Full wwPDB EM Validation Report (i)

Apr 22, 2024 – 10:56 pm BST

PDB ID	:	6ZVI
EMDB ID	:	EMD-11457
Title	:	Mbf1-ribosome complex
Authors	:	Best, K.M.; Denk, T.; Cheng, J.; Thoms, M.; Berninghausen, O.; Beckmann, R.
Deposited on	:	2020-07-24
Resolution	:	3.00 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 (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:

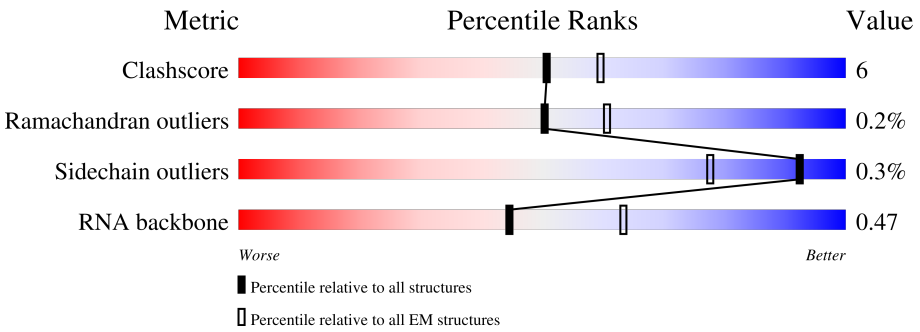
EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 3.00 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 <=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	d	76	70%; 57%, 37%, 7%
2	e	77	75%; 47%, 51%, •
3	f	35	69%; 37%, 54%, 9%
4	h	1758	14%; 68%, 28%, •
5	i	206	17%; 98%, •
6	j	216	27%; 100%
7	k	217	6%; 100%

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Mol	Chain	Length	Quality of chain
8	l	223	23% 98%
9	m	260	9% 99%
10	n	206	15% 99%
11	o	218	31% 99%
12	p	185	50% 98%
13	q	199	14% 94% 6%
14	r	185	20% 97%
15	s	92	29% 98%
16	t	146	11% 99%
17	u	124	90% 98%
18	v	150	99%
19	x	119	30% 98%
20	y	141	7% 99%
21	z	125	38% 98%
22	A	145	19% 82% 18%
23	B	143	17% 89% 11%
24	C	101	42% 86% 13%
25	D	87	20% 95% 5%
26	E	129	92% 8%
27	H	144	83% 17%
28	I	134	24% 78% 21%
29	J	69	35% 84% 16%
30	L	81	23% 83% 17%
31	N	63	21% 86% 14%
32	P	46	22% 96%

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Mol	Chain	Length	Quality of chain
33	Q	73	85% 71% 29%
34	R	313	68% 86% 14%
35	T	111	86% 88% 12%
36	O	53	87% 13%
37	w	128	9% 100%
38	K	97	7% 84% 15%

2 Entry composition (i)

There are 39 unique types of molecules in this entry. The entry contains 80088 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 A/P-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	d	76	1620	723	290	532	75	0	0

- Molecule 2 is a RNA chain called P/E-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	e	77	1644	732	297	538	77	0	0

- Molecule 3 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	f	35	724	325	102	262	35	0	0

- Molecule 4 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
4	h	1758	37455	16745	6624	12328	1758	0	0

- Molecule 5 is a protein called 40S ribosomal protein S0-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	i	206	1583	1017	281	283	2	0	0

- Molecule 6 is a protein called RPS1A isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	j	216	1722	1091	312	315	4	0	0

- Molecule 7 is a protein called RPS2 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	k	217	1635	1047	289	297	2	0	0

- Molecule 8 is a protein called RPS3 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	l	223	1734	1101	313	314	6	0	0

- Molecule 9 is a protein called 40S ribosomal protein S4-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	m	260	2068	1316	389	360	3	0	0

- Molecule 10 is a protein called Rps5p.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	n	206	1609	1007	300	299	3	0	0

- Molecule 11 is a protein called 40S ribosomal protein S6-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	o	218	1755	1102	337	313	3	0	0

- Molecule 12 is a protein called 40S ribosomal protein S7-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
12	p	185	1486	954	266	266	0	0

- Molecule 13 is a protein called 40S ribosomal protein S8-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	q	188	1489	925	298	264	2	0	0

- Molecule 14 is a protein called 40S ribosomal protein S9-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	r	185	1494	943	289	261	1	0	0

- Molecule 15 is a protein called 40S ribosomal protein S10-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	s	92	741	478	121	140	2	0	0

- Molecule 16 is a protein called 40S ribosomal protein S11-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	t	146	1168	747	221	197	3	0	0

- Molecule 17 is a protein called RPS12 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	u	124	890	560	156	172	2	0	0

- Molecule 18 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	v	150	1192	759	224	207	2	0	0

- Molecule 19 is a protein called RPS15 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	x	119	939	595	176	161	7	0	0

- Molecule 20 is a protein called 40S ribosomal protein S16-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
20	y	141	1105	708	203	194	0	0

- Molecule 21 is a protein called 40S ribosomal protein S17-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	z	125	1001	625	188	186	2	0	0

- Molecule 22 is a protein called 40S ribosomal protein S18-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	A	145	1192	743	237	210	2	0	0

- Molecule 23 is a protein called 40S ribosomal protein S19-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	B	143	1112	694	208	208	2	0	0

- Molecule 24 is a protein called RPS20 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	C	101	805	512	145	147	1	0	0

- Molecule 25 is a protein called 40S ribosomal protein S21-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	D	87	684	420	125	137	2	0	0

- Molecule 26 is a protein called RPS22A isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	E	129	1021	650	188	180	3	0	0

- Molecule 27 is a protein called 40S ribosomal protein S23-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	H	144	1121	708	220	191	2	0	0

- Molecule 28 is a protein called 40S ribosomal protein S24-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
28	I	134	1073	676	208	189	0	0

- Molecule 29 is a protein called RPS25A isoform 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
29	J	69	558	357	103	98	0	0

- Molecule 30 is a protein called 40S ribosomal protein S27-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	L	81	610	382	110	113	5	0	0

- Molecule 31 is a protein called RPS28A isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	N	63	497	306	99	91	1	0	0

- Molecule 32 is a protein called 40S ribosomal protein S30-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
32	P	46	370	236	75	59	0	0

- Molecule 33 is a protein called RPS31 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	Q	73	556	352	105	95	4	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	97	ALA	LYS	conflict	UNP A0A6A5PU37

- Molecule 34 is a protein called Guanine nucleotide-binding protein subunit beta-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	R	313	2403	1521	411	463	8	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	161	ALA	LYS	conflict	UNP P38011

- Molecule 35 is a protein called MBF1 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	T	111	870	528	174	167	1	0	0

- Molecule 36 is a protein called RPS29A isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	O	53	442	274	92	72	4	0	0

- Molecule 37 is a protein called 40S ribosomal protein S14-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	w	128	949	582	188	176	3	0	0

- Molecule 38 is a protein called RPS26B isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
38	K	97	769	475	160	129	5	0	0

- Molecule 39 is ZINC ION (three-letter code: ZN) (formula: Zn).

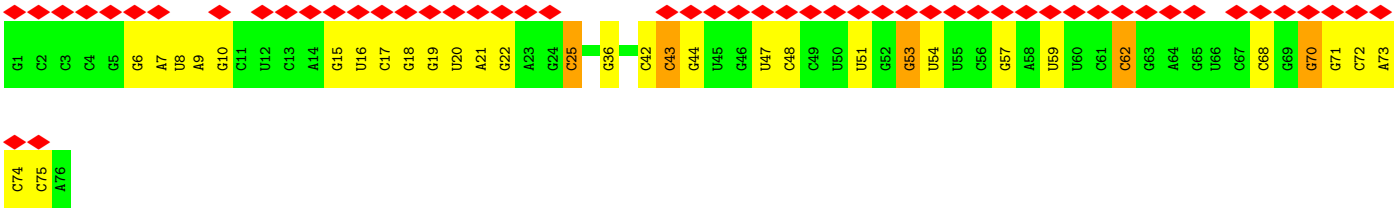
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
39	L	1	1	1	0
39	O	1	Total	Zn	0
			1	1	

3 Residue-property plots (i)

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

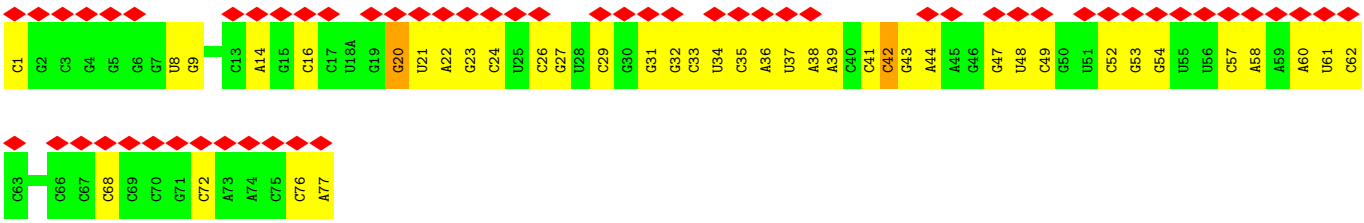
- Molecule 1: A/P-site tRNA

Chain d:



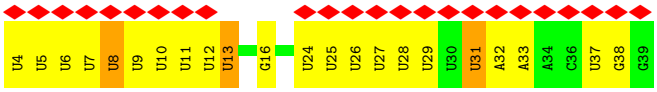
- Molecule 2: P/E-site tRNA

Chain e:



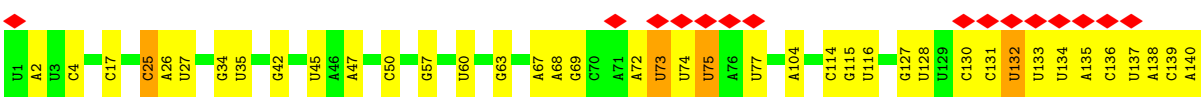
- Molecule 3: mRNA

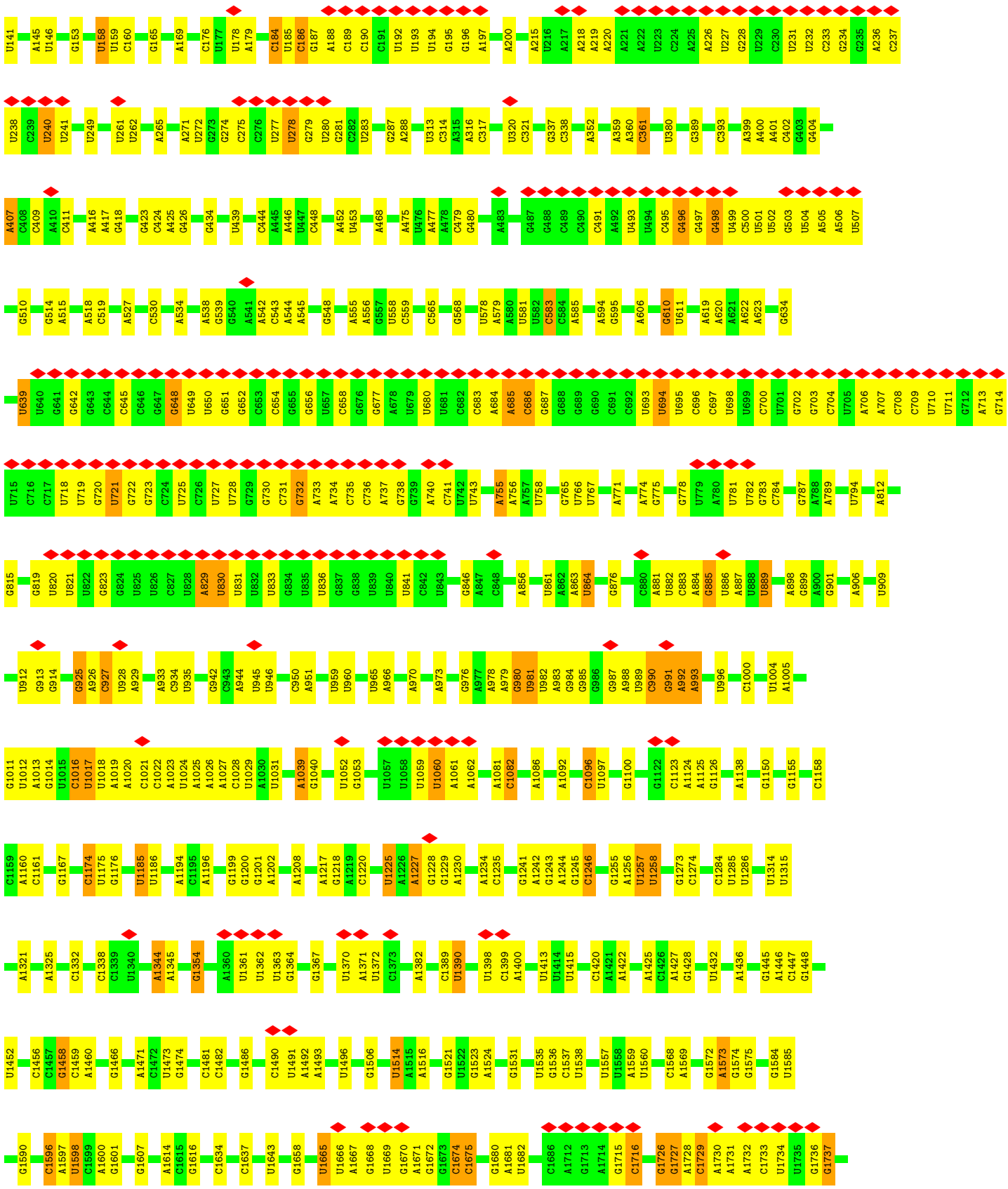
Chain f:



- Molecule 4: 18S rRNA

Chain h:

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U238 C239 U240 U241 U249 U261 U262 A265 A271 U272 C273 G274 C275 C276 U277 U278 G279 U280 G281 C282 U283 G287 A288 U313 C314 A315 A316 C317 U320 C321 G337 C338 A352 A359 A360 C361 U380 G389 C393 A399 A400 A401 C402 G403 C404
A407 C408 C409 A410 C411 A416 A417 G418 G423 C424 A425 G426 G434 U439 C444 A445 A446 U447 C448 A452 U453 A468 A475 U476 A477 A478 C479 G480 A483 G487 G488 C489 C490 C491 A492 U493 U494 C495 G496 G497 G498 U499 C500 U501 U502 G503 U504 A505 A506 U507
G510 G514 A515 A518 C519 A527 C530 A534 A538 G539 G540 A541 A542 C543 A544 A545 G548 A555 A556 G557 U558 C559 C565 G568 U578 A579 A580 U581 U582 C583 C584 A585 A594 G595 A606 G610 U611 A619 A620 A621 A622 A623 G634
U639 U640 G641 G642 G643 C644 C645 C646 G647 G648 U649 U650 G651 G652 C653 C654 G655 G656 U657 C658 G676 G677 A678 U679 U680 U681 C682 C683 A684 A685 C686 G687 G688 G689 G690 C691 C692 U693 U694 U695 C696 C697 U698 U699 C700 U701 G702 G703 C704 U705 A706 A707 C708 C709 U710 U711 G712 A713 G714
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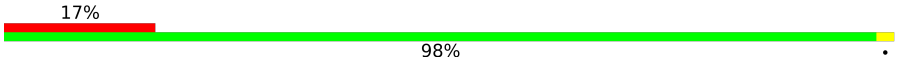
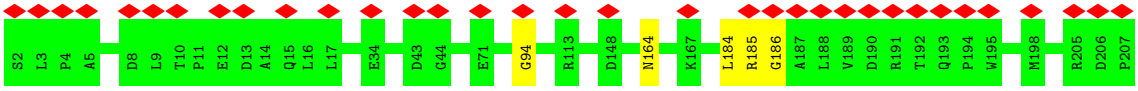
G815 G819 U820 U821 U822 G823 G824 U825 U826 C827 U828 A829 U830 U831 U832 U833 G834 U835 U836 G837 G838 U839 U840 U841 C842 U843 G846 A847 C848 A856 U861 A862 A863 U864 G876 C880 A881 U882 C883 A884 G885 U886 A887 U888 U889 A898 G899 A900 G901 A906 U909
U912 G913 G914 G925 A926 C927 U928 A929 A933 C934 U935 G942 C943 A944 U945 U946 C950 A951 U959 U960 U965 A966 A970 A973 G976 A977 A978 A979 G980 U981 U982 A983 G984 G985 C986 G987 A988 U989 C990 G991 A992 A993 U996 C1000 U1004 A1005
G1011 U1012 A1013 G1014 U1015 C1016 U1017 U1018 A1019 A1020 C1021 C1022 A1023 U1024 A1025 A1026 A1027 C1028 U1029 A1030 U1031 A1039 G1040 U1052 G1053 U1057 U1058 U1059 U1060 A1061 A1062 A1081 C1082 A1086 A1092 C1096 U1097 G1100 G1122 C1123 A1124 A1125 G1126 A1138 G1150 G1155 C1158
C1159 A1160 C1161 G1167 C1174 U1175 G1176 U1185 U1186 A1194 C1195 A1196 G1199 G1200 G1201 A1202 A1208 A1217 G1218 A1219 C1220 U1225 A1226 A1227 G1228 G1229 A1230 A1234 C1235 G1241 A1242 G1243 A1244 G1245 C1246 G1255 A1256 U1257 U1258 G1273 C1274 C1284 U1285 U1286 U1314 U1315
A1321 A1325 C1332 C1338 C1339 U1340 A1344 A1345 G1354 A1360 U1361 U1362 U1363 G1364 G1367 U1370 A1371 U1372 C1373 A1382 C1389 U1390 U1398 C1399 A1400 U1413 U1414 U1415 C1420 A1421 A1422 A1425 C1426 A1427 G1428 U1432 A1436 G1445 A1446 C1447 G1448
U1452 C1456 C1457 G1458 C1459 A1460 G1466 A1471 C1472 U1473 G1474 C1481 C1482 G1486 C1490 U1491 A1492 A1493 U1496 G1506 U1514 A1515 A1516 G1521 U1522 G1523 A1524 G1531 U1535 G1536 C1537 U1538 U1557 U1558 A1559 U1560 C1568 A1569 G1572 A1573 G1574 G1575 G1584 U1585
G1590 C1596 A1597 U1598 C1599 A1600 G1601 G1607 A1614 C1615 G1616 C1634 C1637 U1643 G1658 U1665 U1666 A1667 G1668 U1669 G1670 A1671 G1672 G1673 C1674 C1675 G1680 A1681 U1682 C1686 A1712 G1713 A1714 G1715 C1716 G1726 G1727 A1728 C1729 A1730 A1731 A1732 C1733 U1734 U1735 G1736 G1737

