



wwPDB EM Validation Summary Report ⓘ

Mar 7, 2026 – 12:10 AM UTC

PDB ID : 6ICZ / pdb_00006icz
EMDB ID : EMD-9645
Title : Cryo-EM structure of a human post-catalytic spliceosome (P complex) at 3.0 angstrom
Authors : Zhang, X.; Zhan, X.; Yan, C.; Shi, Y.
Deposited on : 2018-09-07
Resolution : 3.00 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

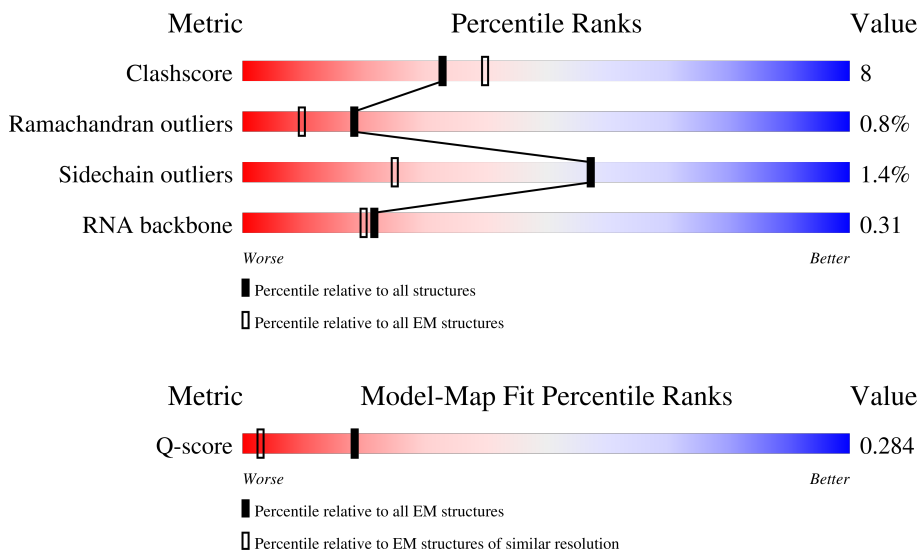
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 3.00 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	14081 (2.50 - 3.50)

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

Mol	Chain	Length	Quality of chain
1	v	148	
2	w	174	
3	u	411	

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Mol	Chain	Length	Quality of chain
4	x	703	96%
5	A	2335	12% 81% 15%
6	B	117	14% 29% 33% 20% 17%
7	C	972	73% 17% 8%
8	E	357	61% 22% 15%
9	F	107	46% 37% 7% 9%
10	G	273	6% 12% 10% 8% 69%
11	H	188	37% 17% 18% 37% 26%
12	J	848	33% 61% 5% 33%
13	L	802	27% 50% 6% 43%
14	M	243	43% 10% 47%
15	N	144	76% 17% 6%
16	O	420	54% 14% 32%
17	P	229	43% 5% 52%
18	R	536	38% 10% 51%
19	S	166	77% 19%
20	T	514	43% 16% 39%
21	U	2752	99%
22	V	908	28% 47% 50%
23	W	579	68% 18% 12%
24	X	184	14% 41% 9% 50%
25	Z	586	33% 8% 59%
26	I	855	57% 59% 6% 34%
27	y	301	24% 26% 74%
28	Q	1485	89% 88% 11%

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Mol	Chain	Length	Quality of chain
29	a	126	44% 64% 36%
29	h	126	56% 63% 36%
30	b	231	28% 36% 63%
30	i	231	33% 35% 63%
31	c	119	52% 67% 31%
31	j	119	47% 67% 31%
32	d	118	56% 75% 7% 18%
32	k	118	57% 66% 6% 28%
33	f	86	63% 85% 14%
33	m	86	58% 83% 15%
34	e	92	60% 82% 14%
34	l	92	62% 73% 12% 14%
35	g	76	71% 92% 5%
35	n	76	74% 74% 16% 9%
36	o	255	59% 51% 12% 36%
37	p	225	36% 37% 58%
38	Y	1220	42% 54% 42%
39	K	225	65% 52% 14% 32%
40	q	504	26% 23% 74%
40	r	504	26% 22% 74%
40	s	504	13% 12% 87%
40	t	504	13% 12% 87%
41	D	2136	81% 79% 19%

2 Entry composition [i](#)

There are 46 unique types of molecules in this entry. The entry contains 97900 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Protein mago nashi homolog 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
1	v	144	711	423	144	144	0	0

- Molecule 2 is a protein called RNA-binding protein 8A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	w	91	445	263	91	91	0	0

- Molecule 3 is a protein called Eukaryotic initiation factor 4A-III.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	u	386	1907	1135	386	386	0	0

- Molecule 4 is a protein called Protein CASC3.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	x	25	124	74	25	25	0	0

- Molecule 5 is a protein called Pre-mRNA-processing-splicing factor 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	A	2253	17837	11432	3157	3177	71	0	0

- Molecule 6 is a RNA chain called U5snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
6	B	97	2040	914	339	690	97	0	0

- Molecule 7 is a protein called 116 kDa U5 small nuclear ribonucleoprotein component.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	C	894	7066	4520	1178	1334	34	0	0

- Molecule 8 is a protein called U5 small nuclear ribonucleoprotein 40 kDa protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	E	303	2366	1487	415	451	13	0	0

- Molecule 9 is a RNA chain called U6snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
9	F	97	2075	928	381	669	97	0	0

- Molecule 10 is a RNA chain called pre-mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
10	G	84	1549	684	218	563	84	0	0

- Molecule 11 is a RNA chain called U2snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
11	H	140	2966	1326	510	990	140	0	0

- Molecule 12 is a protein called Crooked neck-like protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	J	571	3829	2385	720	718	6	0	0

- Molecule 13 is a protein called Cell division cycle 5-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	L	454	3064	1884	596	578	6	0	0

- Molecule 14 is a protein called Pre-mRNA-splicing factor SYF2.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	M	130	Total	C	N	O	S	0	0
			1098	684	204	208	2		

- Molecule 15 is a protein called Protein BUD31 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	N	143	Total	C	N	O	S	0	0
			1184	746	217	209	12		

- Molecule 16 is a protein called Pre-mRNA-splicing factor RBM22.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	O	285	Total	C	N	O	S	0	0
			2296	1442	408	426	20		

- Molecule 17 is a protein called Spliceosome-associated protein CWC15 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	P	110	Total	C	N	O	S	0	0
			929	569	182	176	2		

- Molecule 18 is a protein called SNW domain-containing protein 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	R	261	Total	C	N	O	P	S	0	0
			2073	1300	373	386	2	12		

- Molecule 19 is a protein called Peptidyl-prolyl cis-trans isomerase-like 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	159	Total	C	N	O	S	0	0
			1236	787	215	227	7		

- Molecule 20 is a protein called Pleiotropic regulator 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	313	Total	C	N	O	S	0	0
			2461	1554	447	452	8		

- Molecule 21 is a protein called Serine/arginine repetitive matrix protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	26	Total	C	N	O	S	0	0
			193	120	36	36	1		

- Molecule 22 is a protein called Pre-mRNA-splicing factor CWC22 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	452	Total	C	N	O	S	0	0
			2765	1723	508	523	11		

- Molecule 23 is a protein called Pre-mRNA-processing factor 17.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	W	508	Total	C	N	O	S	0	0
			4122	2623	714	761	24		

- Molecule 24 is a protein called PRKR-interacting protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	X	92	Total	C	N	O	S	0	0
			701	432	133	132	4		

- Molecule 25 is a protein called Pre-mRNA-splicing factor SLU7.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Z	242	Total	C	N	O	S	0	0
			1999	1260	357	374	8		

- Molecule 26 is a protein called Pre-mRNA-splicing factor SYF1.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	I	564	Total	C	N	O	0	0
			2782	1654	564	564		

- Molecule 27 is a protein called Peptidyl-prolyl cis-trans isomerase E.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	y	79	Total	C	N	O	0	0
			390	232	79	79		

- Molecule 28 is a protein called RNA helicase aquarius.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
28	Q	1322	6562	3918	1322	1322	4	0

- Molecule 29 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
29	h	81	398	236	81	81	0	0
29	a	81	399	237	81	81	0	0

- Molecule 30 is a protein called Small nuclear ribonucleoprotein-associated protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
30	i	86	424	252	86	86	0	0
30	b	86	424	252	86	86	0	0

- Molecule 31 is a protein called Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
31	j	82	406	242	82	82	0	0
31	c	82	406	242	82	82	0	0

- Molecule 32 is a protein called Small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
32	k	85	422	252	85	85	0	0
32	d	97	480	286	97	97	0	0

- Molecule 33 is a protein called Small nuclear ribonucleoprotein F.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
33	m	73	356	210	73	73	0	0
33	f	74	361	213	74	74	0	0

- Molecule 34 is a protein called Small nuclear ribonucleoprotein E.

Mol	Chain	Residues	Atoms				AltConf	Trace
34	l	79	Total	C	N	O	0	0
			391	233	79	79		
34	e	79	Total	C	N	O	0	0
			391	233	79	79		

- Molecule 35 is a protein called Small nuclear ribonucleoprotein G.

Mol	Chain	Residues	Atoms				AltConf	Trace
35	n	69	Total	C	N	O	0	0
			339	201	69	69		
35	g	74	Total	C	N	O	0	0
			363	215	74	74		

- Molecule 36 is a protein called U2 small nuclear ribonucleoprotein A'.

Mol	Chain	Residues	Atoms				AltConf	Trace
36	o	162	Total	C	N	O	0	0
			804	480	162	162		

- Molecule 37 is a protein called U2 small nuclear ribonucleoprotein B'.

Mol	Chain	Residues	Atoms				AltConf	Trace
37	p	94	Total	C	N	O	0	0
			464	276	94	94		

- Molecule 38 is a protein called ATP-dependent RNA helicase DHX8.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	Y	713	Total	C	N	O	S	0	0
			2917	1486	716	714	1		

- Molecule 39 is a protein called Pre-mRNA-splicing factor SPF27.

Mol	Chain	Residues	Atoms				AltConf	Trace
39	K	152	Total	C	N	O	0	0
			757	453	152	152		

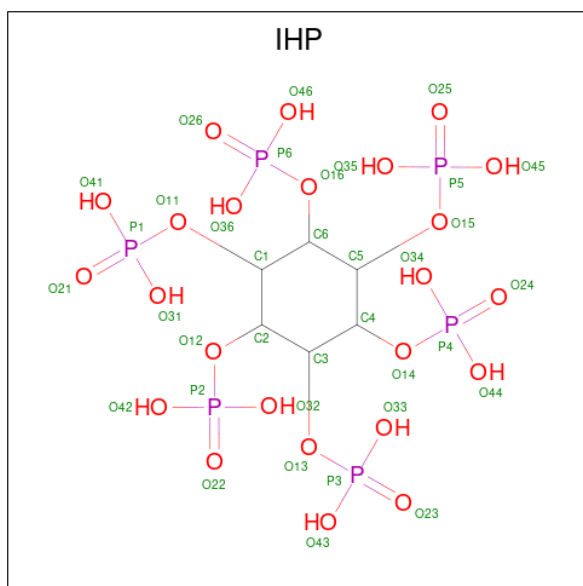
- Molecule 40 is a protein called Pre-mRNA-processing factor 19.

Mol	Chain	Residues	Atoms				AltConf	Trace
40	q	132	Total	C	N	O	0	0
			659	395	132	132		
40	r	131	Total	C	N	O	0	0
			654	392	131	131		
40	s	67	Total	C	N	O	0	0
			335	201	67	67		
40	t	67	Total	C	N	O	0	0
			335	201	67	67		

- Molecule 41 is a protein called U5 small nuclear ribonucleoprotein 200 kDa helicase.

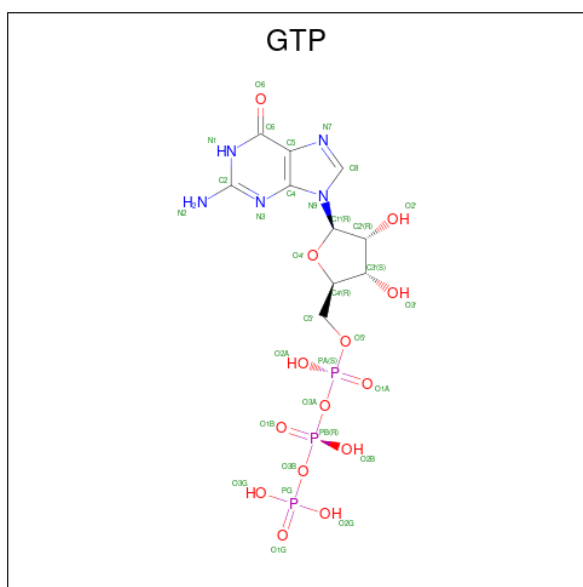
Mol	Chain	Residues	Atoms				AltConf	Trace
41	D	1722	Total	C	N	O	0	0
			8530	5086	1722	1722		

- Molecule 42 is INOSITOL HEXAKISPHOSPHATE (CCD ID: IHP) (formula: $C_6H_{18}O_{24}P_6$).



Mol	Chain	Residues	Atoms				AltConf
42	A	1	Total	C	O	P	0
			36	6	24	6	

- Molecule 43 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



Mol	Chain	Residues	Atoms					AltConf
43	C	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 44 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
44	C	1	Total	Mg	0
			1	1	
44	F	6	Total	Mg	0
			6	6	
44	Q	2	Total	Mg	0
			2	2	

- Molecule 45 is ZINC ION (CCD ID: ZN) (formula: Zn).

