



Full wwPDB EM Validation Report ⓘ

Feb 27, 2023 – 05:21 pm GMT

PDB ID : 8AGW
EMDB ID : EMD-15426
Title : Yeast RQC complex in state D
Authors : Tesina, P.; Buschauer, R.; Beckmann, R.
Deposited on : 2022-07-20
Resolution : 2.60 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:

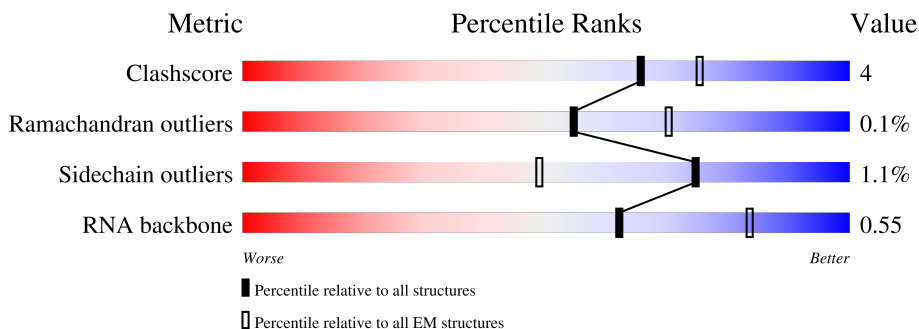
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.32.1

1 Overall quality at a glance

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

The reported resolution of this entry is 2.60 Å.

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




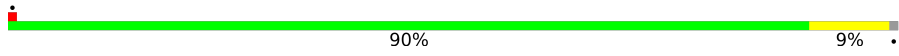

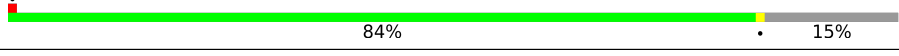
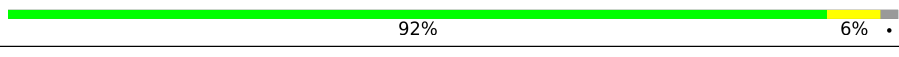
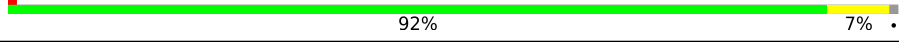
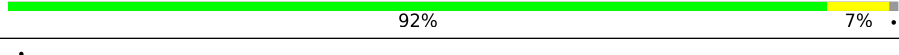

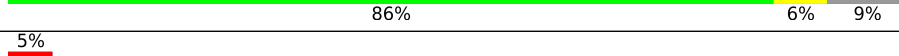
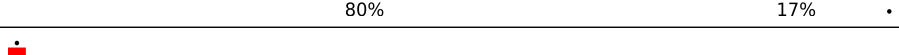
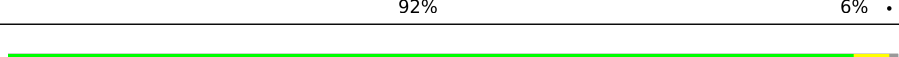
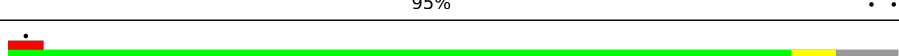

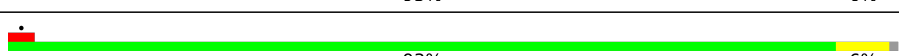
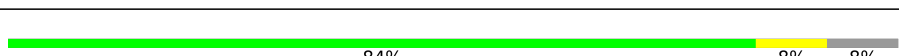
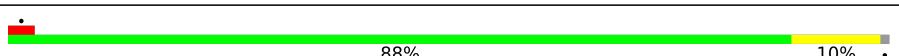
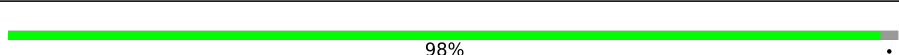

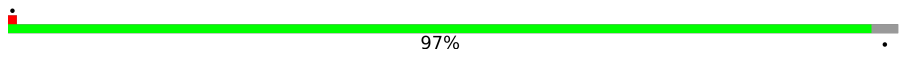
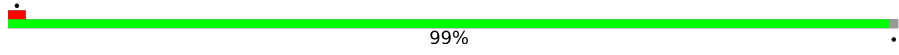

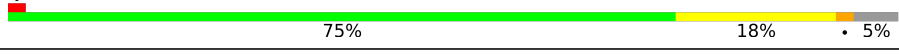

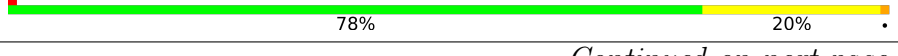

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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

Mol	Chain	Length	Quality of chain
1	A	204	
2	B	199	
3	C	184	
4	D	186	
5	E	189	
6	F	172	
7	G	160	

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Mol	Chain	Length	Quality of chain
8	H	121	 74% 9% 17%
9	I	137	 90% 9%
10	J	155	 37% 59%
11	K	142	 84% 15%
12	L	127	 92% 6%
13	M	136	 92% 7%
14	N	149	 92% 7%
15	O	59	 83% 12%
16	P	105	 86% 6% 9%
17	Q	113	 5% 80% 17%
18	R	130	 92% 6%
19	S	107	 95%
20	T	121	 88% 5% 7%
21	U	120	 93% 6%
22	V	100	 93% 6%
23	W	88	 84% 8% 8%
24	X	78	 88% 10%
25	Y	51	 98%
26	Z	128	 41% 59%
27	b	106	 97%
28	c	92	 99%
29	d	25	 32% 88% 12%
30	f	3395	 75% 18% 5%
31	h	121	 86% 14%
32	i	158	 78% 20%

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Mol	Chain	Length	Quality of chain
33	j	254	97%
34	k	387	99%
35	l	362	99%
36	m	297	98%
37	n	176	94% 5%
38	o	244	91% 9%
39	p	256	89% 9%
40	q	191	98%
41	r	221	98%
42	s	174	95%
43	t	199	96%
44	u	138	97%
45	a	1038	52% 81% 18%
46	e	1562	82% 94%
47	g	245	33% 91% 8%
48	x	76	22% 63% 34%
48	y	76	9% 62% 34%
49	z	165	28% 88% 10%
50	0	312	31% 7% 61%
51	1	17	6% 100%
52	w	217	91% 99%

2 Entry composition [i](#)

There are 55 unique types of molecules in this entry. The entry contains 150269 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 60S ribosomal protein L15-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	203	1720	1077	361	281	1	0	0

- Molecule 2 is a protein called 60S ribosomal protein L16-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	197	1555	1003	289	262	1	197	0

- Molecule 3 is a protein called 60S ribosomal protein L17-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	C	183	1416	879	284	253	0	0

- Molecule 4 is a protein called 60S ribosomal protein L18-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	185	1441	908	290	241	2	0	0

- Molecule 5 is a protein called 60S ribosomal protein L19-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	E	156	1258	781	265	212	0	0

- Molecule 6 is a protein called 60S ribosomal protein L20-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	171	1437	925	266	243	3	0	0

- Molecule 7 is a protein called 60S ribosomal protein L21-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	G	159	1272	802	245	221	4	0	0

- Molecule 8 is a protein called 60S ribosomal protein L22-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
8	H	100	796	516	131	149	0	0

- Molecule 9 is a protein called 60S ribosomal protein L23-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	I	136	1003	628	189	179	7	0	0

- Molecule 10 is a protein called 60S ribosomal protein L24-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	J	63	518	333	102	82	1	0	0

- Molecule 11 is a protein called 60S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	K	121	964	620	169	173	2	0	0

- Molecule 12 is a protein called 60S ribosomal protein L26-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
12	L	125	984	620	191	173	0	0

- Molecule 13 is a protein called 60S ribosomal protein L27-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
13	M	135	1080	701	199	180	0	0

- Molecule 14 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	N	148	1169	747	231	188	3	0	0

- Molecule 15 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	O	58	462	289	100	73		0	0

- Molecule 16 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	P	96	737	476	123	137	1	0	0

- Molecule 17 is a protein called 60S ribosomal protein L31-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	Q	109	876	556	167	152	1	0	0

- Molecule 18 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	R	127	1013	642	205	165	1	0	0

- Molecule 19 is a protein called 60S ribosomal protein L33-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	S	106	850	540	165	144	1	0	0

- Molecule 20 is a protein called 60S ribosomal protein L34-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	T	112	880	545	179	152	4	0	0

- Molecule 21 is a protein called 60S ribosomal protein L35-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	119	Total	C	N	O	S	0	0
			969	615	186	167	1		

- Molecule 22 is a protein called 60S ribosomal protein L36-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	99	Total	C	N	O	S	0	0
			766	478	154	132	2		

- Molecule 23 is a protein called 60S ribosomal protein L37-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	W	81	Total	C	N	O	S	0	0
			645	393	141	106	5		

- Molecule 24 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	X	77	Total	C	N	O	0	0
			612	391	115	106		

- Molecule 25 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Y	50	Total	C	N	O	S	0	0
			436	272	97	65	2		

- Molecule 26 is a protein called Ubiquitin-60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Z	52	Total	C	N	O	S	0	0
			410	254	86	65	5		

- Molecule 27 is a protein called 60S ribosomal protein L42-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	b	103	Total	C	N	O	S	0	0
			824	517	167	135	5		

- Molecule 28 is a protein called 60S ribosomal protein L43-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	c	91	Total	C	N	O	S	0	0
			694	429	138	121	6		

- Molecule 29 is a protein called 60S ribosomal protein L41-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	d	22	Total	C	N	O	S	0	0
			207	127	56	23	1		

- Molecule 30 is a RNA chain called 25S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	f	3216	Total	C	N	O	P	1	0
			68802	30732	12391	22462	3217		

- Molecule 31 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	h	121	Total	C	N	O	P	0	0
			2579	1152	461	845	121		

- Molecule 32 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	i	158	Total	C	N	O	P	0	0
			3353	1500	586	1109	158		

- Molecule 33 is a protein called 60S ribosomal protein L2-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	j	246	Total	C	N	O	S	0	0
			1874	1168	380	325	1		

- Molecule 34 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	k	386	Total	C	N	O	S	0	0
			3075	1950	584	533	8		

- Molecule 35 is a protein called 60S ribosomal protein L4-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	l	361	Total	C	N	O	S	0	0
			2748	1729	522	494	3		

- Molecule 36 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	m	294	Total	C	N	O	S	0	0
			2351	1484	410	455	2		

- Molecule 37 is a protein called 60S ribosomal protein L6-B.

Mol	Chain	Residues	Atoms				AltConf	Trace
37	n	167	Total	C	N	O	0	0
			1307	843	234	230		

- Molecule 38 is a protein called 60S ribosomal protein L7-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	o	222	Total	C	N	O	S	0	0
			1784	1151	324	308	1		

- Molecule 39 is a protein called 60S ribosomal protein L8-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	p	233	Total	C	N	O	S	0	0
			1804	1151	323	327	3		

- Molecule 40 is a protein called 60S ribosomal protein L9-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	q	191	Total	C	N	O	S	0	0
			1508	957	274	273	4		

- Molecule 41 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	r	218	Total	C	N	O	S	0	0
			1764	1117	334	306	7		

- Molecule 42 is a protein called 60S ribosomal protein L11-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	s	169	1346	843	252	247	4	0	0

- Molecule 43 is a protein called 60S ribosomal protein L13-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	t	193	1543	962	315	266		0	0

- Molecule 44 is a protein called 60S ribosomal protein L14-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
44	u	136	1053	675	199	177	2	0	0

- Molecule 45 is a protein called RQC2 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
45	a	848	6573	4191	1139	1226	17	0	0

- Molecule 46 is a protein called E3 ubiquitin-protein ligase listerin.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
46	e	1527	11512	7356	1937	2181	38	0	0

- Molecule 47 is a protein called Eukaryotic translation initiation factor 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
47	g	225	1651	1030	282	332	7	0	0

- Molecule 48 is a RNA chain called Ala tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
48	x	74	1579	702	278	525	74	0	0
48	y	73	1556	692	273	518	73	0	0

- Molecule 49 is a protein called 60S ribosomal protein L12-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
49	z	148	Total	C	N	O	0	0
			728	432	148	148		

- Molecule 50 is a protein called 60S acidic ribosomal protein P0.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	0	121	Total	C	N	O	S	0	0
			961	618	167	173	3		

- Molecule 51 is a protein called CAT-tailed nascent peptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
51	1	17	Total	C	N	O	0	0
			85	51	17	17		

- Molecule 52 is a protein called 60S ribosomal protein L1-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	w	216	Total	C	N	O	S	0	0
			1709	1092	298	310	9		

- Molecule 53 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
53	A	1	Total	Mg	0
			1	1	
53	C	1	Total	Mg	0
			1	1	
53	E	1	Total	Mg	0
			1	1	
53	I	1	Total	Mg	0
			1	1	
53	R	1	Total	Mg	0
			1	1	
53	T	1	Total	Mg	0
			1	1	
53	f	3	Total	Mg	0
			3	3	
53	h	1	Total	Mg	0
			1	1	
53	j	2	Total	Mg	0
			2	2	

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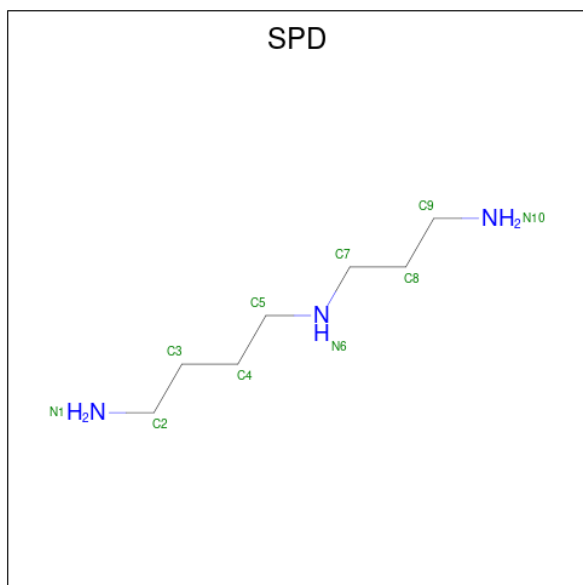
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Mol	Chain	Residues	Atoms		AltConf
53	k	1	Total	Mg	0
			1	1	

- Molecule 54 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
54	T	1	Total	Zn	0
			1	1	
54	W	1	Total	Zn	0
			1	1	
54	Z	1	Total	Zn	0
			1	1	
54	b	1	Total	Zn	0
			1	1	
54	c	1	Total	Zn	0
			1	1	
54	e	2	Total	Zn	0
			2	2	

- Molecule 55 is SPERMIDINE (three-letter code: SPD) (formula: C₇H₁₉N₃).

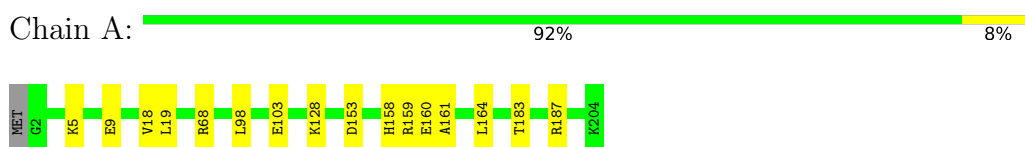


Mol	Chain	Residues	Atoms			AltConf
55	f	1	Total	C	N	0
			10	7	3	

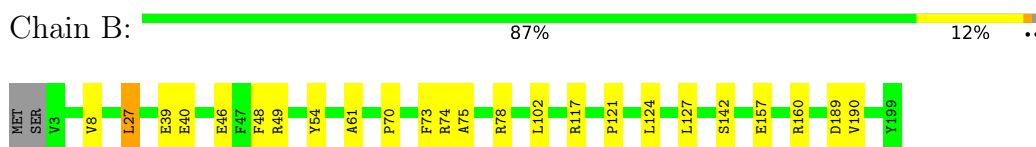
3 Residue-property plots [i](#)

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

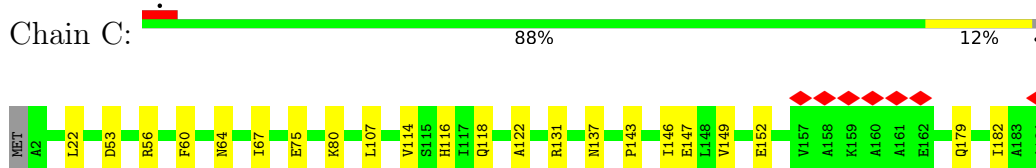
- Molecule 1: 60S ribosomal protein L15-A



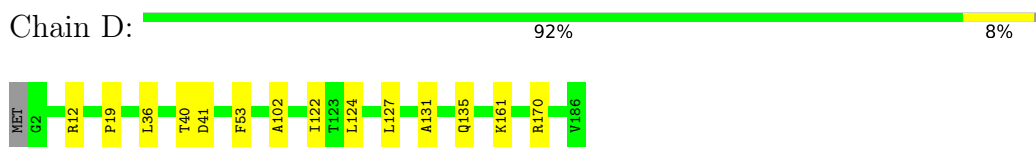
- Molecule 2: 60S ribosomal protein L16-A



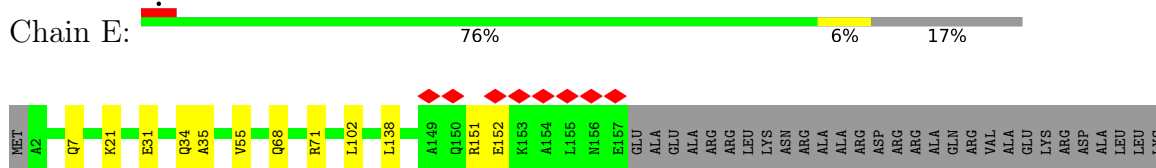
- Molecule 3: 60S ribosomal protein L17-A



- Molecule 4: 60S ribosomal protein L18-A

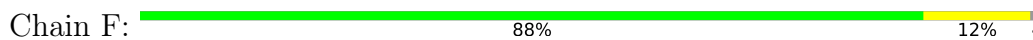


- Molecule 5: 60S ribosomal protein L19-A

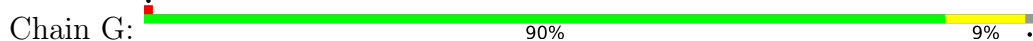


GLU
ASP
ALA

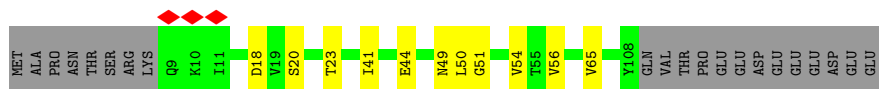
• Molecule 6: 60S ribosomal protein L20-A



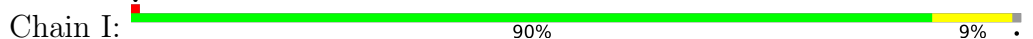
• Molecule 7: 60S ribosomal protein L21-A



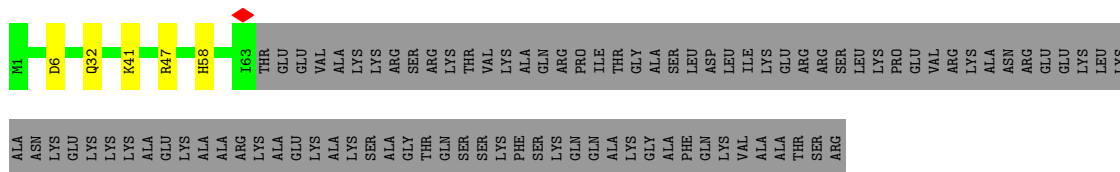
• Molecule 8: 60S ribosomal protein L22-A



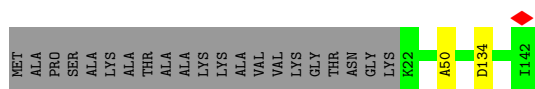
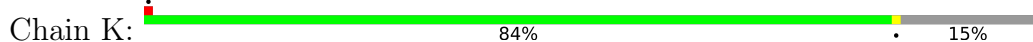
• Molecule 9: 60S ribosomal protein L23-A



