



## Full wwPDB EM Validation Report ⓘ

Nov 10, 2024 – 01:05 am GMT

PDB ID : 7QV3  
EMDB ID : EMD-14159  
Title : Bacillus subtilis MutS2-collided disome complex (MutS2 conf.2; Leading 70S)  
Authors : Filbeck, S.; Pfeffer, S.  
Deposited on : 2022-01-19  
Resolution : 5.14 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

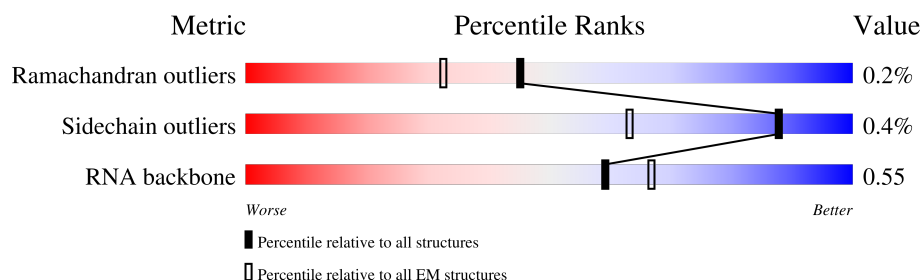
EMDB validation analysis : 0.0.1.dev113  
MolProbity : 4.02b-467  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

# 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 5.14 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.



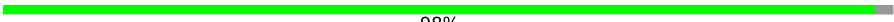
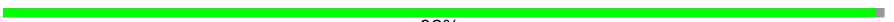












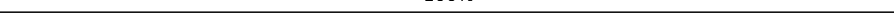
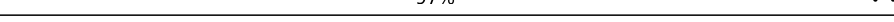
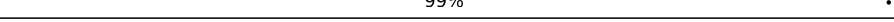
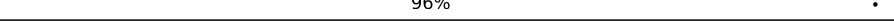
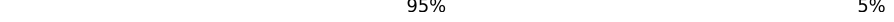
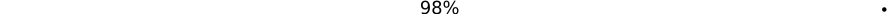


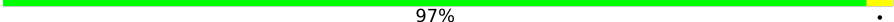
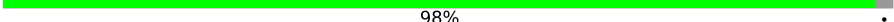
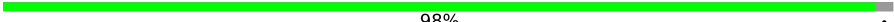
Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . 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	59	
2	1	49	
3	2	44	
4	3	66	
5	4	37	
6	6	66	
7	A	26	
8	B	112	

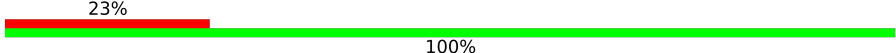
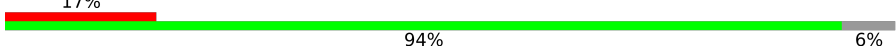
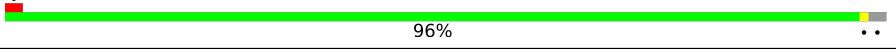
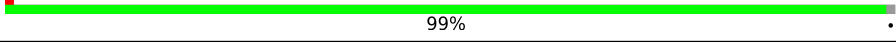
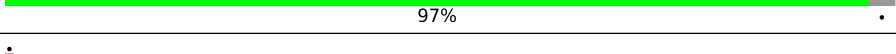
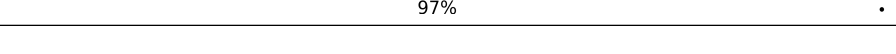
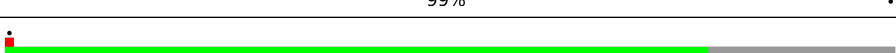
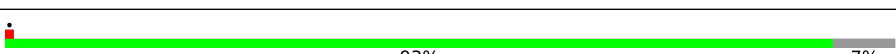
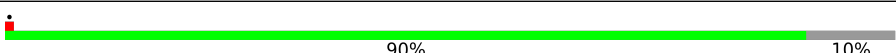
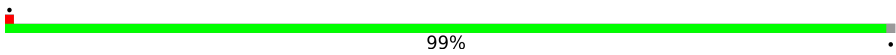

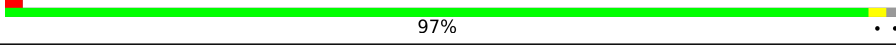
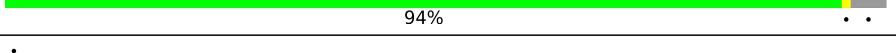
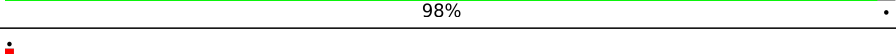
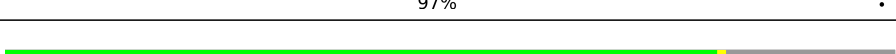
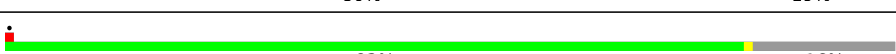
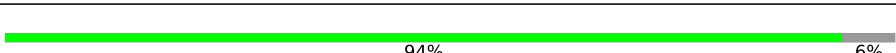
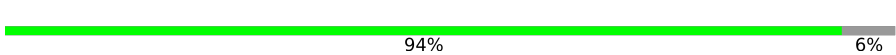




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Mol	Chain	Length	Quality of chain
9	C	277	 98% .
10	D	209	 98% .
11	E	207	 99% .
12	F	179	 97% ..
13	G	179	 98% .
14	H	77	 81% 19%
15	I	24	 33% 100%
16	J	145	 98% .
17	K	122	 100%
18	L	146	 100%
19	M	144	 94% 6%
20	N	120	 99% .
21	O	120	 98% .
22	P	115	 100%
23	Q	119	 97% ..
24	R	102	 99% .
25	S	113	 96% .
26	T	95	 95% 5%
27	U	103	 98% .
28	V	2928	 75% 23% ..
29	W	94	 87% 13%
30	X	149	 11% 97% .
31	Y	66	 98% .
32	Z	59	 98% .
33	a	1533	 83% 17%

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Mol	Chain	Length	Quality of chain
34	b	57	
35	c	218	
36	d	200	
37	e	166	
38	f	95	
39	g	156	
40	h	132	
41	i	130	
42	j	102	
43	k	131	
44	l	138	
45	m	121	
46	n	61	
47	o	89	
48	p	90	
49	q	87	
50	r	79	
51	s	92	
52	t	88	
53	u	62	
54	v	785	
54	w	785	

## 2 Entry composition

There are 54 unique types of molecules in this entry. The entry contains 149707 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	54	Total	C	N	O	S	0	0
			426	262	86	71	7		

- Molecule 2 is a protein called 50S ribosomal protein L33 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	48	Total	C	N	O	S	0	0
			401	244	80	73	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	44	Total	C	N	O	S	0	0
			367	222	89	54	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	64	Total	C	N	O	S	0	0
			512	321	107	82	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	4	37	Total	C	N	O	S	0	0
			296	186	60	45	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	6	63	Total	C	N	O	S	0	0
			499	312	91	91	5		

- Molecule 7 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	A	26	Total	C	N	O	P	0	0
			559	251	106	176	26		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	B	112	Total	C	N	O	P	0	0
			2392	1068	435	778	111		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	C	272	Total	C	N	O	S	0	0
			2083	1296	408	373	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	D	206	Total	C	N	O	S	0	0
			1569	985	289	290	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	E	205	Total	C	N	O	S	0	0
			1561	980	289	290	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	F	176	Total	C	N	O	S	0	0
			1386	882	241	256	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	G	175	Total	C	N	O	S	0	0
			1342	835	248	257	2		

- Molecule 14 is a RNA chain called P-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	H	77	Total	C	N	O	P	0	0
			1643	731	290	545	77		

- Molecule 15 is a protein called Nascent chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	I	24	Total	C	N	O	0	0
			120	72	24	24		

- Molecule 16 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	J	142	Total	C	N	O	S	0	0
			1123	710	206	202	5		

- Molecule 17 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	K	122	Total	C	N	O	S	0	0
			920	571	173	172	4		

- Molecule 18 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	L	146	Total	C	N	O	S	0	0
			1081	671	207	201	2		

- Molecule 19 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	M	135	Total	C	N	O	S	0	0
			1076	690	205	176	5		

- Molecule 20 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	N	119	Total	C	N	O	S	0	0
			953	583	186	180	4		

- Molecule 21 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	O	120	Total	C	N	O	S	0	0
			912	564	176	171	1		

- Molecule 22 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	P	115	Total	C	N	O	S	0	0
			944	600	185	158	1		

- Molecule 23 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Q	117	Total	C	N	O	S	0	0
			940	591	189	156	4		

- Molecule 24 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	R	101	Total	C	N	O		0	0
			786	501	139	146			

- Molecule 25 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	S	109	Total	C	N	O	S	0	0
			842	525	164	150	3		

- Molecule 26 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	T	90	Total	C	N	O	S	0	0
			725	452	134	136	3		

- Molecule 27 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	U	101	Total	C	N	O	S	0	0
			762	478	142	138	4		

- Molecule 28 is a RNA chain called 23S ribosomal RNA.



Mol	Chain	Residues	Atoms					AltConf	Trace
28	V	2887	Total	C	N	O	P	0	0
			61998	27661	11460	19993	2884		

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
V	243	G	A	conflict	GB 1491848961
V	325	A	-	insertion	GB 1491848961
V	326	A	-	insertion	GB 1491848961
V	327	G	-	insertion	GB 1491848961
V	328	G	-	insertion	GB 1491848961
V	640	U	C	conflict	GB 1491848961
V	2232	A	G	conflict	GB 1491848961

- Molecule 29 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms				AltConf	Trace
29	W	82	Total	C	N	O	0	0
			630	390	123	117		

- Molecule 30 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	X	149	Total	C	N	O	S	0	0
			1151	726	205	219	1		

- Molecule 31 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Y	65	Total	C	N	O	S	0	0
			530	328	102	98	2		

- Molecule 32 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Z	58	Total	C	N	O	S	0	0
			455	281	89	84	1		

- Molecule 33 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	a	1533	Total	C	N	O	P	0	0
			32891	14667	6034	10657	1533		

- Molecule 34 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	b	57	Total	C	N	O	S	0	0
			476	295	97	83	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
b	30	ALA	GLN	conflict	UNP P21478

- Molecule 35 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	c	206	Total	C	N	O	S	0	0
			1619	1011	304	301	3		

- Molecule 36 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	d	195	Total	C	N	O	S	0	0
			1568	991	291	284	2		

- Molecule 37 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	e	164	Total	C	N	O	S	0	0
			1218	767	225	224	2		

- Molecule 38 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	f	92	Total	C	N	O	S	0	0
			755	476	132	146	1		

- Molecule 39 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	g	151	Total	C	N	O	S	0	0
			1203	755	224	218	6		

- Molecule 40 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	h	131	Total	C	N	O	S	0	0
			1036	655	191	187	3		

- Molecule 41 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	i	103	Total	C	N	O	S	0	0
			784	485	151	148			

- Molecule 42 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	j	95	Total	C	N	O	S	0	0
			761	479	139	141	2		

- Molecule 43 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	k	118	Total	C	N	O	S	0	0
			871	537	171	161	2		

- Molecule 44 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	l	136	Total	C	N	O	S	0	0
			1052	653	211	186	2		

- Molecule 45 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	m	92	Total	C	N	O	S	0	0
			740	459	145	136			

- Molecule 46 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	n	60	Total	C	N	O	S	0	0
			497	317	98	77	5		

- Molecule 47 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	o	85	Total	C	N	O	S	0	0
			710	436	144	129	1		

- Molecule 48 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	p	88	Total	C	N	O	S	0	0
			695	441	128	124	2		

- Molecule 49 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	q	84	Total	C	N	O	S	0	0
			691	435	128	126	2		

- Molecule 50 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	r	64	Total	C	N	O	S	0	0
			518	332	96	88	2		

- Molecule 51 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	s	77	Total	C	N	O	S	0	0
			624	403	110	109	2		

- Molecule 52 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	t	83	Total	C	N	O	S	0	0
			637	390	130	116	1		

- Molecule 53 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	u	58	Total	C	N	O	S	0	0
			444	275	92	75	2		

- Molecule 54 is a protein called Endonuclease MutS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	v	548	Total	C	N	O	S	0	0
			4289	2680	743	850	16		
54	w	593	Total	C	N	O	S	0	0
			4644	2904	804	919	17		

### 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 L32

Chain 0:  92% 8%



- Molecule 2: 50S ribosomal protein L33 1

Chain 1:  98% .



- Molecule 3: 50S ribosomal protein L34

Chain 2:  100%

There are no outlier residues recorded for this chain.

- Molecule 4: 50S ribosomal protein L35

Chain 3:  97% .



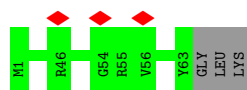
- Molecule 5: 50S ribosomal protein L36

Chain 4:  100%

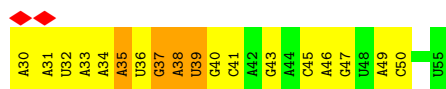
There are no outlier residues recorded for this chain.

- Molecule 6: 50S ribosomal protein L31

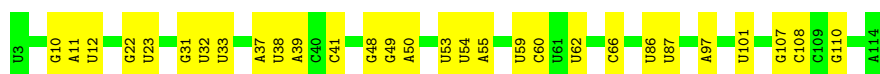
Chain 6:  5% 95% 5%



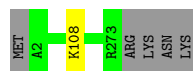
- Molecule 7: mRNA



- Molecule 8: 5S ribosomal RNA



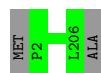
- Molecule 9: 50S ribosomal protein L2



- Molecule 10: 50S ribosomal protein L3



- Molecule 11: 50S ribosomal protein L4



- Molecule 12: 50S ribosomal protein L5



- Molecule 13: 50S ribosomal protein L6





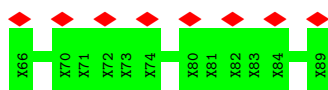
- Molecule 14: P-site tRNA

Chain H: 81% 19%



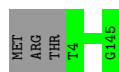
- Molecule 15: Nascent chain

Chain I: 33% 100%



- Molecule 16: 50S ribosomal protein L13

Chain J: 98% .