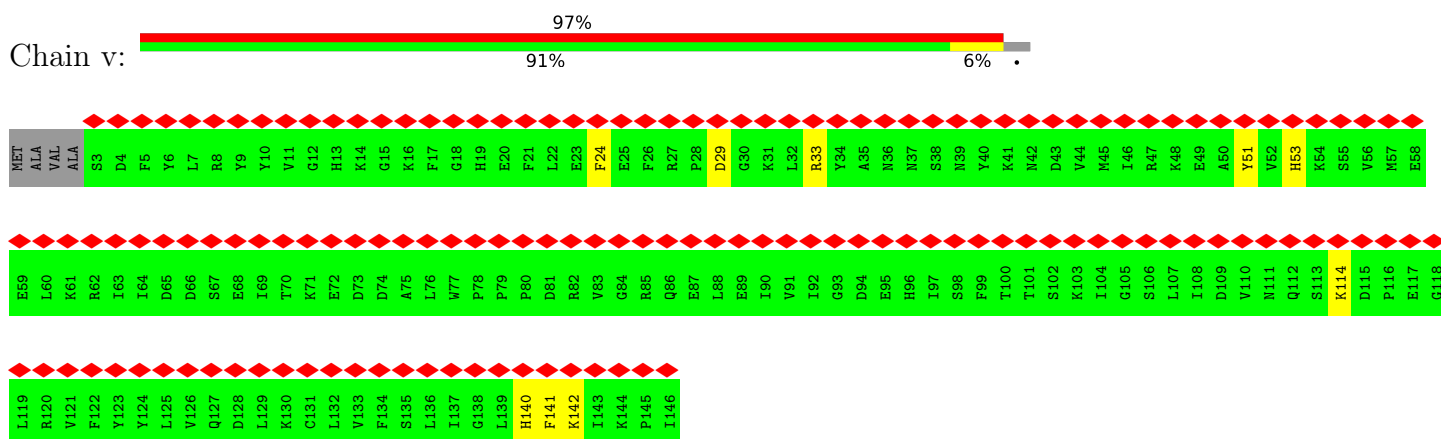
Mol	Chain	Residues	Atoms		AltConf
45	N	3	Total	Zn	0
			3	3	
45	O	3	Total	Zn	0
			3	3	
45	Z	1	Total	Zn	0
			1	1	

- Molecule 46 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).

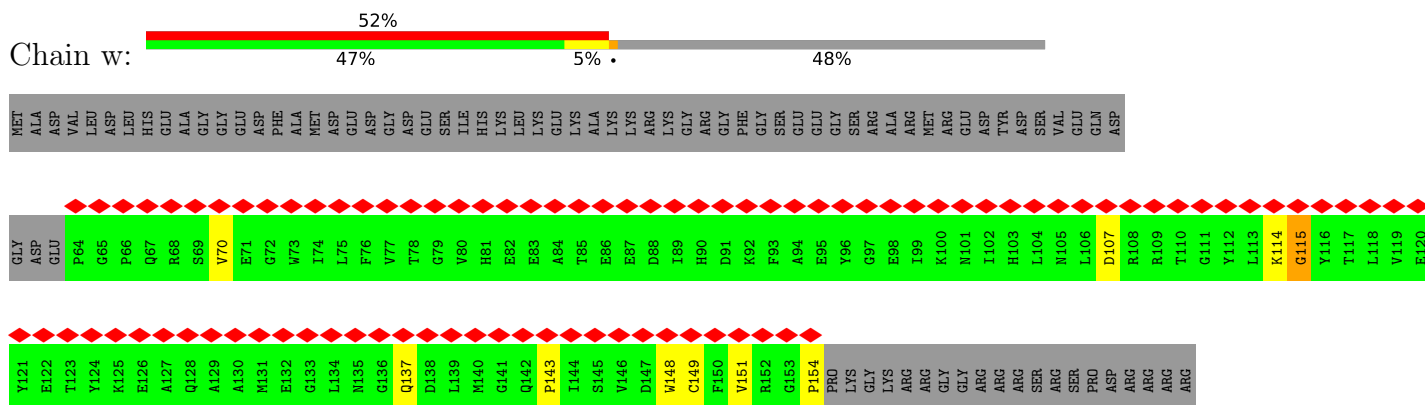
3 Residue-property plots

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

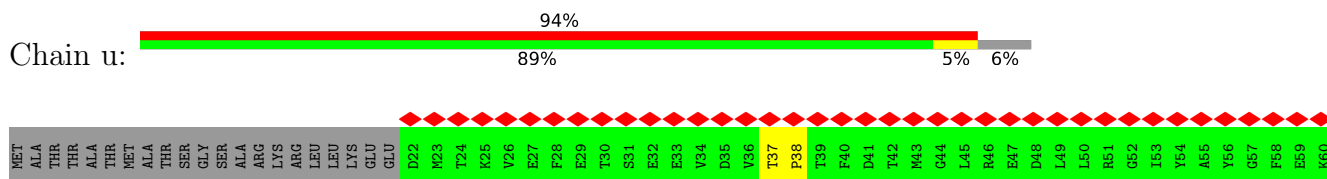
- Molecule 1: Protein mago nashi homolog 2