• Molecule 10: 60S ribosomal protein L24-A

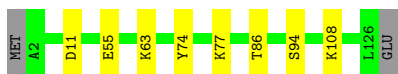


• Molecule 11: 60S ribosomal protein L25



- Molecule 12: 60S ribosomal protein L26-A

Chain L:  92% 6%



- Molecule 13: 60S ribosomal protein L27-A

Chain M:  92% 7%




- Molecule 14: 60S ribosomal protein L28

Chain N:  92% 7%




- Molecule 15: 60S ribosomal protein L29

Chain O:  83% 12%




- Molecule 16: 60S ribosomal protein L30

Chain P:  86% 6% 9%



- Molecule 17: 60S ribosomal protein L31-A

Chain Q:  5% 80% 17%



- Molecule 18: 60S ribosomal protein L32

Chain R:  92% 6%



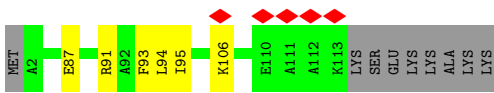
- Molecule 19: 60S ribosomal protein L33-A

Chain S: 95%



- Molecule 20: 60S ribosomal protein L34-A

Chain T: 88% 5% 7%



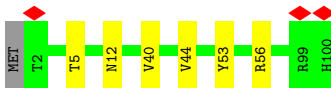
- Molecule 21: 60S ribosomal protein L35-A

Chain U: 93% 6%



- Molecule 22: 60S ribosomal protein L36-A

Chain V: 93% 6%



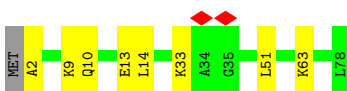
- Molecule 23: 60S ribosomal protein L37-A

Chain W: 84% 8% 8%



- Molecule 24: 60S ribosomal protein L38

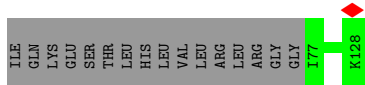
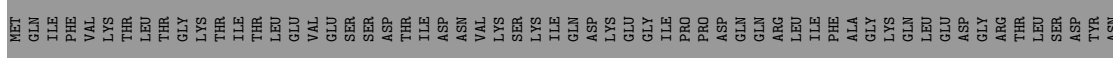
Chain X: 88% 10%



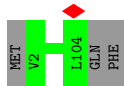
- Molecule 25: 60S ribosomal protein L39



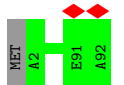
- Molecule 26: Ubiquitin-60S ribosomal protein L40



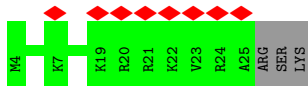
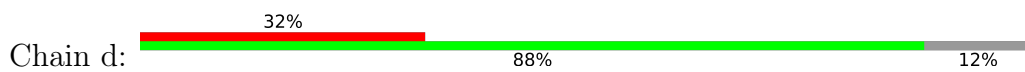
- Molecule 27: 60S ribosomal protein L42-A



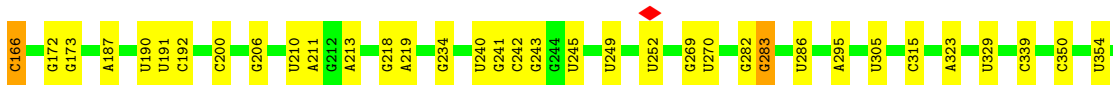
- Molecule 28: 60S ribosomal protein L43-A

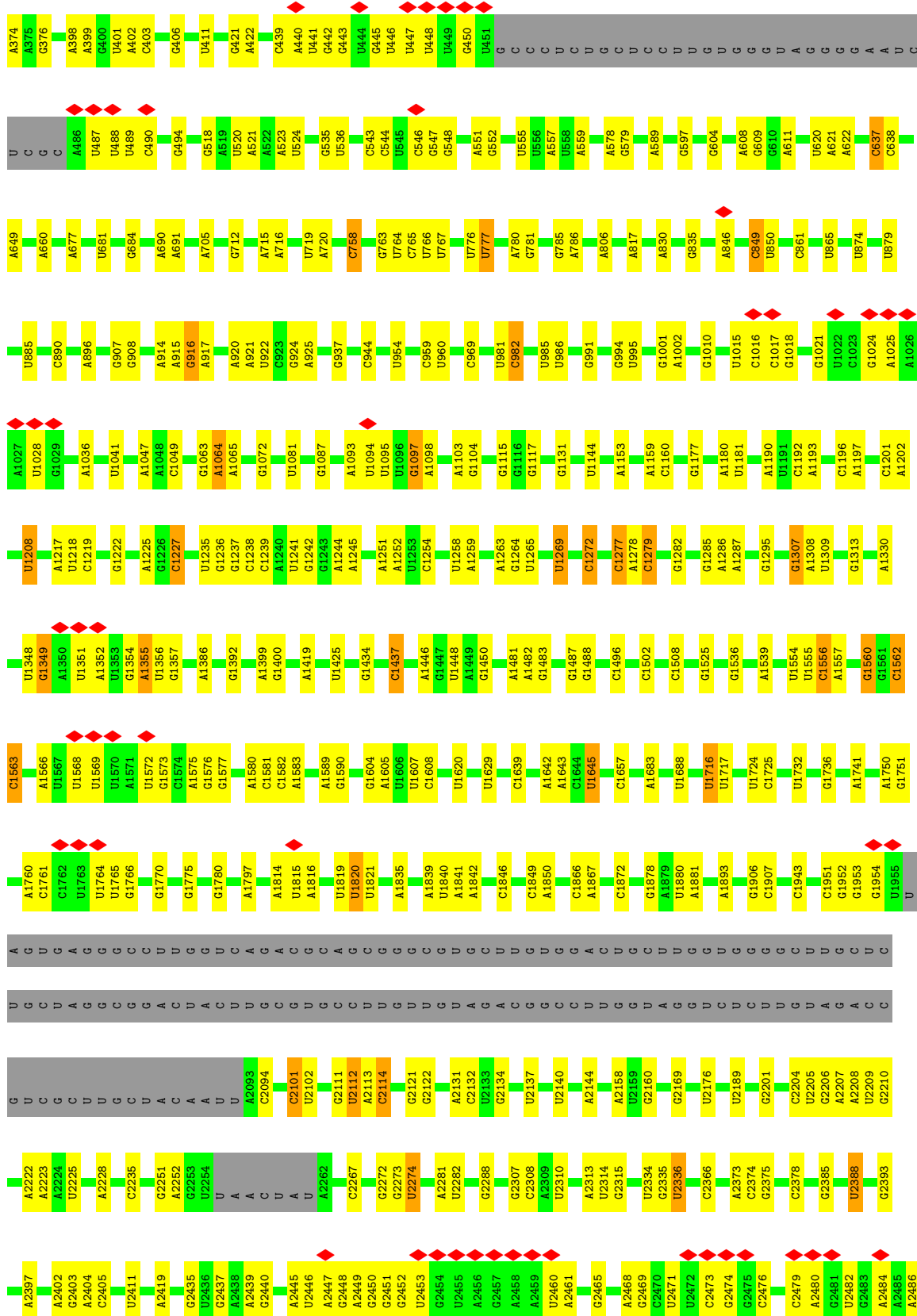


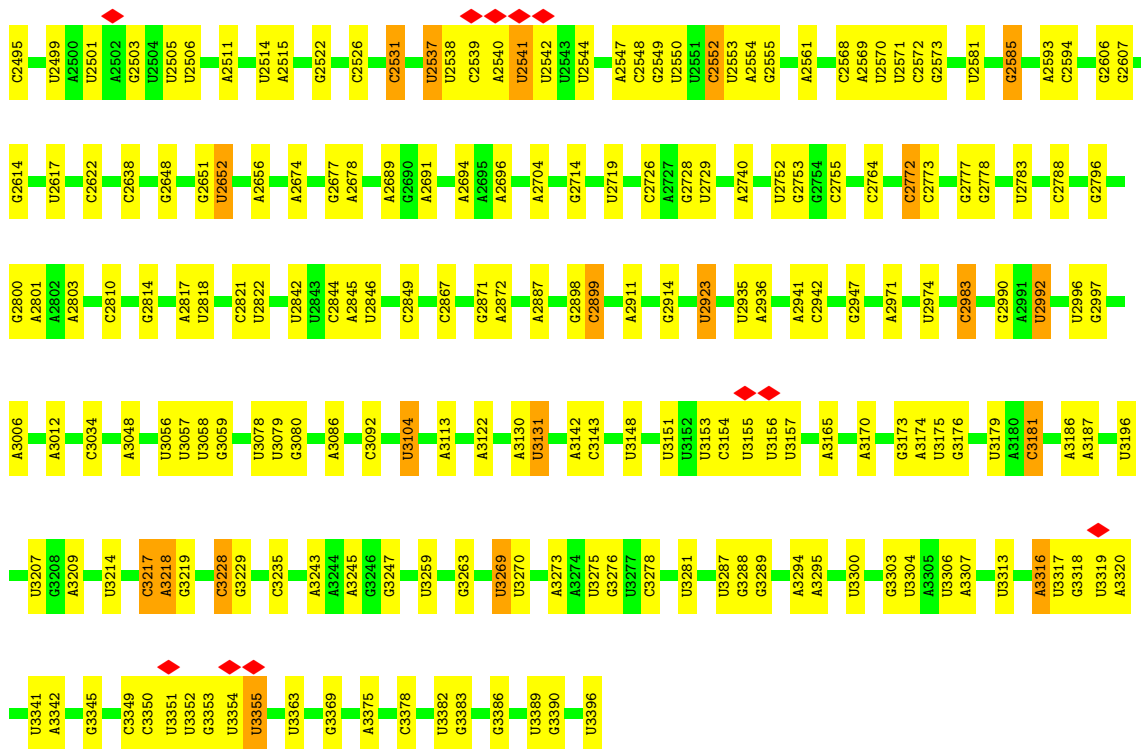
- Molecule 29: 60S ribosomal protein L41-A



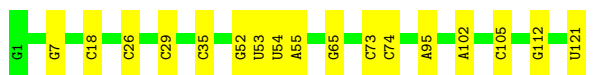
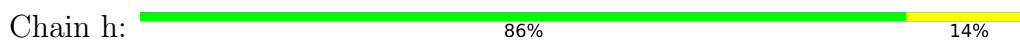
- Molecule 30: 25S rRNA



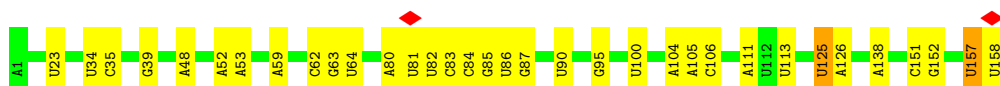
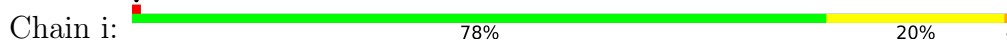




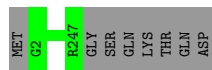
• Molecule 31: 5S rRNA



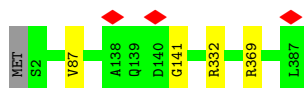
• Molecule 32: 5.8S rRNA



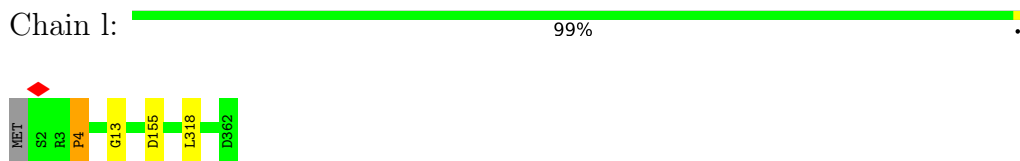
• Molecule 33: 60S ribosomal protein L2-A



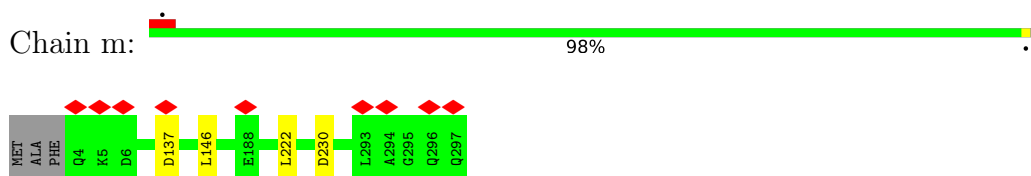
• Molecule 34: 60S ribosomal protein L3



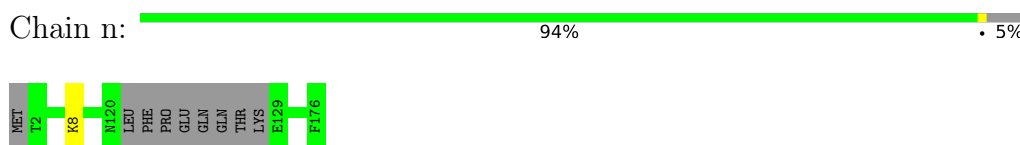
- Molecule 35: 60S ribosomal protein L4-A



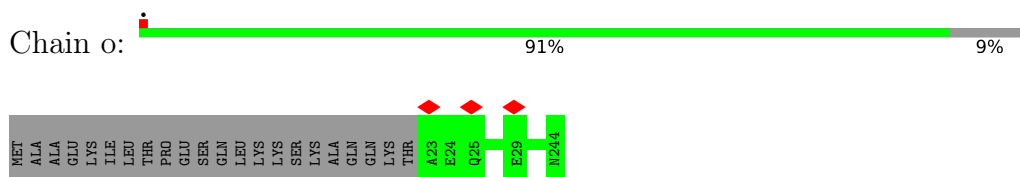
- Molecule 36: 60S ribosomal protein L5



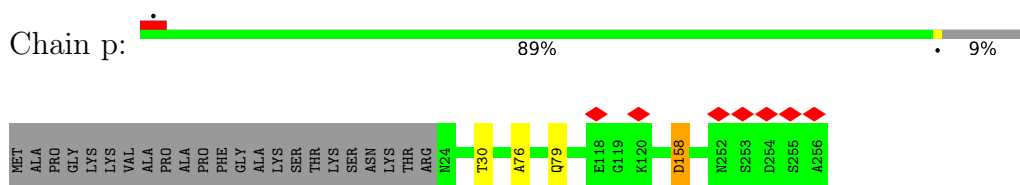
- Molecule 37: 60S ribosomal protein L6-B



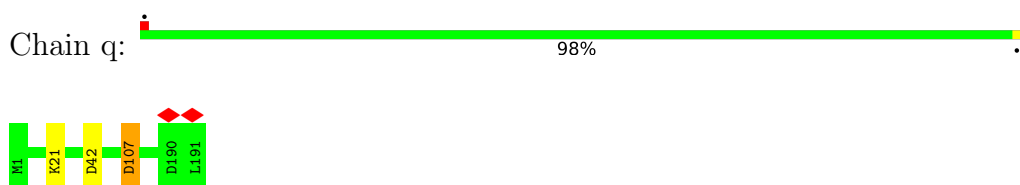
- Molecule 38: 60S ribosomal protein L7-A



- Molecule 39: 60S ribosomal protein L8-A



- Molecule 40: 60S ribosomal protein L9-A

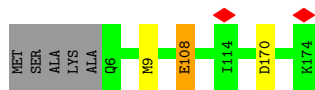


- Molecule 41: 60S ribosomal protein L10

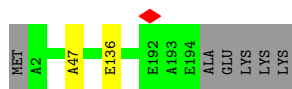




• Molecule 42: 60S ribosomal protein L11-A



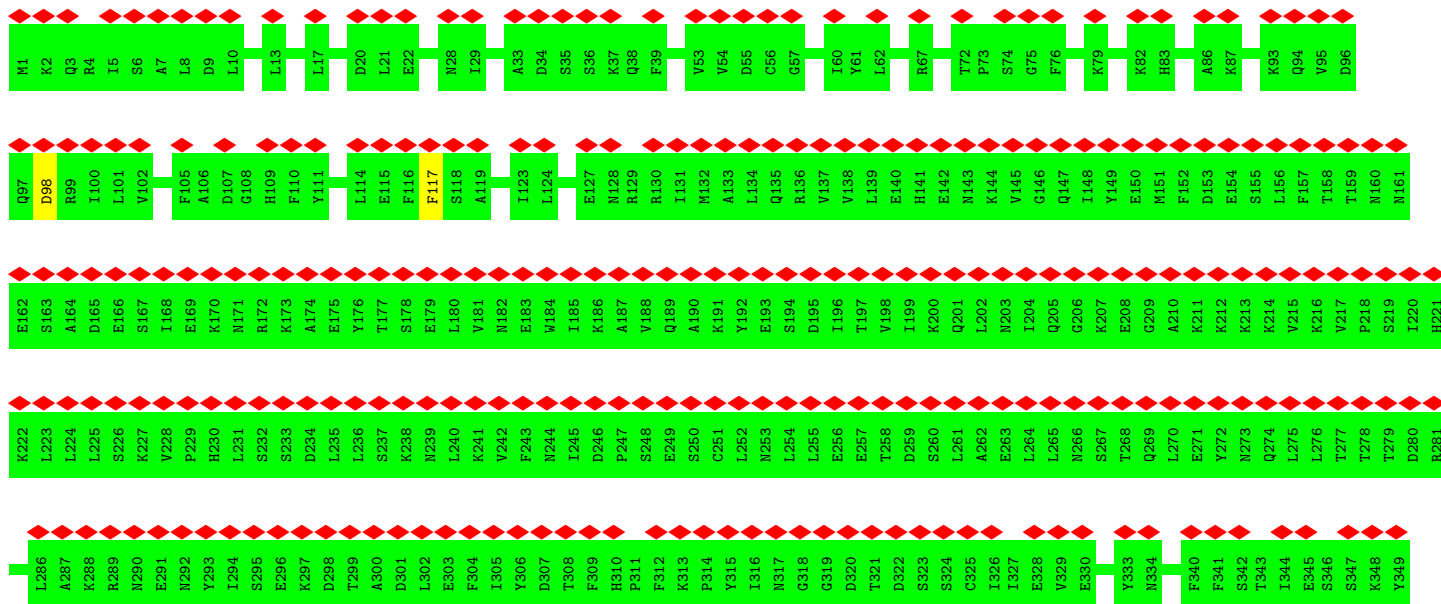
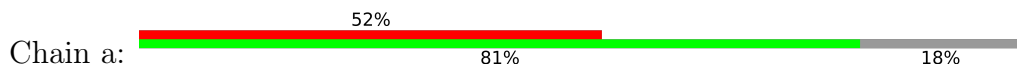
• Molecule 43: 60S ribosomal protein L13-A



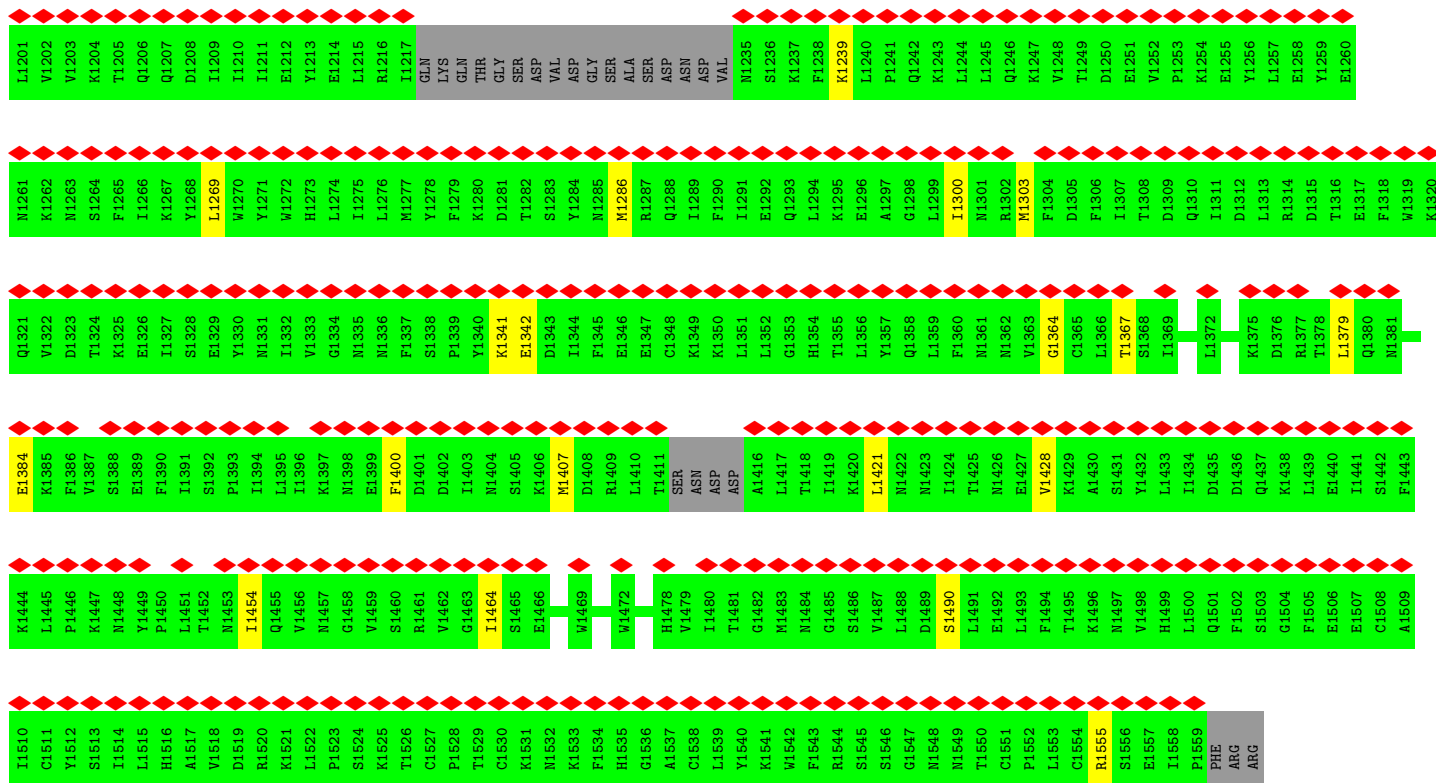
• Molecule 44: 60S ribosomal protein L14-A