- Molecule 17: 50S ribosomal protein L14

Chain K: 100%

There are no outlier residues recorded for this chain.

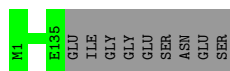
- Molecule 18: 50S ribosomal protein L15

Chain L: 100%

There are no outlier residues recorded for this chain.

- Molecule 19: 50S ribosomal protein L16

Chain M: 94% 6%



- Molecule 20: 50S ribosomal protein L17

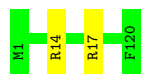
Chain N: 99% .





- Molecule 21: 50S ribosomal protein L18

Chain O:  98%



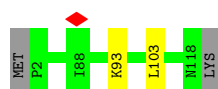
- Molecule 22: 50S ribosomal protein L19

Chain P:  100%

There are no outlier residues recorded for this chain.

- Molecule 23: 50S ribosomal protein L20

Chain Q:  97%



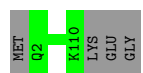
- Molecule 24: 50S ribosomal protein L21

Chain R:  99%



- Molecule 25: 50S ribosomal protein L22

Chain S:  96%



- Molecule 26: 50S ribosomal protein L23

Chain T:  95%



- Molecule 27: 50S ribosomal protein L24

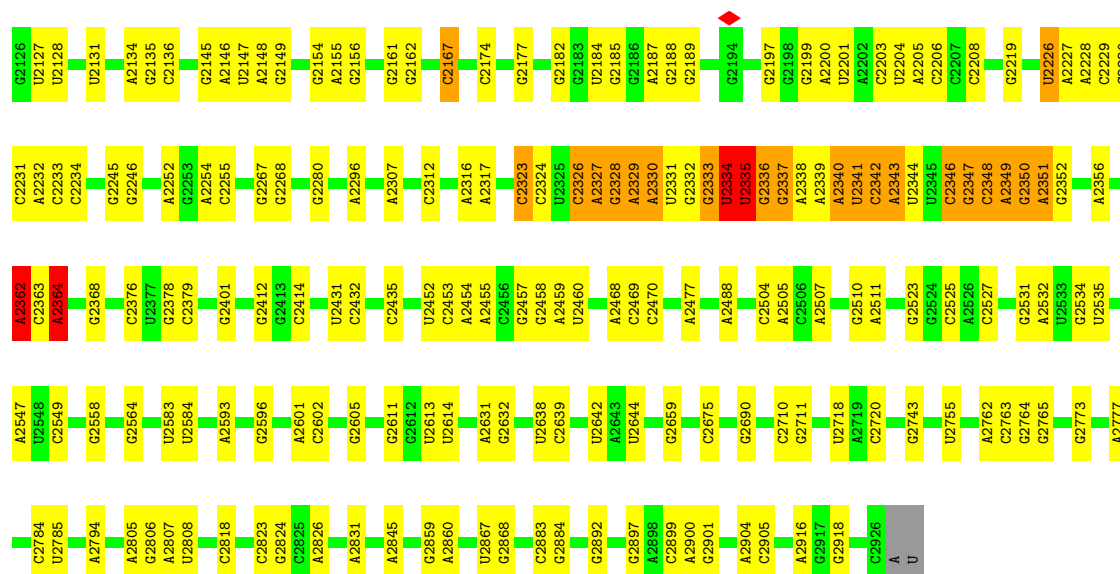
Chain U:  98%



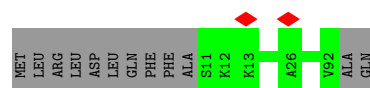
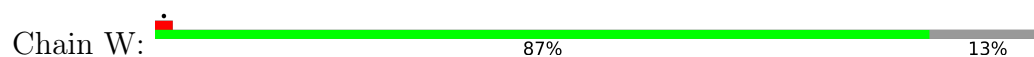
- Molecule 28: 23S ribosomal RNA

Chain V:  75% 23% ..

U1972	G1810	A1631	G1525	C1389	G1259	C1110	A957	C789	A578	U420	C308	G175	G
U1973	C1811	G1632	G1526	A1404	A1260	U1111	A958	A790	5579	A421	U309	G176	G2
U1984	A1813	U1634	C1527	U1527	G1264	A1116	C959	U794	A592	C432	G	A178	U8
C1991	G1828	A1638	U1529	C1415	G1265	G1117	C960	G795	A593	G433	U	A179	A13
C1992	C1829	A1653	G1530	U1417	A1265	C1118	C961	C795	C594	U434	A	C182	
C1993	G1830	A1654	G1531	U1418	A1269	A1119	C962	A811	C594	U434	A	A183	G23
C1996	U1837	A1655	A1532	C1422	C1270	C1120	A964	G822	U598	G443	G	G184	G26
A1999	A1838		U1535	U1535	G1275	C1121	G973	G823	C441	U444	A	C186	U34
A2000	G1843	A1661	A1536	A1424	G1276	C1124	C380	A829	G607	C445	G	C187	
G2001	A1844	A1679	C1539	C1425	A1277	C1125	C380	A829	A616	G458	U	C188	C46
G2009	A1845	A1679	A1540	G1427	G1278	A1426	A987	U831	G617	A459	A	A199	
A2010	G1846	A1691	A1541	U1691	A1293	U1128	A991	G832	A618	U459	C	A200	G51
U2020	A1850	C1693	U1543	G1431	G1296	C1129	G992	A619	A619	G471	A	C201	
G2021	A1858		U1547	A1434	A1305	G1134	A999	U637	U632	A476	A	A202	G60
U2022	C1862	A1697	A1553	U1435	G1306	U1136	A999	G845	A477	A477	G	A207	A71
U2024	U1863	G1698	U	A1553	G1311	G1139	A1005	C852	A647	C482	A329	G215	U74
C2025	G1864	A1700	A1555	A1442	A1312	U1140	A1006	C859	G649	C483	U	A216	G75
A2026	A1877	U1708	A1556	C1447	A1313	A1141	G1007	C859	A658	C491	A342	A219	C76
C2037	A1882		G1557	U1448	A1314	C1148	A1020	A866	A659	U498	A343		U77
G2050	A1883	G1719	C1559	C1449	G1315	G1158	A1027	U874	U662	U498	G344	A224	U78
A2052	G1884	G1726	U1451	C1450	A1323	U1159	C1028	U892	A667	C502	A345	A225	
C2053	A1885	A1727	U1565	C1452	G1324	A1160	A1029	U892	A667	A504	G347	A226	C85
C2054	G1886	U1738	U1567	U1457	A1326	A1161	A1036	G905	A673	G505	U348		C96
	G1887		G1568	U1458	U1327	A1172	A1042	U907	A683	U506	G352	A231	U87
	A1891	A1745	A1569	G1460	A1339	A1173	A1051	A908	C509	C509	G361	G233	U89
A2059	A1895	G1757	U1570	A1465	A1340	U1178	C1052	A908	A689	C509	G367	U242	A91
G2062	U1896	U1758	G1571	U1466	G1342	A1179	C1053	A909	A690	G512	A373	U242	C93
U2063	U1899	U1759	C1573	G1472	C1343	C1180	A1054	A692	U691	A527	A374	G251	U99
G2064	A1760	A1760		A1473	C1344	G1182	A1055	U924	A699	C529	C375	G253	U100
	G1904		C1577	A1472	A1473	G1185	U1068	A925	A699	C529			G101
C2072	A1914	G1775	A	C1474	U1351	C1186	A1059	A925	U700	A530	G382	A258	
C2079	U1915	A1776	A	C1476	U1352	U1187	A1059	G929	G701	A530	C399	A258	A117
	G1935	A1778	A		G1362	A1188	G1068	C931	A702	A537	U	G269	A118
G2084	C1943	G1779	U	U1489	C1364	G1383	A1073	C932	C718	A548	C	G283	U119
G2085		C1780	U	A1490	U1365	U	A1073	U934	C719	A549	U	C284	A124
A2089	A1948	G1781	A	A1499	U1368	C	U1079	A935	U733	G550	C	U285	A125
G2090		G1782	G	U1500	U1369	U	U1079	A935	U733	G550	U	U286	
		A1783	A	U1501	C1370	U	U1091	C936	C764	U554	C	G287	U138
G2098	G1958	G1783	U	G1502	G1371	G1220	A1092	C937	A765	C555	G406	C291	A139
	G1959	G1785	G1589		G1372	A1243	G1093	G938	A765	C556	A407		U141
C2114				A1506	C1372	A1244	G1093	G939	G772	G568	G410	G296	
U2121	A1965	A1791	A1614	U1507	A1375	G1245	A1094	G940	G773	G411	G411	G297	G145
G2122	A1966	G1792	A1617	C1508	A1375	G1245	G1101	U941	G773	A412	C		
A2123	A1967	G1793	A1617		A1375	G1245	G1101	U942	C573	A412	U	U301	A162
U1969	U1968		U1626	C1514	G1384	C1248	G1102	U943	C777	A574	C	A302	U163
A2124	U1969	A1802	U1626	C1515	G1385	U1249	A1103	C944	C787	A575	G417	A418	U164
U2125				A1516	G1385	G1250	U1106	U949	G788	U577	G419	A307	



• Molecule 29: 50S ribosomal protein L27



• Molecule 30: 50S ribosomal protein L9



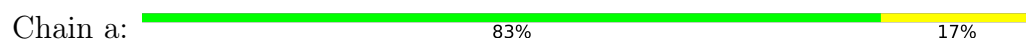
• Molecule 31: 50S ribosomal protein L29

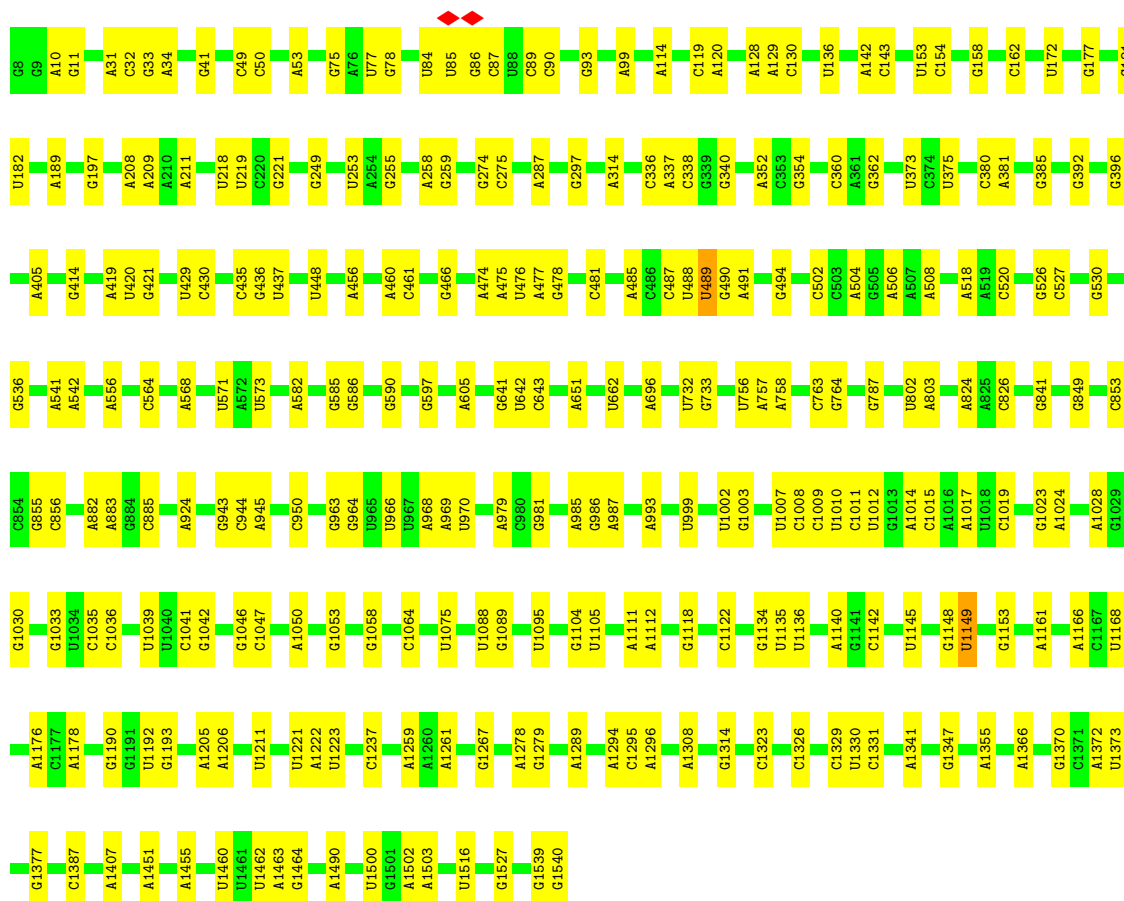


• Molecule 32: 50S ribosomal protein L30



• Molecule 33: 16S ribosomal RNA



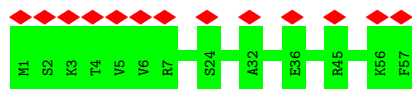


• Molecule 34: 30S ribosomal protein S21

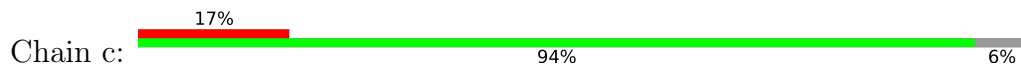


Chain b:

100%



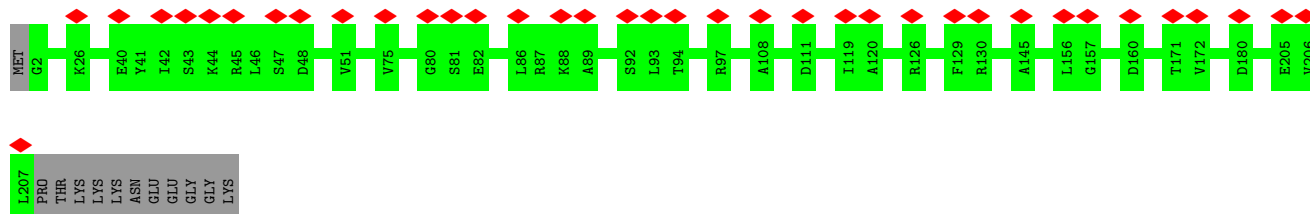
• Molecule 35: 30S ribosomal protein S3



Chain c:

94%

6%



• Molecule 36: 30S ribosomal protein S4

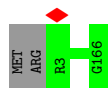


Chain d:

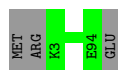
96%



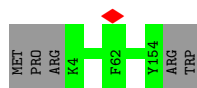
- Molecule 37: 30S ribosomal protein S5



- Molecule 38: 30S ribosomal protein S6



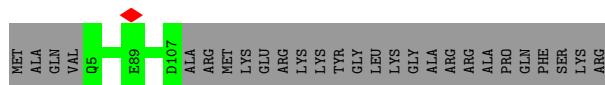
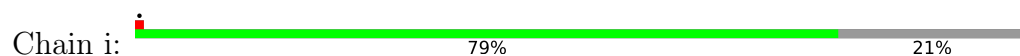
- Molecule 39: 30S ribosomal protein S7



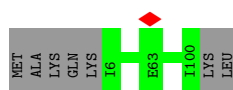
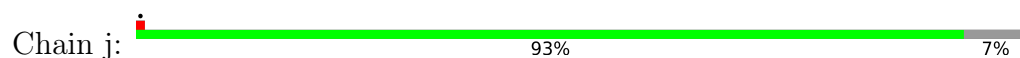
- Molecule 40: 30S ribosomal protein S8



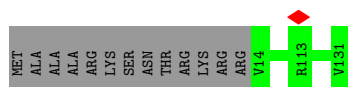
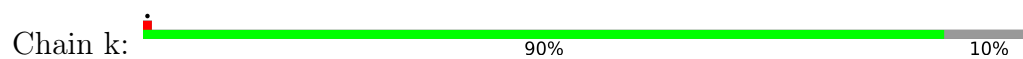
- Molecule 41: 30S ribosomal protein S9



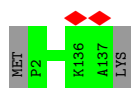
- Molecule 42: 30S ribosomal protein S10



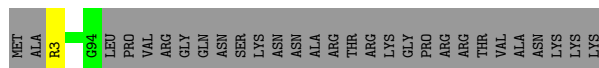
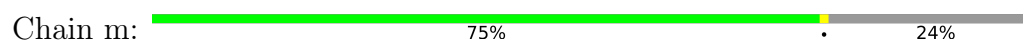
- Molecule 43: 30S ribosomal protein S11



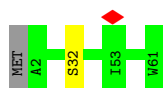
- Molecule 44: 30S ribosomal protein S12



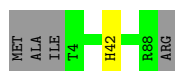
- Molecule 45: 30S ribosomal protein S13



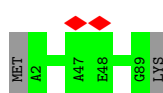
- Molecule 46: 30S ribosomal protein S14



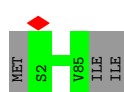
- Molecule 47: 30S ribosomal protein S15




- Molecule 48: 30S ribosomal protein S16

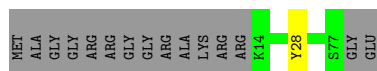


- Molecule 49: 30S ribosomal protein S17




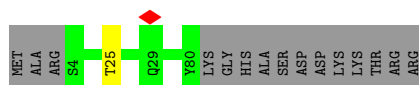
- Molecule 50: 30S ribosomal protein S18

Chain r:  80% 19%



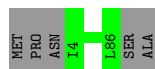
- Molecule 51: 30S ribosomal protein S19

Chain s:  83% 16%



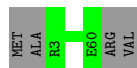
- Molecule 52: 30S ribosomal protein S20

Chain t:  94% 6%



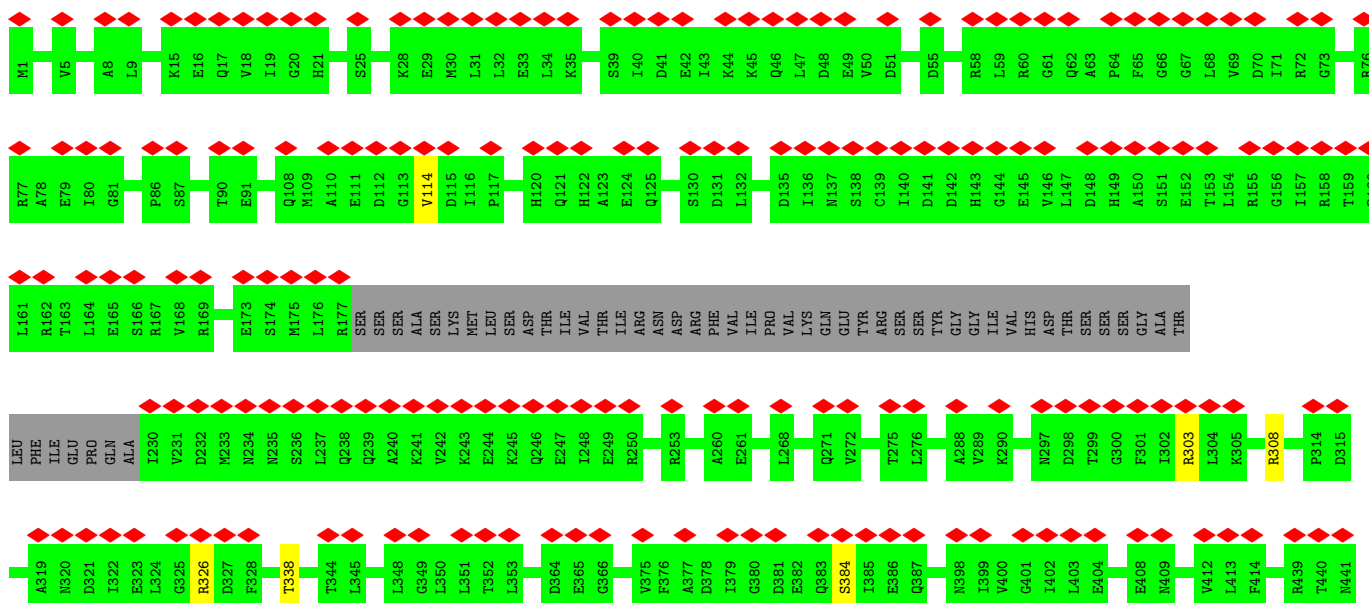
- Molecule 53: 50S ribosomal protein L28

Chain u:  94% 6%



- Molecule 54: Endonuclease MutS2

Chain v:  31% 69% 30%







## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	5078	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 ( $e^-/\text{\AA}^2$ )	46.5	Depositor
Minimum defocus (nm)	750	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.341	Depositor
Minimum map value	-0.207	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.0172	Depositor
Map size (Å)	590.64, 590.64, 590.64	wwPDB
Map dimensions	368, 368, 368	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.605, 1.605, 1.605	Depositor

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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	0.25	0/433	0.41	0/574
2	1	0.25	0/406	0.44	0/540
3	2	0.26	0/370	0.42	0/483
4	3	0.24	0/519	0.41	0/680
5	4	0.25	0/299	0.40	0/393
6	6	0.26	0/509	0.40	0/678
7	A	0.72	2/627 (0.3%)	1.17	8/975 (0.8%)
8	B	0.18	0/2675	0.73	0/4170
9	C	0.25	0/2120	0.43	0/2845
10	D	0.25	0/1591	0.45	0/2132
11	E	0.24	0/1580	0.41	0/2132
12	F	0.39	0/1405	0.66	0/1887
13	G	0.24	0/1360	0.42	0/1832
14	H	0.16	0/1834	0.72	0/2858
16	J	0.24	0/1146	0.41	0/1542
17	K	0.26	0/927	0.45	0/1245
18	L	0.26	0/1093	0.44	0/1457
19	M	0.25	0/1099	0.41	0/1468
20	N	0.23	0/960	0.41	0/1284
21	O	0.30	0/921	0.55	2/1236 (0.2%)
22	P	0.25	0/957	0.43	0/1279
23	Q	0.25	0/952	0.40	0/1266
24	R	0.26	0/797	0.46	0/1070
25	S	0.24	0/851	0.43	0/1146
26	T	0.24	0/731	0.41	0/974
27	U	0.25	0/772	0.43	0/1032
28	V	0.27	0/69444	0.81	91/108334 (0.1%)
29	W	0.25	0/638	0.43	0/847
30	X	0.24	0/1162	0.41	0/1551
31	Y	0.24	0/531	0.37	0/707
32	Z	0.23	0/457	0.43	0/613
33	a	0.20	0/36826	0.73	4/57450 (0.0%)
34	b	0.26	0/480	0.42	0/628
35	c	0.25	0/1641	0.43	0/2208

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
36	d	0.25	0/1598	0.40	0/2147
37	e	0.25	0/1230	0.43	0/1655
38	f	0.24	0/766	0.41	0/1031
39	g	0.23	0/1220	0.38	0/1637
40	h	0.25	0/1048	0.45	0/1407
41	i	0.23	0/794	0.43	0/1074
42	j	0.23	0/773	0.40	0/1044
43	k	0.25	0/885	0.44	0/1196
44	l	0.25	0/1069	0.45	0/1435
45	m	0.23	0/744	0.41	0/994
46	n	0.24	0/507	0.40	0/672
47	o	0.23	0/718	0.42	0/960
48	p	0.25	0/708	0.41	0/950
49	q	0.25	0/699	0.42	0/933
50	r	0.24	0/526	0.40	0/705
51	s	0.24	0/640	0.43	0/861
52	t	0.23	0/639	0.39	0/852
53	u	0.23	0/448	0.46	0/596
54	v	0.52	0/4341	0.77	6/5847 (0.1%)
54	w	0.53	0/4703	0.78	7/6337 (0.1%)
All	All	0.27	2/162169 (0.0%)	0.72	118/241849 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
28	V	0	16
54	w	0	2
All	All	0	18

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	41	C	C1'-N1	5.26	1.56	1.48
7	A	50	C	C1'-N1	5.02	1.56	1.48