• Molecule 5: 40S ribosomal protein S0-A

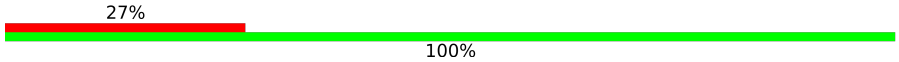
Chain i:

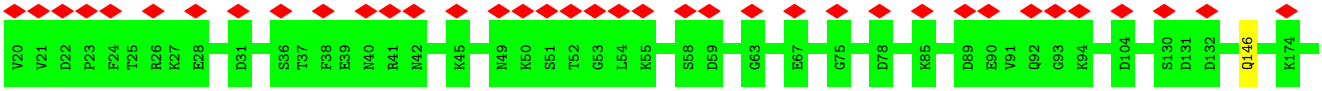


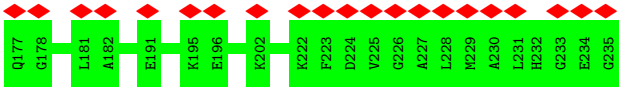


• Molecule 6: RPS1A isoform 1

Chain j:

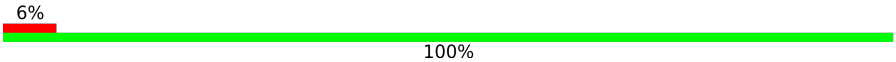






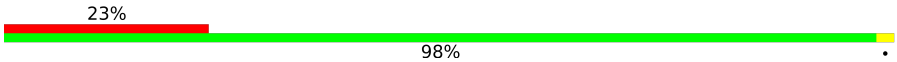
• Molecule 7: RPS2 isoform 1

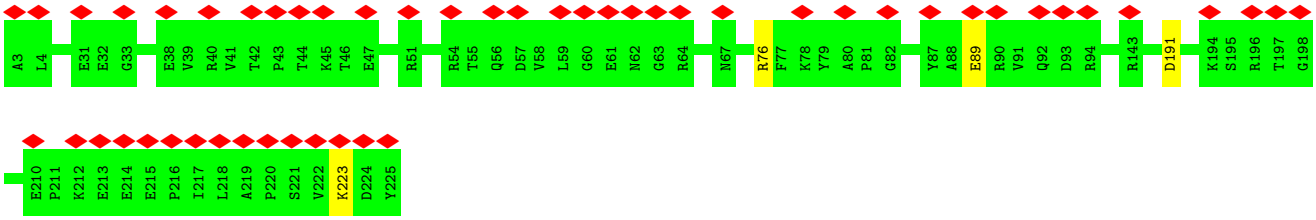
Chain k:



• Molecule 8: RPS3 isoform 1

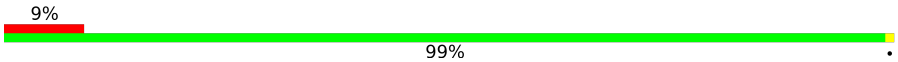
Chain l:

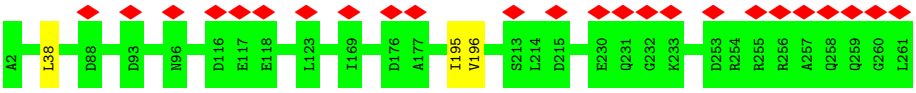




• Molecule 9: 40S ribosomal protein S4-A

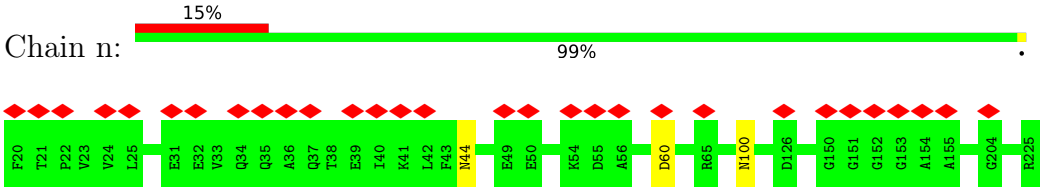
Chain m:





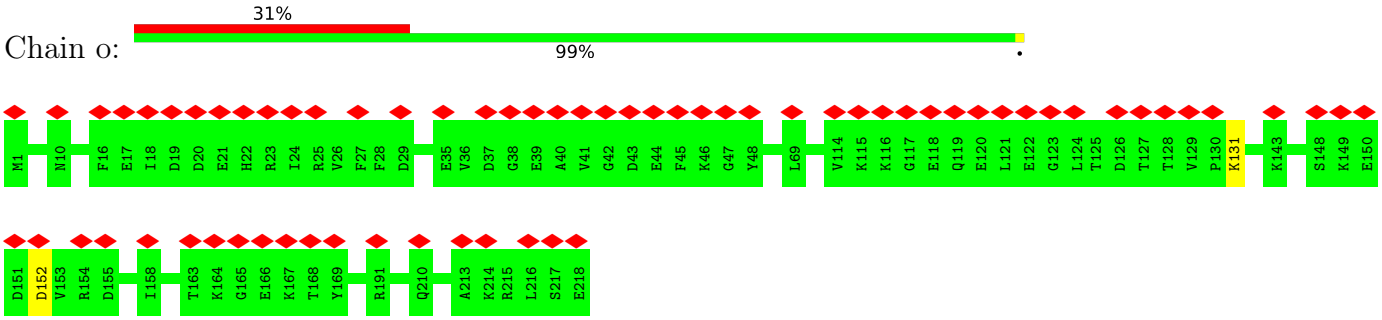
• Molecule 10: Rps5p

Chain n:



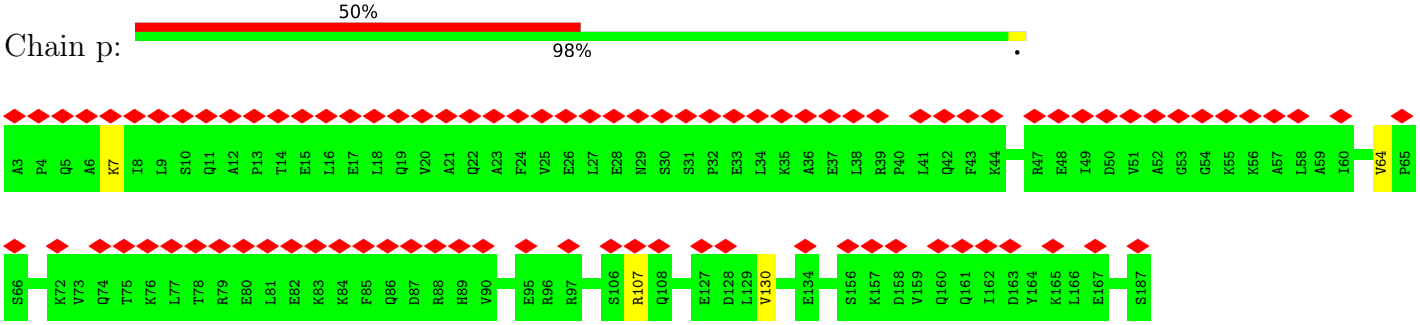
• Molecule 11: 40S ribosomal protein S6-A

Chain o:



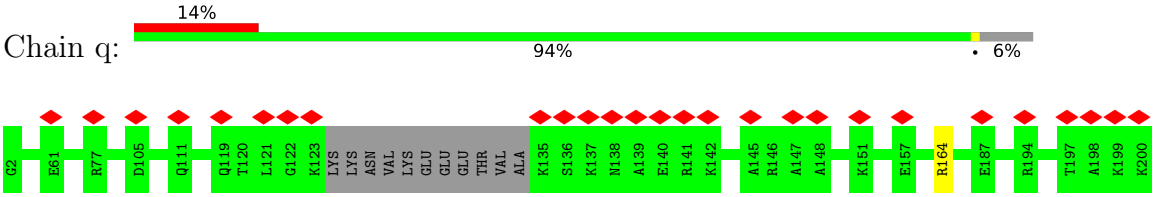
• Molecule 12: 40S ribosomal protein S7-A

Chain p:



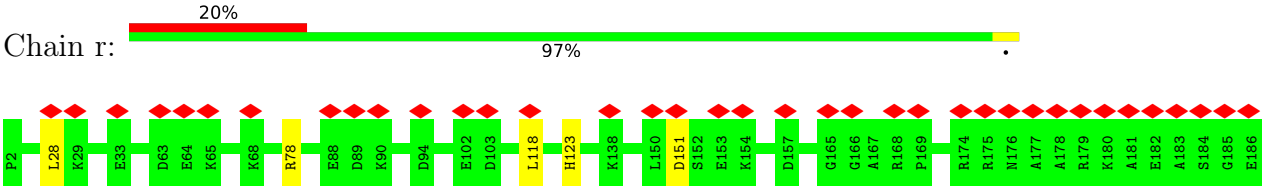
• Molecule 13: 40S ribosomal protein S8-A

Chain q:



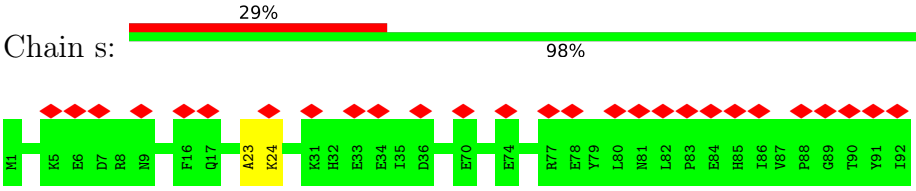
• Molecule 14: 40S ribosomal protein S9-A

Chain r:



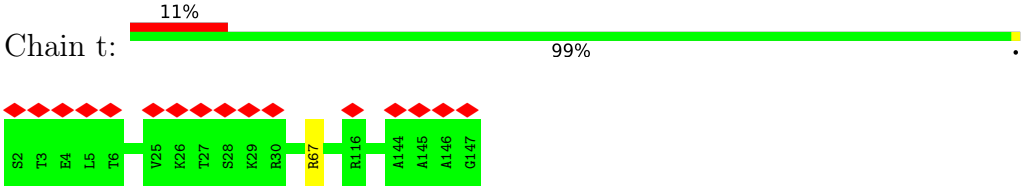
• Molecule 15: 40S ribosomal protein S10-A

Chain s:



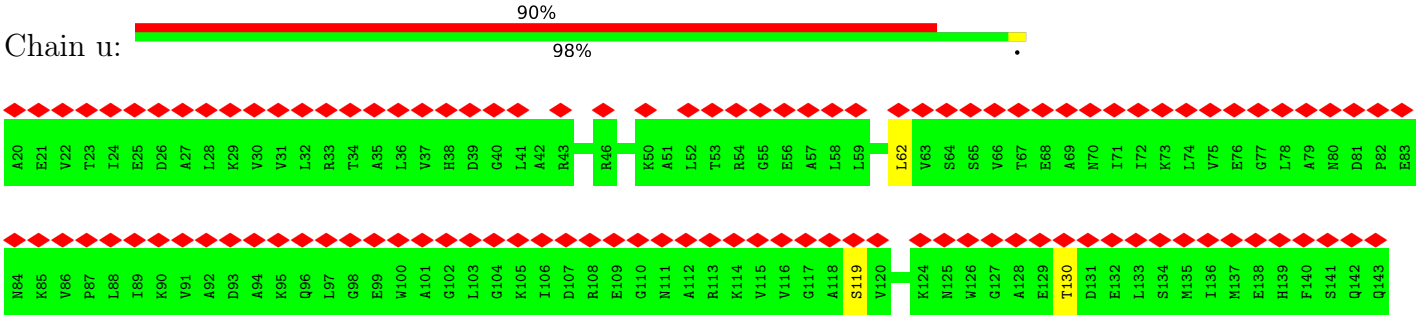
- Molecule 16: 40S ribosomal protein S11-A

Chain t:



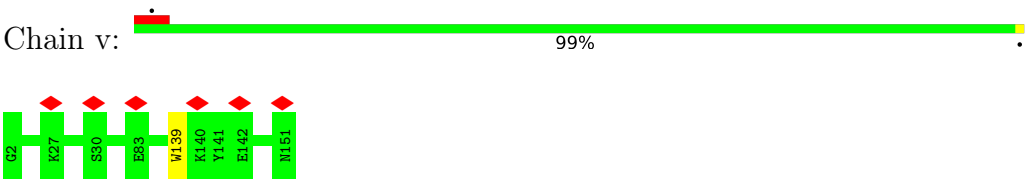
- Molecule 17: RPS12 isoform 1

Chain u:



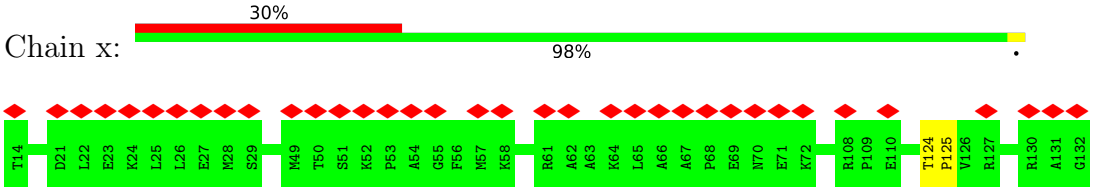
- Molecule 18: 40S ribosomal protein S13

Chain v:



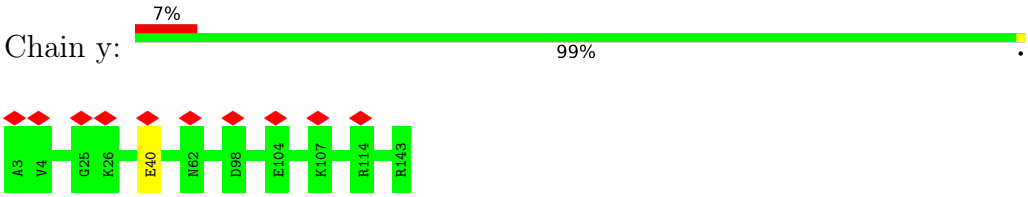
- Molecule 19: RPS15 isoform 1

Chain x:



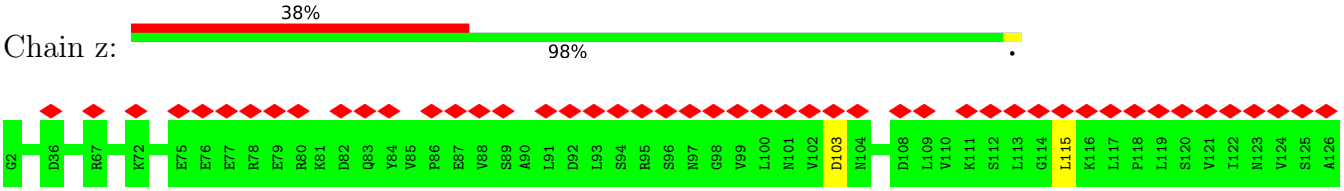
- Molecule 20: 40S ribosomal protein S16-A

Chain y:



- Molecule 21: 40S ribosomal protein S17-A

Chain z:



- Molecule 22: 40S ribosomal protein S18-A

Chain A: 19% 82% 18%

S2 L3 V4 V5 Q6 E7 Q8 G9 S10 F11 Q12 H13 I14 L15 R16 L17 L18 N19 D23 G24 N25 I26 K27 A31 R41 Y42 S43 V46 D51 V52 D53 L54 H55 L61 T62 Q63 L66 E67 R68 Q74 H78 A83 L86 N87 R88 Q89 N90 D91 I92

T93 D97 Y98 H99 T100 L101 D112 I119 R120 A121 G130 R145 A146

• Molecule 23: 40S ribosomal protein S19-A

Chain B: 17% 89% 11%

P2 G3 V6 R7 D8 R24 Q25 G26 K27 L28 E29 V37 K38 T39 S40 S41 R57 N77 K84 S85 R86 P90 N101 L105 E109 K110 I111 G112 I113 I116 K119 R122 R123 E126 N127 G128 Q129 R130 D131 L132 D133 A136 L140 E141

E142 D143 E144

• Molecule 24: RPS20 isoform 1

Chain C: 42% 86% 13%

I19 I20 K21 I22 L26 K32 Q33 L34 E35 I41 V42 K43 N44 A45 E46 Q47 H48 N49 L50 V51 K52 K53 G54 K69 T70 P71 N72 E80 T81 Y82 D92 L93 E94 A95 P96 V97 Q98 I99 V100 K101 R102 I103 T104 Q105 I106 T107 I108 E109 P110 G111 V112 D113 V114 E115

V118 A119

• Molecule 25: 40S ribosomal protein S21-A

Chain D: 20% 95% 5%

M1 E2 N3 D4 K5 G6 Q7 E10 K38 V39 D40 E41 E42 G43 R44 P47 G48 E49 D76 K80 N81 R87

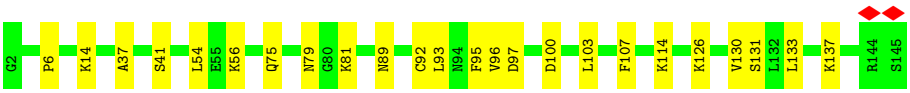
• Molecule 26: RPS22A isoform 1

Chain E: 92% 8%

T2 L26 I27 F50 R57 K60 I61 V62 V63 L93 E115 R118 Y130

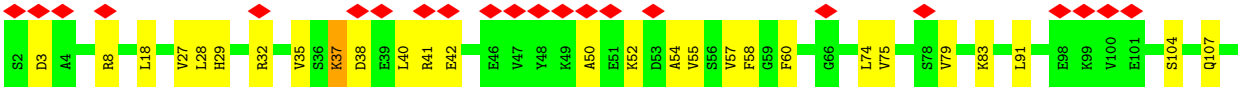
• Molecule 27: 40S ribosomal protein S23-A