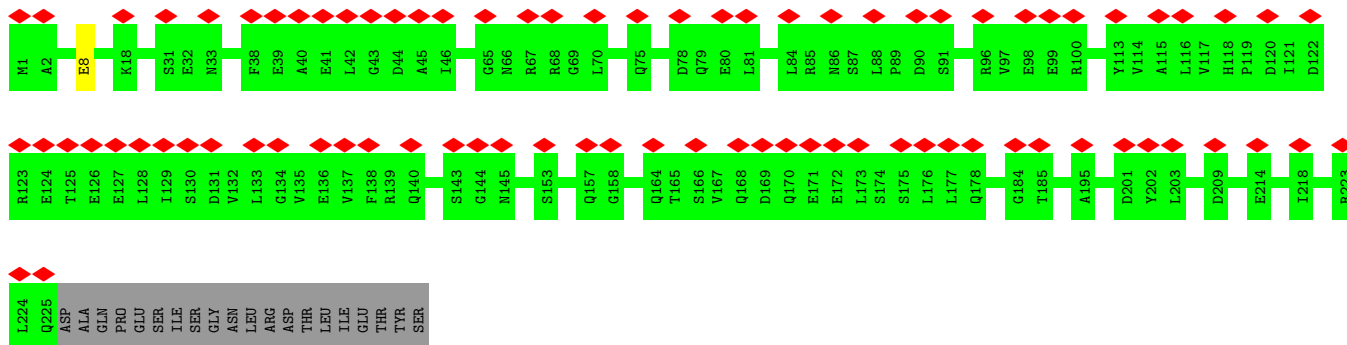
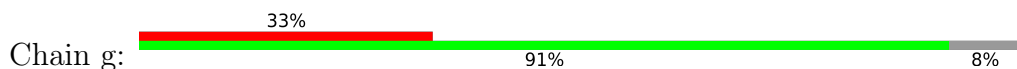
• Molecule 45: RQC2 isoform 1



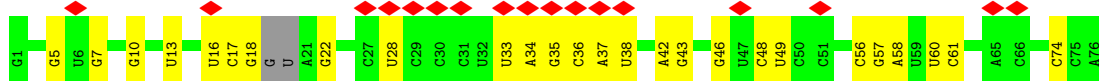
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A1081	D1082	S1083	L1084	S1085	M1086	C1087	Q1088	I1089	T1090	D1091	T1092	L1093	L1094	L1095	L1096	E1097	L1098	R1099	S1100	S1101	C1102	L1103	N1104	L1105	Y1106	E1107	T1108	L1109	S1110	Q1111	GLY	VAL	SER	LYS	ASN	GLY	GLU	ILE	SER	E1122	Y1123	G1124	D1125	E1126	I1127	E1128	E1129	N1130	L1131	I1132	E1133	L1134	M1135	F1136	L1137	N1138	F1139	N1140		
P1021	Q1022	R1023	L1024	M1025	M1026	I1027	F1028	R1029	S1030	I1031	L1032	K1033	W1034	L1035	D1036	S1037	D1038	L1039	A1040	Y1041	E1042	P1043	S1044	F1045	S1046	T1047	V1048	R1049	L1050	L1051	L1052	L1053	D1054	F1055	F1056	T1057	K1058	L1059	M1060	R1061	F1062	E1063	G1064	V1065	M1066	D1067	M1068	G1069	I1070	T1071	A1072	F1073	E1074	L1075	S1076	E1077	R1078	L1079	L1080	
L961	L962	M963	F964	N965	R966	S967	N968	S969	K970	D971	E972	I973	T974	K975	L976	R977	T978	L979	L980	A981	S982	Q983	L984	I985	R986	I987	R988	E989	V990	E991	L992	V993	D994	Q995	E996	F997	K998	S999	L1000	A1001	L1002	L1003	M1004	M1005	L1006	L1007	D1008	I1009	P1010	Q1011	A1012	D1013	K1014	Q1015	F1016	V1017	P1018	I1019	A1020	
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K481	N482	L483	F484	A485	L486	L487	V488	T489	S490	P491	N492	N493	E494	S495	A496	I497	S498	R499	L500	F501	D502	F503	F504	V505	V506	L507	I508	E509	T510	D511	P512	S513	N514	V515	F516	T517	K518	Y519	D520	G521	V522	Y523	D524	E525	L526	N527	Y528	F529	L530	D531	S532	D533	M534	I535	F536	L537	G539	K540		
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L601	A602	T603	M604	N605	E606	L607	D608	M609	D610	I611	V612	Q613	Q614	L615	M616	K617	S618	D619	S620	L621	D622	L623	E624	A625	Q626	I627	E628	D629	F630	M631	K632	M633	Y634	K635	F636	D637	D638	S639	G640	E641	I642	F643	K644	G645	E646	M647	K648	F649	L650	M651	Q652	D653	T654	I655	L656	T657	L658	Y659	R660	
S661	A662	V663	A664	N665	G666	Q667	V668	E669	Q670	F671	C672	A673	V674	L675	S676	K677	L678	D679	E680	F681	D682	F683	S684	T685	L686	L687	L688	N689	T690	D691	F692	L693	S694	C695	A696	L697	Y698	E699	V700	S701	E702	D703	T704	N705	E706	K707	L708	F709	K710	L711	S712	L713	Q714	L715	A716	K717	L718	N719	S720	
E721	I722	A723	N724	K725	L726	A727	Q728	V729	L730	L731	Q732	H733	A734	Q735	V736	Y737	F738	S739	P740	G741	A742	K743	E744	K745	V746	V747	T748	H749	A750	V751	E752	L753	I754	N755	G756	C757	N758	D759	T760	S761	Q762	I763	T764	F765	F766	A767	N768	A769	I770	E771	V772	F773	A774	R775	V776	M777	A778	I780		
D781	Y782	R783	S784	S785	L786	V787	S788	S789	L790	S791	T792	M793	E794	H795	L796	L797	L798	T799	D800	D801	K802	P803	L804	N805	L806	K807	N808	M809	Q810	K811	L812	L813	R814	Y815	A816	L817	F818	L819	D820	A821	L822	L823	D824	A825	L826	P827	E828	R829	R830	M831	N832	H833	L834	V835	A836	F837	L838	T839	V840	
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• Molecule 47: Eukaryotic translation initiation factor 6



• Molecule 48: Ala tRNA

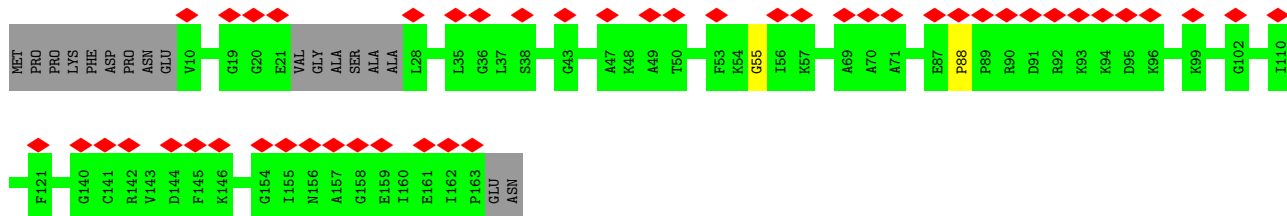
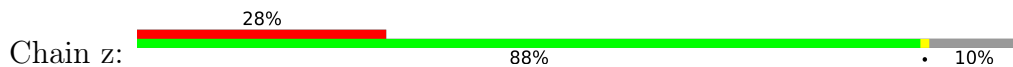


• Molecule 48: Ala tRNA

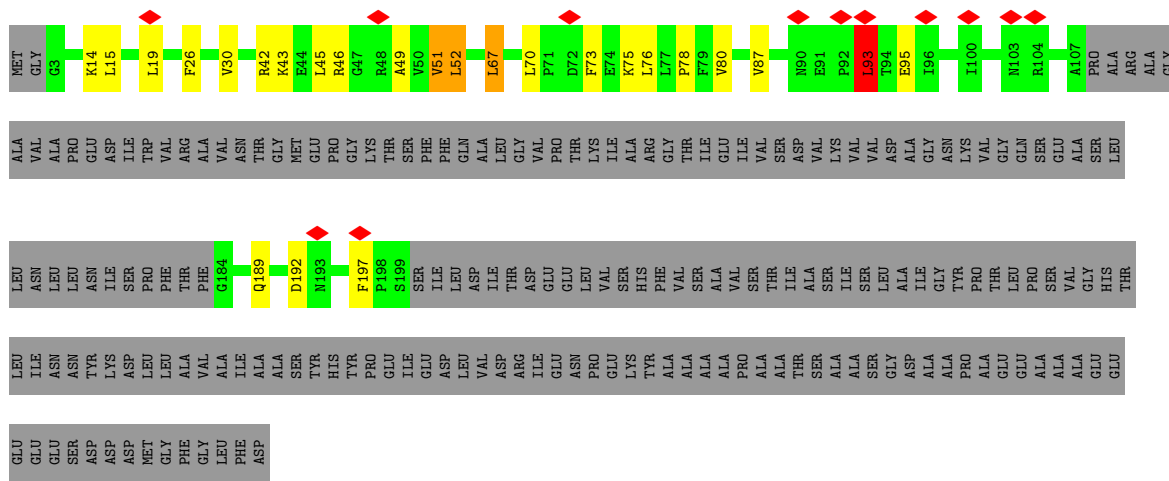




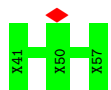
• Molecule 49: 60S ribosomal protein L12-A



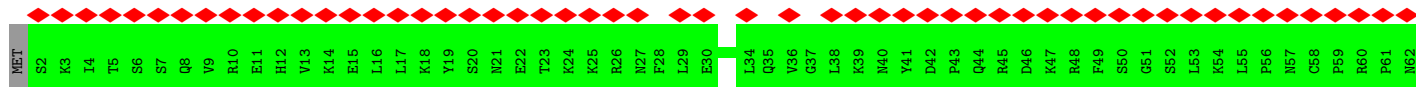
• Molecule 50: 60S acidic ribosomal protein P0



• Molecule 51: CAT-tailed nascent peptide



• Molecule 52: 60S ribosomal protein L1-A



M63	S64	I65	C66	I67	F68	G69	D70	A71	F72	D73	V74	D75	R76	A77	K78	S79	C80	G81	V82	D83	A84	M85	S86	V87	D88	D89	L90	K91	K92	L93	N94	K95	N96	K97	K98	L99	I100	K101	K102	L103	S104	K105	K106	Y107	N108	A109	F110	I111	A112	S113	E114	V115	L116	I117	K118	Q119	V120	P121	R122
L123	L124	G125	P126	Q127	L128	S129	K130	A131	G132	K133	F134	P135	T136	P137	V138	S139	H140	M141	D142	D143	L144	Y145	G146	K147	V148	T149	D150	V151	R152	S153	T154	I155	K156	F157	Q158	L159	K160	K161	V162	L163	C164	L165	A166	V167	A168	V169	G170	M171	V172	E173	M174	E175	E176	D177	V178	L179	V180	N181	Q182
I183	L184	M185	S186	V187	N188	F189	F190	V191	S192	L193	L194	K195	K196	N197	M198	Q199	G202	S203	L204	V205	V206	F214	R215	L216	Y217																																		

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	58513	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	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	3.793	Depositor
Minimum map value	-0.656	Depositor
Average map value	0.021	Depositor
Map value standard deviation	0.131	Depositor
Recommended contour level	0.55	Depositor
Map size (Å)	476.55002, 476.55002, 476.55002	wwPDB
Map dimensions	450, 450, 450	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.059, 1.059, 1.059	Depositor

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: SPD, 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	A	0.39	0/1757	0.70	1/2354 (0.0%)
2	B	0.39	0/1585	0.64	1/2128 (0.0%)
3	C	0.36	0/1439	0.72	2/1938 (0.1%)
4	D	0.34	0/1465	0.67	1/1965 (0.1%)
5	E	0.37	0/1275	0.68	0/1702
6	F	0.38	0/1473	0.65	0/1980
7	G	0.36	0/1296	0.62	0/1739
8	H	0.37	0/812	0.73	3/1099 (0.3%)
9	I	0.35	0/1018	0.64	0/1369
10	J	0.35	0/530	0.63	0/703
11	K	0.41	0/979	0.69	1/1321 (0.1%)
12	L	0.35	0/995	0.68	1/1329 (0.1%)
13	M	0.36	0/1106	0.61	0/1485
14	N	0.40	0/1200	0.62	0/1607
15	O	0.32	0/473	0.72	2/629 (0.3%)
16	P	0.35	0/745	0.67	0/1001
17	Q	0.39	0/890	0.77	2/1196 (0.2%)
18	R	0.32	0/1034	0.59	0/1385
19	S	0.38	0/868	0.61	0/1168
20	T	0.35	0/890	0.67	0/1189
21	U	0.34	0/978	0.65	1/1301 (0.1%)
22	V	0.34	0/772	0.66	0/1026
23	W	0.39	0/660	0.69	0/875
24	X	0.33	0/618	0.78	1/826 (0.1%)
25	Y	0.33	0/443	0.65	0/588
26	Z	0.33	0/416	0.70	0/553
27	b	0.36	0/836	0.66	0/1104
28	c	0.36	0/701	0.67	0/934
29	d	0.26	0/208	0.84	0/267
30	f	0.61	0/77011	1.01	272/120065 (0.2%)
31	h	0.53	0/2883	0.98	8/4491 (0.2%)
32	i	0.61	0/3746	0.96	7/5832 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	j	0.37	0/1908	0.67	0/2564
34	k	0.36	0/3146	0.64	1/4228 (0.0%)
35	l	0.36	0/2800	0.64	2/3790 (0.1%)
36	m	0.34	0/2400	0.67	4/3239 (0.1%)
37	n	0.36	0/1329	0.67	0/1794
38	o	0.37	0/1821	0.61	0/2451
39	p	0.34	0/1836	0.62	2/2481 (0.1%)
40	q	0.37	0/1529	0.68	2/2060 (0.1%)
41	r	0.33	0/1801	0.64	0/2416
42	s	0.33	0/1367	0.70	3/1834 (0.2%)
43	t	0.36	0/1568	0.68	1/2106 (0.0%)
44	u	0.34	0/1068	0.66	1/1438 (0.1%)
45	a	0.31	0/6683	0.57	3/9016 (0.0%)
46	e	0.39	0/11711	0.55	2/15903 (0.0%)
47	g	0.32	0/1672	0.63	0/2281
48	x	0.20	0/1761	0.65	0/2742
48	y	0.23	0/1735	0.65	0/2701
49	z	0.37	0/726	0.60	0/1006
50	0	0.33	0/976	0.55	0/1313
52	w	0.33	0/1736	0.65	0/2332
All	All	0.50	0/160675	0.86	324/234844 (0.1%)

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
15	O	0	1
21	U	0	1
34	k	0	1
35	l	0	2
39	p	0	3
40	q	0	1
44	u	0	1
46	e	0	1
47	g	0	1
All	All	0	12

There are no bond length outliers.

