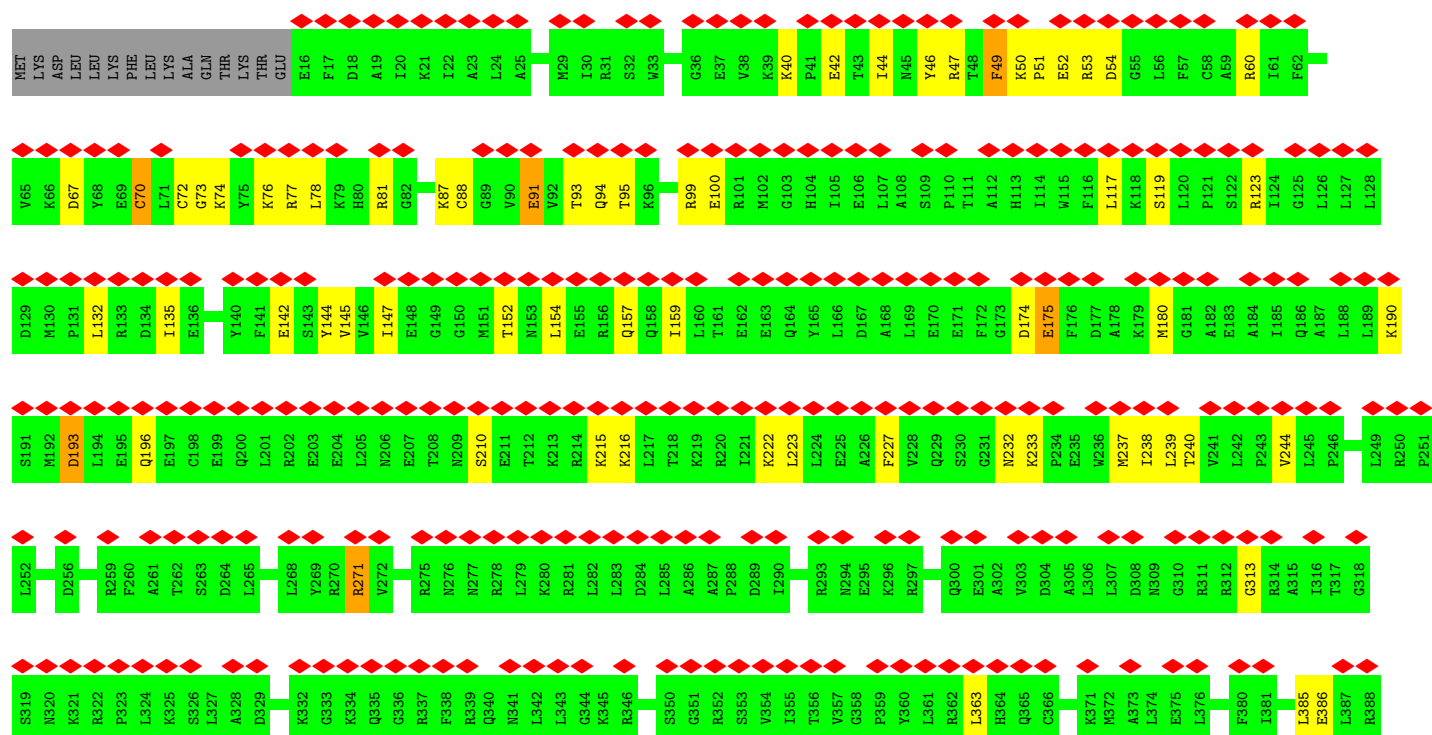
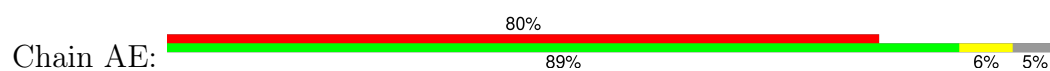




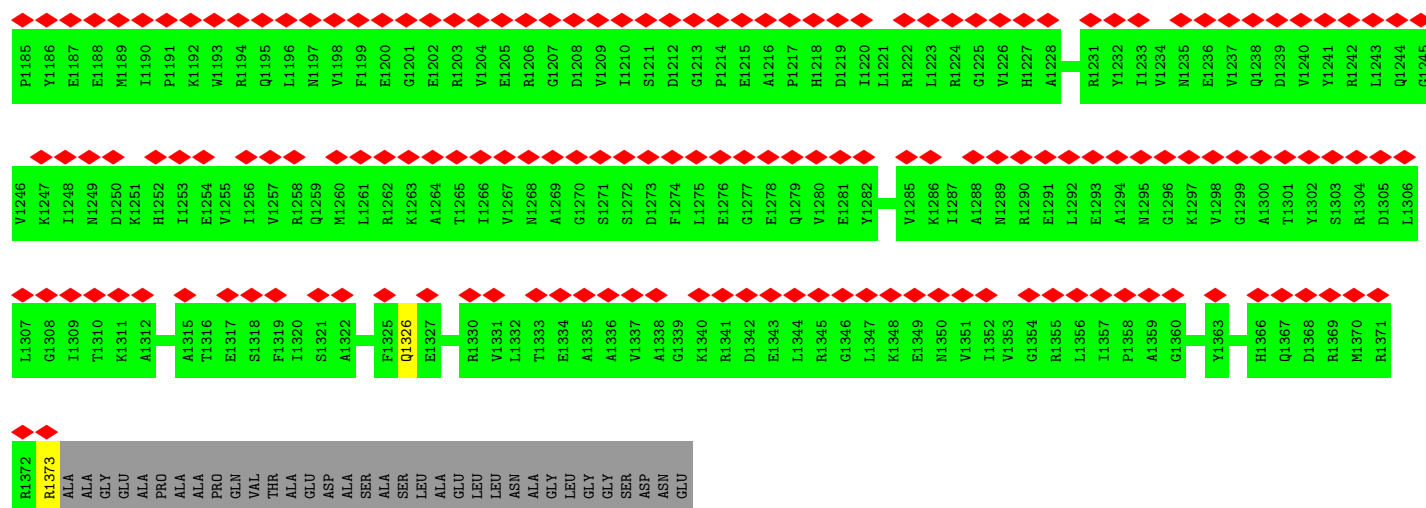
• Molecule 13: DNA-directed RNA polymerase subunit alpha



• Molecule 14: DNA-directed RNA polymerase subunit beta'

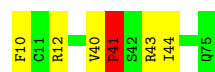


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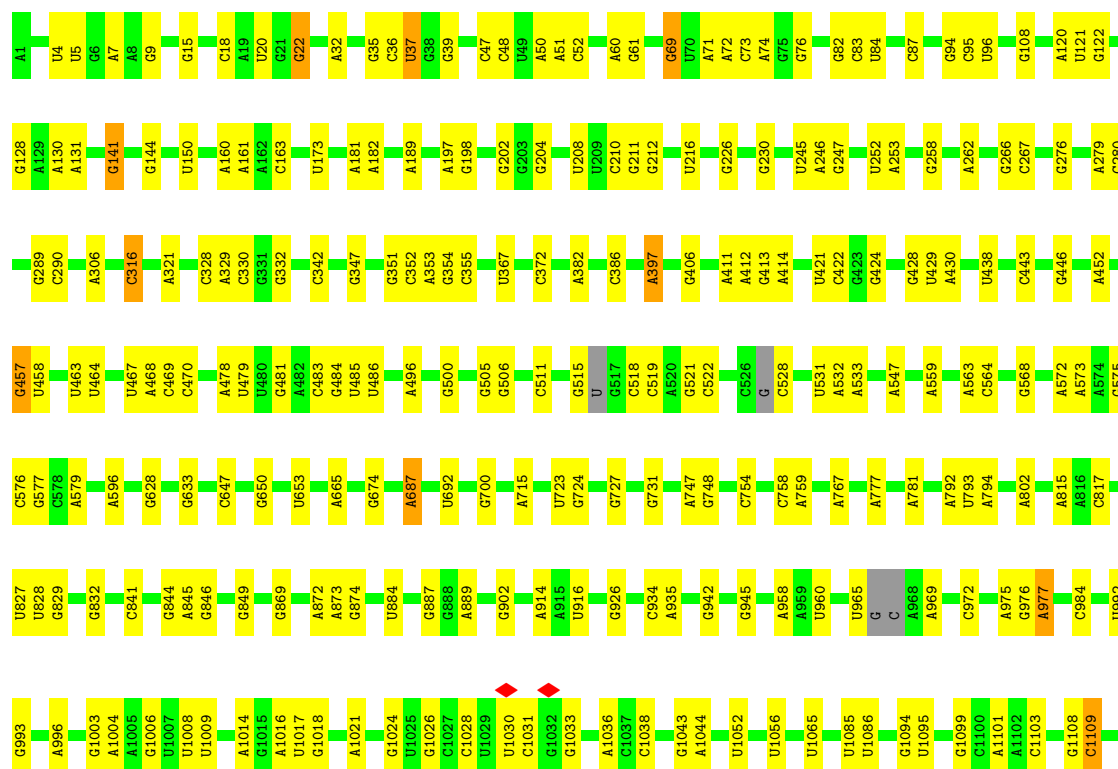
- Molecule 15: 30S ribosomal protein S18

Chain C:



- Molecule 16: 16S rRNA

Chain D:



- Molecule 17: 30S ribosomal protein S20

Chain E: 100%

There are no outlier residues recorded for this chain.

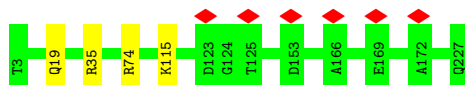
- Molecule 18: 30S ribosomal protein S21

Chain F:  97%

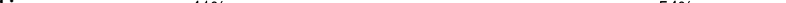


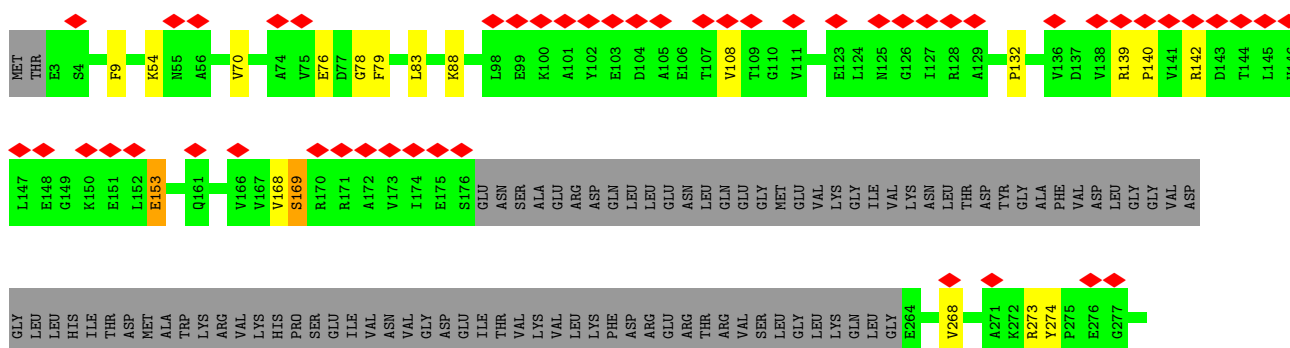
- Molecule 19: 30S ribosomal protein S2

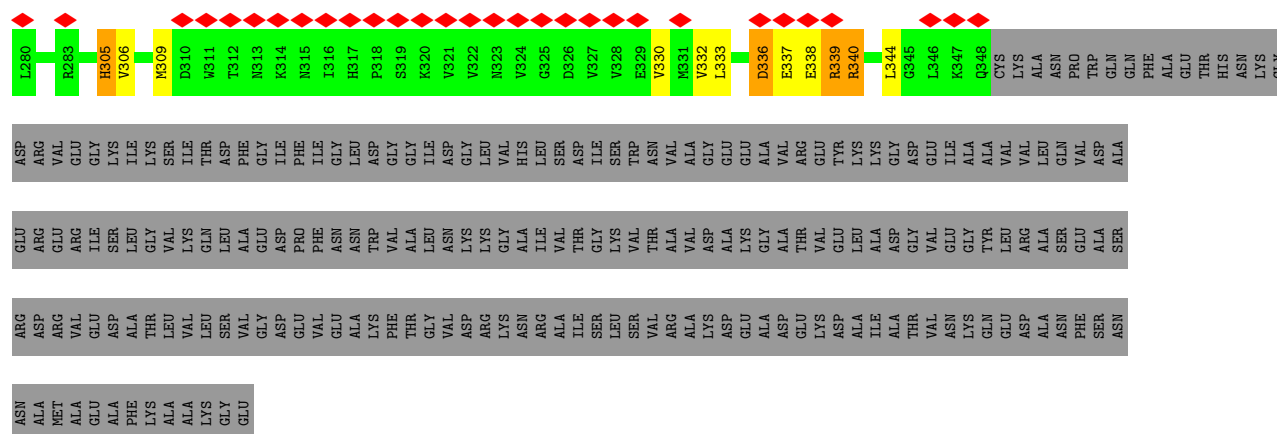
Chain G:  98%



- Molecule 20: 30S ribosomal protein S1

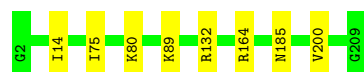
Chain H: 





- Molecule 21: 30S ribosomal protein S3

Chain I: 96%



- Molecule 22: 30S ribosomal protein S4

Chain J: 96%



- Molecule 23: 30S ribosomal protein S5

Chain K: 99%



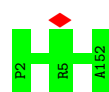
- Molecule 24: 30S ribosomal protein S6

Chain L:  100%

There are no outlier residues recorded for this chain.

- Molecule 25: 30S ribosomal protein S7

Chain M:  100%



- Molecule 26: 30S ribosomal protein S8

Chain N:  100%


There are no outlier residues recorded for this chain.

- Molecule 27: 30S ribosomal protein S9

Chain O:  98% 



- Molecule 28: 30S ribosomal protein S10

Chain P:  90%  10%



- Molecule 29: 30S ribosomal protein S11

Chain Q:  100%



- Molecule 30: 30S ribosomal protein S12

Chain R:  94% 



- Molecule 31: 30S ribosomal protein S14

Chain S:  96% 



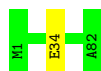
- Molecule 32: 30S ribosomal protein S15

Chain T:  100%

There are no outlier residues recorded for this chain.

- Molecule 33: 30S ribosomal protein S16

Chain U:  99% 



- Molecule 34: 30S ribosomal protein S17

Chain V: 99%



- Molecule 35: 30S ribosomal protein S19

Chain W: 100%

There are no outlier residues recorded for this chain.

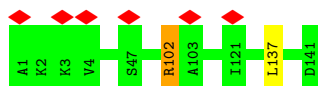
- Molecule 36: 30S ribosomal protein S13

Chain X: 99%



- Molecule 37: 50S ribosomal protein L11

Chain Y: 99%



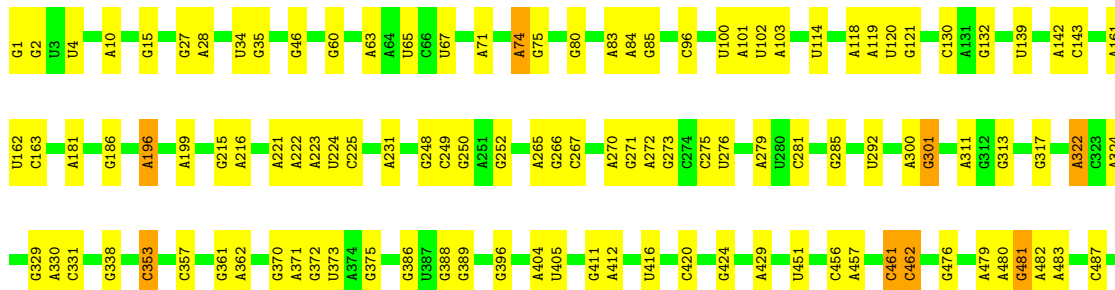
- Molecule 38: 50S ribosomal protein L7/L12

Chain Z: 100%

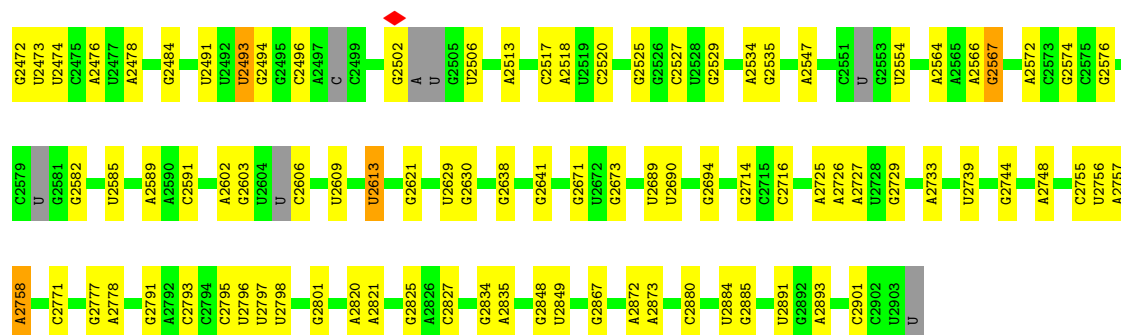
There are no outlier residues recorded for this chain.