All (118) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	V	138	U	OP1-P-O3'	-39.33	18.68	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	V	139	A	OP1-P-OP2	-12.74	100.50	119.60
28	V	2340	A	N1-C6-N6	-11.09	111.95	118.60
28	V	2362	A	N1-C6-N6	-11.09	111.95	118.60
28	V	2364	A	N1-C6-N6	-9.31	113.01	118.60
28	V	2328	G	O4'-C1'-N9	9.20	115.56	108.20
7	A	32	U	P-O3'-C3'	-9.19	108.67	119.70
28	V	2349	A	C1'-O4'-C4'	-8.73	102.92	109.90
28	V	2351	A	N1-C6-N6	-8.41	113.55	118.60
28	V	2339	A	N1-C6-N6	-8.41	113.56	118.60
54	w	544	ARG	NE-CZ-NH1	8.30	124.45	120.30
28	V	1449	C	P-O3'-C3'	-8.30	109.74	119.70
7	A	37	G	P-O3'-C3'	-8.23	109.82	119.70
28	V	1450	C	P-O3'-C3'	-8.17	109.89	119.70
7	A	38	A	P-O3'-C3'	-8.14	109.93	119.70
28	V	1447	C	P-O3'-C3'	-7.96	110.15	119.70
54	w	308	ARG	NE-CZ-NH1	7.89	124.25	120.30
28	V	2327	A	N1-C6-N6	-7.84	113.90	118.60
28	V	2123	A	P-O3'-C3'	-7.79	110.35	119.70
28	V	2351	A	C5-C6-N1	7.79	121.59	117.70
28	V	2346	C	N3-C2-O2	-7.74	116.48	121.90
28	V	2349	A	N1-C6-N6	-7.70	113.98	118.60
28	V	2329	A	C5-C6-N1	7.69	121.54	117.70
28	V	2323	C	N3-C2-O2	-7.62	116.57	121.90
28	V	2330	A	C5-C6-N1	7.51	121.46	117.70
28	V	2340	A	C5-C6-N1	7.51	121.46	117.70
28	V	2342	C	N3-C2-O2	-7.51	116.64	121.90
28	V	2330	A	C5'-C4'-O4'	7.43	118.02	109.10
28	V	2324	C	N3-C2-O2	-7.39	116.73	121.90
28	V	2362	A	C5-C6-N1	7.06	121.23	117.70
54	v	326	ARG	NE-CZ-NH1	7.04	123.82	120.30
28	V	2343	A	N1-C6-N6	-6.98	114.41	118.60
28	V	2349	A	C5-C6-N1	6.97	121.18	117.70
54	v	308	ARG	NE-CZ-NH1	6.92	123.76	120.30
28	V	2339	A	C5-C6-N1	6.90	121.15	117.70
28	V	925	A	N1-C6-N6	-6.89	114.46	118.60
28	V	2323	C	N1-C2-O2	6.89	123.03	118.90
28	V	2328	G	N9-C1'-C2'	-6.78	104.55	112.00
28	V	2350	G	N1-C6-O6	-6.75	115.85	119.90
7	A	35	A	P-O3'-C3'	-6.74	111.62	119.70
28	V	2327	A	C5-C6-N1	6.70	121.05	117.70
28	V	2343	A	C5-C6-N1	6.66	121.03	117.70
28	V	2335	U	O4'-C1'-N1	6.64	113.51	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	V	2349	A	C5'-C4'-O4'	6.58	116.99	109.10
28	V	2343	A	C4-C5-C6	-6.51	113.74	117.00
54	w	439	ARG	NE-CZ-NH1	6.51	123.56	120.30
28	V	2333	G	N3-C2-N2	-6.49	115.35	119.90
28	V	2122	G	P-O3'-C3'	-6.46	111.95	119.70
28	V	2340	A	C4-C5-C6	-6.43	113.78	117.00
28	V	2334	U	N3-C2-O2	-6.38	117.73	122.20
54	w	58	ARG	NE-CZ-NH2	6.37	123.49	120.30
28	V	924	U	O4'-C1'-N1	6.31	113.25	108.20
28	V	2342	C	C5'-C4'-C3'	-6.27	105.97	116.00
54	w	443	ARG	NE-CZ-NH1	6.26	123.43	120.30
28	V	2324	C	N1-C2-O2	6.25	122.65	118.90
28	V	2323	C	O4'-C1'-N1	6.23	113.18	108.20
33	a	1149	U	C2-N1-C1'	6.18	125.11	117.70
28	V	2341	U	O4'-C1'-N1	6.17	113.14	108.20
28	V	2226	U	P-O3'-C3'	-6.10	112.38	119.70
28	V	925	A	C5-C6-N1	6.09	120.75	117.70
28	V	509	C	N3-C2-O2	-6.08	117.64	121.90
28	V	1452	C	P-O3'-C3'	-6.07	112.41	119.70
28	V	2364	A	C5-C6-N1	6.07	120.74	117.70
21	O	17	ARG	NE-CZ-NH1	6.05	123.32	120.30
28	V	2330	A	N1-C6-N6	-6.03	114.98	118.60
7	A	31	A	P-O3'-C3'	-6.01	112.48	119.70
28	V	2362	A	C4-C5-C6	-6.01	114.00	117.00
54	v	443	ARG	NE-CZ-NH1	5.98	123.29	120.30
21	O	14	ARG	NE-CZ-NH1	5.98	123.29	120.30
28	V	420	U	P-O3'-C3'	-5.98	112.53	119.70
28	V	2331	U	C5'-C4'-C3'	-5.97	106.45	116.00
28	V	2335	U	C3'-C2'-C1'	5.95	106.26	101.50
28	V	2342	C	C5'-C4'-O4'	5.94	116.23	109.10
28	V	2348	C	N3-C2-O2	-5.89	117.77	121.90
28	V	2351	A	C4-C5-C6	-5.83	114.08	117.00
28	V	2331	U	C5'-C4'-O4'	5.80	116.06	109.10
28	V	2167	C	N3-C2-O2	-5.79	117.84	121.90
28	V	2339	A	C4-C5-C6	-5.78	114.11	117.00
28	V	2336	G	C3'-C2'-C1'	5.71	106.07	101.50
54	v	303	ARG	NE-CZ-NH1	5.71	123.15	120.30
28	V	2334	U	O4'-C1'-N1	5.71	112.77	108.20
28	V	417	G	P-O3'-C3'	-5.64	112.93	119.70
28	V	138	U	OP2-P-O3'	5.62	117.58	105.20
28	V	1693	C	C2-N1-C1'	-5.57	112.67	118.80
28	V	1693	C	C6-N1-C1'	5.55	127.46	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	V	1451	U	P-O3'-C3'	-5.50	113.10	119.70
28	V	2364	A	O4'-C1'-N9	5.50	112.60	108.20
28	V	2346	C	N1-C2-O2	5.49	122.19	118.90
28	V	2347	G	C5'-C4'-O4'	5.47	115.67	109.10
33	a	489	U	C2-N1-C1'	5.43	124.22	117.70
7	A	30	A	P-O3'-C3'	-5.40	113.22	119.70
28	V	2349	A	N9-C1'-C2'	5.40	121.03	114.00
28	V	419	G	P-O3'-C3'	-5.40	113.22	119.70
54	w	439	ARG	NE-CZ-NH2	-5.38	117.61	120.30
28	V	2037	C	N3-C2-O2	-5.38	118.13	121.90
54	v	308	ARG	NH1-CZ-NH2	-5.37	113.49	119.40
28	V	2333	G	C5'-C4'-C3'	-5.37	107.41	116.00
33	a	1323	C	N1-C2-O2	5.37	122.12	118.90
28	V	2329	A	C4-C5-C6	-5.31	114.34	117.00
28	V	2364	A	C4-C5-C6	-5.28	114.36	117.00
28	V	2329	A	N1-C6-N6	-5.25	115.45	118.60
33	a	763	C	C2-N1-C1'	5.23	124.56	118.80
28	V	2342	C	N1-C2-O2	5.20	122.02	118.90
28	V	2332	G	N1-C6-O6	-5.19	116.78	119.90
54	w	196	ARG	NE-CZ-NH2	5.19	122.89	120.30
7	A	36	U	P-O3'-C3'	-5.19	113.48	119.70
28	V	2327	A	C4-C5-C6	-5.17	114.42	117.00
28	V	2336	G	N3-C4-C5	-5.14	126.03	128.60
54	v	497	ARG	NE-CZ-NH1	5.13	122.87	120.30
28	V	2326	C	N3-C2-O2	-5.09	118.34	121.90
28	V	2346	C	N3-C4-N4	-5.07	114.45	118.00
28	V	2330	A	C4-C5-C6	-5.07	114.46	117.00
28	V	2352	G	N1-C6-O6	-5.06	116.86	119.90
28	V	2350	G	C5-C6-N1	5.06	114.03	111.50
28	V	949	U	O4'-C1'-N1	5.06	112.25	108.20
28	V	2350	G	C5'-C4'-C3'	-5.06	107.91	116.00
7	A	39	U	OP2-P-O3'	5.01	116.22	105.20
28	V	2347	G	C5'-C4'-C3'	-5.01	107.99	116.00

There are no chirality outliers.

All (18) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
28	V	2323	C	Sidechain
28	V	2326	C	Sidechain
28	V	2327	A	Sidechain
28	V	2329	A	Sidechain

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Mol	Chain	Res	Type	Group
28	V	2333	G	Sidechain
28	V	2334	U	Sidechain
28	V	2335	U	Sidechain
28	V	2337	G	Sidechain
28	V	2340	A	Sidechain
28	V	2342	C	Sidechain
28	V	2343	A	Sidechain
28	V	2344	U	Sidechain
28	V	2346	C	Sidechain
28	V	2362	A	Sidechain
28	V	2364	A	Sidechain
28	V	924	U	Sidechain
54	w	308	ARG	Sidechain
54	w	456	TYR	Sidechain

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

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

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	52/59 (88%)	50 (96%)	2 (4%)	0	100	100
2	1	46/49 (94%)	44 (96%)	2 (4%)	0	100	100
3	2	42/44 (96%)	42 (100%)	0	0	100	100
4	3	62/66 (94%)	60 (97%)	2 (3%)	0	100	100
5	4	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
6	6	61/66 (92%)	60 (98%)	1 (2%)	0	100	100
9	C	270/277 (98%)	260 (96%)	10 (4%)	0	100	100
10	D	204/209 (98%)	193 (95%)	11 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	E	203/207 (98%)	193 (95%)	10 (5%)	0	100	100
12	F	174/179 (97%)	161 (92%)	13 (8%)	0	100	100
13	G	173/179 (97%)	165 (95%)	8 (5%)	0	100	100
16	J	140/145 (97%)	133 (95%)	7 (5%)	0	100	100
17	K	120/122 (98%)	117 (98%)	3 (2%)	0	100	100
18	L	144/146 (99%)	139 (96%)	5 (4%)	0	100	100
19	M	133/144 (92%)	132 (99%)	1 (1%)	0	100	100
20	N	117/120 (98%)	113 (97%)	4 (3%)	0	100	100
21	O	118/120 (98%)	113 (96%)	5 (4%)	0	100	100
22	P	113/115 (98%)	108 (96%)	5 (4%)	0	100	100
23	Q	115/119 (97%)	107 (93%)	6 (5%)	2 (2%)	7	35
24	R	99/102 (97%)	88 (89%)	11 (11%)	0	100	100
25	S	107/113 (95%)	102 (95%)	5 (5%)	0	100	100
26	T	88/95 (93%)	87 (99%)	1 (1%)	0	100	100
27	U	99/103 (96%)	92 (93%)	7 (7%)	0	100	100
29	W	80/94 (85%)	76 (95%)	4 (5%)	0	100	100
30	X	147/149 (99%)	135 (92%)	12 (8%)	0	100	100
31	Y	63/66 (96%)	62 (98%)	1 (2%)	0	100	100
32	Z	56/59 (95%)	53 (95%)	3 (5%)	0	100	100
34	b	55/57 (96%)	53 (96%)	2 (4%)	0	100	100
35	c	204/218 (94%)	194 (95%)	10 (5%)	0	100	100
36	d	193/200 (96%)	176 (91%)	17 (9%)	0	100	100
37	e	162/166 (98%)	155 (96%)	7 (4%)	0	100	100
38	f	90/95 (95%)	87 (97%)	3 (3%)	0	100	100
39	g	149/156 (96%)	144 (97%)	5 (3%)	0	100	100
40	h	129/132 (98%)	116 (90%)	13 (10%)	0	100	100
41	i	101/130 (78%)	95 (94%)	6 (6%)	0	100	100
42	j	93/102 (91%)	87 (94%)	6 (6%)	0	100	100
43	k	116/131 (88%)	110 (95%)	6 (5%)	0	100	100
44	l	134/138 (97%)	124 (92%)	10 (8%)	0	100	100
45	m	90/121 (74%)	85 (94%)	5 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
46	n	58/61 (95%)	52 (90%)	5 (9%)	1 (2%)	7	35
47	o	83/89 (93%)	79 (95%)	4 (5%)	0	100	100
48	p	86/90 (96%)	81 (94%)	5 (6%)	0	100	100
49	q	82/87 (94%)	76 (93%)	6 (7%)	0	100	100
50	r	62/79 (78%)	56 (90%)	5 (8%)	1 (2%)	8	37
51	s	75/92 (82%)	69 (92%)	6 (8%)	0	100	100
52	t	81/88 (92%)	79 (98%)	2 (2%)	0	100	100
53	u	56/62 (90%)	54 (96%)	2 (4%)	0	100	100
54	v	544/785 (69%)	527 (97%)	15 (3%)	2 (0%)	30	68
54	w	589/785 (75%)	569 (97%)	16 (3%)	4 (1%)	19	56
All	All	6293/7048 (89%)	5986 (95%)	297 (5%)	10 (0%)	45	78

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
54	v	384	SER
54	w	384	SER
23	Q	103	LEU
50	r	28	TYR
54	w	382	GLU
54	w	114	VAL
54	w	337	ASN
46	n	32	SER
54	v	114	VAL
23	Q	93	LYS

### 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	48/53 (91%)	48 (100%)	0	100	100
2	1	46/47 (98%)	46 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	2	39/39 (100%)	39 (100%)	0	100	100
4	3	54/56 (96%)	54 (100%)	0	100	100
5	4	35/35 (100%)	35 (100%)	0	100	100
6	6	53/55 (96%)	53 (100%)	0	100	100
9	C	220/225 (98%)	219 (100%)	1 (0%)	86	89
10	D	167/170 (98%)	166 (99%)	1 (1%)	84	88
11	E	169/170 (99%)	169 (100%)	0	100	100
12	F	151/154 (98%)	149 (99%)	2 (1%)	65	77
13	G	148/151 (98%)	148 (100%)	0	100	100
16	J	120/123 (98%)	120 (100%)	0	100	100
17	K	101/101 (100%)	101 (100%)	0	100	100
18	L	110/110 (100%)	110 (100%)	0	100	100
19	M	109/116 (94%)	109 (100%)	0	100	100
20	N	99/100 (99%)	99 (100%)	0	100	100
21	O	93/93 (100%)	93 (100%)	0	100	100
22	P	100/100 (100%)	100 (100%)	0	100	100
23	Q	96/98 (98%)	96 (100%)	0	100	100
24	R	83/84 (99%)	83 (100%)	0	100	100
25	S	90/93 (97%)	90 (100%)	0	100	100
26	T	81/85 (95%)	81 (100%)	0	100	100
27	U	85/87 (98%)	85 (100%)	0	100	100
29	W	64/74 (86%)	64 (100%)	0	100	100
30	X	124/124 (100%)	119 (96%)	5 (4%)	27	48
31	Y	56/57 (98%)	56 (100%)	0	100	100
32	Z	52/53 (98%)	52 (100%)	0	100	100
34	b	51/51 (100%)	51 (100%)	0	100	100
35	c	168/178 (94%)	168 (100%)	0	100	100
36	d	169/173 (98%)	167 (99%)	2 (1%)	67	79
37	e	128/130 (98%)	128 (100%)	0	100	100
38	f	81/84 (96%)	81 (100%)	0	100	100
39	g	127/132 (96%)	127 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
40	h	111/112 (99%)	111 (100%)	0	100	100
41	i	81/102 (79%)	81 (100%)	0	100	100
42	j	86/92 (94%)	86 (100%)	0	100	100
43	k	90/100 (90%)	90 (100%)	0	100	100
44	l	114/116 (98%)	114 (100%)	0	100	100
45	m	80/104 (77%)	79 (99%)	1 (1%)	65	77
46	n	53/54 (98%)	53 (100%)	0	100	100
47	o	80/83 (96%)	79 (99%)	1 (1%)	65	77
48	p	74/76 (97%)	74 (100%)	0	100	100
49	q	77/80 (96%)	77 (100%)	0	100	100
50	r	56/64 (88%)	56 (100%)	0	100	100
51	s	69/81 (85%)	68 (99%)	1 (1%)	62	76
52	t	66/70 (94%)	66 (100%)	0	100	100
53	u	47/50 (94%)	47 (100%)	0	100	100
54	v	472/674 (70%)	470 (100%)	2 (0%)	89	91
54	w	513/674 (76%)	510 (99%)	3 (1%)	84	88
All	All	5386/5933 (91%)	5367 (100%)	19 (0%)	88	91

