Full wwPDB EM Validation Report (i)

Nov 26, 2022 – 05:50 PM EST

PDB ID	:	7SYS
EMDB ID	:	EMD-25539
Title	:	Structure of the delta dII IRES eIF2-containing 48S initiation complex, closed conformation. Structure 12(delta dII).
Authors	:	Brown, Z.P.; Abaeva, I.S.; De, S.; Hellen, C.U.T.; Pestova, T.V.; Frank, J.
Deposited on	:	2021-11-25
Resolution	:	3.50 Å(reported)
Based on initial models	:	5FLX, 5K0Y, 4KZZ, 6O85, 6D9J

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 (i) 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 (i)) were used in the production of this report:

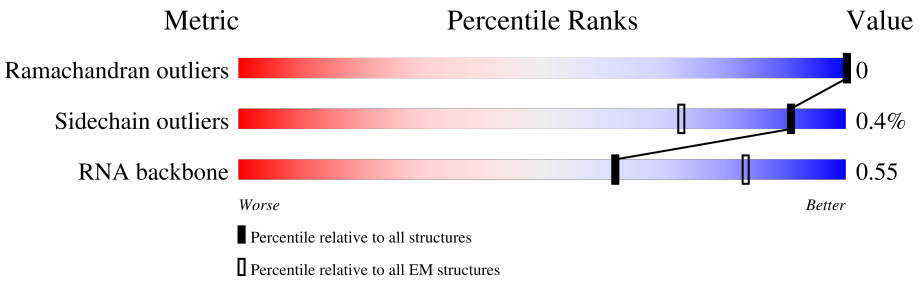
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.50 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	2	1870	72% 18% • 9%
2	A	144	61% 69% 31%
3	B	295	73% • 26%
4	C	264	5% 81% 19%
5	D	221	100%
6	E	281	10% 80% • 19%
7	F	263	99%
8	G	204	5% 93% 6%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	H	249	11% 95% 5%
10	I	432	11% 43% 57%
11	J	208	10% 99%
12	K	194	95% 5%
13	L	149	8% 64% 36%
14	M	158	10% 94%
15	N	132	81% 88% 11%
16	O	151	99%
17	P	168	7% 81% 19%
18	Q	145	10% 83% 17%
19	R	172	83% 17%
20	S	135	12% 97%
21	T	152	14% 93% 5%
22	U	145	97%
23	V	119	20% 84% 16%
24	W	83	99%
25	X	130	99%
26	Y	143	98%
27	Z	131	93% 5%
28	a	124	10% 62% 38%
29	b	101	100%
30	c	84	8% 99%
31	d	69	14% 97%
32	e	56	96%
33	f	133	12% 43% 57%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
34	g	188	28% 36% 64%
35	h	317	8% 98%
36	j	315	6% 56% 42%
37	n	25	20% 100%
38	z	400	9% 34% 14% 53%
39	i	75	24% 80% 19%

2 Entry composition (i)

There are 40 unique types of molecules in this entry. The entry contains 82981 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 RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	2	1697	36227	16170	6504	11857	1696	0	0

- Molecule 2 is a protein called Eukaryotic translation initiation factor 1A, X-chromosomal.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	A	99	798	503	143	148	4	0	0

- Molecule 3 is a protein called uS2 (SA).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	B	217	1710	1086	300	316	8	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	114	THR	ALA	conflict	UNP G1TLT8

- Molecule 4 is a protein called eS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	C	213	1729	1098	309	308	14	0	0

- Molecule 5 is a protein called uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	D	221	1716	1111	295	301	9	0	0

- Molecule 6 is a protein called uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	E	228	1768	1126	318	316	8	0	0

- Molecule 7 is a protein called eS4 (S4 X isoform).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	F	262	2076	1324	386	358	8	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	25	GLY	SER	conflict	UNP G1TK17
F	51	ARG	LYS	conflict	UNP G1TK17
F	78	THR	ALA	conflict	UNP G1TK17
F	156	VAL	MET	conflict	UNP G1TK17

- Molecule 8 is a protein called uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	G	191	1509	943	286	273	7	0	0

- Molecule 9 is a protein called eS6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	H	237	1923	1200	387	329	7	0	0

- Molecule 10 is a protein called eS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	I	185	1488	952	271	264	1	0	0

- Molecule 11 is a protein called eS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	J	206	1691	1061	333	292	5	1	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	47	ARG	GLY	conflict	UNP G1TJW1

- Molecule 12 is a protein called uS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	K	185	1525	969	306	248	2	0	0

- Molecule 13 is a protein called eS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	L	96	810	530	143	131	6	0	0

- Molecule 14 is a protein called uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	M	151	1233	785	231	211	6	0	0

- Molecule 15 is a protein called eS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	N	117	908	570	161	169	8	0	0

- Molecule 16 is a protein called uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	O	149	1202	770	228	203	1	0	0

- Molecule 17 is a protein called uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	P	136	1016	621	199	190	6	0	0

- Molecule 18 is a protein called uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	Q	120	997	635	187	168	7	0	0

- Molecule 19 is a protein called uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	R	142	1128	717	213	195	3	0	0

- Molecule 20 is a protein called eS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	S	132	1068	670	199	195	4	0	0

- Molecule 21 is a protein called uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	T	144	1190	746	241	202	1	0	0

- Molecule 22 is a protein called eS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	U	141	1097	688	211	195	3	0	0

- Molecule 23 is a protein called uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	V	100	795	498	152	141	4	0	0

- Molecule 24 is a protein called eS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	W	83	636	393	117	121	5	0	0

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
W	3	ASN	SER	conflict	UNP G1TM82
W	4	ASP	ASN	conflict	UNP G1TM82
W	33	GLN	PRO	conflict	UNP G1TM82
W	50	PHE	SER	conflict	UNP G1TM82
W	75	ALA	SER	conflict	UNP G1TM82
W	76	ASP	HIS	conflict	UNP G1TM82
W	81	LYS	GLN	conflict	UNP G1TM82

- Molecule 25 is a protein called uS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	X	129	1034	659	193	176	6	0	0

- Molecule 26 is a protein called uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	Y	141	1098	693	219	183	3	0	0

- Molecule 27 is a protein called eS24.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	Z	124	1011	640	198	168	5	0	0

- Molecule 28 is a protein called eS25.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	a	77	614	393	114	106	1	0	0

- Molecule 29 is a protein called eS26.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	b	101	814	507	170	132	5	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
b	28	ARG	CYS	conflict	UNP G1TFE8

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
b	56	ALA	VAL	conflict	UNP G1TFE8

- Molecule 30 is a protein called eS27.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	c	83	651	408	121	115	7	0	0

- Molecule 31 is a protein called eS28.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	d	67	530	321	108	99	2	0	0

- Molecule 32 is a protein called uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	e	55	459	286	94	74	5	0	0

- Molecule 33 is a protein called eS30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	f	57	457	282	101	73	1	0	0

- Molecule 34 is a protein called eS31.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	g	68	555	351	103	94	7	0	0

- Molecule 35 is a protein called Receptor for Activated C Kinase 1 (RACK1).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	h	313	2436	1535	424	465	12	0	0

- Molecule 36 is a protein called Eukaryotic translation initiation factor 2 subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	j	182	1221	781	225	212	3	0	0

- Molecule 37 is a protein called eL41.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	n	25	239	145	64	27	3	0	0

- Molecule 38 is a RNA chain called HCV IRES.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
38	z	188	4017	1789	721	1319	188	0	0

- Molecule 39 is a RNA chain called Met-tRNA-i-Met.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
39	i	75	1604	717	298	515	74	0	0

- Molecule 40 is ZINC ION (three-letter code: ZN) (formula: Zn).

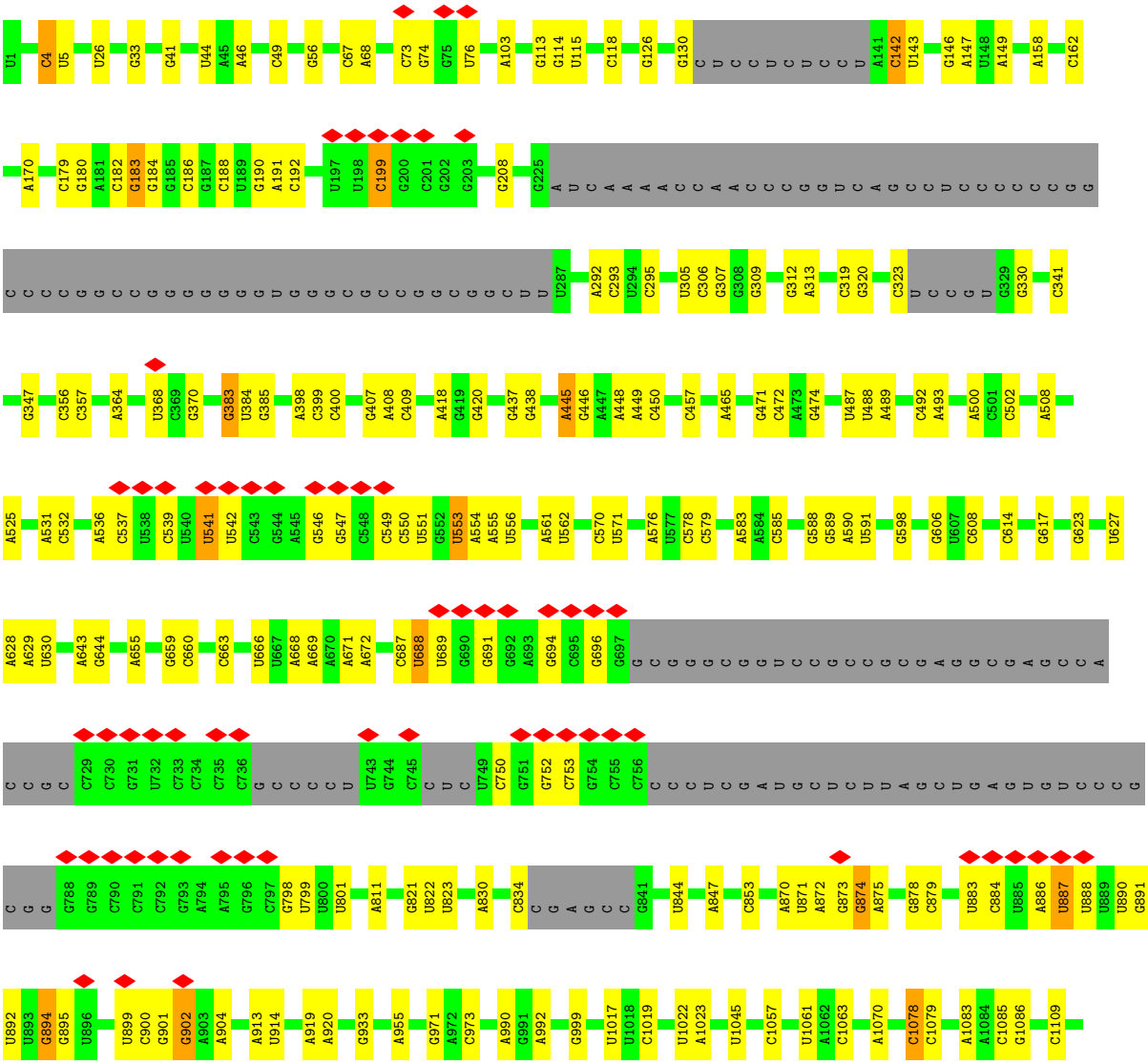
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
40	b	1	1	1	0

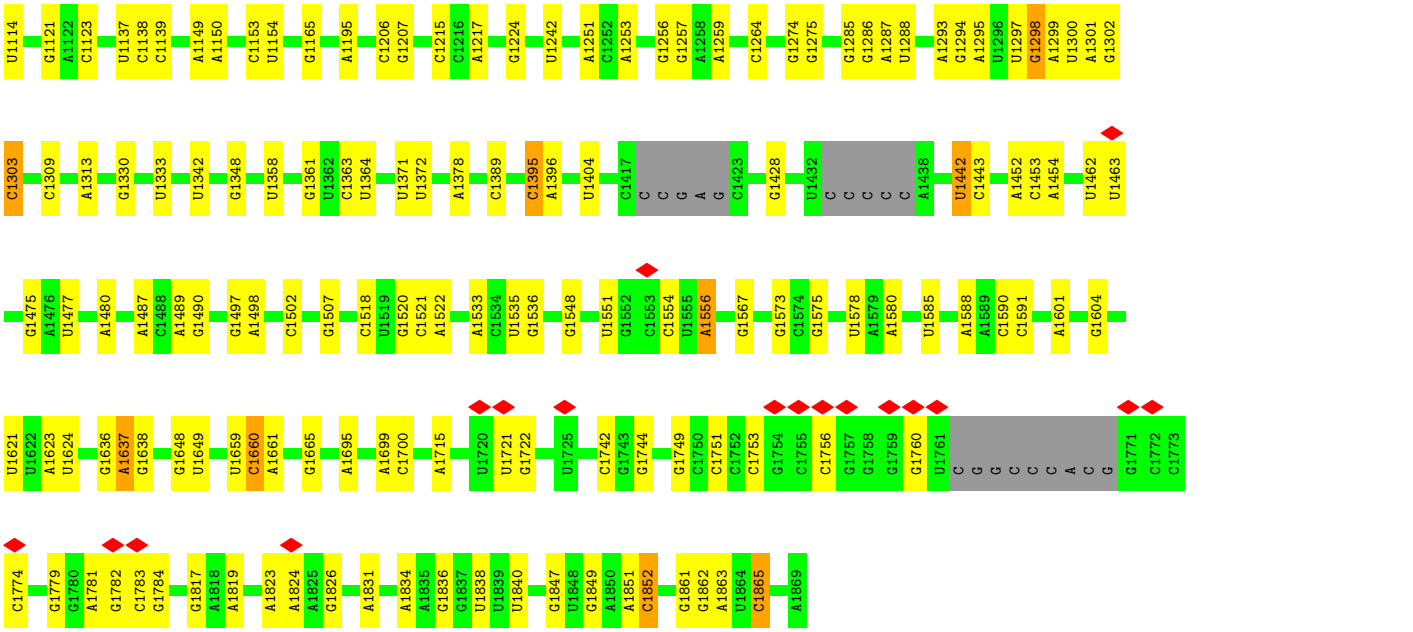
3 Residue-property plots (i)