- Molecule 39: 23S rRNA

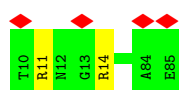
Chain a: 75% 22%



U2344	A2198	G2107	U1991	G1863	A1668	C1536	A1392	U1198	U1065	A899	G757	A613	G491
G2345	U2203	A2108	G1992	U1864	G1674	G1537	A1395	G1210	A1066	A910	A764	A614	G498
C2347	G2204	U2109	U1993	G1869	A1713	A1549	A1395	G1210	G1068	G914	C765	A616	U615
C2350	A2211	U2110	C1997	A1871	U1714	U1554	U1406	G1227	A1069	C915	G775	A621	G500
G2357	A2212	G2112	A2013	A1872	G1715	C1557	G1407	G1236	A1070	U931	G776	A621	A501
G2361	A2225	U2113	A2018	C1881	A1722	C1564	U1409	A1237	C1072	U941	A782	G625	A505
G2361	C2226	G2115	G2018	A1889	C1726	C1564	C1414	G1238	A1073	G942	G784	A627	A508
U2372	U2229	G2116	A2019	C1889	U1729	A1566	U1416	G1248	C1079	C946	G785	A637	C510
G2373	G2230	U2117	A2020	C1893	A1730	A1569	C1417	U1249	A1080	G961	C795	C640	C517
C2374	U2231	U2118	C2021	C1893	G1731	A1569	G1418	A1253	U1081	G954	A783	G646	A509
G2375	U2231	A2119	U2022	C1893	C1732	G1573	C1417	G1256	U1082	U	G784	A647	C510
A2376	G2238	G2121	C2023	G1906	G1733	C1574	A1420	C1270	U1083	G974	A819	A654	A532
G2376	G2239	G2122	G2027	G1907	C1734	C1574	A1420	G1271	A1084	G974	A819	A655	G533
C2380	G2239	G2123	U2028	G1910	U1738	C1577	A1427	A1266	A1085	G956	G805	C645	C527
U2383	U2243	G2124	G2029	U	A1764	U1578	C1428	G1266	A1086	C961	C812	U646	A528
U2384	C2248	A2126	A	A1912	A1787	U1578	C1428	G1266	A1087	G961	C812	U646	A529
U2249	U2249	G2127	A2031	A1913	C1764	A1580	A1433	G1271	U1088	G974	A819	A654	C531
C2385	G2250	G2128	G2032	C1914	C1764	G1581	A1433	A1284	A1088	G974	A819	A654	A532
G2395	G	U2131	A2033	U	A1773	C1582	A1453	G1300	A1088	G974	A819	A654	G533
G2396	G2252	U2132	C2043	A1916	U1775	A1583	A1453	G1301	U1101	A983	U827	A661	G543
U2402	U2257	U2133	G2048	A1918	U1775	U1589	G1459	A1301	G1107	A984	U828	A661	G543
C2403	U2257	A2134	G2049	A1919	A1787	U1590	G1459	G1277	A1111	C992	G831	G664	U546
U2419	A2273	U2139	C2050	G1921	C1787	A1590	U1460	G1277	G1112	C993	G831	G664	A547
U2423	A2278	U2146	A2051	G1922	U1791	C1604	G1478	A1284	U1119	C994	C837	A668	G548
C2428	A2288	C2146	A2052	C1924	U1798	C1604	G1479	G1300	G1122	C995	C838	A676	G549
A2425	C2283	A2147	C2055	G1925	G1799	C1607	G1482	G1301	G1122	A996	A845	A676	C550
A2426	A2284	U2154	G2056	U1926	C1800	A1609	A1490	A1301	U1129	U999	U846	A685	G551
G2427	A2287	G2157	G2057	G1929	A1801	A1610	G1491	U1313	G1131	U1012	C851	A685	C557
G2428	A2288	A2158	A2060	G1930	A1805	G1613	G1492	U1329	U1132	C1013	U702	A685	C557
G2429	A2297	C2159	G2061	A1938	C1806	A1616	C1493	G1339	A1133	U1019	U703	A685	A563
U2431	U2305	C2160	A2062	U	A1807	C1617	U1497	U1344	A1134	A1020	G704	U567	U568
A2435	U2305	C2161	U2068	U1940	C1816	A	C1498	C1345	C1135	A1021	U710	U569	U569
U2441	A2309	G2162	G	U1955	C1816	G1619	C1499	U1345	G1136	U1022	C717	U573	U573
G2444	G2325	A2171	A2070	U1961	A1829	G1622	A1502	U1352	U1141	U1023	G869	A574	A574
G2446	C2326	C2172	A2071	C1961	C1832	A1634	A1503	A1354	A1142	G1026	G876	A575	A575
G2447	A2327	U2172	A2072	C	C1833	A1634	A1504	A1354	G1166	U1033	A877	A586	A586
A2448	C2328	C2173	U2075	U1963	U1834	C1638	A1508	A1359	A1169	U1041	A878	G729	C587
G2448	A2329	A2176	A2080	G1965	G	C1836	A1509	C1363	C1170	G1044	U884	A742	U588
C2456	U2329	U2182	C2084	A1966	U1841	U1647	A1510	G1364	U1173	C1044	C885	A742	U588
U	C2332	A2183	C2089	C1967	A1847	U1648	A1515	G1365	U1174	C1045	A886	A743	A599
G2458	A2333	U2189	C2089	U1970	A1847	G1649	C1526	G1368	A1175	A1046	A887	U744	A599
A2459	U2334	G2190	C2096	U1971	A1848	G1651	C1526	G1368	U1176	G1047	G891	U	A603
A2335	A2335	U2194	C2097	G1972	A1848	G1651	C1526	G1368	G1177	U1060	U891	G	G604
C2463	C2338	G2194	A2097	U1976	G1857	G1659	G1529	A1378	C1178	U1061	U895	U	G605
G2470	C2339	U2194	U2098	U1976	A1858	G1659	C1533	U1379	G1179	U1061	A896	G748	G605
A2471	C2339	U2194	G2100	A1987	U1859	A1665	U1534	G1380	U1180	G1063	C897	G748	A608
							A1535	A1383	G1186	C1064	C898	A752	A609



- Molecule 40: 50S ribosomal protein L27

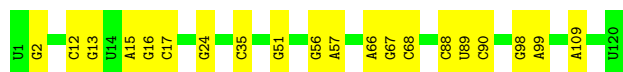
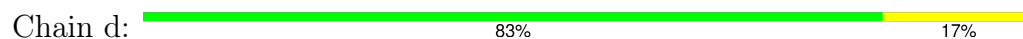


- Molecule 41: 50S ribosomal protein L28



There are no outlier residues recorded for this chain.

- Molecule 42: 5S rRNA



- Molecule 43: 50S ribosomal protein L29



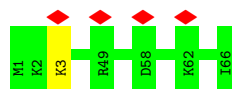
There are no outlier residues recorded for this chain.

- Molecule 44: 50S ribosomal protein L30




There are no outlier residues recorded for this chain.

- Molecule 45: 50S ribosomal protein L31



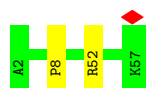
- Molecule 46: 50S ribosomal protein L2

Chain h:  100%



- Molecule 47: 50S ribosomal protein L32

Chain i:  96%



- Molecule 48: 50S ribosomal protein L3

Chain j:  100%



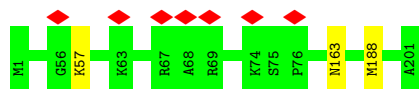
- Molecule 49: 50S ribosomal protein L33

Chain k:  100%

There are no outlier residues recorded for this chain.

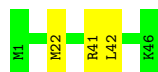
- Molecule 50: 50S ribosomal protein L4

Chain l:  99%



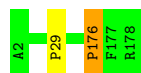
- Molecule 51: 50S ribosomal protein L34

Chain m:  93%



- Molecule 52: 50S ribosomal protein L5

Chain n:  99%



- Molecule 53: 50S ribosomal protein L35

Chain o:  97%



- Molecule 54: 50S ribosomal protein L6

Chain p:  98%



- Molecule 55: 50S ribosomal protein L36

Chain q:  95% 5%



- Molecule 56: 50S ribosomal protein L9

Chain r:  100%



- Molecule 57: 50S ribosomal protein L13

Chain s:  100%

There are no outlier residues recorded for this chain.

- Molecule 58: 50S ribosomal protein L14

Chain t:  100%

There are no outlier residues recorded for this chain.

- Molecule 59: 50S ribosomal protein L15

Chain u:  100%

There are no outlier residues recorded for this chain.

- Molecule 60: 50S ribosomal protein L16

Chain v:  99%



- Molecule 61: 50S ribosomal protein L17

Chain w:  99% .



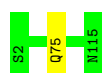
- Molecule 62: 50S ribosomal protein L18

Chain x:  100%

There are no outlier residues recorded for this chain.

- Molecule 63: 50S ribosomal protein L19

Chain y:  99% .



- Molecule 64: 50S ribosomal protein L20

Chain z:  99% .



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	24959	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	45	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	0.093	Depositor
Minimum map value	-0.039	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.007	Depositor
Map size (\AA)	548.05, 548.05, 548.05	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.0961, 1.0961, 1.0961	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.51	0/829	0.70	0/1107
2	1	0.48	0/864	0.62	0/1156
3	2	0.48	0/752	0.63	0/1005
4	3	0.46	0/796	0.65	0/1062
5	4	0.47	0/766	0.60	0/1025
6	5	1.13	6/528 (1.1%)	0.97	1/810 (0.1%)
7	6	1.11	4/603 (0.7%)	0.97	0/926
8	7	0.60	2/681 (0.3%)	0.92	3/1058 (0.3%)
9	9	0.34	0/1131	0.63	1/1524 (0.1%)
10	A	0.55	0/1810	1.28	11/2821 (0.4%)
10	B	0.55	0/1810	1.28	11/2821 (0.4%)
11	AA	0.58	2/10591 (0.0%)	0.75	15/14289 (0.1%)
12	AB	0.43	0/808	0.59	0/1088
13	AC	0.48	0/1808	0.62	1/2450 (0.0%)
13	AD	0.39	0/1789	0.56	0/2425
14	AE	0.50	3/10545 (0.0%)	0.66	4/14236 (0.0%)
15	C	0.88	3/553 (0.5%)	0.86	2/743 (0.3%)
16	D	0.69	9/36610 (0.0%)	1.21	107/57091 (0.2%)
17	E	0.50	0/675	0.64	0/895
18	F	0.53	0/597	0.63	0/792
19	G	0.47	0/1791	0.61	0/2413
20	H	0.57	1/1746 (0.1%)	1.05	13/2382 (0.5%)
21	I	0.44	0/1663	0.71	0/2241
22	J	0.48	0/1665	0.74	0/2227
23	K	0.52	0/1165	0.67	0/1568
24	L	0.54	0/867	0.70	0/1171
25	M	0.51	0/1195	0.63	0/1602
26	N	0.50	0/989	0.68	0/1326
27	O	0.59	0/1034	0.78	0/1375
28	P	0.44	0/800	0.77	0/1082
29	Q	0.47	0/893	0.65	0/1205
30	R	0.72	2/952 (0.2%)	0.80	1/1274 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
31	S	0.48	0/817	0.69	0/1088
32	T	0.47	0/722	0.62	0/964
33	U	0.58	2/659 (0.3%)	0.67	0/884
34	V	0.50	0/657	0.64	0/881
35	W	0.46	0/680	0.62	0/915
36	X	0.43	0/909	0.59	0/1215
37	Y	0.37	0/1046	0.59	2/1410 (0.1%)
38	Z	0.28	0/227	0.47	0/304
39	a	0.69	12/69247 (0.0%)	1.19	226/107985 (0.2%)
40	b	0.49	0/589	0.59	0/779
41	c	0.47	0/635	0.67	0/848
42	d	0.67	0/2872	1.10	2/4478 (0.0%)
43	e	0.44	0/502	0.59	0/667
44	f	0.43	0/452	0.66	0/605
45	g	0.44	0/531	0.62	0/709
46	h	0.61	2/2121 (0.1%)	0.76	4/2852 (0.1%)
47	i	0.65	1/450 (0.2%)	0.86	2/599 (0.3%)
48	j	0.50	0/1586	0.67	0/2134
49	k	0.51	0/433	0.60	0/576
50	l	0.47	0/1571	0.65	1/2113 (0.0%)
51	m	0.55	0/380	0.98	0/498
52	n	0.77	4/1434 (0.3%)	0.91	7/1926 (0.4%)
53	o	0.47	0/513	0.73	0/676
54	p	0.60	3/1333 (0.2%)	0.78	4/1805 (0.2%)
55	q	0.77	1/303 (0.3%)	0.84	1/397 (0.3%)
56	r	0.43	0/1122	0.60	0/1515
57	s	0.50	0/1152	0.64	0/1551
58	t	0.51	0/955	0.69	0/1279
59	u	0.50	0/1062	0.71	0/1413
60	v	0.53	0/1093	0.68	0/1460
61	w	0.51	0/964	0.69	0/1289
62	x	0.46	0/902	0.61	0/1209
63	y	0.54	0/929	0.65	0/1242
64	z	0.53	0/960	0.80	2/1278 (0.2%)
All	All	0.63	57/189114 (0.0%)	1.04	421/278734 (0.2%)

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
9	9	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
11	AA	0	10
14	AE	0	5
20	H	0	1
27	O	0	1
30	R	0	1
36	X	0	1
40	b	0	1
52	n	0	1
53	o	0	1
54	p	0	1
All	All	0	26

All (57) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	C	41	PRO	N-CA	14.00	1.71	1.47
46	h	107	PRO	CG-CD	-14.00	1.04	1.50
30	R	42	PRO	N-CA	13.72	1.70	1.47
52	n	176	PRO	CG-CD	-13.50	1.06	1.50
52	n	29	PRO	CG-CD	-11.86	1.11	1.50
11	AA	374	GLU	C-N	10.40	1.54	1.34
52	n	29	PRO	N-CD	9.34	1.60	1.47
54	p	154	PRO	CG-CD	-8.76	1.21	1.50
6	5	109	DT	O3'-P	8.71	1.71	1.61
7	6	10	DG	C1'-N9	-8.25	1.35	1.47
11	AA	850	ILE	N-CA	-8.17	1.30	1.46
39	a	462	C	C4-C5	-8.11	1.36	1.43
39	a	2013	A	C6-N1	-7.67	1.30	1.35
20	H	169	SER	N-CA	7.49	1.61	1.46
46	h	107	PRO	N-CD	7.40	1.58	1.47
47	i	8	PRO	CG-CD	-7.36	1.26	1.50
6	5	121	DG	C1'-N9	-7.25	1.37	1.47
8	7	19	G	C1'-N9	-7.22	1.36	1.46
16	D	563	A	C6-N1	-7.17	1.30	1.35
39	a	462	C	N1-C6	-7.16	1.32	1.37
39	a	2013	A	C6-N6	-7.03	1.28	1.33
8	7	-7	U	C1'-N1	6.94	1.59	1.48
16	D	397	A	C6-N1	-6.88	1.30	1.35
39	a	1141	U	N3-C4	-6.78	1.32	1.38
52	n	176	PRO	N-CD	6.76	1.57	1.47
16	D	37	U	N3-C4	-6.73	1.32	1.38
15	C	40	VAL	C-N	6.72	1.47	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	p	154	PRO	N-CD	6.68	1.57	1.47
6	5	112	DG	C1'-N9	-6.63	1.38	1.47
6	5	100	DA	C1'-N9	-6.58	1.38	1.47
7	6	21	DA	C1'-N9	-6.51	1.38	1.47
39	a	2613	U	N3-C4	-6.45	1.32	1.38
39	a	1021	A	C6-N1	-6.44	1.31	1.35
55	q	1	MET	N-CA	6.34	1.59	1.46
30	R	41	THR	C-N	6.32	1.46	1.34
39	a	1142	A	C6-N1	-6.24	1.31	1.35
14	AE	93	THR	CA-C	6.22	1.69	1.52
6	5	115	DA	C1'-N9	-6.08	1.38	1.47
6	5	116	DG	C1'-N9	-6.07	1.38	1.47
33	U	34	GLU	CG-CD	5.90	1.60	1.51
14	AE	70	CYS	CA-CB	-5.85	1.41	1.53
7	6	28	DA	C1'-N9	-5.75	1.39	1.47
16	D	1125	U	P-O5'	-5.70	1.54	1.59
33	U	34	GLU	CB-CG	-5.61	1.41	1.52
16	D	1358	U	N3-C4	-5.60	1.33	1.38
16	D	827	U	N3-C4	-5.58	1.33	1.38
16	D	1363	A	C6-N6	-5.40	1.29	1.33
16	D	1363	A	C6-N1	-5.38	1.31	1.35
16	D	563	A	C6-N6	-5.37	1.29	1.33
39	a	1082	U	N3-C4	-5.36	1.33	1.38
39	a	1021	A	C6-N6	-5.30	1.29	1.33
7	6	24	DT	C1'-N1	5.28	1.56	1.49
39	a	1019	U	N3-C4	-5.27	1.33	1.38
15	C	10	PHE	CB-CG	5.16	1.60	1.51
39	a	74	A	C6-N1	-5.11	1.31	1.35
54	p	153	ARG	C-N	-5.05	1.24	1.34
14	AE	801	VAL	CB-CG2	-5.05	1.42	1.52