All (324) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	f	3217	C	N1-C2-O2	12.05	126.13	118.90
30	f	3217	C	C2-N1-C1'	11.35	131.29	118.80
30	f	3217	C	N3-C2-O2	-9.71	115.10	121.90
11	K	134	ASP	CB-CG-OD1	9.66	126.99	118.30
30	f	922	U	C2-N1-C1'	9.31	128.87	117.70
17	Q	84	ASP	CB-CG-OD1	9.27	126.65	118.30
30	f	2531	C	N1-C2-O2	8.90	124.24	118.90
30	f	922	U	N1-C2-O2	8.86	129.00	122.80
30	f	3278	C	N1-C2-O2	8.77	124.16	118.90
30	f	3181	C	N1-C2-O2	8.73	124.14	118.90
30	f	3181	C	C2-N1-C1'	8.49	128.14	118.80
30	f	1279	C	C5-C6-N1	8.31	125.16	121.00
36	m	230	ASP	CB-CG-OD1	8.14	125.63	118.30
30	f	1496	C	C2-N1-C1'	8.09	127.70	118.80
30	f	922	U	N3-C2-O2	-8.09	116.54	122.20
30	f	406	G	O4'-C1'-N9	7.95	114.56	108.20
30	f	1645	U	N3-C2-O2	-7.88	116.69	122.20
30	f	2205	U	N1-C2-O2	7.86	128.30	122.80
30	f	3217	C	C6-N1-C2	-7.85	117.16	120.30
4	D	41	ASP	CB-CG-OD1	7.82	125.33	118.30
30	f	3217	C	C6-N1-C1'	-7.77	111.48	120.80
30	f	2983	C	C2-N1-C1'	7.73	127.30	118.80
30	f	1208	U	N1-C2-O2	7.72	128.21	122.80
30	f	2652	U	N3-C2-O2	-7.59	116.89	122.20
30	f	3278	C	N3-C2-O2	-7.58	116.59	121.90
30	f	3306	U	N3-C2-O2	-7.58	116.89	122.20
30	f	3306	U	C2-N1-C1'	7.57	126.78	117.70
30	f	2541	U	P-O3'-C3'	7.53	128.73	119.70
30	f	3278	C	C2-N1-C1'	7.52	127.08	118.80
30	f	2205	U	N3-C2-O2	-7.50	116.95	122.20
30	f	758	C	C2-N1-C1'	7.46	127.00	118.80
30	f	1277	C	C2-N1-C1'	7.36	126.90	118.80
30	f	2235	C	C2-N1-C1'	7.36	126.90	118.80
30	f	1645	U	N1-C2-O2	7.34	127.94	122.80
30	f	3181	C	N3-C2-O2	-7.33	116.77	121.90
15	O	36	ASP	CB-CG-OD1	7.27	124.84	118.30
30	f	1239	C	C2-N1-C1'	7.23	126.75	118.80
30	f	2531	C	C2-N1-C1'	7.21	126.73	118.80
30	f	1349	G	N3-C4-C5	-7.19	125.00	128.60
42	s	170	ASP	CB-CG-OD1	7.18	124.77	118.30
30	f	1277	C	N1-C2-O2	7.18	123.21	118.90
30	f	1556	C	N1-C2-O2	7.16	123.20	118.90
30	f	1227	C	C2-N1-C1'	7.13	126.65	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	f	2923	U	N1-C2-O2	7.11	127.78	122.80
30	f	2205	U	C2-N1-C1'	7.08	126.20	117.70
30	f	1645	U	C2-N1-C1'	7.07	126.18	117.70
30	f	14	U	O5'-P-OP2	-7.07	99.34	105.70
30	f	1815	U	P-O3'-C3'	7.07	128.18	119.70
30	f	78	U	N3-C2-O2	-7.06	117.26	122.20
39	p	158	ASP	CB-CG-OD1	7.06	124.66	118.30
30	f	1307	G	P-O3'-C3'	7.06	128.17	119.70
30	f	1227	C	N1-C2-O2	7.05	123.13	118.90
30	f	1604	G	C4-N9-C1'	7.05	135.66	126.50
30	f	36	C	N1-C2-O2	7.04	123.12	118.90
30	f	982	C	C2-N1-C1'	7.03	126.54	118.80
30	f	1872	C	N1-C2-O2	7.02	123.11	118.90
30	f	1349	G	C4-N9-C1'	6.96	135.55	126.50
30	f	1272	C	N1-C2-O2	6.91	123.05	118.90
30	f	2405	C	C6-N1-C2	-6.91	117.53	120.30
30	f	1208	U	C2-N1-C1'	6.90	125.98	117.70
30	f	3217	C	C5-C6-N1	6.88	124.44	121.00
30	f	3275	U	OP1-P-O3'	6.87	120.31	105.20
30	f	3235	C	C2-N1-C1'	6.80	126.28	118.80
30	f	3306	U	N1-C2-O2	6.80	127.56	122.80
30	f	2923	U	N3-C2-O2	-6.78	117.46	122.20
12	L	11	ASP	CB-CG-OD1	6.73	124.36	118.30
30	f	2531	C	N3-C2-O2	-6.72	117.20	121.90
30	f	2983	C	N3-C2-O2	-6.71	117.20	121.90
30	f	1227	C	C5-C6-N1	6.69	124.35	121.00
30	f	270	U	N1-C2-O2	6.69	127.48	122.80
30	f	270	U	N3-C2-O2	-6.68	117.52	122.20
30	f	1227	C	C6-N1-C2	-6.66	117.64	120.30
30	f	2537	U	P-O3'-C3'	6.65	127.68	119.70
30	f	3058	U	C2-N1-C1'	6.62	125.65	117.70
30	f	2112	U	OP2-P-O3'	6.61	119.74	105.20
31	h	26	C	N1-C2-O2	6.61	122.87	118.90
30	f	2235	C	C6-N1-C2	-6.60	117.66	120.30
30	f	2189	U	N1-C2-O2	6.57	127.40	122.80
30	f	1239	C	N1-C2-O2	6.55	122.83	118.90
32	i	64	U	N3-C2-O2	-6.55	117.62	122.20
30	f	3034	C	N1-C2-O2	6.54	122.83	118.90
30	f	524	U	N1-C2-O2	6.54	127.38	122.80
30	f	1208	U	N3-C2-O2	-6.51	117.64	122.20
30	f	3214	U	C2-N1-C1'	6.51	125.51	117.70
2	B	27[A]	LEU	CB-CG-CD2	-6.50	99.95	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	f	2101	C	P-O3'-C3'	6.49	127.49	119.70
30	f	2112	U	P-O3'-C3'	6.47	127.46	119.70
31	h	105	C	N1-C2-O2	6.46	122.77	118.90
30	f	2274	U	N1-C2-O2	6.42	127.30	122.80
30	f	2189	U	N3-C2-O2	-6.41	117.72	122.20
44	u	47	ASP	CB-CG-OD1	6.40	124.06	118.30
30	f	1269	U	C2-N1-C1'	6.40	125.38	117.70
30	f	524	U	N3-C2-O2	-6.39	117.72	122.20
30	f	2983	C	N1-C2-O2	6.39	122.74	118.90
30	f	2550	U	N3-C2-O2	-6.37	117.74	122.20
30	f	986	U	N3-C2-O2	-6.37	117.74	122.20
30	f	865	U	N3-C2-O2	-6.33	117.77	122.20
36	m	137	ASP	CB-CG-OD1	6.33	124.00	118.30
30	f	1269	U	N1-C2-O2	6.32	127.23	122.80
35	l	155	ASP	CB-CG-OD1	6.31	123.98	118.30
1	A	153	ASP	CB-CG-OD1	6.30	123.97	118.30
30	f	36	C	N3-C2-O2	-6.30	117.49	121.90
30	f	2617	U	N3-C2-O2	-6.30	117.79	122.20
30	f	1496	C	C6-N1-C2	-6.30	117.78	120.30
30	f	1556	C	N3-C2-O2	-6.30	117.49	121.90
30	f	922	U	C6-N1-C1'	-6.29	112.40	121.20
30	f	2726	C	N3-C2-O2	-6.29	117.50	121.90
21	U	79	ASP	CB-CG-OD1	6.28	123.95	118.30
30	f	2726	C	C2-N1-C1'	6.26	125.69	118.80
30	f	3058	U	N1-C2-O2	6.26	127.19	122.80
45	a	697	LEU	CA-CB-CG	6.25	129.67	115.30
30	f	1269	U	N3-C2-O2	-6.24	117.83	122.20
30	f	192	C	C2-N1-C1'	6.23	125.65	118.80
40	q	42	ASP	CB-CG-OD1	6.22	123.90	118.30
30	f	915	A	C2-N3-C4	6.21	113.71	110.60
30	f	1097	G	P-O3'-C3'	6.21	127.15	119.70
30	f	1716	U	P-O3'-C3'	6.21	127.15	119.70
46	e	437	LYS	N-CA-C	-6.20	94.25	111.00
30	f	3104	U	N1-C2-O2	6.19	127.14	122.80
30	f	1349	G	N3-C4-N9	6.18	129.71	126.00
30	f	1878	G	C4-N9-C1'	6.13	134.47	126.50
30	f	969	C	C6-N1-C2	-6.12	117.85	120.30
30	f	3104	U	N3-C2-O2	-6.12	117.92	122.20
30	f	2388	U	N3-C2-O2	-6.11	117.92	122.20
30	f	637	C	P-O3'-C3'	6.11	127.03	119.70
30	f	1115	G	C4-N9-C1'	6.10	134.43	126.50
30	f	2550	U	C2-N1-C1'	6.09	125.01	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	f	2923	U	C2-N1-C1'	6.08	125.00	117.70
30	f	2132	C	C6-N1-C2	-6.07	117.87	120.30
30	f	2553	U	C2-N1-C1'	6.06	124.98	117.70
30	f	3131	U	C2-N1-C1'	6.05	124.96	117.70
30	f	1604	G	N3-C4-N9	6.04	129.63	126.00
30	f	995	U	N1-C2-O2	6.04	127.03	122.80
30	f	1064	A	P-O3'-C3'	6.03	126.94	119.70
30	f	1907	C	N1-C2-O2	6.02	122.51	118.90
30	f	3181	C	C6-N1-C1'	-6.02	113.58	120.80
30	f	985	U	N3-C2-O2	-6.01	117.99	122.20
30	f	1604	G	C8-N9-C1'	-6.01	119.19	127.00
30	f	1872	C	N3-C2-O2	-6.01	117.69	121.90
30	f	2274	U	C2-N1-C1'	6.00	124.91	117.70
30	f	1556	C	C2-N1-C1'	5.99	125.39	118.80
30	f	2405	C	N3-C2-O2	-5.98	117.71	121.90
30	f	2204	C	C6-N1-C2	-5.98	117.91	120.30
30	f	2132	C	N3-C2-O2	-5.97	117.72	121.90
8	H	18	ASP	CB-CG-OD1	5.97	123.67	118.30
30	f	1279	C	C6-N1-C2	-5.96	117.92	120.30
8	H	51	GLY	C-N-CA	5.95	136.58	121.70
34	k	87	VAL	CG1-CB-CG2	-5.95	101.38	110.90
30	f	3300	U	N3-C2-O2	-5.94	118.04	122.20
30	f	1425	U	N3-C2-O2	-5.93	118.05	122.20
30	f	2531	C	C6-N1-C2	-5.93	117.93	120.30
30	f	142	C	N1-C2-O2	5.90	122.44	118.90
30	f	865	U	N1-C2-O2	5.89	126.93	122.80
30	f	2622	C	N1-C2-O2	5.89	122.43	118.90
31	h	26	C	C6-N1-C2	-5.89	117.94	120.30
32	i	100	U	C2-N1-C1'	5.89	124.76	117.70
30	f	1562	C	P-O3'-C3'	5.88	126.76	119.70
30	f	1355	A	P-O3'-C3'	5.88	126.76	119.70
30	f	2585	G	N3-C4-C5	-5.88	125.66	128.60
30	f	1604	G	N3-C4-C5	-5.87	125.66	128.60
30	f	1820	U	P-O3'-C3'	5.87	126.74	119.70
30	f	2531	C	C5-C6-N1	5.87	123.93	121.00
30	f	2274	U	N3-C2-O2	-5.86	118.10	122.20
30	f	1577	G	N1-C6-O6	-5.85	116.39	119.90
30	f	2652	U	N1-C2-O2	5.83	126.88	122.80
30	f	3048	A	O4'-C1'-N9	5.83	112.86	108.20
30	f	1272	C	N3-C2-O2	-5.82	117.82	121.90
30	f	1437	C	C2-N1-C1'	5.82	125.20	118.80
30	f	2638	C	N1-C2-O2	5.82	122.39	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	f	1525	G	C4-N9-C1'	5.81	134.05	126.50
30	f	3214	U	N3-C2-O2	-5.81	118.13	122.20
30	f	835	G	O4'-C1'-N9	5.81	112.85	108.20
30	f	3350	C	C6-N1-C2	-5.80	117.98	120.30
30	f	3316	A	P-O3'-C3'	5.79	126.65	119.70
42	s	9	MET	CA-CB-CG	5.78	123.13	113.30
30	f	758	C	C6-N1-C2	-5.77	117.99	120.30
30	f	3228	C	P-O3'-C3'	5.76	126.61	119.70
30	f	270	U	C2-N1-C1'	5.76	124.61	117.70
30	f	3034	C	N3-C2-O2	-5.75	117.88	121.90
30	f	354	U	N1-C2-O2	5.74	126.81	122.80
30	f	3218	A	P-O3'-C3'	5.73	126.57	119.70
30	f	1277	C	N3-C2-O2	-5.71	117.90	121.90
30	f	1190	A	C4-N9-C1'	5.71	136.58	126.30
30	f	2899	C	C2-N1-C1'	5.71	125.08	118.80
45	a	117	PHE	N-CA-CB	-5.70	100.33	110.60
30	f	282	G	P-O3'-C3'	5.70	126.54	119.70
46	e	1364	GLY	N-CA-C	5.70	127.34	113.10
32	i	64	U	N1-C2-O2	5.69	126.79	122.80
30	f	916	G	P-O3'-C3'	5.68	126.52	119.70
30	f	97	U	N3-C2-O2	-5.68	118.22	122.20
30	f	2992	U	N3-C2-O2	-5.67	118.23	122.20
30	f	2553	U	C6-N1-C1'	-5.67	113.26	121.20
30	f	2899	C	N3-C2-O2	-5.67	117.93	121.90
30	f	2204	C	C5-C6-N1	5.66	123.83	121.00
8	H	50	LEU	CA-CB-CG	5.66	128.32	115.30
30	f	3058	U	N3-C2-O2	-5.66	118.24	122.20
30	f	2132	C	N1-C2-O2	5.65	122.29	118.90
30	f	2366	C	C2-N1-C1'	5.65	125.01	118.80
30	f	1349	G	C8-N9-C1'	-5.64	119.67	127.00
30	f	1448	U	N3-C2-O2	-5.63	118.26	122.20
30	f	1496	C	C5-C6-N1	5.63	123.82	121.00
30	f	113	C	C2-N1-C1'	5.63	124.99	118.80
3	C	53	ASP	CB-CG-OD1	5.62	123.36	118.30
30	f	2137	U	C2-N1-C1'	5.61	124.43	117.70
30	f	2378	C	C2-N1-C1'	5.59	124.95	118.80
30	f	3057	U	N3-C2-O2	-5.58	118.29	122.20
30	f	2983	C	C6-N1-C2	-5.58	118.07	120.30
30	f	3269	U	P-O3'-C3'	5.58	126.39	119.70
31	h	26	C	N3-C2-O2	-5.55	118.01	121.90
30	f	982	C	N1-C2-O2	5.55	122.23	118.90
30	f	142	C	C6-N1-C2	-5.54	118.08	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	f	777	U	N3-C2-O2	-5.54	118.32	122.20
30	f	1496	C	N1-C2-O2	5.54	122.22	118.90
30	f	2552	C	N1-C2-O2	5.53	122.22	118.90
30	f	2726	C	N1-C2-O2	5.52	122.21	118.90
30	f	2764	C	N1-C2-O2	5.52	122.21	118.90
32	i	125	U	C2-N1-C1'	5.52	124.32	117.70
40	q	107	ASP	CB-CG-OD1	5.52	123.27	118.30
30	f	2366	C	C5-C6-N1	5.51	123.76	121.00
30	f	1554	U	P-O3'-C3'	5.51	126.31	119.70
31	h	35	C	N1-C2-O2	5.51	122.21	118.90
30	f	283	G	N3-C4-N9	5.51	129.31	126.00
30	f	995	U	N3-C2-O2	-5.50	118.35	122.20
30	f	1688	U	N3-C2-O2	-5.50	118.35	122.20
31	h	52	G	P-O3'-C3'	5.50	126.29	119.70
30	f	411	U	N3-C2-O2	-5.49	118.36	122.20
30	f	3214	U	N1-C2-O2	5.49	126.64	122.80
24	X	14	LEU	CA-CB-CG	5.46	127.87	115.30
30	f	315	C	C2-N1-C1'	5.46	124.81	118.80
30	f	2210	G	N3-C4-C5	-5.46	125.87	128.60
30	f	2726	C	C6-N1-C2	-5.46	118.12	120.30
30	f	283	G	C4-N9-C1'	5.44	133.57	126.50
30	f	3355	U	C2-N1-C1'	5.44	124.23	117.70
30	f	986	U	N1-C2-O2	5.43	126.60	122.80
30	f	3153	U	C2-N1-C1'	5.43	124.22	117.70
30	f	1878	G	C8-N9-C1'	-5.41	119.97	127.00
45	a	439	LEU	CA-CB-CG	-5.41	102.86	115.30
30	f	2622	C	N3-C2-O2	-5.41	118.11	121.90
30	f	3057	U	N1-C2-O2	5.41	126.59	122.80
30	f	2585	G	N3-C4-N9	5.41	129.24	126.00
30	f	2552	C	C2-N1-C1'	5.40	124.74	118.80
30	f	2783	U	N3-C2-O2	-5.40	118.42	122.20
30	f	1349	G	C2-N3-C4	5.39	114.60	111.90
30	f	142	C	N3-C2-O2	-5.38	118.14	121.90
30	f	3350	C	P-O3'-C3'	5.38	126.16	119.70
3	C	114	VAL	CG1-CB-CG2	-5.38	102.30	110.90
30	f	3278	C	C6-N1-C1'	-5.36	114.36	120.80
30	f	3349	C	C6-N1-C2	-5.36	118.16	120.30
30	f	1425	U	N1-C2-O2	5.36	126.55	122.80
30	f	1732	U	N1-C2-O2	5.36	126.55	122.80
30	f	1190	A	C2-N3-C4	5.35	113.28	110.60
30	f	1496	C	C6-N1-C1'	-5.35	114.39	120.80
30	f	1560	G	N3-C4-N9	-5.34	122.79	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	f	2336	U	N3-C2-O2	-5.34	118.46	122.20
30	f	915	A	C4-N9-C1'	5.34	135.91	126.30
30	f	78	U	N1-C2-O2	5.34	126.54	122.80
30	f	2114	C	C6-N1-C2	-5.33	118.17	120.30
30	f	1437	C	C6-N1-C2	-5.32	118.17	120.30
30	f	1115	G	C8-N9-C1'	-5.31	120.10	127.00
30	f	3235	C	N1-C2-O2	5.30	122.08	118.90
30	f	890	C	N1-C2-O2	5.30	122.08	118.90
30	f	982	C	C6-N1-C2	-5.30	118.18	120.30
30	f	982	C	C5-C6-N1	5.30	123.65	121.00
43	t	136	GLU	CA-CB-CG	5.30	125.06	113.40
30	f	1277	C	C6-N1-C2	-5.30	118.18	120.30
30	f	1732	U	N3-C2-O2	-5.30	118.49	122.20
31	h	105	C	N3-C2-O2	-5.29	118.20	121.90
30	f	1525	G	C8-N9-C1'	-5.29	120.13	127.00
30	f	2405	C	N1-C2-O2	5.28	122.07	118.90
30	f	1907	C	N3-C2-O2	-5.28	118.21	121.90
30	f	2235	C	N1-C2-O2	5.26	122.06	118.90
32	i	125	U	N1-C2-O2	5.25	126.47	122.80
42	s	108	GLU	CA-CB-CG	5.24	124.93	113.40
30	f	3148	U	N3-C2-O2	-5.24	118.53	122.20
30	f	2568	C	O4'-C1'-N1	5.24	112.39	108.20
30	f	1608	C	C2-N1-C1'	5.24	124.56	118.80
30	f	2366	C	C6-N1-C2	-5.23	118.21	120.30
30	f	2622	C	C6-N1-C2	-5.21	118.22	120.30
30	f	2585	G	C4-N9-C1'	5.20	133.26	126.50
30	f	2235	C	C5-C6-N1	5.20	123.60	121.00
30	f	1239	C	C6-N1-C1'	-5.20	114.56	120.80
30	f	192	C	C6-N1-C2	-5.18	118.23	120.30
30	f	969	C	N3-C2-O2	-5.18	118.28	121.90
31	h	18	C	C2-N1-C1'	5.17	124.49	118.80
30	f	637	C	OP1-P-O3'	5.17	116.58	105.20
30	f	890	C	N3-C2-O2	-5.17	118.28	121.90
30	f	758	C	N1-C2-O2	5.17	122.00	118.90
30	f	954	U	N3-C2-O2	-5.17	118.58	122.20
30	f	849	C	P-O3'-C3'	5.16	125.89	119.70
30	f	2983	C	C6-N1-C1'	-5.15	114.62	120.80
30	f	166	C	C2-N1-C1'	5.15	124.47	118.80
30	f	1563	C	C6-N1-C1'	5.15	126.98	120.80
30	f	915	A	C8-N9-C4	-5.14	103.74	105.80
30	f	149	U	N3-C2-O2	-5.14	118.60	122.20
30	f	1237	G	N3-C4-N9	5.14	129.08	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	f	3181	C	C6-N1-C2	-5.13	118.25	120.30
30	f	2899	C	N1-C2-O2	5.13	121.98	118.90
32	i	100	U	N1-C2-O2	5.12	126.39	122.80
30	f	87	U	N1-C2-O2	5.12	126.39	122.80
30	f	2550	U	N1-C2-O2	5.11	126.38	122.80
30	f	1608	C	C5-C6-N1	5.11	123.55	121.00
36	m	222	LEU	CA-CB-CG	5.10	127.03	115.30
30	f	2772	C	N1-C2-O2	5.10	121.96	118.90
30	f	1951	C	C2-N1-C1'	5.09	124.40	118.80
30	f	2405	C	C2-N1-C1'	5.09	124.40	118.80
35	l	4	PRO	C-N-CA	5.08	134.40	121.70
30	f	1097	G	OP2-P-O3'	5.07	116.36	105.20
17	Q	42	LEU	CA-CB-CG	5.07	126.97	115.30
30	f	2638	C	N3-C2-O2	-5.07	118.35	121.90
30	f	354	U	N3-C2-O2	-5.06	118.66	122.20
30	f	885	U	N3-C2-O2	-5.06	118.66	122.20
32	i	157	U	N1-C2-O2	5.05	126.33	122.80
36	m	146	LEU	CB-CG-CD1	-5.05	102.42	111.00
30	f	1562	C	N3-C2-O2	-5.04	118.37	121.90
15	O	21	ILE	CG1-CB-CG2	-5.04	100.31	111.40
39	p	79	GLN	CA-CB-CG	5.03	124.46	113.40
30	f	1608	C	C6-N1-C2	-5.02	118.29	120.30
30	f	1820	U	OP2-P-O3'	5.02	116.25	105.20
30	f	3355	U	N1-C2-O2	5.02	126.31	122.80
30	f	777	U	N1-C2-O2	5.02	126.31	122.80
30	f	283	G	C8-N9-C1'	-5.01	120.48	127.00
30	f	1355	A	OP2-P-O3'	5.01	116.23	105.20
30	f	3363	U	N3-C2-O2	-5.00	118.70	122.20
30	f	2974	U	N3-C2-O2	-5.00	118.70	122.20

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
15	O	20	GLY	Peptide
21	U	83	LYS	Peptide
46	e	392	GLY	Peptide
47	g	8	GLU	Peptide
34	k	141	GLY	Peptide
35	l	13	GLY	Peptide
35	l	318	LEU	Peptide
39	p	158	ASP	Peptide