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: 18S rRNA

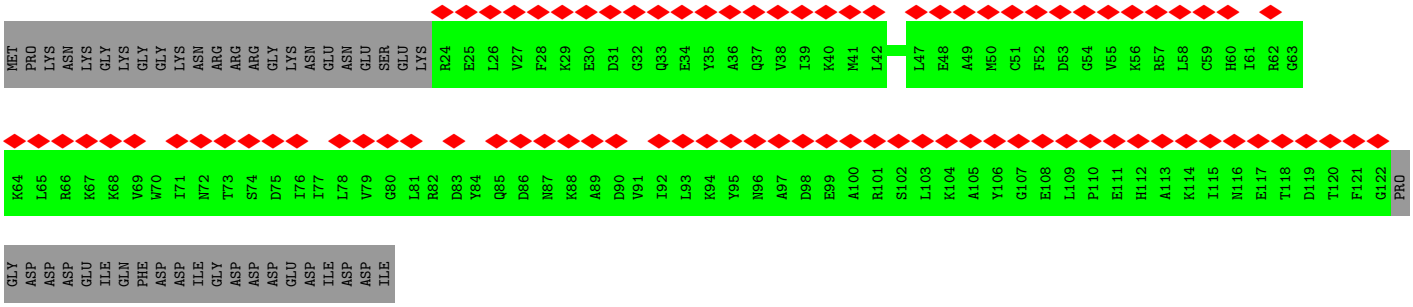
Chain 2:





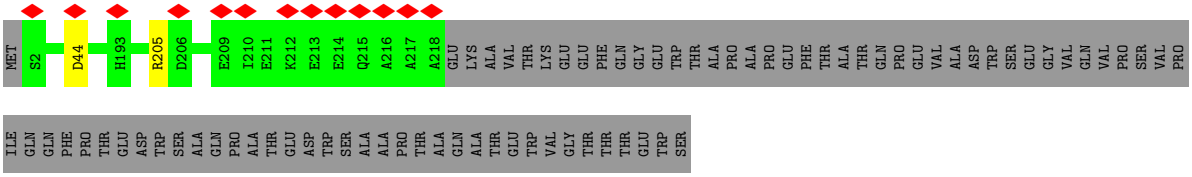
- Molecule 2: Eukaryotic translation initiation factor 1A, X-chromosomal

Chain A:



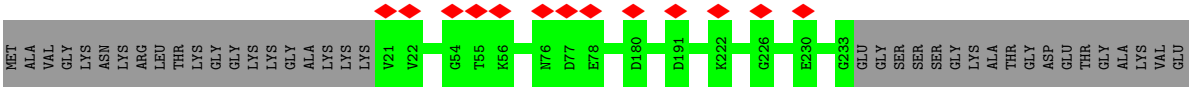
- Molecule 3: uS2 (SA)

Chain B:



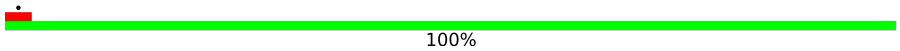
- Molecule 4: eS1

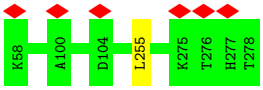
Chain C:



- Molecule 5: uS5

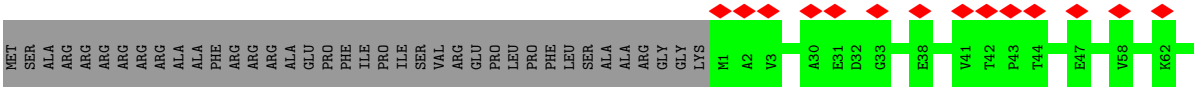
Chain D:

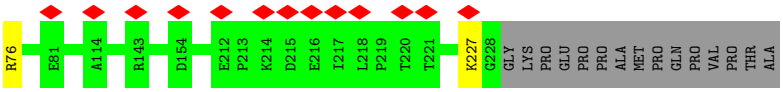




- Molecule 6: uS3

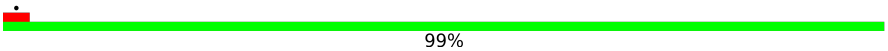
Chain E:

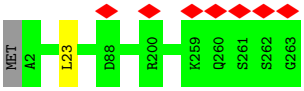




- Molecule 7: eS4 (S4 X isoform)

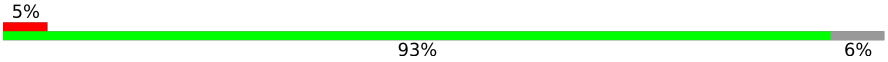
Chain F:

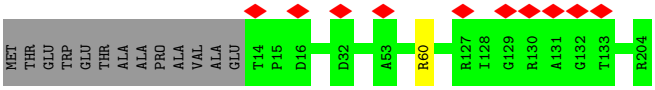




- Molecule 8: uS7

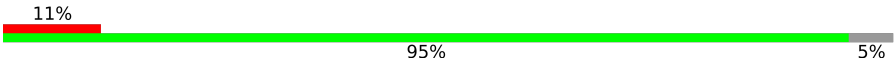
Chain G:

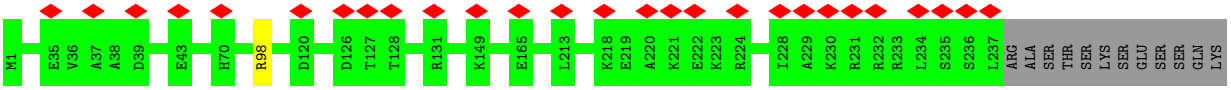




- Molecule 9: eS6

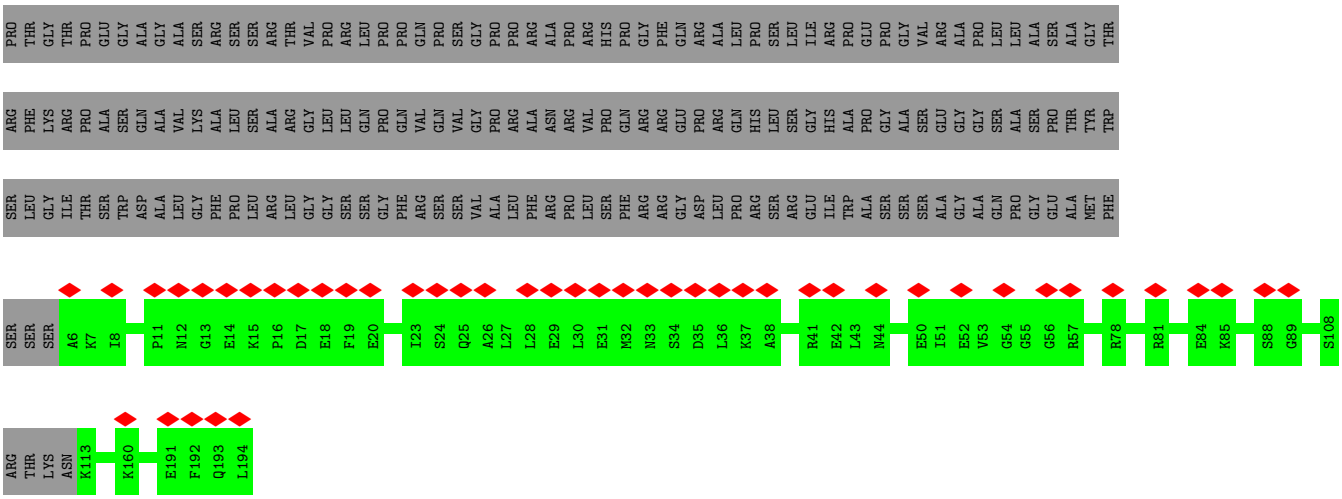
Chain H:





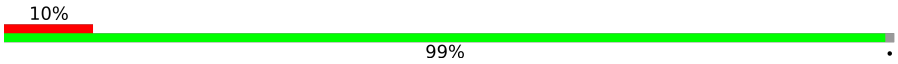
- Molecule 10: eS7

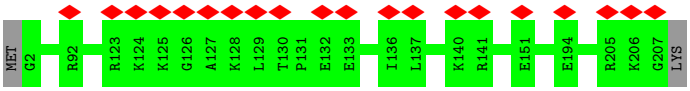
Chain I:



- Molecule 11: eS8

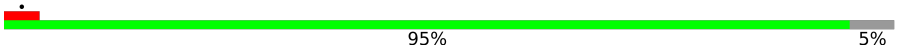
Chain J:

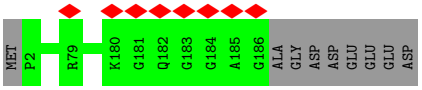




- Molecule 12: uS4

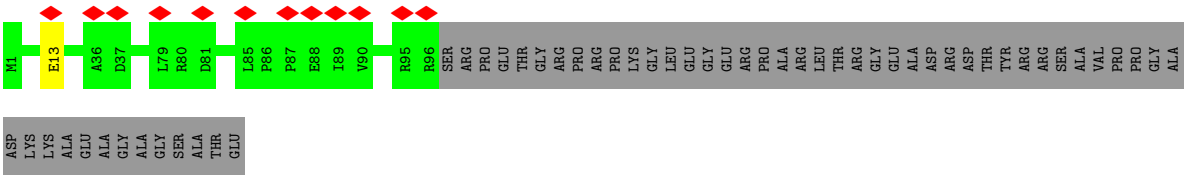
Chain K:





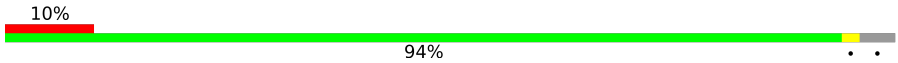
- Molecule 13: eS10

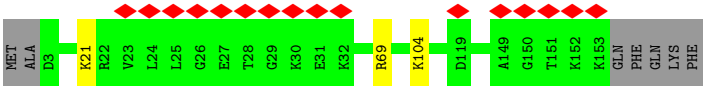
Chain L:



- Molecule 14: uS17

Chain M:



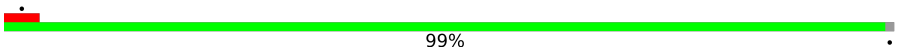


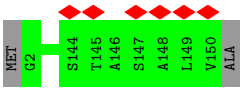
- Molecule 15: eS12

Chain N:

- Molecule 16: uS15

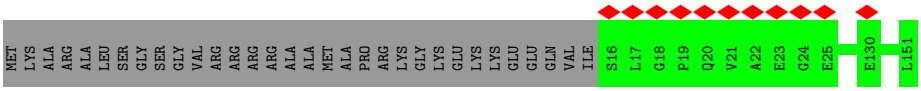
Chain O:





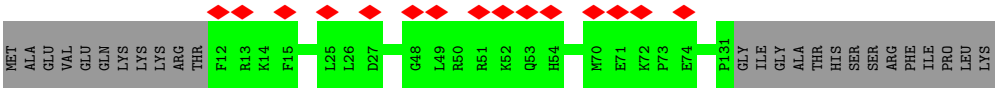
- Molecule 17: uS11

Chain P:



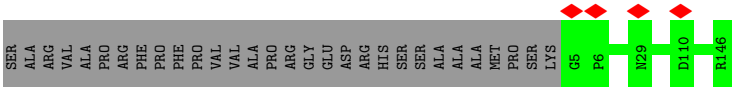
- Molecule 18: uS19

Chain Q:



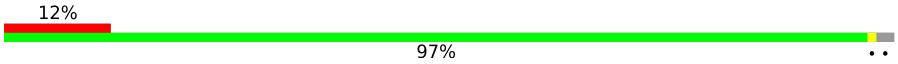
- Molecule 19: uS9

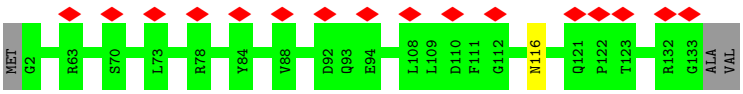
Chain R:



- Molecule 20: eS17

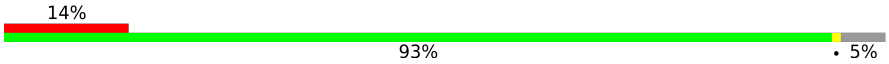
Chain S:

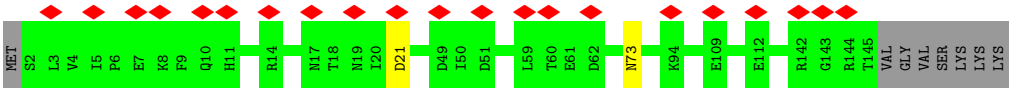




- Molecule 21: uS13

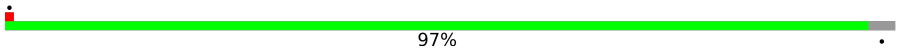
Chain T:

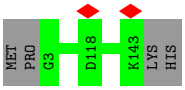




- Molecule 22: eS19

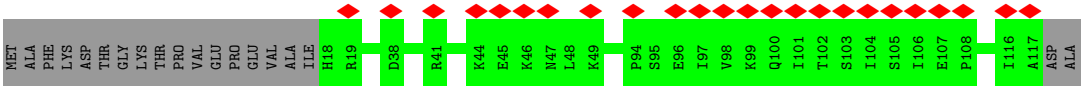
Chain U:





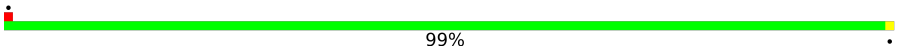
- Molecule 23: uS10

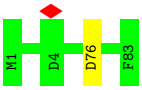
Chain V:



- Molecule 24: eS21

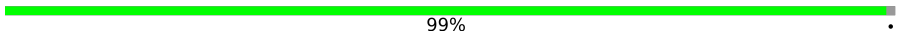
Chain W:





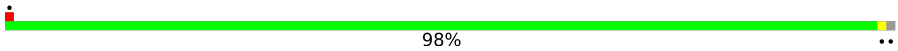
- Molecule 25: uS8

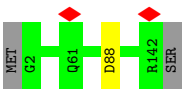
Chain X:



- Molecule 26: uS12

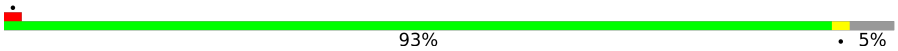
Chain Y:

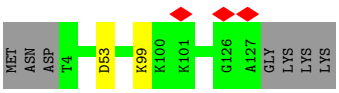




- Molecule 27: eS24

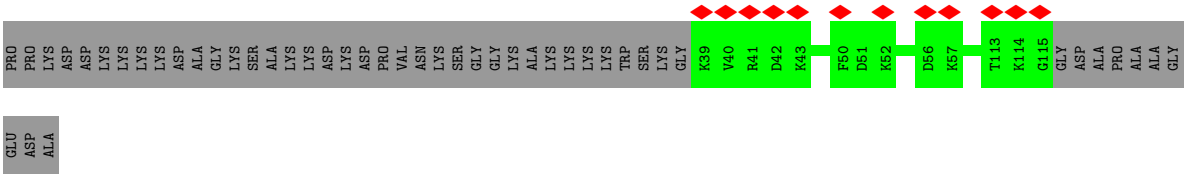
Chain Z:





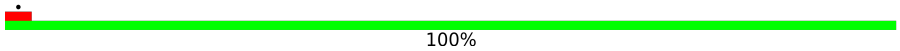
- Molecule 28: eS25

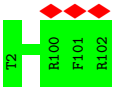
Chain a:



- Molecule 29: eS26

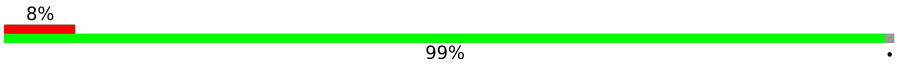
Chain b:

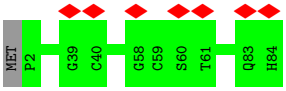




- Molecule 30: eS27

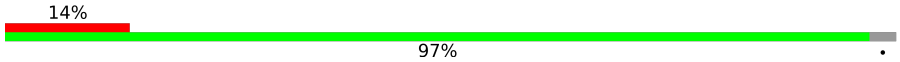
Chain c:

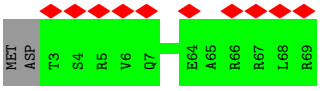




- Molecule 31: eS28

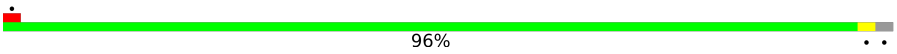
Chain d:

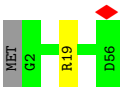




- Molecule 32: uS14

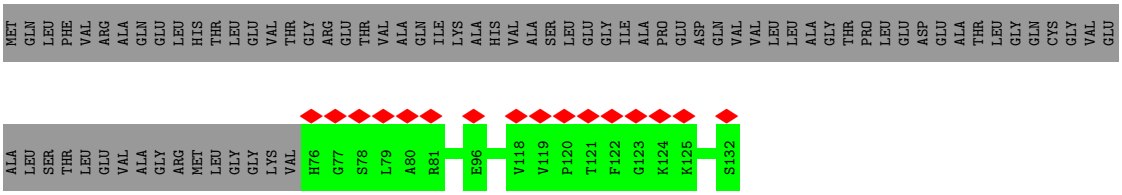
Chain e:





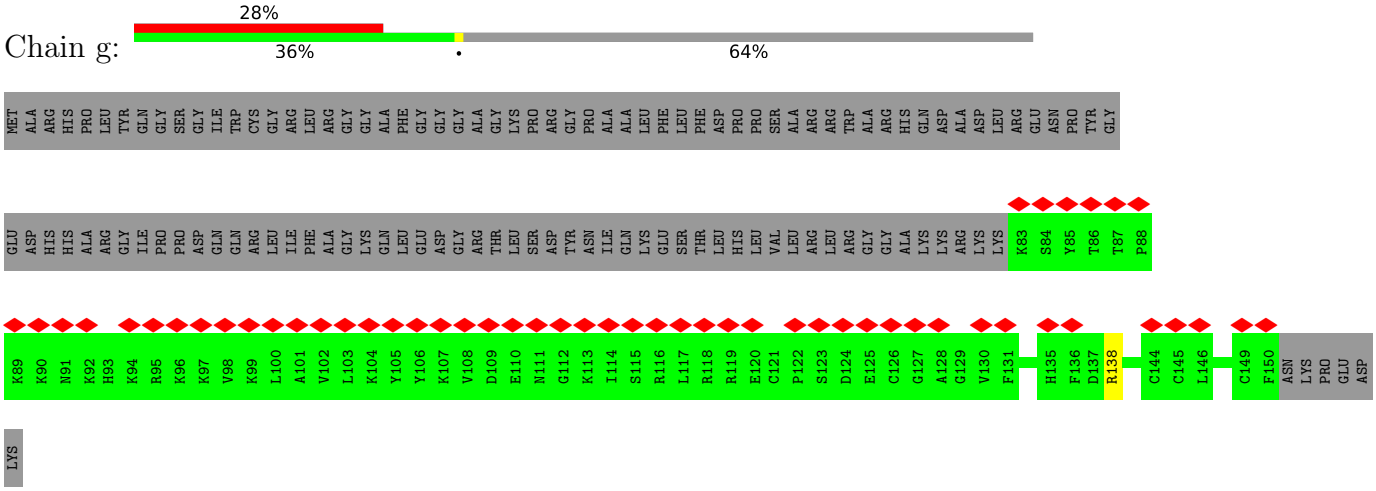
- Molecule 33: eS30

Chain f:



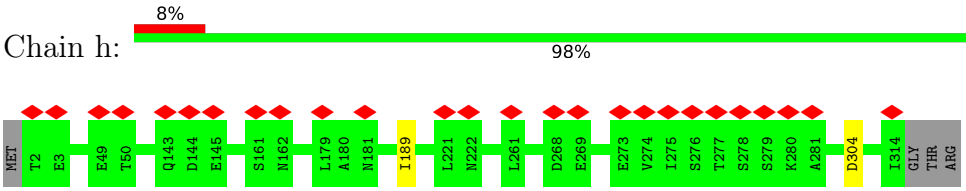
- Molecule 34: eS31

Chain g:



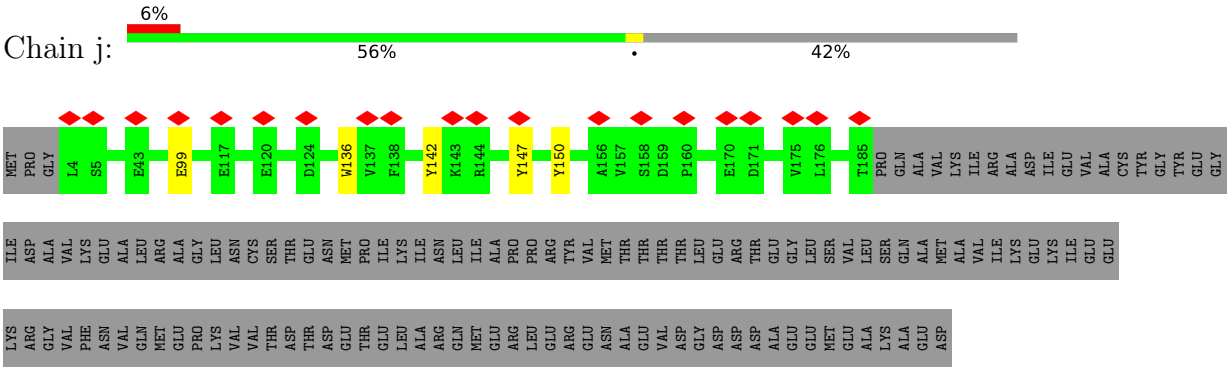
- Molecule 35: Receptor for Activated C Kinase 1 (RACK1)

Chain h:



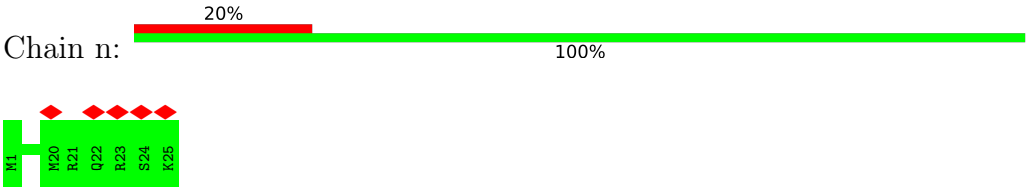
- Molecule 36: Eukaryotic translation initiation factor 2 subunit 1

Chain j:



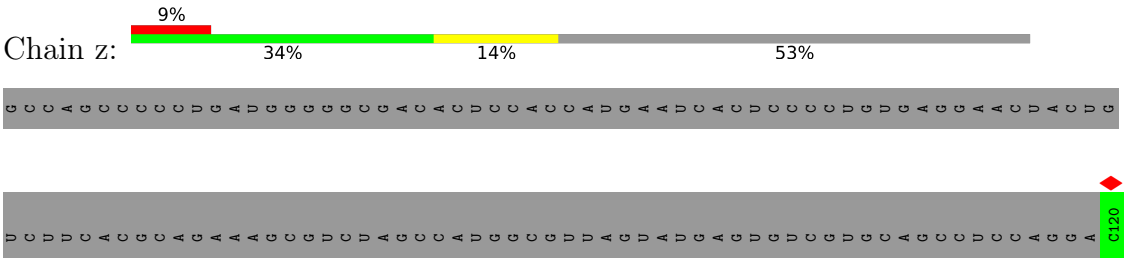
- Molecule 37: eL41

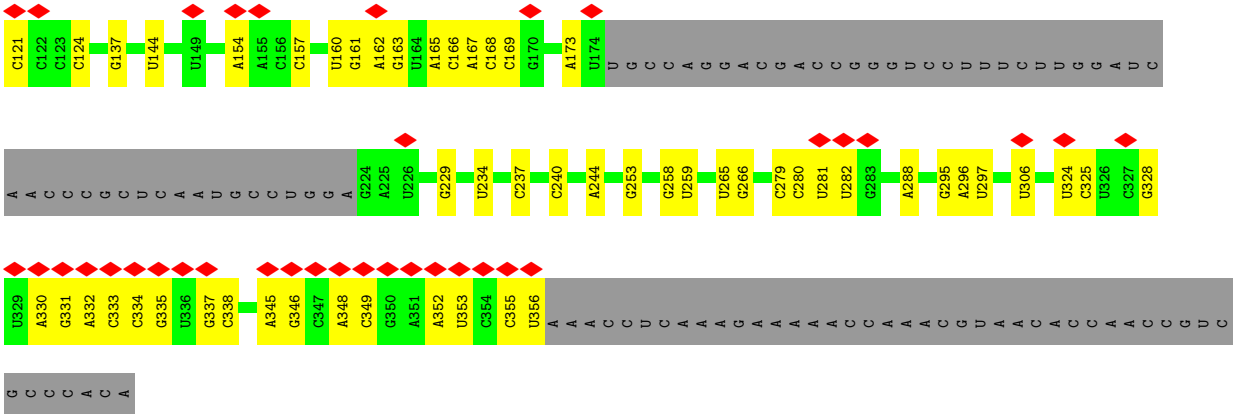
Chain n:



- Molecule 38: HCV IRES

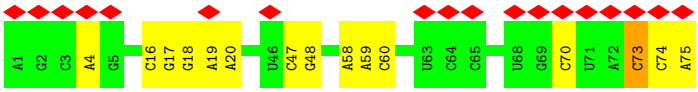
Chain z:





• Molecule 39: Met-tRNA-i-Met

Chain i:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	103813	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	70.9	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	56000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.093	Depositor
Minimum map value	-0.039	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.014	Depositor
Map size (Å)	380.0, 380.0, 380.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.95, 0.95, 0.95	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: 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	2	0.27	0/40506	1.01	185/63123 (0.3%)
2	A	0.26	0/809	0.59	0/1083
3	B	0.28	0/1747	0.65	1/2374 (0.0%)
4	C	0.26	0/1756	0.57	0/2350
5	D	0.27	0/1753	0.55	1/2369 (0.0%)
6	E	0.28	0/1796	0.62	0/2417
7	F	0.26	0/2118	0.57	1/2849 (0.0%)
8	G	0.25	0/1531	0.59	0/2059
9	H	0.25	0/1946	0.60	0/2590
10	I	0.27	0/1510	0.59	0/2022
11	J	0.27	0/1723	0.61	0/2298
12	K	0.27	0/1550	0.63	0/2069
13	L	0.31	0/834	0.63	1/1125 (0.1%)
14	M	0.28	0/1254	0.62	0/1677
15	N	0.28	0/918	0.63	0/1233
16	O	0.25	0/1226	0.56	0/1649
17	P	0.26	0/1029	0.59	0/1380
18	Q	0.28	0/1017	0.63	0/1358
19	R	0.30	0/1146	0.64	0/1534
20	S	0.28	0/1082	0.68	0/1452
21	T	0.27	0/1208	0.66	1/1618 (0.1%)
22	U	0.26	0/1115	0.55	0/1493
23	V	0.24	0/805	0.60	0/1081
24	W	0.27	0/643	0.60	1/860 (0.1%)
25	X	0.27	0/1051	0.58	0/1406
26	Y	0.27	0/1116	0.64	1/1490 (0.1%)
27	Z	0.27	0/1028	0.63	1/1366 (0.1%)
28	a	0.26	0/620	0.66	0/831
29	b	0.27	0/828	0.61	0/1109
30	c	0.26	0/665	0.55	0/891
31	d	0.25	0/532	0.67	0/712
32	e	0.26	0/470	0.59	0/623