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	C	108	LYS
10	D	140	HIS
12	F	122	PHE
12	F	164	GLU
30	X	15	LYS
30	X	25	TYR
30	X	30	LEU
30	X	68	LEU
30	X	75	LEU
36	d	54	LYS
36	d	176	PHE
45	m	3	ARG
47	o	42	HIS
51	s	25	THR
54	v	338	THR

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Mol	Chain	Res	Type
54	v	554	LEU
54	w	196	ARG
54	w	205	TYR
54	w	592	HIS

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

Mol	Chain	Res	Type
36	d	137	GLN
38	f	27	ASN
42	j	78	ASN
48	p	72	ASN
54	v	143	HIS
54	v	235	ASN
54	w	46	GLN
54	w	125	GLN
54	w	239	GLN
54	w	551	HIS

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
14	H	76/77 (98%)	14 (18%)	2 (2%)
28	V	2881/2928 (98%)	634 (22%)	64 (2%)
33	a	1532/1533 (99%)	266 (17%)	0
7	A	25/26 (96%)	12 (48%)	5 (20%)
8	B	111/112 (99%)	28 (25%)	4 (3%)
All	All	4625/4676 (98%)	954 (20%)	75 (1%)

All (954) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
7	A	33	A
7	A	34	A
7	A	35	A
7	A	37	G
7	A	38	A
7	A	39	U
7	A	40	G
7	A	43	G

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Mol	Chain	Res	Type
7	A	45	C
7	A	46	A
7	A	47	G
7	A	49	A
8	B	10	G
8	B	11	A
8	B	12	U
8	B	22	G
8	B	23	U
8	B	31	G
8	B	32	U
8	B	33	U
8	B	38	U
8	B	39	A
8	B	41	C
8	B	48	G
8	B	49	G
8	B	50	A
8	B	53	U
8	B	54	U
8	B	55	A
8	B	59	U
8	B	60	C
8	B	62	U
8	B	66	C
8	B	86	U
8	B	87	U
8	B	97	A
8	B	101	U
8	B	107	G
8	B	108	C
8	B	110	G
14	H	9	A
14	H	17	U
14	H	18	G
14	H	19	U
14	H	21	A
14	H	36	C
14	H	37	A
14	H	48	C
14	H	55	U
14	H	56	C

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Mol	Chain	Res	Type
14	H	70	A
14	H	72	C
14	H	74	C
14	H	76	A
28	V	8	U
28	V	13	A
28	V	23	G
28	V	26	G
28	V	34	U
28	V	46	C
28	V	51	G
28	V	60	G
28	V	71	A
28	V	74	U
28	V	75	G
28	V	76	C
28	V	77	U
28	V	78	U
28	V	79	C
28	V	85	G
28	V	86	C
28	V	87	U
28	V	89	U
28	V	90	A
28	V	92	G
28	V	93	C
28	V	99	U
28	V	100	U
28	V	101	G
28	V	117	A
28	V	119	U
28	V	124	A
28	V	125	A
28	V	141	U
28	V	145	G
28	V	162	A
28	V	164	U
28	V	175	G
28	V	176	A
28	V	177	G
28	V	178	A
28	V	179	A

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Mol	Chain	Res	Type
28	V	182	C
28	V	184	G
28	V	186	C
28	V	187	C
28	V	188	C
28	V	199	A
28	V	200	A
28	V	202	A
28	V	207	A
28	V	215	G
28	V	216	A
28	V	219	A
28	V	224	A
28	V	225	A
28	V	226	A
28	V	231	A
28	V	232	U
28	V	233	G
28	V	234	C
28	V	242	U
28	V	251	G
28	V	252	C
28	V	253	G
28	V	258	A
28	V	269	G
28	V	283	G
28	V	284	C
28	V	286	U
28	V	287	G
28	V	291	C
28	V	296	G
28	V	297	G
28	V	301	U
28	V	302	A
28	V	307	A
28	V	308	C
28	V	310	C
28	V	329	A
28	V	342	A
28	V	344	G
28	V	345	A
28	V	346	G

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Mol	Chain	Res	Type
28	V	348	U
28	V	352	G
28	V	361	G
28	V	367	G
28	V	373	A
28	V	374	A
28	V	375	C
28	V	382	G
28	V	407	A
28	V	410	G
28	V	411	G
28	V	412	A
28	V	418	A
28	V	419	G
28	V	420	U
28	V	421	A
28	V	432	C
28	V	433	G
28	V	434	U
28	V	442	C
28	V	444	U
28	V	445	C
28	V	458	G
28	V	459	A
28	V	471	G
28	V	476	A
28	V	477	A
28	V	482	C
28	V	483	C
28	V	491	C
28	V	498	U
28	V	502	C
28	V	504	A
28	V	506	U
28	V	512	G
28	V	527	A
28	V	528	G
28	V	530	A
28	V	537	A
28	V	548	A
28	V	550	G
28	V	554	U

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Mol	Chain	Res	Type
28	V	555	C
28	V	556	C
28	V	568	G
28	V	573	C
28	V	575	A
28	V	577	U
28	V	578	A
28	V	579	G
28	V	592	A
28	V	593	A
28	V	595	G
28	V	598	U
28	V	599	G
28	V	607	G
28	V	616	A
28	V	617	G
28	V	619	A
28	V	632	U
28	V	647	A
28	V	648	G
28	V	649	G
28	V	658	A
28	V	659	A
28	V	662	U
28	V	667	A
28	V	673	A
28	V	683	A
28	V	690	A
28	V	691	U
28	V	692	A
28	V	699	A
28	V	700	U
28	V	701	G
28	V	702	A
28	V	718	C
28	V	719	C
28	V	733	U
28	V	764	C
28	V	765	A
28	V	773	G
28	V	777	C
28	V	787	C

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Mol	Chain	Res	Type
28	V	788	G
28	V	790	A
28	V	794	U
28	V	795	G
28	V	810	G
28	V	811	A
28	V	822	G
28	V	823	G
28	V	829	A
28	V	831	U
28	V	832	G
28	V	837	U
28	V	845	G
28	V	852	G
28	V	859	C
28	V	866	A
28	V	874	U
28	V	892	U
28	V	906	G
28	V	908	A
28	V	913	A
28	V	914	C
28	V	929	G
28	V	931	C
28	V	933	C
28	V	934	U
28	V	935	A
28	V	936	C
28	V	937	C
28	V	939	G
28	V	940	G
28	V	941	U
28	V	942	U
28	V	943	A
28	V	944	C
28	V	957	A
28	V	959	C
28	V	961	C
28	V	962	C
28	V	964	A
28	V	973	G
28	V	980	C

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Mol	Chain	Res	Type
28	V	987	A
28	V	991	A
28	V	992	G
28	V	999	A
28	V	1005	A
28	V	1007	G
28	V	1020	A
28	V	1027	A
28	V	1029	A
28	V	1036	A
28	V	1042	A
28	V	1051	C
28	V	1053	C
28	V	1054	A
28	V	1055	A
28	V	1058	U
28	V	1059	A
28	V	1068	G
28	V	1073	A
28	V	1079	U
28	V	1091	U
28	V	1094	A
28	V	1101	G
28	V	1102	G
28	V	1103	A
28	V	1106	U
28	V	1110	C
28	V	1111	U
28	V	1116	A
28	V	1117	G
28	V	1118	C
28	V	1119	A
28	V	1121	C
28	V	1124	C
28	V	1125	C
28	V	1126	A
28	V	1127	U
28	V	1128	U
28	V	1134	A
28	V	1139	G
28	V	1148	C
28	V	1158	G

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Mol	Chain	Res	Type
28	V	1159	U
28	V	1160	G
28	V	1161	A
28	V	1173	A
28	V	1178	U
28	V	1179	A
28	V	1180	C
28	V	1181	C
28	V	1182	G
28	V	1185	G
28	V	1187	U
28	V	1188	A
28	V	1243	A
28	V	1244	A
28	V	1245	G
28	V	1248	C
28	V	1249	U
28	V	1251	U
28	V	1259	G
28	V	1260	A
28	V	1264	G
28	V	1265	A
28	V	1270	C
28	V	1275	G
28	V	1276	G
28	V	1278	G
28	V	1293	A
28	V	1296	G
28	V	1306	G
28	V	1311	G
28	V	1312	A
28	V	1313	A
28	V	1315	G
28	V	1323	A
28	V	1325	A
28	V	1326	A
28	V	1327	U
28	V	1339	A
28	V	1340	A
28	V	1341	U
28	V	1343	C
28	V	1344	C

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Mol	Chain	Res	Type
28	V	1351	U
28	V	1352	U
28	V	1362	G
28	V	1364	C
28	V	1365	U
28	V	1368	U
28	V	1369	C
28	V	1370	C
28	V	1371	G
28	V	1372	C
28	V	1375	A
28	V	1384	C
28	V	1385	G
28	V	1389	C
28	V	1404	A
28	V	1415	C
28	V	1417	A
28	V	1418	U
28	V	1422	C
28	V	1423	A
28	V	1425	C
28	V	1426	A
28	V	1427	G
28	V	1431	G
28	V	1434	A
28	V	1435	U
28	V	1436	U
28	V	1442	A
28	V	1449	C
28	V	1450	C
28	V	1457	U
28	V	1459	U
28	V	1460	G
28	V	1465	A
28	V	1466	U
28	V	1472	G
28	V	1473	A
28	V	1475	G
28	V	1476	C
28	V	1489	U
28	V	1490	A
28	V	1499	A

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Mol	Chain	Res	Type
28	V	1500	U
28	V	1501	U
28	V	1502	G
28	V	1506	A
28	V	1507	U
28	V	1508	C
28	V	1514	C
28	V	1516	A
28	V	1525	G
28	V	1526	G
28	V	1527	C
28	V	1528	U
28	V	1529	G
28	V	1530	G
28	V	1531	G
28	V	1532	A
28	V	1536	A
28	V	1539	C
28	V	1540	A
28	V	1542	A
28	V	1543	U
28	V	1547	U
28	V	1553	A
28	V	1557	G
28	V	1558	G
28	V	1559	C
28	V	1560	U
28	V	1566	G
28	V	1568	G
28	V	1570	U
28	V	1571	G
28	V	1573	C
28	V	1614	A
28	V	1617	A
28	V	1626	U
28	V	1632	G
28	V	1634	U
28	V	1638	A
28	V	1653	A
28	V	1655	A
28	V	1661	A
28	V	1679	A

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Mol	Chain	Res	Type
28	V	1691	A
28	V	1692	U
28	V	1693	C
28	V	1696	G
28	V	1697	A
28	V	1699	A
28	V	1700	A
28	V	1708	U
28	V	1719	G
28	V	1727	A
28	V	1738	U
28	V	1745	A
28	V	1757	G
28	V	1758	U
28	V	1759	U
28	V	1760	A
28	V	1761	G
28	V	1775	G
28	V	1776	A
28	V	1778	A
28	V	1779	G
28	V	1780	C
28	V	1781	C
28	V	1782	G
28	V	1785	G
28	V	1791	A
28	V	1792	G
28	V	1793	G
28	V	1802	A
28	V	1810	G
28	V	1811	C
28	V	1813	A
28	V	1829	C
28	V	1830	G
28	V	1837	U
28	V	1838	A
28	V	1843	G
28	V	1845	A
28	V	1846	G
28	V	1850	A
28	V	1858	A
28	V	1862	C

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Mol	Chain	Res	Type
28	V	1864	G
28	V	1877	A
28	V	1883	A
28	V	1885	A
28	V	1887	G
28	V	1891	G
28	V	1895	A
28	V	1899	U
28	V	1904	G
28	V	1915	U
28	V	1935	G
28	V	1943	C
28	V	1948	A
28	V	1958	G
28	V	1959	G
28	V	1965	A
28	V	1966	A
28	V	1967	A
28	V	1968	U
28	V	1969	U
28	V	1973	U
28	V	1984	U
28	V	1992	C
28	V	1993	G
28	V	1996	C
28	V	1999	A
28	V	2000	A
28	V	2001	G
28	V	2010	A
28	V	2020	U
28	V	2022	U
28	V	2023	C
28	V	2025	C
28	V	2026	A
28	V	2050	G
28	V	2051	U
28	V	2052	A
28	V	2054	C
28	V	2059	A
28	V	2060	A
28	V	2061	G
28	V	2062	A

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Mol	Chain	Res	Type
28	V	2064	G
28	V	2072	C
28	V	2079	C
28	V	2084	C
28	V	2085	G
28	V	2089	A
28	V	2090	G
28	V	2098	G
28	V	2114	C
28	V	2121	U
28	V	2122	G
28	V	2123	A
28	V	2125	U
28	V	2128	U
28	V	2131	U
28	V	2134	A
28	V	2135	G
28	V	2136	C
28	V	2145	G
28	V	2146	A
28	V	2147	U
28	V	2148	A
28	V	2149	G
28	V	2154	G
28	V	2156	G
28	V	2161	G
28	V	2162	G
28	V	2167	C
28	V	2174	C
28	V	2177	G
28	V	2182	G
28	V	2184	U
28	V	2185	G
28	V	2187	A
28	V	2188	G
28	V	2189	G
28	V	2197	G
28	V	2199	G
28	V	2200	A
28	V	2201	U
28	V	2203	C
28	V	2204	U

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Mol	Chain	Res	Type
28	V	2205	A
28	V	2206	C
28	V	2208	C
28	V	2219	G
28	V	2226	U
28	V	2227	A
28	V	2228	A
28	V	2229	C
28	V	2230	C
28	V	2231	C
28	V	2232	A
28	V	2233	C
28	V	2234	C
28	V	2245	G
28	V	2246	G
28	V	2252	A
28	V	2254	A
28	V	2255	C
28	V	2267	G
28	V	2268	G
28	V	2280	G
28	V	2296	A
28	V	2307	A
28	V	2312	C
28	V	2316	A
28	V	2317	A
28	V	2328	G
28	V	2330	A
28	V	2334	U
28	V	2335	U
28	V	2336	G
28	V	2337	G
28	V	2338	A
28	V	2341	U
28	V	2347	G
28	V	2348	C
28	V	2350	G
28	V	2351	A
28	V	2356	A
28	V	2362	A
28	V	2363	C
28	V	2364	A