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Mol	Chain	Res	Type	Group
39	p	30	THR	Peptide
39	p	76	ALA	Peptide
40	q	21	LYS	Peptide
44	u	12	TRP	Peptide

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1720	0	1779	9	0
2	B	1555	0	1659	13	0
3	C	1416	0	1433	11	0
4	D	1441	0	1543	7	0
5	E	1258	0	1342	6	0
6	F	1437	0	1475	14	0
7	G	1272	0	1312	9	0
8	H	796	0	812	4	0
9	I	1003	0	1048	7	0
10	J	518	0	542	3	0
11	K	964	0	1025	1	0
12	L	984	0	1075	4	0
13	M	1080	0	1122	5	0
14	N	1169	0	1211	7	0
15	O	462	0	491	5	0
16	P	737	0	792	3	0
17	Q	876	0	912	9	0
18	R	1013	0	1077	5	0
19	S	850	0	880	2	0
20	T	880	0	942	3	0
21	U	969	0	1078	3	0
22	V	766	0	842	4	0
23	W	645	0	645	4	0
24	X	612	0	682	3	0
25	Y	436	0	475	0	0
26	Z	410	0	442	0	0
27	b	824	0	888	0	0
28	c	694	0	734	0	0
29	d	207	0	250	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	f	68802	0	34573	0	0
31	h	2579	0	1304	0	0
32	i	3353	0	1695	0	0
33	j	1874	0	1943	0	0
34	k	3075	0	3142	0	0
35	l	2748	0	2859	0	0
36	m	2351	0	2294	0	0
37	n	1307	0	1377	0	0
38	o	1784	0	1862	0	0
39	p	1804	0	1877	0	0
40	q	1508	0	1572	0	0
41	r	1764	0	1804	0	0
42	s	1346	0	1370	0	0
43	t	1543	0	1608	0	0
44	u	1053	0	1149	0	0
45	a	6573	0	6471	0	0
46	e	11512	0	10772	0	0
47	g	1651	0	1613	0	0
48	x	1579	0	800	0	0
48	y	1556	0	788	0	0
49	z	728	0	337	0	0
50	0	961	0	979	11	0
51	1	85	0	21	0	0
52	w	1709	0	1797	0	0
53	A	1	0	0	0	0
53	C	1	0	0	0	0
53	E	1	0	0	0	0
53	I	1	0	0	0	0
53	R	1	0	0	0	0
53	T	1	0	0	0	0
53	f	3	0	0	0	0
53	h	1	0	0	0	0
53	j	2	0	0	0	0
53	k	1	0	0	0	0
54	T	1	0	0	0	0
54	W	1	0	0	0	0
54	Z	1	0	0	0	0
54	b	1	0	0	0	0
54	c	1	0	0	0	0
54	e	2	0	0	0	0
55	f	10	0	19	0	0
All	All	150269	0	112534	143	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (143) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:16:ALA:O	15:O:20:GLY:HA3	1.69	0.90
15:O:16:ALA:O	15:O:20:GLY:CA	2.36	0.73
23:W:21:ARG:HE	23:W:39:TYR:HB2	1.58	0.69
50:O:26:PHE:HB2	50:O:87:VAL:HB	1.73	0.69
2:B:46[A]:GLU:HB3	2:B:49[A]:ARG:HG3	1.75	0.68
7:G:84:TYR:HB2	15:O:24:PRO:HD3	1.78	0.64
2:B:27[A]:LEU:HD21	2:B:102[A]:LEU:HB2	1.80	0.63
13:M:27:LYS:HB3	13:M:42:LEU:HB2	1.81	0.62
9:I:14:SER:O	9:I:81:GLN:NE2	2.33	0.62
6:F:80:ARG:HH21	6:F:87:THR:HG21	1.66	0.60
50:O:192:ASP:HB2	50:O:197:PHE:HE2	1.67	0.59
6:F:8:GLN:HB3	6:F:64:ILE:HD11	1.85	0.59
1:A:183:THR:HG22	1:A:187:ARG:HB2	1.85	0.59
21:U:5:LYS:HB2	21:U:8:GLU:HG2	1.84	0.58
6:F:77:VAL:HG22	6:F:126:VAL:HG23	1.85	0.58
50:O:43:LYS:HA	50:O:46:ARG:HG2	1.86	0.57
11:K:50:ALA:HB1	21:U:66:VAL:HG11	1.86	0.57
17:Q:4:LEU:O	17:Q:79:ARG:NH2	2.38	0.56
17:Q:55:LEU:HB2	17:Q:95:PRO:HD3	1.86	0.56
20:T:87:GLU:OE1	20:T:91:ARG:NH1	2.39	0.55
18:R:19:ARG:HD3	18:R:33:ARG:HB2	1.89	0.55
50:O:42:ARG:HG2	50:O:51:VAL:HG11	1.88	0.55
2:B:157[A]:GLU:OE1	2:B:160[A]:ARG:NH2	2.40	0.55
17:Q:9:THR:HG23	17:Q:109:VAL:HG23	1.88	0.54
14:N:95:SER:OG	14:N:98:THR:OG1	2.25	0.54
8:H:56:VAL:HG12	8:H:65:VAL:HG22	1.88	0.53
7:G:17:ARG:HG2	7:G:22:HIS:HA	1.90	0.53
10:J:6:ASP:OD1	10:J:32:GLN:N	2.40	0.53
2:B:75[A]:ALA:HB3	2:B:78[A]:ARG:HG2	1.91	0.53
6:F:96:ASP:OD1	6:F:97:VAL:N	2.38	0.52
2:B:61[A]:ALA:HA	2:B:70[A]:PRO:HD2	1.90	0.52
8:H:44:GLU:OE2	8:H:49:ASN:ND2	2.41	0.52
10:J:47:ARG:HH21	10:J:58:HIS:HB2	1.73	0.52
6:F:77:VAL:HG11	6:F:106:LEU:HD22	1.92	0.52
6:F:80:ARG:HB2	6:F:122:HIS:HB2	1.91	0.52
3:C:118:GLN:NE2	3:C:147:GLU:OE2	2.39	0.52
9:I:94:TYR:OH	10:J:41:LYS:NZ	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:36:LEU:O	4:D:40:THR:OG1	2.27	0.52
14:N:100:PRO:HG2	14:N:123:VAL:HG23	1.93	0.51
7:G:99:SER:HG	7:G:101:CYS:HG	1.57	0.51
7:G:136:ARG:HD2	7:G:139:ARG:HH12	1.74	0.51
1:A:103:GLU:HG3	1:A:160:GLU:HB2	1.93	0.50
15:O:23:LYS:HG3	15:O:24:PRO:HD2	1.93	0.50
3:C:107:LEU:HD12	3:C:152:GLU:HG3	1.92	0.50
2:B:74[A]:ARG:O	2:B:142[A]:SER:OG	2.23	0.50
17:Q:77:ARG:HD2	17:Q:89:LEU:HD13	1.94	0.49
3:C:60:PHE:HB3	3:C:64:ASN:HB3	1.93	0.49
2:B:46[A]:GLU:HG3	2:B:48[A]:PHE:H	1.77	0.49
16:P:30:THR:HG23	16:P:91:SER:HB2	1.95	0.49
6:F:155:ARG:HB2	6:F:172:TYR:HD1	1.77	0.49
16:P:9:SER:OG	16:P:10:ILE:N	2.39	0.49
14:N:94:ALA:HA	14:N:121:VAL:HG23	1.95	0.49
7:G:108:ARG:O	7:G:112:ASN:HB2	2.12	0.48
17:Q:80:ASN:OD1	17:Q:81:GLU:N	2.45	0.48
4:D:131:ALA:HB1	4:D:135:GLN:H	1.79	0.48
19:S:49:ILE:HD11	19:S:71:VAL:HG22	1.96	0.48
4:D:102:ALA:HA	4:D:122:ILE:O	2.14	0.48
13:M:133:LYS:HE3	13:M:135:ARG:HD3	1.96	0.48
6:F:93:GLU:HG3	6:F:140:VAL:HG11	1.95	0.48
13:M:23:VAL:HG12	13:M:45:GLY:HA3	1.94	0.47
3:C:22:LEU:HD12	3:C:146:ILE:HD12	1.97	0.47
17:Q:75:ILE:HG12	17:Q:93:VAL:HG22	1.96	0.47
4:D:19:PRO:HB3	4:D:53:PHE:HA	1.96	0.47
50:O:26:PHE:HZ	50:O:93:LEU:HA	1.80	0.47
9:I:18:PRO:HA	9:I:51:ALA:HA	1.97	0.47
5:E:21:LYS:HE3	5:E:55:VAL:HA	1.97	0.47
5:E:151:ARG:NH2	5:E:152:GLU:OE2	2.45	0.47
4:D:170:ARG:HD2	14:N:57:GLY:HA3	1.97	0.47
1:A:5:LYS:HE2	22:V:40:VAL:HG21	1.97	0.47
3:C:67:ILE:HD11	3:C:80:LYS:HB3	1.98	0.46
5:E:68:GLN:OE1	5:E:71:ARG:NH2	2.43	0.46
15:O:55:ALA:O	15:O:59:LYS:HB3	2.16	0.46
12:L:55:GLU:HB2	12:L:108:LYS:HB3	1.98	0.46
12:L:74:TYR:HB3	12:L:77:LYS:HB2	1.98	0.46
13:M:28:PRO:O	13:M:29:HIS:ND1	2.48	0.46
18:R:9:ILE:HG12	18:R:63:THR:HG23	1.97	0.46
2:B:39[A]:GLU:HG2	2:B:40[A]:GLU:HG2	1.97	0.46
18:R:60:ASN:HB3	18:R:63:THR:HB	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:96:LYS:HB2	14:N:96:LYS:HE2	1.70	0.46
1:A:159:ARG:HB3	1:A:164:LEU:HB2	1.98	0.45
6:F:22:PRO:O	7:G:146:ASN:ND2	2.38	0.45
13:M:22:LYS:NZ	13:M:132:SER:O	2.47	0.45
19:S:14:LEU:HD11	19:S:31:LYS:HB2	1.98	0.45
17:Q:44:MET:O	17:Q:77:ARG:NH1	2.49	0.45
22:V:53:TYR:HA	22:V:56:ARG:HG2	1.99	0.45
9:I:38:ALA:HB3	9:I:59:MET:HB2	1.99	0.44
24:X:10:GLN:HA	24:X:13:GLU:HG2	1.99	0.44
2:B:127[A]:LEU:HD22	6:F:156:VAL:HG13	2.00	0.44
6:F:80:ARG:HG3	6:F:124:LEU:HD21	1.99	0.44
6:F:80:ARG:HD2	7:G:155:PRO:HA	2.00	0.44
9:I:129:VAL:O	9:I:133:SER:HB3	2.17	0.44
14:N:36:GLY:HA3	14:N:40:HIS:CE1	2.53	0.44
50:0:45:LEU:HB3	50:0:49:ALA:HB3	1.99	0.44
17:Q:46:THR:HG22	17:Q:48:ASP:H	1.82	0.43
4:D:161:LYS:HA	4:D:161:LYS:HD3	1.82	0.43
8:H:20:SER:HA	8:H:23:THR:HG22	2.00	0.43
23:W:58:THR:OG1	23:W:59:THR:N	2.51	0.43
50:0:15:LEU:O	50:0:19:LEU:HG	2.18	0.43
9:I:117:PRO:HA	9:I:135:VAL:HG13	2.00	0.43
50:0:75:LYS:O	50:0:78:PRO:HD2	2.19	0.43
4:D:124:LEU:HD13	4:D:127:LEU:HD23	2.01	0.43
23:W:27:PHE:HA	23:W:34:CYS:HA	2.01	0.43
24:X:2:ALA:N	24:X:51:LEU:O	2.51	0.43
1:A:68:ARG:HA	1:A:98:LEU:HD21	2.01	0.43
1:A:158:HIS:HB3	1:A:161:ALA:HB3	2.00	0.43
3:C:56:ARG:NH2	3:C:75:GLU:OE2	2.51	0.43
2:B:54[A]:TYR:OH	2:B:73[A]:PHE:O	2.37	0.43
5:E:102:LEU:HD22	5:E:138:LEU:HD22	2.01	0.43
18:R:3:SER:OG	18:R:4:LEU:N	2.51	0.43
3:C:179:GLN:HA	3:C:182:ILE:HG22	2.00	0.42
9:I:80:ARG:HB2	9:I:99:ALA:HB3	2.00	0.42
12:L:86:THR:OG1	12:L:94:SER:OG	2.36	0.42
6:F:95:ARG:HB2	6:F:140:VAL:HG23	2.00	0.42
50:0:14:LYS:HE3	50:0:52:LEU:HD11	2.00	0.42
50:0:70:LEU:HB3	50:0:73:PHE:CD1	2.55	0.42
21:U:78:LYS:HA	21:U:81:ARG:HG2	2.00	0.42
6:F:32:SER:HB2	6:F:36:ILE:HD12	2.01	0.42
8:H:41:ILE:HG21	8:H:54:VAL:HG21	2.02	0.42
24:X:33:LYS:HA	24:X:33:LYS:HD3	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:0:67:LEU:HD22	50:0:67:LEU:HA	1.85	0.42
3:C:182:ILE:HD12	3:C:182:ILE:HA	1.85	0.42
16:P:73:GLY:N	16:P:76:GLU:OE2	2.42	0.42
20:T:95:ILE:HD13	20:T:95:ILE:HG21	1.81	0.42
3:C:116:HIS:HB3	3:C:149:VAL:HB	2.02	0.41
1:A:98:LEU:HD22	1:A:128:LYS:HD2	2.02	0.41
7:G:102:ARG:HD2	7:G:102:ARG:HA	1.77	0.41
12:L:63:LYS:HA	12:L:63:LYS:HD3	1.92	0.41
3:C:122:ALA:HB3	3:C:143:PRO:HB2	2.01	0.41
22:V:5:THR:HG23	22:V:12:ASN:HB2	2.03	0.41
2:B:8[A]:VAL:HG12	2:B:117[A]:ARG:HG3	2.03	0.41
3:C:131:ARG:HG3	3:C:137:ASN:ND2	2.36	0.41
5:E:7:GLN:NE2	5:E:35:ALA:O	2.53	0.41
14:N:75:LEU:HD23	14:N:75:LEU:HA	1.92	0.41
1:A:9:GLU:HG3	22:V:44:VAL:HG21	2.03	0.41
2:B:121[A]:PRO:HA	2:B:124[A]:LEU:HD12	2.03	0.41
17:Q:20:LEU:HD11	17:Q:32:ALA:HB2	2.03	0.41
18:R:4:LEU:HD12	18:R:5:PRO:HD2	2.01	0.41
2:B:189[A]:ASP:OD1	2:B:190[A]:VAL:N	2.53	0.40
1:A:18:VAL:HG13	1:A:19:LEU:HD12	2.02	0.40
20:T:93:PHE:HD2	20:T:94:LEU:HD22	1.86	0.40
5:E:31:GLU:HA	5:E:34:GLN:HB2	2.03	0.40
23:W:43:LYS:HB2	23:W:43:LYS:HE3	1.91	0.40
7:G:73:GLY:HA2	7:G:89:LEU:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [\(i\)](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	201/204 (98%)	190 (94%)	11 (6%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	195/199 (98%)	192 (98%)	3 (2%)	0	100	100
3	C	181/184 (98%)	172 (95%)	9 (5%)	0	100	100
4	D	183/186 (98%)	176 (96%)	7 (4%)	0	100	100
5	E	154/189 (82%)	151 (98%)	3 (2%)	0	100	100
6	F	169/172 (98%)	163 (96%)	6 (4%)	0	100	100
7	G	157/160 (98%)	149 (95%)	8 (5%)	0	100	100
8	H	98/121 (81%)	93 (95%)	5 (5%)	0	100	100
9	I	134/137 (98%)	132 (98%)	2 (2%)	0	100	100
10	J	61/155 (39%)	61 (100%)	0	0	100	100
11	K	119/142 (84%)	118 (99%)	1 (1%)	0	100	100
12	L	123/127 (97%)	119 (97%)	4 (3%)	0	100	100
13	M	133/136 (98%)	126 (95%)	7 (5%)	0	100	100
14	N	146/149 (98%)	136 (93%)	10 (7%)	0	100	100
15	O	56/59 (95%)	52 (93%)	3 (5%)	1 (2%)	8	16
16	P	94/105 (90%)	93 (99%)	1 (1%)	0	100	100
17	Q	107/113 (95%)	98 (92%)	9 (8%)	0	100	100
18	R	125/130 (96%)	123 (98%)	2 (2%)	0	100	100
19	S	104/107 (97%)	101 (97%)	3 (3%)	0	100	100
20	T	110/121 (91%)	108 (98%)	2 (2%)	0	100	100
21	U	117/120 (98%)	112 (96%)	5 (4%)	0	100	100
22	V	97/100 (97%)	93 (96%)	4 (4%)	0	100	100
23	W	79/88 (90%)	75 (95%)	4 (5%)	0	100	100
24	X	75/78 (96%)	74 (99%)	1 (1%)	0	100	100
25	Y	48/51 (94%)	46 (96%)	2 (4%)	0	100	100
26	Z	50/128 (39%)	47 (94%)	3 (6%)	0	100	100
27	b	101/106 (95%)	95 (94%)	6 (6%)	0	100	100
28	c	89/92 (97%)	85 (96%)	4 (4%)	0	100	100
29	d	20/25 (80%)	19 (95%)	1 (5%)	0	100	100
33	j	244/254 (96%)	226 (93%)	18 (7%)	0	100	100
34	k	384/387 (99%)	363 (94%)	21 (6%)	0	100	100
35	l	359/362 (99%)	329 (92%)	29 (8%)	1 (0%)	41	64

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	m	292/297 (98%)	277 (95%)	15 (5%)	0	100	100
37	n	163/176 (93%)	155 (95%)	8 (5%)	0	100	100
38	o	220/244 (90%)	207 (94%)	13 (6%)	0	100	100
39	p	231/256 (90%)	220 (95%)	11 (5%)	0	100	100
40	q	189/191 (99%)	174 (92%)	14 (7%)	1 (0%)	29	52
41	r	216/221 (98%)	206 (95%)	10 (5%)	0	100	100
42	s	167/174 (96%)	161 (96%)	5 (3%)	1 (1%)	25	47
43	t	191/199 (96%)	174 (91%)	16 (8%)	1 (0%)	29	52
44	u	134/138 (97%)	125 (93%)	9 (7%)	0	100	100
45	a	842/1038 (81%)	827 (98%)	15 (2%)	0	100	100
46	e	1519/1562 (97%)	1497 (99%)	20 (1%)	2 (0%)	51	75
47	g	223/245 (91%)	215 (96%)	8 (4%)	0	100	100
49	z	144/165 (87%)	135 (94%)	7 (5%)	2 (1%)	11	22
50	0	117/312 (38%)	116 (99%)	0	1 (1%)	17	35
52	w	214/217 (99%)	211 (99%)	3 (1%)	0	100	100
All	All	9175/10122 (91%)	8817 (96%)	348 (4%)	10 (0%)	54	75

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
49	z	88	PRO
46	e	437	LYS
46	e	855	PRO
35	l	4	PRO
40	q	107	ASP
42	s	108	GLU
50	0	93	LEU
15	O	21	ILE
43	t	47	ALA
49	z	55	GLY

