Full wwPDB EM Validation Report ⓘ

Nov 20, 2022 – 06:08 am GMT

PDB ID	:	5GAP
EMDB ID	:	EMD-8014
Title	:	Body region of the U4/U6.U5 tri-snRNP
Authors	:	Nguyen, T.H.D.; Galej, W.P.; Oubridge, C.; Bai, X.C.; Newman, A.; Scheres, S.; Nagai, K.
Deposited on	:	2015-12-15
Resolution	:	3.60 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

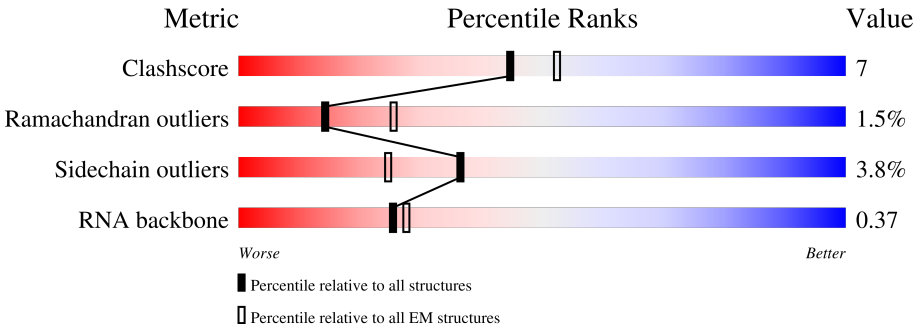
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance

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

The reported resolution of this entry is 3.60 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	67	42% 37% 19%
2	W	112	23% 17% 10% 50%
3	U	214	6% 91%
4	x	82	100%
5	A	2413	47% 9% 44%
6	H	465	59% 18% 23%
7	J	899	64% 16% 19%

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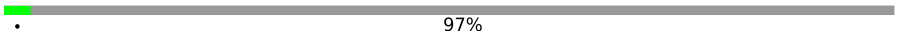
Mol	Chain	Length	Quality of chain
8	D	143	
9	F	494	
10	G	469	
11	K	126	
12	B	2163	

2 Entry composition (i)

There are 12 unique types of molecules in this entry. The entry contains 31576 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 U4 snRNA, 5' region, nucleotides 1-67.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	V	67	1426	637	247	475	67	0	0

- Molecule 2 is a RNA chain called U6 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	W	56	1190	533	210	391	56	0	0

- Molecule 3 is a RNA chain called U5 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	U	20	414	186	64	144	20	0	0

- Molecule 4 is a protein called unknown protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	x	82	410	246	82	82	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	A	1349	11066	7094	1901	2031	40	0	0

- Molecule 6 is a protein called U4/U6 small nuclear ribonucleoprotein PRP4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	H	357	2789	1743	501	532	13	0	0

- Molecule 7 is a protein called Pre-mRNA-splicing factor 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	J	729	Total	C	N	O	S	0	0
			5822	3726	992	1079	25		

- Molecule 8 is a protein called Spliceosomal protein DIB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	D	140	Total	C	N	O	S	0	0
			1151	728	200	212	11		

- Molecule 9 is a protein called Pre-mRNA-processing factor 31.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	F	415	Total	C	N	O	S	0	0
			3218	2052	575	580	11		

- Molecule 10 is a protein called U4/U6 small nuclear ribonucleoprotein PRP3.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	G	318	Total	C	N	O	S	0	0
			2632	1659	469	488	16		

- Molecule 11 is a protein called 13 kDa ribonucleoprotein-associated protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	124	Total	C	N	O	S	0	0
			936	597	161	174	4		

- Molecule 12 is a protein called Pre-mRNA-splicing helicase BRR2.

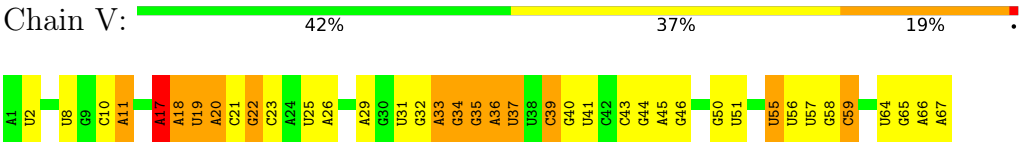
Mol	Chain	Residues	Atoms					AltConf	Trace
12	B	71	Total	C	N	O	S	0	0
			522	326	89	106	1		

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.

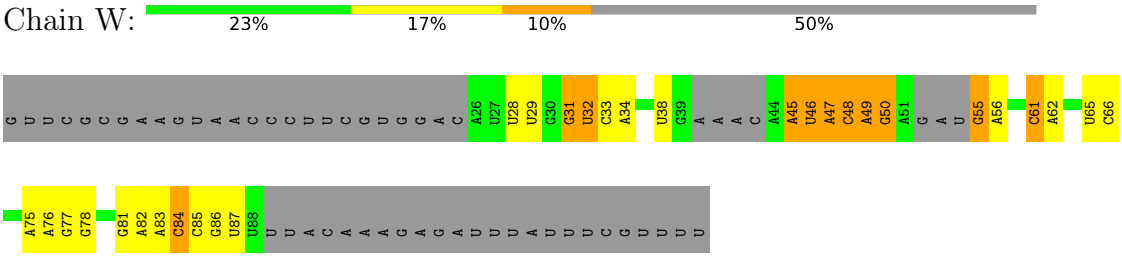
• Molecule 1: U4 snRNA, 5' region, nucleotides 1-67

Chain V:



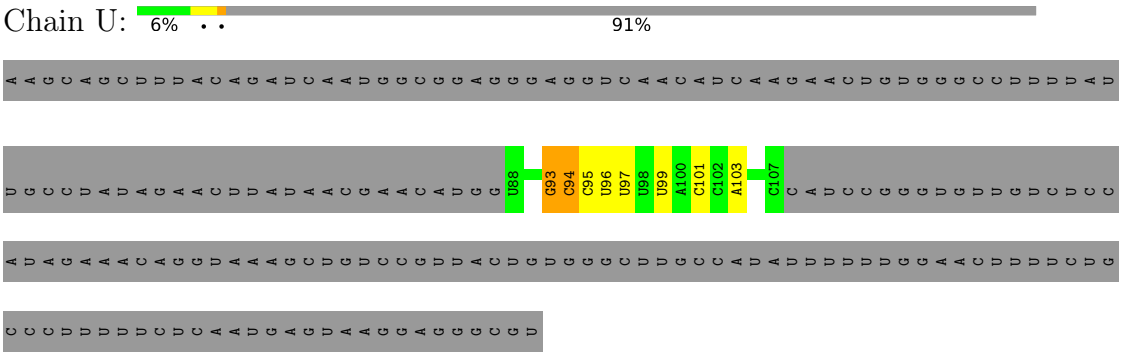
• Molecule 2: U6 snRNA

Chain W:



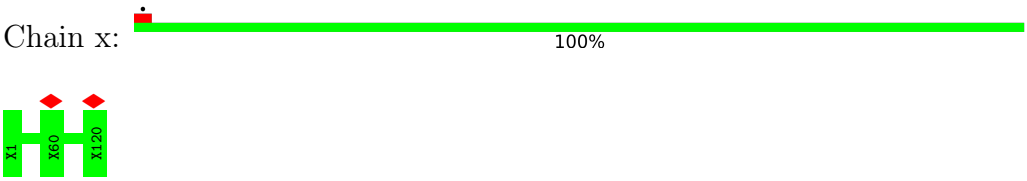
• Molecule 3: U5 snRNA

Chain U:



• Molecule 4: unknown protein

Chain x:



- Molecule 5: Pre-mRNA-splicing factor 8

Chain A: 47% 9% 44%

MET SER GLY LEU PRO PRO PRO PRO PRO GLY PHE GLU GLU ASP SER ASP LEU ALA LEU PRO PRO PRO PRO PRO PRO PRO PRO GLY TYR GLU ILE GLU GLU LEU ASP ASN PRO MET VAL PRO SER SER VAL ASN GLU ASP THR PHE LEU PRO PRO PRO PRO PRO PRO PRO SER ASN PHE GLU

ILE ASN ALA GLU GLU ILE VAL ASP PHE THR LEU PRO PRO PRO PRO PRO PRO PRO GLY LEU ASP GLU LEU GLU THR LYS ALA GLU LYS LYS VAL GLU LEU HIS GLY LYS ARG LYS LEU ASP ILE GLY LYS ASP THR PHE VAL THR ARG LYS SER ARG LYS ARG ALA LYS LYS MET THR LYS