All (421) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	D	37	U	C5-C4-O4	34.28	146.47	125.90
39	a	1141	U	C5-C4-O4	33.53	146.02	125.90
16	D	1358	U	C5-C4-O4	31.93	145.06	125.90
16	D	37	U	N3-C4-O4	-31.78	97.16	119.40
39	a	1019	U	C5-C4-O4	31.05	144.53	125.90
16	D	884	U	C5-C4-O4	30.65	144.29	125.90
39	a	2613	U	C5-C4-O4	30.51	144.21	125.90
39	a	1082	U	C5-C4-O4	30.37	144.12	125.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	D	827	U	C5-C4-O4	30.05	143.93	125.90
39	a	1141	U	N3-C4-O4	-29.54	98.72	119.40
16	D	1358	U	N3-C4-O4	-29.48	98.77	119.40
39	a	1082	U	N3-C4-O4	-29.35	98.85	119.40
16	D	884	U	N3-C4-O4	-29.14	99.00	119.40
16	D	827	U	N3-C4-O4	-28.93	99.15	119.40
39	a	1019	U	N3-C4-O4	-28.47	99.47	119.40
39	a	2613	U	N3-C4-O4	-27.18	100.38	119.40
39	a	1021	A	N1-C6-N6	-21.07	105.96	118.60
39	a	1142	A	N1-C6-N6	-20.61	106.24	118.60
16	D	397	A	N1-C6-N6	-20.37	106.38	118.60
16	D	563	A	N1-C6-N6	-19.01	107.19	118.60
39	a	1086	A	N1-C6-N6	-18.66	107.41	118.60
39	a	2013	A	N1-C6-N6	-18.32	107.61	118.60
39	a	462	C	C5-C6-N1	17.71	129.85	121.00
46	h	107	PRO	N-CD-CG	-16.88	77.88	103.20
52	n	29	PRO	N-CD-CG	-16.56	78.36	103.20
16	D	872	A	N1-C6-N6	-16.48	108.71	118.60
54	p	154	PRO	N-CD-CG	-16.45	78.52	103.20
39	a	462	C	C6-N1-C2	-16.28	113.79	120.30
52	n	176	PRO	N-CD-CG	-15.69	79.67	103.20
16	D	1363	A	N1-C6-N6	-15.28	109.44	118.60
10	A	39	C	C4-C5-C6	15.00	124.90	117.40
10	B	39	C	C4-C5-C6	14.94	124.87	117.40
39	a	2756	U	N3-C4-O4	-14.19	109.47	119.40
39	a	67	U	N3-C4-O4	-13.59	109.89	119.40
64	z	55	ARG	NE-CZ-NH2	12.85	126.73	120.30
39	a	1021	A	C5-C6-N6	12.68	133.85	123.70
16	D	397	A	C5-C6-N6	12.26	133.51	123.70
10	A	39	C	N3-C4-C5	-12.24	117.00	121.90
10	B	39	C	N3-C4-C5	-12.18	117.03	121.90
39	a	1086	A	C5-C6-N6	11.51	132.91	123.70
39	a	1142	A	C5-C6-N6	11.35	132.78	123.70
39	a	1141	U	C2-N3-C4	11.32	133.79	127.00
16	D	563	A	C5-C6-N6	11.22	132.68	123.70
11	AA	1250	SER	C-N-CA	11.18	149.66	121.70
64	z	55	ARG	NE-CZ-NH1	-10.71	114.94	120.30
47	i	8	PRO	N-CD-CG	-10.18	87.94	103.20
16	D	1125	U	O5'-P-OP2	-10.11	96.60	105.70
20	H	169	SER	N-CA-C	10.02	138.04	111.00
15	C	41	PRO	CA-N-CD	-10.00	97.50	111.50
39	a	461	C	N1-C2-O2	9.80	124.78	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	a	1082	U	N1-C2-N3	-9.68	109.09	114.90
39	a	1082	U	C2-N3-C4	9.67	132.81	127.00
39	a	2496	C	N3-C2-O2	-9.53	115.23	121.90
39	a	974	G	O4'-C1'-N9	9.51	115.81	108.20
14	AE	271	ARG	NE-CZ-NH2	-9.39	115.61	120.30
11	AA	375	PRO	CA-N-CD	-9.30	98.48	111.50
39	a	2013	A	C5-C6-N6	9.08	130.97	123.70
39	a	2496	C	N1-C2-O2	9.03	124.32	118.90
16	D	1363	A	C5-C6-N6	9.00	130.90	123.70
39	a	1082	U	C4-C5-C6	-8.91	114.36	119.70
16	D	37	U	C2-N3-C4	8.88	132.33	127.00
39	a	1019	U	C2-N3-C4	8.88	132.33	127.00
16	D	397	A	N1-C2-N3	-8.77	124.92	129.30
16	D	872	A	C5-C6-N6	8.75	130.70	123.70
20	H	88	LYS	C-N-CA	8.72	143.50	121.70
39	a	2756	U	C5-C4-O4	8.61	131.07	125.90
39	a	729	G	O4'-C1'-N9	8.49	114.99	108.20
16	D	1358	U	C2-N3-C4	8.46	132.08	127.00
39	a	2013	A	N1-C2-N3	-8.39	125.10	129.30
39	a	2758	A	N1-C6-N6	-8.38	113.57	118.60
39	a	1141	U	N1-C2-N3	-8.32	109.91	114.90
11	AA	995	ASP	O-C-N	-8.26	109.49	122.70
39	a	67	U	C5-C4-O4	8.18	130.81	125.90
39	a	74	A	N1-C6-N6	-8.12	113.72	118.60
11	AA	376	PRO	N-CA-CB	-8.02	93.67	103.30
52	n	29	PRO	CA-CB-CG	-7.99	88.82	104.00
52	n	176	PRO	CA-N-CD	-7.97	100.34	111.50
16	D	1358	U	N1-C2-N3	-7.96	110.12	114.90
16	D	1145	A	N9-C4-C5	-7.87	102.65	105.80
30	R	42	PRO	CA-N-CD	-7.85	100.51	111.50
54	p	154	PRO	CA-CB-CG	-7.73	89.31	104.00
46	h	107	PRO	CA-N-CD	-7.67	100.75	111.50
52	n	29	PRO	CA-N-CD	-7.62	100.83	111.50
16	D	37	U	N1-C2-N3	-7.60	110.34	114.90
20	H	305	HIS	N-CA-C	7.47	131.18	111.00
39	a	2013	A	C5-C6-N1	7.45	121.42	117.70
39	a	1141	U	C4-C5-C6	-7.44	115.24	119.70
39	a	2613	U	C2-N3-C4	7.42	131.45	127.00
39	a	143	C	N1-C2-O2	7.36	123.32	118.90
39	a	196	A	O4'-C1'-N9	7.36	114.09	108.20
39	a	2013	A	N9-C4-C5	-7.30	102.88	105.80
10	B	39	C	C5-C6-N1	-7.29	117.36	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	D	754	C	N1-C2-O2	7.26	123.26	118.90
10	A	39	C	C5-C6-N1	-7.25	117.37	121.00
16	D	1016	A	N1-C6-N6	7.24	122.94	118.60
16	D	37	U	C4-C5-C6	-7.24	115.36	119.70
8	7	-8	A	OP2-P-O3'	7.21	121.06	105.20
39	a	357	C	N3-C2-O2	-7.20	116.86	121.90
39	a	910	A	N1-C6-N6	-7.19	114.28	118.60
10	B	76	A	O4'-C1'-N9	7.11	113.88	108.20
39	a	461	C	C2-N1-C1'	7.01	126.52	118.80
39	a	1019	U	N1-C2-N3	-6.99	110.70	114.90
10	A	76	A	O4'-C1'-N9	6.99	113.79	108.20
39	a	2641	G	N3-C4-N9	-6.99	121.81	126.00
10	A	37	A	C5-C6-N6	6.95	129.26	123.70
39	a	2329	U	C5-C6-N1	6.94	126.17	122.70
16	D	1145	A	C4-C5-N7	6.92	114.16	110.70
11	AA	855	PRO	N-CA-CB	-6.89	95.02	102.60
10	B	37	A	C5-C6-N6	6.87	129.20	123.70
39	a	1638	C	N1-C2-O2	6.82	122.99	118.90
39	a	1044	C	C6-N1-C2	6.81	123.03	120.30
8	7	-8	A	O3'-P-O5'	-6.78	91.11	104.00
39	a	1816	C	C6-N1-C2	6.75	123.00	120.30
39	a	2771	C	N1-C2-O2	6.74	122.94	118.90
11	AA	995	ASP	CA-C-N	6.74	132.02	117.20
39	a	2758	A	C5-C6-N6	6.73	129.08	123.70
16	D	884	U	C2-N3-C4	6.72	131.03	127.00
39	a	1021	A	N1-C2-N3	-6.69	125.95	129.30
46	h	107	PRO	CA-CB-CG	-6.67	91.33	104.00
39	a	461	C	C6-N1-C1'	-6.62	112.85	120.80
39	a	1832	C	N1-C2-O2	6.61	122.86	118.90
39	a	357	C	N1-C2-O2	6.59	122.86	118.90
39	a	2606	C	N3-C2-O2	-6.59	117.28	121.90
10	A	37	A	N1-C6-N6	-6.59	114.64	118.60
10	A	71	C	C2-N1-C1'	6.59	126.05	118.80
10	B	71	C	C2-N1-C1'	6.58	126.04	118.80
39	a	1604	C	N1-C2-O2	6.58	122.85	118.90
39	a	1142	A	C5-C6-N1	6.57	120.98	117.70
39	a	1170	C	C2-N1-C1'	6.56	126.01	118.80
16	D	1191	A	N1-C6-N6	6.54	122.52	118.60
16	D	1145	A	C5-C6-N1	6.52	120.96	117.70
39	a	1499	C	C6-N1-C2	-6.50	117.70	120.30
39	a	2374	C	N1-C2-O2	6.50	122.80	118.90
10	B	37	A	N1-C6-N6	-6.48	114.71	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	H	339	ARG	C-N-CA	6.47	137.87	121.70
39	a	2638	G	O4'-C1'-N9	6.47	113.37	108.20
39	a	2673	G	N3-C2-N2	-6.46	115.38	119.90
16	D	1358	U	C4-C5-C6	-6.46	115.83	119.70
39	a	1857	G	O4'-C1'-N9	6.46	113.37	108.20
11	AA	935	THR	CA-CB-OG1	-6.44	95.48	109.00
39	a	2756	U	N3-C4-C5	6.44	118.46	114.60
16	D	1016	A	C5-C6-N6	-6.43	118.56	123.70
39	a	704	G	O4'-C1'-N9	6.39	113.31	108.20
10	A	61	C	N1-C2-O2	6.37	122.72	118.90
16	D	1140	C	C6-N1-C2	6.37	122.85	120.30
16	D	884	U	C4-C5-C6	-6.37	115.88	119.70
39	a	2013	A	C4-C5-N7	6.37	113.88	110.70
39	a	1019	U	C4-C5-C6	-6.35	115.89	119.70
39	a	2159	G	N1-C6-O6	-6.34	116.09	119.90
16	D	1125	U	C2-N1-C1'	6.34	125.31	117.70
39	a	1557	C	C6-N1-C2	6.34	122.83	120.30
6	5	109	DT	P-O3'-C3'	6.32	127.28	119.70
16	D	1208	C	C6-N1-C2	6.29	122.82	120.30
16	D	869	G	N3-C4-C5	6.27	131.74	128.60
39	a	1893	C	N3-C4-N4	-6.27	113.61	118.00
39	a	462	C	N1-C2-O2	6.26	122.66	118.90
39	a	322	A	N1-C6-N6	-6.25	114.85	118.60
16	D	674	G	C8-N9-C4	-6.24	103.90	106.40
39	a	2591	C	N1-C2-O2	6.24	122.64	118.90
39	a	837	C	N3-C2-O2	-6.23	117.54	121.90
13	AC	117	HIS	CB-CA-C	-6.23	97.95	110.40
39	a	992	C	C6-N1-C2	6.20	122.78	120.30
39	a	1012	U	N3-C4-O4	6.20	123.74	119.40
55	q	34	LYS	CD-CE-NZ	6.18	125.92	111.70
39	a	910	A	C8-N9-C4	6.15	108.26	105.80
11	AA	849	GLU	C-N-CA	6.13	137.02	121.70
39	a	65	U	C5-C6-N1	6.13	125.76	122.70
10	B	61	C	N1-C2-O2	6.12	122.57	118.90
39	a	2050	C	N3-C2-O2	-6.12	117.62	121.90
39	a	2013	A	C4-C5-C6	-6.10	113.95	117.00
39	a	301	G	N3-C4-C5	6.10	131.65	128.60
39	a	462	C	C2-N1-C1'	6.08	125.49	118.80
16	D	1363	A	N1-C2-N3	-6.07	126.27	129.30
39	a	2756	U	C4-C5-C6	-6.06	116.06	119.70
52	n	176	PRO	N-CA-CB	-6.05	95.94	102.60
39	a	462	C	N3-C4-C5	-6.04	119.49	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	a	2050	C	N1-C2-O2	6.03	122.52	118.90
39	a	1806	C	N1-C2-O2	6.03	122.52	118.90
16	D	1344	C	N3-C2-O2	-6.03	117.68	121.90
39	a	1	G	C4-N9-C1'	6.02	134.33	126.50
39	a	1	G	C8-N9-C1'	-6.01	119.19	127.00
39	a	221	A	O4'-C1'-N9	6.00	113.00	108.20
16	D	754	C	N3-C2-O2	-6.00	117.70	121.90
39	a	1638	C	N3-C2-O2	-6.00	117.70	121.90
54	p	154	PRO	N-CA-CB	-5.99	96.01	102.60
11	AA	1004	ASP	CB-CA-C	5.98	122.37	110.40
20	H	140	PRO	N-CA-CB	5.98	110.47	103.30
16	D	674	G	N7-C8-N9	5.97	116.09	113.10
39	a	1	G	N3-C4-N9	5.97	129.58	126.00
16	D	1124	G	C5'-C4'-O4'	-5.95	101.96	109.10
16	D	18	C	C6-N1-C2	5.95	122.68	120.30
39	a	2606	C	N1-C2-O2	5.94	122.47	118.90
39	a	2161	C	N1-C2-O2	5.94	122.46	118.90
16	D	1125	U	OP1-P-OP2	5.93	128.50	119.60
16	D	1125	U	C5-C4-O4	-5.92	122.35	125.90
39	a	1012	U	C5-C4-O4	-5.91	122.35	125.90
11	AA	727	VAL	N-CA-C	-5.91	95.05	111.00
11	AA	943	LYS	CA-C-O	-5.91	107.69	120.10
20	H	336	ASP	CB-CA-C	-5.90	98.60	110.40
39	a	67	U	N3-C4-C5	5.90	118.14	114.60
16	D	1125	U	N3-C4-O4	5.89	123.52	119.40
16	D	1150	A	C8-N9-C4	-5.89	103.44	105.80
20	H	330	VAL	N-CA-C	5.88	126.88	111.00
39	a	527	C	N3-C4-N4	-5.88	113.88	118.00
39	a	487	C	N3-C2-O2	-5.87	117.79	121.90
11	AA	943	LYS	CA-C-N	5.85	130.07	117.20
39	a	1798	U	C2-N1-C1'	-5.84	110.69	117.70
39	a	557	C	C6-N1-C2	5.84	122.64	120.30
46	h	107	PRO	N-CA-CB	-5.83	96.19	102.60
39	a	2834	G	N3-C4-N9	-5.82	122.51	126.00
20	H	132	PRO	N-CA-CB	5.81	110.28	103.30
16	D	1340	A	C5'-C4'-O4'	5.81	116.07	109.10
15	C	41	PRO	N-CD-CG	5.78	111.87	103.20
20	H	168	VAL	C-N-CA	5.78	136.15	121.70
39	a	2827	C	C6-N1-C2	5.78	122.61	120.30
14	AE	903	LEU	C-N-CA	5.77	136.13	121.70
16	D	290	C	C6-N1-C2	5.77	122.61	120.30
16	D	528	C	N1-C2-O2	5.77	122.36	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	D	827	U	C4-C5-C6	-5.76	116.24	119.70
39	a	2	G	C4-N9-C1'	5.76	133.98	126.50
39	a	876	C	C6-N1-C2	5.75	122.60	120.30
39	a	2110	G	N3-C4-C5	-5.75	125.72	128.60
39	a	2641	G	N3-C4-C5	5.75	131.48	128.60
39	a	942	G	C2-N3-C4	-5.74	109.03	111.90
16	D	872	A	C5-C6-N1	5.73	120.57	117.70
39	a	281	C	N3-C2-O2	-5.73	117.89	121.90
39	a	2795	C	C6-N1-C2	5.73	122.59	120.30
16	D	1124	G	O5'-P-OP2	-5.71	100.56	105.70
42	d	12	C	N3-C4-N4	-5.70	114.01	118.00
39	a	1379	U	C5-C4-O4	5.70	129.32	125.90
39	a	2374	C	N3-C2-O2	-5.69	117.92	121.90
20	H	344	LEU	CA-CB-CG	5.68	128.35	115.30
39	a	2096	C	C6-N1-C2	5.68	122.57	120.30
16	D	141	G	N9-C4-C5	-5.67	103.13	105.40
39	a	942	G	N3-C4-C5	5.67	131.44	128.60
39	a	1414	C	C2-N1-C1'	-5.67	112.57	118.80
39	a	838	C	N1-C2-O2	5.66	122.30	118.90
39	a	2061	G	O4'-C1'-N9	5.66	112.73	108.20
39	a	1170	C	C6-N1-C1'	-5.66	114.01	120.80
16	D	22	G	N3-C2-N2	-5.64	115.95	119.90
39	a	1363	C	N3-C4-N4	-5.63	114.06	118.00
16	D	1127	G	C5-C6-O6	-5.63	125.22	128.60
16	D	60	A	O4'-C1'-N9	5.62	112.70	108.20
16	D	35	G	C4-N9-C1'	5.62	133.81	126.50
16	D	647	C	C6-N1-C2	5.62	122.55	120.30
39	a	2591	C	C2-N1-C1'	5.62	124.98	118.80
16	D	1208	C	N3-C4-C5	5.61	124.15	121.90
16	D	1109	C	N1-C1'-C2'	-5.61	105.83	112.00
14	AE	363	LEU	CA-CB-CG	5.59	128.15	115.30
39	a	462	C	N3-C2-O2	-5.58	117.99	121.90
39	a	1021	A	C4-C5-C6	-5.58	114.21	117.00
39	a	1577	C	C6-N1-C2	5.58	122.53	120.30
39	a	1775	U	C5-C4-O4	-5.58	122.56	125.90
39	a	2493	U	C5-C4-O4	-5.58	122.56	125.90
39	a	995	C	N3-C4-N4	5.57	121.90	118.00
39	a	1479	G	N3-C4-N9	-5.56	122.66	126.00
39	a	2727	A	N9-C4-C5	-5.56	103.58	105.80
39	a	1354	A	N1-C6-N6	5.53	121.92	118.60
39	a	161	A	N1-C6-N6	5.53	121.92	118.60
39	a	487	C	N1-C2-O2	5.53	122.22	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	D	781	A	N1-C6-N6	5.53	121.92	118.60
39	a	231	A	C8-N9-C4	-5.52	103.59	105.80
39	a	2380	C	N1-C2-O2	5.52	122.21	118.90
39	a	1549	A	N1-C6-N6	-5.52	115.29	118.60
39	a	74	A	C5-C6-N6	5.50	128.10	123.70
16	D	1191	A	C5-C6-N6	-5.50	119.30	123.70
39	a	498	G	N3-C2-N2	-5.49	116.06	119.90
16	D	977	A	N1-C6-N6	5.47	121.88	118.60
39	a	1270	C	N1-C2-O2	-5.46	115.62	118.90
39	a	1166	G	N3-C2-N2	-5.46	116.08	119.90
39	a	2771	C	C2-N1-C1'	5.45	124.80	118.80
39	a	273	G	N9-C4-C5	-5.45	103.22	105.40
11	AA	1233	LEU	CA-CB-CG	5.45	127.83	115.30
37	Y	102	ARG	NE-CZ-NH2	5.45	123.02	120.30
52	n	176	PRO	CA-CB-CG	-5.45	93.65	104.00
39	a	143	C	N3-C2-O2	-5.45	118.09	121.90
16	D	1363	A	C4-C5-C6	-5.45	114.28	117.00
39	a	2444	G	N1-C6-O6	-5.45	116.63	119.90
39	a	819	A	N9-C4-C5	-5.43	103.63	105.80
39	a	1433	A	N1-C6-N6	5.43	121.86	118.60
16	D	1344	C	N1-C2-O2	5.41	122.15	118.90
39	a	1906	G	C4-N9-C1'	5.41	133.54	126.50
39	a	910	A	C4-C5-C6	-5.41	114.30	117.00
16	D	715	A	N1-C6-N6	5.40	121.84	118.60
39	a	2493	U	C6-N1-C1'	-5.40	113.64	121.20
16	D	386	C	N3-C2-O2	-5.40	118.12	121.90
16	D	1103	C	N1-C2-O2	5.40	122.14	118.90
39	a	130	C	C6-N1-C2	5.39	122.45	120.30
47	i	8	PRO	CA-CB-CG	-5.39	93.76	104.00
39	a	2	G	C8-N9-C1'	-5.39	120.00	127.00
16	D	1480	A	N9-C4-C5	-5.38	103.65	105.80
39	a	625	G	N3-C2-N2	5.38	123.67	119.90
50	l	188	MET	CG-SD-CE	5.37	108.79	100.20
54	p	154	PRO	CA-N-CD	-5.37	103.99	111.50
16	D	1113	C	N1-C2-O2	5.36	122.12	118.90
16	D	1363	A	N9-C4-C5	-5.36	103.66	105.80
16	D	316	C	N1-C2-O2	5.35	122.11	118.90
16	D	1220	G	N3-C4-N9	-5.35	122.79	126.00
16	D	715	A	C5-C6-N6	-5.35	119.42	123.70
39	a	1277	G	N9-C4-C5	-5.35	103.26	105.40
39	a	2248	C	N1-C2-O2	5.35	122.11	118.90
16	D	1314	C	N1-C2-O2	5.34	122.11	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	a	2089	C	C6-N1-C2	5.34	122.44	120.30
39	a	2248	C	N3-C2-O2	-5.33	118.17	121.90
39	a	2463	C	C6-N1-C2	5.32	122.43	120.30
39	a	1906	G	C8-N9-C1'	-5.32	120.08	127.00
10	B	60	U	P-O3'-C3'	5.32	126.08	119.70
39	a	1395	A	O4'-C1'-N9	5.32	112.45	108.20
9	9	79	PRO	CA-N-CD	-5.31	104.06	111.50
16	D	342	C	C6-N1-C2	5.31	122.42	120.30
39	a	605	G	N3-C4-N9	-5.31	122.81	126.00
39	a	1726	C	C6-N1-C2	5.30	122.42	120.30
16	D	1323	G	C6-C5-N7	-5.28	127.23	130.40
16	D	330	C	N3-C4-C5	5.28	124.01	121.90
11	AA	728	ASP	N-CA-C	5.28	125.25	111.00
39	a	1533	C	N1-C2-O2	5.26	122.06	118.90
39	a	27	G	O4'-C1'-N9	5.25	112.40	108.20
10	A	60	U	P-O3'-C3'	5.25	126.00	119.70
16	D	1316	G	N3-C4-N9	-5.25	122.85	126.00
39	a	1503	A	N9-C4-C5	-5.24	103.70	105.80
10	B	31	G	O4'-C1'-N9	5.24	112.39	108.20
39	a	2084	C	C6-N1-C2	5.24	122.39	120.30
39	a	2048	G	C4-N9-C1'	5.23	133.30	126.50
39	a	2517	C	N3-C2-O2	-5.23	118.24	121.90
39	a	2901	C	N3-C2-O2	-5.23	118.24	121.90
39	a	353	C	N1-C2-O2	5.23	122.04	118.90
16	D	1124	G	OP2-P-O3'	-5.22	93.71	105.20
37	Y	137	LEU	CA-CB-CG	5.22	127.30	115.30
39	a	231	A	N7-C8-N9	5.22	116.41	113.80
39	a	462	C	C4-C5-C6	-5.21	114.79	117.40
39	a	1574	C	C6-N1-C2	5.21	122.39	120.30
16	D	470	C	N1-C2-O2	5.21	122.03	118.90
39	a	2472	G	N3-C4-C5	5.21	131.20	128.60
39	a	2827	C	N3-C4-C5	5.21	123.98	121.90
8	7	-5	U	C2'-C3'-O3'	5.20	122.03	113.70
16	D	141	G	C8-N9-C4	5.20	108.48	106.40
39	a	2567	G	N1-C2-N2	-5.20	111.52	116.20
39	a	2257	U	C5-C4-O4	-5.19	122.78	125.90
39	a	1142	A	C4-C5-C6	-5.19	114.41	117.00
16	D	1134	G	N3-C4-C5	5.19	131.19	128.60
16	D	767	A	N1-C6-N6	5.19	121.71	118.60
39	a	2641	G	C6-C5-N7	5.19	133.51	130.40
39	a	1379	U	N3-C4-O4	-5.18	115.77	119.40
39	a	795	C	C6-N1-C2	5.18	122.37	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	a	2159	G	C5-C6-O6	5.18	131.71	128.60
39	a	2527	C	C6-N1-C2	5.18	122.37	120.30
20	H	169	SER	N-CA-CB	-5.17	102.74	110.50
39	a	500	G	N3-C4-N9	-5.17	122.90	126.00
11	AA	817	LEU	CB-CG-CD2	-5.16	102.22	111.00
39	a	1564	C	C2-N1-C1'	5.16	124.48	118.80
39	a	2190	G	C8-N9-C4	-5.16	104.33	106.40
39	a	605	G	N3-C2-N2	-5.16	116.29	119.90
16	D	20	U	C2-N3-C4	-5.16	123.91	127.00
16	D	161	A	N1-C6-N6	-5.15	115.51	118.60
16	D	1248	A	N1-C6-N6	-5.15	115.51	118.60
16	D	1323	G	N3-C4-N9	5.15	129.09	126.00
39	a	2848	G	O4'-C1'-N9	5.15	112.32	108.20
10	B	71	C	C6-N1-C1'	-5.15	114.62	120.80
39	a	2284	A	N9-C4-C5	-5.15	103.74	105.80
39	a	313	G	N3-C2-N2	5.15	123.50	119.90
39	a	1086	A	N1-C2-N3	-5.14	126.73	129.30
10	A	31	G	O4'-C1'-N9	5.14	112.31	108.20
16	D	1466	C	N1-C2-O2	5.14	121.98	118.90
10	A	71	C	C6-N1-C1'	-5.12	114.66	120.80
39	a	281	C	N1-C2-O2	5.12	121.97	118.90
39	a	517	C	C6-N1-C2	5.12	122.35	120.30
39	a	851	C	C6-N1-C2	5.12	122.35	120.30
39	a	2473	U	N1-C2-O2	5.12	126.38	122.80
16	D	69	G	N9-C4-C5	-5.12	103.35	105.40
16	D	36	C	C6-N1-C2	5.10	122.34	120.30
39	a	993	G	N3-C4-N9	-5.10	122.94	126.00
39	a	742	A	C5-C6-N1	5.10	120.25	117.70
42	d	12	C	C6-N1-C2	5.10	122.34	120.30
39	a	2119	A	N1-C6-N6	-5.10	115.54	118.60
39	a	2332	C	N3-C4-N4	-5.10	114.43	118.00
39	a	1573	G	N3-C2-N2	-5.10	116.33	119.90
39	a	2473	U	C2-N1-C1'	5.10	123.82	117.70
39	a	2161	C	N3-C2-O2	-5.10	118.33	121.90
39	a	1198	U	C6-N1-C2	-5.09	117.94	121.00
39	a	1198	U	N3-C2-O2	-5.09	118.63	122.20
16	D	1333	A	N1-C6-N6	5.09	121.66	118.60
39	a	2493	U	C5'-C4'-O4'	5.09	115.21	109.10
16	D	280	C	N3-C4-N4	-5.09	114.44	118.00
39	a	1816	C	N3-C4-C5	5.09	123.94	121.90
16	D	438	U	O4'-C1'-N1	5.09	112.27	108.20
16	D	687	A	O4'-C1'-N9	5.08	112.27	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	a	2338	C	C6-N1-C2	5.08	122.33	120.30
16	D	230	G	N3-C4-N9	-5.08	122.95	126.00
16	D	827	U	C2-N3-C4	5.08	130.05	127.00
39	a	752	A	N1-C6-N6	5.08	121.64	118.60
39	a	1773	A	N9-C1'-C2'	-5.08	106.42	112.00
39	a	2357	G	N3-C4-C5	5.08	131.14	128.60
39	a	2613	U	C4-C5-C6	-5.07	116.66	119.70
16	D	457	G	N9-C4-C5	-5.07	103.37	105.40
39	a	1504	A	C8-N9-C4	5.07	107.83	105.80
16	D	1220	G	N3-C4-C5	5.07	131.13	128.60
39	a	121	G	N9-C4-C5	-5.06	103.38	105.40
39	a	2198	A	N1-C6-N6	-5.06	115.57	118.60
39	a	1339	G	N3-C2-N2	5.05	123.44	119.90
14	AE	807	LEU	CB-CG-CD2	-5.05	102.41	111.00
16	D	1158	C	N3-C4-C5	-5.05	119.88	121.90
39	a	300	A	C8-N9-C4	5.05	107.82	105.80
16	D	1016	A	N9-C4-C5	-5.05	103.78	105.80
39	a	476	G	N3-C4-C5	5.05	131.13	128.60
39	a	2385	C	N1-C2-O2	5.05	121.93	118.90
16	D	35	G	N7-C8-N9	5.04	115.62	113.10
16	D	443	C	C6-N1-C2	5.04	122.31	120.30
39	a	121	G	N3-C4-N9	5.04	129.02	126.00
39	a	819	A	C8-N9-C4	5.03	107.81	105.80
39	a	1581	G	C8-N9-C1'	-5.03	120.46	127.00
39	a	1920	C	N3-C4-C5	5.03	123.91	121.90
20	H	332	VAL	N-CA-C	5.03	124.57	111.00
20	H	153	GLU	N-CA-C	-5.02	97.44	111.00
39	a	1313	U	C2-N1-C1'	5.02	123.73	117.70
16	D	754	C	C2-N1-C1'	5.01	124.32	118.80
39	a	1408	G	C4-N9-C1'	5.01	133.02	126.50
16	D	483	C	N3-C2-O2	-5.01	118.39	121.90
39	a	2322	A	N1-C6-N6	-5.01	115.60	118.60
39	a	481	G	O4'-C1'-N9	5.00	112.20	108.20
39	a	1805	A	N1-C6-N6	-5.00	115.60	118.60
39	a	1848	A	N1-C6-N6	-5.00	115.60	118.60