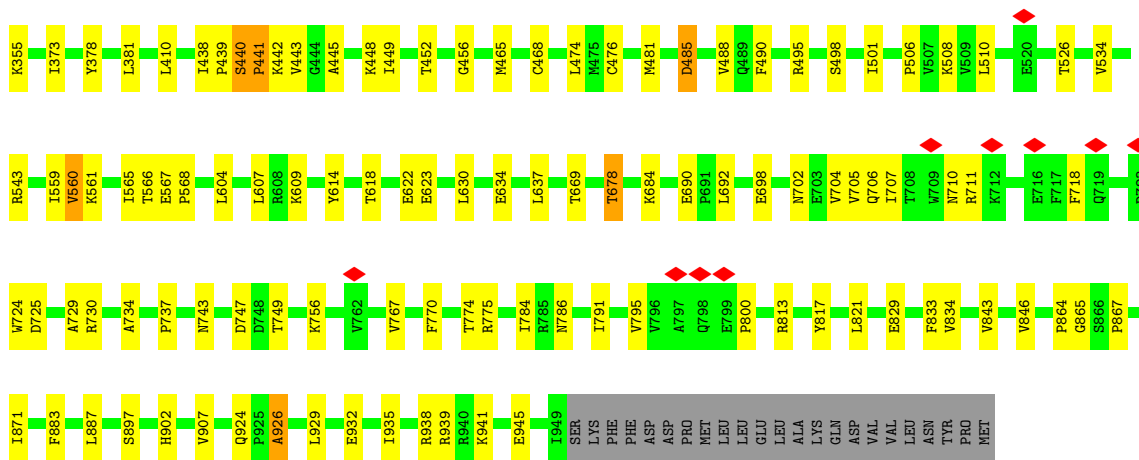


- Molecule 2: RNA-binding protein 8A

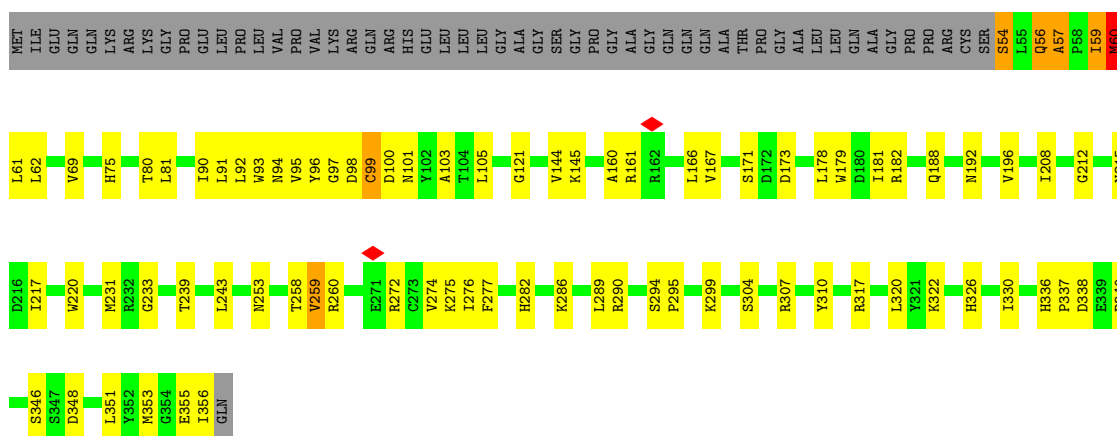


- Molecule 3: Eukaryotic initiation factor 4A-III

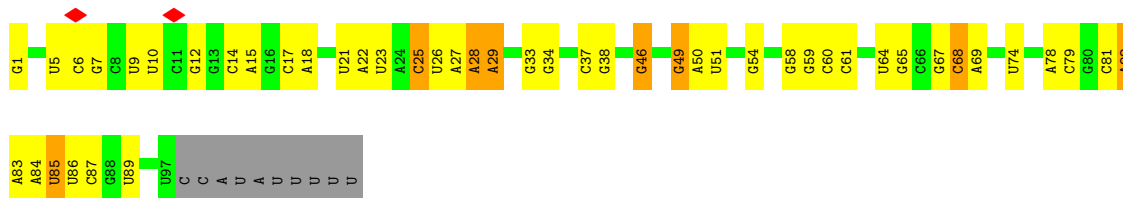




• Molecule 8: U5 small nuclear ribonucleoprotein 40 kDa protein

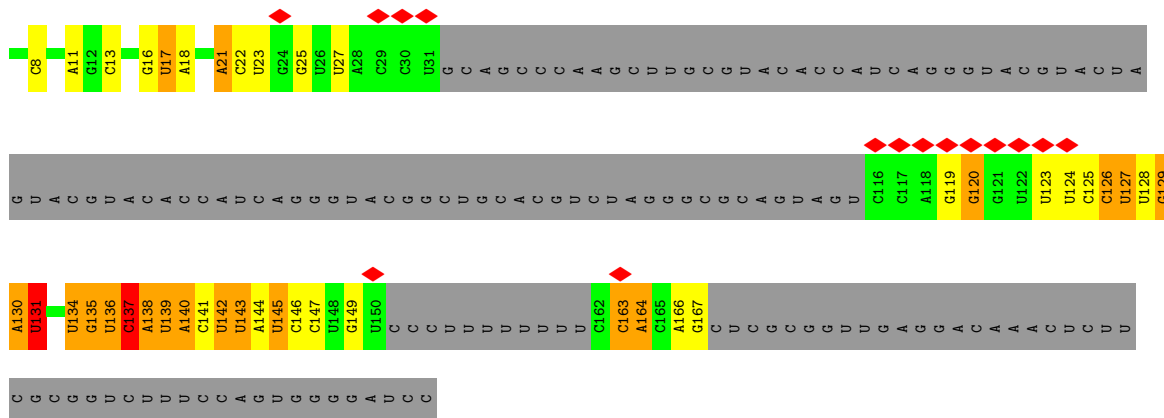


• Molecule 9: U6snRNA

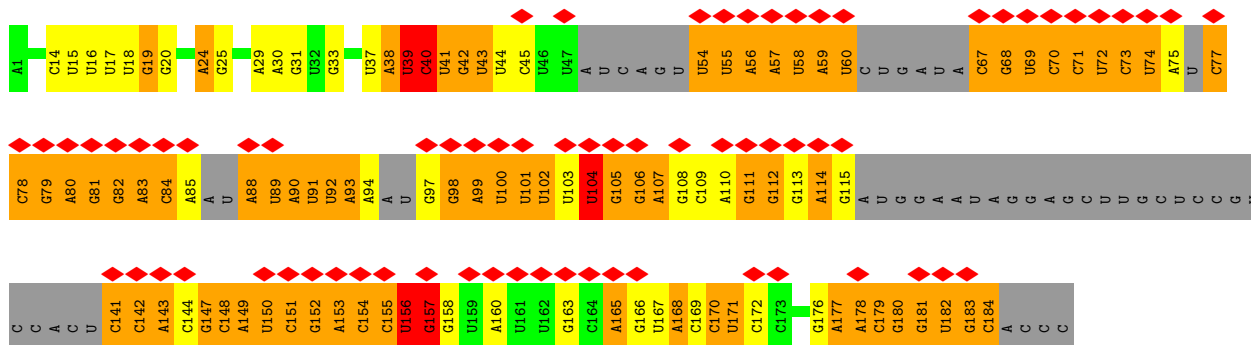


• Molecule 10: pre-mRNA

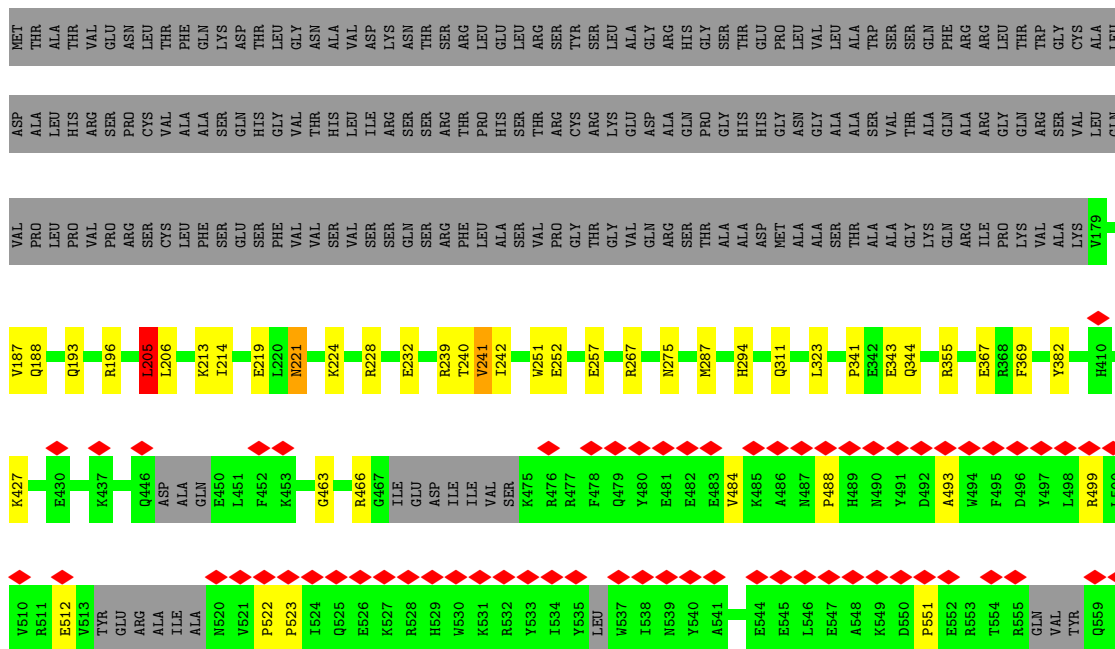


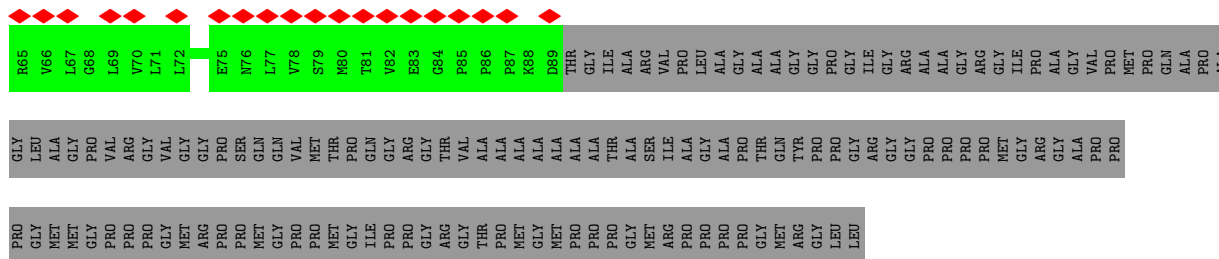


• Molecule 11: U2snRNA

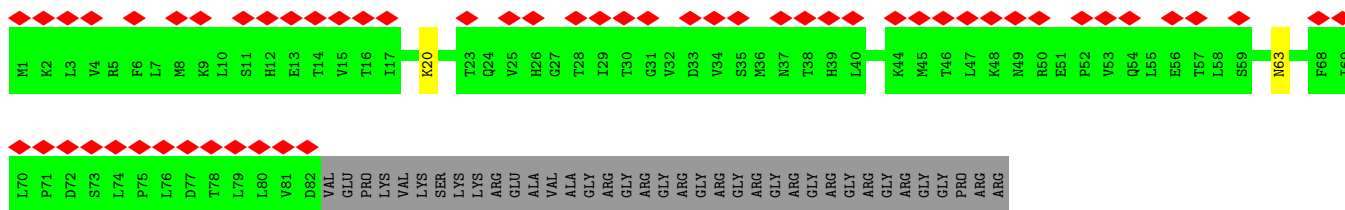


• Molecule 12: Crooked neck-like protein 1

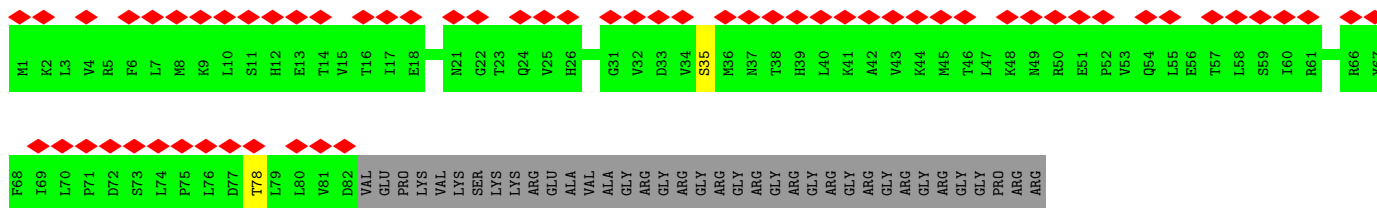




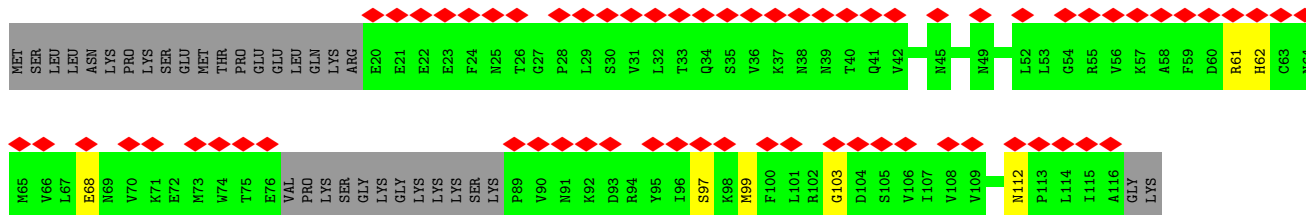
• Molecule 31: Small nuclear ribonucleoprotein Sm D1



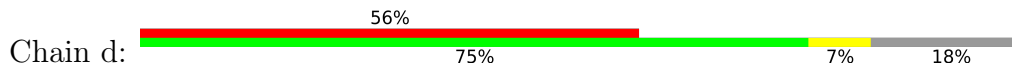
• Molecule 31: Small nuclear ribonucleoprotein Sm D1

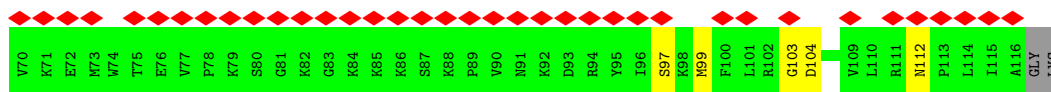


• Molecule 32: Small nuclear ribonucleoprotein Sm D2

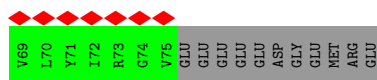
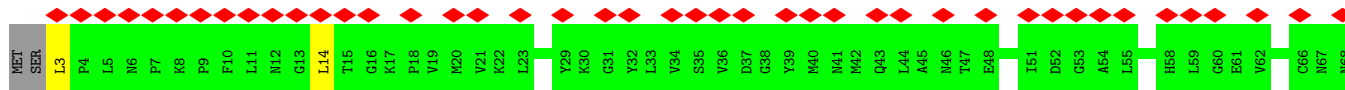
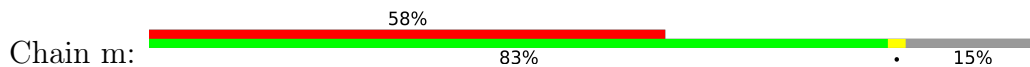


• Molecule 32: Small nuclear ribonucleoprotein Sm D2

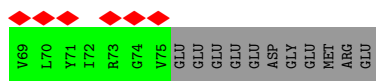
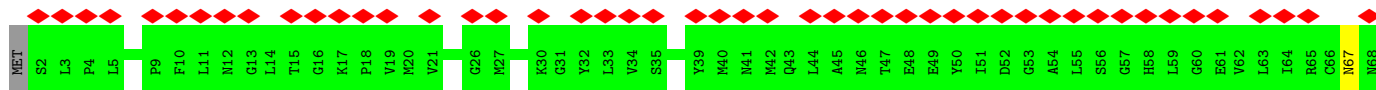
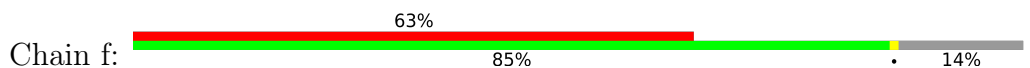




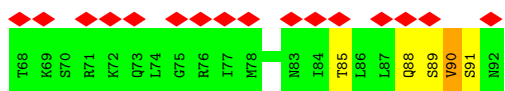
• Molecule 33: Small nuclear ribonucleoprotein F



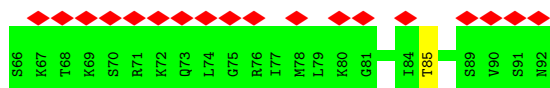
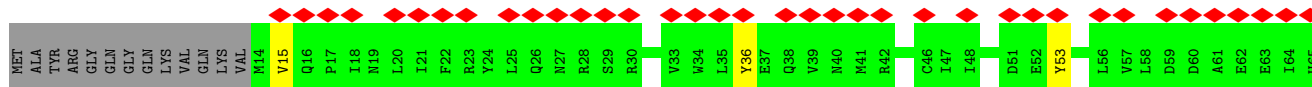
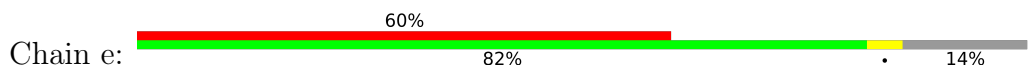
• Molecule 33: Small nuclear ribonucleoprotein F



• Molecule 34: Small nuclear ribonucleoprotein E



• Molecule 34: Small nuclear ribonucleoprotein E



• Molecule 35: Small nuclear ribonucleoprotein G

A1501	H1501	Q1441	P1381	Y1321	P1261	E1201	K1141	M1081	S1021	A961	L901	W841	G781
H1502	H1502	R1442	M1382	Q1322	L1262	L1202	K1142	V1082	S1022	L962	N902	T842	F782
H1503	H1503	K1443	E1383	D1323	T1263	T1203	I1143	Y1083	T1023	M963	A903	E843	A783
L1504	L1504	N1444	A1384	K1324	I1204	I1204	E1144	V1084	F1024	L964	E904	L844	I784
G1505	G1505	V1445	L1385	F1325	P1265	T1205	K1145	T1085	K1025	D965	I905	G845	H785
C1506	C1506	Q1446	A1386	P1326	Y1266	P1206	K1146	Q1086	M1026	K966	V906	A846	H786
S1507	S1507	L1447	E1387	F1327	F1267	D1207	M1147	Q1087	I1027	M967	L907	L847	A787
A1508	A1508	T1448	Q1388	F1328	I1268	F1208	F1148	A1088	T1028	N968	G908	D848	G788
T1509	T1509	N1449	N1389	N1329	P1269	Q1209	P1149	G1089	V1029	L969	N909	L849	M789
S1510	S1510	L1450	V1390	P1330	V1270	W1210	F1150	R1090	F1030	V970	V910	L850	T790
T1511	T1511	F1451	M1391	I1331	V1271	D1211	E1151	L1091	E1031	K971	Q911	Q851	R791
F1512	F1512	V1452	D1392	Q1332	S1272	E1212	R1152	M1092	E1032	Y972	N912	M852	V792
M1513	M1513	V1453	W1393	T1333	D1273	K1213	L1153	R1093	E1033	D973	A913	L853	D793
F1514	F1514	D1454	V1394	Q1334	V1274	V1214	Y1154	A1094	K1034	K974	K914	G854	R794
H1515	H1515	E1455	E1395	V1335	W1275	H1215	D1155	I1095	L1035	K975	D915	R855	T795
P1516	P1516	V1456	K1396	F1336	L1276	G1216	L1156	F1096	E1036	T976	A916	A856	L796
M1517	M1517	H1457	F1397	T1337	C1277	S1217	M1157	E1097	I1037	G977	V917	G857	V797
V1518	V1518	L1458	Q1398	T1338	S1278	S1218	H1158	I1098	Q1038	N978	N918	E858	E798
R1519	R1519	I1459	D1399	V1339	E1279	E1219	M1159	V1099	K1039	F979	W919	P859	D799
P1520	P1520	G1460	R1400	Y1340	T1280	A1220	E1160	L1100	L1040	Q980	L920	Q860	L800
V1521	V1521	G1461	L1401	N1341	Q1281	F1221	I1161	M1101	L1041	Y981	G921	Y861	F801
P1522	P1522	E1462	M1402	S1342	L1282	G1162	G1162	N1102	E1042	T982	Y922	D862	A802
L1523	L1523	N1463	K1403	D1343	P1283	I1223	E1163	G1103	E983	T983	A923	T863	D803
E1524	E1524	G1464	K1404	D1344	V1284	L1224	L1164	W1104	V1044	L984	Y924	K864	K804
L1525	L1525	P1465	V1405	N1345	S1285	V1225	I1165	A1105	P1045	G985	L925	G865	H805
H1526	H1526	V1466	V1406	F1346	F1286	E1226	R1166	I1106	L1046	R986	Y926	G866	I806
I1527	I1527	L1467	L1407	F1347	A1287	D1227	M1167	Q1107	P1047	T987	I927	G867	Q807
Q1528	Q1528	E1468	L1408	V1348	H1288	V1228	P1168	T1108	V1048	A988	R928	I868	V808
F1529	F1529	V1469	T1409	G1349	L1289	D1229	K1169	D1109	K1049	S989	M929	L869	L809
M1530	M1530	G1470	G1410	A1350	I1290	S1230	M1170	K1110	E1050	H990	L930	I870	V810
S1531	S1531	C1471	E1411	P1351	L1291	E1231	G1171	T1111	S1051	Y991	R931	T871	S811
I1532	I1532	S1472	T1412	T1352	P1292	V1232	K1172	L1112	E1052	Y992	S932	S872	T812
S1533	S1533	R1473	S1413	G1353	E1293	I1233	T1173	M1113	E1053	T993	P933	H873	A813
H1534	H1534	M1474	T1414	S1354	K1294	L1234	I1174	L1114	E1054	T994	T934	G874	T814
T1535	T1535	R1475	D1415	G1355	Y1295	H1235	H1175	C1115	P1055	N995	L935	E875	L815
Q1536	Q1536	Y1476	L1416	K1356	P1296	H1236	K1176	K1116	S1056	D996	Y936	L876	A816
T1537	T1537	I1477	K1417	T1357	P1297	E1237	Y1177	M1117	A1057	T997	G937	Q877	W817
R1538	R1538	S1478	L1418	I1358	P1298	V1238	V1178	I1118	K1058	V998	I938	E878	G818
L1539	L1539	S1479	L1419	C1359	T1299	F1239	H1179	D1119	I1059	Q999	S939	Y879	V819
L1540	L1540	Q1480	G1420	A1360	E1300	L1240	L1180	K1120	M1060	T1000	H940	L880	N820
M1541	M1541	I1481	K1421	E1361	L1301	L1241	F1181	R1121	V1061	Y1001	D941	S881	L821
S1542	S1542	E1482	K1422	F1362	L1302	K1242	P1182	M1122	L1062	M1002	D942	L882	R822
A1543	A1543	R1483	M1423	A1363	D1303	A1243	K1183	W1123	L063	Q1003	L943	L883	A823
K1544	K1544	P1484	I1424	I1364	L1304	K1244	L1184	Q1124	Q1064	L1004	K944	N884	H824
P1545	P1545	I1485	I1425	L1365	Q1305	Y1245	E1185	M1125	A1065	L1005	G945	Q885	T825
V1546	V1546	R1486	I1426	F1366	P1306	E1246	L1186	S1126	F1066	K1006	D946	Q886	V826
Y1547	Y1547	I1487	S1427	M1367	L1307	Q1247	S1187	C1127	I1067	P1007	P947	L887	I827
H1548	H1548	V1488	L1428	L1368	P1308	D1248	V1188	P1128	S1068	T1008	L948	P888	I828
A1549	A1549	A1489	P1429	L1369	V1309	E1249	H1189	L1129	Q1069	L1009	L949	P889	K829
I1550	I1550	L1490	E1430	Q1370	S1310	H1250	L1190	R1130	L1070	S1010	E890	G830	G829
T1551	T1551	S1491	K1431	S1371	A1311	L1251	Q1191	Q1131	K1071	E1011	Q951	S891	T831
K1552	K1552	S1492	W1432	S1372	L1312	I1252	P1192	F1132	L1072	I1012	R952	Q892	Q832
H1553	H1553	S1493	D1433	E1373	R1313	T1253	I1193	K1133	E1073	E1013	R953	M893	G833
S1554	S1554	L1494	I1434	G1374	M1314	F1254	T1194	R1134	G1074	L1014	L954	Y894	Y834
P1555	P1555	S1495	L1435	R1375	S1315	F1255	L1195	L1135	F1075	F1015	D955	S895	S835
K1556	K1556	N1496	S1436	C1376	A1316	V1256	S1196	P1136	A1076	R1016	L956	K896	P836
L1557	L1557	A1497	R1437	V1377	F1317	P1257	T1197	E1137	L1077	V1017	V957	L897	E837
V1558	V1558	K1498	L1438	Y1378	E1318	V1258	L1198	I1138	M1078	F1018	P898	E838	K838
V1559	V1559	D1499	W1439	I1379	S1319	F1259	K1199	V1139	A1079	S1019	D899	G839	G840
I1560	I1560	V1500	K1440	T1380	L1320	E1260	V1200	V1140	D1080	L1020	A960	M900	R840