LYS ALA LYS ARG SER ASN LEU TYR THR PRO LYS ALA GLU MET PRO PRO GLU HIS LEU ARG LYS ILE ILE ASN THR HIS SER ASP MET ALA SER LYS MET TYR ASN THR ASP LYS LYS ALA PHE LEU GLY ALA LEU LYS TYR LEU PRO HIS ALA ILE LEU LYS LEU LEU GLU ASN MET PRO

HIS PRO TRP GLU GLN ALA LYS GLU VAL LYS VAL LEU TYR HIS THR SER GLY ALA ILE THR PHE VAL ASN GLU THR PRO ARG VAL ILE GLU PRO VAL TYR THR ALA GLN TRP SER ALA THR TRP ILE ALA MET ARG ARG GLU LYS ARG ASP ARG THR HIS PHE LYS ARG MET ARG PHE PRO

PRO PHE ASP ASP ASP GLU PRO PRO LEU SER TYR GLU GLN HIS ILE GLU ASN ILE GLU PRO LEU ASP PRO ILE ASN LEU PRO LEU ASP SER GLN ASP ASP GLU TYR VAL LYS ASP TRP LEU TYR ASP SER ARG PRO LEU GLU GLU ASP SER LYS LYS VAL ASN GLY THR SER TYR LYS LYS

TRP SER PHE ASP LEU PRO GLU MET SER ASN LEU TYR ARG LEU SER THR PRO LEU ARG ASP GLU VAL THR ASP LYS ASN TYR TYR TYR LEU PHE ASP LYS LYS SER PHE PHE ASN GLY LYS ALA LEU ASN ASN ALA ILE PRO GLY GLY PRO LYS PHE GLU PRO LEU TYR PRO ARG GLU GLU

GLU GLU ASP TYR ASN GLU PHE ASN SER ILE ASP ARG VAL ILE PHE ARG VAL PRO ILE ARG SER GLU TYR LYS VAL ALA PHE PRO HIS LEU TYR ASN SER ARG PRO ARG SER VAL ARG ILE PRO TRP TYR ASN ASN PRO VAL SER CYS ILE ILE GLN ASN ASP GLU GLU TYR ASP THR PRO

ALA LEU PHE PHE ASP PRO SER LEU ASN PRO ILE PRO HIS PHE ILE ASP ASN ASN SER SER LEU ASN VAL SER ASN THR LYS GLU ASN GLY ASP PHE THR LEU PRO GLU ASP PHE ALA PRO LEU LEU ALA GLU GLU GLU GLU LEU ILE LEU PRO ASN THR LYS ASP ALA MET SER LEU TYR

HIS SER PRO PHE PRO PHE ASN ARG THR LYS GLY LYS MET VAL ARG ALA GLN ASP VAL ALA LEU ALA LYS LYS TRP PHE LEU GLN HIS PRO ASP GLU GLU TYR PRO VAL LYS VAL LYS VAL SER TYR GLN LYS LEU LEU LYS ASN TYR VAL LEU ASN GLU LEU HIS PRO THR LEU PRO THR

ASN HIS ASN LYS THR LYS LEU LEU LYS SER LEU LYS ASN THR LYS TYR PHE GLN GLN THR THR ILE ASP TRP VAL GLU ALA GLY LEU GLN LEU CYS ARG GLN GLY HIS ASN MET LEU ASN LEU LEU ILE HIS ARG LYS GLY LEU THR TYR LEU HIS LEU ASP TYR ASN PHE ASN LEU LYS

PRO THR LYS THR LEU THR THR LYS GLU ARG LYS LYS SER ARG LEU GLY ASN SER PHE HIS LEU MET ARG GLU LEU LEU LYS MET MET LYS LEU ILE VAL ASP THR HIS VAL GLN PHE ARG LEU GLY ASN VAL ASP ALA PHE GLN LEU ALA ASP GLY ILE HIS TYR ILE LEU ASN HIS ILE

GLY GLN LEU THR GLY ILE TYR ARG TYR LYS TYR LYS VAL MET HIS GLN ILE ARG ALA CYS LYS ASP LEU LYS HIS ILE ILE TYR TYR LYS PHE ASN LYS ASN LEU GLY LYS GLY PRO GLY CYS GLY PHE TRP GLN PRO ALA TRP ARG VAL TRP LEU ASN PHE LEU ARG GLY THR ILE PRO

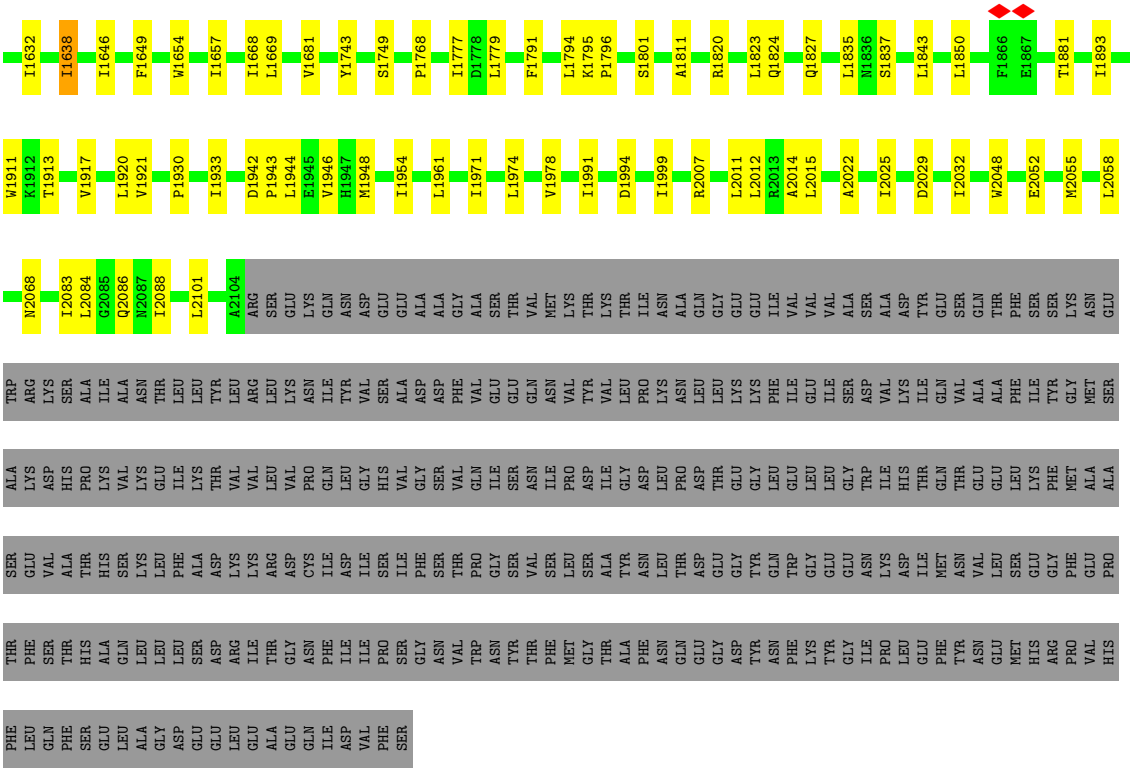
LEU LEU GLU ARG TYR ILE GLY ASN LEU ILE THR ARG GLN PHE GLU GLY ARG SER ASN GLU ILE VAL LYS THR THR THR LYS GLN ARG LEU D751 A752 Y753 Y754 D755 L756 E757 L758 V762 D765 E788 I808 I811 I816 K817 S818 K819 W823 V824 S825 R831

L852 T853 I857 I874 I882 L914 L919 V922 Y923 L939 A943 P947 T950 T960 M971 M972 I978 S979 P980 V981 Y982 I990 D1004 P1010 N1011 W1012 P1021 P1022 L1023 L1024 V1025 Y1026 K1027 W1028 T1029 I1032 I1038 W1039 A1047 V1048

L1049 L1050 F1063 T1064 L1065 L1066 N1067 L1070 I1073 I1082 T1083 A1084 K1085 N1086 N1087 V1088 V1089 F1092 K1093 D1094 M1095 V1098 L1103 I1104 L1107 I1113 F1114 Q1115 Y1116 L1125 L1126 Y1161 M1170 T1183 I1216 N1221 I1230 L1238 V1250 Y1251 N1254