5.3.2 Protein sidechains [i](#)

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	A	175/176 (99%)	175 (100%)	0	100	100
2	B	160/162 (99%)	160 (100%)	0	100	100
3	C	138/146 (94%)	138 (100%)	0	100	100
4	D	150/151 (99%)	149 (99%)	1 (1%)	84	94
5	E	129/154 (84%)	129 (100%)	0	100	100
6	F	155/156 (99%)	155 (100%)	0	100	100
7	G	135/137 (98%)	134 (99%)	1 (1%)	84	94
8	H	87/107 (81%)	87 (100%)	0	100	100
9	I	104/105 (99%)	104 (100%)	0	100	100
10	J	54/129 (42%)	54 (100%)	0	100	100
11	K	104/118 (88%)	104 (100%)	0	100	100
12	L	108/110 (98%)	108 (100%)	0	100	100
13	M	112/116 (97%)	112 (100%)	0	100	100
14	N	117/119 (98%)	117 (100%)	0	100	100
15	O	46/47 (98%)	45 (98%)	1 (2%)	52	76
16	P	81/88 (92%)	81 (100%)	0	100	100
17	Q	92/97 (95%)	92 (100%)	0	100	100
18	R	107/111 (96%)	107 (100%)	0	100	100
19	S	90/91 (99%)	90 (100%)	0	100	100
20	T	95/103 (92%)	94 (99%)	1 (1%)	73	88
21	U	104/105 (99%)	104 (100%)	0	100	100
22	V	80/82 (98%)	80 (100%)	0	100	100
23	W	67/71 (94%)	67 (100%)	0	100	100
24	X	68/69 (99%)	66 (97%)	2 (3%)	42	68
25	Y	45/46 (98%)	45 (100%)	0	100	100
26	Z	45/116 (39%)	45 (100%)	0	100	100
27	b	87/91 (96%)	87 (100%)	0	100	100
28	c	71/72 (99%)	71 (100%)	0	100	100
29	d	20/23 (87%)	20 (100%)	0	100	100
33	j	189/196 (96%)	189 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
34	k	320/323 (99%)	318 (99%)	2 (1%)	86	95
35	l	288/289 (100%)	288 (100%)	0	100	100
36	m	241/245 (98%)	241 (100%)	0	100	100
37	n	139/155 (90%)	138 (99%)	1 (1%)	84	94
38	o	186/205 (91%)	186 (100%)	0	100	100
39	p	187/208 (90%)	187 (100%)	0	100	100
40	q	168/171 (98%)	168 (100%)	0	100	100
41	r	185/187 (99%)	183 (99%)	2 (1%)	73	88
42	s	145/150 (97%)	145 (100%)	0	100	100
43	t	154/159 (97%)	154 (100%)	0	100	100
44	u	107/109 (98%)	107 (100%)	0	100	100
45	a	677/949 (71%)	676 (100%)	1 (0%)	93	98
46	e	1151/1451 (79%)	1093 (95%)	58 (5%)	24	47
47	g	180/211 (85%)	180 (100%)	0	100	100
50	o	104/254 (41%)	95 (91%)	9 (9%)	10	20
52	w	197/198 (100%)	196 (100%)	1 (0%)	88	96
All	All	7444/8558 (87%)	7364 (99%)	80 (1%)	74	88

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	D	12	ARG
7	G	83	ARG
15	O	33	LYS
20	T	106	LYS
24	X	9	LYS
24	X	63	LYS
34	k	332	ARG
34	k	369	ARG
37	n	8	LYS
41	r	112	GLN
41	r	144	ASN
45	a	98	ASP
46	e	8	THR
46	e	105	VAL
46	e	125	ILE

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Mol	Chain	Res	Type
46	e	169	LEU
46	e	205	GLU
46	e	254	ASN
46	e	271	LEU
46	e	277	MET
46	e	299	THR
46	e	309	VAL
46	e	319	THR
46	e	327	THR
46	e	364	SER
46	e	400	GLU
46	e	707	LYS
46	e	710	LYS
46	e	731	LEU
46	e	733	HIS
46	e	754	ILE
46	e	770	ILE
46	e	780	ILE
46	e	797	LEU
46	e	799	THR
46	e	807	LYS
46	e	826	LEU
46	e	867	PHE
46	e	904	VAL
46	e	910	SER
46	e	924	VAL
46	e	933	LEU
46	e	978	THR
46	e	989	GLU
46	e	1032	LEU
46	e	1059	LEU
46	e	1102	CYS
46	e	1149	THR
46	e	1164	LEU
46	e	1175	PHE
46	e	1179	LEU
46	e	1189	ASN
46	e	1239	LYS
46	e	1269	LEU
46	e	1286	MET
46	e	1300	ILE
46	e	1303	MET

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Mol	Chain	Res	Type
46	e	1341	LYS
46	e	1342	GLU
46	e	1367	THR
46	e	1379	LEU
46	e	1384	GLU
46	e	1400	PHE
46	e	1407	MET
46	e	1421	LEU
46	e	1428	VAL
46	e	1454	ILE
46	e	1464	ILE
46	e	1490	SER
46	e	1555	ARG
50	0	30	VAL
50	0	51	VAL
50	0	52	LEU
50	0	67	LEU
50	0	76	LEU
50	0	80	VAL
50	0	93	LEU
50	0	95	GLU
50	0	189	GLN
52	w	98	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
45	a	599	GLN
46	e	160	ASN
46	e	189	ASN
46	e	226	ASN
46	e	233	ASN
46	e	251	ASN
46	e	397	ASN
46	e	805	ASN
46	e	902	ASN
46	e	1141	GLN
46	e	1288	GLN
46	e	1455	GLN
46	e	1457	ASN
46	e	1477	GLN
46	e	1499	HIS

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Mol	Chain	Res	Type
46	e	1501	GLN
47	g	9	ASN
50	0	36	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
30	f	3211/3395 (94%)	600 (18%)	0
31	h	120/121 (99%)	12 (10%)	0
32	i	157/158 (99%)	32 (20%)	0
48	x	72/76 (94%)	26 (36%)	0
48	y	71/76 (93%)	26 (36%)	0
All	All	3631/3826 (94%)	696 (19%)	0

All (696) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
30	f	6	A
30	f	13	A
30	f	14	U
30	f	26	A
30	f	40	A
30	f	43	A
30	f	49	A
30	f	59	G
30	f	60	A
30	f	65	A
30	f	66	A
30	f	92	G
30	f	99	A
30	f	109	A
30	f	110	G
30	f	111	C
30	f	116	A
30	f	120	G
30	f	121	A
30	f	122	A
30	f	133	U
30	f	134	U
30	f	135	C
30	f	136	G

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Mol	Chain	Res	Type
30	f	156	G
30	f	157	A
30	f	165	A
30	f	166	C
30	f	172	G
30	f	173	G
30	f	187	A
30	f	190	U
30	f	191	U
30	f	200	C
30	f	206	G
30	f	210	U
30	f	211	A
30	f	213	A
30	f	218	G
30	f	219	A
30	f	234	G
30	f	240	U
30	f	241	G
30	f	242	C
30	f	243	G
30	f	245	U
30	f	249	U
30	f	252	U
30	f	269	G
30	f	283	G
30	f	286	U
30	f	295	A
30	f	305	U
30	f	323	A
30	f	329	U
30	f	339	C
30	f	350	C
30	f	374	A
30	f	376	G
30	f	398	A
30	f	399	A
30	f	401	U
30	f	402	A
30	f	403	C
30	f	421	G
30	f	422	A

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Mol	Chain	Res	Type
30	f	439	C
30	f	440	A
30	f	441	U
30	f	442	G
30	f	443	G
30	f	445	G
30	f	446	U
30	f	447	U
30	f	448	U
30	f	450	G
30	f	487	U
30	f	488	U
30	f	489	U
30	f	490	C
30	f	494	G
30	f	518	G
30	f	520	U
30	f	521	A
30	f	523	A
30	f	535	G
30	f	536	U
30	f	543	C
30	f	544	C
30	f	546	C
30	f	547	G
30	f	548	G
30	f	551	A
30	f	552	G
30	f	555	U
30	f	557	A
30	f	559	A
30	f	578	A
30	f	579	G
30	f	589	A
30	f	597	G
30	f	604	G
30	f	608	A
30	f	609	G
30	f	611	A
30	f	620	U
30	f	621	A
30	f	622	A

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Mol	Chain	Res	Type
30	f	637	C
30	f	638	C
30	f	649	A
30	f	660	A
30	f	677	A
30	f	681	U
30	f	684	G
30	f	690	A
30	f	691	A
30	f	705	A
30	f	712	G
30	f	715	A
30	f	716	A
30	f	719	U
30	f	720	A
30	f	758	C
30	f	763	G
30	f	764	U
30	f	765	C
30	f	766	U
30	f	767	U
30	f	776	U
30	f	777	U
30	f	780	A
30	f	781	G
30	f	785	G
30	f	786	A
30	f	806	A
30	f	817	A
30	f	830	A
30	f	846	A
30	f	849	C
30	f	850	U
30	f	861	C
30	f	874	U
30	f	879	U
30	f	896	A
30	f	907	G
30	f	908	G
30	f	914	A
30	f	916	G
30	f	917	A

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Mol	Chain	Res	Type
30	f	920	A
30	f	921	A
30	f	924	G
30	f	925	A
30	f	937	G
30	f	944	C
30	f	959	C
30	f	960	U
30	f	981	U
30	f	982	C
30	f	991	G
30	f	994	G
30	f	1001	G
30	f	1002	A
30	f	1010	G
30	f	1015	U
30	f	1016	C
30	f	1017	C
30	f	1018	G
30	f	1021	G
30	f	1024	G
30	f	1025	A
30	f	1028	U
30	f	1036	A
30	f	1041	U
30	f	1047	A
30	f	1049	C
30	f	1063	G
30	f	1064	A
30	f	1065	A
30	f	1072	G
30	f	1081	U
30	f	1087	G
30	f	1093	A
30	f	1094	U
30	f	1095	U
30	f	1097	G
30	f	1098	A
30	f	1103	A
30	f	1104	G
30	f	1117	G
30	f	1131	G

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Mol	Chain	Res	Type
30	f	1144	U
30	f	1153	A
30	f	1159	A
30	f	1160	C
30	f	1177	G
30	f	1180	A
30	f	1181	U
30	f	1192	C
30	f	1193	A
30	f	1196	C
30	f	1197	A
30	f	1201	C
30	f	1202	A
30	f	1208	U
30	f	1217	A
30	f	1218	U
30	f	1219	C
30	f	1222	G
30	f	1225	A
30	f	1227	C
30	f	1235	U
30	f	1236	G
30	f	1238	C
30	f	1241	U
30	f	1242	G
30	f	1244	A
30	f	1245	A
30	f	1251	A
30	f	1252	A
30	f	1254	C
30	f	1258	U
30	f	1259	A
30	f	1263	A
30	f	1264	G
30	f	1265	U
30	f	1269	U
30	f	1272	C
30	f	1277	C
30	f	1278	A
30	f	1279	C
30	f	1282	G
30	f	1285	G

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Mol	Chain	Res	Type
30	f	1286	A
30	f	1287	A
30	f	1295	G
30	f	1307	G
30	f	1308	A
30	f	1309	U
30	f	1313	G
30	f	1330	A
30	f	1348	U
30	f	1349	G
30	f	1351	U
30	f	1352	A
30	f	1354	G
30	f	1355	A
30	f	1356	U
30	f	1357	G
30	f	1386	A
30	f	1392	G
30	f	1399	A
30	f	1400	G
30	f	1419	A
30	f	1434	G
30	f	1437	C
30	f	1446	A
30	f	1450	G
30	f	1481	A
30	f	1482	A
30	f	1483	G
30	f	1487	G
30	f	1488	G
30	f	1502	C
30	f	1508	C
30	f	1536	G
30	f	1539	A
30	f	1555	U
30	f	1556	C
30	f	1557	A
30	f	1560	G
30	f	1562	C
30	f	1563	C
30	f	1566	A
30	f	1568	U

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Mol	Chain	Res	Type
30	f	1569	U
30	f	1572	U
30	f	1573	G
30	f	1575	A
30	f	1576	G
30	f	1580	A
30	f	1581	C
30	f	1582	C
30	f	1583	A
30	f	1589	A
30	f	1590	G
30	f	1605	A
30	f	1607	U
30	f	1620	U
30	f	1629	U
30	f	1639	C
30	f	1642	A
30	f	1643	A
30	f	1645	U
30	f	1657	C
30	f	1683	A
30	f	1716	U
30	f	1717	U
30	f	1724	U
30	f	1725	C
30	f	1736	G
30	f	1741	A
30	f	1750	A
30	f	1751	G
30	f	1760	A
30	f	1761	C
30	f	1764	U
30	f	1765	U
30	f	1766	G
30	f	1770	G
30	f	1775	G
30	f	1780	G
30	f	1797	A
30	f	1814	A
30	f	1816	A
30	f	1819	U
30	f	1820	U

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Mol	Chain	Res	Type
30	f	1821	U
30	f	1835	A
30	f	1839	A
30	f	1840	U
30	f	1841	A
30	f	1842	A
30	f	1846	C
30	f	1849	C
30	f	1850	A
30	f	1866	C
30	f	1867	A
30	f	1880	U
30	f	1881	A
30	f	1893	A
30	f	1906	G
30	f	1943	C
30	f	1952	G
30	f	1953	G
30	f	1954	G
30	f	2094	C
30	f	2101	C
30	f	2102	U
30	f	2111	G
30	f	2112	U
30	f	2113	A
30	f	2114	C
30	f	2121	G
30	f	2122	G
30	f	2131	A
30	f	2134	G
30	f	2140	U
30	f	2144	A
30	f	2158	A
30	f	2160	G
30	f	2169	G
30	f	2176	U
30	f	2201	G
30	f	2206	G
30	f	2207	A
30	f	2208	A
30	f	2209	U
30	f	2222	A

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Mol	Chain	Res	Type
30	f	2223	A
30	f	2225	U
30	f	2228	A
30	f	2251	G
30	f	2252	A
30	f	2267	C
30	f	2272	G
30	f	2273	G
30	f	2274	U
30	f	2281	A
30	f	2282	U
30	f	2288	G
30	f	2307	G
30	f	2308	C
30	f	2310	U
30	f	2313	A
30	f	2314	U
30	f	2315	G
30	f	2334	U
30	f	2335	G
30	f	2336	U
30	f	2373	A
30	f	2374	C
30	f	2375	G
30	f	2385	G
30	f	2388	U
30	f	2393	G
30	f	2397	A
30	f	2402	A
30	f	2403	G
30	f	2404	A
30	f	2411	U
30	f	2419	A
30	f	2435	G
30	f	2437	G
30	f	2439	A
30	f	2440	G
30	f	2445	A
30	f	2446	U
30	f	2447	A
30	f	2448	G
30	f	2449	A

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Mol	Chain	Res	Type
30	f	2450	G
30	f	2451	G
30	f	2452	G
30	f	2453	U
30	f	2460	U
30	f	2461	A
30	f	2465	G
30	f	2468	A
30	f	2469	G
30	f	2471	U
30	f	2473	C
30	f	2474	G
30	f	2476	C
30	f	2479	C
30	f	2480	A
30	f	2482	U
30	f	2484	A
30	f	2486	A
30	f	2487	U
30	f	2494	A
30	f	2495	C
30	f	2499	U
30	f	2501	U
30	f	2503	G
30	f	2505	U
30	f	2506	U
30	f	2511	A
30	f	2514	U
30	f	2515	A
30	f	2522	G
30	f	2526	C
30	f	2531	C
30	f	2537	U
30	f	2538	U
30	f	2539	C
30	f	2540	A
30	f	2541	U
30	f	2542	U
30	f	2544	U
30	f	2547	A
30	f	2548	C
30	f	2549	G

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Mol	Chain	Res	Type
30	f	2552	C
30	f	2554	A
30	f	2555	G
30	f	2561	A
30	f	2569	A
30	f	2570	U
30	f	2571	U
30	f	2572	C
30	f	2573	G
30	f	2581	U
30	f	2585	G
30	f	2593	A
30	f	2594	C
30	f	2606	G
30	f	2607	G
30	f	2614	G
30	f	2648	G
30	f	2651	G
30	f	2652	U
30	f	2656	A
30	f	2674	A
30	f	2677	G
30	f	2678	A
30	f	2689	A
30	f	2691	A
30	f	2694	A
30	f	2696	A
30	f	2704	A
30	f	2714	G
30	f	2719	U
30	f	2728	G
30	f	2729	U
30	f	2740	A
30	f	2752	U
30	f	2753	G
30	f	2755	C
30	f	2772	C
30	f	2773	C
30	f	2777	G
30	f	2778	G
30	f	2788	C
30	f	2796	G

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Mol	Chain	Res	Type
30	f	2800	G
30	f	2801	A
30	f	2803	A
30	f	2810	C
30	f	2814	G
30	f	2817	A
30	f	2818	U
30	f	2821	C
30	f	2822	U
30	f	2842	U
30	f	2844	C
30	f	2845	A
30	f	2846	U
30	f	2849	C
30	f	2867	C
30	f	2871	G
30	f	2872	A
30	f	2887	A
30	f	2898	G
30	f	2899	C
30	f	2911	A
30	f	2914	G
30	f	2923	U
30	f	2935	U
30	f	2936	A
30	f	2941	A
30	f	2942	C
30	f	2947	G
30	f	2971	A
30	f	2983	C
30	f	2990	G
30	f	2992	U
30	f	2996	U
30	f	2997	G
30	f	3006	A
30	f	3012	A
30	f	3056	U
30	f	3059	G
30	f	3078	U
30	f	3079	U
30	f	3080	G
30	f	3086	A

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Mol	Chain	Res	Type
30	f	3092	C
30	f	3104	U
30	f	3113	A
30	f	3122	A
30	f	3130	A
30	f	3131	U
30	f	3142	A
30	f	3143	C
30	f	3151	U
30	f	3154	C
30	f	3155	U
30	f	3156	U
30	f	3157	U
30	f	3165	A
30	f	3170	A
30	f	3173	G
30	f	3174	A
30	f	3175	U
30	f	3176	G
30	f	3179	U
30	f	3181	C
30	f	3186	A
30	f	3187	A
30	f	3196	U
30	f	3207	U
30	f	3209	A
30	f	3217	C
30	f	3218	A
30	f	3219	G
30	f	3228	C
30	f	3229	G
30	f	3243	A
30	f	3245	A
30	f	3247	G
30	f	3259	U
30	f	3263	G
30	f	3269	U
30	f	3270	U
30	f	3273	A
30	f	3276	G
30	f	3281	U
30	f	3287	U

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Mol	Chain	Res	Type
30	f	3288	G
30	f	3289	G
30	f	3294	A
30	f	3295	A
30	f	3303	G
30	f	3304	U
30	f	3307	A
30	f	3313	U
30	f	3316	A
30	f	3317	U
30	f	3318	G
30	f	3319	U
30	f	3320	A
30	f	3341	U
30	f	3342	A
30	f	3345	G
30	f	3351	U
30	f	3352	U
30	f	3353	G
30	f	3354	U
30	f	3355	U
30	f	3369	G
30	f	3375	A
30	f	3378	C
30	f	3382	U
30	f	3383	G
30	f	3386	G
30	f	3389	U
30	f	3390	G
30	f	3396	U
31	h	7	G
31	h	29	C
31	h	53	U
31	h	54	U
31	h	55	A
31	h	65	G
31	h	73	C
31	h	74	C
31	h	95	A
31	h	102	A
31	h	112	G
31	h	121	U

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Mol	Chain	Res	Type
32	i	23	U
32	i	34	U
32	i	35	C
32	i	39	G
32	i	48	A
32	i	52	A
32	i	53	A
32	i	59	A
32	i	62	C
32	i	63	G
32	i	80	A
32	i	81	U
32	i	82	U
32	i	83	C
32	i	84	C
32	i	85	G
32	i	86	U
32	i	87	G
32	i	90	U
32	i	95	G
32	i	104	A
32	i	105	A
32	i	106	C
32	i	111	A
32	i	113	U
32	i	125	U
32	i	126	A
32	i	138	A
32	i	151	C
32	i	152	G
32	i	157	U
32	i	158	U
48	x	5	G
48	x	7	G
48	x	10	G
48	x	13	U
48	x	16	U
48	x	17	C
48	x	18	G
48	x	22	G
48	x	28	U
48	x	33	U

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Mol	Chain	Res	Type
48	x	34	A
48	x	35	G
48	x	36	C
48	x	37	A
48	x	38	U
48	x	42	A
48	x	43	G
48	x	46	G
48	x	48	C
48	x	49	U
48	x	56	C
48	x	57	G
48	x	58	A
48	x	60	U
48	x	61	C
48	x	74	C
48	y	5	G
48	y	7	G
48	y	8	U
48	y	9	G
48	y	13	U
48	y	16	U
48	y	17	C
48	y	22	G
48	y	23	C
48	y	36	C
48	y	38	U
48	y	43	G
48	y	44	A
48	y	46	G
48	y	47	U
48	y	48	C
48	y	51	C
48	y	52	G
48	y	53	G
48	y	56	C
48	y	57	G
48	y	58	A
48	y	59	U
48	y	61	C
48	y	75	C
48	y	76	A

There are no RNA pucker outliers to report.

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 21 ligands modelled in this entry, 20 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
55	SPD	f	3401	-	9,9,9	0.32	0	8,8,8	0.86	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
55	SPD	f	3401	-	-	5/7/7/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
55	f	3401	SPD	C3-C4-C5-N6

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Mol	Chain	Res	Type	Atoms
55	f	3401	SPD	N6-C7-C8-C9
55	f	3401	SPD	C2-C3-C4-C5
55	f	3401	SPD	C8-C7-N6-C5
55	f	3401	SPD	C4-C5-N6-C7

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 [i](#)

There are no chain breaks in this entry.