A2101	H2102	M2103	Y2104	T2105	L2106	Y2107	F2108	M2109	S2110	D2111	A2112	Y2113	M2114	G2115	C2116	D2117	Q2118	E2119	Y2120	K2121	F2122	S2123	V2124	D2125	VAL	LYS	GLU	ALA	GLU	THR	SER	ASP	SER	ASP																										
L2041	E2042	R2043	E2044	E2045	E2046	V2047	T2048	G2049	P2050	V2051	L2052	A2053	P2054	L2055	F2056	P2057	Q2058	K2059	R2060	E2061	E2062	G2063	W2064	W2065	W2066	V2067	I2068	G2069	D2070	A2071	K2072	S2073	N2074	S2075	L2076	I2077	S2078	I2079	K2080	R2081	L2082	T2083	L2084	Q2085	Q2086	K2087	A2088	K2089	V2090	K2091	L2092	D2093	F2094	V2095	A2096	F2097	A2098	T2099	G2100	
R1861	H1862	H1863	E1864	D1865	M1866	L1867	L1868	V1869	Q1870	L1871	A1872	Q1873	K1874	V1875	P1876	H1877	K1878	L1879	M1880	M1881	P1882	K1883	F1884	M1885	D1886	P1887	H1888	V1889	M1890	Q1891	L1892	M1893	L1894	L1895	Q1896	A1897	H1898	L1899	S1900	R1901	M1902	Q1903	L1904	S1905	A1906	E1907	L1908	Q1909	S1910	D1911	T1912	E1913	E1914	I1915	L1916	S1917	K1918	A1919	I1920	
C1801	I1802	S1803	I1804	E1805	D1806	E1807	M1808	V1809	V1810	A1811	P1812	L1813	M1814	L1815	Q1816	I1817	I1818	A1819	A1820	Y1821	Y1822	Y1823	I1824	M1825	I1826	T1827	T1828	I1829	E1830	L1831	F1832	S1833	M1834	S1835	L1836	M1837	A1838	K1839	T1840	K1841	R1842	R1843	G1844	L1845	I1846	E1847	I1848	I1849	S1850	M1851	A1852	A1853	E1854	Y1855	E1856	M1857	I1858	P1859	I1860	
V1741	T1742	K1743	T1744	I1745	E1746	M1747	K1748	Q1749	D1750	A1751	V1752	D1753	Y1754	L1755	T1756	M1757	F1758	I1759	L1760	Y1761	R1762	R1763	M1764	T1765	Q1766	M1767	P1768	M1769	Y1770	Y1771	M1772	L1773	Q1774	G1775	I1776	S1777	H1778	R1779	H1780	L1781	D1782	D1783	H1784	L1785	L1786	E1787	L1788	V1789	H1790	Q1791	T1792	L1793	S1794	D1795	L1796	E1797	Q1798	S1799	K1800	
I1681	Y1682	D1683	V1684	L1685	Q1686	M1687	V1688	H1689	H1690	A1691	M1692	R1693	P1694	L1695	Q1696	D1697	D1698	E1699	G1700	I1701	C1702	V1703	I1704	M1705	C1706	Q1707	G1708	S1709	K1710	M1711	D1712	F1713	P1714	M1715	K1716	F1717	L1718	Y1719	E1720	P1721	L1722	P1723	V1724	E1725	S1726	H1727	L1728	D1729	H1730	M1731	M1732	H1733	D1734	H1735	F1736	M1737	A1738	E1739	I1740	
H1621	E1622	G1623	L1624	S1625	P1626	M1627	E1628	R1629	R1630	L1631	V1632	E1633	Q1634	L1635	F1636	S1637	S1638	G1639	A1640	I1641	Q1642	V1643	V1644	V1645	A1646	S1647	R1648	S1649	L1650	C1651	G1652	G1653	M1654	N1655	V1656	A1657	I1658	P1659	H1660	V1661	I1662	I1663	K1664	M1665	T1666	Q1667	Y1668	Y1669	N1670	G1671	K1672	I1673	H1674	A1675	Y1676	V1677	D1678	Y1679	P1680	
V1561	F1562	V1563	P1564	S1565	R1566	K1567	Q1568	T1569	R1570	L1571	T1572	A1573	I1574	D1575	I1576	L1577	T1578	T1579	C1580	A1581	A1582	D1583	I1584	Q1585	R1586	Q1587	R1588	F1589	L1590	H1591	C1592	T1593	E1594	K1595	D1596	L1597	I1598	I1599	P1599	Y1600	L1601	E1602	K1603	L1604	S1605	D1606	S1607	T1608	L1609	K1610	E1611	T1612	L1613	L1614	M1615	G1616	V1617	G1618	Y1619	L1620

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	143320	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	45	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.552	Depositor
Minimum map value	-0.288	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.011	Depositor
Recommended contour level	0.03	Depositor
Map size (\AA)	535.2, 535.2, 535.2	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.338, 1.338, 1.338	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: IHP, SEP, GTP, ZN, ATP, MG

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	v	0.46	0/710	1.03	3/987 (0.3%)
2	w	0.46	0/444	1.21	4/614 (0.7%)
3	u	0.51	0/1906	1.20	13/2653 (0.5%)
4	x	0.53	0/123	1.12	0/170
5	A	0.52	1/18287 (0.0%)	0.81	25/24842 (0.1%)
6	B	0.48	1/2274 (0.0%)	0.61	2/3535 (0.1%)
7	C	1.55	10/7225 (0.1%)	0.86	18/9818 (0.2%)
8	E	0.30	0/2420	0.77	3/3281 (0.1%)
9	F	0.47	0/2323	0.59	0/3619
10	G	0.41	0/1716	0.78	5/2656 (0.2%)
11	H	0.79	24/3305 (0.7%)	1.29	46/5130 (0.9%)
12	J	0.48	0/3870	0.86	15/5252 (0.3%)
13	L	0.47	1/3091 (0.0%)	0.83	10/4178 (0.2%)
14	M	0.39	0/1119	0.72	0/1497
15	N	1.04	1/1210 (0.1%)	0.99	5/1622 (0.3%)
16	O	0.40	0/2344	0.74	2/3163 (0.1%)
17	P	0.41	0/943	0.70	0/1255
18	R	0.46	0/2091	0.81	2/2809 (0.1%)
19	S	0.29	0/1268	0.62	0/1714
20	T	0.63	0/2526	0.94	7/3443 (0.2%)
21	U	0.29	0/196	0.64	0/265
22	V	0.39	0/2784	0.77	0/3791
23	W	0.36	0/4230	0.82	7/5713 (0.1%)
24	X	0.30	0/714	0.64	0/959
25	Z	0.34	0/2049	0.80	6/2757 (0.2%)
26	I	0.53	0/2749	0.96	20/3773 (0.5%)
27	y	0.43	0/389	1.01	0/540
28	Q	0.38	0/6565	0.86	4/9143 (0.0%)
29	a	0.78	0/397	1.00	0/549
29	h	0.78	0/396	0.99	0/547
30	b	0.85	0/423	1.14	3/587 (0.5%)
30	i	0.84	0/423	1.14	3/587 (0.5%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
31	c	0.88	0/405	1.12	1/563 (0.2%)
31	j	0.87	0/405	1.11	0/563
32	d	1.12	0/479	1.25	1/666 (0.2%)
32	k	1.14	0/420	1.24	1/583 (0.2%)
33	f	1.20	0/360	1.25	0/497
33	m	1.21	1/355 (0.3%)	1.24	0/490
34	e	1.04	0/390	1.24	1/542 (0.2%)
34	l	1.00	0/390	1.33	2/542 (0.4%)
35	g	0.86	0/362	1.08	1/501 (0.2%)
35	n	0.80	0/337	1.05	1/465 (0.2%)
36	o	0.98	0/803	2.25	43/1119 (3.8%)
37	p	0.93	0/463	1.85	6/643 (0.9%)
38	Y	0.82	0/2917	1.65	22/3670 (0.6%)
39	K	0.62	1/753 (0.1%)	1.07	3/1046 (0.3%)
40	q	0.63	0/658	0.97	3/919 (0.3%)
40	r	0.57	0/653	1.07	6/912 (0.7%)
40	s	0.50	0/334	0.91	0/466
40	t	0.56	0/334	0.82	0/466
41	D	0.56	0/8529	1.12	27/11891 (0.2%)
All	All	0.68	40/99857 (0.0%)	0.96	321/137993 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
5	A	0	6
7	C	0	7
8	E	0	1
11	H	0	1
12	J	0	3
14	M	0	1
16	O	0	1
17	P	0	1
18	R	0	2
20	T	0	3
23	W	0	3
25	Z	0	2
32	d	0	1
32	k	0	1
38	Y	0	15

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Mol	Chain	#Chirality outliers	#Planarity outliers
41	D	0	1
All	All	0	49

The worst 5 of 40 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	104	LEU	CB-CG	55.56	2.64	1.53
7	C	172	PHE	CE1-CZ	53.27	2.98	1.38
7	C	172	PHE	CD1-CE1	52.29	2.95	1.38
7	C	172	PHE	CD2-CE2	51.50	2.93	1.38
7	C	172	PHE	CE2-CZ	50.12	2.89	1.38

The worst 5 of 321 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	104	LEU	CD1-CG-CD2	-12.80	82.65	110.80
10	G	131	U	C2'-C3'-O3'	-12.13	95.51	113.70
7	C	104	LEU	CA-CB-CG	11.85	157.76	116.30
5	A	624	GLY	CA-C-N	10.96	131.27	119.87
5	A	624	GLY	C-N-CA	10.96	131.27	119.87

There are no chirality outliers.