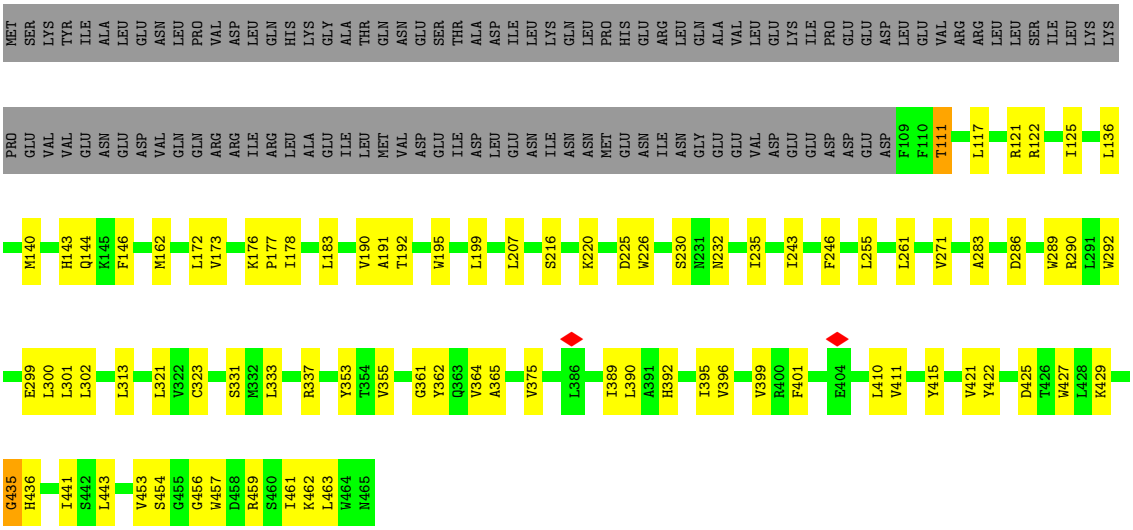
M1262 R1268 P1271 M1275 E1276 E1277 V1278 N1281 D1282 W1286 L1302 F1312 G1318 I1319 L1320 M1321 A1322 S1323 G1324 W1335 L1339 L1342 F1343 T1344 E1354 P1355 L1360 R1366 I1367 Q1368 K1372 L1375 F1383 P1384 P1385 A1386 V1387 L1394 A1402

I1407 L1412 S1413 W1414 A1427 GLY MET THR HIS GLU D1433 I1437 F1451 W1458 Y1461 L1494 D1505 R1512 K1535 L1536 W1537 Y1542 V1546 I1553 E1558 H1559 T1560 A1578 S1599 Q1600 I1601 P1602 R1605 F1606 T1607 L1608 W1609 W1610 T1613 I1614 F1623



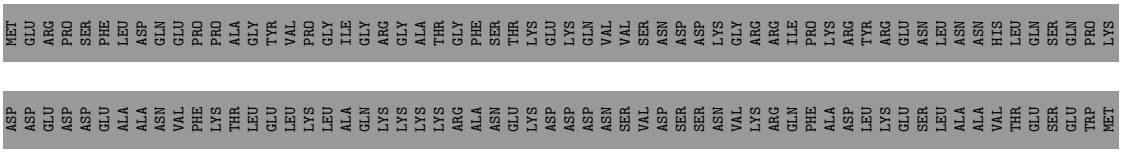
• Molecule 6: U4/U6 small nuclear ribonucleoprotein PRP4

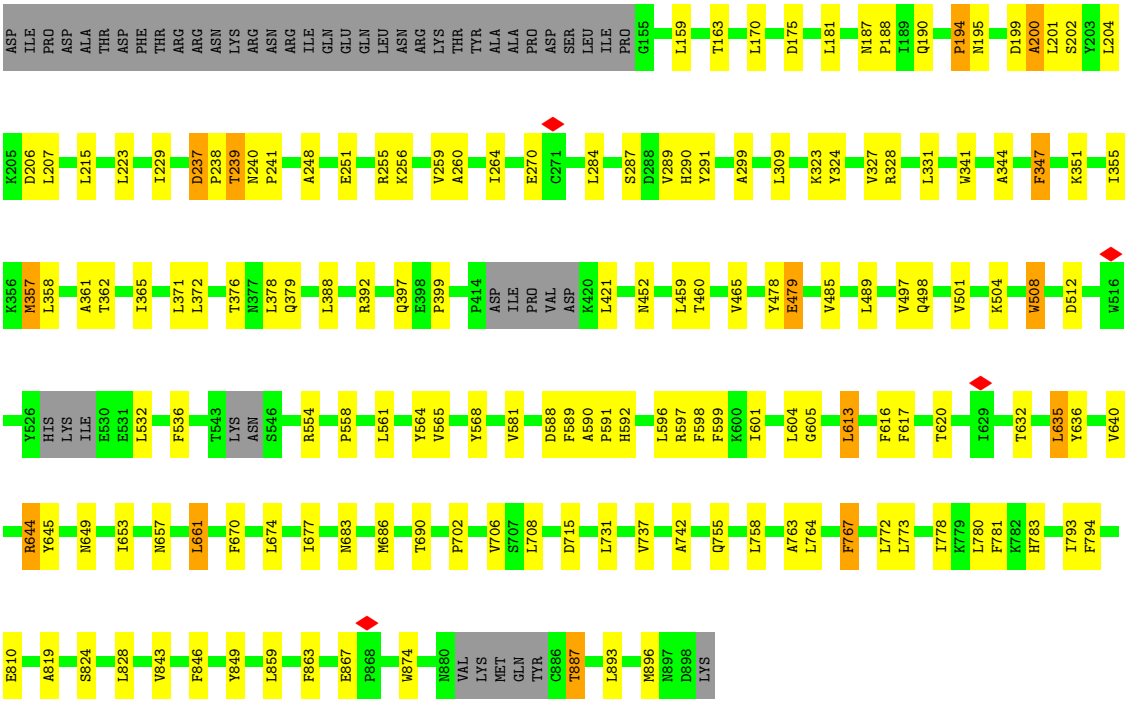
Chain H:



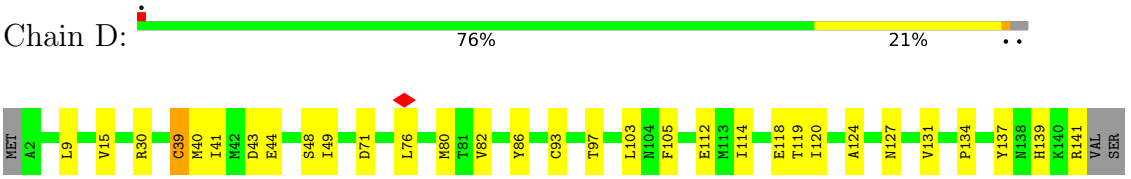
• Molecule 7: Pre-mRNA-splicing factor 6

Chain J:

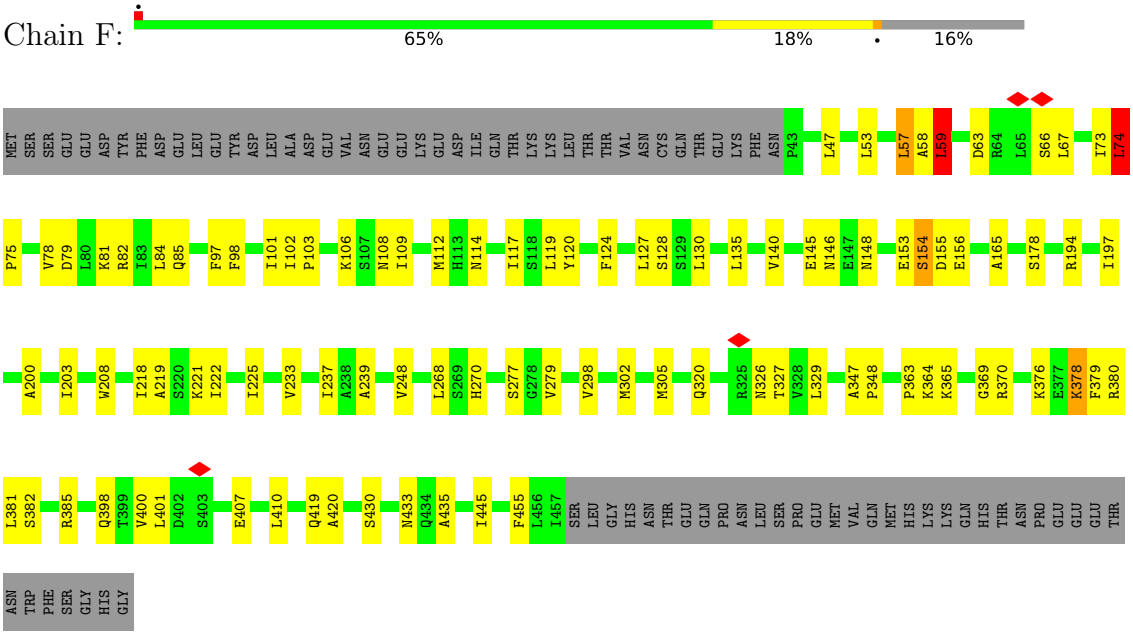




• Molecule 8: Spliceosomal protein DIB1

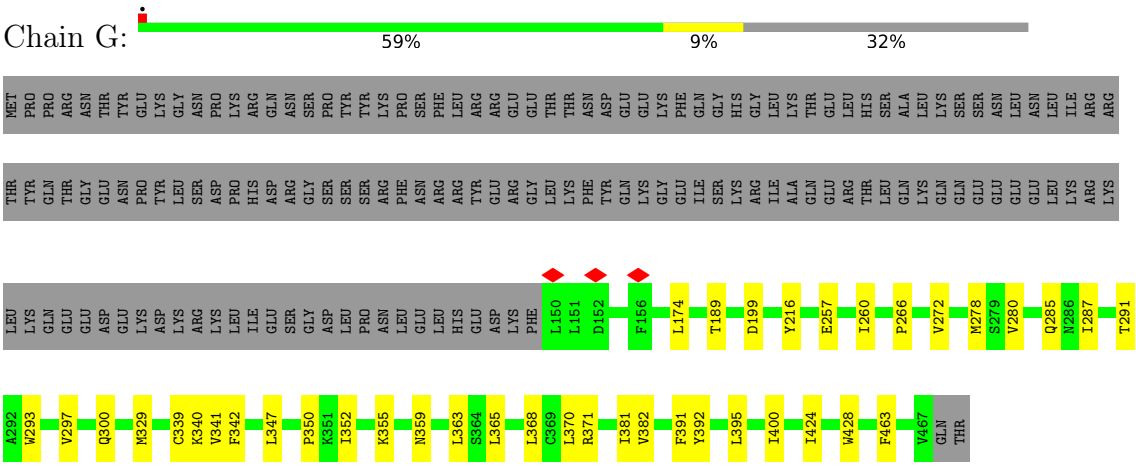


• Molecule 9: Pre-mRNA-processing factor 31



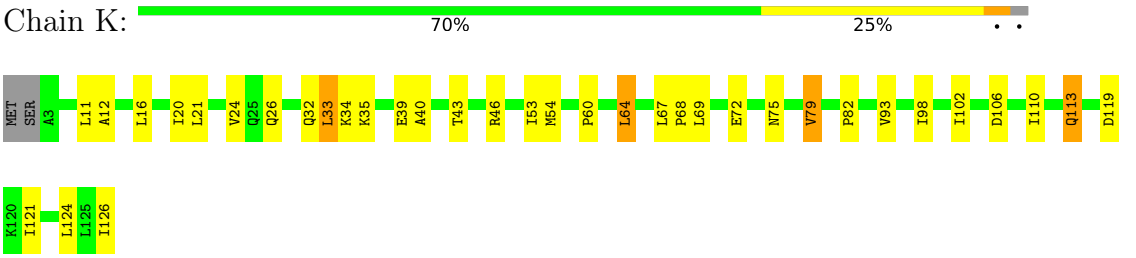
• Molecule 10: U4/U6 small nuclear ribonucleoprotein PRP3

Chain G:



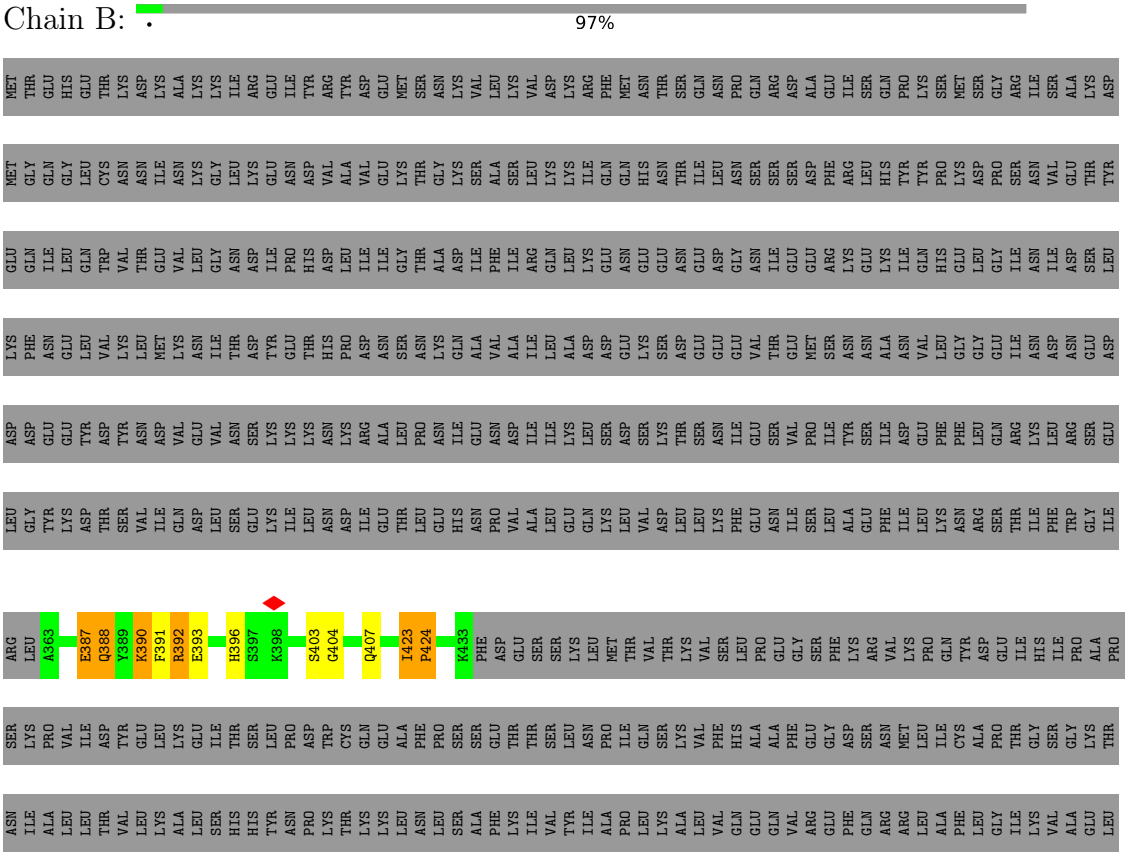
• Molecule 11: 13 kDa ribonucleoprotein-associated protein

Chain K:



• Molecule 12: Pre-mRNA-splicing helicase BRR2

Chain B:



THR GLY ASP SER ARG LEU SER ARG LYS GLN ILE ASP GLU THR GLN VAL LEU VAL SER THR PRO GLU LYS TRP ASP ILE THR THR ARG ASN SER ASN ASN LEU ALA ILE VAL GLU LEU VAL ARG LEU LEU ILE ILE ASP GLU ILE HIS LEU LEU HIS ASP ASP ARG GLY PRO VAL LEU GLU

SER ILE VAL ALA ARG THR PHE TRP ALA SER LYS TYR GLY GLN GLU TYR PRO ARG ILE ILE GLY LEU SER ALA THR LEU PRO ASN TYR GLU ASP VAL GLY ARG PHE LEU ARG VAL PRO LYS GLU GLY LEU PHE TYR PHE ASP SER SER PHE ARG PRO CYS PRO LEU SER GLN GLN PHE CYS

GLY ILE LYS GLU ARG ASN SER LEU LYS LYS LEU LYS ALA MET ASN ASP ALA CYS TYR GLU LYS VAL LEU GLU SER ILE ASN GLU GLY ASN GLN ILE ILE VAL PHE VAL HIS SER ARG LYS GLU THR SER ARG THR ALA THR TRP LEU LYS ASN LYS PHE ALA GLU GLU ASN ILE THR HIS

LYS LEU THR LYS ASN ASP ALA GLY SER LYS GLN ILE LEU LYS THR GLU ALA ALA ASN VAL LEU ASP PRO SER LEU ARG LYS LEU ILE GLU SER GLY ILE GLY THR HIS HIS ALA GLY LEU THR ARG SER ASP ARG SER LEU SER GLU ASP LEU PHE ALA ASP GLY LEU LEU GLN VAL LEU

VAL CYS THR ALA THR LEU ALA TRP GLY VAL ASN LEU PRO ALA HIS THR VAL ILE ILE LYS GLY THR ASP VAL TYR SER PRO GLU LYS GLY SER TRP GLU GLN LEU SER PRO GLN ASP VAL LEU GLN MET LEU GLY ARG ALA GLY ARG PRO ARG TYR ASP THR PHE GLY GLU GLY ILE ILE

ILE THR ASP GLN SER ASN VAL GLN TYR TYR LEU SER VAL LEU ASN GLN GLN LEU PRO ILE GLU SER GLN PHE VAL SER LYS LEU VAL ASP ASN LEU ASN ALA GLU VAL VAL ALA GLY ASN ILE LYS CYS ARG ASN ASP ALA VAL ASN TRP LEU ALA TYR THR TYR LEU TYR VAL ARG MET