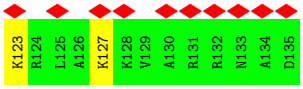
Chain H: 83% 17%



• Molecule 28: 40S ribosomal protein S24-A

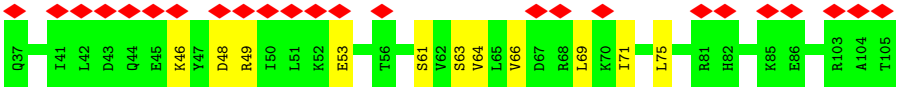
Chain I:





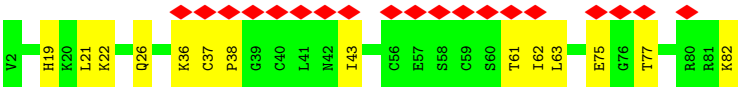
• Molecule 29: RPS25A isoform 1

Chain J:



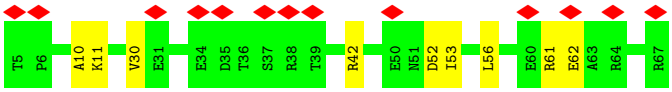
• Molecule 30: 40S ribosomal protein S27-A

Chain L:



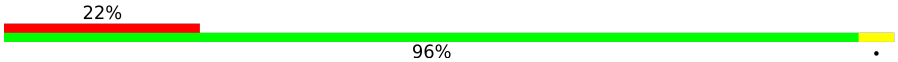
• Molecule 31: RPS28A isoform 1

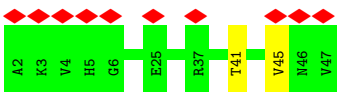
Chain N:



• Molecule 32: 40S ribosomal protein S30-A

Chain P:



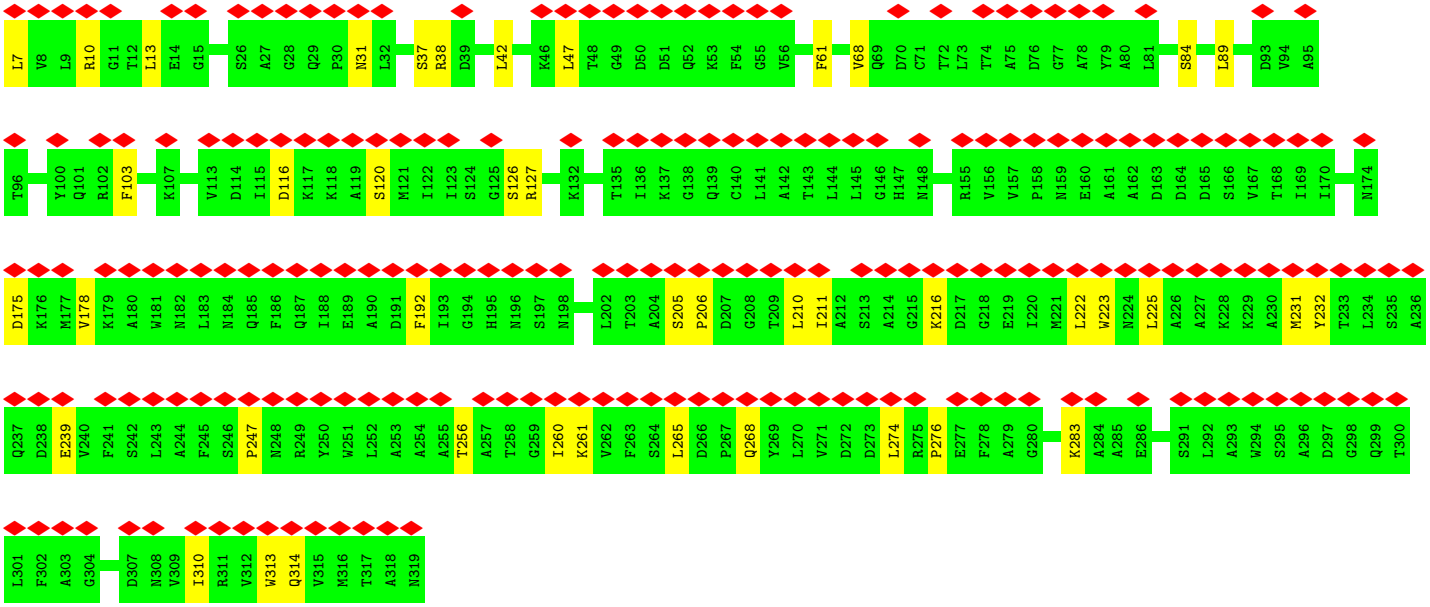


• Molecule 33: RPS31 isoform 1

Chain Q:

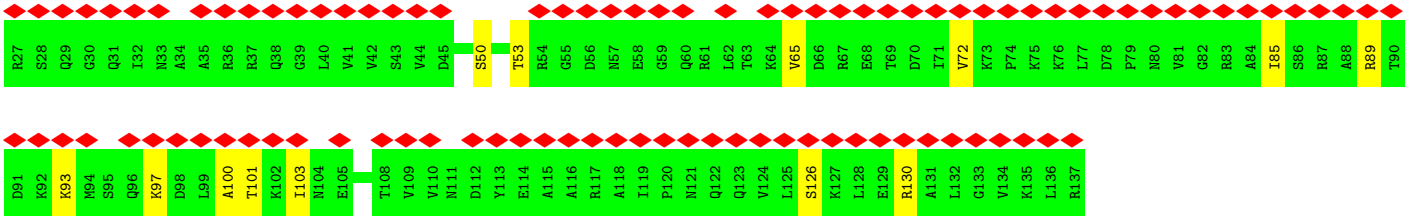
• Molecule 34: Guanine nucleotide-binding protein subunit beta-like protein

Chain R:



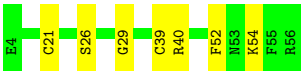
• Molecule 35: MBF1 isoform 1

Chain T:



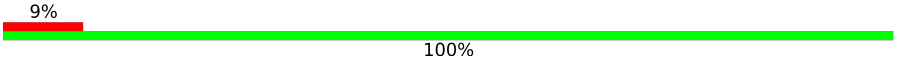
• Molecule 36: RPS29A isoform 1

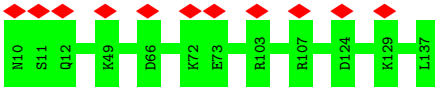
Chain O:



• Molecule 37: 40S ribosomal protein S14-B

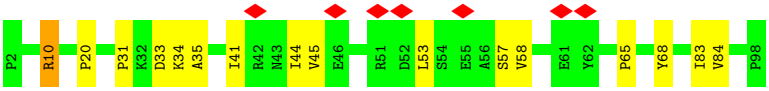
Chain w:





- Molecule 38: RPS26B isoform 1

Chain K:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	57350	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 ($e^-/Å^2$)	28	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.298	Depositor
Minimum map value	-0.090	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.014	Depositor
Recommended contour level	0.06	Depositor
Map size (Å)	423.6, 423.6, 423.6	wwPDB
Map dimensions	400, 400, 400	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: 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	d	0.42	0/1810	1.06	7/2821 (0.2%)
2	e	0.54	1/1836 (0.1%)	1.33	23/2859 (0.8%)
3	f	0.65	1/802 (0.1%)	1.08	9/1238 (0.7%)
4	h	0.78	2/41890 (0.0%)	1.08	264/65269 (0.4%)
5	i	0.38	0/1623	0.62	0/2222
6	j	0.36	0/1748	0.58	0/2352
7	k	0.41	0/1665	0.59	0/2263
8	l	0.38	0/1759	0.61	1/2368 (0.0%)
9	m	0.40	0/2109	0.59	1/2839 (0.0%)
10	n	0.36	0/1629	0.62	1/2202 (0.0%)
11	o	0.33	0/1779	0.57	1/2379 (0.0%)
12	p	0.33	0/1511	0.59	0/2036
13	q	0.39	0/1514	0.54	0/2021
14	r	0.38	0/1519	0.61	3/2035 (0.1%)
15	s	0.40	0/757	0.63	0/1022
16	t	0.47	0/1194	0.56	0/1610
17	u	0.30	0/898	0.74	1/1220 (0.1%)
18	v	0.41	0/1215	0.54	0/1638
19	x	0.36	0/959	0.54	0/1288
20	y	0.43	0/1125	0.61	0/1510
21	z	0.34	0/1011	0.63	2/1355 (0.1%)
22	A	0.34	0/1211	0.59	1/1628 (0.1%)
23	B	0.42	0/1130	0.57	0/1517
24	C	0.38	0/815	0.59	0/1102
25	D	0.42	0/693	0.62	0/935
26	E	0.47	0/1038	0.60	1/1395 (0.1%)
27	H	0.42	0/1139	0.58	0/1518
28	I	0.38	0/1087	0.59	0/1449
29	J	0.36	0/566	0.64	0/761
30	L	0.36	0/620	0.68	0/838
31	N	0.41	0/499	0.71	2/670 (0.3%)
32	P	0.41	0/376	0.56	0/499

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	Q	0.36	0/567	0.83	1/764 (0.1%)
34	R	0.32	0/2456	0.58	0/3343
35	T	0.31	0/875	0.65	0/1170
36	O	0.48	0/452	0.54	0/600
37	w	0.41	0/960	0.64	0/1290
38	K	0.45	0/782	0.64	0/1047
All	All	0.61	4/85619 (0.0%)	0.92	318/125073 (0.3%)

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
5	i	0	3
6	j	0	1
7	k	0	1
8	l	0	1
9	m	0	1
10	n	0	2
12	p	0	2
14	r	0	1
15	s	0	1
17	u	0	1
19	x	0	1
20	y	0	1
22	A	0	2
24	C	0	1
27	H	0	1
30	L	0	1
33	Q	0	2
35	T	0	1
38	K	0	1
All	All	0	25

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	e	1	C	OP3-P	-10.66	1.48	1.61
3	f	4	U	OP3-P	-10.49	1.48	1.61
4	h	993	A	N9-C4	5.62	1.41	1.37
4	h	976	G	C2-N3	-5.40	1.28	1.32