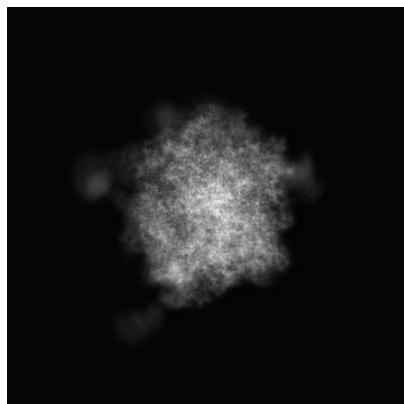
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-15426. These allow visual inspection of the internal detail of the map and identification of artifacts.

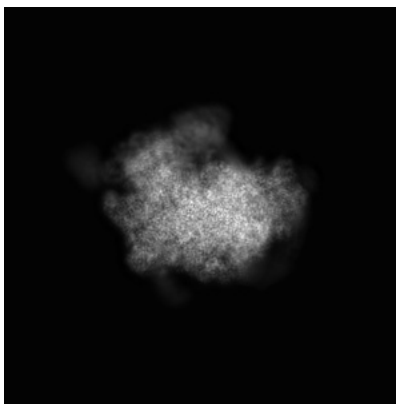
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

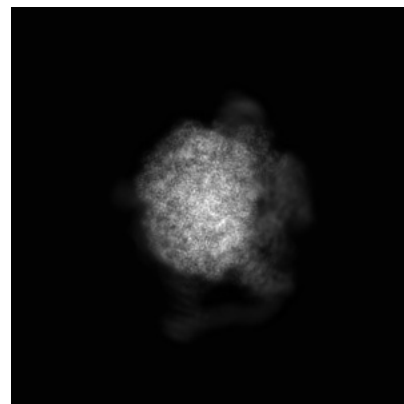
6.1.1 Primary map



X

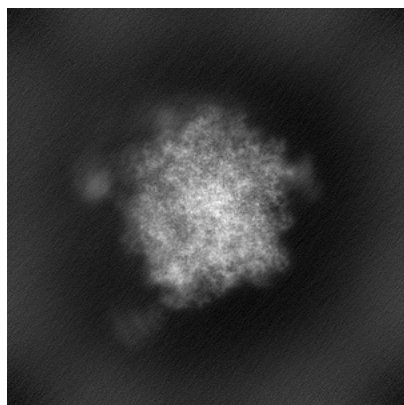


Y

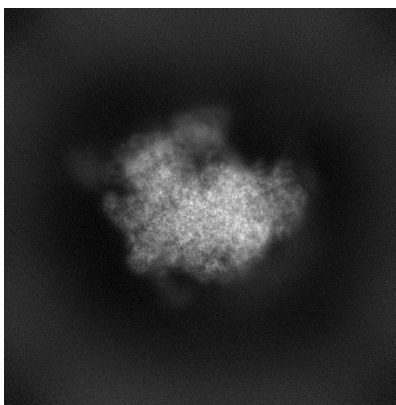


Z

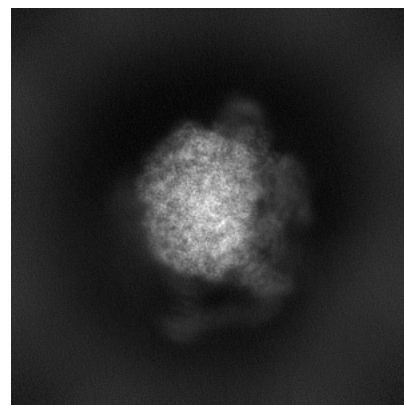
6.1.2 Raw map



X



Y

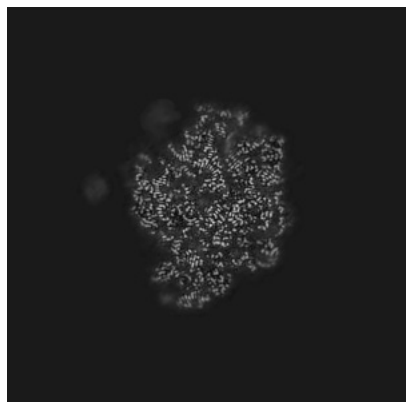


Z

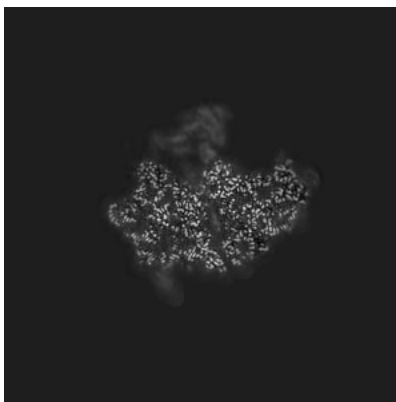
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

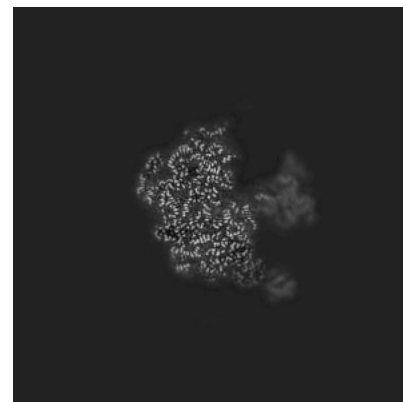
6.2.1 Primary map



X Index: 225

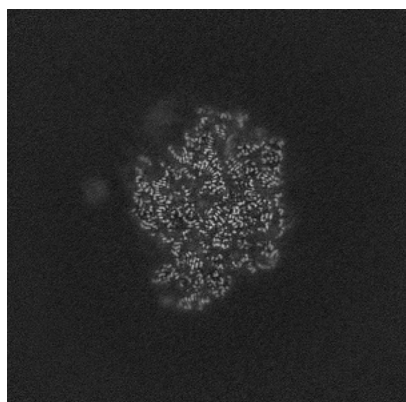


Y Index: 225

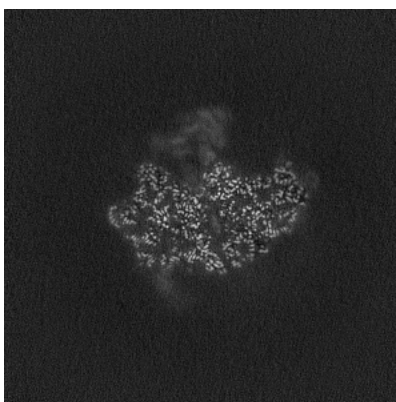


Z Index: 225

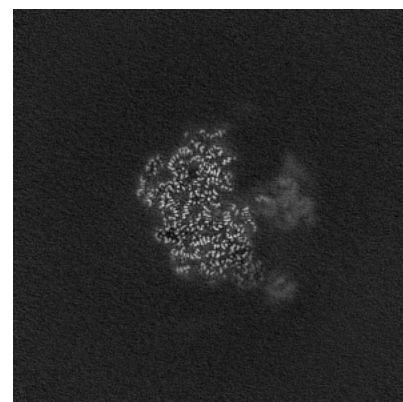
6.2.2 Raw map



X Index: 225



Y Index: 225

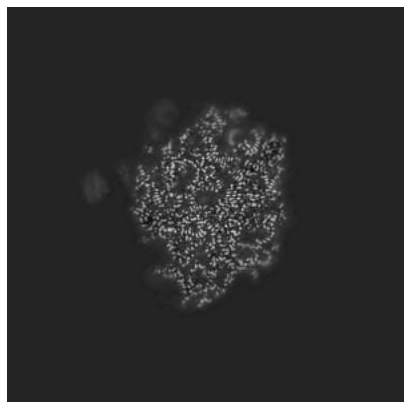


Z Index: 225

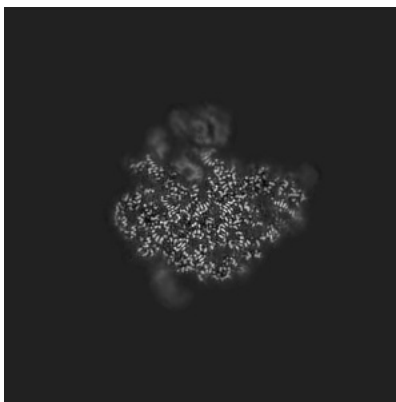
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

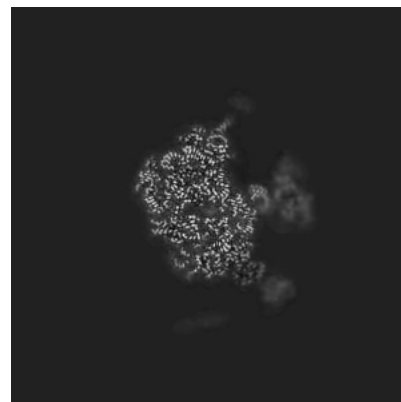
6.3.1 Primary map



X Index: 219

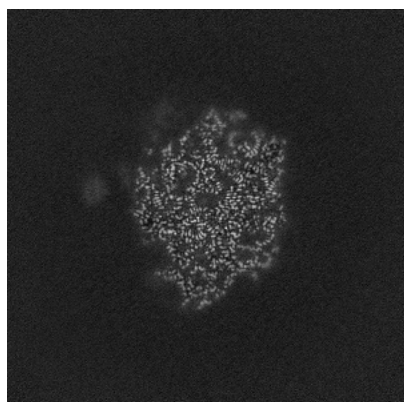


Y Index: 237

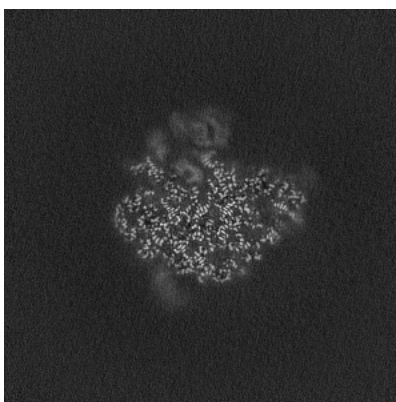


Z Index: 230

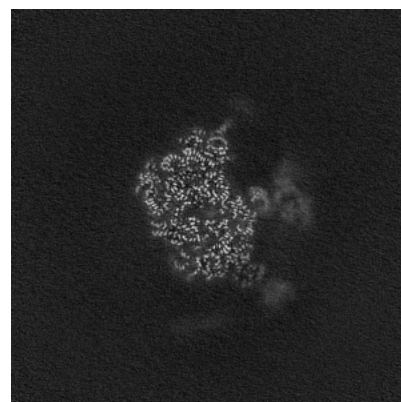
6.3.2 Raw map



X Index: 219



Y Index: 237

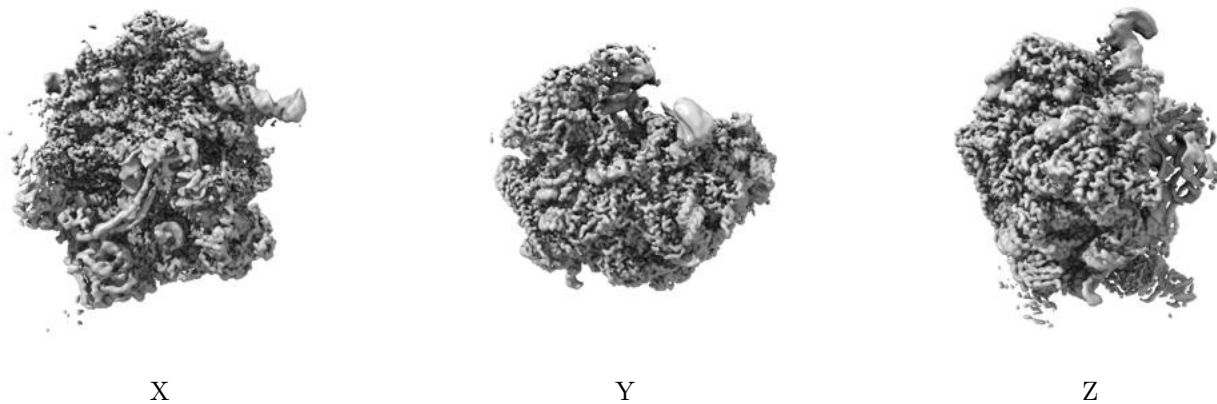


Z Index: 230

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

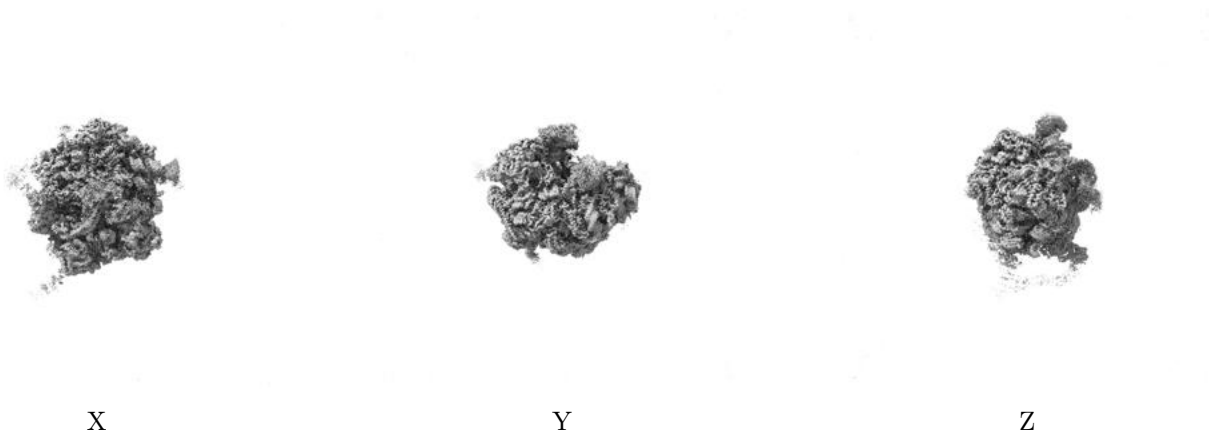
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.55. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



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

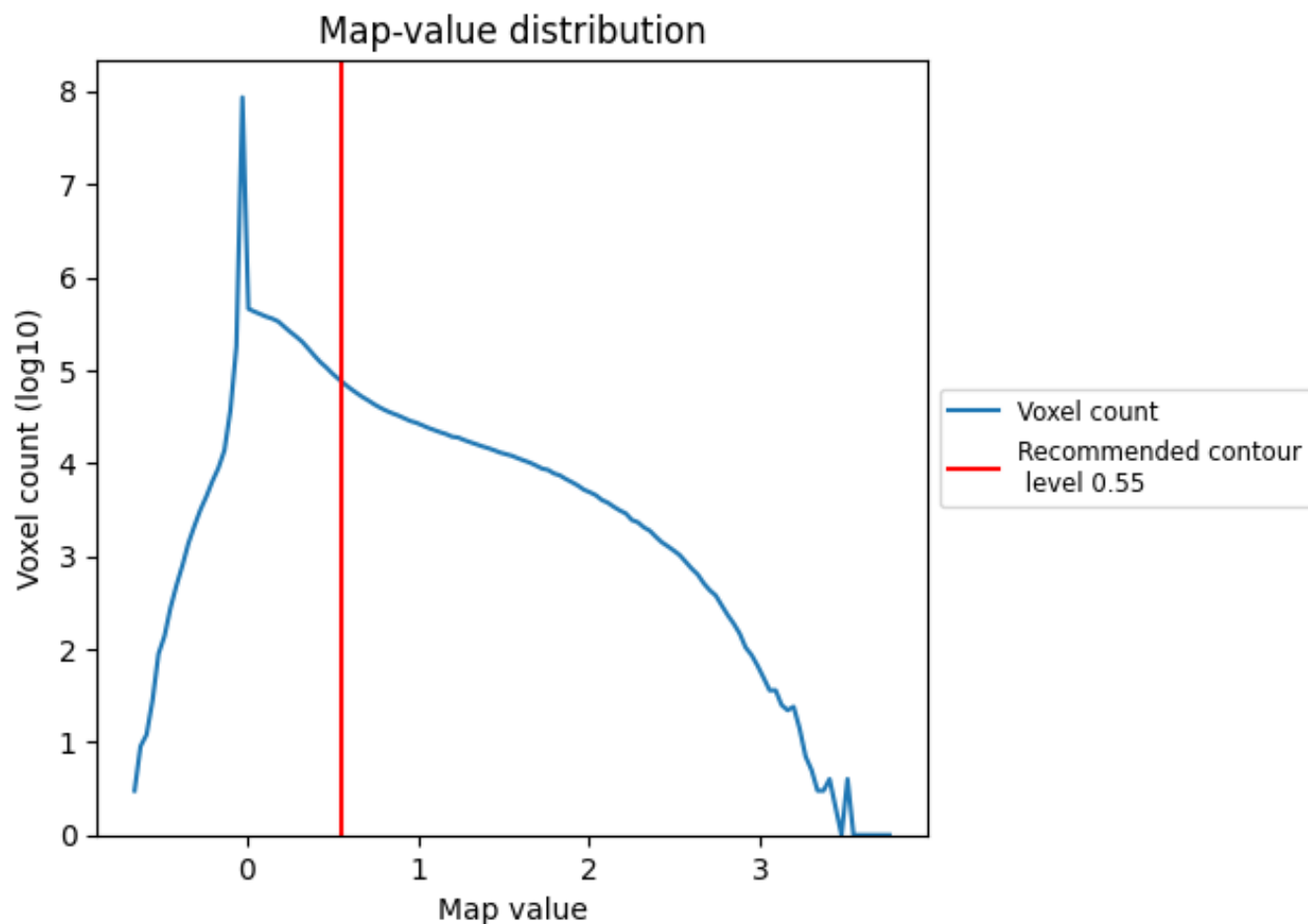
6.5 Mask visualisation [i](#)

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

7 Map analysis [i](#)

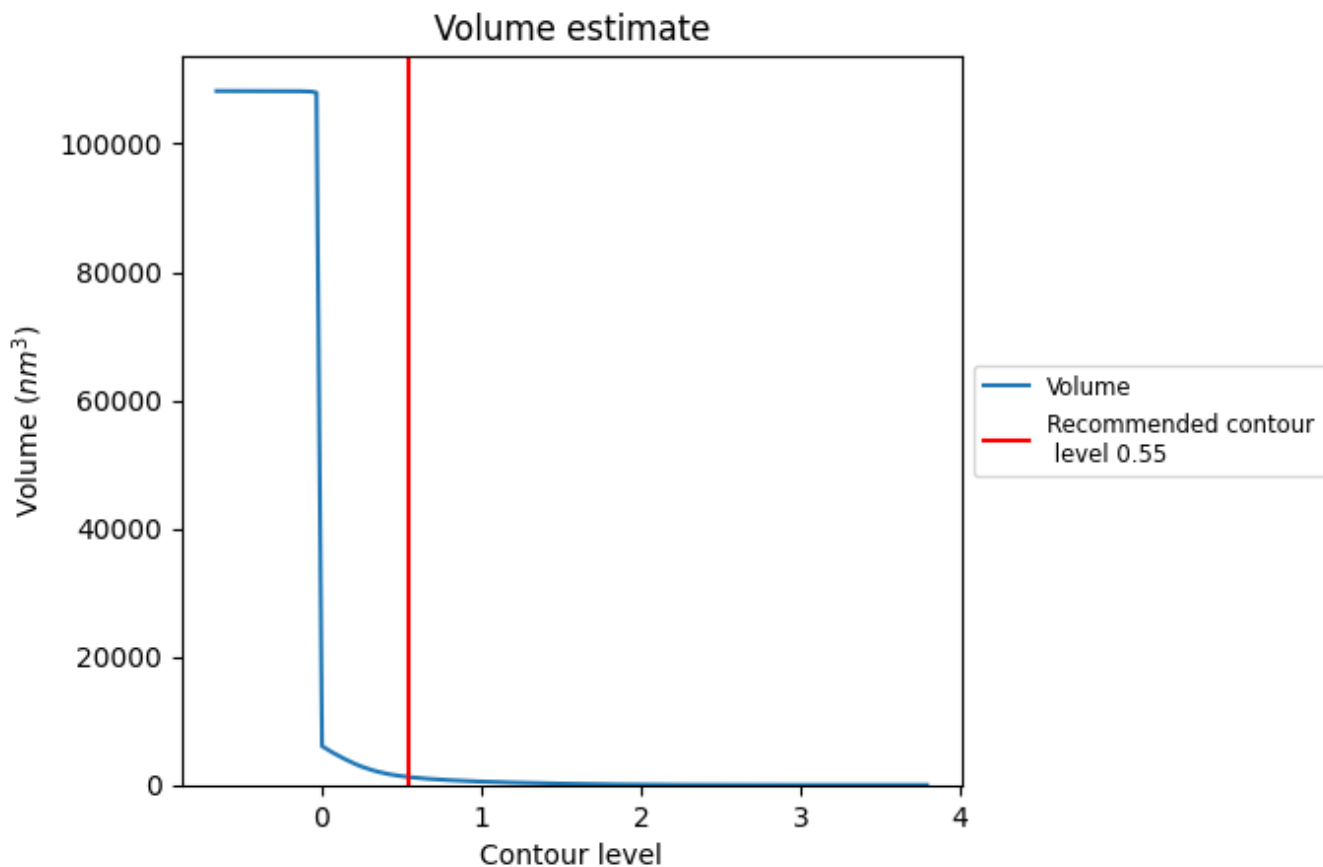
This section contains the results of statistical analysis of the map.