LEU ALA SER PRO MET LEU TYR LYS VAL PRO ASP ILE SER SER ASP GLY GLN LEU LYS LYS PHE ARG GLU SER LEU VAL HIS SER ALA LEU CYS ILE LEU LYS GLU GLN GLU LEU VAL LEU TYR ASP ALA GLU ASN ASP VAL ILE GLU ALA THR ASP LEU GLY ASN ILE ALA SER SER PHE

TYR ILE ASN HIS ALA SER MET ASP VAL TYR ASN ARG GLU LEU ASP GLU HIS THR THR GLN ILE ASP LEU PHE ARG ILE PHE SER MET SER GLU GLU PHE LYS TYR VAL SER VAL ARG TYR GLU GLU LYS ARG GLU LEU LYS GLN LEU LEU GLU LYS ALA PRO ILE PRO ILE ARG GLU ASP

ILE ASP ASP PRO LEU ALA LYS VAL ASN VAL LEU LEU GLN SER TYR PHE SER GLN LEU LYS PHE GLU GLY PHE ALA LEU ASN SER ASP ILE VAL PHE ILE HIS GLN ASN ALA GLY ARG LEU LEU ARG ALA MET PHE GLU ILE CYS LEU LYS ARG GLY TRP GLY HIS PRO THR ARG MET LEU

LEU ASN LEU CYS LYS SER ALA THR THR LYS MET TRP PRO THR ASN CYS PRO LEU ARG GLN PHE LYS THR CYS PRO VAL GLU VAL ILE LYS ARG LEU GLU ALA SER THR VAL PRO TRP GLY ASP TYR LEU GLN LEU GLU THR PRO ALA GLU VAL GLY ARG ALA ILE ARG SER GLU LYS TYR

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ASP SER ILE LEU TYR TYR ASP VAL LEU PHE ILE THR PRO ASP ILE VAL GLY HIS GLU PHE THR LEU SER PHE THR TYR GLU LEU LYS GLN HIS ASN GLN ASN ASN LEU PRO PRO ASN PHE PHE LEU THR LEU ILE SER GLU ASN TRP TRP HIS SER GLU PHE GLU ILE PRO VAL SER PHE

ASN GLY PHE LYS LEU PRO LYS LYS PHE PRO PRO PRO THR PRO LEU LEU GLU ASN ILE SER ILE SER THR SER GLU LEU GLY ASN ASP ASP PHE SER GLU VAL PHE GLU PHE LYS THR PHE ASN LYS ILE GLN SER GLN VAL PHE GLU SER LEU TYR ASN SER ASN ASP SER VAL PHE VAL

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GLY ASN ASP PRO SER LEU ASN LEU LYS LEU LEU ALA LYS SER HIS VAL LEU LEU ALA THR PRO VAL GLN PHE GLU LEU LEU SER ARG ARG TRP ARG GLN ARG LYS ASN ILE GLN SER LEU GLU LEU MET ILE TYR ASP ASP ALA HIS GLU ILE SER GLN GLY VAL TYR GLY ALA VAL TYR

GLU THR LEU ILE SER ARG MET ILE PHE ILE ALA THR GLN LEU GLU LYS LYS ILE ARG PHE VAL CYS LEU SER ASN CYS LEU ALA ASN ALA ARG ASP PHE GLY GLU TRP ALA GLY MET THR LYS SER ASN ILE TYR ASN PHE SER PRO SER GLU ARG ILE GLU PRO LEU GLU ILE ASN ILE

GLN SER PHE LYS ASP VAL GLU HIS ILE SER PHE ASN PHE SER MET LEU GLN MET ALA PHE GLU ALA SER ALA ALA ALA ALA GLY ASN ARG ASN SER SER SER VAL PHE LEU PRO SER ARG LYS ASP CYS MET GLU VAL ALA SER ALA PHE MET LYS PHE SER LYS ALA ILE GLU TRP ASP

MET LEU ASN VAL GLU GLU GLN GLN ILE VAL PRO TYR ILE GLU LYS LEU THR ASP GLY HIS LEU ARG ALA PRO LEU LYS HIS GLY VAL GLY ILE LEU TYR LYS GLY MET ALA SER ASN ASP GLU ARG ILE VAL LYS ARG LEU TYR GLU TYR GLY ALA VAL SER VAL LEU LEU ILE SER LYS

ASP CYS SER ALA PHE ALA CYS LYS THR ASP GLU VAL ILE ILE LEU GLY THR ASN LEU TYR ASP GLY ALA GLU HIS LYS TYR MET PRO TYR THR ILE ASN GLU LEU LEU GLU MET VAL GLY LEU ALA SER GLY ASN ASP SER MET ALA GLY LYS VAL LEU ILE LEU THR SER HIS ASN MET

LYS ALA TYR TYR LYS LYS PHE LEU ILE GLU PRO LEU PRO THR GLU SER TYR LEU GLN TYR ILE ILE HIS ASP THR LEU ASN ASN GLU ILE ALA ASN SER ILE ILE GLN SER LYS GLN ASP CYS VAL ASP TRP PHE THR TYR SER TYR PHE TYR ARG ARG ILE HIS VAL ASN PRO SER TYR

TYR GLY VAL ARG ASP THR SER PRO HIS GLY ILE SER VAL PHE LEU SER ASN LEU VAL GLU THR CYS LEU ASN ASP LEU VAL GLU SER SER PHE ILE GLU ILE ASP ASP THR GLU ALA GLU VAL THR ALA GLU VAL ASN GLY GLY ASP ASP GLU ALA THR GLU ILE ILE SER THR LEU SER

ASN GLY LEU ILE ALA SER HIS TYR GLY VAL SER PHE PHE THR ILE GLN SER PHE VAL SER SER LEU SER ASN THR SER THR LEU LYS ASN MET LEU TYR VAL LEU SER THR ALA VAL GLU PHE GLU SER VAL PRO LEU ARG LYS GLY ASP ARG ALA LEU LEU VAL LYS LEU SER LYS ARG

LEU PRO LEU ARG PHE PRO GLU HIS THR SER SER GLY SER VAL SER PHE LYS VAL PHE LEU LEU LEU GLN ALA TYR PHE SER ARG LEU GLU LEU PRO VAL ASP PHE GLN ASN ASP LEU LYS ASP ILE LEU GLU LYS VAL VAL PRO LEU ILE ASN VAL VAL VAL ASP ILE LEU SER ALA ASN

GLY TYR LEU ASN ALA THR THR ALA MET ASP LEU ALA GLN MET LEU ILE GLN GLY VAL TRP ASP VAL ASP ASN PRO LEU ARG GLN ILE PRO HIS PHE ASN ASN LYS ILE LEU GLU LYS CYS LYS GLU ILE ASN VAL GLU THR VAL TYR ASP ILE MET ALA LEU GLU ASP GLU GLU ARG ASP

GLU ILE LEU THR LEU THR ASP SER GLN LEU ALA GLN VAL ALA ALA PHE VAL ASN ASN TYR PRO ASN VAL GLU LEU THR TYR SER LEU ASN ASN SER ASP SER LEU ILE SER GLY VAL LYS GLN LYS ILE THR ILE GLN LEU THR ARG ASP VAL GLU PRO GLU ASN LEU GLN VAL THR SER

GLU LYS TYR PRO PHE ASP LYS LEU GLU SER TRP TRP LEU VAL LEU GLY GLU VAL SER LYS LYS GLU LEU TYR ALA ILE LYS LYS VAL THR LEU ASN LYS GLU THR GLN GLN TYR GLU LEU GLU PHE ASP THR PRO THR SER GLY LYS HIS ASN LEU THR ILE TRP CYS VAL CYS ASP SER

TYR LEU ASP ALA ASP LYS GLU LEU SER PHE GLU ILE ASN VAL LYS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	140155	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	38	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	35714	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.326	Depositor
Minimum map value	-0.232	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	543.39996, 543.39996, 543.39996	wwPDB
Map dimensions	380, 380, 380	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.43, 1.43, 1.43	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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	0.36	0/1593	0.79	1/2480 (0.0%)
2	W	0.38	0/1328	0.84	2/2061 (0.1%)
3	U	0.32	0/459	0.76	0/710
5	A	0.42	1/11327 (0.0%)	0.73	2/15348 (0.0%)
6	H	0.38	0/2845	0.71	0/3843
7	J	0.44	0/5934	0.80	2/8039 (0.0%)
8	D	0.42	0/1172	0.75	1/1578 (0.1%)
9	F	0.43	0/3273	0.80	2/4413 (0.0%)
10	G	0.41	0/2687	0.69	0/3611
11	K	0.45	0/949	0.81	0/1292
12	B	0.42	0/529	0.69	0/716
All	All	0.42	1/32096 (0.0%)	0.76	10/44091 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
5	A	0	3
9	F	0	1
12	B	0	1
All	All	0	5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	825	SER	CB-OG	5.40	1.49	1.42