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Mol	Chain	Res	Type
28	V	2368	G
28	V	2376	C
28	V	2378	G
28	V	2379	C
28	V	2401	G
28	V	2412	G
28	V	2414	C
28	V	2431	U
28	V	2432	C
28	V	2435	C
28	V	2452	U
28	V	2453	C
28	V	2454	A
28	V	2455	A
28	V	2457	G
28	V	2458	G
28	V	2459	A
28	V	2460	U
28	V	2469	C
28	V	2470	C
28	V	2477	A
28	V	2488	A
28	V	2504	C
28	V	2505	A
28	V	2507	A
28	V	2511	A
28	V	2523	G
28	V	2525	C
28	V	2527	C
28	V	2531	G
28	V	2532	A
28	V	2534	G
28	V	2535	U
28	V	2547	A
28	V	2549	C
28	V	2558	G
28	V	2564	G
28	V	2583	U
28	V	2584	U
28	V	2593	A
28	V	2596	G
28	V	2601	A

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Mol	Chain	Res	Type
28	V	2602	C
28	V	2605	G
28	V	2611	G
28	V	2613	U
28	V	2614	U
28	V	2631	A
28	V	2632	G
28	V	2638	U
28	V	2639	C
28	V	2642	U
28	V	2644	U
28	V	2659	G
28	V	2675	C
28	V	2690	G
28	V	2711	G
28	V	2718	U
28	V	2720	C
28	V	2743	G
28	V	2755	U
28	V	2762	A
28	V	2763	C
28	V	2764	G
28	V	2765	G
28	V	2773	G
28	V	2777	A
28	V	2784	C
28	V	2785	U
28	V	2794	A
28	V	2806	G
28	V	2807	A
28	V	2808	U
28	V	2818	C
28	V	2823	C
28	V	2824	G
28	V	2826	A
28	V	2831	A
28	V	2845	A
28	V	2859	G
28	V	2860	A
28	V	2867	U
28	V	2868	G
28	V	2884	G

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Mol	Chain	Res	Type
28	V	2892	G
28	V	2897	G
28	V	2899	C
28	V	2900	A
28	V	2901	G
28	V	2905	C
28	V	2916	A
28	V	2918	G
33	a	10	A
33	a	11	G
33	a	31	A
33	a	32	C
33	a	33	G
33	a	34	A
33	a	41	G
33	a	49	C
33	a	50	C
33	a	53	A
33	a	75	G
33	a	77	U
33	a	78	G
33	a	84	U
33	a	85	U
33	a	86	G
33	a	87	C
33	a	89	C
33	a	90	C
33	a	93	G
33	a	99	A
33	a	114	A
33	a	119	C
33	a	120	A
33	a	128	A
33	a	129	A
33	a	130	C
33	a	136	U
33	a	142	A
33	a	143	C
33	a	153	U
33	a	154	C
33	a	158	G
33	a	162	C

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Mol	Chain	Res	Type
33	a	172	U
33	a	177	G
33	a	181	G
33	a	182	U
33	a	189	A
33	a	197	G
33	a	208	A
33	a	209	A
33	a	211	A
33	a	218	U
33	a	219	U
33	a	221	G
33	a	249	G
33	a	253	U
33	a	255	G
33	a	258	A
33	a	259	G
33	a	274	G
33	a	275	C
33	a	287	A
33	a	297	G
33	a	314	A
33	a	336	C
33	a	337	A
33	a	338	C
33	a	340	G
33	a	352	A
33	a	354	G
33	a	360	C
33	a	362	G
33	a	373	U
33	a	375	U
33	a	380	C
33	a	381	A
33	a	385	G
33	a	392	G
33	a	396	G
33	a	405	A
33	a	414	G
33	a	419	A
33	a	420	U
33	a	421	G

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Mol	Chain	Res	Type
33	a	429	U
33	a	430	C
33	a	435	C
33	a	436	G
33	a	437	U
33	a	448	U
33	a	456	A
33	a	460	A
33	a	461	C
33	a	466	G
33	a	474	A
33	a	475	A
33	a	476	U
33	a	477	A
33	a	478	G
33	a	481	C
33	a	485	A
33	a	487	C
33	a	488	U
33	a	489	U
33	a	490	G
33	a	491	A
33	a	494	G
33	a	502	C
33	a	504	A
33	a	506	A
33	a	508	A
33	a	518	A
33	a	520	C
33	a	526	G
33	a	527	C
33	a	530	G
33	a	536	G
33	a	541	A
33	a	542	A
33	a	556	A
33	a	564	C
33	a	568	A
33	a	571	U
33	a	573	U
33	a	582	A
33	a	585	G

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Mol	Chain	Res	Type
33	a	586	G
33	a	590	G
33	a	597	G
33	a	605	A
33	a	641	G
33	a	642	U
33	a	643	C
33	a	651	A
33	a	662	U
33	a	696	A
33	a	732	U
33	a	733	G
33	a	756	U
33	a	757	A
33	a	758	A
33	a	764	G
33	a	787	G
33	a	802	U
33	a	803	A
33	a	824	A
33	a	826	C
33	a	841	G
33	a	849	G
33	a	853	C
33	a	855	G
33	a	856	C
33	a	882	A
33	a	883	A
33	a	885	C
33	a	924	A
33	a	943	G
33	a	944	C
33	a	945	A
33	a	950	C
33	a	963	G
33	a	964	G
33	a	966	U
33	a	968	A
33	a	969	A
33	a	970	U
33	a	979	A
33	a	981	G

*Continued on next page...*



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Mol	Chain	Res	Type
33	a	985	A
33	a	986	G
33	a	987	A
33	a	993	A
33	a	999	U
33	a	1002	U
33	a	1003	G
33	a	1007	U
33	a	1008	C
33	a	1009	C
33	a	1010	U
33	a	1011	C
33	a	1012	U
33	a	1014	A
33	a	1015	C
33	a	1017	A
33	a	1019	C
33	a	1023	G
33	a	1024	A
33	a	1028	A
33	a	1030	G
33	a	1033	G
33	a	1035	C
33	a	1036	C
33	a	1039	U
33	a	1041	C
33	a	1042	G
33	a	1046	G
33	a	1047	C
33	a	1050	A
33	a	1053	G
33	a	1058	G
33	a	1064	C
33	a	1075	U
33	a	1088	U
33	a	1089	G
33	a	1095	U
33	a	1104	G
33	a	1105	U
33	a	1111	A
33	a	1112	A
33	a	1118	G

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Mol	Chain	Res	Type
33	a	1122	C
33	a	1134	G
33	a	1135	U
33	a	1136	U
33	a	1140	A
33	a	1142	C
33	a	1145	U
33	a	1148	G
33	a	1149	U
33	a	1153	G
33	a	1161	A
33	a	1166	A
33	a	1168	U
33	a	1176	A
33	a	1178	A
33	a	1190	G
33	a	1192	U
33	a	1193	G
33	a	1205	A
33	a	1206	A
33	a	1211	U
33	a	1221	U
33	a	1222	A
33	a	1223	U
33	a	1237	C
33	a	1259	A
33	a	1261	A
33	a	1267	G
33	a	1278	A
33	a	1279	G
33	a	1289	A
33	a	1294	A
33	a	1295	C
33	a	1296	A
33	a	1308	A
33	a	1314	G
33	a	1326	C
33	a	1329	C
33	a	1330	U
33	a	1331	C
33	a	1341	A
33	a	1347	G

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Mol	Chain	Res	Type
33	a	1355	A
33	a	1366	A
33	a	1370	G
33	a	1372	A
33	a	1373	U
33	a	1377	G
33	a	1387	C
33	a	1407	A
33	a	1451	A
33	a	1455	A
33	a	1460	U
33	a	1462	U
33	a	1463	A
33	a	1464	G
33	a	1490	A
33	a	1500	U
33	a	1502	A
33	a	1503	A
33	a	1516	U
33	a	1527	G
33	a	1539	G
33	a	1540	G

All (75) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
7	A	33	A
7	A	34	A
7	A	38	A
7	A	39	U
7	A	45	C
8	B	31	G
8	B	37	A
8	B	48	G
8	B	49	G
14	H	47	U
14	H	55	U
28	V	88	G
28	V	183	A
28	V	252	C
28	V	347	G
28	V	411	G

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Mol	Chain	Res	Type
28	V	441	C
28	V	444	U
28	V	549	A
28	V	554	U
28	V	689	A
28	V	772	G
28	V	810	G
28	V	905	G
28	V	1093	G
28	V	1172	A
28	V	1243	A
28	V	1244	A
28	V	1250	G
28	V	1264	G
28	V	1269	A
28	V	1275	G
28	V	1305	A
28	V	1351	U
28	V	1435	U
28	V	1448	U
28	V	1507	U
28	V	1525	G
28	V	1527	C
28	V	1529	G
28	V	1530	G
28	V	1535	U
28	V	1565	U
28	V	1567	U
28	V	1570	U
28	V	1631	A
28	V	1726	G
28	V	1757	G
28	V	1784	A
28	V	1828	G
28	V	1882	A
28	V	1914	A
28	V	1972	U
28	V	1991	C
28	V	2009	G
28	V	2022	U
28	V	2127	U
28	V	2155	A

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Mol	Chain	Res	Type
28	V	2205	A
28	V	2254	A
28	V	2316	A
28	V	2335	U
28	V	2336	G
28	V	2349	A
28	V	2364	A
28	V	2452	U
28	V	2454	A
28	V	2468	A
28	V	2510	G
28	V	2534	G
28	V	2631	A
28	V	2710	C
28	V	2805	A
28	V	2883	C
28	V	2904	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](#)

There are no ligands in this entry.

#### 5.7 Other polymers [i](#)

There are no such residues in this entry.

#### 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

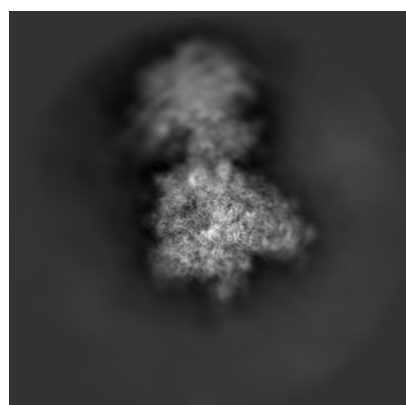
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14159. These allow visual inspection of the internal detail of the map and identification of artifacts.

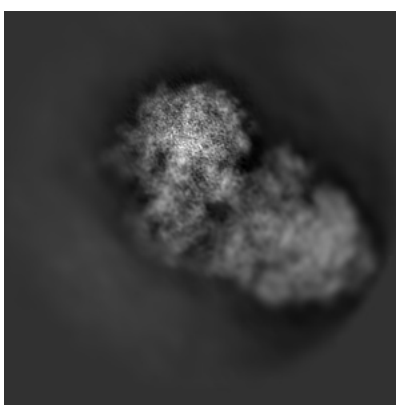
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

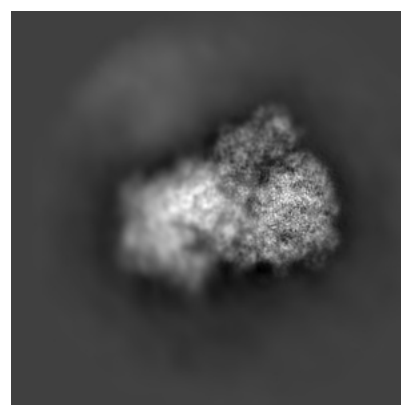
#### 6.1.1 Primary map



X



Y

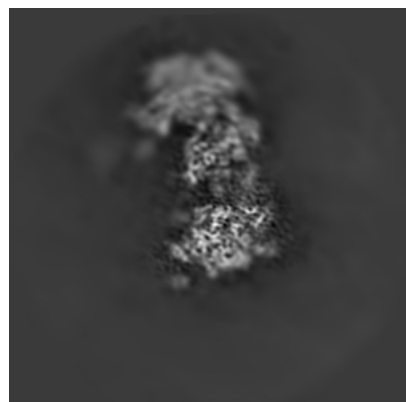


Z

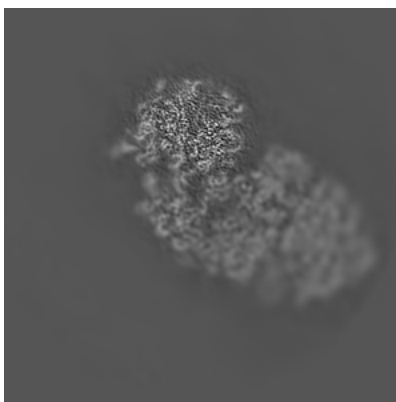
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

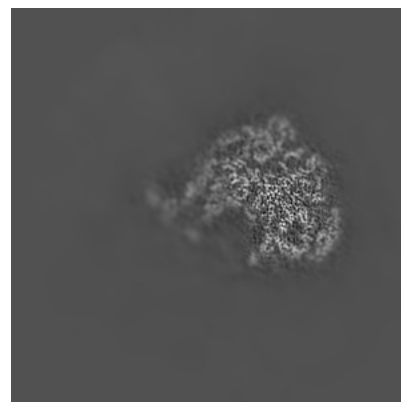
#### 6.2.1 Primary map



X Index: 184



Y Index: 184

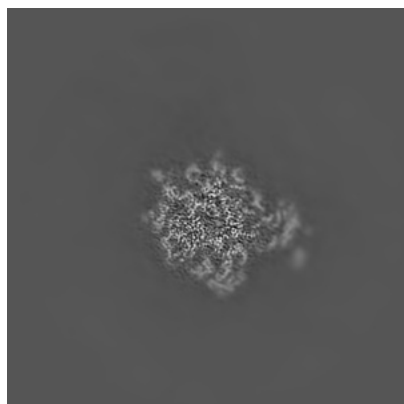


Z Index: 184

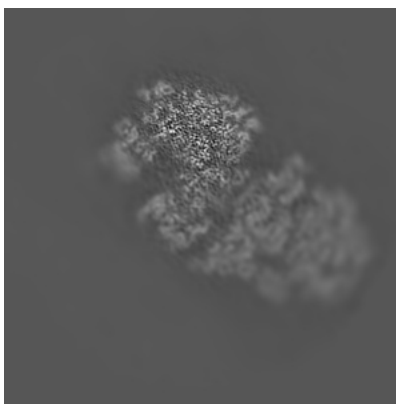
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