5 of 49 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	A	1070	ASP	Peptide
5	A	1091	TYR	Peptide
5	A	1209	HIS	Peptide
5	A	851	SER	Peptide
5	A	941	LYS	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	v	711	0	299	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	w	445	0	203	6	0
3	u	1907	0	845	2	0
4	x	124	0	51	0	0
5	A	17837	0	17053	242	0
6	B	2040	0	1034	66	0
7	C	7066	0	7084	131	0
8	E	2366	0	2303	67	0
9	F	2075	0	1048	27	0
10	G	1549	0	784	51	0
11	H	2966	0	1505	256	0
12	J	3829	0	2907	40	0
13	L	3064	0	2521	53	0
14	M	1098	0	1082	24	0
15	N	1184	0	1189	41	0
16	O	2296	0	2284	36	0
17	P	929	0	910	7	0
18	R	2073	0	2119	37	0
19	S	1236	0	1210	25	0
20	T	2461	0	2420	70	0
21	U	193	0	196	5	0
22	V	2765	0	1955	17	0
23	W	4122	0	4031	154	0
24	X	701	0	631	56	0
25	Z	1999	0	1951	35	0
26	I	2782	0	1245	54	0
27	y	390	0	190	1	0
28	Q	6562	0	2836	6	0
29	a	399	0	173	0	0
29	h	398	0	172	1	0
30	b	424	0	179	1	0
30	i	424	0	179	3	0
31	c	406	0	170	1	0
31	j	406	0	170	3	0
32	d	480	0	200	8	0
32	k	422	0	175	5	0
33	f	361	0	158	1	0
33	m	356	0	156	1	0
34	e	391	0	163	5	0
34	l	391	0	163	28	0
35	g	363	0	160	4	0
35	n	339	0	145	45	0
36	o	804	0	350	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	p	464	0	205	16	0
38	Y	2917	0	857	15	0
39	K	757	0	338	52	0
40	q	659	0	296	23	0
40	r	654	0	294	33	0
40	s	335	0	168	5	0
40	t	335	0	168	8	0
41	D	8530	0	3747	12	0
42	A	36	0	6	3	0
43	C	32	0	12	2	0
44	C	1	0	0	0	0
44	F	6	0	0	0	0
44	Q	2	0	0	0	0
45	N	3	0	0	0	0
45	O	3	0	0	0	0
45	Z	1	0	0	0	0
46	Q	31	0	12	0	0
All	All	97900	0	70702	1400	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 8.

The worst 5 of 1400 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)
23:W:266:ARG:HB2	34:l:16:GLN:CB	1.23	1.64
7:C:104:LEU:CG	7:C:104:LEU:CD1	1.74	1.61
12:J:466:ARG:CB	26:I:607:GLY:HA2	1.44	1.47
23:W:257:ILE:HG13	35:n:10:LYS:CB	1.47	1.45
23:W:264:ASN:HB3	35:n:35:ASP:CA	1.43	1.44

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	v	142/148 (96%)	138 (97%)	4 (3%)	0	100	100
2	w	89/174 (51%)	87 (98%)	1 (1%)	1 (1%)	11	43
3	u	384/411 (93%)	372 (97%)	9 (2%)	3 (1%)	16	50
4	x	23/703 (3%)	22 (96%)	1 (4%)	0	100	100
5	A	2247/2335 (96%)	2091 (93%)	147 (6%)	9 (0%)	30	65
7	C	892/972 (92%)	798 (90%)	90 (10%)	4 (0%)	30	65
8	E	301/357 (84%)	273 (91%)	28 (9%)	0	100	100
12	J	530/848 (62%)	491 (93%)	32 (6%)	7 (1%)	9	38
13	L	436/802 (54%)	405 (93%)	27 (6%)	4 (1%)	14	48
14	M	128/243 (53%)	124 (97%)	3 (2%)	1 (1%)	16	50
15	N	141/144 (98%)	126 (89%)	13 (9%)	2 (1%)	9	36
16	O	283/420 (67%)	260 (92%)	22 (8%)	1 (0%)	30	65
17	P	104/229 (45%)	86 (83%)	15 (14%)	3 (3%)	3	20
18	R	255/536 (48%)	229 (90%)	24 (9%)	2 (1%)	16	50
19	S	157/166 (95%)	148 (94%)	9 (6%)	0	100	100
20	T	311/514 (60%)	281 (90%)	23 (7%)	7 (2%)	5	25
21	U	24/2752 (1%)	23 (96%)	1 (4%)	0	100	100
22	V	444/908 (49%)	429 (97%)	14 (3%)	1 (0%)	43	76
23	W	506/579 (87%)	441 (87%)	60 (12%)	5 (1%)	12	45
24	X	90/184 (49%)	84 (93%)	6 (7%)	0	100	100
25	Z	238/586 (41%)	214 (90%)	24 (10%)	0	100	100
26	I	498/855 (58%)	481 (97%)	10 (2%)	7 (1%)	9	36
27	y	77/301 (26%)	75 (97%)	2 (3%)	0	100	100
28	Q	1308/1485 (88%)	1282 (98%)	26 (2%)	0	100	100
29	a	77/126 (61%)	76 (99%)	1 (1%)	0	100	100
29	h	77/126 (61%)	76 (99%)	1 (1%)	0	100	100
30	b	84/231 (36%)	82 (98%)	2 (2%)	0	100	100
30	i	84/231 (36%)	82 (98%)	2 (2%)	0	100	100
31	c	80/119 (67%)	77 (96%)	3 (4%)	0	100	100
31	j	80/119 (67%)	77 (96%)	3 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
32	d	95/118 (80%)	91 (96%)	4 (4%)	0	100	100
32	k	81/118 (69%)	78 (96%)	3 (4%)	0	100	100
33	f	72/86 (84%)	69 (96%)	3 (4%)	0	100	100
33	m	71/86 (83%)	68 (96%)	3 (4%)	0	100	100
34	e	77/92 (84%)	76 (99%)	1 (1%)	0	100	100
34	l	77/92 (84%)	76 (99%)	1 (1%)	0	100	100
35	g	72/76 (95%)	70 (97%)	2 (3%)	0	100	100
35	n	65/76 (86%)	59 (91%)	4 (6%)	2 (3%)	3	19
36	o	160/255 (63%)	146 (91%)	12 (8%)	2 (1%)	9	38
37	p	92/225 (41%)	90 (98%)	2 (2%)	0	100	100
38	Y	709/1220 (58%)	616 (87%)	61 (9%)	32 (4%)	2	12
39	K	144/225 (64%)	129 (90%)	8 (6%)	7 (5%)	1	10
40	q	130/504 (26%)	119 (92%)	7 (5%)	4 (3%)	3	19
40	r	129/504 (26%)	119 (92%)	8 (6%)	2 (2%)	7	34
40	s	65/504 (13%)	62 (95%)	2 (3%)	1 (2%)	8	35
40	t	65/504 (13%)	64 (98%)	0	1 (2%)	8	35
41	D	1720/2136 (80%)	1633 (95%)	84 (5%)	3 (0%)	43	76
All	All	13914/24425 (57%)	12995 (93%)	808 (6%)	111 (1%)	18	50

5 of 111 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	u	383	ASN
15	N	36	PRO
18	R	233	PRO
20	T	343	PRO
20	T	458	SER

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	A	1795/2108 (85%)	1783 (99%)	12 (1%)	76	86
7	C	793/866 (92%)	788 (99%)	5 (1%)	78	88
8	E	259/300 (86%)	253 (98%)	6 (2%)	44	74
12	J	241/751 (32%)	240 (100%)	1 (0%)	84	90
13	L	208/709 (29%)	206 (99%)	2 (1%)	68	84
14	M	117/209 (56%)	115 (98%)	2 (2%)	53	78
15	N	130/130 (100%)	124 (95%)	6 (5%)	24	58
16	O	255/361 (71%)	251 (98%)	4 (2%)	55	79
17	P	99/203 (49%)	99 (100%)	0	100	100
18	R	219/457 (48%)	215 (98%)	4 (2%)	51	77
19	S	129/134 (96%)	129 (100%)	0	100	100
20	T	269/441 (61%)	260 (97%)	9 (3%)	33	67
21	U	21/2432 (1%)	20 (95%)	1 (5%)	23	57
22	V	140/838 (17%)	134 (96%)	6 (4%)	26	60
23	W	447/502 (89%)	440 (98%)	7 (2%)	55	79
24	X	62/157 (40%)	58 (94%)	4 (6%)	15	47
25	Z	214/520 (41%)	211 (99%)	3 (1%)	59	80
38	Y	8/1085 (1%)	4 (50%)	4 (50%)	0	0
All	All	5406/12203 (44%)	5330 (99%)	76 (1%)	57	80

5 of 76 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
22	V	597	PRO
25	Z	166	LYS
23	W	257	ILE
24	X	104	LYS
38	Y	411	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 95 such sidechains are listed below:

Mol	Chain	Res	Type
13	L	211	ASN
18	R	71	GLN
14	M	172	HIS
16	O	79	ASN

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Mol	Chain	Res	Type
18	R	279	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
10	G	82/273 (30%)	44 (53%)	7 (8%)
11	H	133/188 (70%)	45 (33%)	9 (6%)
6	B	96/117 (82%)	46 (47%)	8 (8%)
9	F	96/107 (89%)	33 (34%)	6 (6%)
All	All	407/685 (59%)	168 (41%)	30 (7%)

5 of 168 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
6	B	9	G
6	B	10	U
6	B	13	C
6	B	19	A
6	B	20	G

5 of 30 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
10	G	-12	G
11	H	106	G
10	G	21	A
11	H	168	A
11	H	100	U

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	SEP	R	232	18	8,9,10	1.52	1 (12%)	7,12,14	1.81	1 (14%)
18	SEP	R	224	18	8,9,10	0.84	0	7,12,14	1.54	1 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	SEP	R	232	18	-	2/6/8/10	-
18	SEP	R	224	18	-	1/6/8/10	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	R	232	SEP	P-O1P	3.33	1.60	1.50

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	R	232	SEP	OG-CB-CA	4.37	112.39	108.14
18	R	224	SEP	OG-CB-CA	-2.59	105.63	108.14

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	R	232	SEP	N-CA-CB-OG
18	R	232	SEP	C-CA-CB-OG
18	R	224	SEP	CB-OG-P-O1P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 19 ligands modelled in this entry, 16 are monoatomic - leaving 3 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
42	IHP	A	3000	-	36,36,36	0.84	0	60,60,60	1.08	2 (3%)
46	ATP	Q	1501	44	32,33,33	2.06	7 (21%)	48,52,52	1.89	16 (33%)
43	GTP	C	1500	44	33,34,34	1.00	2 (6%)	50,54,54	1.60	9 (18%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
42	IHP	A	3000	-	-	5/30/54/54	0/1/1/1
46	ATP	Q	1501	44	-	4/22/38/38	0/3/3/3
43	GTP	C	1500	44	-	4/22/38/38	0/3/3/3

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	Q	1501	ATP	PB-O3B	7.43	1.67	1.59
46	Q	1501	ATP	C6-N6	4.57	1.45	1.34
46	Q	1501	ATP	C4-N3	3.31	1.40	1.34
46	Q	1501	ATP	C2'-C3'	-2.82	1.45	1.53
46	Q	1501	ATP	C3'-C4'	-2.24	1.47	1.53

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	Q	1501	ATP	C5-C4-N3	-4.96	119.89	126.72
43	C	1500	GTP	C5-C4-N3	-4.54	121.16	128.39
43	C	1500	GTP	C2-N3-C4	4.53	120.10	112.30
46	Q	1501	ATP	N3-C2-N1	-4.33	122.02	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	Q	1501	ATP	N3-C4-N9	3.79	133.62	127.17

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

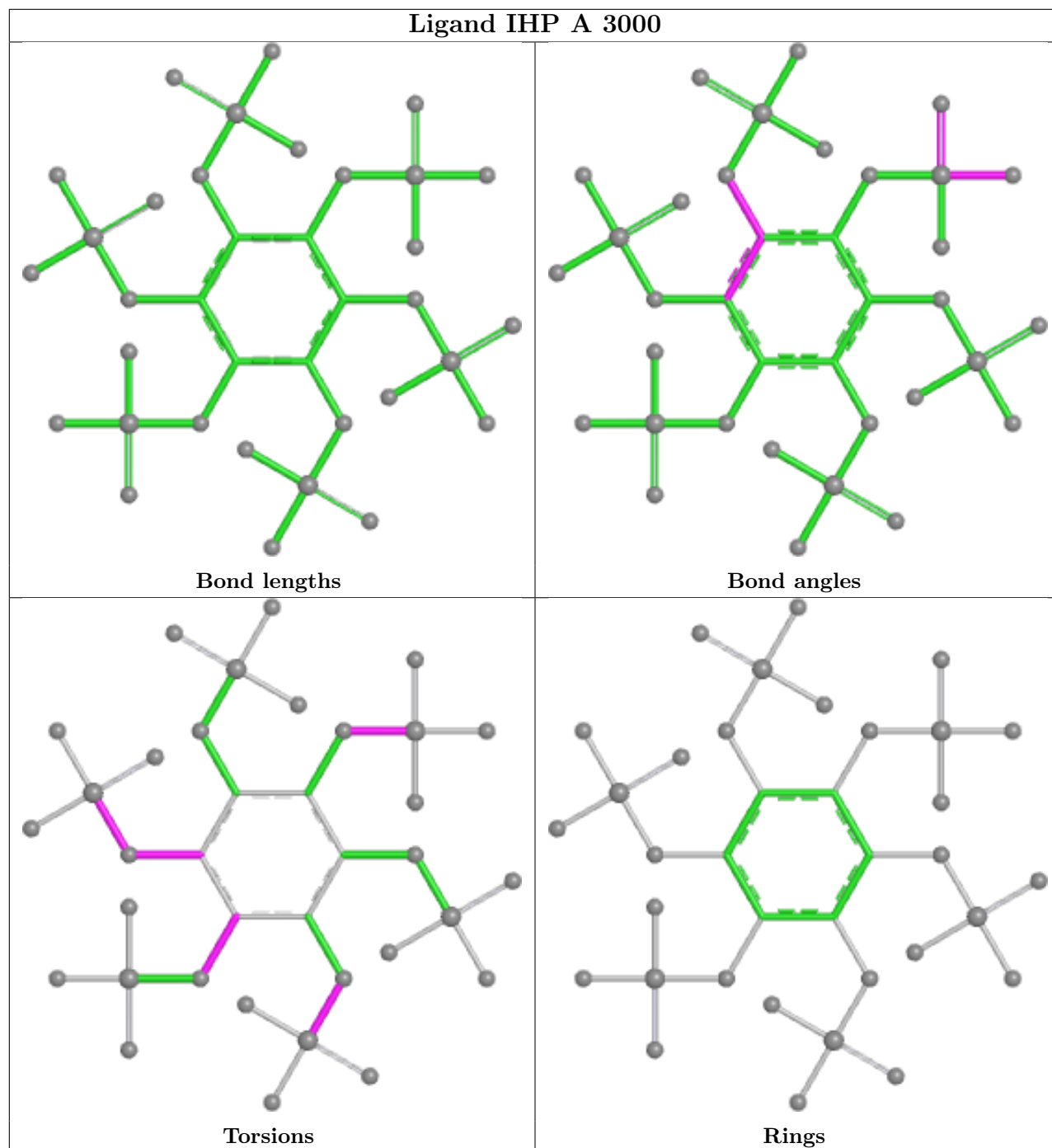
Mol	Chain	Res	Type	Atoms
43	C	1500	GTP	PB-O3B-PG-O3G
46	Q	1501	ATP	C5'-O5'-PA-O1A
46	Q	1501	ATP	C5'-O5'-PA-O2A
46	Q	1501	ATP	C5'-O5'-PA-O3A
43	C	1500	GTP	C3'-C4'-C5'-O5'