All (318) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	h	989	U	C5-C6-N1	11.79	128.60	122.70
4	h	1027	A	N1-C6-N6	-11.56	111.66	118.60
4	h	990	C	C5-C6-N1	11.39	126.70	121.00
4	h	989	U	C2-N1-C1'	11.34	131.30	117.70
2	e	33	C	N1-C2-O2	11.17	125.60	118.90
2	e	41	C	N1-C2-O2	11.03	125.52	118.90
4	h	453	U	C2-N1-C1'	10.87	130.75	117.70
4	h	976	G	N1-C2-N2	10.55	125.70	116.20
4	h	1729	C	C5-C6-N1	10.53	126.27	121.00
4	h	453	U	N1-C2-O2	10.49	130.14	122.80
4	h	993	A	C8-N9-C4	-10.46	101.62	105.80
4	h	75	U	C2-N1-C1'	10.33	130.10	117.70
4	h	75	U	N1-C2-O2	10.13	129.89	122.80
4	h	976	G	C2-N3-C4	9.76	116.78	111.90
4	h	980	G	C4-N9-C1'	9.72	139.13	126.50
4	h	978	A	C8-N9-C4	-9.66	101.94	105.80
2	e	41	C	C2-N1-C1'	9.65	129.42	118.80
4	h	989	U	C6-N1-C2	-9.50	115.30	121.00
2	e	42	C	C6-N1-C2	-9.42	116.53	120.30
4	h	990	C	N1-C2-O2	9.33	124.50	118.90
4	h	453	U	N3-C2-O2	-9.33	115.67	122.20
4	h	989	U	N3-C2-O2	-9.33	115.67	122.20
4	h	75	U	N3-C2-O2	-9.30	115.69	122.20
4	h	1082	C	C2-N1-C1'	9.18	128.89	118.80
4	h	1560	U	N3-C2-O2	-9.04	115.88	122.20
4	h	989	U	N1-C2-O2	8.96	129.07	122.80
4	h	990	C	C6-N1-C2	-8.84	116.77	120.30
4	h	990	C	C4-C5-C6	-8.82	112.99	117.40
2	e	42	C	C5-C6-N1	8.80	125.40	121.00
4	h	1012	U	N3-C4-O4	-8.78	113.25	119.40
4	h	491	C	N3-C2-O2	-8.75	115.77	121.90
4	h	980	G	C8-N9-C1'	-8.74	115.64	127.00
4	h	980	G	N3-C4-N9	8.64	131.18	126.00
4	h	287	G	O4'-C1'-N9	8.60	115.08	108.20
4	h	976	G	N3-C2-N2	-8.60	113.88	119.90
4	h	683	C	N3-C2-O2	-8.55	115.91	121.90
4	h	991	G	N9-C4-C5	-8.55	101.98	105.40
4	h	581	U	C2-N1-C1'	8.36	127.73	117.70
4	h	976	G	C6-C5-N7	8.35	135.41	130.40
4	h	581	U	N3-C2-O2	-8.28	116.41	122.20
4	h	1014	G	C5-C6-N1	8.24	115.62	111.50
4	h	1012	U	C5-C4-O4	8.14	130.78	125.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	h	581	U	N1-C2-O2	8.07	128.45	122.80
4	h	728	U	C2-N1-C1'	8.04	127.35	117.70
4	h	1390	U	C2-N1-C1'	8.03	127.33	117.70
2	e	41	C	N3-C2-O2	-7.96	116.33	121.90
10	n	60	ASP	CB-CG-OD1	7.86	125.37	118.30
4	h	1473	U	C2-N1-C1'	7.67	126.91	117.70
4	h	1389	C	C2-N1-C1'	7.65	127.22	118.80
4	h	728	U	N1-C2-O2	7.63	128.15	122.80
4	h	683	C	N1-C2-O2	7.58	123.45	118.90
4	h	980	G	N3-C4-C5	-7.56	124.82	128.60
4	h	993	A	N7-C8-N9	7.55	117.57	113.80
4	h	965	U	C2-N1-C1'	7.53	126.74	117.70
4	h	1258	U	N3-C2-O2	-7.50	116.95	122.20
4	h	965	U	N3-C2-O2	-7.45	116.98	122.20
4	h	1458	G	C4-N9-C1'	7.38	136.10	126.50
4	h	991	G	C8-N9-C4	7.34	109.34	106.40
4	h	1285	U	C2-N1-C1'	7.30	126.47	117.70
3	f	13	U	C2-N1-C1'	7.30	126.46	117.70
4	h	1027	A	C5-C6-N6	7.28	129.53	123.70
4	h	889	U	C5-C6-N1	7.24	126.32	122.70
4	h	1039	A	O4'-C1'-N9	7.24	113.99	108.20
2	e	33	C	N3-C2-O2	-7.22	116.84	121.90
4	h	453	U	C6-N1-C1'	-7.20	111.12	121.20
4	h	990	C	N3-C4-C5	7.18	124.77	121.90
4	h	1258	U	C2-N1-C1'	7.18	126.32	117.70
4	h	1246	C	N1-C2-O2	7.17	123.20	118.90
4	h	978	A	N7-C8-N9	7.12	117.36	113.80
4	h	934	C	C2-N1-C1'	7.09	126.60	118.80
4	h	184	C	C2-N1-C1'	7.08	126.59	118.80
4	h	1246	C	C2-N1-C1'	7.06	126.57	118.80
4	h	1598	U	C5-C6-N1	7.03	126.22	122.70
4	h	1420	C	C6-N1-C2	-7.00	117.50	120.30
4	h	1082	C	C6-N1-C1'	-6.97	112.44	120.80
4	h	1560	U	C2-N1-C1'	6.97	126.06	117.70
4	h	728	U	N3-C2-O2	-6.96	117.33	122.20
26	E	93	LEU	CA-CB-CG	6.96	131.30	115.30
4	h	1258	U	N1-C2-O2	6.95	127.66	122.80
4	h	864	U	N3-C2-O2	-6.94	117.34	122.20
4	h	864	U	C2-N1-C1'	6.94	126.03	117.70
4	h	75	U	C6-N1-C1'	-6.93	111.50	121.20
4	h	1458	G	N3-C4-N9	6.91	130.15	126.00
4	h	730	G	C4-N9-C1'	6.91	135.48	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	h	885	G	N1-C6-O6	-6.90	115.76	119.90
4	h	990	C	C2-N1-C1'	6.87	126.36	118.80
4	h	767	U	N3-C2-O2	-6.87	117.39	122.20
4	h	1096	C	N1-C2-O2	6.86	123.02	118.90
4	h	1082	C	N1-C2-O2	6.86	123.02	118.90
4	h	1274	C	N1-C2-O2	6.85	123.01	118.90
4	h	927	C	C2-N1-C1'	6.85	126.33	118.80
4	h	1456	C	N3-C2-O2	-6.83	117.12	121.90
4	h	639	U	N3-C2-O2	-6.83	117.42	122.20
4	h	927	C	C6-N1-C2	-6.83	117.57	120.30
4	h	1274	C	C2-N1-C1'	6.82	126.30	118.80
2	e	31	G	N3-C4-N9	6.80	130.08	126.00
2	e	26	C	N1-C2-O2	6.78	122.97	118.90
2	e	41	C	C6-N1-C1'	-6.75	112.71	120.80
3	f	8	U	C2-N1-C1'	6.74	125.79	117.70
4	h	1560	U	N1-C2-O2	6.72	127.50	122.80
4	h	1227	A	OP2-P-O3'	6.68	119.90	105.20
4	h	1481	C	C6-N1-C2	-6.66	117.64	120.30
4	h	965	U	N1-C2-O2	6.64	127.45	122.80
4	h	1390	U	N1-C2-O2	6.63	127.44	122.80
4	h	864	U	N1-C2-O2	6.62	127.43	122.80
4	h	1458	G	C8-N9-C1'	-6.61	118.41	127.00
33	Q	91	ILE	CG1-CB-CG2	-6.58	96.91	111.40
4	h	991	G	C5-C6-O6	-6.58	124.65	128.60
4	h	1596	C	C2-N1-C1'	6.58	126.04	118.80
4	h	993	A	O4'-C1'-N9	6.57	113.45	108.20
1	d	53	G	N1-C6-O6	-6.50	116.00	119.90
4	h	1012	U	N1-C2-O2	6.47	127.33	122.80
4	h	934	C	N1-C2-O2	6.46	122.78	118.90
3	f	13	U	N1-C2-O2	6.46	127.32	122.80
4	h	976	G	N9-C4-C5	6.46	107.98	105.40
4	h	1729	C	C6-N1-C2	-6.45	117.72	120.30
4	h	861	U	C2-N1-C1'	6.43	125.41	117.70
4	h	498	G	N7-C8-N9	6.42	116.31	113.10
4	h	1227	A	P-O3'-C3'	6.40	127.38	119.70
4	h	990	C	C5-C4-N4	-6.40	115.72	120.20
2	e	42	C	C2-N1-C1'	6.39	125.83	118.80
4	h	976	G	C8-N9-C1'	6.37	135.29	127.00
4	h	730	G	N3-C4-C5	-6.35	125.42	128.60
4	h	730	G	N3-C4-N9	6.34	129.81	126.00
2	e	20	G	O4'-C1'-N9	-6.34	103.13	108.20
4	h	741	C	C6-N1-C2	-6.33	117.77	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	h	991	G	C4-C5-N7	6.33	113.33	110.80
4	h	1000	C	C2-N1-C1'	6.33	125.76	118.80
4	h	1473	U	N1-C2-O2	6.31	127.22	122.80
4	h	158	U	P-O3'-C3'	6.28	127.23	119.70
4	h	1742	U	C2-N1-C1'	6.26	125.21	117.70
4	h	453	U	C5-C6-N1	6.26	125.83	122.70
4	h	491	C	C6-N1-C2	-6.26	117.80	120.30
4	h	639	U	C2-N1-C1'	6.24	125.19	117.70
4	h	720	G	OP1-P-O3'	6.23	118.91	105.20
4	h	1285	U	N1-C2-O2	6.23	127.16	122.80
2	e	42	C	N1-C2-O2	6.23	122.64	118.90
4	h	380	U	N1-C2-O2	6.22	127.16	122.80
4	h	1389	C	C6-N1-C2	-6.22	117.81	120.30
3	f	31	U	N3-C2-O2	-6.21	117.85	122.20
4	h	991	G	N1-C6-O6	6.20	123.62	119.90
4	h	1285	U	N3-C2-O2	-6.20	117.86	122.20
1	d	43	C	O5'-P-OP1	6.19	118.13	110.70
4	h	830	U	O4'-C1'-N1	6.17	113.14	108.20
4	h	959	U	N1-C2-O2	6.17	127.12	122.80
4	h	1572	G	C4-N9-C1'	6.16	134.50	126.50
2	e	42	C	N3-C2-O2	-6.15	117.60	121.90
4	h	1674	C	C6-N1-C2	-6.14	117.84	120.30
4	h	583	C	C2-N1-C1'	6.14	125.55	118.80
2	e	41	C	C6-N1-C2	-6.13	117.85	120.30
4	h	639	U	N1-C2-O2	6.11	127.08	122.80
4	h	479	C	N1-C2-O2	6.08	122.55	118.90
8	l	191	ASP	CB-CG-OD2	6.08	123.77	118.30
4	h	829	A	P-O3'-C3'	6.08	126.99	119.70
4	h	139	C	P-O3'-C3'	6.05	126.96	119.70
17	u	62	LEU	CA-CB-CG	6.04	129.19	115.30
4	h	1013	A	O4'-C1'-N9	6.03	113.03	108.20
4	h	530	C	N1-C2-O2	6.03	122.52	118.90
4	h	720	G	P-O3'-C3'	6.02	126.92	119.70
4	h	959	U	N3-C2-O2	-6.00	118.00	122.20
4	h	1458	G	N3-C4-C5	-6.00	125.60	128.60
4	h	925	G	N3-C2-N2	-5.99	115.71	119.90
3	f	13	U	N3-C2-O2	-5.99	118.01	122.20
21	z	103	ASP	CB-CG-OD2	5.93	123.64	118.30
4	h	981	U	N3-C2-O2	-5.93	118.05	122.20
4	h	721	U	O5'-P-OP1	-5.93	100.37	105.70
4	h	158	U	OP1-P-O3'	5.92	118.22	105.20
4	h	959	U	C2-N1-C1'	5.92	124.80	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	h	685	A	P-O3'-C3'	5.92	126.80	119.70
4	h	1257	U	N3-C2-O2	-5.91	118.06	122.20
4	h	407	A	N1-C6-N6	5.91	122.15	118.60
2	e	33	C	C2-N1-C1'	5.88	125.26	118.80
4	h	990	C	N3-C2-O2	-5.88	117.79	121.90
4	h	1473	U	N3-C2-O2	-5.87	118.09	122.20
4	h	1675	C	N3-C2-O2	-5.87	117.79	121.90
2	e	72	C	C5-C6-N1	5.85	123.93	121.00
4	h	116	U	N3-C2-O2	-5.85	118.11	122.20
4	h	648	G	C4-N9-C1'	5.83	134.07	126.50
4	h	498	G	C8-N9-C4	-5.82	104.07	106.40
4	h	1246	C	N3-C2-O2	-5.82	117.82	121.90
4	h	1012	U	N3-C2-O2	-5.82	118.13	122.20
4	h	976	G	N1-C2-N3	-5.82	120.41	123.90
4	h	1096	C	C2-N1-C1'	5.80	125.19	118.80
4	h	1390	U	C6-N1-C1'	-5.79	113.09	121.20
4	h	767	U	C2-N1-C1'	5.77	124.62	117.70
4	h	976	G	C4-N9-C1'	-5.76	119.00	126.50
4	h	1285	U	C5-C6-N1	5.76	125.58	122.70
3	f	8	U	N1-C2-O2	5.75	126.82	122.80
4	h	380	U	N3-C2-O2	-5.74	118.18	122.20
4	h	648	G	C8-N9-C1'	-5.74	119.54	127.00
4	h	1535	U	N3-C2-O2	-5.73	118.19	122.20
4	h	1420	C	N3-C2-O2	-5.72	117.90	121.90
4	h	1332	C	C2-N1-C1'	5.71	125.08	118.80
4	h	730	G	C8-N9-C1'	-5.70	119.59	127.00
4	h	1456	C	C2-N1-C1'	5.69	125.06	118.80
4	h	1174	C	O4'-C1'-N1	5.69	112.75	108.20
4	h	885	G	C6-N1-C2	-5.68	121.69	125.10
2	e	41	C	C5-C6-N1	5.68	123.84	121.00
14	r	28	LEU	CA-CB-CG	5.67	128.34	115.30
4	h	1185	U	C2-N1-C1'	5.66	124.50	117.70
4	h	989	U	C6-N1-C1'	-5.66	113.28	121.20
4	h	1274	C	N3-C2-O2	-5.66	117.94	121.90
4	h	1716	C	C2-N1-C1'	5.66	125.03	118.80
4	h	1674	C	C2-N1-C1'	5.65	125.02	118.80
4	h	73	U	P-O3'-C3'	5.63	126.45	119.70
4	h	1665	U	C2-N1-C1'	5.63	124.45	117.70
4	h	1568	C	P-O3'-C3'	5.62	126.45	119.70
2	e	68	C	N1-C2-O2	5.62	122.27	118.90
4	h	1027	A	N9-C4-C5	5.62	108.05	105.80
4	h	1344	A	P-O3'-C3'	5.60	126.42	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	f	31	U	N1-C2-O2	5.60	126.72	122.80
4	h	1014	G	N3-C4-N9	5.60	129.36	126.00
4	h	1225	U	N1-C2-O2	5.60	126.72	122.80
4	h	1014	G	C4-C5-N7	5.59	113.04	110.80
4	h	1060	U	N1-C2-O2	5.59	126.72	122.80
4	h	925	G	P-O3'-C3'	5.59	126.41	119.70
1	d	25	C	N1-C2-O2	5.58	122.25	118.90
4	h	946	U	N1-C2-O2	5.57	126.70	122.80
4	h	1017	U	O5'-P-OP1	5.56	117.38	110.70
4	h	1473	U	C6-N1-C1'	-5.55	113.44	121.20
4	h	1573	A	P-O3'-C3'	5.54	126.34	119.70
2	e	26	C	C5-C6-N1	5.53	123.76	121.00
2	e	68	C	N3-C2-O2	-5.52	118.04	121.90
4	h	1257	U	N1-C2-O2	5.51	126.66	122.80
1	d	62	C	C2-N1-C1'	5.51	124.86	118.80
4	h	979	A	O4'-C1'-N9	5.51	112.61	108.20
4	h	1017	U	C6-N1-C2	-5.50	117.70	121.00
4	h	767	U	N1-C2-O2	5.49	126.64	122.80
4	h	1389	C	C5-C6-N1	5.48	123.74	121.00
4	h	1783	C	C2-N1-C1'	5.47	124.82	118.80
4	h	686	C	C6-N1-C2	-5.47	118.11	120.30
4	h	530	C	N3-C2-O2	-5.47	118.07	121.90
4	h	1246	C	C6-N1-C1'	-5.46	114.25	120.80
4	h	132	U	P-O3'-C3'	5.46	126.25	119.70
4	h	758	U	N1-C2-O2	5.46	126.62	122.80
4	h	1614	A	O4'-C1'-N9	5.45	112.56	108.20
4	h	694	U	C2-N1-C1'	5.44	124.23	117.70
4	h	946	U	C2-N1-C1'	5.44	124.22	117.70
4	h	934	C	C6-N1-C1'	-5.43	114.28	120.80
4	h	1456	C	N1-C2-O2	5.43	122.16	118.90
4	h	1674	C	N1-C2-O2	5.43	122.16	118.90
22	A	53	ASP	CB-CG-OD2	5.43	123.18	118.30
4	h	1060	U	N3-C2-O2	-5.42	118.41	122.20
14	r	151	ASP	CB-CG-OD2	5.40	123.16	118.30
4	h	755	A	P-O3'-C3'	5.37	126.15	119.70
9	m	38	LEU	CA-CB-CG	5.37	127.65	115.30
4	h	75	U	C5-C6-N1	5.37	125.39	122.70
4	h	1726	G	C3'-C2'-C1'	5.36	105.79	101.50
14	r	118	LEU	CA-CB-CG	5.36	127.64	115.30
4	h	1514	U	N1-C2-O2	5.36	126.55	122.80
4	h	1796	C	N3-C2-O2	-5.35	118.16	121.90
3	f	8	U	N3-C2-O2	-5.34	118.46	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	h	283	U	N1-C2-O2	5.33	126.53	122.80
31	N	52	ASP	CB-CG-OD2	5.33	123.10	118.30
4	h	889	U	C6-N1-C2	-5.33	117.80	121.00
4	h	1274	C	C6-N1-C1'	-5.30	114.44	120.80
4	h	886	U	C5-C6-N1	5.29	125.34	122.70
4	h	1235	C	N1-C2-O2	5.29	122.07	118.90
4	h	1235	C	C2-N1-C1'	5.28	124.61	118.80
4	h	610	G	C4-N9-C1'	5.26	133.34	126.50
4	h	186	C	C2-N1-C1'	5.24	124.57	118.80
4	h	741	C	N3-C2-O2	-5.24	118.23	121.90
4	h	1246	C	O4'-C1'-N1	5.23	112.39	108.20
1	d	36	G	N3-C2-N2	-5.22	116.24	119.90
4	h	1060	U	C2-N1-C1'	5.22	123.97	117.70
4	h	1481	C	C5-C6-N1	5.22	123.61	121.00
4	h	721	U	P-O3'-C3'	5.22	125.96	119.70
4	h	1535	U	P-O3'-C3'	5.21	125.96	119.70
4	h	25	C	P-O3'-C3'	5.21	125.95	119.70
4	h	1017	U	N3-C2-O2	-5.20	118.56	122.20
4	h	417	A	P-O3'-C3'	5.20	125.94	119.70
4	h	581	U	C6-N1-C1'	-5.20	113.93	121.20
4	h	728	U	C6-N1-C1'	-5.20	113.92	121.20
4	h	496	G	N3-C4-N9	5.19	129.12	126.00
4	h	639	U	O4'-C1'-N1	5.19	112.35	108.20
1	d	70	G	N1-C6-O6	-5.18	116.79	119.90
3	f	31	U	C2-N1-C1'	5.18	123.91	117.70
4	h	992	A	O4'-C1'-N9	5.17	112.33	108.20
4	h	1514	U	N3-C2-O2	-5.17	118.58	122.20
4	h	1675	C	N1-C2-O2	5.17	122.00	118.90
4	h	278	U	P-O3'-C3'	5.16	125.89	119.70
4	h	980	G	C6-C5-N7	-5.15	127.31	130.40
4	h	980	G	N7-C8-N9	5.14	115.67	113.10
4	h	1285	U	C6-N1-C2	-5.13	117.92	121.00
4	h	361	C	C6-N1-C2	-5.13	118.25	120.30
4	h	1354	G	C4-N9-C1'	5.13	133.17	126.50
4	h	1572	G	C8-N9-C1'	-5.13	120.33	127.00
4	h	491	C	N1-C2-O2	5.12	121.97	118.90
4	h	380	U	C2-N1-C1'	5.12	123.84	117.70
4	h	1390	U	N3-C2-O2	-5.12	118.62	122.20
4	h	1737	G	C4-N9-C1'	5.11	133.15	126.50
4	h	389	G	N1-C6-O6	-5.10	116.84	119.90
2	e	72	C	C6-N1-C2	-5.10	118.26	120.30
4	h	1727	G	P-O3'-C3'	5.09	125.81	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	h	686	C	C5-C6-N1	5.09	123.54	121.00
4	h	240	U	P-O3'-C3'	5.08	125.80	119.70
31	N	62	GLU	CA-CB-CG	5.08	124.58	113.40
1	d	62	C	C6-N1-C2	-5.08	118.27	120.30
2	e	24	C	N1-C2-O2	5.08	121.94	118.90
4	h	732	G	C4-N9-C1'	5.07	133.09	126.50
4	h	976	G	C4-C5-N7	-5.07	108.77	110.80
4	h	992	A	C8-N9-C4	-5.07	103.77	105.80
4	h	927	C	C5-C6-N1	5.07	123.53	121.00
4	h	35	U	N3-C2-O2	-5.06	118.66	122.20
4	h	1225	U	N3-C2-O2	-5.06	118.66	122.20
4	h	1585	U	N1-C2-O2	5.06	126.34	122.80
4	h	991	G	C6-C5-N7	-5.06	127.36	130.40
4	h	925	G	OP1-P-O3'	5.06	116.32	105.20
4	h	1560	U	C6-N1-C2	-5.05	117.97	121.00
4	h	885	G	C5-C6-N1	5.05	114.03	111.50
4	h	993	A	N3-C4-C5	-5.04	123.27	126.80
4	h	184	C	C6-N1-C1'	-5.01	114.78	120.80
4	h	1000	C	N3-C2-O2	-5.01	118.39	121.90
4	h	1016	C	C6-N1-C2	-5.01	118.30	120.30
4	h	1596	C	N1-C2-O2	5.01	121.91	118.90
21	z	115	LEU	CA-CB-CG	5.01	126.82	115.30
11	o	152	ASP	CB-CG-OD1	5.01	122.81	118.30
4	h	1161	C	C5-C6-N1	5.00	123.50	121.00

There are no chirality outliers.

All (25) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
22	A	101	LEU	Peptide
22	A	90	ASN	Peptide
24	C	70	THR	Peptide
27	H	89	ASN	Peptide
38	K	10	ARG	Peptide
30	L	75	GLU	Peptide
33	Q	106	TYR	Peptide
33	Q	97	ALA	Peptide
35	T	93	LYS	Peptide
5	i	184	LEU	Peptide
5	i	186	GLY	Peptide
5	i	94	GLY	Peptide
6	j	146	GLN	Peptide

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Mol	Chain	Res	Type	Group
7	k	106	ASP	Peptide
8	l	89	GLU	Peptide
9	m	195	ILE	Peptide
10	n	100	ASN	Peptide
10	n	44	ASN	Peptide
12	p	130	VAL	Peptide
12	p	64	VAL	Peptide
14	r	123	HIS	Peptide
15	s	23	ALA	Peptide
17	u	119	SER	Peptide
19	x	124	THR	Peptide
20	y	40	GLU	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	d	1620	0	822	0	0
2	e	1644	0	836	0	0
3	f	724	0	364	0	0
4	h	37455	0	18846	0	0
5	i	1583	0	1578	0	0
6	j	1722	0	1793	0	0
7	k	1635	0	1723	0	0
8	l	1734	0	1817	0	0
9	m	2068	0	2154	0	0
10	n	1609	0	1675	0	0
11	o	1755	0	1846	0	0
12	p	1486	0	1576	0	0
13	q	1489	0	1525	0	0
14	r	1494	0	1573	0	0
15	s	741	0	691	0	0
16	t	1168	0	1233	0	0
17	u	890	0	887	0	0
18	v	1192	0	1255	0	0
19	x	939	0	968	0	0
20	y	1105	0	1166	0	0
21	z	1001	0	1063	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	A	1192	0	1222	11	0
23	B	1112	0	1124	10	0
24	C	805	0	874	9	0
25	D	684	0	672	3	0
26	E	1021	0	1060	5	0
27	H	1121	0	1196	12	0
28	I	1073	0	1132	17	0
29	J	558	0	598	6	0
30	L	610	0	631	10	0
31	N	497	0	535	4	0
32	P	370	0	413	1	0
33	Q	556	0	552	10	0
34	R	2403	0	2353	28	0
35	T	870	0	917	6	0
36	O	442	0	431	6	0
37	w	949	0	985	0	0
38	K	769	0	818	9	0
39	L	1	0	0	0	0
39	O	1	0	0	0	0
All	All	80088	0	60904	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 6.