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	J	613	LEU	CA-CB-CG	7.12	131.69	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	979	SER	C-N-CD	-6.95	105.32	120.60
1	V	17	A	C2'-C3'-O3'	6.90	124.74	113.70
2	W	55	G	C2'-C3'-O3'	5.73	122.87	113.70
9	F	74	LEU	CA-CB-CG	5.58	128.14	115.30
9	F	155	ASP	N-CA-C	5.34	125.42	111.00
7	J	532	LEU	CA-CB-CG	5.30	127.49	115.30
8	D	103	LEU	CA-CB-CG	5.26	127.41	115.30
2	W	48	C	C2'-C3'-O3'	5.21	122.04	113.70
5	A	831	ARG	NE-CZ-NH1	5.10	122.85	120.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	A	1278	VAL	Peptide
5	A	1994	ASP	Peptide
5	A	979	SER	Peptide
12	B	423	ILE	Peptide
9	F	154	SER	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	1426	0	716	22	0
2	W	1190	0	603	14	0
3	U	414	0	213	4	0
4	x	410	0	89	0	0
5	A	11066	0	11078	138	0
6	H	2789	0	2725	53	0
7	J	5822	0	5792	103	0
8	D	1151	0	1138	17	0
9	F	3218	0	3297	53	0
10	G	2632	0	2599	27	0
11	K	936	0	987	24	0
12	B	522	0	506	5	0
All	All	31576	0	29743	413	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 7.