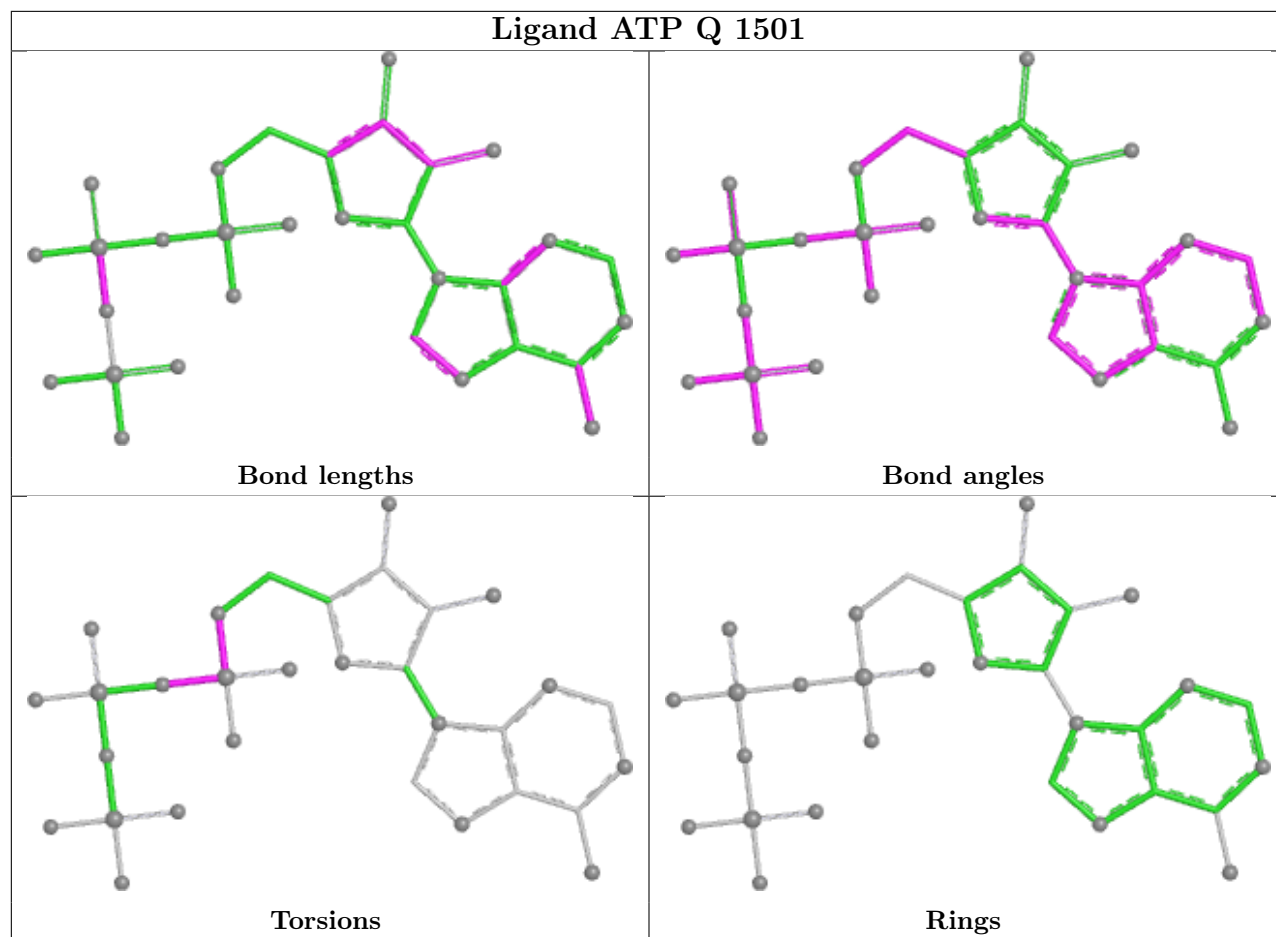
There are no ring outliers.

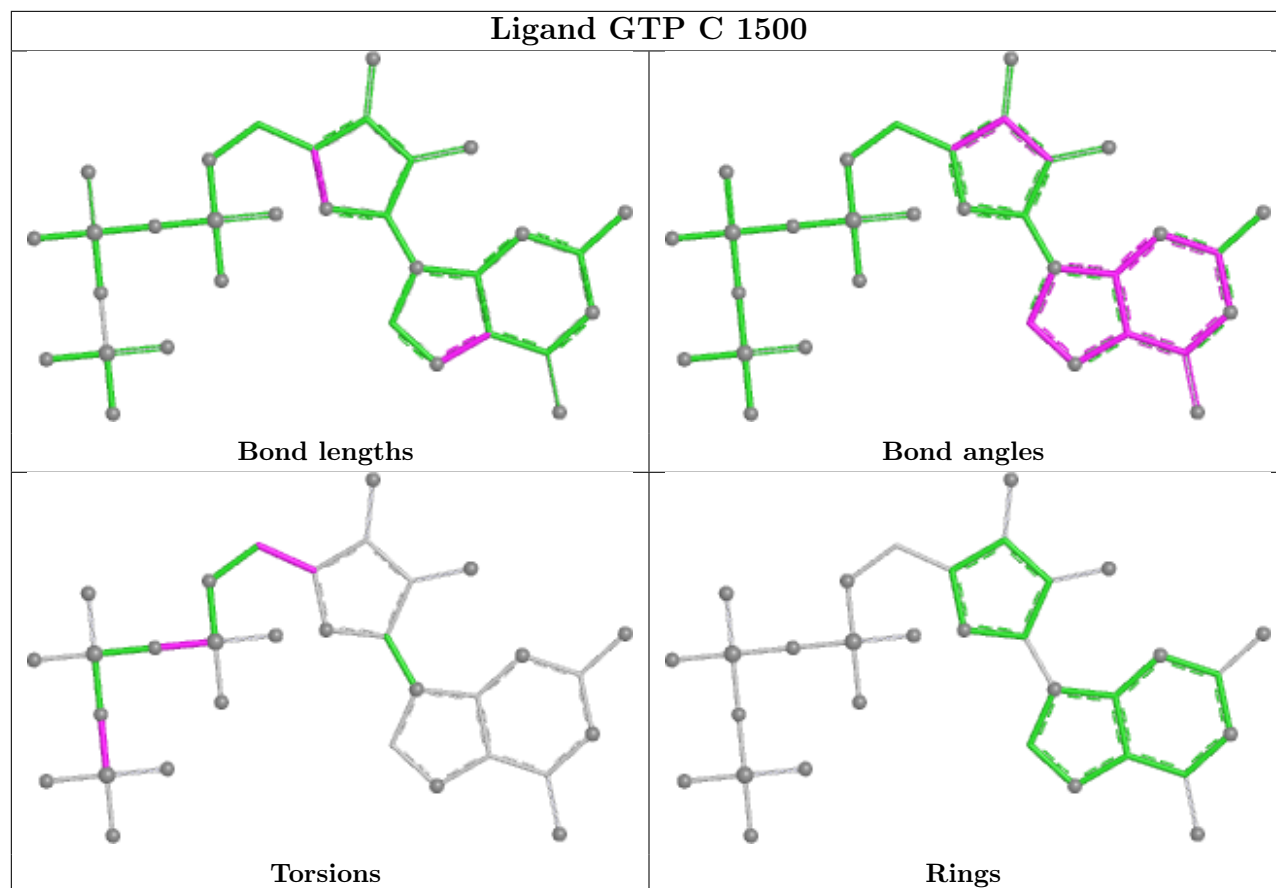
2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
42	A	3000	IHP	3	0
43	C	1500	GTP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







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.

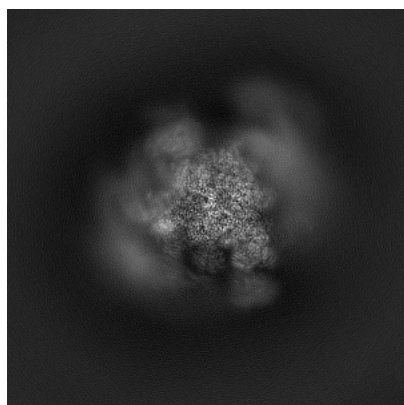
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9645. These allow visual inspection of the internal detail of the map and identification of artifacts.

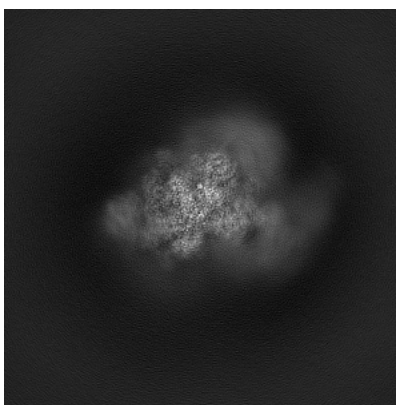
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

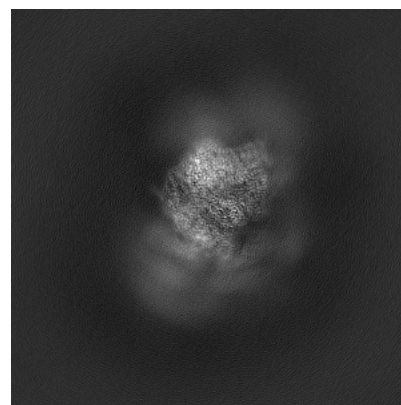
6.1.1 Primary map



X



Y

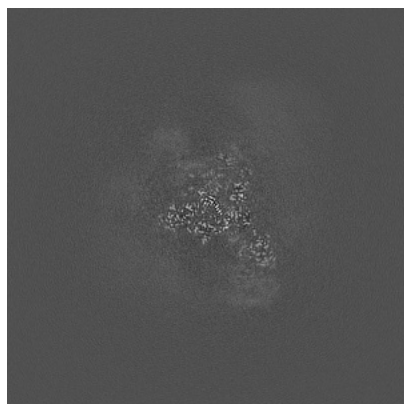


Z

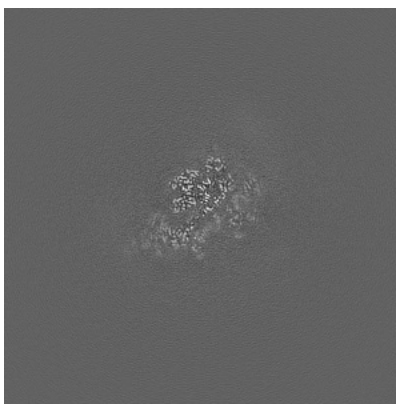
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

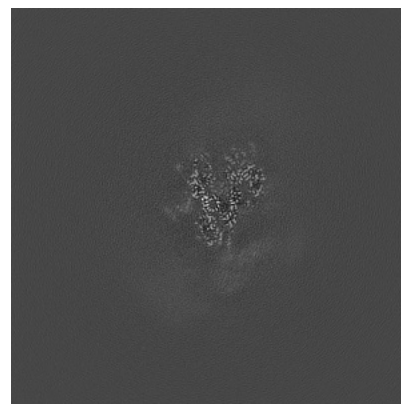
6.2.1 Primary map



X Index: 200



Y Index: 200

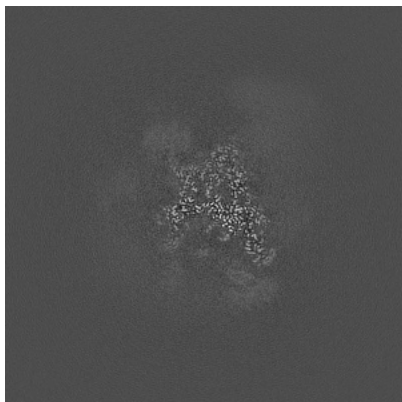


Z Index: 200

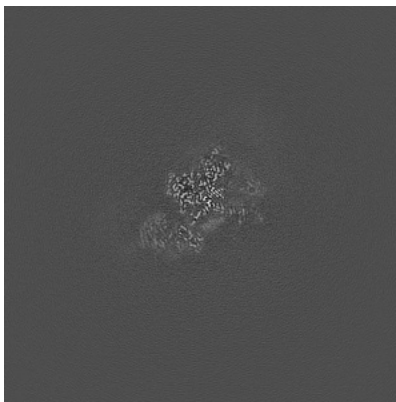
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