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)
28:I:27:VAL:HG21	28:I:35:VAL:HG21	1.74	0.69
34:R:205:SER:HB3	34:R:210:LEU:HB2	1.75	0.68
34:R:13:LEU:HB2	34:R:310:ILE:HB	1.75	0.68
25:D:38:LYS:HD3	25:D:49:GLU:HG2	1.75	0.68
28:I:57:VAL:HB	28:I:60:PHE:HE2	1.59	0.67
33:Q:107:LYS:NZ	33:Q:115:THR:OG1	2.28	0.66
24:C:69:LYS:HE2	24:C:80:GLU:HG3	1.78	0.65
23:B:57:ARG:NH2	23:B:101:ASN:OD1	2.30	0.64
30:L:38:PRO:HD3	30:L:77:THR:HG22	1.79	0.63
24:C:70:THR:O	36:O:40:ARG:NH1	2.32	0.62
27:H:56:LYS:NZ	27:H:96:VAL:O	2.32	0.61
28:I:55:VAL:HG12	28:I:75:VAL:HG22	1.82	0.61
23:B:105:LEU:HD13	23:B:122:ARG:HD2	1.83	0.60
38:K:41:ILE:HD12	38:K:68:TYR:HD2	1.65	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:Q:105:TYR:O	33:Q:118:ARG:NH2	2.35	0.60
22:A:92:ILE:HG23	22:A:93:THR:HG23	1.84	0.59
26:E:115:GLU:HA	26:E:118:ARG:HG2	1.84	0.59
28:I:27:VAL:HG11	28:I:35:VAL:HG11	1.84	0.58
38:K:44:ILE:HD12	38:K:65:PRO:HG2	1.85	0.58
34:R:42:LEU:HB2	34:R:61:PHE:HB2	1.84	0.58
33:Q:132:LEU:HD23	33:Q:139:LEU:HB3	1.86	0.58
35:T:85:ILE:HG22	35:T:89:ARG:HE	1.67	0.58
34:R:265:LEU:O	34:R:268:GLN:NE2	2.36	0.57
23:B:77:ASN:OD1	23:B:101:ASN:ND2	2.37	0.57
27:H:79:ASN:HB3	27:H:81:LYS:HG3	1.86	0.57
22:A:17:LEU:HD11	22:A:66:LEU:HD22	1.88	0.56
24:C:106:ILE:HG13	24:C:107:THR:HG23	1.87	0.56
30:L:61:THR:OG1	30:L:62:ILE:N	2.38	0.56
22:A:27:LYS:HE3	22:A:55:HIS:HA	1.88	0.56
34:R:206:PRO:HG3	34:R:247:PRO:HA	1.88	0.56
38:K:10:ARG:HB2	38:K:34:LYS:HA	1.88	0.56
28:I:50:ALA:HB1	28:I:54:ALA:HB3	1.88	0.56
28:I:41:ARG:NH2	28:I:52:LYS:O	2.38	0.56
33:Q:123:ASN:ND2	33:Q:125:THR:OG1	2.39	0.55
22:A:88:ARG:HE	22:A:91:ASP:HB2	1.72	0.54
23:B:41:SER:O	23:B:84:LYS:NZ	2.30	0.53
27:H:37:ALA:O	27:H:41:SER:OG	2.26	0.53
24:C:80:GLU:OE2	36:O:54:LYS:NZ	2.41	0.52
34:R:37:SER:OG	34:R:38:ARG:N	2.43	0.52
23:B:113:ILE:HG13	23:B:128:GLY:HA2	1.90	0.52
34:R:276:PRO:HG3	34:R:313:TRP:HZ2	1.75	0.51
38:K:34:LYS:HG2	38:K:35:ALA:H	1.74	0.51
27:H:133:LEU:HD22	27:H:137:LYS:HE3	1.93	0.50
26:E:27:ILE:HD11	26:E:61:ILE:HD12	1.93	0.49
34:R:256:THR:HG21	34:R:261:LYS:HD3	1.93	0.49
30:L:36:LYS:HZ2	30:L:43:ILE:HD13	1.78	0.49
28:I:42:GLU:HG2	28:I:52:LYS:HZ3	1.77	0.48
34:R:231:MET:HG2	34:R:232:TYR:HD1	1.77	0.48
35:T:65:VAL:HG12	35:T:72:VAL:HG21	1.94	0.48
35:T:97:LYS:O	35:T:101:THR:OG1	2.27	0.48
26:E:26:LEU:HD21	26:E:60:LYS:HD3	1.95	0.48
28:I:58:PHE:HE1	28:I:74:LEU:HD23	1.78	0.48
28:I:38:ASP:OD2	28:I:52:LYS:NZ	2.43	0.47
34:R:260:ILE:HB	34:R:274:LEU:HB2	1.96	0.47
34:R:116:ASP:OD2	34:R:120:SER:OG	2.27	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:L:37:CYS:HB3	30:L:63:LEU:HD21	1.96	0.47
34:R:10:ARG:HH12	34:R:314:GLN:HB3	1.79	0.47
22:A:130:GLY:O	22:A:145:ARG:NH1	2.47	0.47
22:A:43:SER:HA	22:A:46:VAL:HG22	1.96	0.47
38:K:20:PRO:HA	38:K:31:PRO:HA	1.97	0.46
24:C:82:TYR:HB3	36:O:52:PHE:HB3	1.98	0.46
22:A:83:ALA:HA	22:A:86:LEU:HD23	1.98	0.46
28:I:104:SER:OG	28:I:107:GLN:OE1	2.31	0.46
31:N:10:ALA:HB1	31:N:30:VAL:HB	1.98	0.46
34:R:10:ARG:NH2	34:R:314:GLN:OE1	2.48	0.46
38:K:45:VAL:HG11	38:K:53:LEU:HD22	1.98	0.46
34:R:175:ASP:OD1	34:R:175:ASP:N	2.45	0.45
34:R:210:LEU:HD12	34:R:222:LEU:HD12	1.98	0.45
34:R:211:ILE:HB	34:R:223:TRP:HB2	1.98	0.45
22:A:26:ILE:HG13	22:A:31:ALA:HB2	1.97	0.45
28:I:3:ASP:N	28:I:3:ASP:OD1	2.50	0.45
36:O:21:CYS:HB2	36:O:39:CYS:SG	2.56	0.45
24:C:26:LEU:HB3	24:C:34:LEU:HD11	1.99	0.44
34:R:178:VAL:HB	34:R:192:PHE:HB2	1.99	0.44
30:L:19:HIS:HB3	30:L:22:LYS:HG2	1.99	0.44
38:K:83:ILE:HG13	38:K:84:VAL:HG23	2.00	0.44
27:H:93:LEU:HA	27:H:96:VAL:HG12	1.98	0.44
28:I:37:LYS:HA	28:I:40:LEU:HD13	2.00	0.44
33:Q:116:LYS:HA	33:Q:116:LYS:HD3	1.81	0.44
33:Q:123:ASN:ND2	33:Q:148:TYR:OH	2.50	0.44
38:K:57:SER:OG	38:K:58:VAL:O	2.34	0.44
23:B:6:VAL:HG12	23:B:136:ALA:HB2	1.99	0.44
27:H:130:VAL:HG23	27:H:131:SER:H	1.82	0.44
31:N:11:LYS:HB3	31:N:53:ILE:HD13	2.00	0.44
34:R:231:MET:HG2	34:R:232:TYR:CD1	2.52	0.44
28:I:29:HIS:HB2	28:I:32:ARG:HB2	1.98	0.44
30:L:36:LYS:NZ	30:L:43:ILE:HD13	2.33	0.44
34:R:216:LYS:HA	34:R:239:GLU:HG2	2.00	0.44
27:H:54:LEU:HD11	27:H:75:GLN:HB2	2.00	0.43
35:T:126:SER:OG	35:T:130:ARG:NH1	2.40	0.43
29:J:48:ASP:OD1	29:J:48:ASP:N	2.50	0.43
30:L:82:LYS:HD2	30:L:82:LYS:HA	1.82	0.43
33:Q:130:VAL:HG11	33:Q:143:LYS:HB2	2.00	0.43
27:H:97:ASP:N	27:H:100:ASP:OD2	2.45	0.43
29:J:61:SER:H	29:J:64:VAL:HB	1.82	0.43
31:N:56:LEU:HA	31:N:56:LEU:HD23	1.75	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:O:26:SER:HB2	36:O:39:CYS:SG	2.59	0.43
26:E:50:PHE:HB3	26:E:63:VAL:HG13	2.00	0.43
33:Q:135:HIS:O	33:Q:136:LYS:HD2	2.19	0.43
34:R:89:LEU:HB2	34:R:103:PHE:HB2	2.00	0.43
33:Q:121:CYS:SG	33:Q:122:SER:N	2.92	0.43
23:B:86:ARG:NE	23:B:90:PRO:O	2.50	0.43
27:H:6:PRO:HG3	27:H:14:LYS:HG2	1.99	0.43
27:H:103:LEU:HD13	27:H:126:LYS:HD3	2.01	0.43
34:R:283:LYS:H	34:R:283:LYS:HD2	1.84	0.43
35:T:50:SER:HB2	35:T:53:THR:HB	2.01	0.43
34:R:126:SER:OG	34:R:127:ARG:N	2.52	0.43
34:R:31:ASN:HA	34:R:47:LEU:HD12	2.00	0.42
25:D:5:LYS:HE2	25:D:5:LYS:HB3	1.83	0.42
29:J:49:ARG:NH2	29:J:53:GLU:OE2	2.52	0.42
22:A:86:LEU:HD13	22:A:99:HIS:HB2	2.01	0.42
23:B:110:LYS:HE2	23:B:110:LYS:HB2	1.92	0.42
24:C:49:ASN:N	24:C:49:ASN:OD1	2.53	0.42
28:I:8:ARG:HH22	28:I:28:LEU:HB2	1.85	0.42
27:H:92:CYS:HA	27:H:95:PHE:HD2	1.83	0.42
23:B:37:VAL:HG12	23:B:39:THR:H	1.85	0.42
33:Q:123:ASN:HB3	33:Q:126:CYS:HB2	2.01	0.42
24:C:96:PRO:HG2	24:C:99:ILE:HG12	2.02	0.41
28:I:127:LYS:HE2	28:I:127:LYS:HB3	1.96	0.41
29:J:71:ILE:HG12	29:J:75:LEU:HB3	2.02	0.41
34:R:7:LEU:HD12	34:R:7:LEU:HA	1.92	0.41
24:C:95:ALA:HB1	24:C:99:ILE:HD11	2.01	0.41
31:N:42:ARG:HH12	31:N:61:ARG:H	1.67	0.41
29:J:46:LYS:NZ	29:J:69:LEU:HB3	2.35	0.41
30:L:63:LEU:HD23	30:L:63:LEU:HA	1.91	0.41
38:K:33:ASP:OD1	38:K:34:LYS:N	2.53	0.41
35:T:100:ALA:HA	35:T:103:ILE:HG12	2.03	0.41
36:O:29:GLY:O	36:O:40:ARG:N	2.47	0.41
32:P:41:THR:O	32:P:45:VAL:HG13	2.20	0.41
28:I:18:LEU:HD23	28:I:18:LEU:HA	1.89	0.41
29:J:63:SER:HA	29:J:66:VAL:HG22	2.02	0.41
30:L:21:LEU:HD23	30:L:21:LEU:HA	2.66	0.41
34:R:10:ARG:NH1	34:R:314:GLN:HB3	2.35	0.41
34:R:116:ASP:N	34:R:116:ASP:OD1	2.54	0.41
22:A:11:PHE:HZ	22:A:25:ASN:HB3	1.85	0.41
22:A:119:ILE:HG23	22:A:121:ALA:H	1.86	0.41
28:I:83:LYS:HE3	28:I:91:LEU:HD13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:R:211:ILE:HD11	34:R:225:LEU:HB3	2.03	0.41
25:D:4:ASP:OD1	25:D:4:ASP:N	2.54	0.40
23:B:105:LEU:HD23	23:B:105:LEU:HA	1.87	0.40
27:H:107:PHE:CE2	27:H:114:LYS:HB3	2.56	0.40
34:R:68:VAL:HA	34:R:84:SER:HA	2.03	0.40
26:E:57:ARG:NH2	30:L:26:GLN:HE21	2.20	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	
5	i	204/206 (99%)	181 (89%)	22 (11%)	1 (0%)	29	68
6	j	214/216 (99%)	207 (97%)	7 (3%)	0	100	100
7	k	215/217 (99%)	211 (98%)	4 (2%)	0	100	100
8	l	221/223 (99%)	209 (95%)	12 (5%)	0	100	100
9	m	258/260 (99%)	249 (96%)	8 (3%)	1 (0%)	34	72
10	n	204/206 (99%)	193 (95%)	11 (5%)	0	100	100
11	o	216/218 (99%)	208 (96%)	8 (4%)	0	100	100
12	p	183/185 (99%)	173 (94%)	10 (6%)	0	100	100
13	q	184/199 (92%)	182 (99%)	2 (1%)	0	100	100
14	r	183/185 (99%)	173 (94%)	10 (6%)	0	100	100
15	s	90/92 (98%)	76 (84%)	13 (14%)	1 (1%)	14	50
16	t	144/146 (99%)	138 (96%)	6 (4%)	0	100	100
17	u	122/124 (98%)	102 (84%)	19 (16%)	1 (1%)	19	57
18	v	148/150 (99%)	143 (97%)	4 (3%)	1 (1%)	22	60
19	x	117/119 (98%)	110 (94%)	6 (5%)	1 (1%)	17	55

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	y	139/141 (99%)	131 (94%)	8 (6%)	0	100	100
21	z	123/125 (98%)	122 (99%)	1 (1%)	0	100	100
22	A	143/145 (99%)	132 (92%)	11 (8%)	0	100	100
23	B	141/143 (99%)	139 (99%)	2 (1%)	0	100	100
24	C	99/101 (98%)	94 (95%)	3 (3%)	2 (2%)	7	34
25	D	85/87 (98%)	81 (95%)	4 (5%)	0	100	100
26	E	127/129 (98%)	124 (98%)	3 (2%)	0	100	100
27	H	142/144 (99%)	134 (94%)	8 (6%)	0	100	100
28	I	132/134 (98%)	125 (95%)	5 (4%)	2 (2%)	10	42
29	J	67/69 (97%)	64 (96%)	3 (4%)	0	100	100
30	L	79/81 (98%)	70 (89%)	9 (11%)	0	100	100
31	N	61/63 (97%)	59 (97%)	2 (3%)	0	100	100
32	P	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
33	Q	71/73 (97%)	58 (82%)	13 (18%)	0	100	100
34	R	311/313 (99%)	307 (99%)	4 (1%)	0	100	100
35	T	109/111 (98%)	96 (88%)	13 (12%)	0	100	100
36	O	51/53 (96%)	51 (100%)	0	0	100	100
37	w	126/128 (98%)	116 (92%)	10 (8%)	0	100	100
38	K	95/97 (98%)	87 (92%)	8 (8%)	0	100	100
All	All	4848/4929 (98%)	4588 (95%)	250 (5%)	10 (0%)	50	82

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
19	x	125	PRO
24	C	71	PRO
24	C	72	ASN
18	v	139	TRP
5	i	164	ASN
15	s	24	LYS
28	I	37	LYS
17	u	130	THR
28	I	79	VAL
9	m	196	VAL

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	
5	i	165/173 (95%)	164 (99%)	1 (1%)	86	95
6	j	192/192 (100%)	192 (100%)	0	100	100
7	k	176/176 (100%)	176 (100%)	0	100	100
8	l	182/182 (100%)	180 (99%)	2 (1%)	73	90
9	m	221/221 (100%)	221 (100%)	0	100	100
10	n	173/173 (100%)	173 (100%)	0	100	100
11	o	187/187 (100%)	186 (100%)	1 (0%)	88	96
12	p	165/165 (100%)	163 (99%)	2 (1%)	71	90
13	q	150/160 (94%)	149 (99%)	1 (1%)	84	94
14	r	158/158 (100%)	157 (99%)	1 (1%)	86	95
15	s	73/85 (86%)	73 (100%)	0	100	100
16	t	129/129 (100%)	128 (99%)	1 (1%)	81	93
17	u	88/100 (88%)	88 (100%)	0	100	100
18	v	127/127 (100%)	127 (100%)	0	100	100
19	x	98/98 (100%)	98 (100%)	0	100	100
20	y	117/117 (100%)	117 (100%)	0	100	100
21	z	113/113 (100%)	113 (100%)	0	100	100
22	A	128/128 (100%)	126 (98%)	2 (2%)	62	86
23	B	115/115 (100%)	115 (100%)	0	100	100
24	C	94/94 (100%)	94 (100%)	0	100	100
25	D	74/74 (100%)	74 (100%)	0	100	100
26	E	110/110 (100%)	110 (100%)	0	100	100
27	H	119/119 (100%)	119 (100%)	0	100	100
28	I	112/112 (100%)	111 (99%)	1 (1%)	78	92
29	J	61/61 (100%)	61 (100%)	0	100	100
30	L	70/70 (100%)	70 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
31	N	56/56 (100%)	56 (100%)	0	100	100
32	P	39/39 (100%)	39 (100%)	0	100	100
33	Q	56/63 (89%)	55 (98%)	1 (2%)	59	85
34	R	255/256 (100%)	255 (100%)	0	100	100
35	T	95/95 (100%)	95 (100%)	0	100	100
36	O	47/47 (100%)	47 (100%)	0	100	100
37	w	97/97 (100%)	97 (100%)	0	100	100
38	K	83/83 (100%)	83 (100%)	0	100	100
All	All	4125/4175 (99%)	4112 (100%)	13 (0%)	92	97

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	i	185	ARG
8	l	76	ARG
8	l	223	LYS
11	o	131	LYS
12	p	7	LYS
12	p	107	ARG
13	q	164	ARG
14	r	78	ARG
16	t	67	ARG
22	A	41	ARG
22	A	74	GLN
28	I	123	LYS
33	Q	92	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
8	l	74	GLN
9	m	67	GLN
10	n	131	GLN
12	p	5	GLN
21	z	48	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	d	75/76 (98%)	32 (42%)	0
2	e	76/77 (98%)	33 (43%)	0
3	f	33/35 (94%)	21 (63%)	0
4	h	1754/1758 (99%)	506 (28%)	0
All	All	1938/1946 (99%)	592 (30%)	0

All (592) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	d	6	G
1	d	7	A
1	d	8	U
1	d	9	A
1	d	10	G
1	d	15	G
1	d	16	U
1	d	17	C
1	d	18	G
1	d	19	G
1	d	20	U
1	d	21	A
1	d	22	G
1	d	25	C
1	d	42	C
1	d	43	C
1	d	44	G
1	d	47	U
1	d	48	C
1	d	51	U
1	d	53	G
1	d	54	U
1	d	57	G
1	d	59	U
1	d	62	C
1	d	68	C
1	d	70	G
1	d	71	G
1	d	72	C
1	d	73	A
1	d	74	C
1	d	75	C
2	e	8	U
2	e	9	G