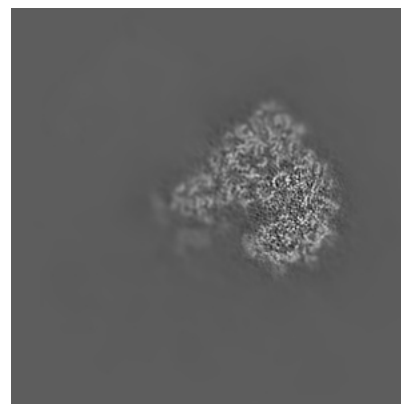
### 6.3.1 Primary map



X Index: 254



Y Index: 196

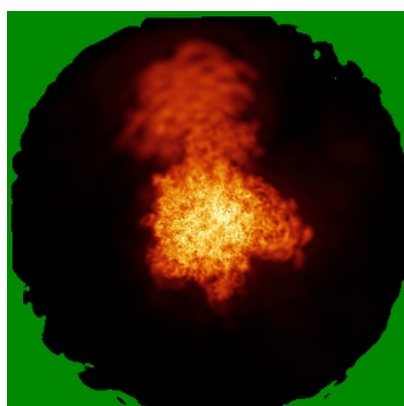


Z Index: 169

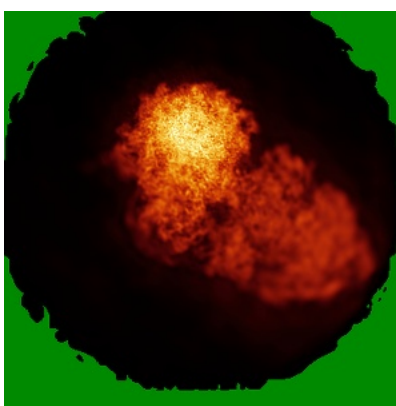
The images above show the largest variance slices of the map in three orthogonal directions.

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

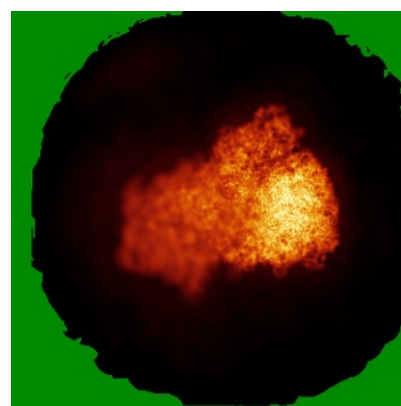
### 6.4.1 Primary map



X



Y

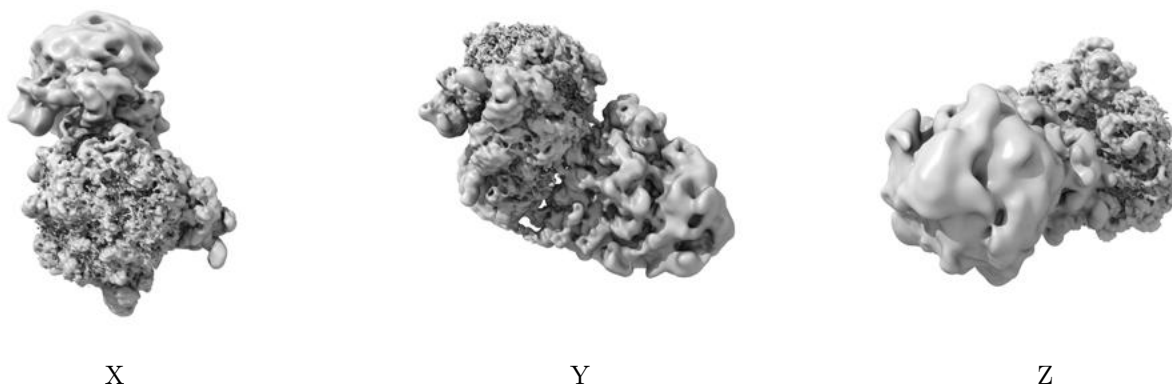


Z

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 0.0172. 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](#)

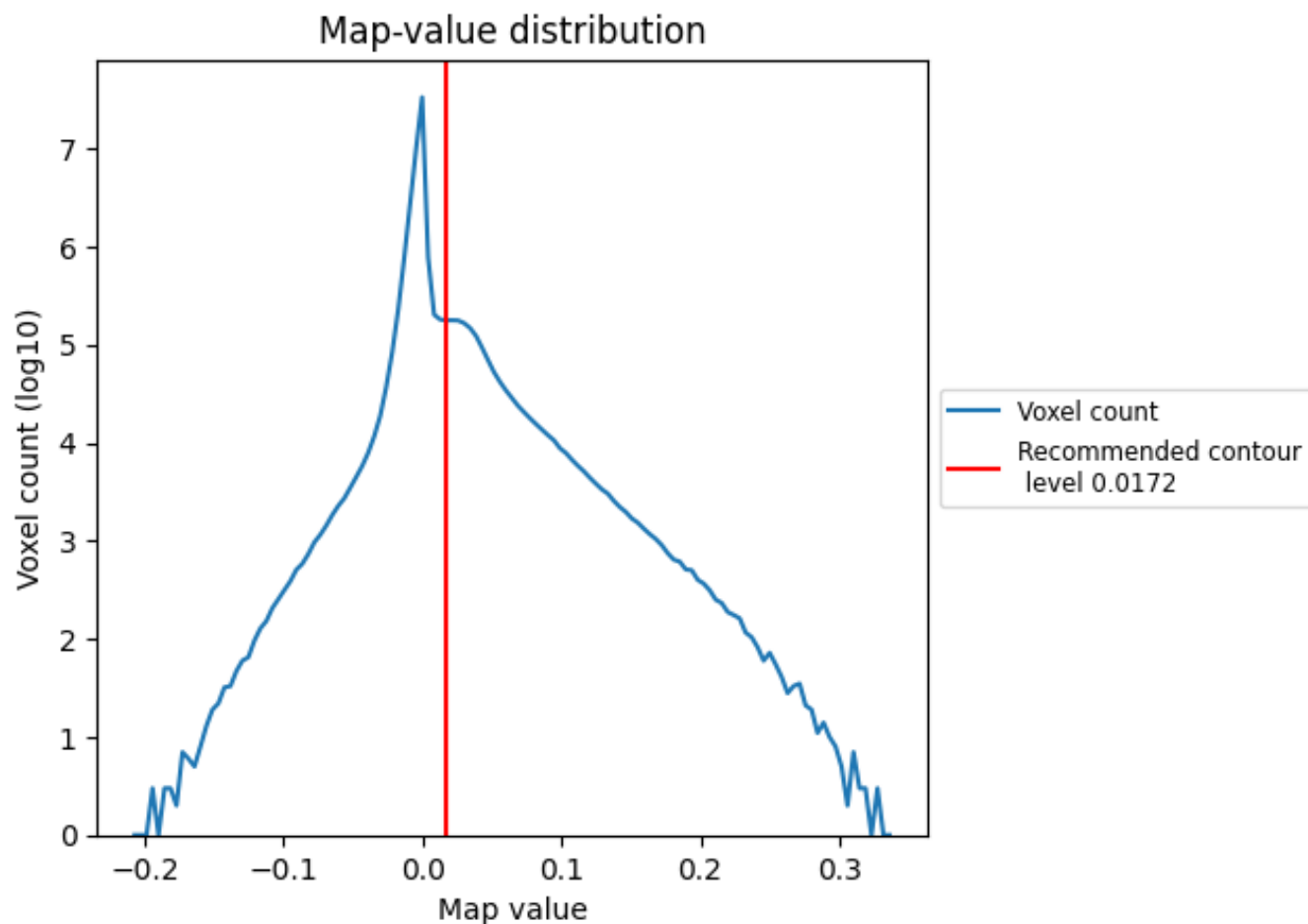
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

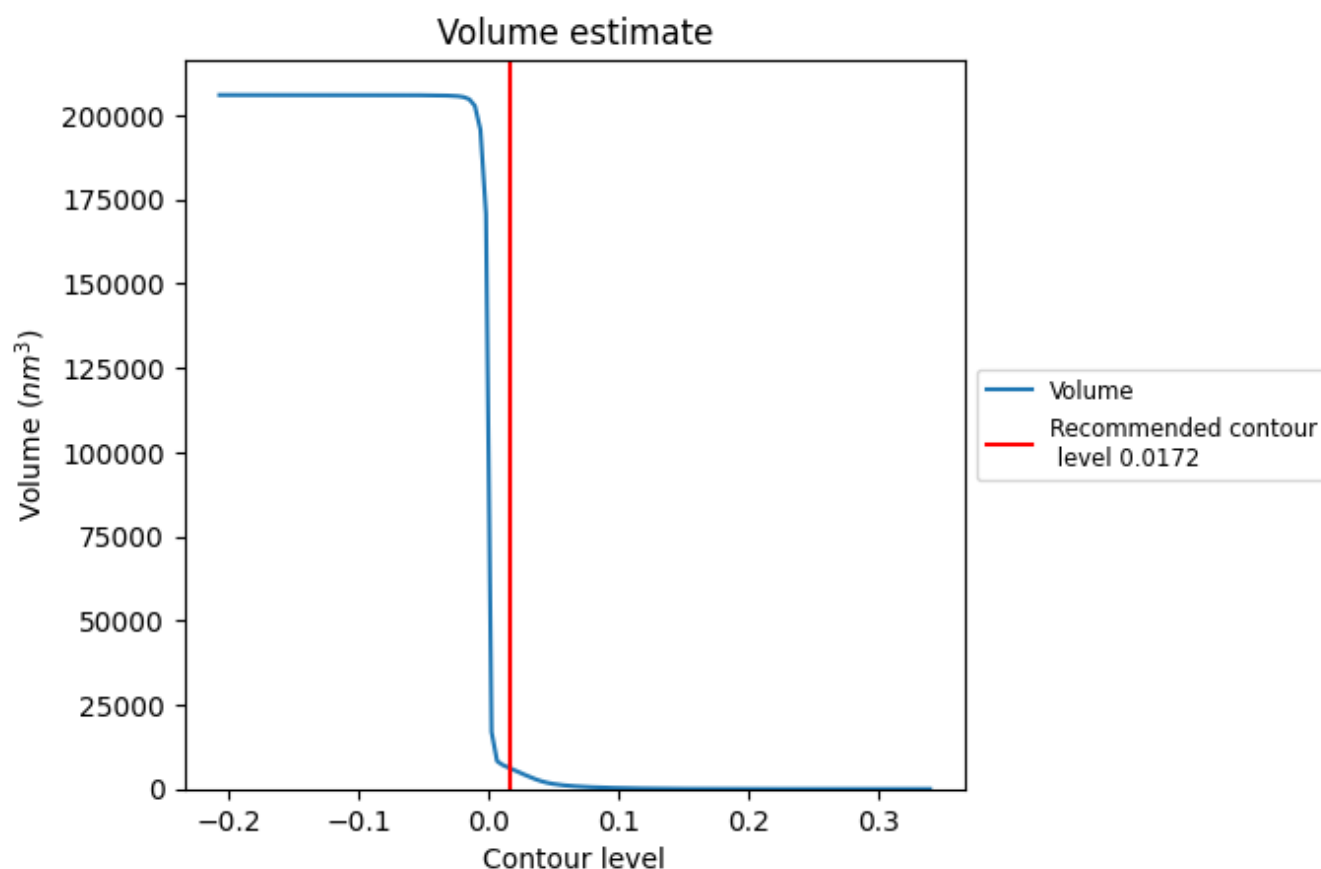
This section contains the results of statistical analysis of the map.