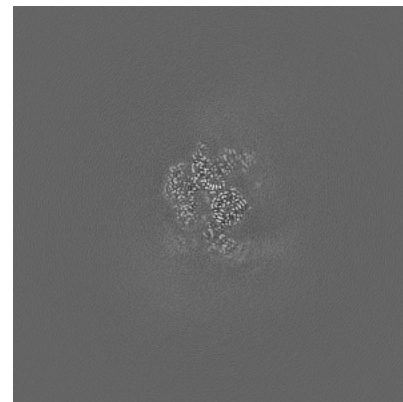
6.3.1 Primary map



X Index: 193



Y Index: 205

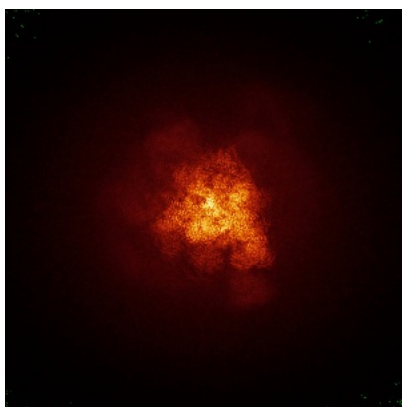


Z Index: 180

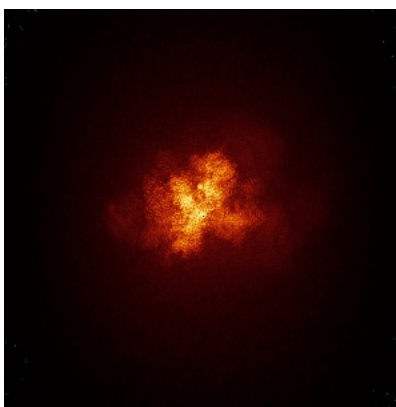
The images above show the largest variance slices of the map in three orthogonal directions.

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

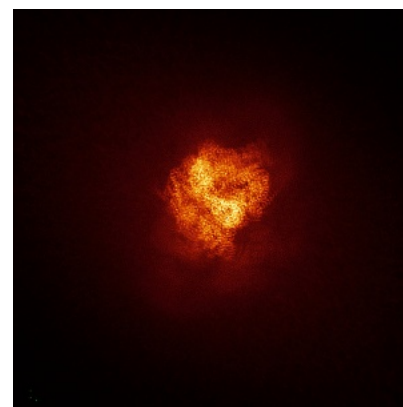
6.4.1 Primary map



X



Y

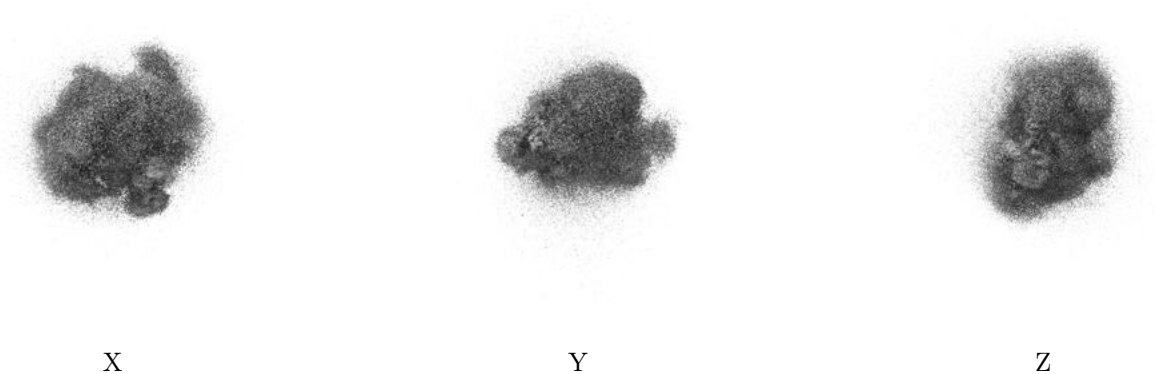


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

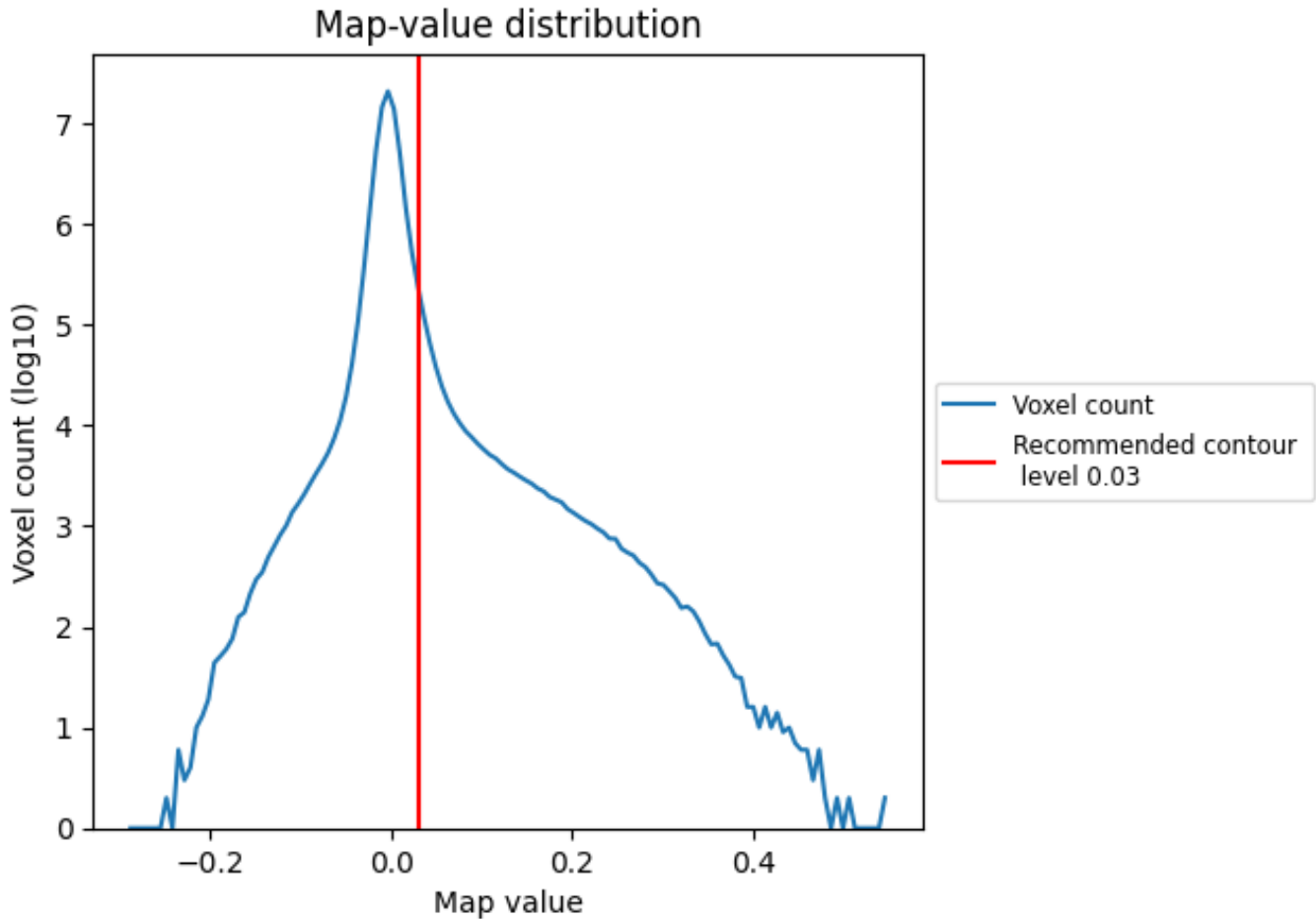
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

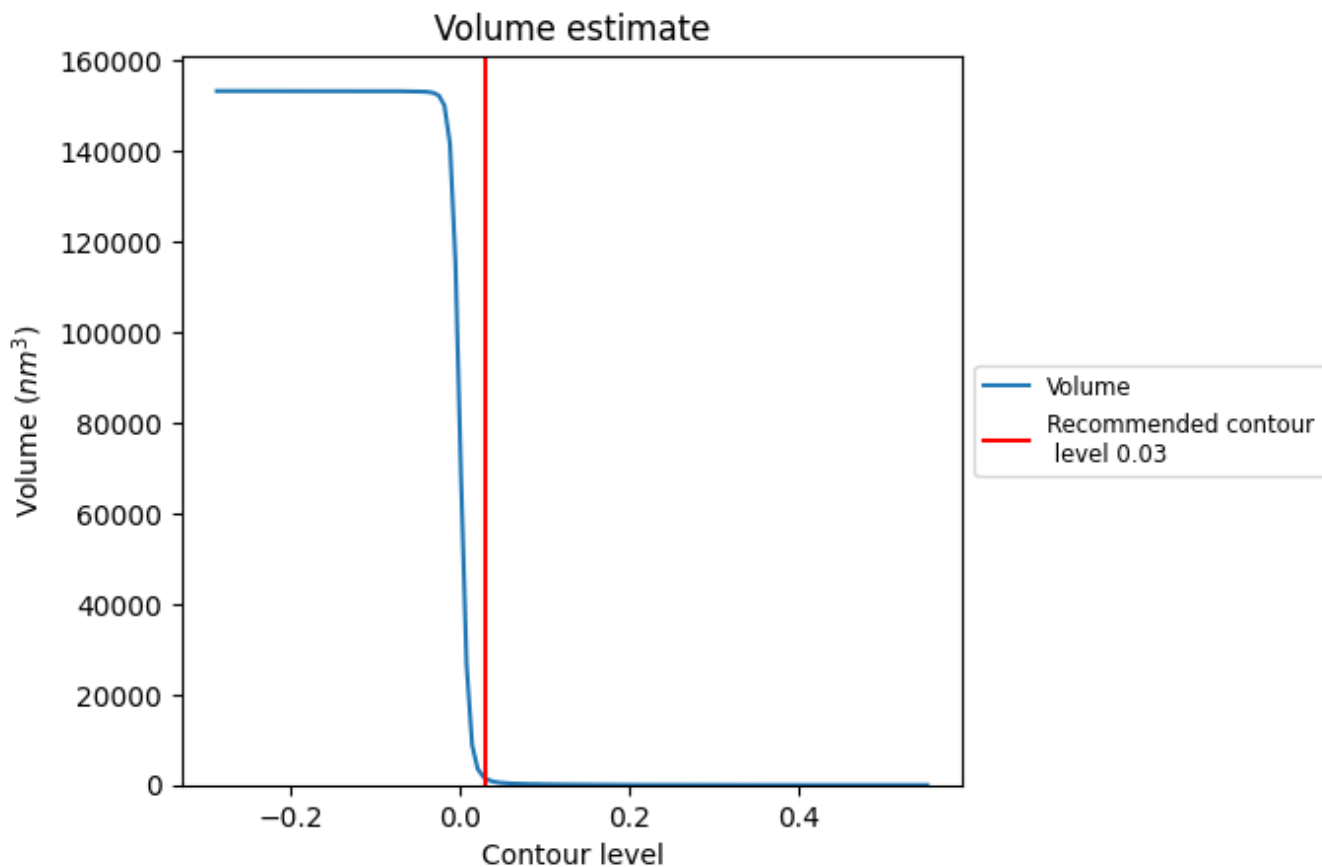
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