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Mol	Chain	Res	Type
2	e	14	A
2	e	16	C
2	e	20	G
2	e	21	U
2	e	22	A
2	e	23	G
2	e	27	G
2	e	29	C
2	e	32	G
2	e	34	U
2	e	35	C
2	e	36	A
2	e	37	U
2	e	38	A
2	e	39	A
2	e	42	C
2	e	43	G
2	e	44	A
2	e	47	G
2	e	48	U
2	e	49	C
2	e	52	C
2	e	53	G
2	e	54	G
2	e	57	C
2	e	58	A
2	e	60	A
2	e	61	U
2	e	62	C
2	e	76	C
2	e	77	A
3	f	5	U
3	f	6	U
3	f	7	U
3	f	8	U
3	f	9	U
3	f	10	U
3	f	11	U
3	f	12	U
3	f	13	U
3	f	16	G
3	f	24	U

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Mol	Chain	Res	Type
3	f	25	U
3	f	26	U
3	f	27	U
3	f	28	U
3	f	29	U
3	f	31	U
3	f	32	A
3	f	33	A
3	f	37	U
3	f	38	G
4	h	2	A
4	h	4	C
4	h	17	C
4	h	25	C
4	h	26	A
4	h	27	U
4	h	34	G
4	h	42	G
4	h	45	U
4	h	47	A
4	h	50	C
4	h	57	G
4	h	60	U
4	h	63	G
4	h	67	A
4	h	68	A
4	h	69	G
4	h	72	A
4	h	73	U
4	h	74	U
4	h	75	U
4	h	77	U
4	h	104	A
4	h	114	C
4	h	115	G
4	h	127	G
4	h	128	U
4	h	130	C
4	h	131	C
4	h	132	U
4	h	133	U
4	h	134	U

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Mol	Chain	Res	Type
4	h	135	A
4	h	136	C
4	h	137	U
4	h	138	A
4	h	140	A
4	h	141	U
4	h	145	A
4	h	146	U
4	h	153	G
4	h	158	U
4	h	159	U
4	h	160	C
4	h	165	G
4	h	169	A
4	h	176	C
4	h	178	U
4	h	179	A
4	h	184	C
4	h	185	U
4	h	186	C
4	h	187	G
4	h	188	A
4	h	189	C
4	h	190	C
4	h	192	U
4	h	193	U
4	h	194	U
4	h	195	G
4	h	196	G
4	h	197	A
4	h	200	A
4	h	215	A
4	h	218	A
4	h	219	A
4	h	220	A
4	h	226	A
4	h	227	U
4	h	228	G
4	h	231	U
4	h	232	U
4	h	233	C
4	h	234	G

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Mol	Chain	Res	Type
4	h	236	A
4	h	237	C
4	h	238	U
4	h	240	U
4	h	241	U
4	h	249	U
4	h	261	U
4	h	262	U
4	h	265	A
4	h	271	A
4	h	272	U
4	h	274	G
4	h	275	C
4	h	277	U
4	h	278	U
4	h	279	G
4	h	280	U
4	h	281	G
4	h	288	A
4	h	313	U
4	h	314	C
4	h	316	A
4	h	317	C
4	h	320	U
4	h	321	C
4	h	337	G
4	h	338	C
4	h	352	A
4	h	359	A
4	h	360	A
4	h	361	C
4	h	393	C
4	h	399	A
4	h	400	A
4	h	401	A
4	h	402	C
4	h	404	G
4	h	407	A
4	h	409	C
4	h	411	C
4	h	416	A
4	h	418	G

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Mol	Chain	Res	Type
4	h	423	G
4	h	424	C
4	h	425	A
4	h	426	G
4	h	434	G
4	h	439	U
4	h	444	C
4	h	446	A
4	h	448	C
4	h	452	A
4	h	468	A
4	h	475	A
4	h	477	A
4	h	480	G
4	h	493	U
4	h	495	C
4	h	496	G
4	h	497	G
4	h	498	G
4	h	499	U
4	h	500	C
4	h	501	U
4	h	502	U
4	h	503	G
4	h	504	U
4	h	505	A
4	h	506	A
4	h	507	U
4	h	510	G
4	h	514	G
4	h	515	A
4	h	518	A
4	h	519	C
4	h	527	A
4	h	534	A
4	h	538	A
4	h	539	G
4	h	542	A
4	h	543	C
4	h	544	A
4	h	545	A
4	h	548	G

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Mol	Chain	Res	Type
4	h	555	A
4	h	556	A
4	h	558	U
4	h	559	C
4	h	565	C
4	h	568	G
4	h	578	U
4	h	579	A
4	h	583	C
4	h	585	A
4	h	594	A
4	h	595	G
4	h	606	A
4	h	610	G
4	h	611	U
4	h	619	A
4	h	620	A
4	h	622	A
4	h	623	A
4	h	634	G
4	h	639	U
4	h	642	G
4	h	645	C
4	h	648	G
4	h	649	U
4	h	650	U
4	h	651	G
4	h	652	G
4	h	654	C
4	h	656	G
4	h	658	C
4	h	677	G
4	h	680	U
4	h	684	A
4	h	685	A
4	h	686	C
4	h	687	G
4	h	693	U
4	h	694	U
4	h	695	U
4	h	696	C
4	h	697	C

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Mol	Chain	Res	Type
4	h	698	U
4	h	700	C
4	h	702	G
4	h	703	G
4	h	704	C
4	h	706	A
4	h	707	A
4	h	708	C
4	h	709	C
4	h	710	U
4	h	711	U
4	h	713	A
4	h	714	G
4	h	718	U
4	h	719	U
4	h	721	U
4	h	722	G
4	h	723	G
4	h	725	U
4	h	727	U
4	h	731	C
4	h	732	G
4	h	733	A
4	h	734	A
4	h	735	C
4	h	736	C
4	h	737	A
4	h	738	G
4	h	740	A
4	h	743	U
4	h	755	A
4	h	756	A
4	h	765	G
4	h	766	U
4	h	771	A
4	h	774	A
4	h	775	G
4	h	778	G
4	h	781	U
4	h	782	U
4	h	783	G
4	h	784	C

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Mol	Chain	Res	Type
4	h	787	G
4	h	789	A
4	h	794	U
4	h	812	A
4	h	815	G
4	h	819	G
4	h	820	U
4	h	821	U
4	h	823	G
4	h	829	A
4	h	830	U
4	h	831	U
4	h	833	U
4	h	836	U
4	h	841	U
4	h	846	G
4	h	856	A
4	h	863	A
4	h	864	U
4	h	876	G
4	h	881	A
4	h	882	U
4	h	883	C
4	h	884	A
4	h	885	G
4	h	887	A
4	h	889	U
4	h	898	A
4	h	899	G
4	h	901	G
4	h	906	A
4	h	909	U
4	h	912	U
4	h	913	G
4	h	914	G
4	h	925	G
4	h	926	A
4	h	927	C
4	h	928	U
4	h	929	A
4	h	933	A
4	h	935	U

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Mol	Chain	Res	Type
4	h	942	G
4	h	944	A
4	h	945	U
4	h	950	C
4	h	951	A
4	h	960	U
4	h	966	A
4	h	970	A
4	h	973	A
4	h	980	G
4	h	981	U
4	h	982	U
4	h	983	A
4	h	984	G
4	h	985	G
4	h	987	G
4	h	988	A
4	h	990	C
4	h	991	G
4	h	992	A
4	h	993	A
4	h	996	U
4	h	1004	U
4	h	1005	A
4	h	1011	G
4	h	1016	C
4	h	1017	U
4	h	1018	U
4	h	1019	A
4	h	1020	A
4	h	1021	C
4	h	1022	C
4	h	1023	A
4	h	1024	U
4	h	1025	A
4	h	1026	A
4	h	1028	C
4	h	1029	U
4	h	1031	U
4	h	1039	A
4	h	1040	G
4	h	1052	U

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Mol	Chain	Res	Type
4	h	1053	G
4	h	1059	U
4	h	1060	U
4	h	1061	A
4	h	1062	A
4	h	1081	A
4	h	1082	C
4	h	1086	A
4	h	1092	A
4	h	1096	C
4	h	1097	U
4	h	1100	G
4	h	1123	C
4	h	1124	A
4	h	1125	A
4	h	1126	G
4	h	1138	A
4	h	1150	G
4	h	1155	G
4	h	1158	C
4	h	1160	A
4	h	1167	G
4	h	1174	C
4	h	1175	U
4	h	1176	G
4	h	1185	U
4	h	1186	U
4	h	1194	A
4	h	1196	A
4	h	1199	G
4	h	1200	G
4	h	1201	G
4	h	1202	A
4	h	1208	A
4	h	1217	A
4	h	1218	G
4	h	1220	C
4	h	1225	U
4	h	1227	A
4	h	1228	G
4	h	1229	G
4	h	1230	A

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Mol	Chain	Res	Type
4	h	1234	A
4	h	1241	G
4	h	1242	A
4	h	1243	G
4	h	1244	A
4	h	1245	G
4	h	1246	C
4	h	1255	G
4	h	1256	A
4	h	1257	U
4	h	1258	U
4	h	1273	G
4	h	1284	C
4	h	1286	U
4	h	1314	U
4	h	1315	U
4	h	1321	A
4	h	1325	A
4	h	1338	C
4	h	1344	A
4	h	1345	A
4	h	1354	G
4	h	1361	U
4	h	1362	U
4	h	1363	U
4	h	1364	G
4	h	1367	G
4	h	1370	U
4	h	1371	A
4	h	1372	U
4	h	1382	A
4	h	1390	U
4	h	1398	U
4	h	1399	C
4	h	1400	A
4	h	1413	U
4	h	1415	U
4	h	1422	A
4	h	1425	A
4	h	1427	A
4	h	1428	G
4	h	1432	U

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Mol	Chain	Res	Type
4	h	1436	A
4	h	1445	G
4	h	1446	A
4	h	1447	C
4	h	1448	G
4	h	1452	U
4	h	1458	G
4	h	1459	C
4	h	1460	A
4	h	1466	G
4	h	1471	A
4	h	1474	G
4	h	1482	C
4	h	1486	G
4	h	1490	C
4	h	1491	U
4	h	1492	A
4	h	1493	A
4	h	1496	U
4	h	1506	G
4	h	1514	U
4	h	1516	A
4	h	1521	G
4	h	1523	G
4	h	1524	A
4	h	1531	G
4	h	1536	G
4	h	1537	C
4	h	1538	U
4	h	1557	U
4	h	1559	A
4	h	1569	A
4	h	1573	A
4	h	1574	G
4	h	1575	G
4	h	1584	G
4	h	1590	G
4	h	1596	C
4	h	1597	A
4	h	1598	U
4	h	1600	A
4	h	1601	G

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Mol	Chain	Res	Type
4	h	1607	G
4	h	1616	G
4	h	1634	C
4	h	1637	C
4	h	1643	U
4	h	1658	G
4	h	1665	U
4	h	1666	U
4	h	1667	A
4	h	1668	G
4	h	1669	U
4	h	1670	G
4	h	1671	A
4	h	1672	G
4	h	1674	C
4	h	1675	C
4	h	1680	G
4	h	1681	A
4	h	1682	U
4	h	1715	G
4	h	1716	C
4	h	1726	G
4	h	1727	G
4	h	1728	A
4	h	1729	C
4	h	1730	A
4	h	1731	A
4	h	1732	A
4	h	1733	C
4	h	1734	U
4	h	1736	G
4	h	1737	G
4	h	1743	U
4	h	1744	A
4	h	1747	G
4	h	1750	A
4	h	1755	A
4	h	1756	A
4	h	1757	G
4	h	1760	G
4	h	1762	A
4	h	1766	A

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Mol	Chain	Res	Type
4	h	1767	G
4	h	1769	U
4	h	1780	G
4	h	1781	A
4	h	1782	A
4	h	1792	G
4	h	1793	G
4	h	1794	A
4	h	1795	U
4	h	1796	C
4	h	1799	U
4	h	1800	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 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
4	h	3
3	f	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	h	1686:C	O3'	1712:A	P	17.71
1	h	658:C	O3'	676:G	P	17.06
1	f	33:A	O3'	34:A	P	3.69
1	h	540:G	O3'	541:A	P	3.24

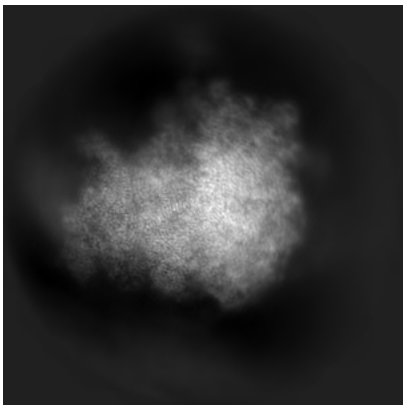
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-11457. These allow visual inspection of the internal detail of the map and identification of artifacts.

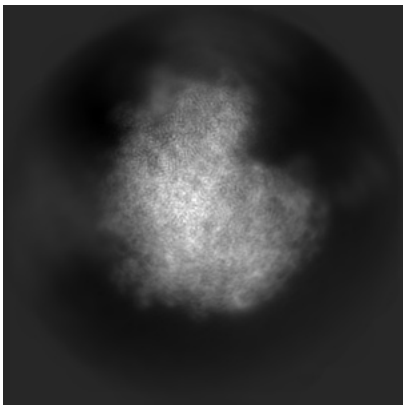
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

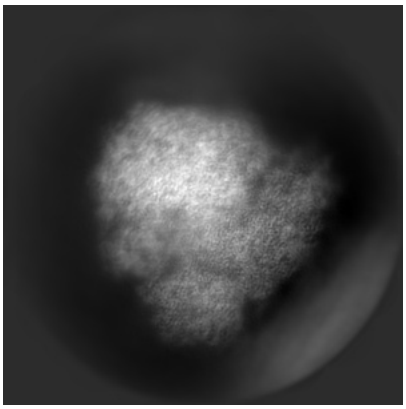
6.1.1 Primary map



X

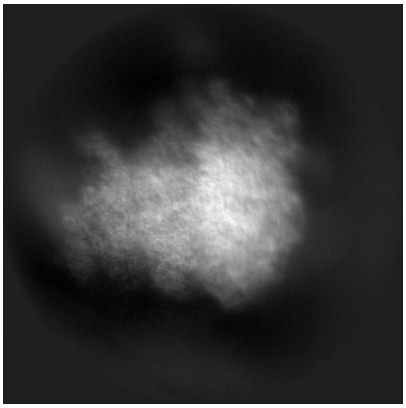


Y

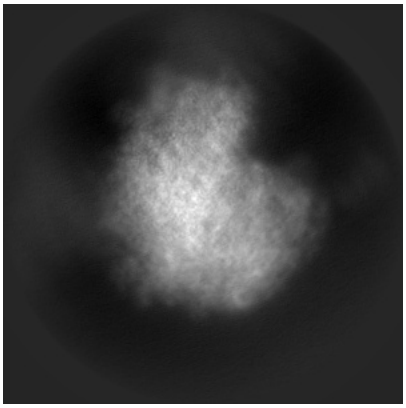


Z

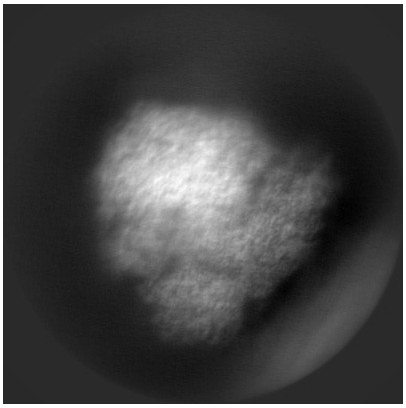
6.1.2 Raw map



X



Y

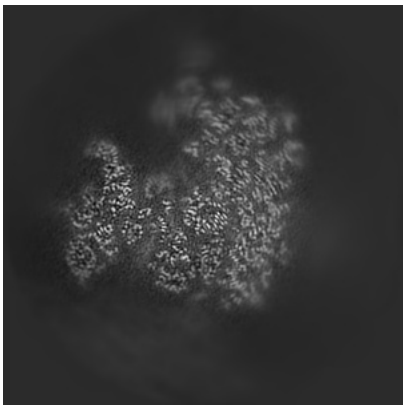


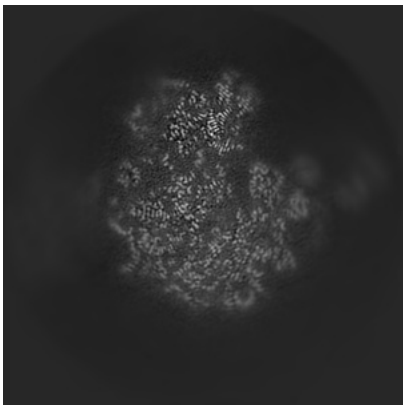
Z

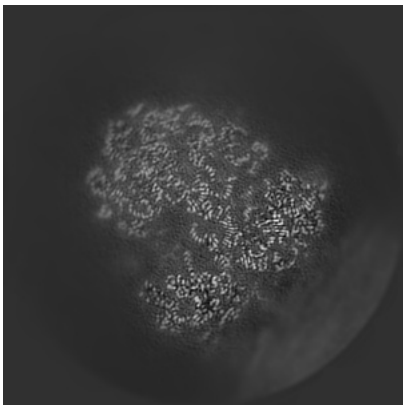
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