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	f	0.26	0/462	0.59	0/607
34	g	0.30	0/567	0.59	0/753
35	h	0.26	0/2493	0.61	2/3394 (0.1%)
36	j	0.39	1/1239 (0.1%)	0.66	3/1680 (0.2%)
37	n	0.29	0/240	0.71	0/305
38	z	0.26	0/4488	0.97	5/6995 (0.1%)
39	i	0.24	0/1795	0.89	1/2798 (0.0%)
All	All	0.27	1/88616 (0.0%)	0.85	204/129023 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	j	136	TRP	CD2-CE2	5.92	1.48	1.41

All (204) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2	1852	C	N1-C2-O2	16.60	128.86	118.90
1	2	1852	C	N3-C2-O2	-15.27	111.21	121.90
1	2	1852	C	C2-N1-C1'	12.74	132.82	118.80
1	2	1852	C	C6-N1-C2	-11.53	115.69	120.30
1	2	630	U	C2-N1-C1'	10.94	130.83	117.70
1	2	630	U	N1-C2-O2	10.51	130.16	122.80
1	2	1078	C	N1-C2-O2	10.50	125.20	118.90
1	2	630	U	N3-C2-O2	-10.02	115.19	122.20
1	2	1453	C	N1-C2-O2	9.78	124.77	118.90
1	2	853	C	N1-C2-O2	9.60	124.66	118.90
1	2	1139	C	N1-C2-O2	9.59	124.66	118.90
1	2	1453	C	C2-N1-C1'	9.57	129.33	118.80
1	2	1078	C	N3-C2-O2	-9.57	115.20	121.90
1	2	1591	C	N1-C2-O2	9.46	124.58	118.90
1	2	1206	C	N1-C2-O2	9.36	124.51	118.90
1	2	1206	C	C2-N1-C1'	9.00	128.70	118.80
1	2	1139	C	C2-N1-C1'	8.92	128.62	118.80
1	2	457	C	N3-C2-O2	-8.67	115.83	121.90
1	2	853	C	C2-N1-C1'	8.42	128.06	118.80
1	2	1063	C	N1-C2-O2	8.39	123.94	118.90
1	2	1700	C	C2-N1-C1'	8.39	128.03	118.80
36	j	136	TRP	CD2-CE3-CZ3	8.33	129.63	118.80
1	2	293	C	N1-C2-O2	8.29	123.88	118.90
1	2	1123	C	N1-C2-O2	8.20	123.82	118.90
1	2	1624	U	C2-N1-C1'	8.02	127.33	117.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2	585	C	N1-C2-O2	7.98	123.69	118.90
1	2	853	C	N3-C2-O2	-7.84	116.41	121.90
1	2	1520	G	C4-N9-C1'	7.83	136.67	126.50
1	2	1442	U	N1-C2-O2	7.79	128.26	122.80
1	2	1852	C	C6-N1-C1'	-7.79	111.45	120.80
1	2	1591	C	C2-N1-C1'	7.75	127.32	118.80
1	2	1139	C	N3-C2-O2	-7.68	116.52	121.90
1	2	1453	C	N3-C2-O2	-7.64	116.56	121.90
1	2	1591	C	N3-C2-O2	-7.61	116.57	121.90
1	2	1442	U	N3-C2-O2	-7.61	116.88	122.20
1	2	539	C	N1-C2-O2	7.51	123.41	118.90
1	2	1078	C	C6-N1-C2	-7.45	117.32	120.30
1	2	1298	G	N3-C4-N9	7.40	130.44	126.00
1	2	1700	C	N1-C2-O2	7.37	123.32	118.90
1	2	293	C	C2-N1-C1'	7.28	126.81	118.80
1	2	1298	G	C4-N9-C1'	7.28	135.96	126.50
1	2	1852	C	C5-C6-N1	7.22	124.61	121.00
1	2	1206	C	N3-C2-O2	-7.18	116.87	121.90
1	2	1520	G	N3-C4-N9	7.17	130.30	126.00
26	Y	88	ASP	CB-CG-OD1	7.14	124.73	118.30
1	2	578	C	N1-C2-O2	7.13	123.18	118.90
1	2	1022	U	C2-N1-C1'	7.11	126.23	117.70
1	2	1303	C	N1-C2-O2	7.10	123.16	118.90
3	B	44	ASP	CB-CG-OD1	7.09	124.68	118.30
1	2	894	G	C4-N9-C1'	7.08	135.71	126.50
21	T	21	ASP	CB-CG-OD1	7.07	124.66	118.30
1	2	183	G	N3-C4-C5	-7.00	125.10	128.60
1	2	1520	G	N3-C4-C5	-7.00	125.10	128.60
1	2	630	U	C6-N1-C1'	-6.98	111.43	121.20
1	2	1591	C	C6-N1-C2	-6.89	117.55	120.30
1	2	1442	U	C2-N1-C1'	6.84	125.91	117.70
1	2	1123	C	N3-C2-O2	-6.84	117.11	121.90
1	2	853	C	C6-N1-C2	-6.84	117.56	120.30
1	2	894	G	N3-C4-C5	-6.82	125.19	128.60
1	2	1624	U	N1-C2-O2	6.73	127.51	122.80
1	2	1624	U	N3-C2-O2	-6.69	117.52	122.20
1	2	894	G	N3-C4-N9	6.65	129.99	126.00
1	2	1453	C	C6-N1-C1'	-6.65	112.82	120.80
1	2	1298	G	C8-N9-C1'	-6.64	118.37	127.00
1	2	1063	C	N3-C2-O2	-6.63	117.26	121.90
1	2	1520	G	C8-N9-C1'	-6.61	118.41	127.00
1	2	1303	C	C2-N1-C1'	6.56	126.02	118.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2	688	U	P-O3'-C3'	6.55	127.56	119.70
7	F	23	LEU	CA-CB-CG	6.53	130.32	115.30
1	2	183	G	C4-N9-C1'	6.50	134.96	126.50
1	2	659	G	C4-N9-C1'	6.50	134.95	126.50
1	2	1847	G	N1-C6-O6	-6.50	116.00	119.90
1	2	1063	C	C2-N1-C1'	6.49	125.94	118.80
1	2	118	C	N1-C2-O2	6.47	122.78	118.90
38	z	124	C	N1-C2-O2	6.47	122.78	118.90
1	2	1389	C	C2-N1-C1'	6.46	125.91	118.80
1	2	1057	C	C2-N1-C1'	6.45	125.90	118.80
1	2	1298	G	N3-C4-C5	-6.44	125.38	128.60
1	2	585	C	C2-N1-C1'	6.44	125.88	118.80
1	2	553	U	P-O3'-C3'	6.43	127.42	119.70
1	2	541	U	N1-C2-O2	6.41	127.28	122.80
1	2	1865	C	N1-C2-O2	6.39	122.74	118.90
1	2	457	C	C6-N1-C2	-6.35	117.76	120.30
1	2	1123	C	C2-N1-C1'	6.33	125.76	118.80
5	D	255	LEU	CA-CB-CG	6.32	129.83	115.30
1	2	1019	C	N1-C2-O2	6.32	122.69	118.90
1	2	293	C	N3-C2-O2	-6.31	117.48	121.90
1	2	585	C	N3-C2-O2	-6.30	117.49	121.90
1	2	973	C	N1-C2-O2	6.29	122.68	118.90
1	2	1139	C	C6-N1-C2	-6.29	117.78	120.30
1	2	1395	C	P-O3'-C3'	6.26	127.22	119.70
1	2	199	C	N1-C2-O2	6.25	122.65	118.90
1	2	1206	C	C6-N1-C1'	-6.25	113.30	120.80
1	2	1590	C	N1-C2-O2	6.24	122.64	118.90
27	Z	53	ASP	CB-CG-OD2	6.20	123.88	118.30
1	2	4	C	C2-N1-C1'	6.19	125.61	118.80
1	2	1637	A	P-O3'-C3'	6.17	127.11	119.70
1	2	183	G	C2-N3-C4	6.15	114.97	111.90
1	2	1078	C	C2-N1-C1'	6.14	125.56	118.80
1	2	1847	G	C5-C6-O6	6.14	132.28	128.60
1	2	1453	C	C6-N1-C2	-6.13	117.85	120.30
1	2	630	U	C5-C6-N1	6.12	125.76	122.70
1	2	1079	C	N1-C2-O2	6.12	122.57	118.90
1	2	1443	C	N1-C2-O2	6.09	122.55	118.90
38	z	160	U	N3-C2-O2	-6.05	117.96	122.20
1	2	541	U	N3-C2-O2	-6.04	117.97	122.20
1	2	1139	C	C6-N1-C1'	-6.02	113.58	120.80
1	2	887	U	N1-C2-O2	6.01	127.01	122.80
1	2	1123	C	C6-N1-C2	-6.01	117.90	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2	356	C	C2-N1-C1'	6.00	125.39	118.80
39	i	73	C	P-O3'-C3'	5.99	126.88	119.70
1	2	1865	C	C2-N1-C1'	5.98	125.38	118.80
24	W	76	ASP	CB-CG-OD2	5.98	123.68	118.30
1	2	578	C	N3-C2-O2	-5.97	117.72	121.90
1	2	1700	C	C6-N1-C1'	-5.96	113.64	120.80
1	2	1389	C	C6-N1-C2	-5.96	117.92	120.30
1	2	383	G	P-O3'-C3'	5.95	126.84	119.70
1	2	445	A	P-O3'-C3'	5.92	126.81	119.70
1	2	539	C	C2-N1-C1'	5.92	125.31	118.80
1	2	1753	C	N3-C2-O2	-5.91	117.77	121.90
36	j	99	GLU	CA-CB-CG	5.90	126.39	113.40
1	2	887	U	C2-N1-C1'	5.90	124.78	117.70
1	2	884	C	N1-C2-O2	5.88	122.43	118.90
1	2	539	C	N3-C2-O2	-5.88	117.78	121.90
1	2	894	G	C8-N9-C1'	-5.87	119.37	127.00
1	2	579	C	N1-C2-O2	5.86	122.42	118.90
1	2	1063	C	C6-N1-C2	-5.83	117.97	120.30
1	2	1206	C	C6-N1-C2	-5.82	117.97	120.30
1	2	1389	C	N1-C2-O2	5.82	122.39	118.90
1	2	1660	C	C2-N1-C1'	5.81	125.20	118.80
1	2	1518	C	C2-N1-C1'	5.79	125.17	118.80
1	2	879	C	N1-C2-O2	5.78	122.37	118.90
1	2	1700	C	N3-C2-O2	-5.77	117.86	121.90
1	2	570	C	N1-C2-O2	5.74	122.34	118.90
1	2	356	C	N1-C2-O2	5.73	122.34	118.90
1	2	295	C	N1-C2-O2	5.72	122.33	118.90
1	2	183	G	N3-C4-N9	5.71	129.43	126.00
1	2	1303	C	N3-C2-O2	-5.69	117.92	121.90
35	h	304	ASP	CB-CG-OD1	5.69	123.42	118.30
1	2	1057	C	N1-C2-O2	5.68	122.31	118.90
1	2	1591	C	C5-C6-N1	5.64	123.82	121.00
1	2	179	C	N1-C2-O2	5.60	122.26	118.90
1	2	630	U	C6-N1-C2	-5.57	117.66	121.00
1	2	1556	A	C2-N3-C4	5.56	113.38	110.60
1	2	1742	C	N1-C2-O2	5.56	122.24	118.90
1	2	585	C	C6-N1-C2	-5.56	118.08	120.30
1	2	4	C	N1-C2-O2	5.54	122.23	118.90
1	2	1395	C	OP1-P-O3'	5.53	117.37	105.20
1	2	1019	C	N3-C2-O2	-5.53	118.03	121.90
1	2	457	C	N1-C2-N3	5.53	123.07	119.20
1	2	823	U	C2-N1-C1'	5.52	124.32	117.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	L	13	GLU	CA-CB-CG	5.51	125.52	113.40
1	2	659	G	C8-N9-C1'	-5.50	119.85	127.00
1	2	874	G	P-O3'-C3'	5.50	126.29	119.70
1	2	1453	C	C5-C6-N1	5.47	123.74	121.00
1	2	1624	U	O4'-C1'-N1	5.47	112.58	108.20
1	2	902	G	C5-C6-O6	5.46	131.88	128.60
1	2	659	G	N3-C4-N9	5.45	129.27	126.00
1	2	853	C	C5-C6-N1	5.42	123.71	121.00
1	2	1442	U	C5-C6-N1	5.41	125.41	122.70
1	2	1389	C	C5-C6-N1	5.38	123.69	121.00
1	2	853	C	C6-N1-C1'	-5.38	114.35	120.80
1	2	4	C	C6-N1-C2	-5.35	118.16	120.30
1	2	887	U	N3-C2-O2	-5.34	118.46	122.20
1	2	142	C	N1-C2-O2	5.32	122.09	118.90
1	2	539	C	C6-N1-C2	-5.30	118.18	120.30
1	2	1206	C	C5-C6-N1	5.30	123.65	121.00
1	2	659	G	N3-C4-C5	-5.28	125.96	128.60
38	z	160	U	N1-C2-O2	5.28	126.50	122.80
1	2	1636	G	C4-N9-C1'	5.28	133.37	126.50
1	2	973	C	N3-C2-O2	-5.27	118.21	121.90
1	2	1079	C	N3-C2-O2	-5.27	118.21	121.90
1	2	1847	G	N3-C2-N2	5.22	123.55	119.90
1	2	118	C	N3-C2-O2	-5.20	118.26	121.90
1	2	884	C	N3-C2-O2	-5.19	118.27	121.90
1	2	1649	U	N1-C2-O2	5.18	126.43	122.80
1	2	541	U	C2-N1-C1'	5.17	123.91	117.70
1	2	1590	C	N3-C2-O2	-5.17	118.28	121.90
1	2	571	U	N1-C2-O2	5.16	126.41	122.80
1	2	1022	U	N1-C2-O2	5.15	126.40	122.80
1	2	1865	C	N3-C2-O2	-5.13	118.31	121.90
1	2	1852	C	C2-N3-C4	5.13	122.47	119.90
1	2	687	C	N1-C2-O2	5.11	121.96	118.90
1	2	1298	G	C2-N3-C4	5.11	114.45	111.90
1	2	1590	C	C6-N1-C2	-5.10	118.26	120.30
35	h	189	ILE	CG1-CB-CG2	-5.10	100.17	111.40
1	2	341	C	N1-C2-O2	5.10	121.96	118.90
1	2	1660	C	N1-C2-O2	5.10	121.96	118.90
1	2	1139	C	C5-C6-N1	5.09	123.55	121.00
1	2	1288	U	N3-C2-O2	-5.07	118.65	122.20
38	z	124	C	N3-C2-O2	-5.07	118.35	121.90
1	2	1636	G	N3-C4-C5	-5.06	126.07	128.60
1	2	199	C	N3-C2-O2	-5.05	118.36	121.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2	183	G	C8-N9-C1'	-5.05	120.44	127.00
38	z	124	C	C2-N1-C1'	5.04	124.35	118.80
1	2	666	U	C2-N1-C1'	5.04	123.75	117.70
1	2	884	C	N3-C4-N4	-5.04	114.48	118.00
1	2	1636	G	N3-C4-N9	5.03	129.02	126.00
1	2	1206	C	O4'-C1'-N1	5.03	112.22	108.20
1	2	1502	C	N1-C2-O2	5.03	121.92	118.90
36	j	136	TRP	CE2-CD2-CE3	5.02	124.72	118.70
1	2	1624	U	C6-N1-C1'	-5.01	114.19	121.20
1	2	188	C	C2-N1-C1'	5.01	124.31	118.80
1	2	1057	C	N3-C2-O2	-5.00	118.40	121.90