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.

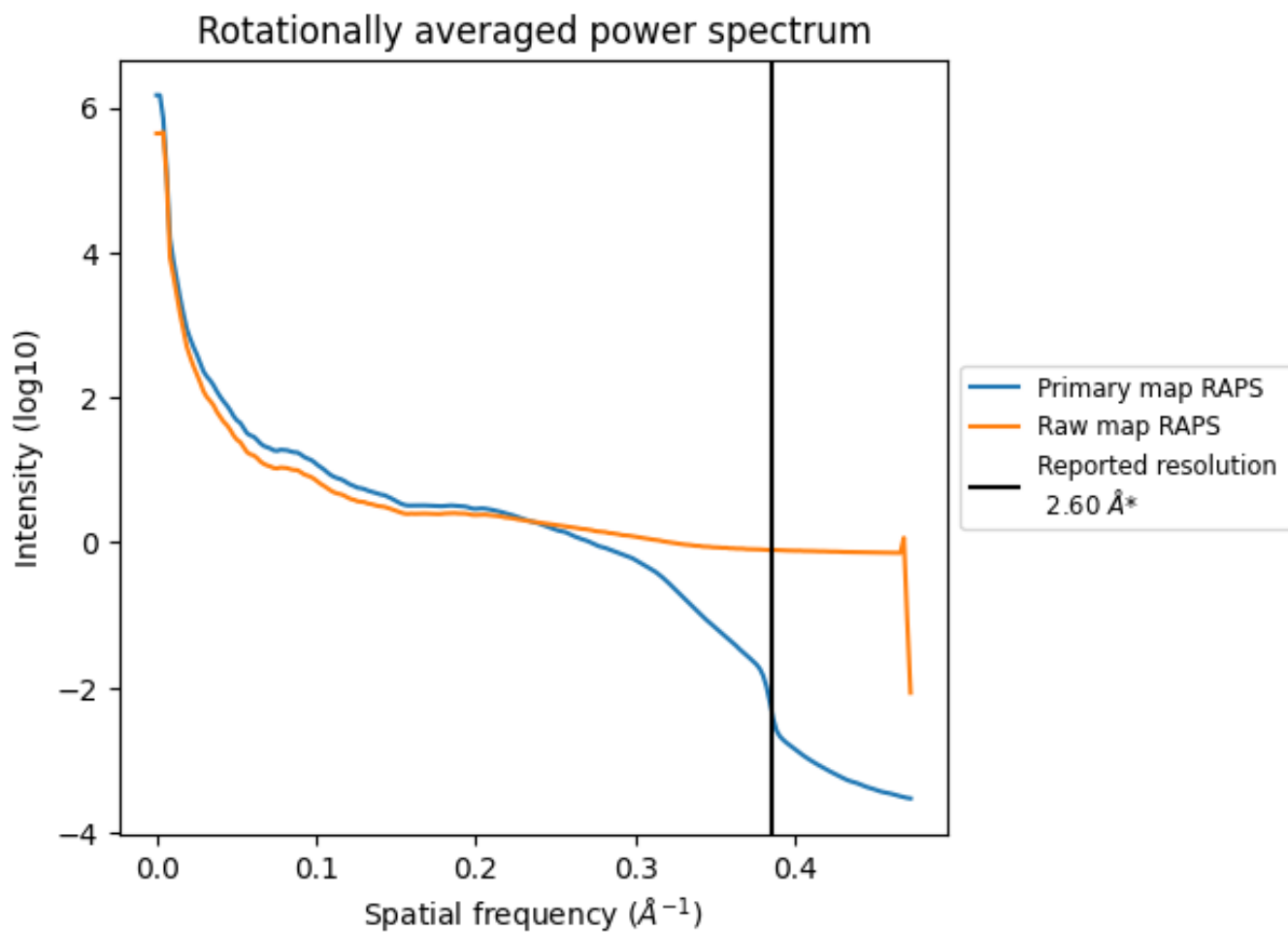
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 1231 nm^3 ; this corresponds to an approximate mass of 1112 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 i

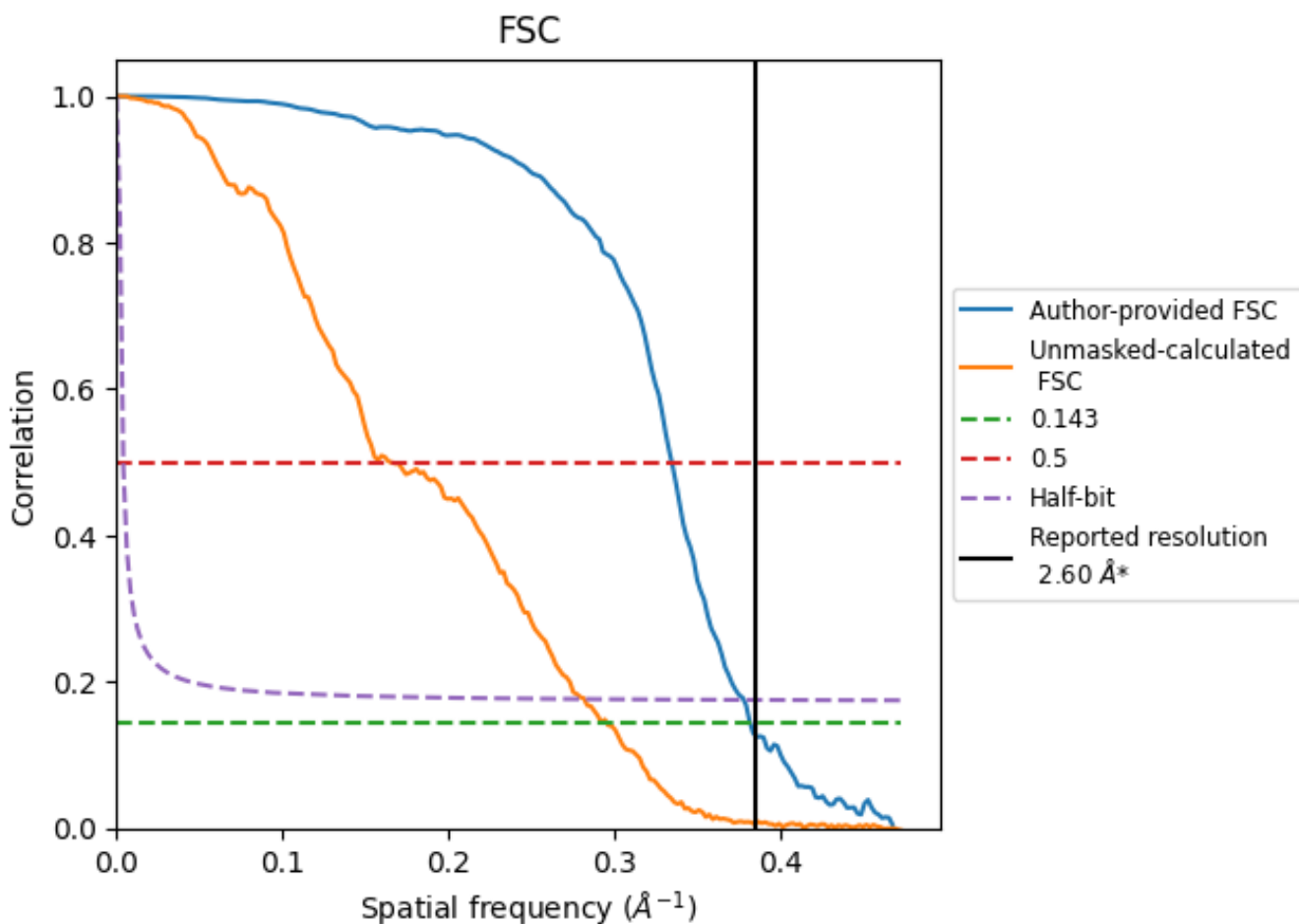


*Reported resolution corresponds to spatial frequency of 0.385 \AA^{-1}

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



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

8.2 Resolution estimates [i](#)

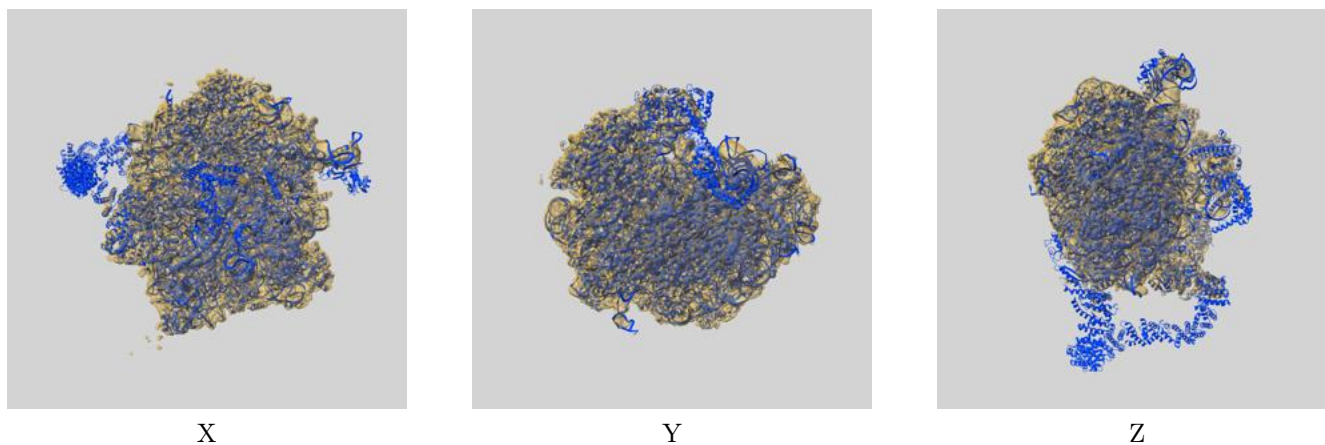
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.60	-	-
Author-provided FSC curve	2.62	2.99	2.65
Unmasked-calculated*	3.39	6.07	3.55

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.39 differs from the reported value 2.6 by more than 10 %

9 Map-model fit [i](#)

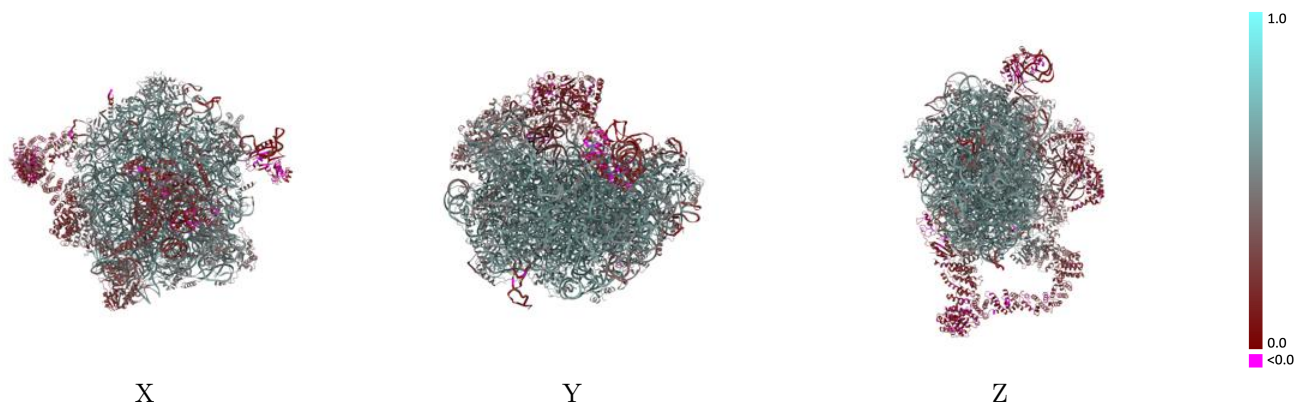
This section contains information regarding the fit between EMDB map EMD-15426 and PDB model 8AGW. Per-residue inclusion information can be found in section 3 on page 14.

9.1 Map-model overlay [i](#)



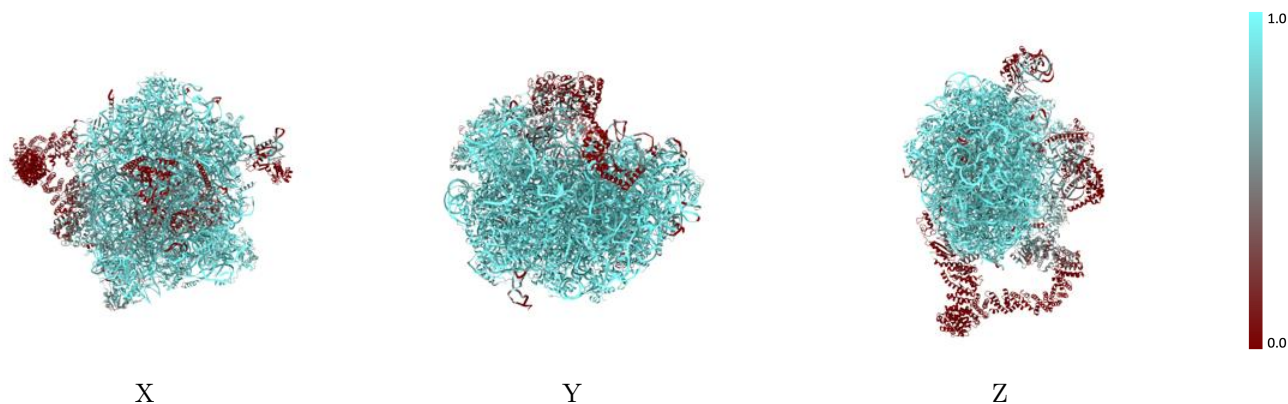
The images above show the 3D surface view of the map at the recommended contour level 0.55 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



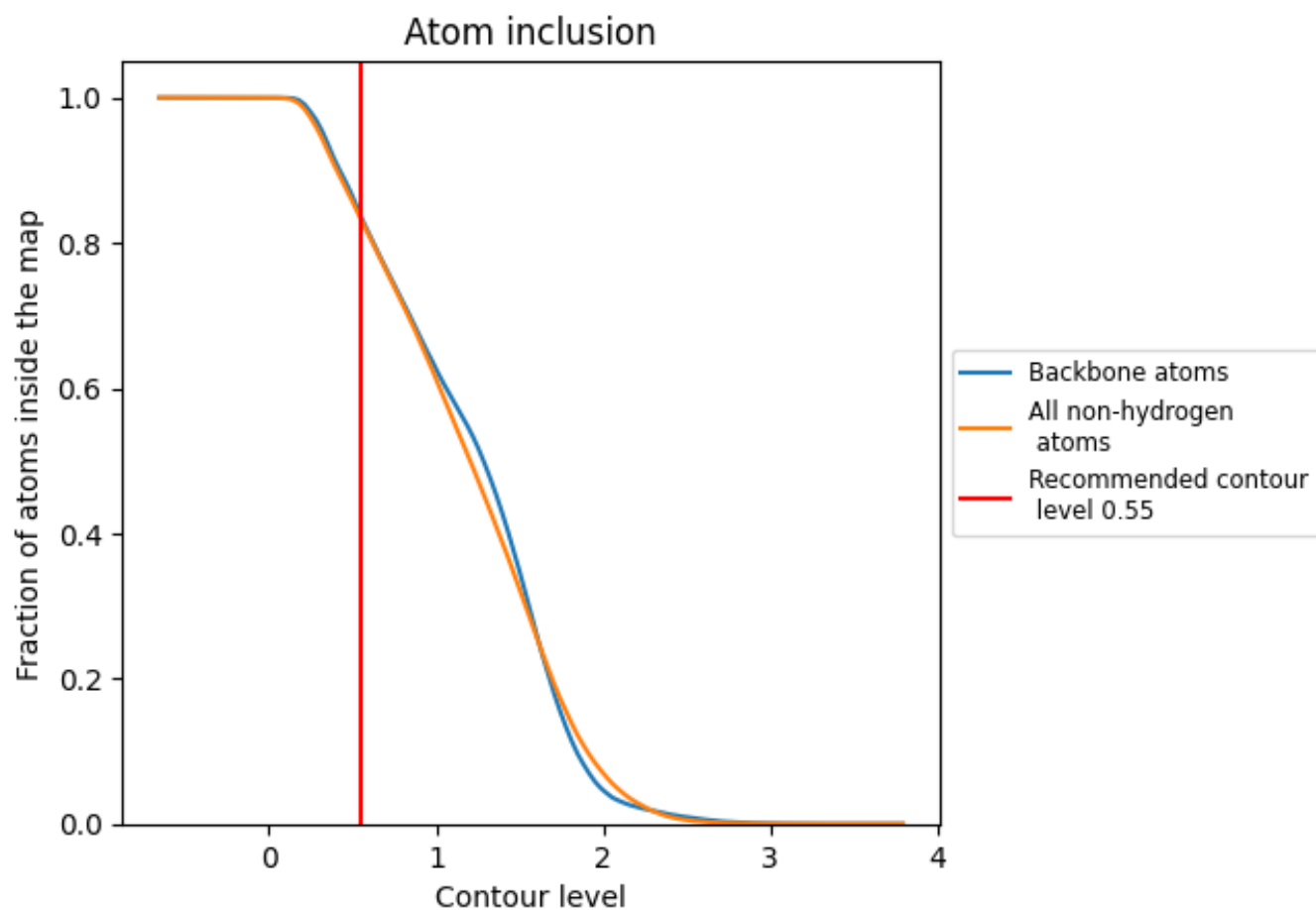
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.55).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 83% 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 (0.55) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8325	 0.5020
0	 0.6227	 0.2810
1	 0.9059	 0.4570
A	 0.9786	 0.6090
B	 0.9505	 0.5820
C	 0.9322	 0.5860
D	 0.9491	 0.5800
E	 0.8871	 0.5450
F	 0.9340	 0.5750
G	 0.9110	 0.5620
H	 0.8133	 0.4670
I	 0.9224	 0.5690
J	 0.9223	 0.5700
K	 0.9204	 0.5680
L	 0.9352	 0.5660
M	 0.8801	 0.5230
N	 0.9482	 0.5880
O	 0.9093	 0.5330
P	 0.8538	 0.5240
Q	 0.8824	 0.5500
R	 0.9514	 0.5960
S	 0.9671	 0.6090
T	 0.9215	 0.5680
U	 0.9183	 0.5520
V	 0.9027	 0.5180
W	 0.9952	 0.6250
X	 0.8130	 0.4940
Y	 0.9711	 0.5990
Z	 0.9295	 0.5650
a	 0.2798	 0.1930
b	 0.9094	 0.5700
c	 0.9164	 0.5660
d	 0.5000	 0.3930
e	 0.1376	 0.1850
f	 0.9678	 0.5670



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Chain	Atom inclusion	Q-score
g	0.4687	0.4560
h	0.9934	0.5710
i	0.9833	0.5960
j	0.9587	0.6030
k	0.9458	0.5800
l	0.9371	0.5730
m	0.8558	0.4820
n	0.8821	0.5280
o	0.9386	0.5660
p	0.8781	0.5160
q	0.9108	0.5430
r	0.9040	0.5460
s	0.8142	0.4390
t	0.9206	0.5600
u	0.9269	0.5460
w	0.0766	0.0750
x	0.5598	0.2560
y	0.7969	0.2340
z	0.6126	0.3040