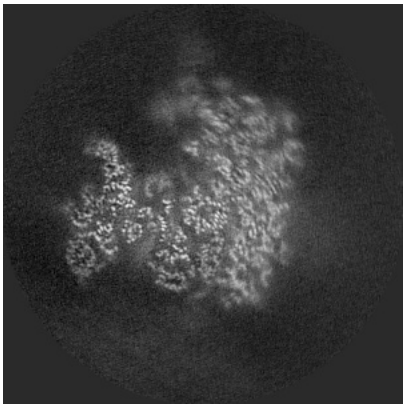
6.2.1 Primary map

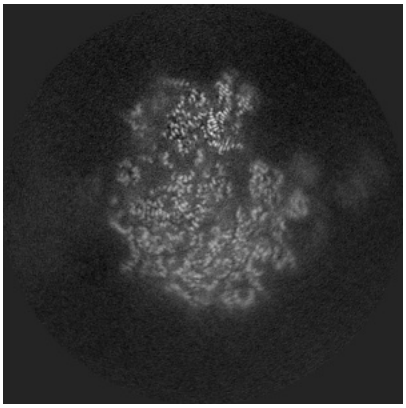

X Index: 200

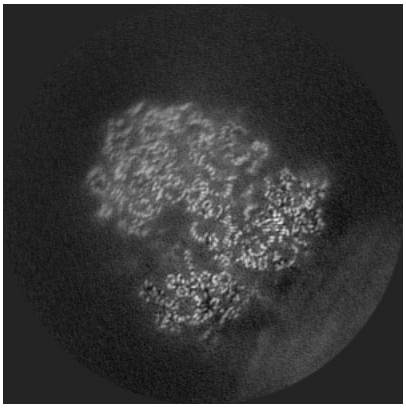

Y Index: 200


Z Index: 200

6.2.2 Raw map


X Index: 200

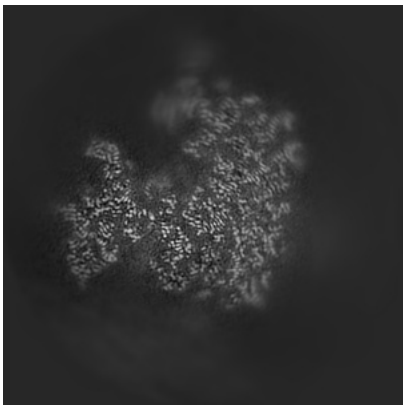

Y Index: 200

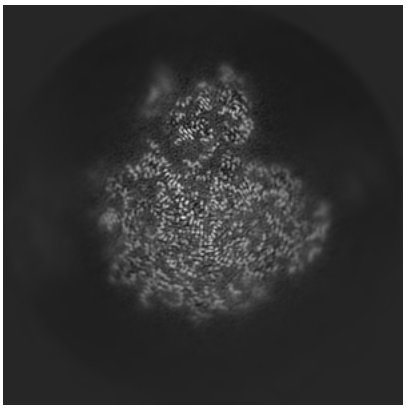

Z Index: 200

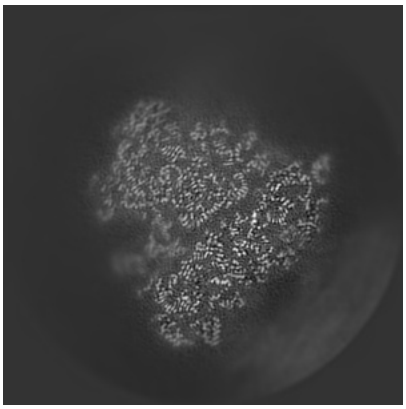
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

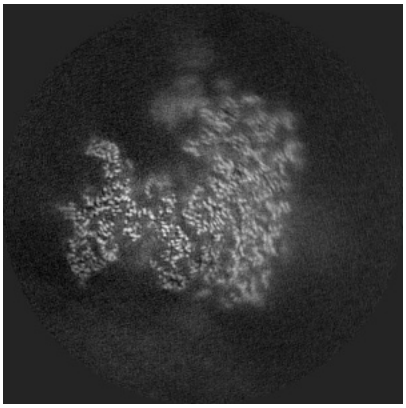
6.3.1 Primary map

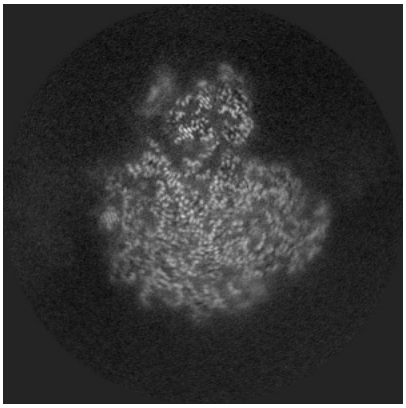

X Index: 202

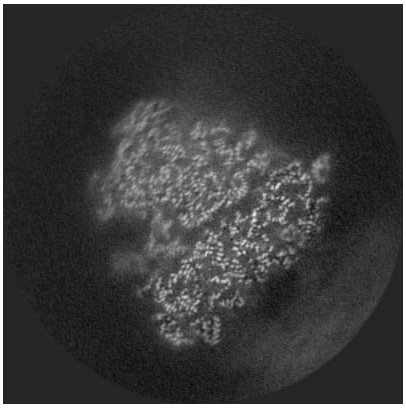

Y Index: 217


Z Index: 186

6.3.2 Raw map


X Index: 202

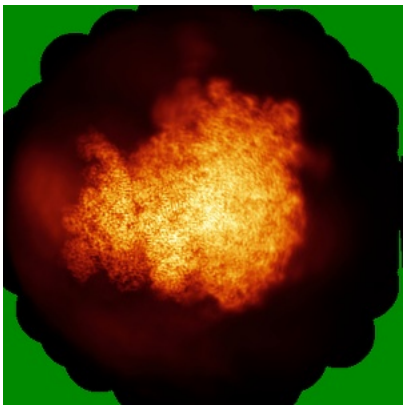

Y Index: 217

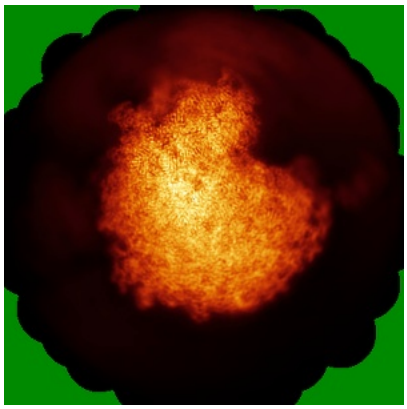

Z Index: 186

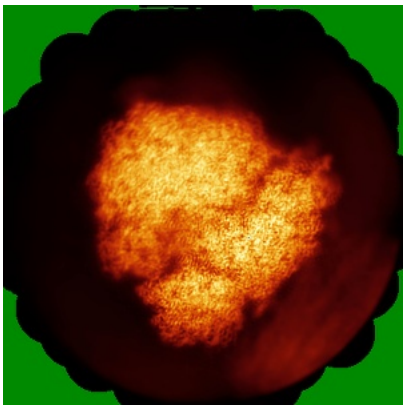
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

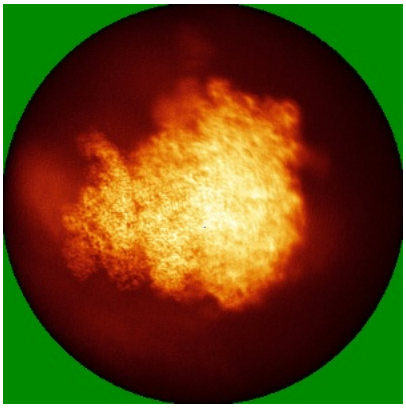
6.4.1 Primary map

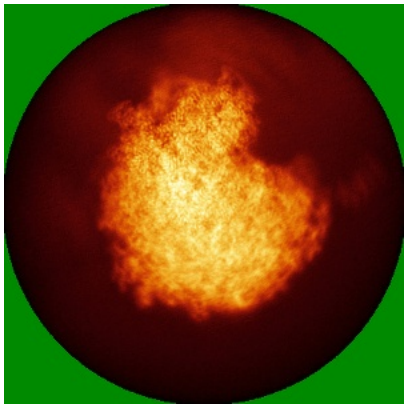

X

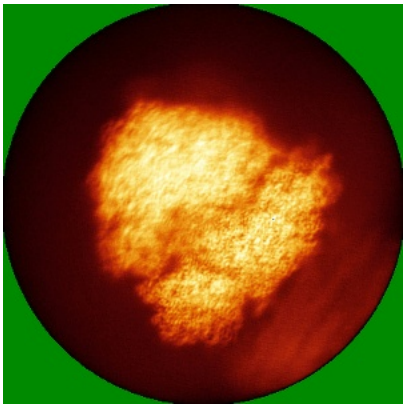

Y


Z

6.4.2 Raw map


X

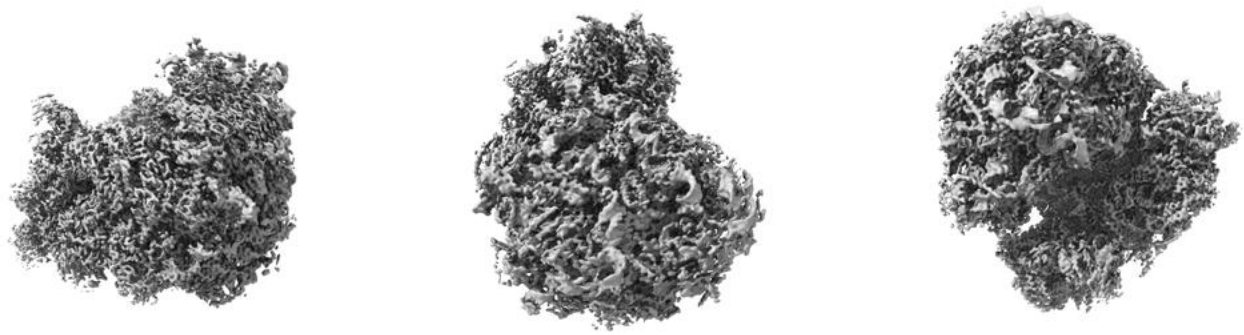

Y


Z

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

6.5 Orthogonal surface views (i)

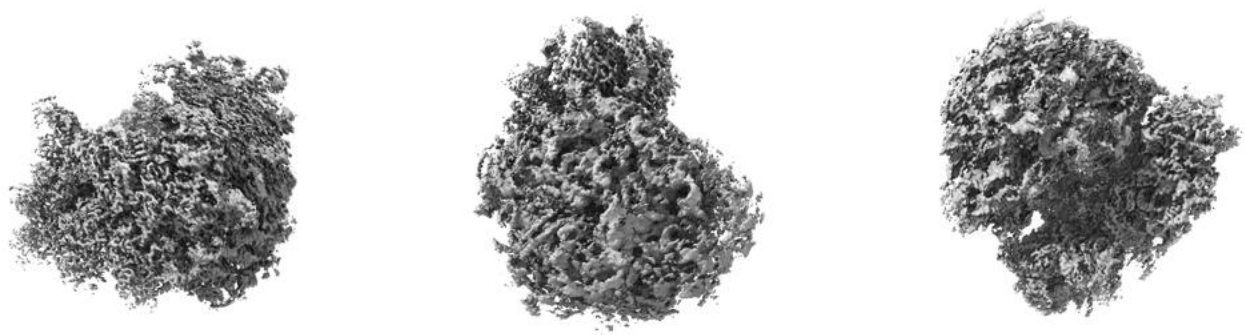
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.06. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 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.

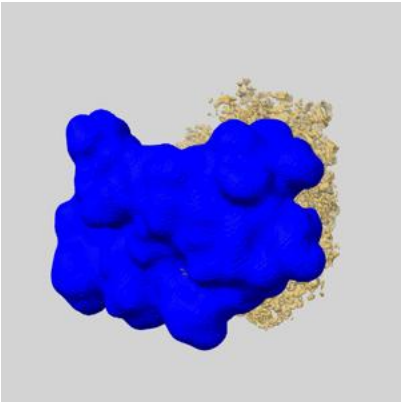
6.6 Mask visualisation (i)

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

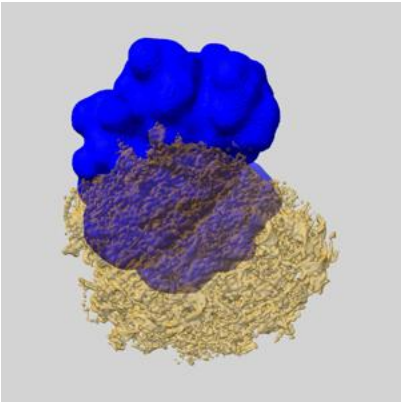
A mask typically either:

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

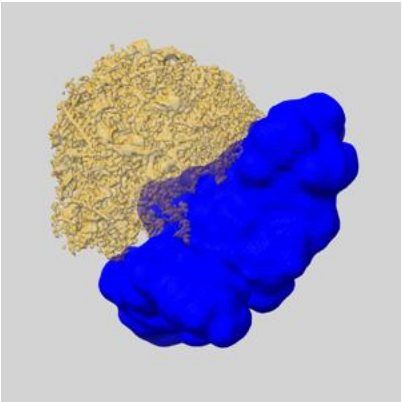
6.6.1 emd_11457_msk_1.map (i)



X



Y

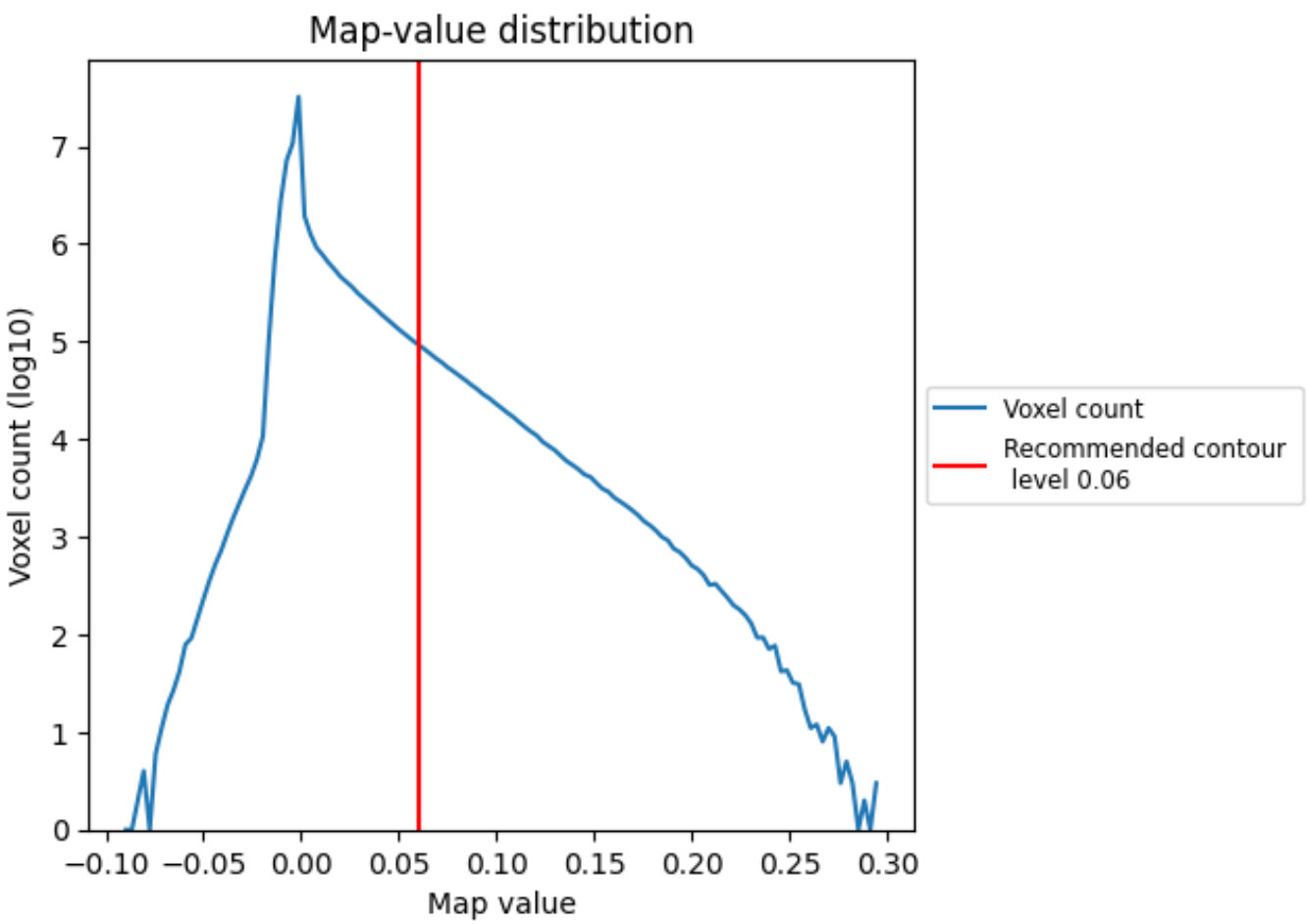


Z

7 Map analysis (i)

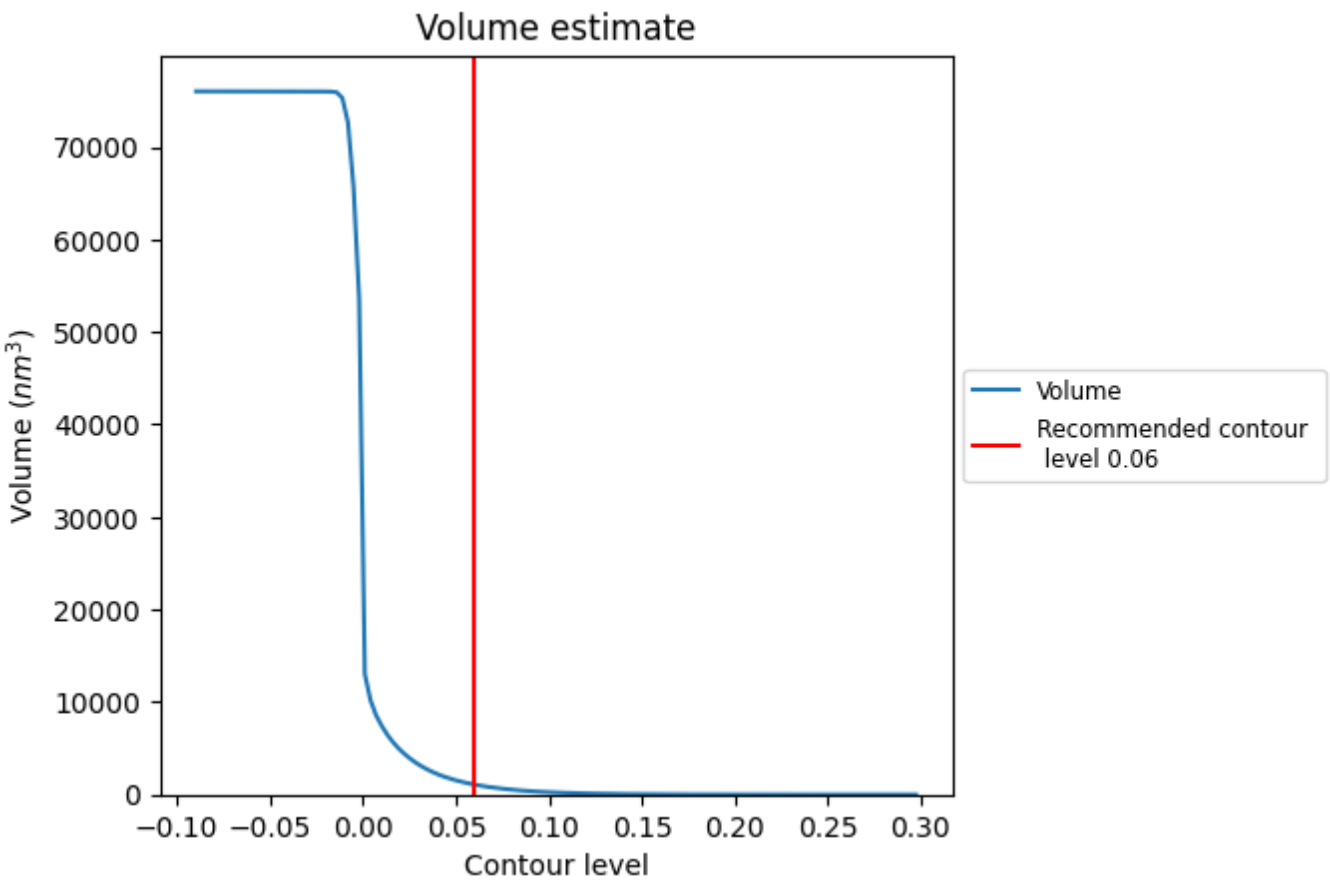
This section contains the results of statistical analysis of the map.