All (413) 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)
5:A:1578:ALA:HB1	5:A:1602:PRO:HB3	1.40	1.02
5:A:1275:MET:HE2	5:A:1281:ASN:ND2	1.92	0.84
10:G:272:VAL:HG12	10:G:280:VAL:HG21	1.59	0.81
5:A:1067:ASN:HB2	5:A:1083:THR:HG21	1.64	0.80
7:J:199:ASP:O	7:J:201:LEU:N	2.14	0.79
9:F:347:ALA:HB1	9:F:348:PRO:HD2	1.69	0.74
7:J:598:PHE:HA	7:J:601:ILE:HD12	1.68	0.74
11:K:16:LEU:HD21	11:K:124:LEU:HD11	1.69	0.74
11:K:24:VAL:HG13	11:K:33:LEU:CD1	2.19	0.72
6:H:441:ILE:HG22	6:H:456:GLY:HA2	1.69	0.72
7:J:361:ALA:HB1	7:J:371:LEU:HD13	1.72	0.72
1:V:18:A:OP2	9:F:378:LYS:NZ	2.24	0.70
7:J:849:TYR:CD2	7:J:859:LEU:HD11	2.27	0.70
8:D:86:TYR:CD2	8:D:124:ALA:HB1	2.27	0.69
5:A:960:THR:HG21	9:F:455:PHE:CZ	2.29	0.68
5:A:1668:ILE:HD13	5:A:1801:SER:HB3	1.76	0.68
5:A:1050:LEU:HD22	5:A:1170:MET:HE3	1.77	0.67
5:A:1946:VAL:HG21	7:J:229:ILE:HG21	1.77	0.66
11:K:16:LEU:CD2	11:K:124:LEU:HD11	2.25	0.66
7:J:264:ILE:HD13	7:J:284:LEU:HD11	1.78	0.66
7:J:863:PHE:CE1	7:J:893:LEU:HD11	2.32	0.65
5:A:1835:LEU:HD21	5:A:1843:LEU:HD11	1.79	0.64
9:F:135:LEU:HD22	9:F:208:TRP:CD1	2.33	0.64
7:J:351:LYS:O	7:J:355:ILE:HG13	1.98	0.64
7:J:251:GLU:OE2	7:J:259:VAL:HG23	1.99	0.62
7:J:597:ARG:HE	7:J:620:THR:HG22	1.64	0.62
7:J:601:ILE:HD13	7:J:640:VAL:HG11	1.80	0.62
9:F:74:LEU:HB3	9:F:75:PRO:HD3	1.80	0.62
3:U:93:G:N1	3:U:94:C:C4	2.68	0.62
9:F:53:LEU:HD22	9:F:73:ILE:HG12	1.81	0.62
11:K:24:VAL:HG22	11:K:102:ILE:HD11	1.82	0.61
5:A:1342:LEU:CD2	5:A:1360:LEU:HD21	2.30	0.61
6:H:411:VAL:HG12	6:H:443:LEU:HD21	1.81	0.61
5:A:1063:PHE:CE1	5:A:1086:ASN:HB3	2.35	0.61
5:A:1089:VAL:HG22	5:A:1098:VAL:HG22	1.82	0.61
7:J:452:ASN:CB	7:J:497:VAL:HG21	2.30	0.61
9:F:127:LEU:HD11	9:F:140:VAL:HG11	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:283:ALA:HB2	6:H:313:LEU:HG	1.83	0.61
5:A:1559:HIS:HB3	5:A:1613:THR:HG21	1.82	0.60
5:A:2025:ILE:HD12	5:A:2058:LEU:HD22	1.83	0.60
11:K:64:LEU:CD2	11:K:98:ILE:HD13	2.31	0.60
5:A:1578:ALA:CB	5:A:1602:PRO:HB3	2.25	0.60
6:H:192:THR:HG21	6:H:461:ILE:CD1	2.32	0.60
2:W:31:G:H4'	2:W:32:U:OP1	2.01	0.60
1:V:58:G:H2'	1:V:59:C:O4'	2.02	0.60
7:J:204:LEU:HD23	9:F:433:ASN:HD22	1.66	0.60
9:F:233:VAL:HG11	9:F:237:ILE:HG21	1.84	0.59
5:A:1971:ILE:HD11	5:A:2012:LEU:HD21	1.83	0.59
5:A:1082:ILE:HD13	5:A:1113:ILE:HD11	1.84	0.59
3:U:93:G:N2	3:U:94:C:C2	2.70	0.59
7:J:465:VAL:HG11	7:J:501:VAL:HG22	1.84	0.59
7:J:702:PRO:O	7:J:706:VAL:HG23	2.02	0.59
6:H:395:ILE:HD11	6:H:415:TYR:CD1	2.38	0.59
7:J:613:LEU:O	7:J:617:PHE:CD2	2.56	0.59
10:G:342:PHE:HB3	10:G:424:ILE:HD11	1.85	0.59
7:J:590:ALA:HB3	7:J:591:PRO:HD3	1.85	0.58
9:F:218:ILE:O	9:F:222:ILE:HG23	2.04	0.58
10:G:341:VAL:HG11	10:G:463:PHE:CD1	2.39	0.58
7:J:341:TRP:CD1	7:J:365:ILE:HD11	2.39	0.58
8:D:86:TYR:CG	8:D:124:ALA:HB1	2.38	0.58
5:A:1023:LEU:HD13	5:A:1451:PHE:CD1	2.39	0.58
6:H:375:VAL:HG11	6:H:427:TRP:CH2	2.39	0.58
5:A:1092:PHE:O	5:A:1093:LYS:C	2.42	0.57
7:J:204:LEU:HD22	9:F:380:ARG:O	2.04	0.57
7:J:758:LEU:HD21	11:K:75:ASN:HB2	1.86	0.57
7:J:536:PHE:HB3	7:J:564:TYR:CZ	2.40	0.57
6:H:162:MET:HB3	6:H:421:VAL:HG21	1.87	0.57
5:A:1312:PHE:CE2	5:A:1360:LEU:HD23	2.40	0.56
10:G:368:LEU:HD13	10:G:370:LEU:HD13	1.87	0.56
5:A:808:ILE:O	5:A:811:ILE:HG22	2.05	0.56
5:A:1599:SER:O	5:A:1602:PRO:HD2	2.05	0.56
2:W:84:C:H3'	10:G:350:PRO:HB3	1.88	0.56
10:G:365:LEU:HD22	10:G:382:VAL:HG12	1.88	0.56
5:A:1275:MET:CE	5:A:1281:ASN:CG	2.74	0.55
5:A:1275:MET:HE3	5:A:1281:ASN:CG	2.27	0.55
5:A:1394:LEU:HD11	5:A:1553:ILE:HD13	1.88	0.55
11:K:64:LEU:HD22	11:K:98:ILE:HD13	1.88	0.55
12:B:387:GLU:O	12:B:388:GLN:CB	2.54	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1339:LEU:HD21	5:A:1402:ALA:HB2	1.88	0.55
7:J:327:VAL:HG11	7:J:344:ALA:HB2	1.89	0.55
7:J:846:PHE:CD1	7:J:859:LEU:HD13	2.42	0.55
5:A:1961:LEU:HG	5:A:2084:LEU:HG	1.88	0.55
7:J:215:LEU:HD13	9:F:398:GLN:NE2	2.22	0.55
9:F:98:PHE:HA	9:F:101:ILE:HG22	1.88	0.55
1:V:10:C:H2'	1:V:11:A:O4'	2.06	0.54
5:A:882:ILE:CD1	5:A:1238:LEU:HD21	2.37	0.54
10:G:352:ILE:HD12	10:G:400:ILE:HG23	1.89	0.54
11:K:54:MET:HB3	11:K:64:LEU:HD11	1.89	0.54
1:V:58:G:C6	1:V:59:C:C4	2.96	0.54
2:W:49:A:O2'	2:W:50:G:OP2	2.22	0.54
5:A:831:ARG:NH2	5:A:978:ILE:HG23	2.22	0.54
9:F:194:ARG:O	9:F:197:ILE:HG13	2.08	0.54
7:J:616:PHE:O	7:J:620:THR:HG23	2.06	0.54
5:A:874:ILE:HD13	5:A:1065:LEU:HD22	1.90	0.53
9:F:329:LEU:HD22	11:K:60:PRO:HG3	1.90	0.53
7:J:204:LEU:CD1	9:F:381:LEU:HD23	2.38	0.53
11:K:39:GLU:O	11:K:43:THR:HG23	2.08	0.53
6:H:390:LEU:HB3	10:G:428:TRP:CE3	2.43	0.53
5:A:1921:VAL:HG21	5:A:1948:MET:HE1	1.91	0.53
7:J:299:ALA:HB1	7:J:309:LEU:HD13	1.90	0.53
12:B:423:ILE:HG23	12:B:424:PRO:HD3	1.91	0.53
7:J:617:PHE:CD2	7:J:644:ARG:CZ	2.91	0.53
5:A:1354:GLU:N	5:A:1355:PRO:CD	2.72	0.53
7:J:204:LEU:HD23	9:F:433:ASN:ND2	2.23	0.53
2:W:77:G:H2'	2:W:78:G:O4'	2.09	0.53
5:A:1946:VAL:HG21	7:J:229:ILE:CG2	2.39	0.52
6:H:436:HIS:HA	6:H:462:LYS:HE3	1.90	0.52
11:K:40:ALA:O	11:K:43:THR:OG1	2.21	0.52
7:J:215:LEU:HD13	9:F:398:GLN:HE22	1.74	0.52
5:A:1791:PHE:CE2	5:A:1794:LEU:HD22	2.44	0.52
7:J:781:PHE:CZ	7:J:793:ILE:HG13	2.45	0.52
9:F:106:LYS:O	9:F:109:ILE:HG22	2.09	0.52
5:A:939:LEU:HD21	9:F:445:ILE:HD11	1.92	0.52
7:J:376:THR:HG22	7:J:388:LEU:HD13	1.91	0.51
7:J:737:VAL:HG22	7:J:767:PHE:CD1	2.44	0.51
5:A:753:TYR:HB2	8:D:41:ILE:HD11	1.92	0.51
5:A:1063:PHE:CZ	5:A:1086:ASN:HB3	2.46	0.51
7:J:561:LEU:HB3	7:J:596:LEU:HD21	1.92	0.51
9:F:268:LEU:HD13	9:F:270:HIS:CE1	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1600:GLN:NE2	8:D:134:PRO:O	2.43	0.51
6:H:192:THR:HG21	6:H:461:ILE:HD13	1.92	0.51
7:J:204:LEU:HD11	9:F:381:LEU:HD23	1.92	0.51
7:J:601:ILE:HG12	7:J:617:PHE:CZ	2.46	0.51
7:J:605:GLY:HA3	7:J:887:THR:HG21	1.92	0.51
9:F:145:GLU:HG3	9:F:197:ILE:HD11	1.91	0.51
11:K:24:VAL:HG13	11:K:33:LEU:HD11	1.93	0.51
1:V:35:G:N2	1:V:43:C:C2	2.79	0.51
5:A:1669:LEU:HB3	5:A:1681:VAL:HG21	1.93	0.51
5:A:2015:LEU:HD23	5:A:2022:ALA:HB3	1.93	0.51
6:H:207:LEU:HD22	6:H:463:LEU:HG	1.91	0.51
7:J:201:LEU:O	7:J:202:SER:C	2.49	0.51
10:G:382:VAL:HG21	10:G:392:TYR:CD2	2.45	0.51
9:F:57:LEU:HD21	9:F:108:ASN:HA	1.92	0.51
3:U:93:G:C2	3:U:94:C:C4	2.99	0.51
5:A:982:TYR:CD2	5:A:1104:ILE:HG23	2.46	0.51
5:A:1066:LEU:HD11	5:A:1113:ILE:HG23	1.93	0.51
5:A:1387:VAL:HG12	5:A:1610:TRP:CE3	2.46	0.51
9:F:74:LEU:HD13	9:F:78:VAL:HB	1.93	0.51
6:H:246:PHE:HB3	6:H:255:LEU:HD22	1.93	0.50
7:J:661:LEU:HD22	7:J:670:PHE:HB3	1.92	0.50
11:K:53:ILE:HD11	11:K:102:ILE:HG12	1.92	0.50