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	A	97/144 (67%)	92 (95%)	5 (5%)	0	100	100
3	B	215/295 (73%)	202 (94%)	13 (6%)	0	100	100
4	C	211/264 (80%)	198 (94%)	13 (6%)	0	100	100
5	D	219/221 (99%)	216 (99%)	3 (1%)	0	100	100
6	E	226/281 (80%)	219 (97%)	7 (3%)	0	100	100
7	F	260/263 (99%)	250 (96%)	10 (4%)	0	100	100
8	G	189/204 (93%)	181 (96%)	8 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	H	235/249 (94%)	231 (98%)	4 (2%)	0	100	100
10	I	181/432 (42%)	173 (96%)	8 (4%)	0	100	100
11	J	205/208 (99%)	191 (93%)	14 (7%)	0	100	100
12	K	183/194 (94%)	181 (99%)	2 (1%)	0	100	100
13	L	94/149 (63%)	86 (92%)	8 (8%)	0	100	100
14	M	149/158 (94%)	136 (91%)	13 (9%)	0	100	100
15	N	115/132 (87%)	106 (92%)	9 (8%)	0	100	100
16	O	147/151 (97%)	145 (99%)	2 (1%)	0	100	100
17	P	134/168 (80%)	122 (91%)	12 (9%)	0	100	100
18	Q	118/145 (81%)	111 (94%)	7 (6%)	0	100	100
19	R	140/172 (81%)	134 (96%)	6 (4%)	0	100	100
20	S	130/135 (96%)	117 (90%)	13 (10%)	0	100	100
21	T	142/152 (93%)	137 (96%)	5 (4%)	0	100	100
22	U	139/145 (96%)	134 (96%)	5 (4%)	0	100	100
23	V	98/119 (82%)	94 (96%)	4 (4%)	0	100	100
24	W	81/83 (98%)	78 (96%)	3 (4%)	0	100	100
25	X	127/130 (98%)	124 (98%)	3 (2%)	0	100	100
26	Y	139/143 (97%)	137 (99%)	2 (1%)	0	100	100
27	Z	122/131 (93%)	119 (98%)	3 (2%)	0	100	100
28	a	75/124 (60%)	73 (97%)	2 (3%)	0	100	100
29	b	99/101 (98%)	96 (97%)	3 (3%)	0	100	100
30	c	81/84 (96%)	77 (95%)	4 (5%)	0	100	100
31	d	65/69 (94%)	60 (92%)	5 (8%)	0	100	100
32	e	53/56 (95%)	51 (96%)	2 (4%)	0	100	100
33	f	55/133 (41%)	54 (98%)	1 (2%)	0	100	100
34	g	66/188 (35%)	60 (91%)	6 (9%)	0	100	100
35	h	311/317 (98%)	298 (96%)	13 (4%)	0	100	100
36	j	180/315 (57%)	173 (96%)	7 (4%)	0	100	100
37	n	23/25 (92%)	23 (100%)	0	0	100	100
All	All	5104/6280 (81%)	4879 (96%)	225 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	
2	A	84/123 (68%)	84 (100%)	0	100	100
3	B	180/245 (74%)	179 (99%)	1 (1%)	86	94
4	C	194/231 (84%)	194 (100%)	0	100	100
5	D	187/187 (100%)	187 (100%)	0	100	100
6	E	190/232 (82%)	188 (99%)	2 (1%)	73	88
7	F	224/225 (100%)	224 (100%)	0	100	100
8	G	161/170 (95%)	160 (99%)	1 (1%)	86	94
9	H	207/218 (95%)	206 (100%)	1 (0%)	88	94
10	I	165/360 (46%)	165 (100%)	0	100	100
11	J	179/180 (99%)	179 (100%)	0	100	100
12	K	161/168 (96%)	161 (100%)	0	100	100
13	L	87/125 (70%)	87 (100%)	0	100	100
14	M	136/142 (96%)	133 (98%)	3 (2%)	52	78
15	N	99/108 (92%)	98 (99%)	1 (1%)	76	88
16	O	130/131 (99%)	130 (100%)	0	100	100
17	P	106/130 (82%)	106 (100%)	0	100	100
18	Q	109/130 (84%)	109 (100%)	0	100	100
19	R	117/140 (84%)	117 (100%)	0	100	100
20	S	119/121 (98%)	118 (99%)	1 (1%)	81	91
21	T	125/132 (95%)	124 (99%)	1 (1%)	81	91
22	U	111/116 (96%)	111 (100%)	0	100	100
23	V	92/107 (86%)	92 (100%)	0	100	100
24	W	67/67 (100%)	67 (100%)	0	100	100
25	X	112/113 (99%)	112 (100%)	0	100	100
26	Y	113/115 (98%)	113 (100%)	0	100	100
27	Z	107/113 (95%)	106 (99%)	1 (1%)	78	90

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
28	a	68/102 (67%)	68 (100%)	0	100	100
29	b	88/88 (100%)	88 (100%)	0	100	100
30	c	75/76 (99%)	75 (100%)	0	100	100
31	d	60/62 (97%)	60 (100%)	0	100	100
32	e	48/49 (98%)	47 (98%)	1 (2%)	53	79
33	f	47/106 (44%)	47 (100%)	0	100	100
34	g	61/154 (40%)	60 (98%)	1 (2%)	62	83
35	h	272/275 (99%)	272 (100%)	0	100	100
36	j	84/280 (30%)	81 (96%)	3 (4%)	35	66
37	n	24/24 (100%)	24 (100%)	0	100	100
All	All	4389/5345 (82%)	4372 (100%)	17 (0%)	91	96

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	B	205	ARG
6	E	76	ARG
6	E	227	LYS
8	G	60	ARG
9	H	98	ARG
14	M	21	LYS
14	M	69	ARG
14	M	104	LYS
15	N	96	ARG
20	S	116	ASN
21	T	73	ASN
27	Z	99	LYS
32	e	19	ARG
34	g	138	ARG
36	j	142	TYR
36	j	147	TYR
36	j	150	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
13	L	44	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
14	M	141	ASN
21	T	72	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1685/1870 (90%)	307 (18%)	10 (0%)
38	z	186/400 (46%)	52 (27%)	0
39	i	74/75 (98%)	15 (20%)	0
All	All	1945/2345 (82%)	374 (19%)	10 (0%)

All (374) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	4	C
1	2	5	U
1	2	26	U
1	2	33	G
1	2	41	G
1	2	44	U
1	2	46	A
1	2	49	C
1	2	56	G
1	2	67	C
1	2	68	A
1	2	73	C
1	2	74	G
1	2	76	U
1	2	103	A
1	2	113	G
1	2	114	G
1	2	115	U
1	2	126	G
1	2	130	G
1	2	142	C
1	2	143	U
1	2	146	G
1	2	147	A
1	2	149	A
1	2	158	A
1	2	162	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2	170	A
1	2	180	G
1	2	182	C
1	2	183	G
1	2	184	G
1	2	186	C
1	2	190	G
1	2	191	A
1	2	192	C
1	2	199	C
1	2	208	G
1	2	292	A
1	2	305	U
1	2	306	C
1	2	307	G
1	2	309	G
1	2	312	G
1	2	313	A
1	2	319	C
1	2	320	G
1	2	323	C
1	2	330	G
1	2	347	G
1	2	357	C
1	2	364	A
1	2	368	U
1	2	370	G
1	2	383	G
1	2	384	U
1	2	385	G
1	2	398	A
1	2	399	C
1	2	400	C
1	2	407	G
1	2	408	A
1	2	409	C
1	2	418	A
1	2	420	G
1	2	437	G
1	2	438	G
1	2	446	G
1	2	448	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2	449	A
1	2	450	C
1	2	465	A
1	2	471	G
1	2	472	C
1	2	474	G
1	2	487	U
1	2	488	U
1	2	489	A
1	2	492	C
1	2	493	A
1	2	500	A
1	2	502	C
1	2	508	A
1	2	525	A
1	2	531	A
1	2	532	C
1	2	536	A
1	2	537	C
1	2	541	U
1	2	542	U
1	2	546	G
1	2	547	G
1	2	549	C
1	2	550	C
1	2	551	U
1	2	554	A
1	2	555	A
1	2	556	U
1	2	561	A
1	2	562	U
1	2	576	A
1	2	583	A
1	2	588	G
1	2	589	G
1	2	590	A
1	2	591	U
1	2	598	G
1	2	606	G
1	2	608	C
1	2	614	C
1	2	617	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2	623	G
1	2	627	U
1	2	628	A
1	2	629	A
1	2	643	A
1	2	644	G
1	2	655	A
1	2	660	C
1	2	663	C
1	2	668	A
1	2	669	A
1	2	671	A
1	2	672	A
1	2	689	U
1	2	691	G
1	2	694	G
1	2	696	G
1	2	750	C
1	2	752	G
1	2	753	C
1	2	798	G
1	2	799	U
1	2	801	U
1	2	811	A
1	2	821	G
1	2	822	U
1	2	830	A
1	2	834	C
1	2	844	U
1	2	847	A
1	2	870	A
1	2	871	U
1	2	872	A
1	2	873	G
1	2	874	G
1	2	875	A
1	2	878	G
1	2	883	U
1	2	886	A
1	2	887	U
1	2	888	U
1	2	890	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2	891	G
1	2	892	U
1	2	894	G
1	2	895	G
1	2	899	U
1	2	900	C
1	2	901	G
1	2	902	G
1	2	904	A
1	2	913	A
1	2	914	U
1	2	919	A
1	2	920	A
1	2	933	G
1	2	955	A
1	2	971	G
1	2	990	A
1	2	992	A
1	2	999	G
1	2	1017	U
1	2	1023	A
1	2	1045	U
1	2	1061	U
1	2	1070	A
1	2	1078	C
1	2	1083	A
1	2	1085	C
1	2	1086	G
1	2	1109	C
1	2	1114	U
1	2	1121	G
1	2	1138	C
1	2	1149	A
1	2	1150	A
1	2	1153	C
1	2	1154	U
1	2	1165	G
1	2	1195	A
1	2	1207	G
1	2	1215	C
1	2	1217	A
1	2	1224	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2	1242	U
1	2	1251	A
1	2	1253	A
1	2	1256	G
1	2	1257	G
1	2	1259	A
1	2	1264	C
1	2	1274	G
1	2	1275	G
1	2	1285	G
1	2	1286	G
1	2	1287	A
1	2	1293	A
1	2	1294	G
1	2	1295	A
1	2	1297	U
1	2	1298	G
1	2	1299	A
1	2	1300	U
1	2	1301	A
1	2	1302	G
1	2	1303	C
1	2	1309	C
1	2	1313	A
1	2	1330	G
1	2	1333	U
1	2	1342	U
1	2	1348	G
1	2	1358	U
1	2	1361	G
1	2	1363	C
1	2	1364	U
1	2	1371	U
1	2	1372	U
1	2	1378	A
1	2	1396	A
1	2	1404	U
1	2	1428	G
1	2	1442	U
1	2	1452	A
1	2	1454	A
1	2	1462	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2	1463	U
1	2	1475	G
1	2	1477	U
1	2	1480	A
1	2	1487	A
1	2	1489	A
1	2	1490	G
1	2	1497	G
1	2	1498	A
1	2	1507	G
1	2	1521	C
1	2	1522	A
1	2	1533	A
1	2	1535	U
1	2	1536	G
1	2	1548	G
1	2	1551	U
1	2	1554	C
1	2	1556	A
1	2	1567	G
1	2	1573	G
1	2	1575	G
1	2	1578	U
1	2	1580	A
1	2	1585	U
1	2	1588	A
1	2	1601	A
1	2	1604	G
1	2	1621	U
1	2	1623	A
1	2	1637	A
1	2	1638	G
1	2	1648	G
1	2	1659	U
1	2	1660	C
1	2	1661	A
1	2	1665	G
1	2	1695	A
1	2	1699	A
1	2	1715	A
1	2	1721	U
1	2	1722	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2	1744	G
1	2	1749	G
1	2	1751	C
1	2	1756	C
1	2	1760	G
1	2	1774	C
1	2	1779	G
1	2	1781	A
1	2	1782	G
1	2	1783	C
1	2	1784	G
1	2	1817	G
1	2	1819	A
1	2	1823	A
1	2	1824	A
1	2	1826	G
1	2	1831	A
1	2	1834	A
1	2	1836	G
1	2	1838	U
1	2	1840	U
1	2	1849	G
1	2	1851	A
1	2	1852	C
1	2	1861	G
1	2	1862	G
1	2	1863	A
1	2	1865	C
38	z	121	C
38	z	137	G
38	z	144	U
38	z	154	A
38	z	157	C
38	z	161	G
38	z	162	A
38	z	163	G
38	z	165	A
38	z	166	C
38	z	167	A
38	z	168	C
38	z	169	C
38	z	173	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
38	z	229	G
38	z	234	U
38	z	237	C
38	z	240	C
38	z	244	A
38	z	253	G
38	z	258	G
38	z	259	U
38	z	265	U
38	z	266	G
38	z	279	C
38	z	280	C
38	z	281	U
38	z	282	U
38	z	288	A
38	z	295	G
38	z	296	A
38	z	297	U
38	z	306	U
38	z	324	U
38	z	325	C
38	z	328	G
38	z	330	A
38	z	331	G
38	z	332	A
38	z	333	C
38	z	334	C
38	z	335	G
38	z	337	G
38	z	338	C
38	z	345	A
38	z	346	G
38	z	348	A
38	z	349	C
38	z	352	A
38	z	353	U
38	z	355	C
38	z	356	U
39	i	4	A
39	i	16	C
39	i	17	G
39	i	18	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
39	i	19	A
39	i	20	A
39	i	47	C
39	i	48	G
39	i	58	A
39	i	59	A
39	i	60	C
39	i	70	C
39	i	73	C
39	i	74	C
39	i	75	A