There are no chirality outliers.

All (26) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
9	9	107	GLU	Peptide
9	9	79	PRO	Peptide

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Mol	Chain	Res	Type	Group
9	9	92	ALA	Peptide
11	AA	1134	GLN	Peptide
11	AA	1157	GLN	Peptide
11	AA	1158	LYS	Peptide
11	AA	205	PRO	Peptide
11	AA	594	VAL	Peptide
11	AA	595	THR	Peptide
11	AA	596	ASP	Mainchain
11	AA	696	ASP	Peptide
11	AA	746	ALA	Peptide
11	AA	853	ASP	Mainchain
14	AE	1184	ASP	Peptide
14	AE	1326	GLN	Peptide
14	AE	313	GLY	Peptide
14	AE	416	ILE	Peptide
14	AE	804	ALA	Peptide
20	H	274	TYR	Peptide
27	O	12	ARG	Peptide
30	R	44	LYS	Peptide
36	X	65	VAL	Peptide
40	b	11	ARG	Peptide
52	n	176	PRO	Peptide
53	o	31	HIS	Peptide
54	p	47	ASP	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.

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	101/103 (98%)	89 (88%)	12 (12%)	0	100	100
2	1	108/110 (98%)	99 (92%)	9 (8%)	0	100	100
3	2	92/94 (98%)	87 (95%)	5 (5%)	0	100	100
4	3	101/103 (98%)	93 (92%)	7 (7%)	1 (1%)	13	44
5	4	92/94 (98%)	82 (89%)	10 (11%)	0	100	100
9	9	146/148 (99%)	112 (77%)	33 (23%)	1 (1%)	19	51
11	AA	1318/1342 (98%)	1149 (87%)	137 (10%)	32 (2%)	5	30
12	AB	94/181 (52%)	88 (94%)	6 (6%)	0	100	100
13	AC	228/230 (99%)	215 (94%)	11 (5%)	2 (1%)	14	47
13	AD	226/230 (98%)	212 (94%)	14 (6%)	0	100	100
14	AE	1329/1407 (94%)	1199 (90%)	121 (9%)	9 (1%)	19	51
15	C	64/66 (97%)	59 (92%)	4 (6%)	1 (2%)	8	37
17	E	84/86 (98%)	82 (98%)	2 (2%)	0	100	100
18	F	68/70 (97%)	68 (100%)	0	0	100	100
19	G	223/225 (99%)	201 (90%)	22 (10%)	0	100	100
20	H	255/557 (46%)	187 (73%)	56 (22%)	12 (5%)	2	19
21	I	206/208 (99%)	197 (96%)	8 (4%)	1 (0%)	25	57
22	J	203/205 (99%)	198 (98%)	5 (2%)	0	100	100
23	K	154/156 (99%)	140 (91%)	13 (8%)	1 (1%)	22	54
24	L	102/104 (98%)	95 (93%)	7 (7%)	0	100	100
25	M	149/151 (99%)	142 (95%)	7 (5%)	0	100	100
26	N	127/129 (98%)	110 (87%)	17 (13%)	0	100	100
27	O	125/127 (98%)	111 (89%)	14 (11%)	0	100	100
28	P	97/99 (98%)	88 (91%)	8 (8%)	1 (1%)	13	44
29	Q	115/117 (98%)	104 (90%)	11 (10%)	0	100	100
30	R	117/124 (94%)	105 (90%)	11 (9%)	1 (1%)	14	47
31	S	98/100 (98%)	95 (97%)	2 (2%)	1 (1%)	13	44
32	T	86/88 (98%)	82 (95%)	4 (5%)	0	100	100
33	U	80/82 (98%)	74 (92%)	6 (8%)	0	100	100
34	V	78/80 (98%)	67 (86%)	11 (14%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
35	W	81/83 (98%)	75 (93%)	6 (7%)	0	100	100
36	X	114/116 (98%)	100 (88%)	14 (12%)	0	100	100
37	Y	139/141 (99%)	121 (87%)	18 (13%)	0	100	100
38	Z	28/30 (93%)	27 (96%)	1 (4%)	0	100	100
40	b	74/76 (97%)	67 (90%)	7 (10%)	0	100	100
41	c	75/77 (97%)	69 (92%)	6 (8%)	0	100	100
43	e	60/62 (97%)	58 (97%)	2 (3%)	0	100	100
44	f	56/58 (97%)	51 (91%)	5 (9%)	0	100	100
45	g	64/66 (97%)	58 (91%)	6 (9%)	0	100	100
46	h	269/271 (99%)	241 (90%)	28 (10%)	0	100	100
47	i	54/56 (96%)	49 (91%)	5 (9%)	0	100	100
48	j	207/209 (99%)	188 (91%)	19 (9%)	0	100	100
49	k	50/52 (96%)	48 (96%)	2 (4%)	0	100	100
50	l	199/201 (99%)	184 (92%)	15 (8%)	0	100	100
51	m	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
52	n	175/177 (99%)	161 (92%)	14 (8%)	0	100	100
53	o	62/64 (97%)	54 (87%)	7 (11%)	1 (2%)	8	37
54	p	173/175 (99%)	156 (90%)	16 (9%)	1 (1%)	22	54
55	q	36/38 (95%)	33 (92%)	3 (8%)	0	100	100
56	r	147/149 (99%)	136 (92%)	11 (8%)	0	100	100
57	s	140/142 (99%)	127 (91%)	13 (9%)	0	100	100
58	t	121/123 (98%)	108 (89%)	13 (11%)	0	100	100
59	u	142/144 (99%)	132 (93%)	10 (7%)	0	100	100
60	v	134/136 (98%)	121 (90%)	13 (10%)	0	100	100
61	w	117/119 (98%)	109 (93%)	8 (7%)	0	100	100
62	x	114/116 (98%)	110 (96%)	4 (4%)	0	100	100
63	y	112/114 (98%)	104 (93%)	8 (7%)	0	100	100
64	z	115/117 (98%)	107 (93%)	8 (7%)	0	100	100
All	All	9368/9974 (94%)	8467 (90%)	836 (9%)	65 (1%)	21	51