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.

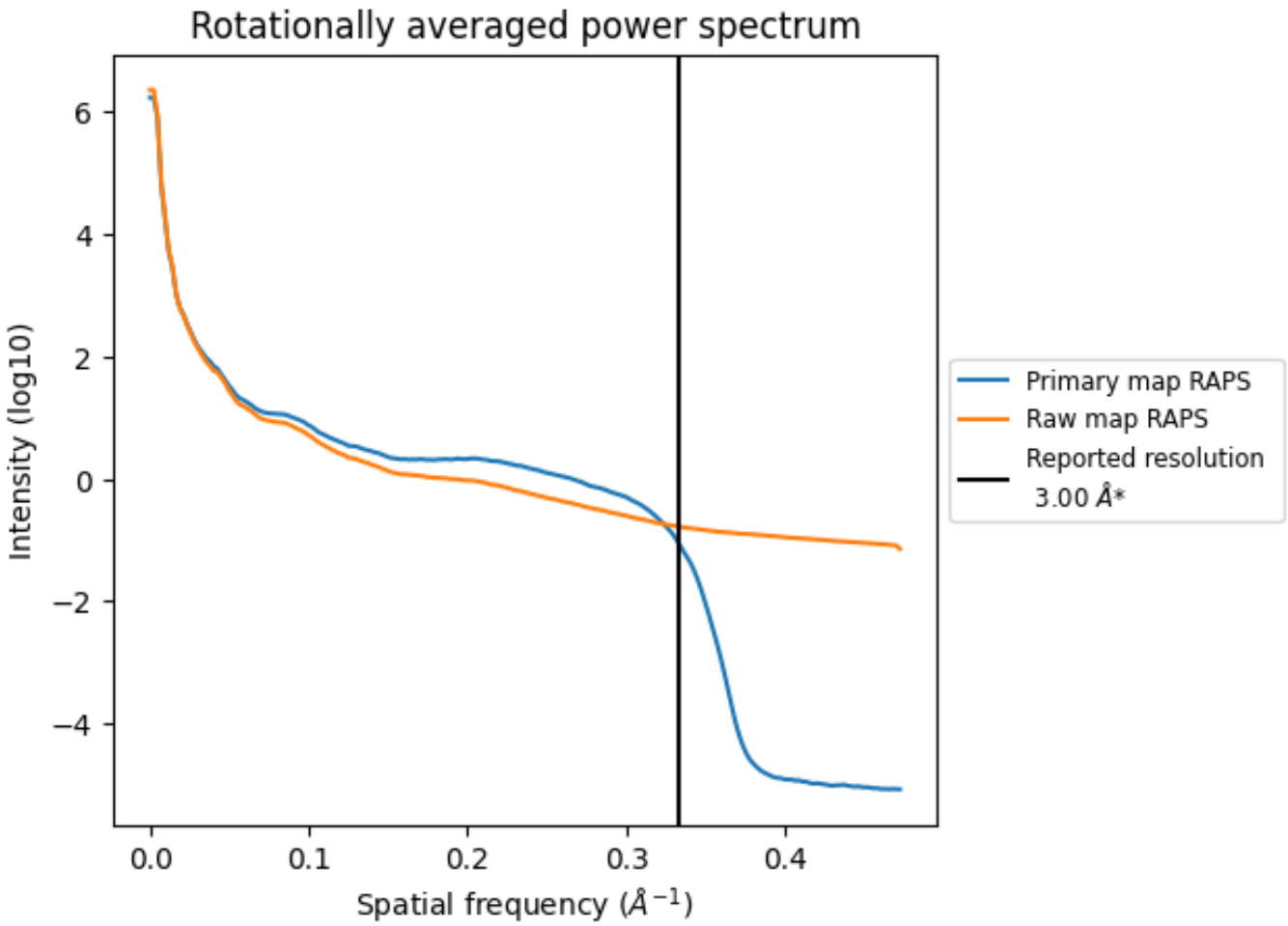
7.2 Volume estimate (i)



The volume at the recommended contour level is 1080 nm^3; this corresponds to an approximate mass of 976 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)

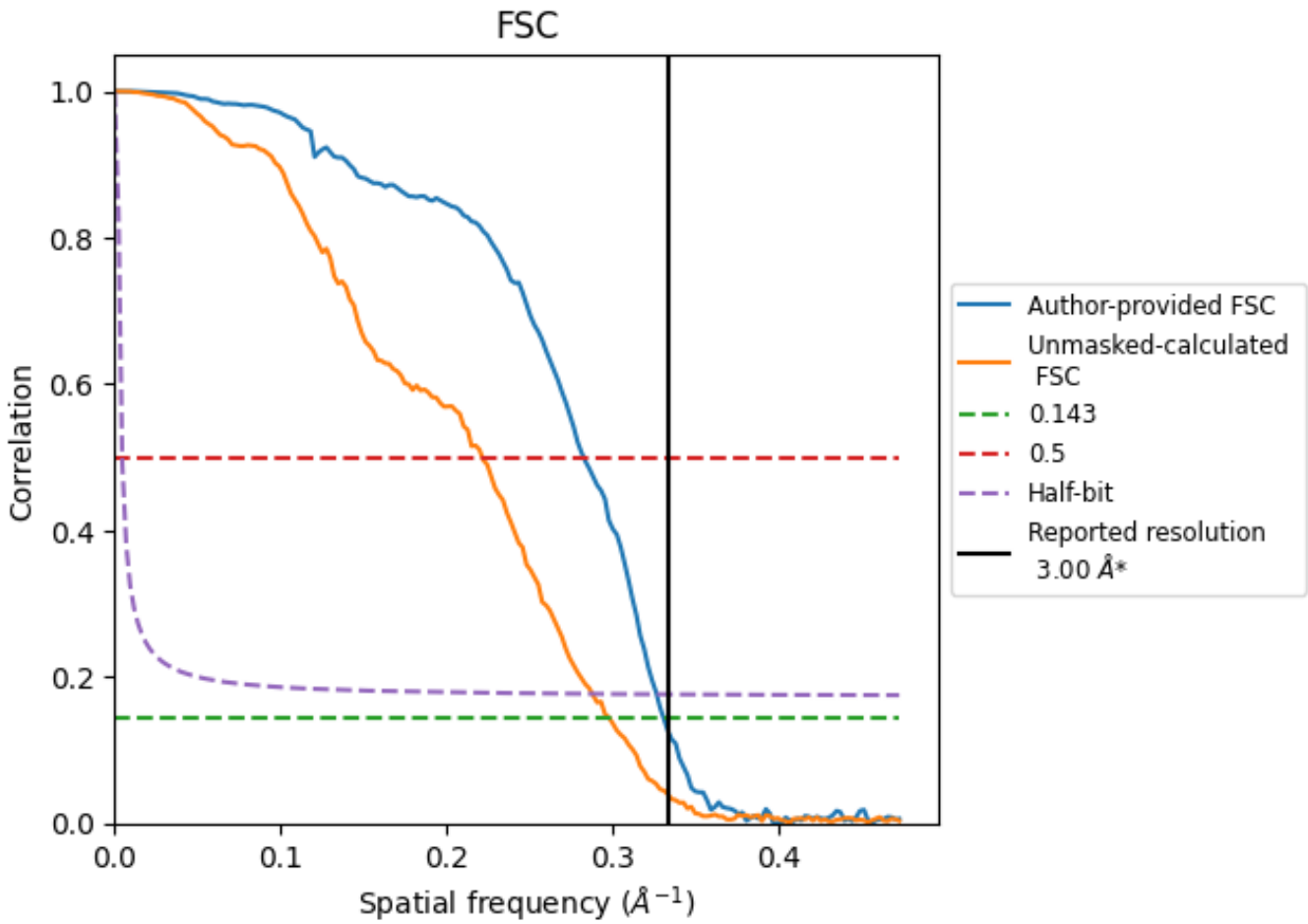


*Reported resolution corresponds to spatial frequency of 0.333 Å^{-1}

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 0.333 Å^{-1}

8.2 Resolution estimates (i)

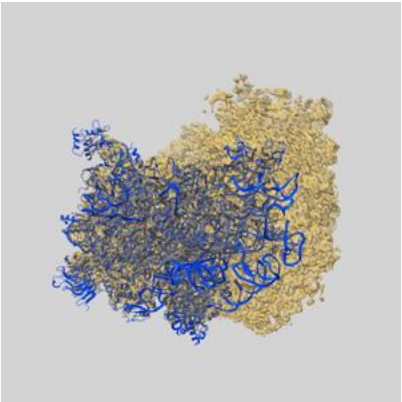
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	3.03	3.54	3.07
Unmasked-calculated*	3.36	4.52	3.48

*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 3.36 differs from the reported value 3.0 by more than 10 %

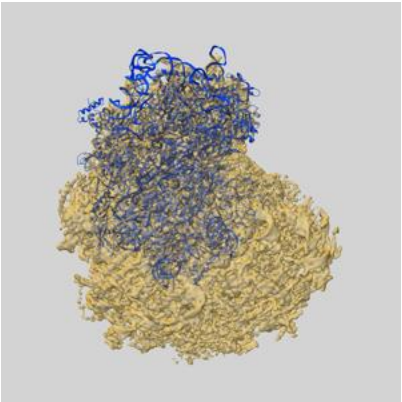
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-11457 and PDB model 6ZVI. Per-residue inclusion information can be found in section 3 on page 11.

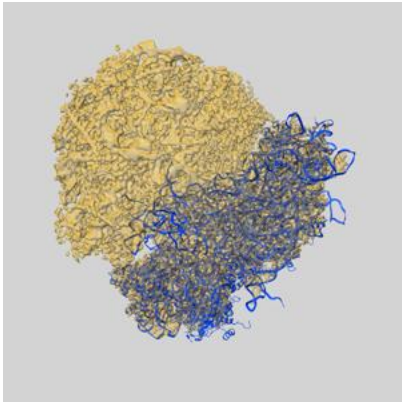
9.1 Map-model overlay (i)



X



Y



Z

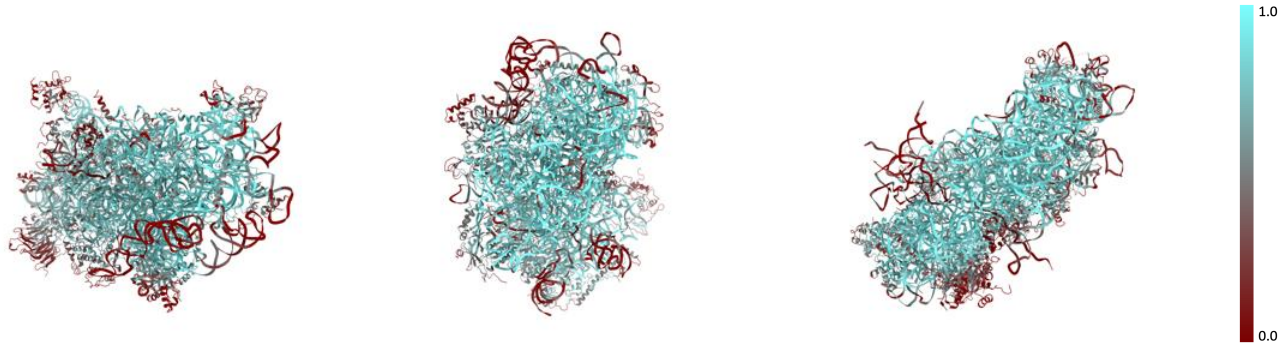
The images above show the 3D surface view of the map at the recommended contour level 0.06 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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.

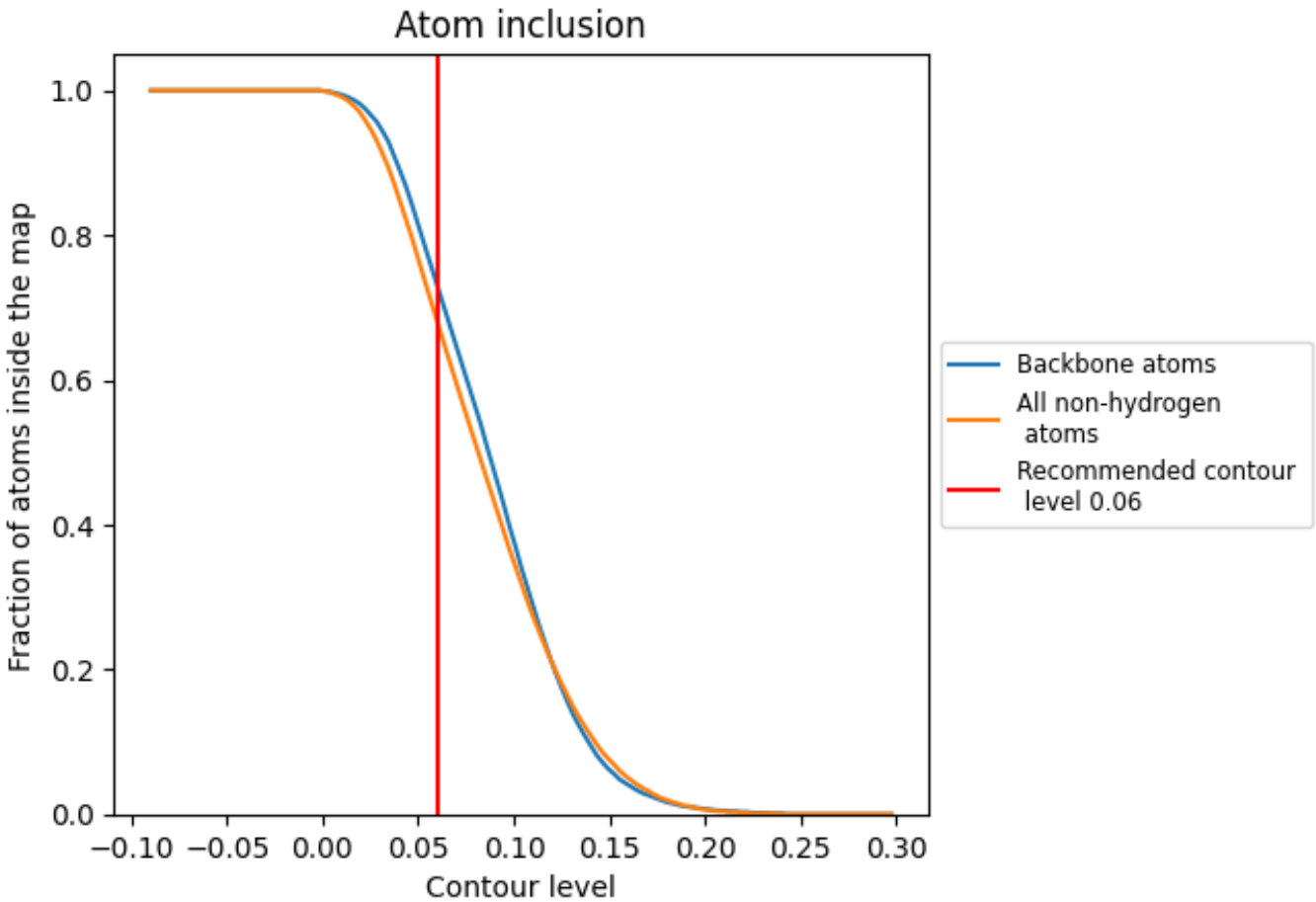
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.06).

9.4 Atom inclusion (i)



At the recommended contour level, 73% of all backbone atoms, 68% 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 (0.06) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6800	0.5110
A	0.6250	0.5280
B	0.6590	0.5490
C	0.5040	0.4940
D	0.6430	0.5620
E	0.8850	0.6060
H	0.8470	0.5930
I	0.5790	0.5260
J	0.5170	0.5120
K	0.8050	0.5720
L	0.5950	0.5380
N	0.5930	0.5240
O	0.9060	0.6000
P	0.6150	0.5020
Q	0.1950	0.3810
R	0.2820	0.4860
T	0.1610	0.4210
d	0.2640	0.2940
e	0.2520	0.1280
f	0.3260	0.3330
h	0.8080	0.5230
i	0.5930	0.5490
j	0.5910	0.5260
k	0.7540	0.5790
l	0.5890	0.5310
m	0.7280	0.5680
n	0.6370	0.5320
o	0.5260	0.5000
p	0.3890	0.4780
q	0.7210	0.5450
r	0.6420	0.5240
s	0.5780	0.5110
t	0.8040	0.5770
u	0.1000	0.3290
v	0.7910	0.5780

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
w	0.6880	0.5460
x	0.5690	0.5170
y	0.6920	0.5570
z	0.4990	0.5140