All (10) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	383	G
1	2	445	A
1	2	553	U
1	2	561	A
1	2	688	U
1	2	874	G
1	2	886	A
1	2	1137	U
1	2	1395	C
1	2	1637	A

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

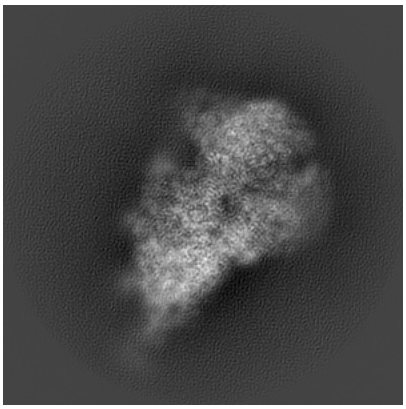
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-25539. These allow visual inspection of the internal detail of the map and identification of artifacts.

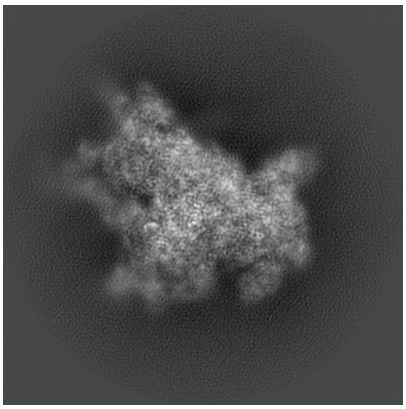
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

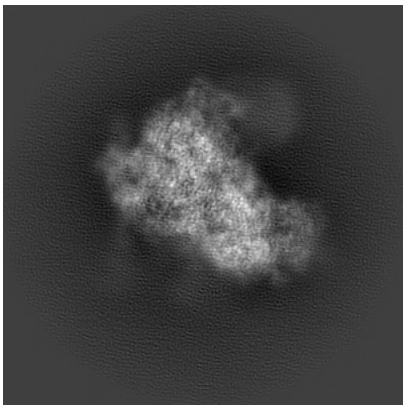
6.1.1 Primary map



X

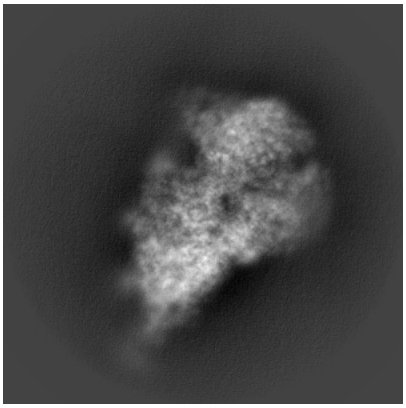


Y

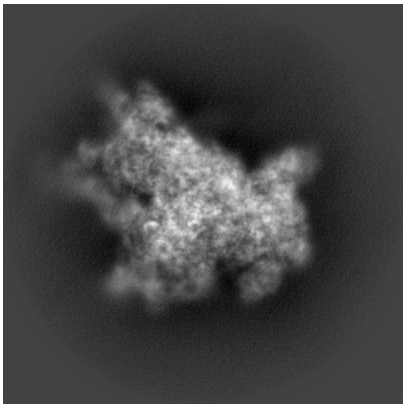


Z

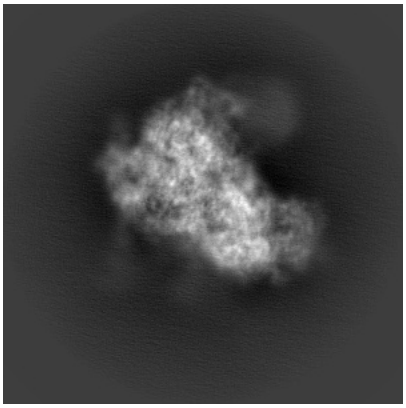
6.1.2 Raw map



X



Y

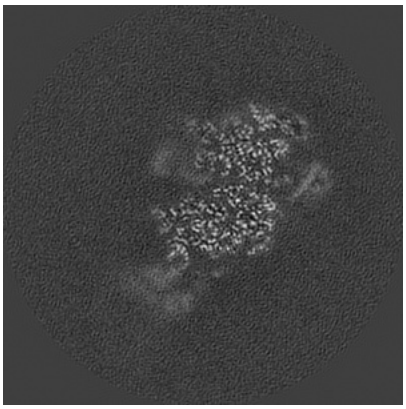


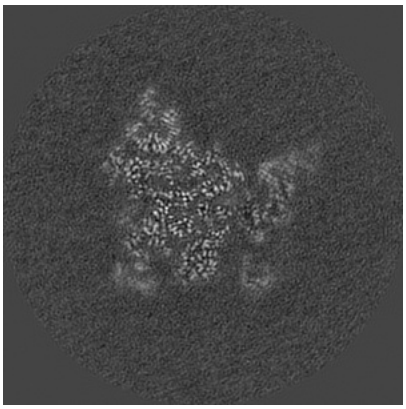
Z

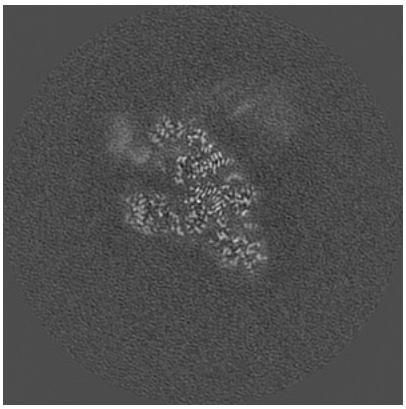
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

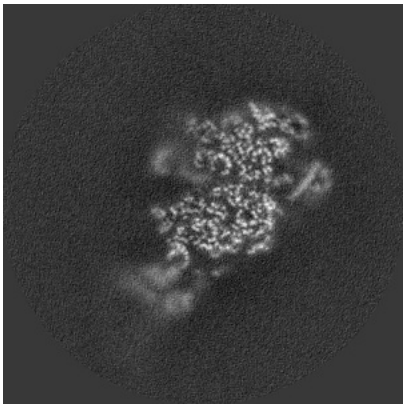
6.2.1 Primary map

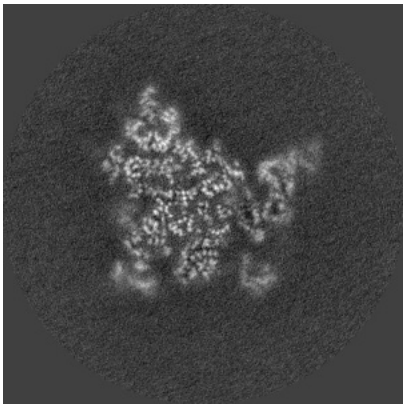

X Index: 200

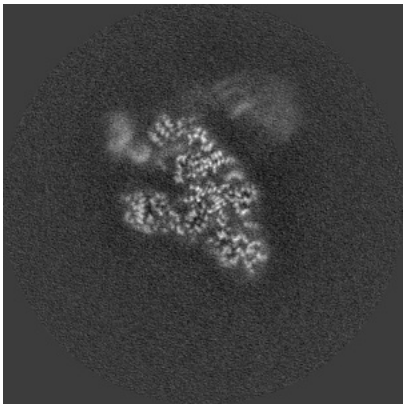

Y Index: 200


Z Index: 200

6.2.2 Raw map


X Index: 200

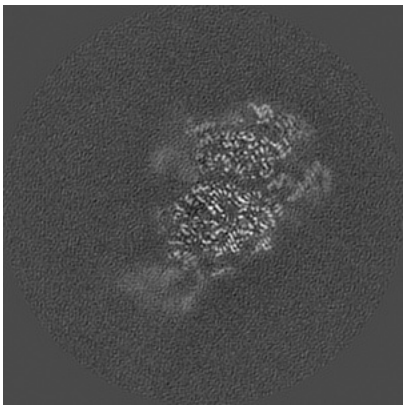

Y Index: 200

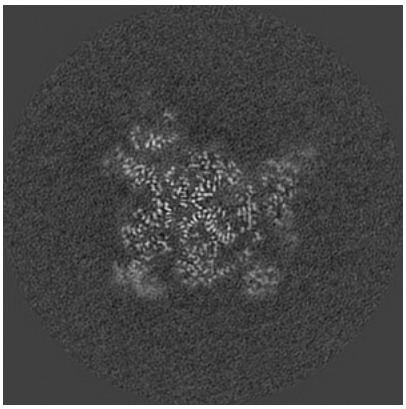

Z Index: 200

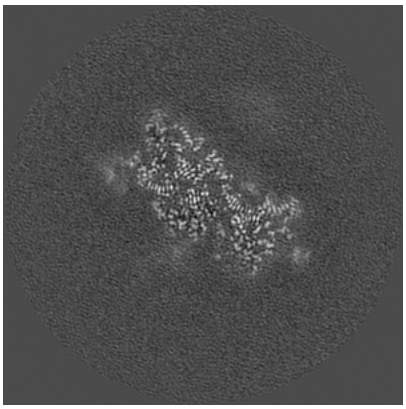
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

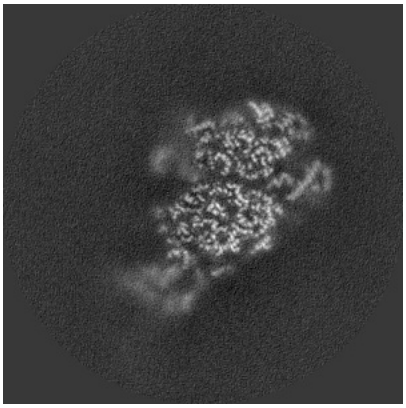
6.3.1 Primary map

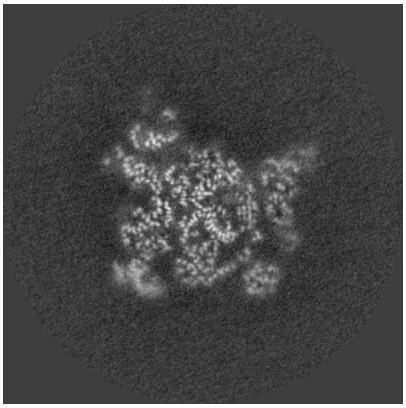

X Index: 197

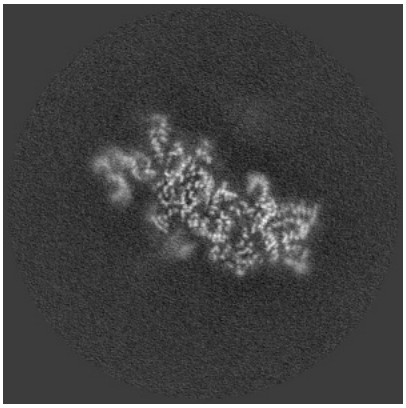

Y Index: 206


Z Index: 165

6.3.2 Raw map


X Index: 198

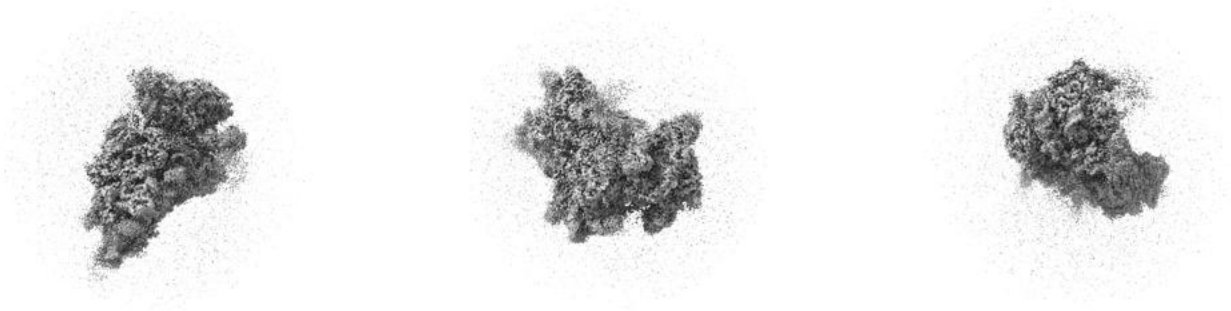

Y Index: 206


Z Index: 153

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.014. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map