All (65) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	AA	596	ASP
11	AA	853	ASP
11	AA	859	GLU
11	AA	862	LEU
11	AA	873	ILE
11	AA	937	ASP
11	AA	993	PRO
20	H	76	GLU
20	H	139	ARG
20	H	153	GLU
20	H	169	SER
20	H	306	VAL
20	H	340	ARG
31	S	96	LEU
11	AA	375	PRO
11	AA	856	ASN
11	AA	870	ILE
11	AA	940	GLU
11	AA	985	GLU
11	AA	1003	THR
11	AA	1158	LYS
14	AE	175	GLU
20	H	108	VAL
20	H	309	MET
20	H	333	LEU
53	o	32	ILE
11	AA	376	PRO
11	AA	723	VAL
11	AA	728	ASP
11	AA	935	THR
11	AA	980	VAL
11	AA	1005	GLU
11	AA	1045	GLY
13	AC	164	ASP
13	AC	165	GLU
14	AE	51	PRO
14	AE	805	GLN
20	H	78	GLY
20	H	142	ARG
28	P	58	ASN
30	R	45	PRO
11	AA	850	ILE
11	AA	943	LYS

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Mol	Chain	Res	Type
11	AA	995	ASP
14	AE	174	ASP
14	AE	193	ASP
21	I	80	LYS
54	p	48	ASN
9	9	79	PRO
11	AA	917	SER
11	AA	991	LYS
11	AA	997	TRP
11	AA	1044	PRO
14	AE	91	GLU
15	C	41	PRO
20	H	70	VAL
14	AE	49	PHE
14	AE	73	GLY
14	AE	904	ALA
23	K	91	GLY
11	AA	697	LYS
11	AA	1159	VAL
11	AA	1317	PRO
4	3	55	PRO
11	AA	933	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	84/84 (100%)	84 (100%)	0	100	100
2	1	93/93 (100%)	93 (100%)	0	100	100
3	2	81/81 (100%)	81 (100%)	0	100	100
4	3	84/84 (100%)	84 (100%)	0	100	100
5	4	78/78 (100%)	78 (100%)	0	100	100
9	9	112/112 (100%)	111 (99%)	1 (1%)	75	84
11	AA	1140/1157 (98%)	1039 (91%)	101 (9%)	8	31

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	AB	86/158 (54%)	84 (98%)	2 (2%)	45	64
13	AC	198/198 (100%)	182 (92%)	16 (8%)	9	34
13	AD	196/198 (99%)	194 (99%)	2 (1%)	73	82
14	AE	1120/1168 (96%)	1051 (94%)	69 (6%)	15	42
15	C	57/57 (100%)	53 (93%)	4 (7%)	12	39
17	E	65/65 (100%)	65 (100%)	0	100	100
18	F	60/60 (100%)	58 (97%)	2 (3%)	33	57
19	G	187/187 (100%)	183 (98%)	4 (2%)	48	67
20	H	137/461 (30%)	125 (91%)	12 (9%)	8	32
21	I	171/171 (100%)	164 (96%)	7 (4%)	26	52
22	J	172/172 (100%)	163 (95%)	9 (5%)	19	46
23	K	119/119 (100%)	118 (99%)	1 (1%)	79	85
24	L	91/91 (100%)	91 (100%)	0	100	100
25	M	124/124 (100%)	124 (100%)	0	100	100
26	N	104/104 (100%)	104 (100%)	0	100	100
27	O	105/105 (100%)	103 (98%)	2 (2%)	52	70
28	P	86/86 (100%)	77 (90%)	9 (10%)	5	25
29	Q	90/90 (100%)	90 (100%)	0	100	100
30	R	101/104 (97%)	101 (100%)	0	100	100
31	S	83/83 (100%)	80 (96%)	3 (4%)	30	55
32	T	76/76 (100%)	76 (100%)	0	100	100
33	U	65/65 (100%)	65 (100%)	0	100	100
34	V	74/74 (100%)	73 (99%)	1 (1%)	62	76
35	W	72/72 (100%)	72 (100%)	0	100	100
36	X	94/94 (100%)	94 (100%)	0	100	100
37	Y	109/109 (100%)	108 (99%)	1 (1%)	75	84
38	Z	26/26 (100%)	26 (100%)	0	100	100
40	b	58/58 (100%)	57 (98%)	1 (2%)	56	73
41	c	67/67 (100%)	67 (100%)	0	100	100
43	e	54/54 (100%)	54 (100%)	0	100	100
44	f	48/48 (100%)	48 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
45	g	59/59 (100%)	58 (98%)	1 (2%)	56	73
46	h	216/216 (100%)	216 (100%)	0	100	100
47	i	47/47 (100%)	46 (98%)	1 (2%)	48	67
48	j	164/164 (100%)	163 (99%)	1 (1%)	84	90
49	k	47/47 (100%)	47 (100%)	0	100	100
50	l	165/165 (100%)	163 (99%)	2 (1%)	67	79
51	m	38/38 (100%)	35 (92%)	3 (8%)	10	36
52	n	148/148 (100%)	148 (100%)	0	100	100
53	o	51/51 (100%)	51 (100%)	0	100	100
54	p	136/136 (100%)	136 (100%)	0	100	100
55	q	34/34 (100%)	34 (100%)	0	100	100
56	r	114/114 (100%)	114 (100%)	0	100	100
57	s	116/116 (100%)	116 (100%)	0	100	100
58	t	104/104 (100%)	104 (100%)	0	100	100
59	u	103/103 (100%)	103 (100%)	0	100	100
60	v	109/109 (100%)	107 (98%)	2 (2%)	54	71
61	w	99/99 (100%)	98 (99%)	1 (1%)	73	82
62	x	86/86 (100%)	86 (100%)	0	100	100
63	y	99/99 (100%)	98 (99%)	1 (1%)	73	82
64	z	89/89 (100%)	89 (100%)	0	100	100
All	All	7791/8257 (94%)	7532 (97%)	259 (3%)	35	57

All (259) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	9	125	ARG
11	AA	376	PRO
11	AA	723	VAL
11	AA	728	ASP
11	AA	731	ARG
11	AA	752	ASN
11	AA	817	LEU
11	AA	840	SER
11	AA	844	LYS
11	AA	845	LEU

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Mol	Chain	Res	Type
11	AA	851	THR
11	AA	854	ILE
11	AA	855	PRO
11	AA	857	VAL
11	AA	862	LEU
11	AA	864	LYS
11	AA	865	LEU
11	AA	866	ASP
11	AA	867	GLU
11	AA	868	SER
11	AA	871	VAL
11	AA	873	ILE
11	AA	876	GLU
11	AA	884	VAL
11	AA	886	LYS
11	AA	890	LYS
11	AA	912	ASP
11	AA	913	VAL
11	AA	914	LYS
11	AA	918	LEU
11	AA	933	VAL
11	AA	936	ARG
11	AA	939	VAL
11	AA	941	LYS
11	AA	943	LYS
11	AA	944	ARG
11	AA	949	GLU
11	AA	950	GLU
11	AA	951	MET
11	AA	952	GLN
11	AA	953	LEU
11	AA	954	LYS
11	AA	955	GLN
11	AA	957	LYS
11	AA	958	LYS
11	AA	959	ASP
11	AA	960	LEU
11	AA	962	GLU
11	AA	963	GLU
11	AA	964	LEU
11	AA	965	GLN
11	AA	967	LEU

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Mol	Chain	Res	Type
11	AA	968	GLU
11	AA	971	LEU
11	AA	973	SER
11	AA	974	ARG
11	AA	979	LEU
11	AA	980	VAL
11	AA	985	GLU
11	AA	988	LYS
11	AA	989	LEU
11	AA	991	LYS
11	AA	992	LEU
11	AA	994	ARG
11	AA	995	ASP
11	AA	997	TRP
11	AA	998	LEU
11	AA	999	GLU
11	AA	1002	LEU
11	AA	1005	GLU
11	AA	1006	GLU
11	AA	1007	LYS
11	AA	1008	GLN
11	AA	1009	ASN
11	AA	1010	GLN
11	AA	1013	GLN
11	AA	1019	ASP
11	AA	1020	GLU
11	AA	1022	LYS
11	AA	1023	HIS
11	AA	1024	GLU
11	AA	1025	PHE
11	AA	1026	GLU
11	AA	1027	LYS
11	AA	1029	LEU
11	AA	1032	LYS
11	AA	1034	ARG
11	AA	1035	LYS
11	AA	1038	GLN
11	AA	1041	ASP
11	AA	1042	LEU
11	AA	1046	VAL
11	AA	1047	LEU
11	AA	1048	LYS

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Mol	Chain	Res	Type
11	AA	1151	LEU
11	AA	1159	VAL
11	AA	1250	SER
11	AA	1252	SER
11	AA	1253	LEU
11	AA	1254	VAL
11	AA	1256	GLN
11	AA	1259	LEU
12	AB	21	ARG
12	AB	47	GLU
13	AC	12	ARG
13	AC	62	ASP
13	AC	65	LEU
13	AC	72	GLU
13	AC	91	ARG
13	AC	134	THR
13	AC	158	ARG
13	AC	159	ILE
13	AC	160	HIS
13	AC	162	GLU
13	AC	163	GLU
13	AC	165	GLU
13	AC	166	ARG
13	AC	168	ILE
13	AC	170	ARG
13	AC	171	LEU
13	AD	12	ARG
13	AD	208	ASN
14	AE	40	LYS
14	AE	42	GLU
14	AE	44	ILE
14	AE	46	TYR
14	AE	47	ARG
14	AE	49	PHE
14	AE	50	LYS
14	AE	52	GLU
14	AE	53	ARG
14	AE	54	ASP
14	AE	60	ARG
14	AE	67	ASP
14	AE	70	CYS
14	AE	72	CYS

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Mol	Chain	Res	Type
14	AE	74	LYS
14	AE	76	LYS
14	AE	77	ARG
14	AE	78	LEU
14	AE	81	ARG
14	AE	87	LYS
14	AE	88	CYS
14	AE	91	GLU
14	AE	94	GLN
14	AE	95	THR
14	AE	99	ARG
14	AE	100	GLU
14	AE	117	LEU
14	AE	119	SER
14	AE	123	ARG
14	AE	132	LEU
14	AE	135	ILE
14	AE	142	GLU
14	AE	144	TYR
14	AE	145	VAL
14	AE	147	ILE
14	AE	152	THR
14	AE	154	LEU
14	AE	157	GLN
14	AE	159	ILE
14	AE	175	GLU
14	AE	180	MET
14	AE	190	LYS
14	AE	193	ASP
14	AE	196	GLN
14	AE	210	SER
14	AE	215	LYS
14	AE	216	LYS
14	AE	222	LYS
14	AE	223	LEU
14	AE	227	PHE
14	AE	232	ASN
14	AE	233	LYS
14	AE	237	MET
14	AE	238	ILE
14	AE	239	LEU
14	AE	240	THR

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Mol	Chain	Res	Type
14	AE	244	VAL
14	AE	271	ARG
14	AE	385	LEU
14	AE	386	GLU
14	AE	390	LEU
14	AE	393	THR
14	AE	394	ILE
14	AE	395	LYS
14	AE	514	THR
14	AE	709	ARG
14	AE	836	ARG
14	AE	1172	LYS
14	AE	1373	ARG
15	C	12	ARG
15	C	41	PRO
15	C	43	ARG
15	C	44	ILE
18	F	55	ARG
18	F	66	ARG
19	G	19	GLN
19	G	35	ARG
19	G	74	ARG
19	G	115	LYS
20	H	9	PHE
20	H	54	LYS
20	H	79	PHE
20	H	83	LEU
20	H	268	VAL
20	H	273	ARG
20	H	305	HIS
20	H	336	ASP
20	H	337	GLU
20	H	338	GLU
20	H	339	ARG
20	H	340	ARG
21	I	14	ILE
21	I	75	ILE
21	I	89	LYS
21	I	132	ARG
21	I	164	ARG
21	I	185	ASN
21	I	200	VAL

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Mol	Chain	Res	Type
22	J	47	ARG
22	J	48	LEU
22	J	83	LYS
22	J	95	GLU
22	J	104	ARG
22	J	116	GLN
22	J	138	SER
22	J	143	VAL
22	J	166	GLU
23	K	96	MET
27	O	12	ARG
27	O	106	ARG
28	P	5	ARG
28	P	17	LEU
28	P	24	GLU
28	P	25	ILE
28	P	27	GLU
28	P	37	ARG
28	P	72	ARG
28	P	87	LEU
28	P	89	ARG
31	S	85	ARG
31	S	97	LYS
31	S	98	LYS
34	V	77	ARG
37	Y	102	ARG
40	b	14	ARG
45	g	3	LYS
47	i	52	ARG
48	j	173	GLN
50	l	57	LYS
50	l	163	ASN
51	m	22	MET
51	m	41	ARG
51	m	42	LEU
60	v	10	ARG
60	v	44	ARG
61	w	63	ARG
63	y	75	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
2	1	9	HIS
4	3	69	ASN
11	AA	1236	ASN
15	C	31	ASN
15	C	74	HIS
23	K	70	ASN
27	O	81	HIS
29	Q	40	ASN
31	S	66	GLN
33	U	9	HIS
37	Y	104	GLN
41	c	6	GLN
41	c	34	HIS
43	e	41	HIS
44	f	20	HIS
45	g	6	HIS
46	h	15	HIS
46	h	134	ASN
47	i	4	GLN
47	i	5	GLN
47	i	41	HIS
48	j	173	GLN
49	k	46	HIS
50	l	9	GLN
50	l	62	GLN
51	m	29	GLN
54	p	38	ASN
54	p	115	HIS
56	r	18	GLN
60	v	13	HIS
61	w	73	ASN
64	z	14	HIS
64	z	20	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
10	A	75/76 (98%)	30 (40%)	8 (10%)
10	B	75/76 (98%)	30 (40%)	8 (10%)
16	D	1514/1542 (98%)	304 (20%)	10 (0%)
39	a	2859/2904 (98%)	582 (20%)	0
42	d	119/120 (99%)	19 (15%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
8	7	28/29 (96%)	18 (64%)	3 (10%)
All	All	4670/4747 (98%)	983 (21%)	29 (0%)

All (983) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
8	7	-6	G
8	7	-5	U
8	7	-4	U
8	7	-2	U
8	7	-1	U
8	7	0	U
8	7	1	U
8	7	2	U
8	7	3	U
8	7	4	U
8	7	5	U
8	7	7	G
8	7	8	A
8	7	9	U
8	7	10	U
8	7	11	U
8	7	12	G
8	7	13	G
10	A	2	G
10	A	6	G
10	A	7	G
10	A	8	U
10	A	10	G
10	A	13	C
10	A	14	A
10	A	15	G
10	A	16	C
10	A	17	C
10	A	18	G
10	A	19	G
10	A	20	U
10	A	21	A
10	A	23	C
10	A	46	G
10	A	47	U
10	A	48	C

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Mol	Chain	Res	Type
10	A	49	G
10	A	52	G
10	A	57	A
10	A	58	A
10	A	59	A
10	A	60	U
10	A	61	C
10	A	66	C
10	A	69	C
10	A	71	C
10	A	73	A
10	A	76	A
10	B	2	G
10	B	6	G
10	B	7	G
10	B	8	U
10	B	10	G
10	B	13	C
10	B	14	A
10	B	15	G
10	B	16	C
10	B	17	C
10	B	18	G
10	B	19	G
10	B	20	U
10	B	21	A
10	B	23	C
10	B	46	G
10	B	47	U
10	B	48	C
10	B	49	G
10	B	52	G
10	B	57	A
10	B	58	A
10	B	59	A
10	B	60	U
10	B	61	C
10	B	66	C
10	B	69	C
10	B	71	C
10	B	73	A
10	B	76	A

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Mol	Chain	Res	Type
16	D	4	U
16	D	5	U
16	D	7	A
16	D	9	G
16	D	15	G
16	D	22	G
16	D	32	A
16	D	37	U
16	D	39	G
16	D	47	C
16	D	48	C
16	D	50	A
16	D	51	A
16	D	52	C
16	D	61	G
16	D	69	G
16	D	71	A
16	D	72	A
16	D	73	C
16	D	74	A
16	D	76	G
16	D	82	G
16	D	83	C
16	D	84	U
16	D	87	C
16	D	94	G
16	D	95	C
16	D	96	U
16	D	108	G
16	D	120	A
16	D	121	U
16	D	122	G
16	D	128	G
16	D	130	A
16	D	131	A
16	D	141	G
16	D	144	G
16	D	150	U
16	D	160	A
16	D	163	C
16	D	173	U
16	D	181	A

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Mol	Chain	Res	Type
16	D	182	A
16	D	189	A
16	D	197	A
16	D	198	G
16	D	202	G
16	D	204	G
16	D	208	U
16	D	210	C
16	D	211	G
16	D	212	G
16	D	216	U
16	D	226	G
16	D	245	U
16	D	246	A
16	D	247	G
16	D	252	U
16	D	253	A
16	D	258	G
16	D	262	A
16	D	266	G
16	D	267	C
16	D	276	G
16	D	279	A
16	D	289	G
16	D	306	A
16	D	316	C
16	D	321	A
16	D	328	C
16	D	329	A
16	D	332	G
16	D	347	G
16	D	351	G
16	D	352	C
16	D	353	A
16	D	354	G
16	D	355	C
16	D	367	U
16	D	372	C
16	D	382	A
16	D	397	A
16	D	406	G
16	D	411	A

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Mol	Chain	Res	Type
16	D	412	A
16	D	413	G
16	D	414	A
16	D	421	U
16	D	422	C
16	D	424	G
16	D	429	U
16	D	430	A
16	D	446	G
16	D	452	A
16	D	457	G
16	D	458	U
16	D	463	U
16	D	464	U
16	D	467	U
16	D	468	A
16	D	469	C
16	D	478	A
16	D	479	U
16	D	481	G
16	D	484	G
16	D	485	U
16	D	486	U
16	D	496	A
16	D	500	G
16	D	505	G
16	D	506	G
16	D	511	C
16	D	515	G
16	D	518	C
16	D	519	C
16	D	521	G
16	D	522	C
16	D	531	U
16	D	532	A
16	D	533	A
16	D	547	A
16	D	559	A
16	D	564	C
16	D	568	G
16	D	572	A
16	D	573	A