### 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.

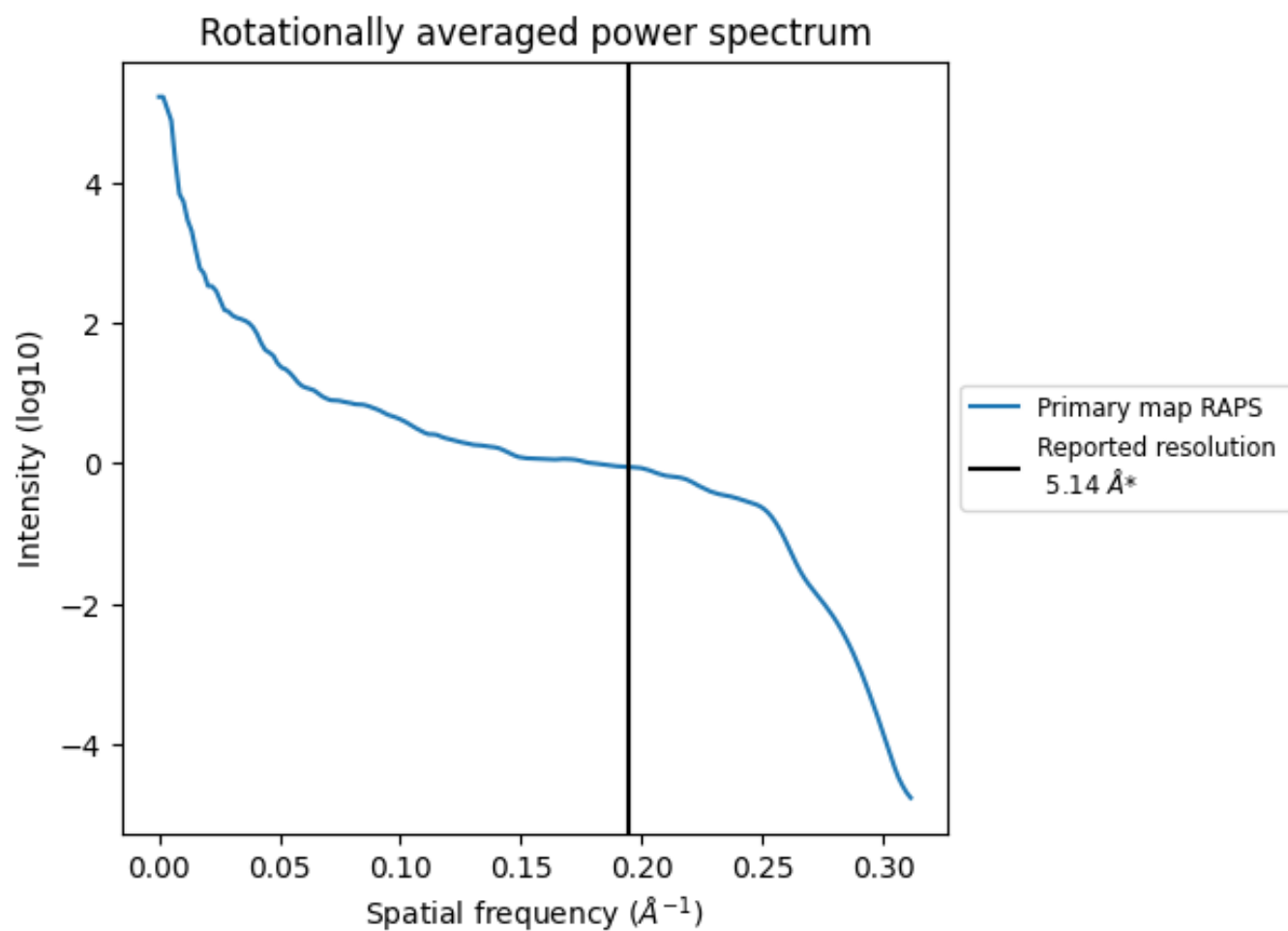
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 6043  $\text{nm}^3$ ; this corresponds to an approximate mass of 5459 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 0.195 Å<sup>-1</sup>

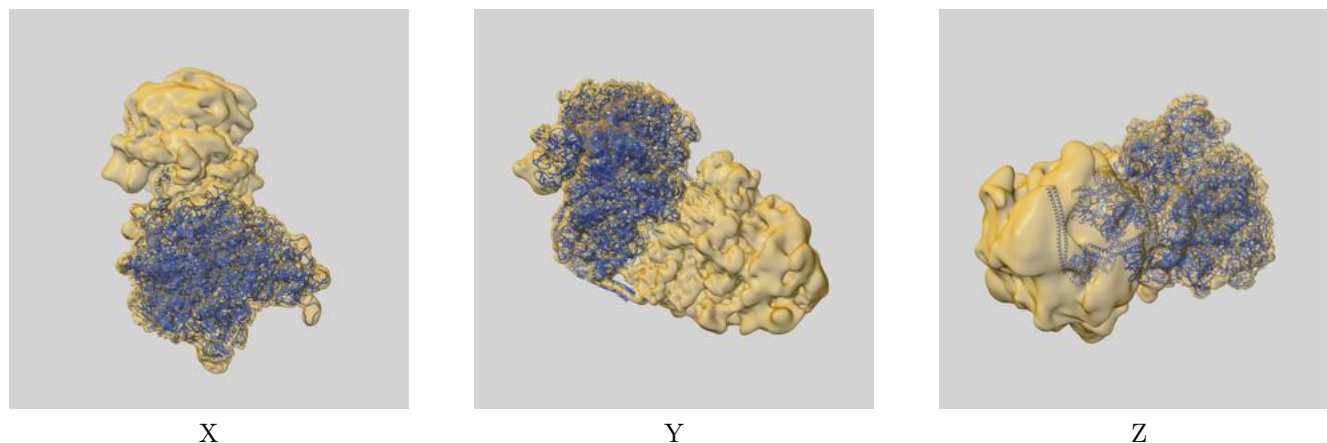
## 8 Fourier-Shell correlation ⓘ

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

## 9 Map-model fit [i](#)

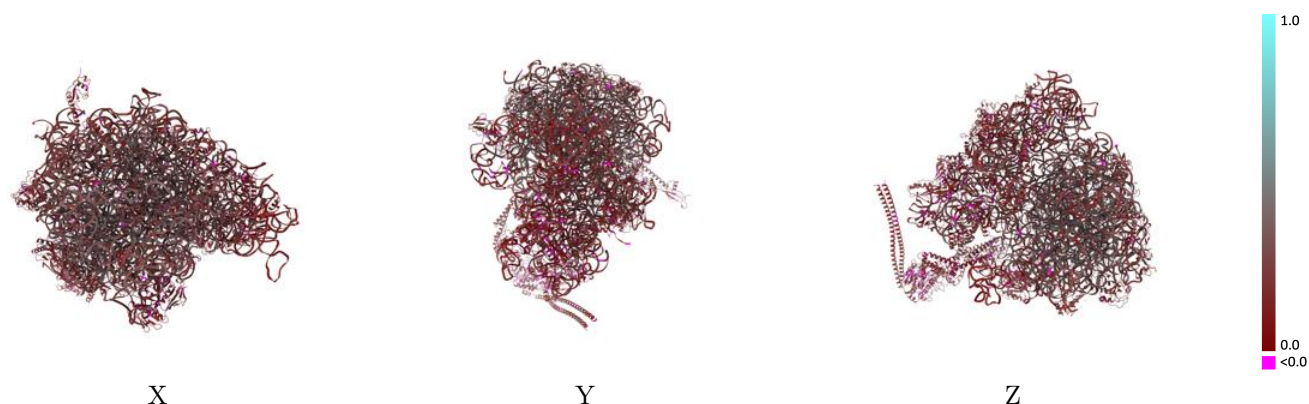
This section contains information regarding the fit between EMDB map EMD-14159 and PDB model 7QV3. Per-residue inclusion information can be found in section 3 on page 14.

### 9.1 Map-model overlay [i](#)



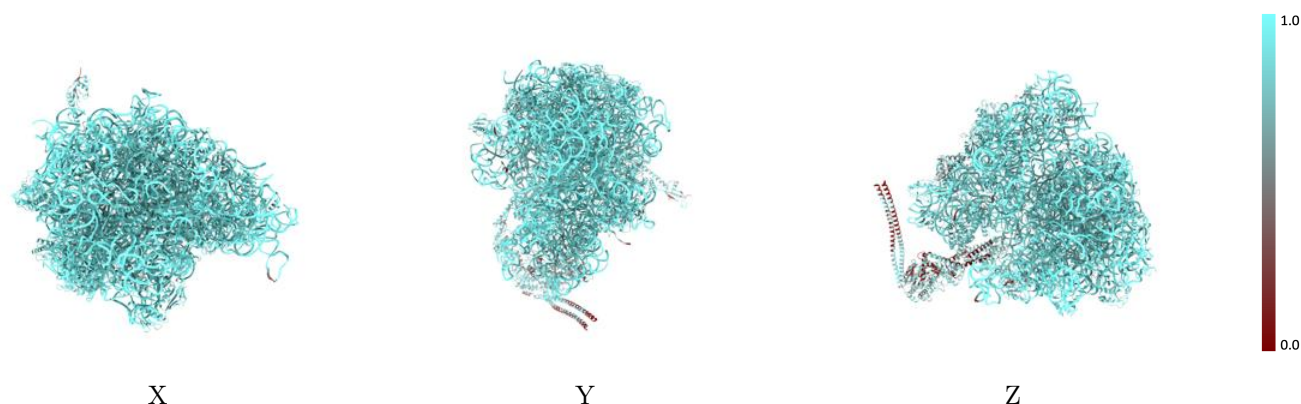
The images above show the 3D surface view of the map at the recommended contour level 0.0172 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



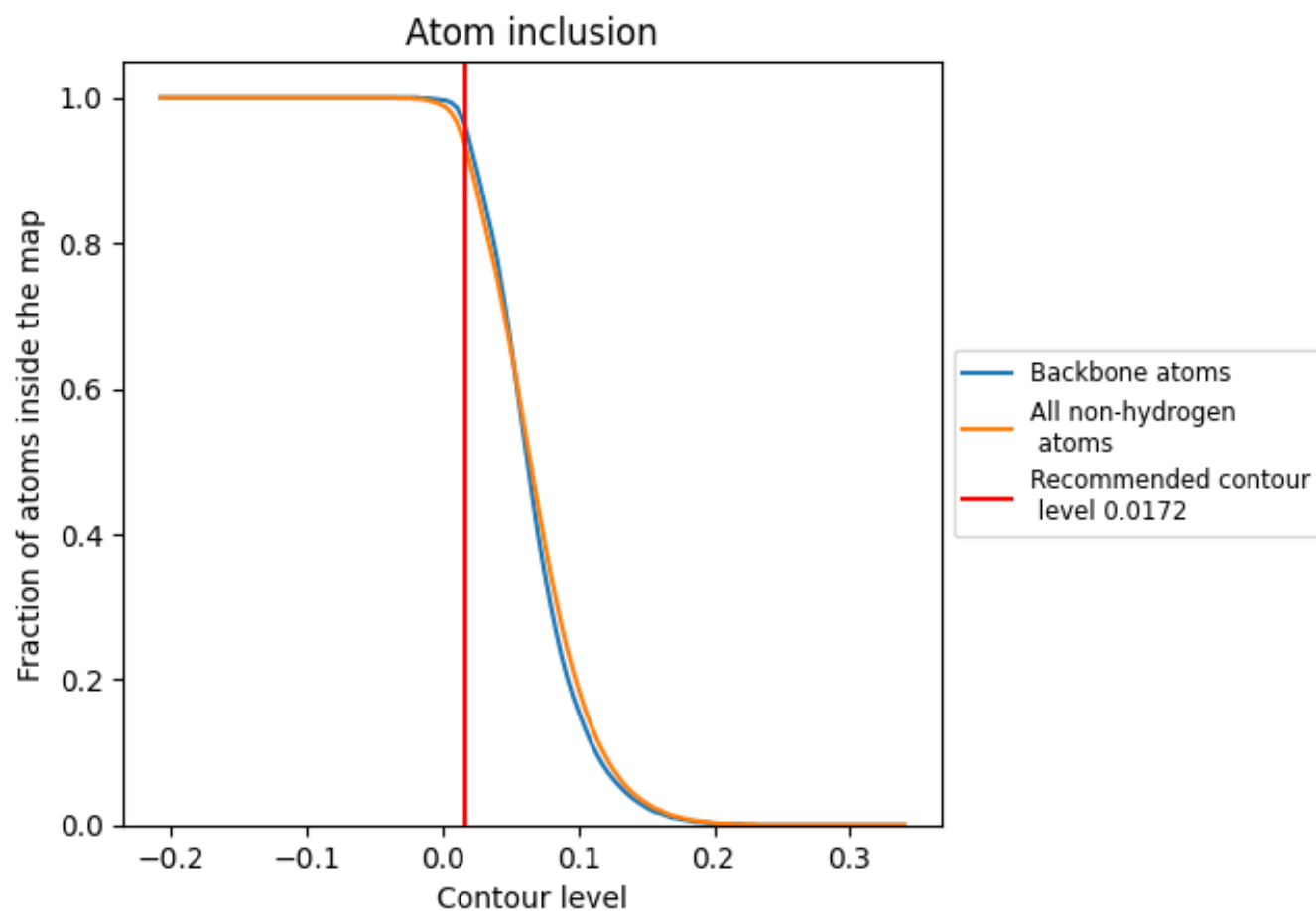
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0172).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 93% 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 (0.0172) and Q-score for the entire model and for each chain.











































Chain	Atom inclusion	Q-score
All	 0.9340	 0.2480
0	 0.9080	 0.3000
1	 0.9220	 0.2440
2	 0.8960	 0.3180
3	 0.9000	 0.3550
4	 0.8550	 0.2090
6	 0.9300	 0.1610
A	 0.7980	 0.1250
B	 0.9940	 0.2530
C	 0.8930	 0.3170
D	 0.9070	 0.3090
E	 0.9200	 0.2620
F	 0.9030	 0.1500
G	 0.9260	 0.1810
H	 0.9700	 0.2330
I	 0.6500	 0.1160
J	 0.9230	 0.2970
K	 0.8720	 0.3210
L	 0.9260	 0.2840
M	 0.9100	 0.2600
N	 0.9120	 0.2830
O	 0.9260	 0.1790
P	 0.8950	 0.2790
Q	 0.9150	 0.2940
R	 0.9560	 0.2990
S	 0.8960	 0.2950
T	 0.9030	 0.2850
U	 0.9440	 0.2500
V	 0.9780	 0.3050
W	 0.8800	 0.2850
X	 0.7510	 0.1500
Y	 0.9530	 0.1900
Z	 0.9240	 0.2580
a	 0.9880	 0.2230
b	 0.6450	 0.1060



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Chain	Atom inclusion	Q-score
c	 0.6960	 0.1140
d	 0.8750	 0.1380
e	 0.8590	 0.1790
f	 0.8440	 0.1720
g	 0.8630	 0.1620
h	 0.8830	 0.1770
i	 0.9120	 0.1440
j	 0.9070	 0.1250
k	 0.8780	 0.2000
l	 0.8990	 0.1720
m	 0.9100	 0.1630
n	 0.8380	 0.1000
o	 0.8880	 0.1610
p	 0.8790	 0.1400
q	 0.8990	 0.1600
r	 0.8530	 0.1970
s	 0.9610	 0.1090
t	 0.8920	 0.1630
u	 0.8840	 0.2900
v	 0.4980	 0.0920
w	 0.7590	 0.1080