X Y Z

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

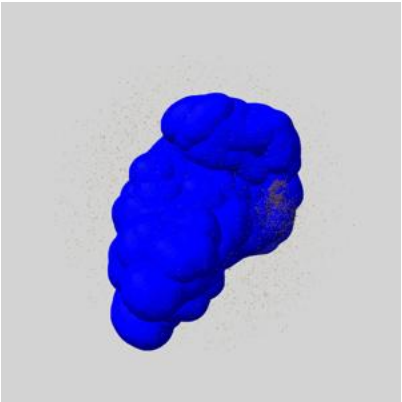
6.5 Mask visualisation (i)

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

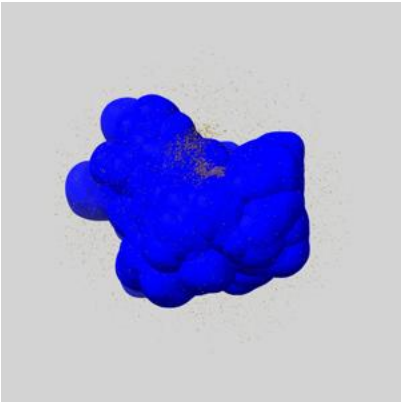
A mask typically either:

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

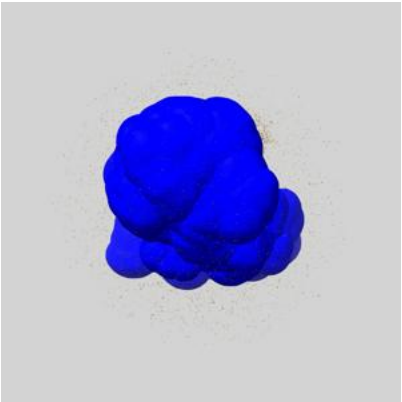
6.5.1 emd_25539_msk_1.map (i)



X



Y

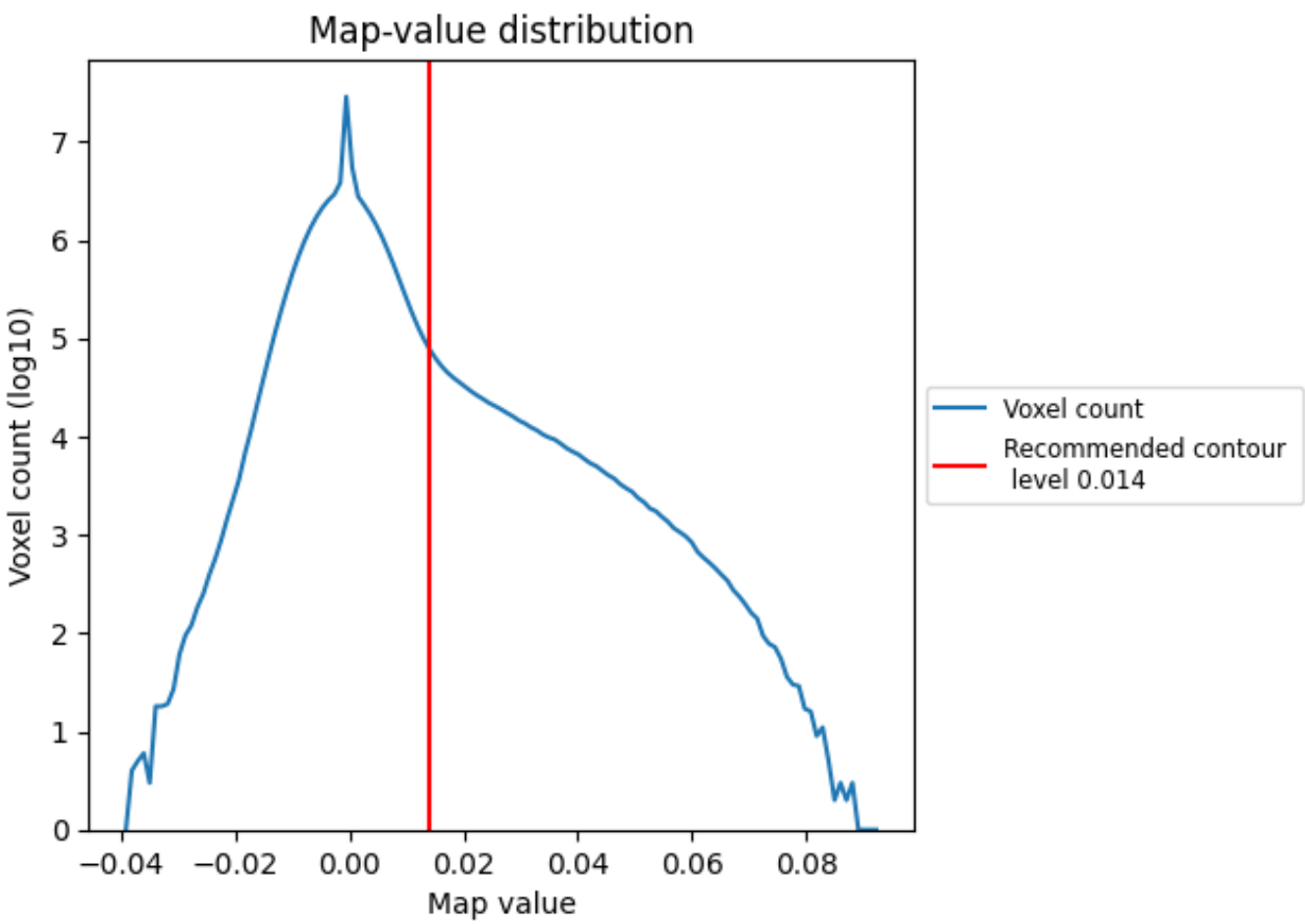


Z

7 Map analysis (i)

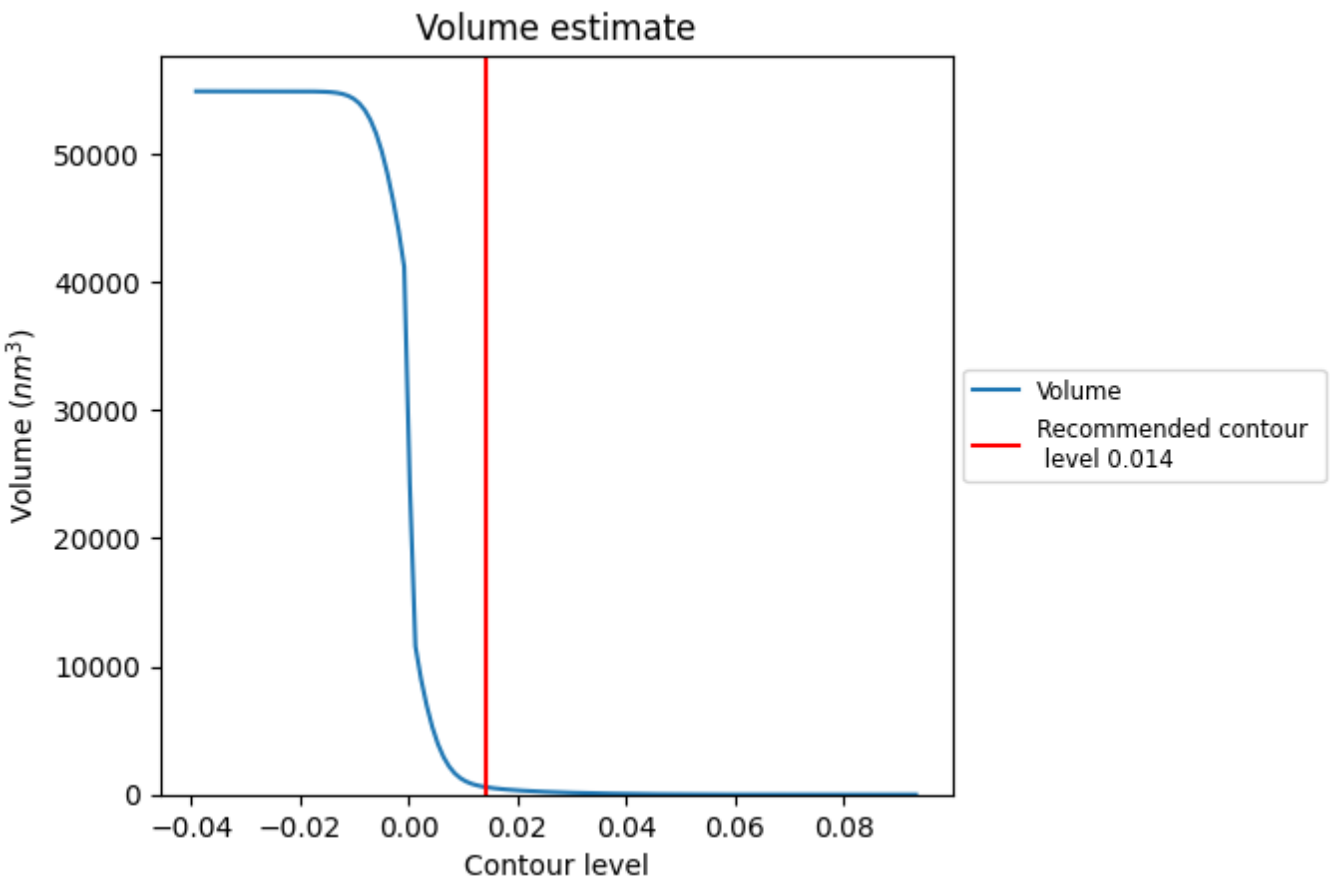
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

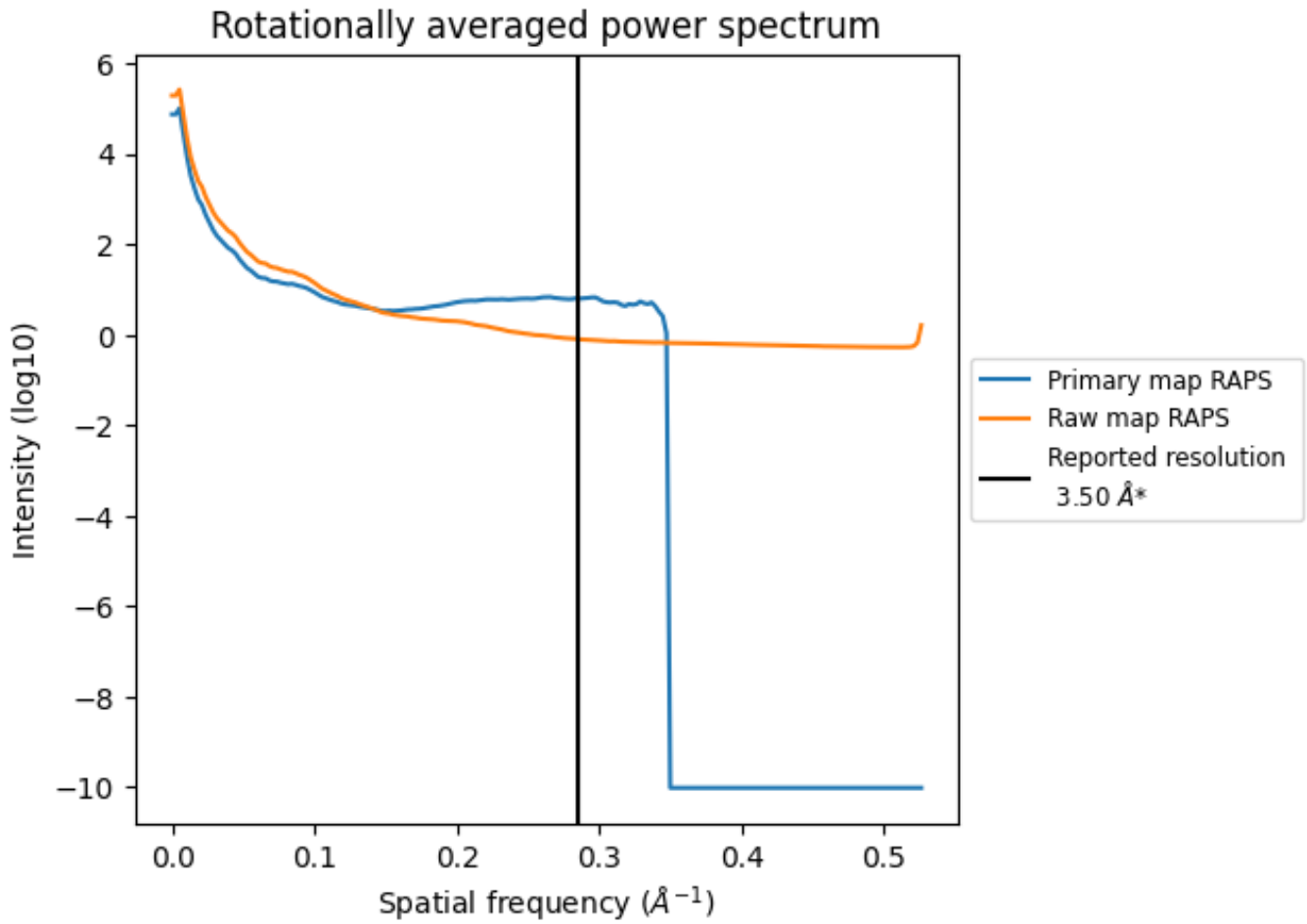
7.2 Volume estimate (i)



The volume at the recommended contour level is 594 nm^3; this corresponds to an approximate mass of 536 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)