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Mol	Chain	Res	Type
16	D	575	G
16	D	576	C
16	D	577	G
16	D	579	A
16	D	596	A
16	D	628	G
16	D	633	G
16	D	650	G
16	D	653	U
16	D	665	A
16	D	687	A
16	D	692	U
16	D	700	G
16	D	723	U
16	D	724	G
16	D	727	G
16	D	731	G
16	D	747	A
16	D	748	G
16	D	759	A
16	D	777	A
16	D	792	A
16	D	793	U
16	D	794	A
16	D	802	A
16	D	815	A
16	D	817	C
16	D	828	U
16	D	829	G
16	D	832	G
16	D	841	C
16	D	844	G
16	D	845	A
16	D	846	G
16	D	849	G
16	D	874	G
16	D	887	G
16	D	889	A
16	D	902	G
16	D	914	A
16	D	916	U
16	D	926	G

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Mol	Chain	Res	Type
16	D	934	C
16	D	935	A
16	D	942	G
16	D	945	G
16	D	958	A
16	D	960	U
16	D	965	U
16	D	969	A
16	D	972	C
16	D	975	A
16	D	976	G
16	D	977	A
16	D	984	C
16	D	992	U
16	D	993	G
16	D	996	A
16	D	1003	G
16	D	1004	A
16	D	1006	G
16	D	1008	U
16	D	1009	U
16	D	1014	A
16	D	1017	U
16	D	1018	G
16	D	1021	A
16	D	1024	G
16	D	1026	G
16	D	1028	C
16	D	1030	U
16	D	1031	C
16	D	1033	G
16	D	1036	A
16	D	1038	C
16	D	1043	G
16	D	1044	A
16	D	1052	U
16	D	1056	U
16	D	1065	U
16	D	1085	U
16	D	1086	U
16	D	1094	G
16	D	1095	U

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Mol	Chain	Res	Type
16	D	1099	G
16	D	1101	A
16	D	1108	G
16	D	1124	G
16	D	1125	U
16	D	1131	G
16	D	1133	G
16	D	1135	U
16	D	1136	C
16	D	1137	C
16	D	1139	G
16	D	1140	C
16	D	1141	C
16	D	1142	G
16	D	1143	G
16	D	1145	A
16	D	1146	A
16	D	1151	A
16	D	1152	A
16	D	1154	G
16	D	1158	C
16	D	1159	U
16	D	1167	A
16	D	1171	A
16	D	1175	G
16	D	1176	A
16	D	1179	A
16	D	1184	G
16	D	1193	G
16	D	1196	A
16	D	1197	A
16	D	1201	A
16	D	1206	G
16	D	1213	A
16	D	1215	G
16	D	1224	U
16	D	1227	A
16	D	1234	C
16	D	1238	A
16	D	1239	A
16	D	1252	A
16	D	1254	A

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Mol	Chain	Res	Type
16	D	1256	A
16	D	1257	A
16	D	1260	G
16	D	1275	A
16	D	1276	G
16	D	1279	G
16	D	1280	A
16	D	1285	A
16	D	1286	U
16	D	1287	A
16	D	1299	A
16	D	1302	C
16	D	1303	C
16	D	1305	G
16	D	1312	G
16	D	1317	C
16	D	1320	C
16	D	1322	C
16	D	1338	G
16	D	1343	G
16	D	1346	A
16	D	1347	G
16	D	1353	G
16	D	1363	A
16	D	1368	A
16	D	1370	G
16	D	1378	C
16	D	1379	G
16	D	1381	U
16	D	1396	A
16	D	1397	C
16	D	1398	A
16	D	1404	C
16	D	1419	G
16	D	1429	A
16	D	1432	G
16	D	1441	A
16	D	1446	A
16	D	1452	C
16	D	1453	G
16	D	1475	G
16	D	1487	G

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Mol	Chain	Res	Type
16	D	1493	A
16	D	1494	G
16	D	1497	G
16	D	1503	A
16	D	1506	U
16	D	1507	A
16	D	1517	G
16	D	1529	G
16	D	1530	G
16	D	1534	A
39	a	4	U
39	a	10	A
39	a	15	G
39	a	28	A
39	a	34	U
39	a	35	G
39	a	46	G
39	a	60	G
39	a	63	A
39	a	71	A
39	a	74	A
39	a	75	G
39	a	80	G
39	a	83	A
39	a	84	A
39	a	85	G
39	a	96	C
39	a	100	U
39	a	101	A
39	a	102	U
39	a	103	A
39	a	114	U
39	a	118	A
39	a	119	A
39	a	120	U
39	a	132	G
39	a	139	U
39	a	142	A
39	a	162	U
39	a	163	C
39	a	181	A
39	a	186	G

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Mol	Chain	Res	Type
39	a	196	A
39	a	199	A
39	a	215	G
39	a	216	A
39	a	222	A
39	a	223	A
39	a	224	U
39	a	225	C
39	a	248	G
39	a	249	C
39	a	250	G
39	a	252	G
39	a	265	A
39	a	266	G
39	a	267	C
39	a	270	A
39	a	271	G
39	a	272	A
39	a	275	C
39	a	276	U
39	a	279	A
39	a	285	G
39	a	292	U
39	a	301	G
39	a	311	A
39	a	317	G
39	a	322	A
39	a	324	A
39	a	329	G
39	a	330	A
39	a	331	C
39	a	338	G
39	a	353	C
39	a	361	G
39	a	362	A
39	a	370	G
39	a	371	A
39	a	372	G
39	a	373	U
39	a	375	G
39	a	386	G
39	a	388	G

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Mol	Chain	Res	Type
39	a	389	G
39	a	396	G
39	a	404	A
39	a	405	U
39	a	411	G
39	a	412	A
39	a	416	U
39	a	420	C
39	a	424	G
39	a	429	A
39	a	451	U
39	a	456	C
39	a	457	A
39	a	461	C
39	a	462	C
39	a	479	A
39	a	480	A
39	a	481	G
39	a	482	A
39	a	483	A
39	a	491	G
39	a	499	U
39	a	501	A
39	a	505	A
39	a	508	A
39	a	509	C
39	a	510	C
39	a	522	A
39	a	529	A
39	a	531	C
39	a	532	A
39	a	533	G
39	a	543	G
39	a	546	U
39	a	547	A
39	a	548	G
39	a	549	G
39	a	551	G
39	a	563	A
39	a	567	U
39	a	569	U
39	a	573	U

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Mol	Chain	Res	Type
39	a	574	A
39	a	575	A
39	a	586	A
39	a	588	U
39	a	594	U
39	a	599	A
39	a	603	A
39	a	608	A
39	a	609	A
39	a	613	A
39	a	614	A
39	a	615	U
39	a	616	A
39	a	621	A
39	a	627	A
39	a	637	A
39	a	640	C
39	a	642	U
39	a	645	C
39	a	646	U
39	a	647	G
39	a	654	A
39	a	655	A
39	a	661	A
39	a	664	G
39	a	668	A
39	a	676	A
39	a	685	A
39	a	686	U
39	a	702	U
39	a	710	U
39	a	717	C
39	a	726	G
39	a	729	G
39	a	730	A
39	a	738	G
39	a	757	G
39	a	764	A
39	a	765	C
39	a	775	G
39	a	776	G
39	a	782	A

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Mol	Chain	Res	Type
39	a	784	G
39	a	785	G
39	a	800	A
39	a	805	G
39	a	812	C
39	a	819	A
39	a	827	U
39	a	828	U
39	a	831	G
39	a	845	A
39	a	846	U
39	a	857	G
39	a	858	G
39	a	859	G
39	a	866	A
39	a	869	G
39	a	878	A
39	a	884	U
39	a	885	C
39	a	887	A
39	a	891	G
39	a	895	U
39	a	896	A
39	a	897	C
39	a	899	A
39	a	910	A
39	a	914	G
39	a	915	C
39	a	931	U
39	a	941	A
39	a	946	C
39	a	953	G
39	a	961	C
39	a	973	A
39	a	974	G
39	a	983	A
39	a	984	A
39	a	994	C
39	a	995	C
39	a	996	A
39	a	999	U
39	a	1012	U

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Mol	Chain	Res	Type
39	a	1013	C
39	a	1022	G
39	a	1023	U
39	a	1026	G
39	a	1033	U
39	a	1041	G
39	a	1045	C
39	a	1046	A
39	a	1047	G
39	a	1060	U
39	a	1062	G
39	a	1064	C
39	a	1066	U
39	a	1067	A
39	a	1068	G
39	a	1070	A
39	a	1071	G
39	a	1073	A
39	a	1074	G
39	a	1079	C
39	a	1081	U
39	a	1083	U
39	a	1084	A
39	a	1087	G
39	a	1088	A
39	a	1101	U
39	a	1107	G
39	a	1111	A
39	a	1112	G
39	a	1119	U
39	a	1122	G
39	a	1129	A
39	a	1130	U
39	a	1132	U
39	a	1133	A
39	a	1134	A
39	a	1135	C
39	a	1136	G
39	a	1141	U
39	a	1142	A
39	a	1169	A
39	a	1170	C

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Mol	Chain	Res	Type
39	a	1173	U
39	a	1174	U
39	a	1175	A
39	a	1176	U
39	a	1177	G
39	a	1178	C
39	a	1179	G
39	a	1180	U
39	a	1186	G
39	a	1210	G
39	a	1227	G
39	a	1236	G
39	a	1238	G
39	a	1248	G
39	a	1249	U
39	a	1253	A
39	a	1255	U
39	a	1256	G
39	a	1265	A
39	a	1266	G
39	a	1271	G
39	a	1272	A
39	a	1273	U
39	a	1284	A
39	a	1300	G
39	a	1301	A
39	a	1329	U
39	a	1344	U
39	a	1345	C
39	a	1352	U
39	a	1359	A
39	a	1365	A
39	a	1368	G
39	a	1378	A
39	a	1379	U
39	a	1380	G
39	a	1383	A
39	a	1392	A
39	a	1395	A
39	a	1406	U
39	a	1408	G
39	a	1409	U

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Mol	Chain	Res	Type
39	a	1416	G
39	a	1417	C
39	a	1419	A
39	a	1420	A
39	a	1427	A
39	a	1428	C
39	a	1452	G
39	a	1453	A
39	a	1459	G
39	a	1460	U
39	a	1478	G
39	a	1482	G
39	a	1490	A
39	a	1491	G
39	a	1493	C
39	a	1497	U
39	a	1502	A
39	a	1503	A
39	a	1508	A
39	a	1509	A
39	a	1510	G
39	a	1515	A
39	a	1526	C
39	a	1529	G
39	a	1534	U
39	a	1535	A
39	a	1536	C
39	a	1537	G
39	a	1554	U
39	a	1566	A
39	a	1569	A
39	a	1578	U
39	a	1580	A
39	a	1581	G
39	a	1583	A
39	a	1589	U
39	a	1590	A
39	a	1607	C
39	a	1608	A
39	a	1610	A
39	a	1613	G
39	a	1616	A

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Mol	Chain	Res	Type
39	a	1622	G
39	a	1634	A
39	a	1646	C
39	a	1647	U
39	a	1648	U
39	a	1649	G
39	a	1651	G
39	a	1659	G
39	a	1665	A
39	a	1668	A
39	a	1674	G
39	a	1713	A
39	a	1714	U
39	a	1715	G
39	a	1722	A
39	a	1729	U
39	a	1730	C
39	a	1732	C
39	a	1738	G
39	a	1754	A
39	a	1764	C
39	a	1773	A
39	a	1787	A
39	a	1791	A
39	a	1799	G
39	a	1800	C
39	a	1801	A
39	a	1808	A
39	a	1816	C
39	a	1829	A
39	a	1833	C
39	a	1841	U
39	a	1847	A
39	a	1848	A
39	a	1858	A
39	a	1859	U
39	a	1863	G
39	a	1864	U
39	a	1869	G
39	a	1870	C
39	a	1872	A
39	a	1881	C

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Mol	Chain	Res	Type
39	a	1889	A
39	a	1907	G
39	a	1913	A
39	a	1914	C
39	a	1919	A
39	a	1920	C
39	a	1922	G
39	a	1923	U
39	a	1925	C
39	a	1926	U
39	a	1929	G
39	a	1930	G
39	a	1938	A
39	a	1955	U
39	a	1960	A
39	a	1965	C
39	a	1967	C
39	a	1970	A
39	a	1971	U
39	a	1972	G
39	a	1976	U
39	a	1987	A
39	a	1991	U
39	a	1992	G
39	a	1993	U
39	a	1997	C
39	a	2018	G
39	a	2020	A
39	a	2021	C
39	a	2022	U
39	a	2023	C
39	a	2027	G
39	a	2033	A
39	a	2043	C
39	a	2052	A
39	a	2055	C
39	a	2056	G
39	a	2057	G
39	a	2060	A
39	a	2061	G
39	a	2062	A
39	a	2072	C

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Mol	Chain	Res	Type
39	a	2080	A
39	a	2097	A
39	a	2099	U
39	a	2100	G
39	a	2107	G
39	a	2108	A
39	a	2110	G
39	a	2111	U
39	a	2112	G
39	a	2113	U
39	a	2115	G
39	a	2116	G
39	a	2117	A
39	a	2118	U
39	a	2121	G
39	a	2122	U
39	a	2124	G
39	a	2125	G
39	a	2126	A
39	a	2127	G
39	a	2128	G
39	a	2131	U
39	a	2132	U
39	a	2133	G
39	a	2134	A
39	a	2139	U
39	a	2146	C
39	a	2147	A
39	a	2154	A
39	a	2157	G
39	a	2158	A
39	a	2159	G
39	a	2161	C
39	a	2162	G
39	a	2163	A
39	a	2164	C
39	a	2165	C
39	a	2171	A
39	a	2172	U
39	a	2176	A
39	a	2182	U
39	a	2183	A

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Mol	Chain	Res	Type
39	a	2189	U
39	a	2190	G
39	a	2193	G
39	a	2194	U
39	a	2198	A
39	a	2203	U
39	a	2204	G
39	a	2211	A
39	a	2212	A
39	a	2225	A
39	a	2226	C
39	a	2229	U
39	a	2231	U
39	a	2238	G
39	a	2239	G
39	a	2243	U
39	a	2250	G
39	a	2273	A
39	a	2278	A
39	a	2283	C
39	a	2287	A
39	a	2288	A
39	a	2297	A
39	a	2305	U
39	a	2309	A
39	a	2322	A
39	a	2325	G
39	a	2327	A
39	a	2333	A
39	a	2335	A
39	a	2339	C
39	a	2344	U
39	a	2345	G
39	a	2347	C
39	a	2350	C
39	a	2361	G
39	a	2372	U
39	a	2376	A
39	a	2383	G
39	a	2385	C
39	a	2395	C
39	a	2396	G

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Mol	Chain	Res	Type
39	a	2402	U
39	a	2403	C
39	a	2419	U
39	a	2423	U
39	a	2424	C
39	a	2425	A
39	a	2426	A
39	a	2428	G
39	a	2429	G
39	a	2430	A
39	a	2431	U
39	a	2435	A
39	a	2441	U
39	a	2448	A
39	a	2459	A
39	a	2463	C
39	a	2470	G
39	a	2474	U
39	a	2476	A
39	a	2478	A
39	a	2484	G
39	a	2491	U
39	a	2493	U
39	a	2494	G
39	a	2502	G
39	a	2506	U
39	a	2513	A
39	a	2518	A
39	a	2520	C
39	a	2525	G
39	a	2529	G
39	a	2534	A
39	a	2535	G
39	a	2547	A
39	a	2554	U
39	a	2564	A
39	a	2566	A
39	a	2567	G
39	a	2572	A
39	a	2574	G
39	a	2576	G
39	a	2582	G

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Mol	Chain	Res	Type
39	a	2585	U
39	a	2589	A
39	a	2602	A
39	a	2603	G
39	a	2609	U
39	a	2613	U
39	a	2621	G
39	a	2629	U
39	a	2630	G
39	a	2671	G
39	a	2689	U
39	a	2690	U
39	a	2694	G
39	a	2714	G
39	a	2716	C
39	a	2725	A
39	a	2726	A
39	a	2729	G
39	a	2733	A
39	a	2739	U
39	a	2744	G
39	a	2748	A
39	a	2755	C
39	a	2757	A
39	a	2758	A
39	a	2777	G
39	a	2778	A
39	a	2791	G
39	a	2793	C
39	a	2796	U
39	a	2797	U
39	a	2798	U
39	a	2801	G
39	a	2820	A
39	a	2821	A
39	a	2825	G
39	a	2835	A
39	a	2849	U
39	a	2867	G
39	a	2872	A
39	a	2873	A
39	a	2880	C

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Mol	Chain	Res	Type
39	a	2884	U
39	a	2885	G
39	a	2891	U
39	a	2893	A
42	d	2	G
42	d	13	G
42	d	15	A
42	d	16	G
42	d	17	C
42	d	24	G
42	d	35	C
42	d	51	G
42	d	56	G
42	d	57	A
42	d	66	A
42	d	67	G
42	d	68	C
42	d	88	C
42	d	89	U
42	d	90	C
42	d	98	G
42	d	99	A
42	d	109	A

All (29) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
8	7	-5	U
8	7	1	U
8	7	11	U
10	A	6	G
10	A	9	G
10	A	12	G
10	A	22	G
10	A	46	G
10	A	48	C
10	A	57	A
10	A	60	U
10	B	6	G
10	B	9	G
10	B	12	G
10	B	22	G

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Mol	Chain	Res	Type
10	B	46	G
10	B	48	C
10	B	57	A
10	B	60	U
16	D	197	A
16	D	428	G
16	D	496	A
16	D	758	C
16	D	873	A
16	D	992	U
16	D	1109	C
16	D	1145	A
16	D	1492	A
16	D	1493	A

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

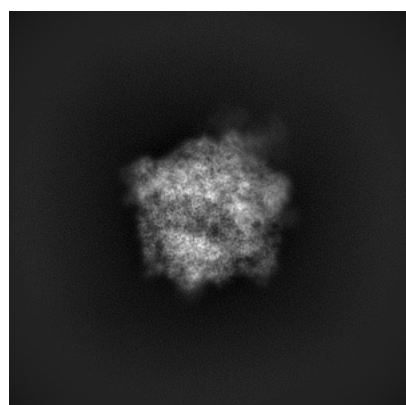
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-21386. These allow visual inspection of the internal detail of the map and identification of artifacts.