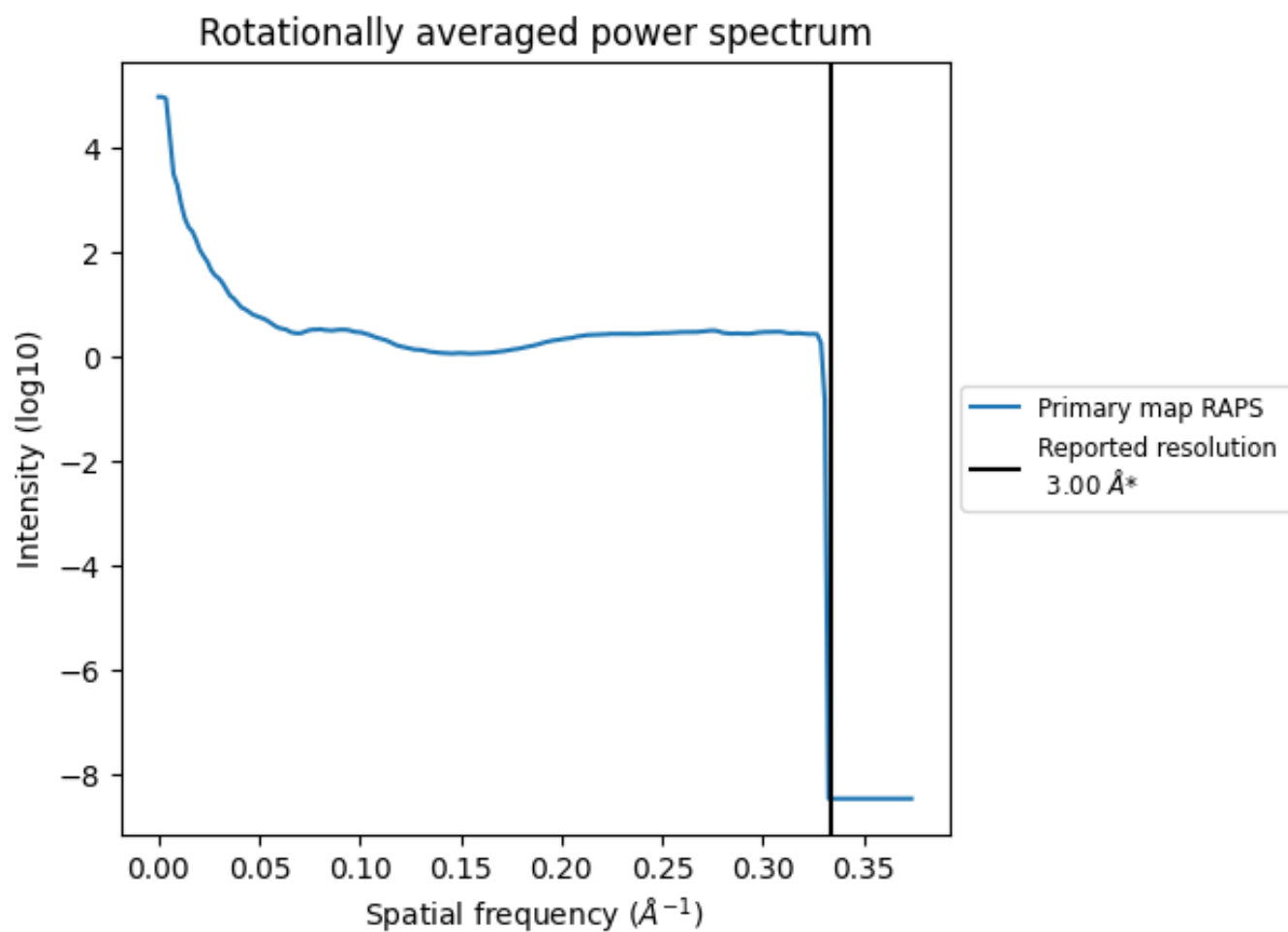
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1504 nm^3 ; this corresponds to an approximate mass of 1358 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 \AA^{-1}

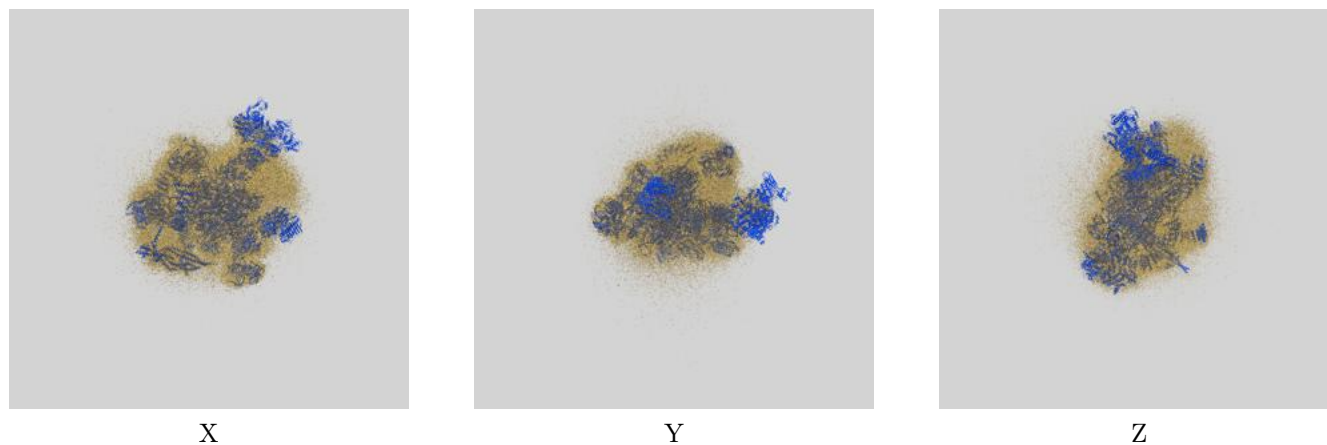
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

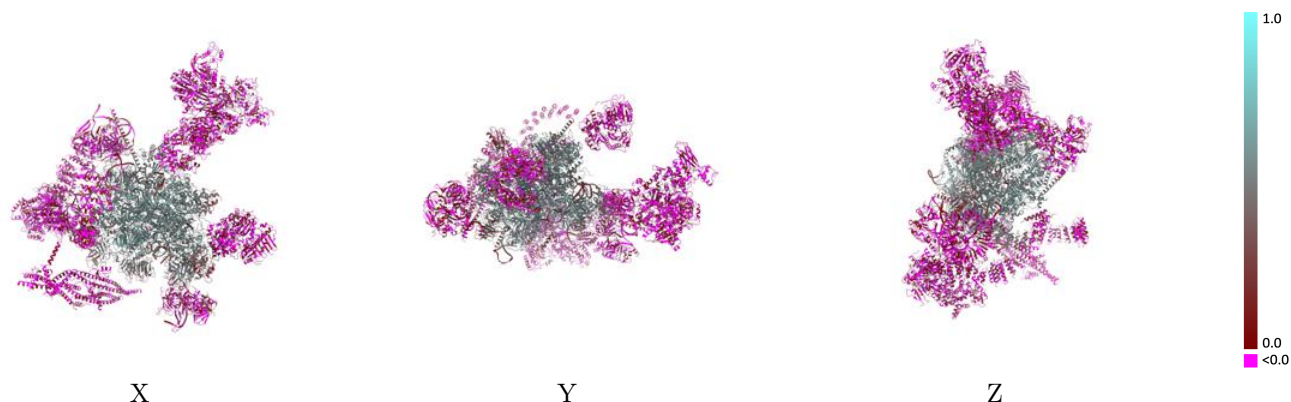
This section contains information regarding the fit between EMDB map EMD-9645 and PDB model 6ICZ. Per-residue inclusion information can be found in section 3 on page 14.

9.1 Map-model overlay [i](#)



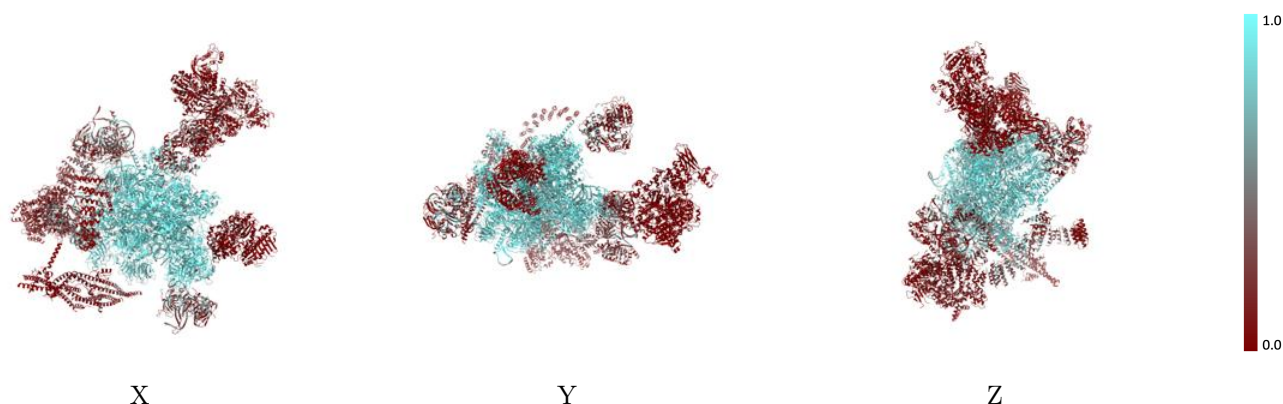
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



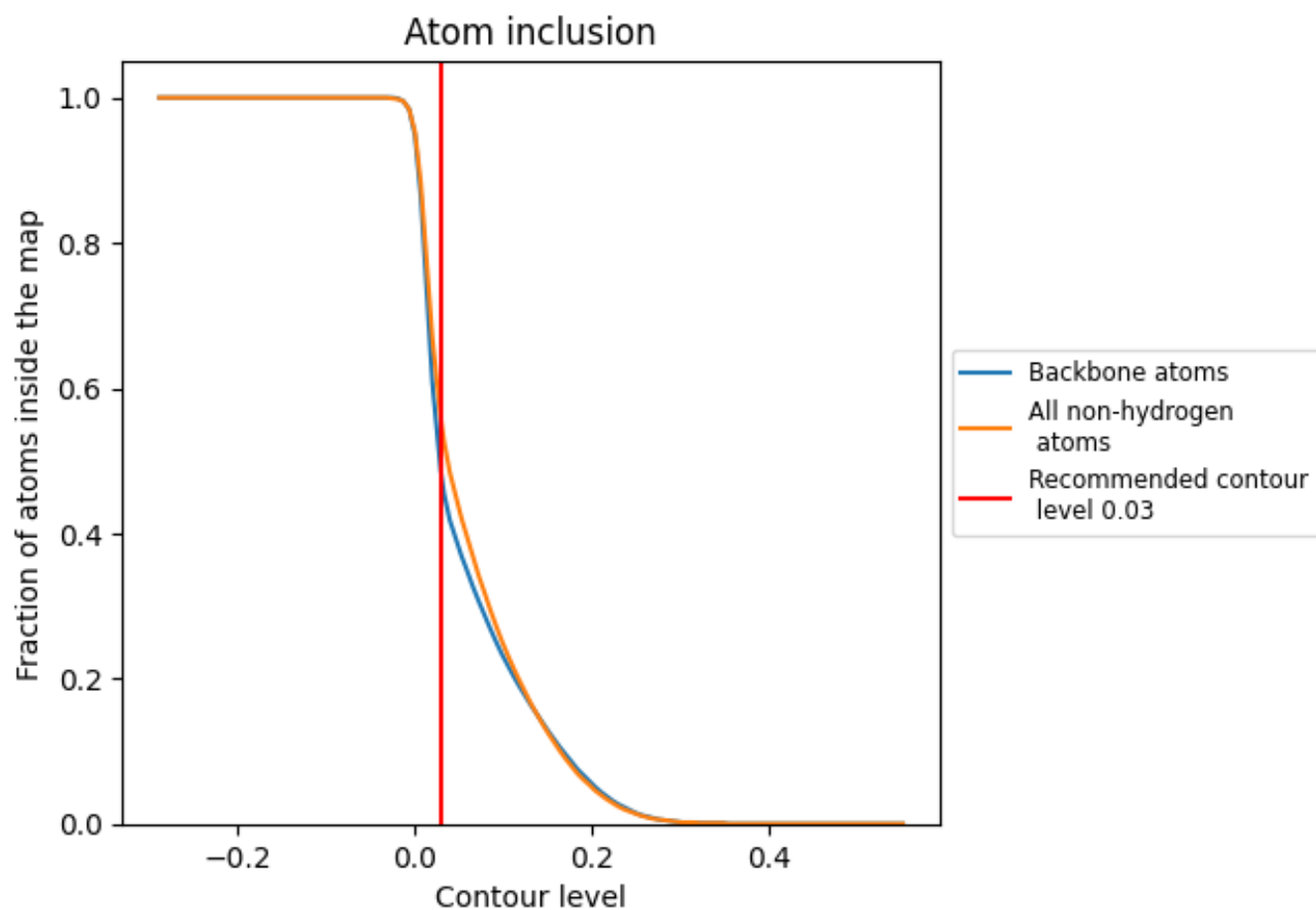
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.03).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 49% of all backbone atoms, 56% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary



































The table lists the average atom inclusion at the recommended contour level (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5600	 0.2840
A	 0.8720	 0.5070
B	 0.7660	 0.3530
C	 0.8960	 0.4650
D	 0.0170	 0.0020
E	 0.8600	 0.4140
F	 0.9330	 0.4850
G	 0.7650	 0.3440
H	 0.4880	 0.1340
I	 0.2180	 0.0190
J	 0.5970	 0.3190
K	 0.1120	 -0.0060
L	 0.6000	 0.3280
M	 0.8730	 0.4830
N	 0.9350	 0.5390
O	 0.8170	 0.4200
P	 0.8340	 0.4750
Q	 0.0290	 0.0020
R	 0.8770	 0.4780
S	 0.8670	 0.4200
T	 0.9650	 0.5840
U	 0.8240	 0.5200
V	 0.4890	 0.2780
W	 0.8310	 0.4190
X	 0.5930	 0.3250
Y	 0.2630	 0.0450
Z	 0.7970	 0.4390
a	 0.3460	 0.0120
b	 0.3260	 0.0300
c	 0.2930	 0.0150
d	 0.3210	 0.0150
e	 0.3220	 0.0560
f	 0.3020	 0.0360
g	 0.3000	 0.0160
h	 0.1990	 -0.0100



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Chain	Atom inclusion	Q-score
i	 0.2030	 0.0080
j	 0.3640	 0.0370
k	 0.2940	 -0.0060
l	 0.3040	 0.0530
m	 0.3820	 0.0410
n	 0.2270	 -0.0020
o	 0.1490	 0.0120
p	 0.2390	 -0.0180
q	 0.0430	 -0.0060
r	 0.0690	 0.0010
s	 0.1190	 0.0440
t	 0.0570	 -0.0170
u	 0.0290	 -0.0080
v	 0.0010	 0.0100
w	 0.0000	 0.0450
x	 0.0000	 0.0520
y	 0.1870	 -0.0070