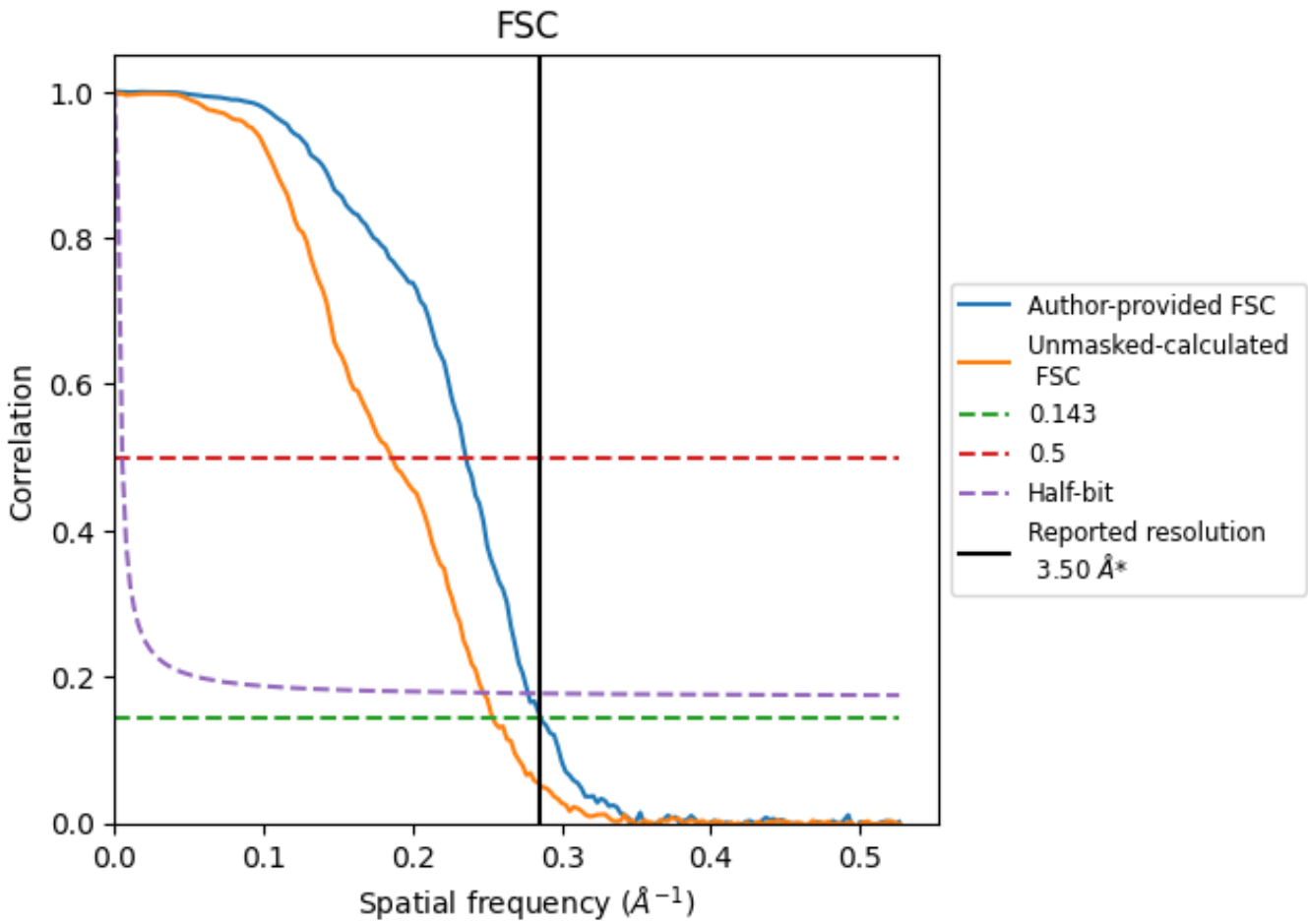


*Reported resolution corresponds to spatial frequency of 0.286 Å^{-1}

8 Fourier-Shell correlation (i)

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

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.286 Å^{-1}

8.2 Resolution estimates (i)

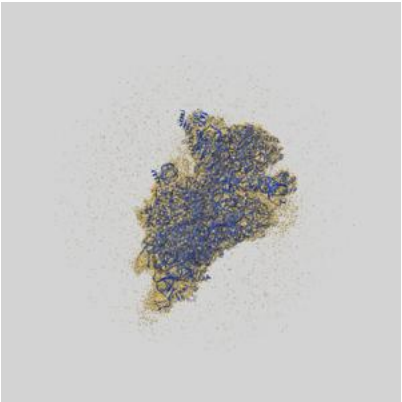
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	3.50	4.24	3.61
Unmasked-calculated*	3.94	5.38	4.04

*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 3.94 differs from the reported value 3.5 by more than 10 %

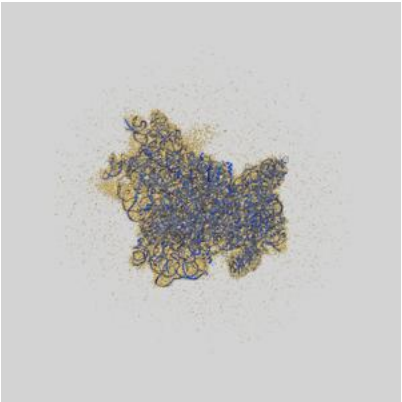
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-25539 and PDB model 7SYS. Per-residue inclusion information can be found in section 3 on page 12.

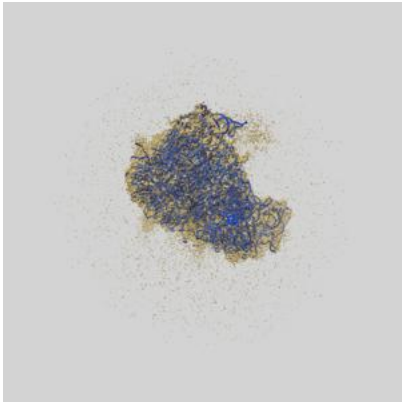
9.1 Map-model overlay (i)



X



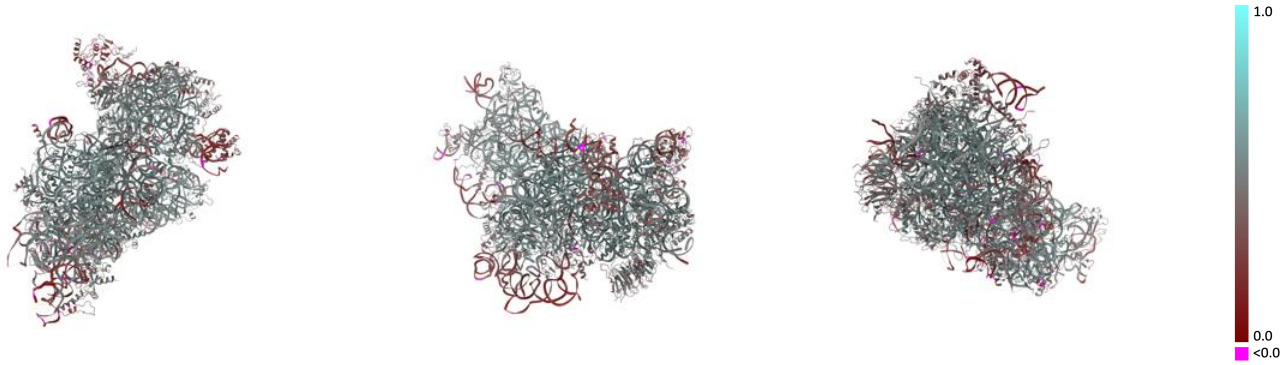
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.014 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.

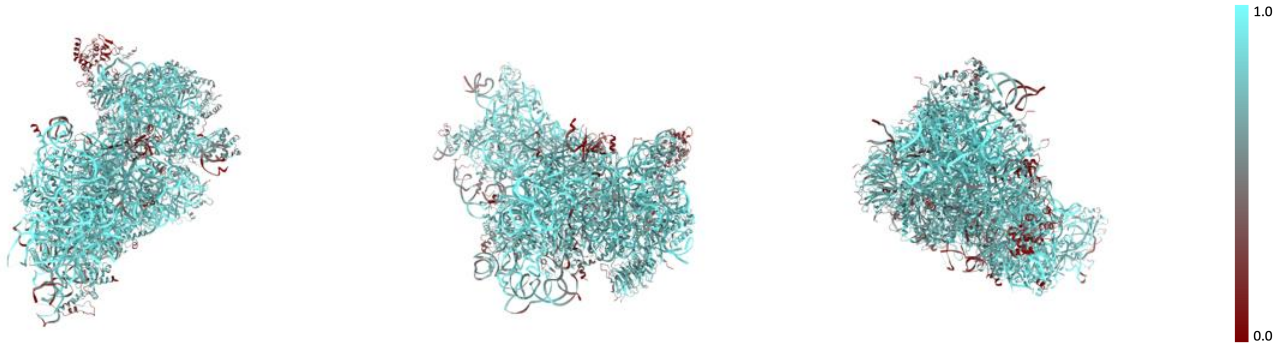
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according 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.

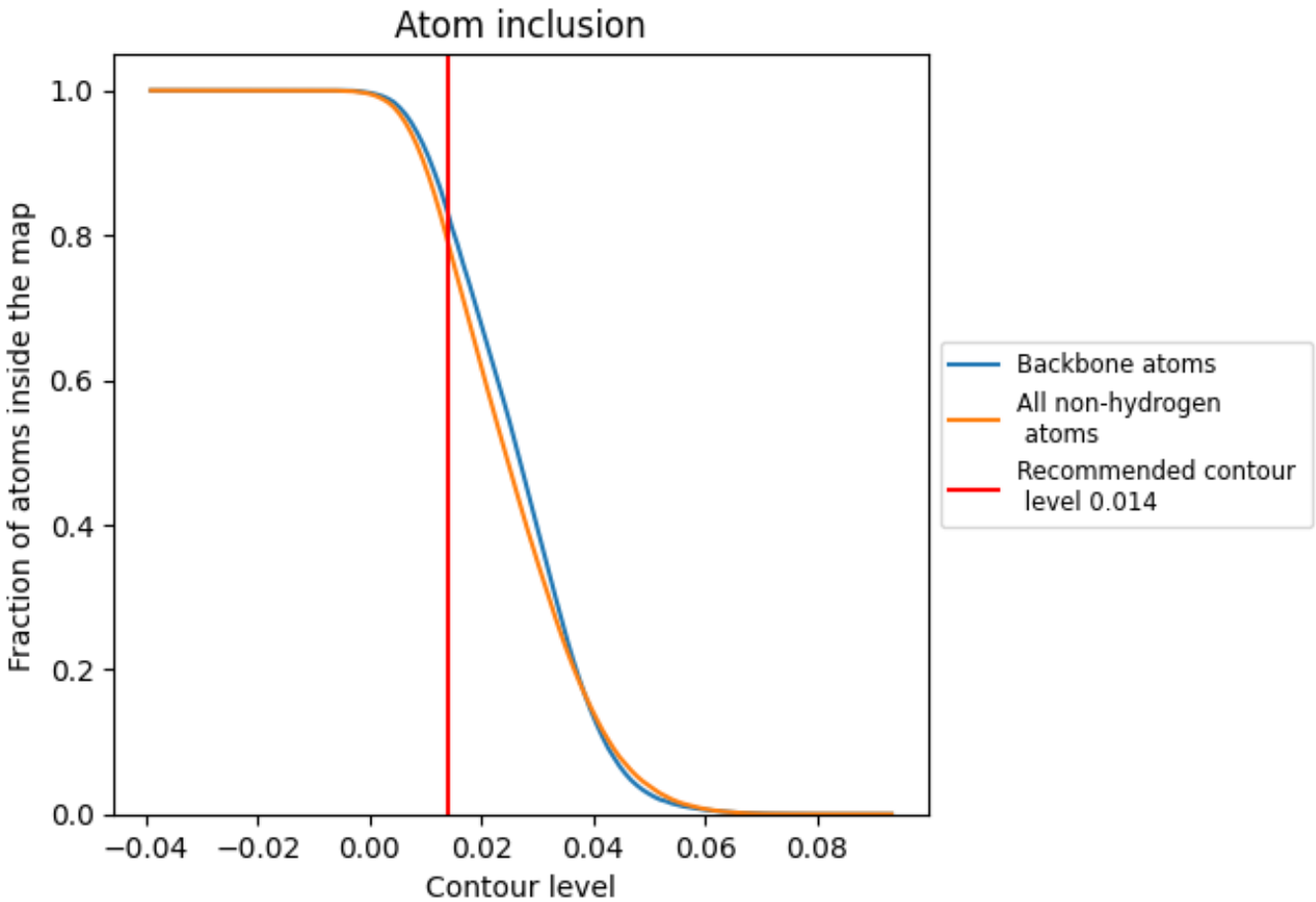
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.014).

9.4 Atom inclusion (i)



At the recommended contour level, 83% of all backbone atoms, 79% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.014) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7898	0.4690
2	0.8881	0.4940
A	0.1553	0.3060
B	0.7993	0.5130
C	0.7899	0.5090
D	0.8029	0.5200
E	0.6759	0.4730
F	0.8222	0.5230
G	0.7793	0.5090
H	0.7326	0.4290
I	0.5777	0.4350
J	0.7437	0.4750
K	0.8068	0.5070
L	0.6911	0.4320
M	0.7696	0.5110
N	0.1644	0.2440
O	0.8259	0.5220
P	0.7852	0.5040
Q	0.6891	0.4110
R	0.8288	0.5150
S	0.7283	0.4680
T	0.6865	0.4480
U	0.8435	0.5110
V	0.6447	0.4690
W	0.8199	0.5280
X	0.8554	0.5460
Y	0.7955	0.5230
Z	0.8247	0.4950
a	0.5893	0.4370
b	0.8223	0.5300
c	0.7637	0.4910
d	0.6850	0.4770
e	0.8594	0.5370
f	0.6500	0.4670
g	0.2500	0.2910

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
h	0.7202	0.4450
i	0.6552	0.3160
j	0.6896	0.3880
n	0.7018	0.4730
z	0.6176	0.2600