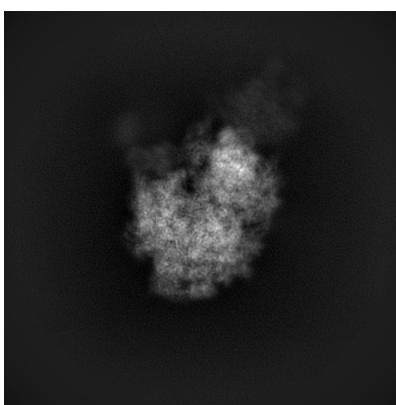
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

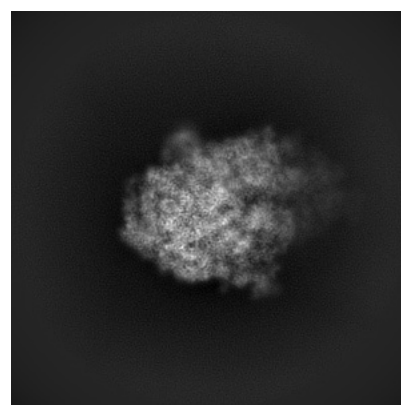
6.1.1 Primary map



X



Y

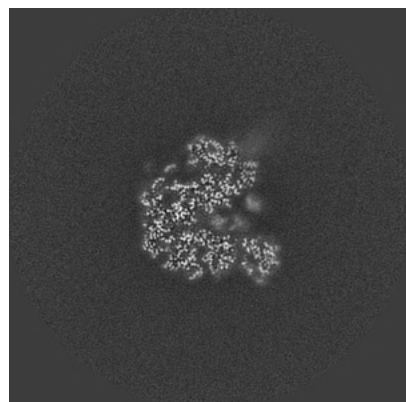


Z

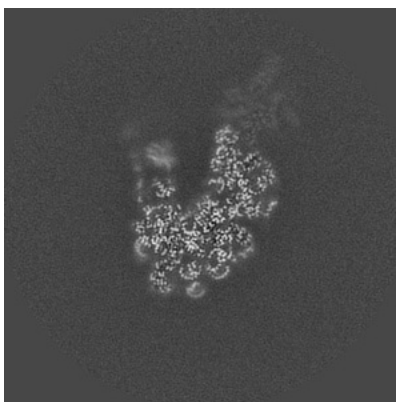
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

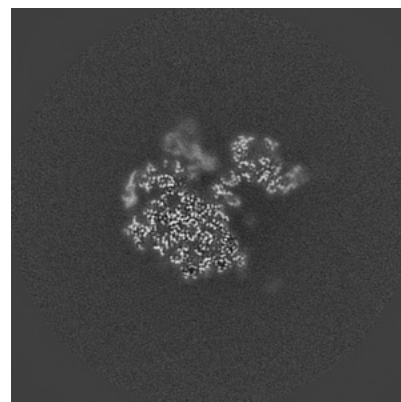
6.2.1 Primary map



X Index: 250



Y Index: 250

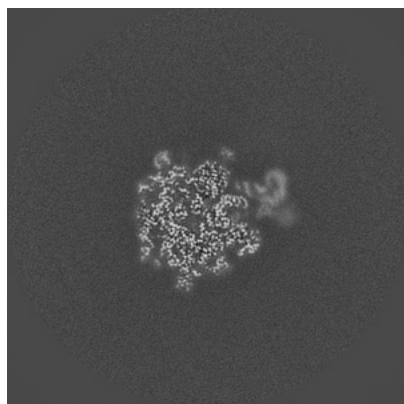


Z Index: 250

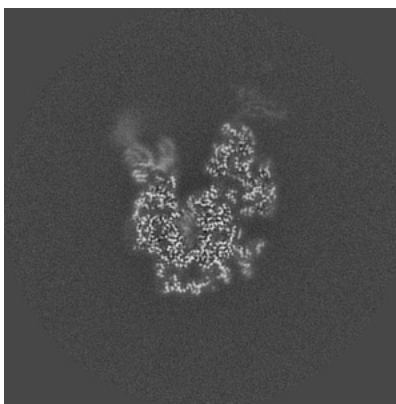
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

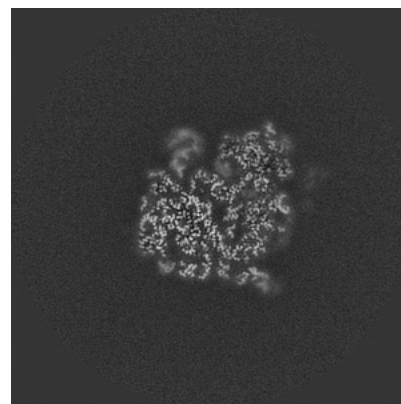
6.3.1 Primary map



X Index: 215



Y Index: 233

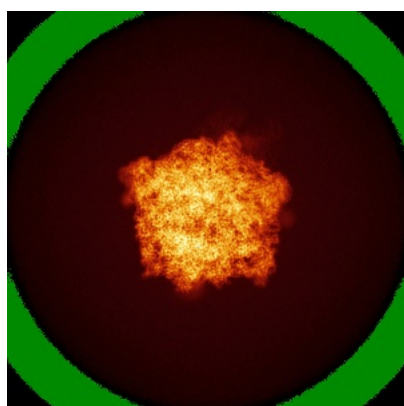


Z Index: 271

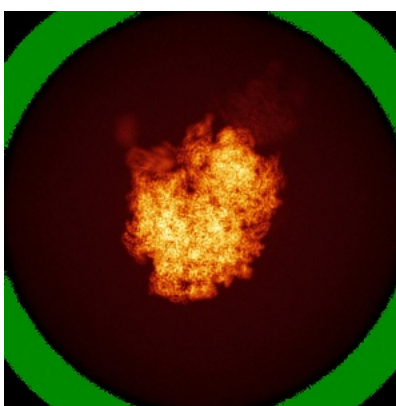
The images above show the largest variance slices of the map in three orthogonal directions.

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

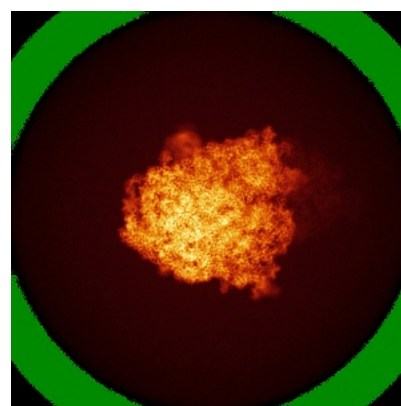
6.4.1 Primary map



X



Y

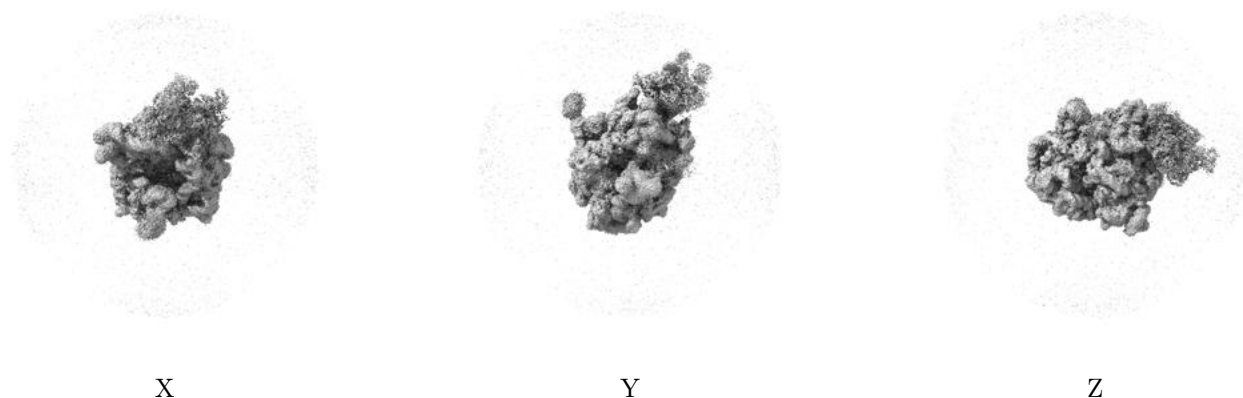


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.007. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

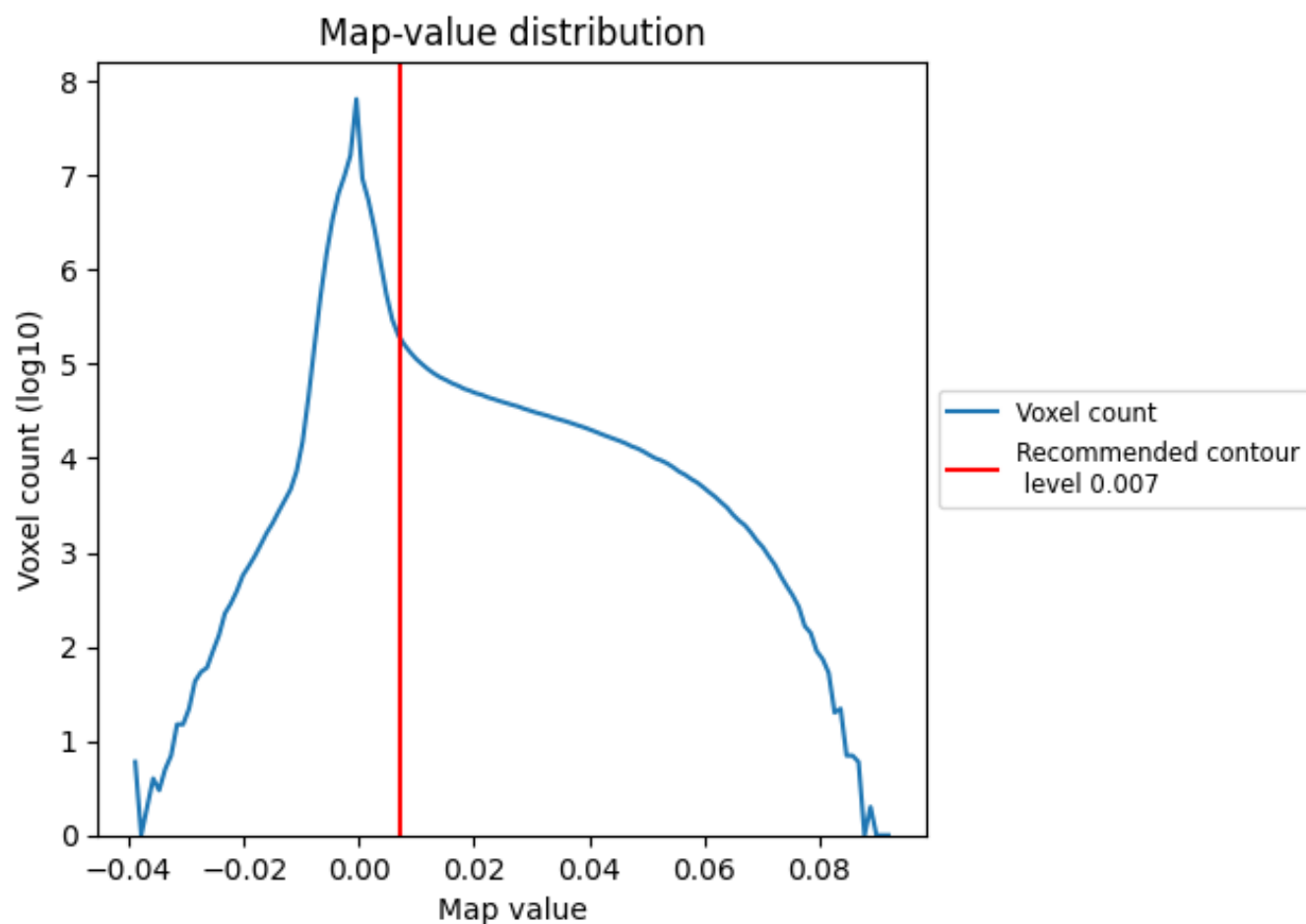
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

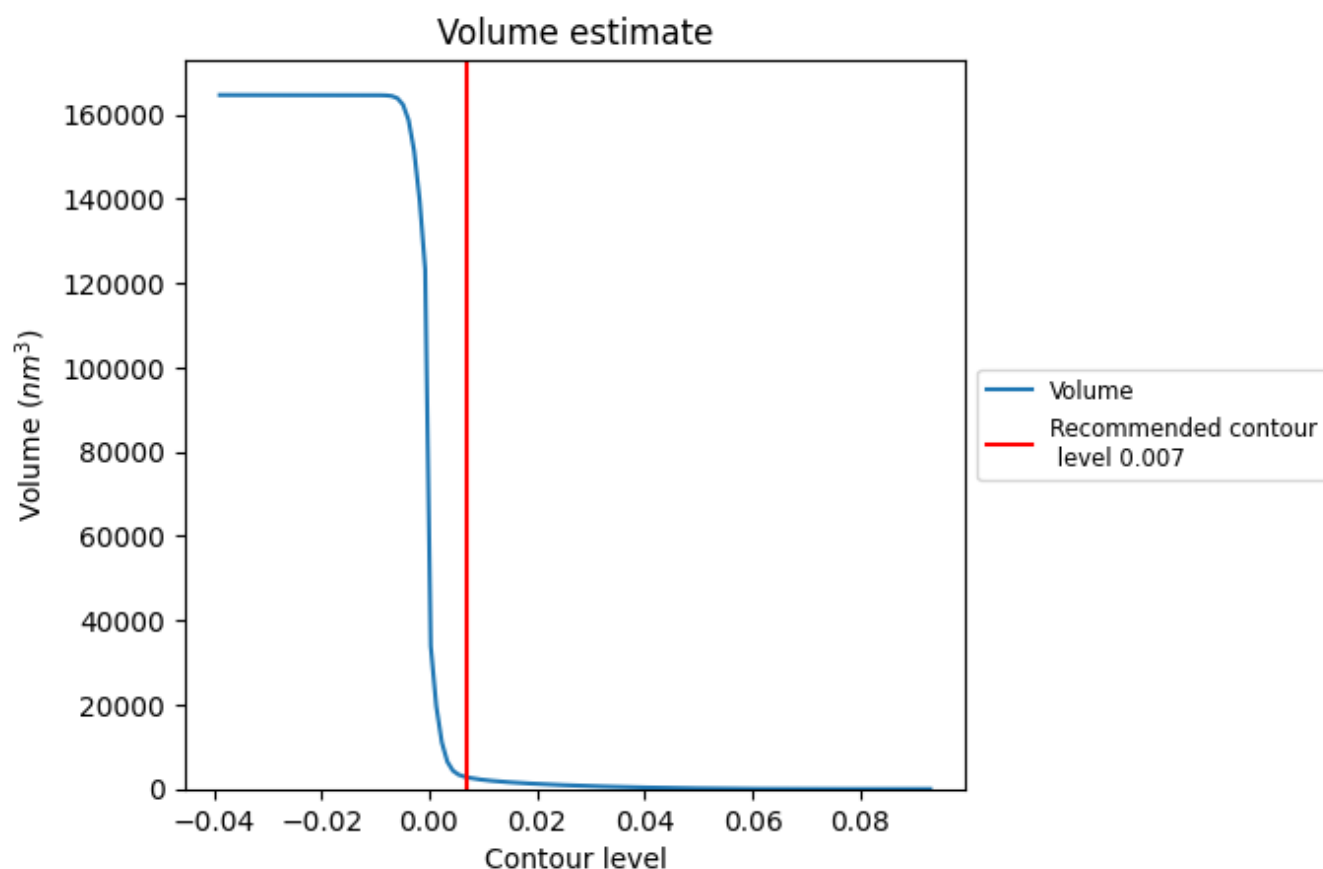
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

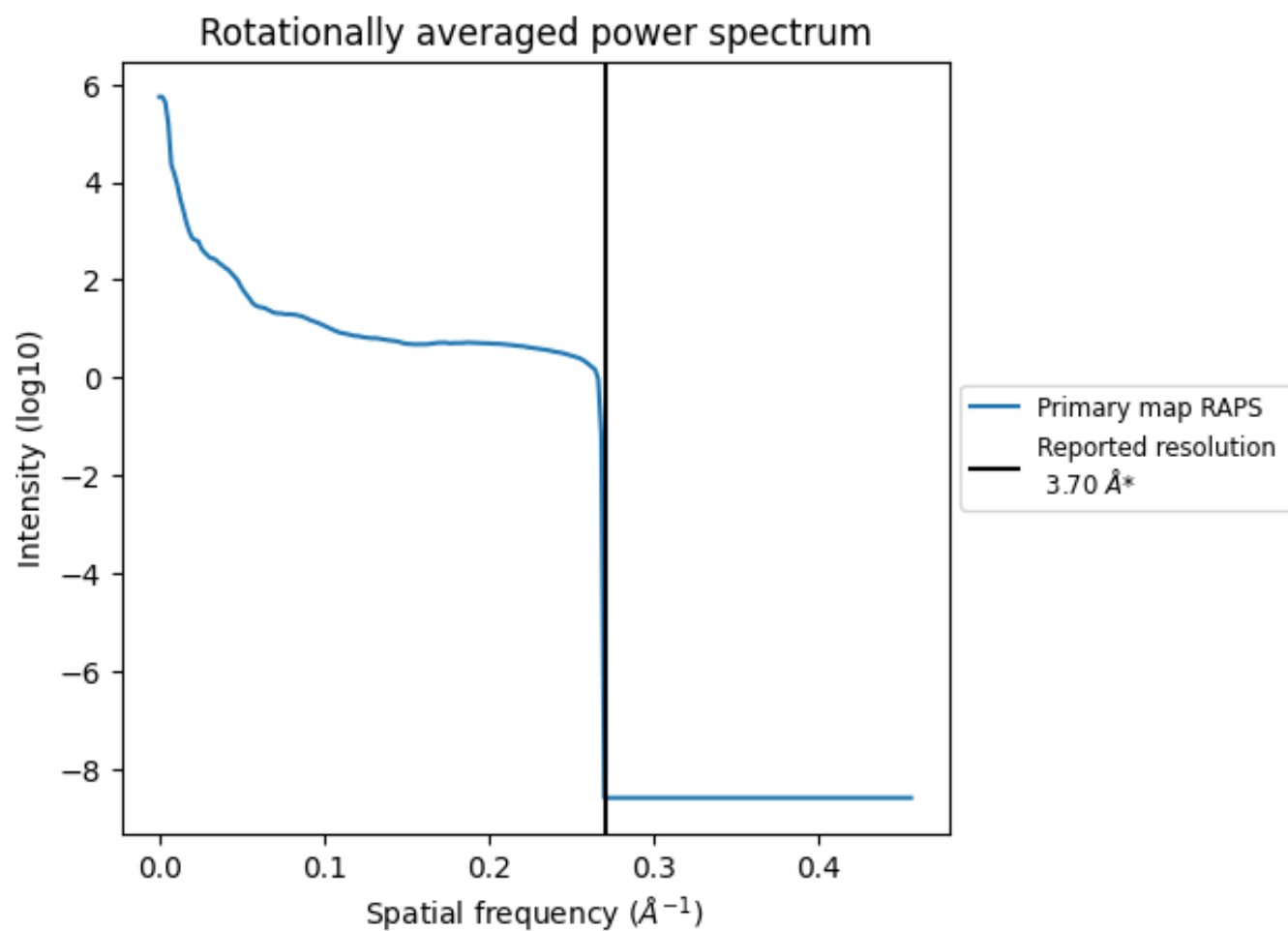
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2788 nm^3 ; this corresponds to an approximate mass of 2518 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 ⓘ

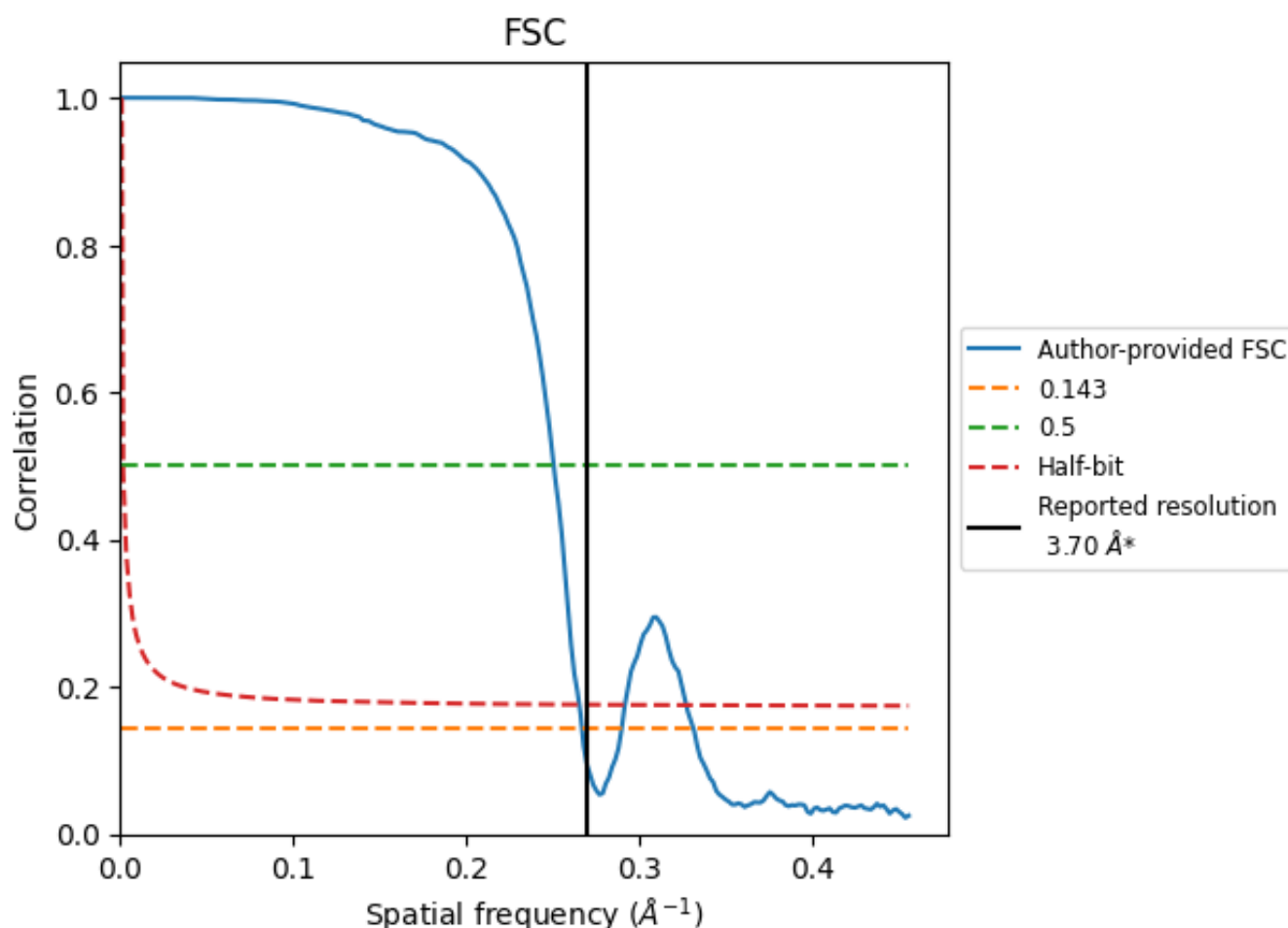


*Reported resolution corresponds to spatial frequency of 0.270 Å⁻¹

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 0.270 \AA^{-1}

8.2 Resolution estimates [i](#)

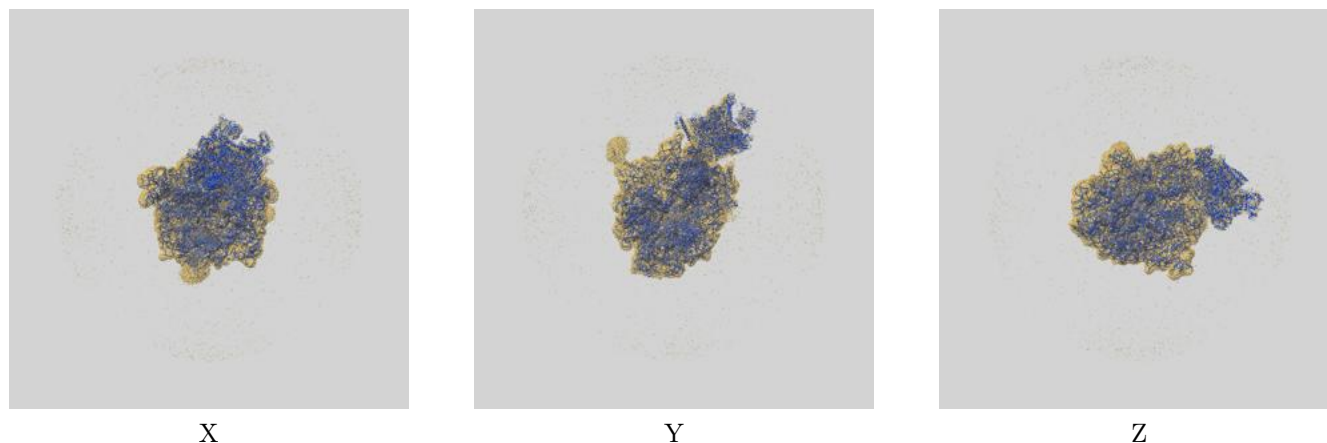
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	3.74	3.99	3.77
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

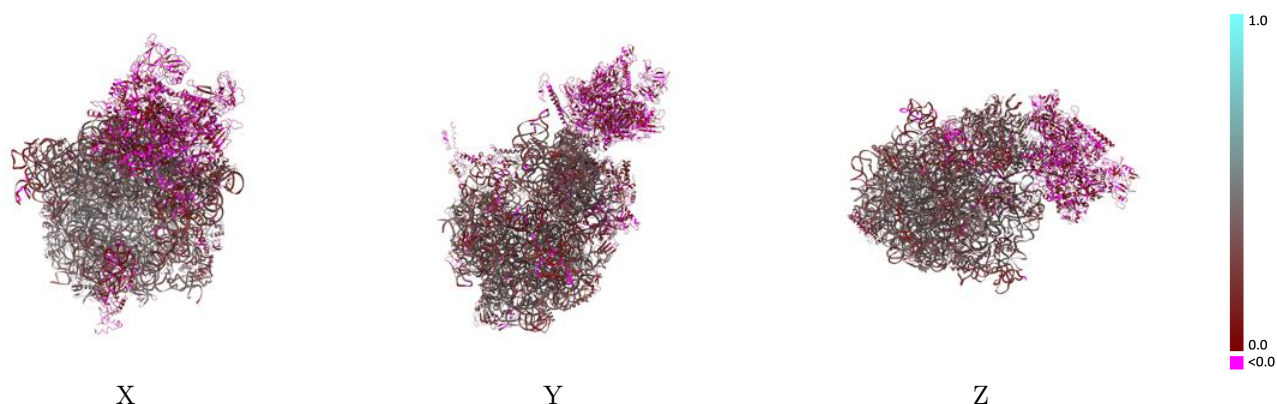
This section contains information regarding the fit between EMDB map EMD-21386 and PDB model 6VU3. Per-residue inclusion information can be found in section [3](#) on page [16](#).

9.1 Map-model overlay [i](#)



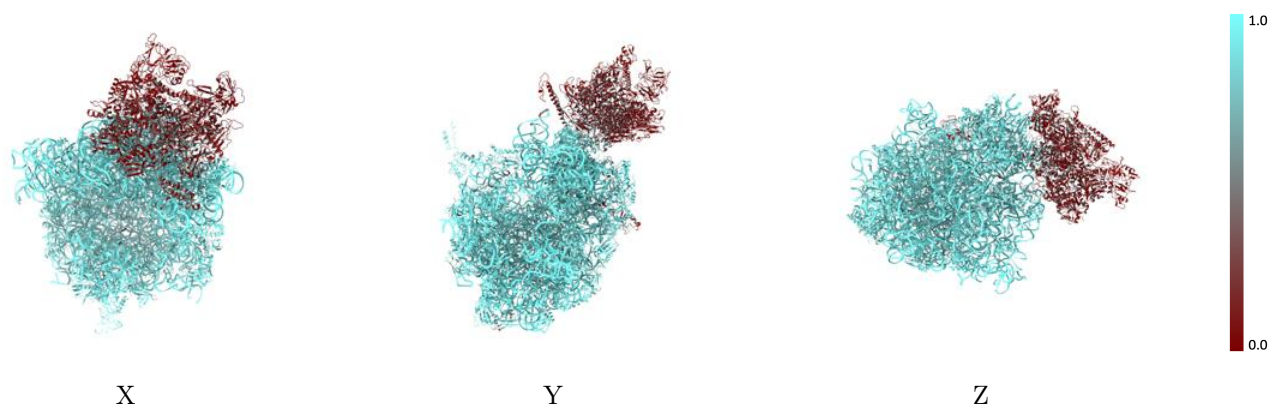
The images above show the 3D surface view of the map at the recommended contour level 0.007 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



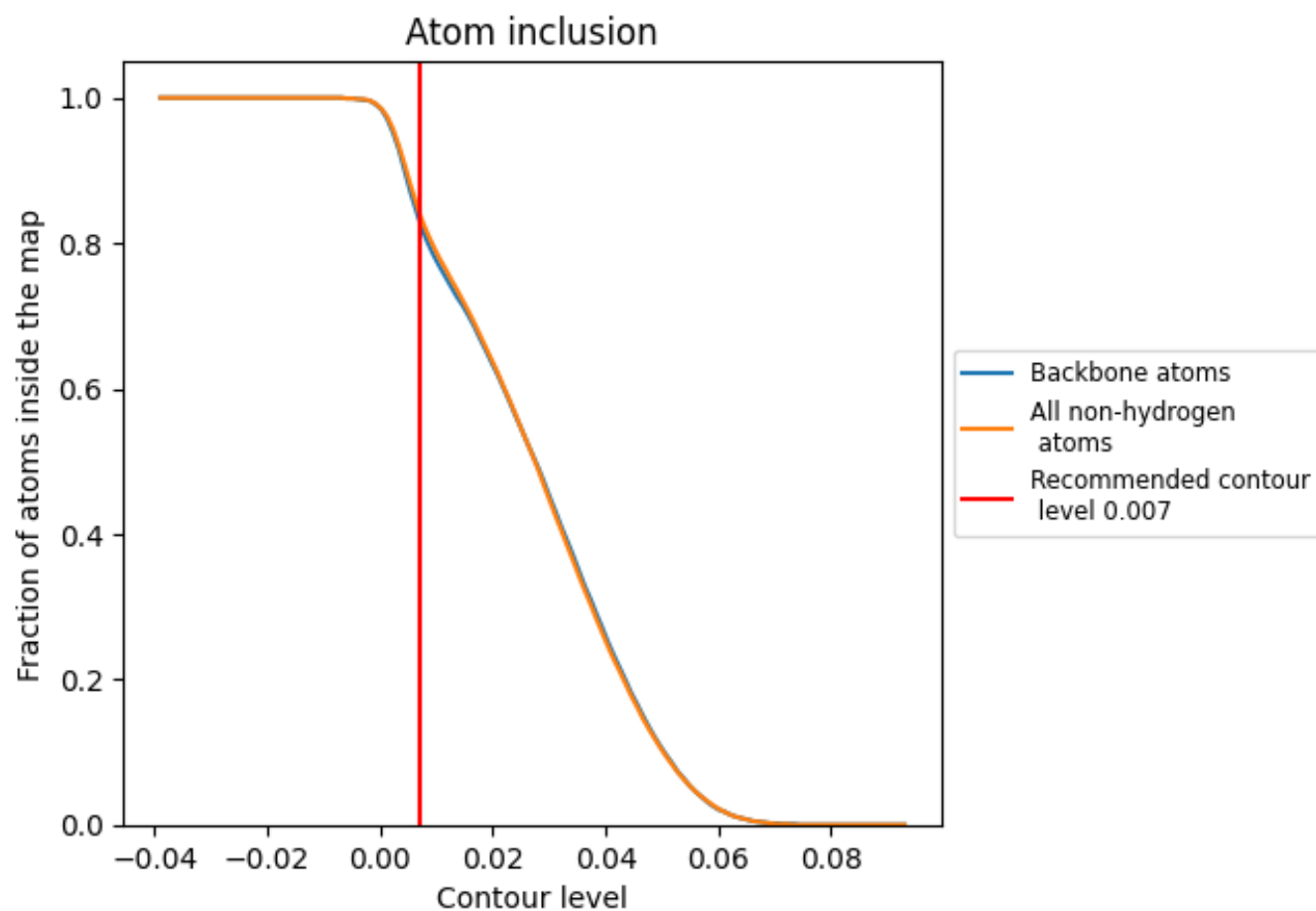
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.007).







































































9.4 Atom inclusion ⓘ



At the recommended contour level, 83% of all backbone atoms, 84% 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 (0.007) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8420	 0.2760
0	 0.8630	 0.1500
1	 0.9110	 0.3400
2	 0.9110	 0.2660
3	 0.6280	 0.0310
4	 0.9420	 0.3370
5	 0.2100	 0.0920
6	 0.3360	 0.0790
7	 0.6430	 0.0640
9	 0.9420	 0.1200
A	 0.9890	 0.2070
AA	 0.2260	 0.0620
AB	 0.1630	 0.1010
AC	 0.2250	 0.0630
AD	 0.1360	 0.0640
AE	 0.1910	 0.0790
B	 0.9170	 0.1670
C	 0.8680	 0.1580
D	 0.9890	 0.3430
E	 0.9480	 0.3300
F	 0.8230	 0.0680
G	 0.8700	 0.1600
H	 0.6290	 0.0360
I	 0.9350	 0.3890
J	 0.9180	 0.2940
K	 0.8750	 0.1820
L	 0.9190	 0.2480
M	 0.9170	 0.2680
N	 0.8870	 0.2180
O	 0.9100	 0.1900
P	 0.9310	 0.3190
Q	 0.9030	 0.2490
R	 0.8880	 0.2860
S	 0.9110	 0.2460
T	 0.9130	 0.2380



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Chain	Atom inclusion	Q-score
U	 0.9280	 0.2700
V	 0.8810	 0.2100
W	 0.9460	 0.3250
X	 0.9290	 0.3180
Y	 0.8830	 0.0510
Z	 0.9210	 0.0010
a	 0.9850	 0.3450
b	 0.8550	 0.1810
c	 0.9150	 0.3260
d	 0.9950	 0.3210
e	 0.8850	 0.1590
f	 0.9130	 0.3480
g	 0.8400	 0.0960
h	 0.9530	 0.4140
i	 0.8760	 0.2890
j	 0.9270	 0.3660
k	 0.8900	 0.2720
l	 0.8740	 0.2520
m	 0.9270	 0.3560
n	 0.9300	 0.2780
o	 0.9230	 0.3850
p	 0.9530	 0.3550
q	 0.9310	 0.3900
r	 0.8750	 0.2450
s	 0.9260	 0.3160
t	 0.9250	 0.3760
u	 0.9430	 0.3710
v	 0.9300	 0.3530
w	 0.9210	 0.2700
x	 0.9270	 0.2180
y	 0.9090	 0.2750
z	 0.9060	 0.2850