5:A:788:GLU:HB2	7:J:181:LEU:HD23	1.93	0.50
5:A:1318:GLY:O	5:A:1321:MET:O	2.30	0.50
7:J:778:ILE:HG23	7:J:794:PHE:CE1	2.47	0.50
5:A:1578:ALA:HB1	5:A:1602:PRO:CB	2.28	0.50
5:A:1387:VAL:HG12	5:A:1610:TRP:CD2	2.47	0.50
9:F:298:VAL:HG12	9:F:302:MET:HB2	1.92	0.50
9:F:102:ILE:N	9:F:103:PRO:CD	2.75	0.50
6:H:111:THR:HG22	10:G:216:TYR:HB3	1.94	0.49
11:K:26:GLN:HB3	11:K:110:ILE:HG21	1.94	0.49
7:J:372:LEU:O	7:J:376:THR:HG23	2.12	0.49
1:V:21:C:H2'	1:V:22:G:O4'	2.12	0.49
5:A:1560:THR:HG21	5:A:1609:TRP:NE1	2.27	0.49
5:A:1893:ILE:HD12	5:A:1978:VAL:HG22	1.95	0.49
6:H:425:ASP:HB2	10:G:174:LEU:HD23	1.93	0.49
9:F:320:GLN:HE22	9:F:326:ASN:HB3	1.78	0.49
6:H:122:ARG:O	6:H:125:ILE:HG12	2.13	0.49
7:J:601:ILE:HG12	7:J:617:PHE:CE1	2.47	0.49
10:G:368:LEU:HD11	10:G:381:ILE:HD12	1.94	0.49
6:H:390:LEU:HD13	10:G:428:TRP:HB2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:J:465:VAL:CG1	7:J:501:VAL:HG22	2.43	0.49
5:A:1183:THR:HG23	5:A:1221:ASN:HB3	1.94	0.49
5:A:1933:ILE:HG21	5:A:1944:LEU:HD21	1.94	0.49
1:V:34:G:H2'	1:V:35:G:O4'	2.12	0.49
5:A:1791:PHE:CZ	5:A:1794:LEU:HD22	2.47	0.49
9:F:112:MET:HE1	9:F:203:ILE:HD12	1.95	0.49
7:J:195:ASN:O	7:J:199:ASP:N	2.46	0.49
7:J:207:LEU:HD12	9:F:382:SER:CB	2.43	0.49
1:V:22:G:C2	1:V:23:C:C2	3.00	0.48
7:J:248:ALA:HA	7:J:264:ILE:HD11	1.94	0.48
7:J:251:GLU:HB3	7:J:260:ALA:HB2	1.96	0.48
7:J:341:TRP:CE3	7:J:361:ALA:HB2	2.48	0.48
10:G:347:LEU:HD11	10:G:371:ARG:HD3	1.93	0.48
6:H:121:ARG:O	6:H:125:ILE:HG23	2.14	0.48
6:H:243:ILE:HG13	6:H:261:LEU:HD13	1.94	0.48
7:J:239:THR:N	7:J:240:ASN:HA	2.28	0.48
7:J:674:LEU:CD2	7:J:690:THR:HG21	2.43	0.48
5:A:1010:PRO:HG2	5:A:1012:TRP:CZ2	2.49	0.48
6:H:459:ARG:NH2	11:K:72:GLU:O	2.46	0.48
1:V:22:G:C6	1:V:23:C:C4	3.02	0.48
5:A:1275:MET:CE	5:A:1281:ASN:ND2	2.70	0.48
7:J:190:GLN:O	7:J:194:PRO:HD2	2.13	0.48
5:A:1657:ILE:HA	5:A:1811:ALA:CB	2.44	0.48
7:J:170:LEU:HD13	7:J:175:ASP:OD2	2.14	0.48
12:B:404:GLY:O	12:B:407:GLN:HB2	2.13	0.48
5:A:1050:LEU:HD22	5:A:1170:MET:CE	2.42	0.48
6:H:176:LYS:HB3	6:H:177:PRO:HD2	1.95	0.48
7:J:256:LYS:HD2	7:J:259:VAL:HG22	1.96	0.48
7:J:674:LEU:HD22	7:J:690:THR:HG21	1.96	0.48
8:D:93:CYS:SG	8:D:120:ILE:HG21	2.54	0.48
11:K:54:MET:SD	11:K:64:LEU:CD1	3.02	0.48
5:A:1286:TRP:CZ2	5:A:1302:LEU:HD11	2.49	0.47
7:J:187:ASN:N	7:J:188:PRO:HD2	2.28	0.47
9:F:225:ILE:HG22	9:F:248:VAL:HG21	1.96	0.47
5:A:1407:ILE:HG21	5:A:1412:LEU:HD21	1.94	0.47
7:J:378:LEU:HD13	7:J:379:GLN:HA	1.96	0.47
5:A:1126:LEU:HD21	5:A:1161:TYR:CG	2.50	0.47
5:A:1820:ARG:O	5:A:1824:GLN:N	2.44	0.47
1:V:58:G:C5	1:V:59:C:C5	3.03	0.47
5:A:1974:LEU:O	5:A:1978:VAL:HG23	2.14	0.47
5:A:2052:GLU:OE1	10:G:291:THR:OG1	2.31	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:35:G:C2	1:V:43:C:C2	3.03	0.47
1:V:58:G:C2	1:V:59:C:C2	3.03	0.47
5:A:765:ASP:CG	7:J:163:THR:HG21	2.35	0.47
5:A:853:THR:O	5:A:857:ILE:HG12	2.14	0.47
7:J:645:TYR:O	7:J:649:ASN:N	2.46	0.47
9:F:130:LEU:HD11	9:F:178:SER:HB3	1.97	0.47
9:F:320:GLN:HE22	9:F:326:ASN:CB	2.28	0.47
5:A:1414:TRP:HA	5:A:1558:GLU:HG2	1.95	0.47
8:D:30:ARG:HA	8:D:82:VAL:HG12	1.95	0.47
5:A:1632:ILE:HD11	5:A:1649:PHE:CE1	2.49	0.47
5:A:1777:ILE:N	5:A:1777:ILE:HD12	2.30	0.47
6:H:125:ILE:HG22	6:H:337:ARG:HB3	1.95	0.47
6:H:435:GLY:N	7:J:731:LEU:HD13	2.30	0.47
11:K:67:LEU:N	11:K:68:PRO:CD	2.76	0.47
9:F:277:SER:HB2	9:F:279:VAL:HG12	1.95	0.47
10:G:293:TRP:O	10:G:297:VAL:HG13	2.15	0.47
1:V:50:G:C6	1:V:51:U:N3	2.83	0.47
7:J:324:TYR:CD1	7:J:347:PHE:CE2	3.03	0.47
5:A:756:LEU:HD13	8:D:44:GLU:HG3	1.97	0.46
5:A:1632:ILE:HD11	5:A:1649:PHE:CD1	2.49	0.46
6:H:289:TRP:CD2	6:H:313:LEU:HD21	2.50	0.46
6:H:321:LEU:HD11	6:H:333:LEU:HB3	1.97	0.46
7:J:498:GLN:HE21	7:J:498:GLN:N	2.13	0.46
5:A:1601:ILE:N	5:A:1602:PRO:CD	2.79	0.46
5:A:1542:TYR:O	5:A:1546:VAL:HG23	2.16	0.46
7:J:323:LYS:O	7:J:327:VAL:HG23	2.16	0.46
11:K:79:VAL:HG13	11:K:121:ILE:HG12	1.98	0.46
5:A:1372:LYS:HG2	5:A:1383:PHE:CE2	2.51	0.46
5:A:1605:ARG:HG2	5:A:1823:LEU:HA	1.98	0.46
7:J:238:PRO:C	7:J:240:ASN:HA	2.35	0.46
5:A:819:LYS:O	5:A:823:TRP:N	2.48	0.46
6:H:176:LYS:HB3	6:H:177:PRO:CD	2.46	0.46
7:J:289:VAL:HG23	7:J:290:HIS:N	2.31	0.46
1:V:37:U:H2'	1:V:39:C:C5	2.51	0.45
9:F:219:ALA:HA	9:F:239:ALA:HB2	1.97	0.45
5:A:1368:GLN:O	5:A:1372:LYS:HG3	2.16	0.45
6:H:235:ILE:HD11	6:H:243:ILE:HG13	1.98	0.45
6:H:365:ALA:HB2	6:H:375:VAL:HG13	1.98	0.45
7:J:706:VAL:HG22	7:J:742:ALA:CB	2.46	0.45
5:A:1115:GLN:HA	5:A:1115:GLN:OE1	2.17	0.45
7:J:568:TYR:CZ	7:J:581:VAL:HG21	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:54:MET:CG	11:K:64:LEU:HD11	2.46	0.45
5:A:914:LEU:HD22	5:A:1505:ASP:HB2	1.97	0.45
5:A:971:MET:HG3	5:A:979:SER:HA	1.99	0.45
5:A:1948:MET:HE3	5:A:1954:ILE:HD12	1.98	0.45
7:J:159:LEU:O	7:J:163:THR:HG23	2.17	0.45
7:J:504:LYS:HG3	7:J:508:TRP:CZ3	2.51	0.45
2:W:49:A:C5	5:A:1646:ILE:HD13	2.51	0.45
5:A:1413:SER:N	5:A:1743:TYR:OH	2.50	0.45
6:H:173:VAL:HB	6:H:178:ILE:HD11	1.98	0.45
5:A:1335:TRP:CD1	5:A:1367:ILE:HG13	2.50	0.45
5:A:1911:TRP:CH2	5:A:1943:PRO:HA	2.52	0.45
6:H:323:CYS:SG	6:H:355:VAL:HG21	2.57	0.45
5:A:1092:PHE:O	5:A:1095:MET:N	2.50	0.45
5:A:1795:LYS:N	5:A:1796:PRO:CD	2.79	0.45
11:K:20:ILE:HD13	11:K:79:VAL:HG21	1.99	0.45
5:A:1614:ILE:HG22	5:A:1638:ILE:HD13	1.99	0.45
6:H:177:PRO:HB3	6:H:457:TRP:HA	1.99	0.45
6:H:243:ILE:HG12	6:H:261:LEU:HB2	1.99	0.45
8:D:9:LEU:HD13	8:D:15:VAL:HA	1.98	0.45
5:A:1850:LEU:HD12	5:A:1930:PRO:HG3	1.98	0.45
6:H:395:ILE:HD11	6:H:415:TYR:CE1	2.52	0.45
9:F:112:MET:CE	9:F:203:ILE:HD12	2.46	0.45
2:W:50:G:N3	2:W:50:G:C2'	2.80	0.44
5:A:1375:LEU:HD22	5:A:1607:THR:HG23	1.98	0.44
7:J:763:ALA:HB1	7:J:773:LEU:CD1	2.47	0.44
1:V:8:U:O2'	12:B:390:LYS:NZ	2.46	0.44
5:A:755:ASP:OD1	5:A:756:LEU:N	2.50	0.44
5:A:919:LEU:HD13	5:A:990:ILE:HD13	1.99	0.44
5:A:1021:PRO:O	5:A:1025:VAL:HG23	2.17	0.44
5:A:1946:VAL:CG2	7:J:229:ILE:HG21	2.47	0.44
6:H:117:LEU:HD13	6:H:301:LEU:HD12	1.98	0.44
7:J:478:TYR:O	7:J:479:GLU:CB	2.66	0.44
2:W:61:C:H2'	2:W:62:A:H8	1.82	0.44
5:A:1025:VAL:HG22	5:A:1262:MET:HG2	2.00	0.44
6:H:195:TRP:CG	6:H:220:LYS:HG3	2.52	0.44
6:H:390:LEU:HD13	10:G:428:TRP:CG	2.53	0.44
6:H:392:HIS:HD2	6:H:396:VAL:HG22	1.82	0.44
5:A:1085:LYS:O	5:A:1088:VAL:HG13	2.17	0.44
9:F:47:LEU:HD13	9:F:97:PHE:HB3	1.99	0.44
7:J:780:LEU:O	7:J:783:HIS:HB2	2.18	0.44
9:F:59:LEU:HD21	9:F:66:SER:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:D:97:THR:O	8:D:141:ARG:NH2	2.51	0.44
8:D:97:THR:HG21	8:D:105:PHE:CE1	2.53	0.44
6:H:183:LEU:HD23	6:H:190:VAL:HB	1.99	0.44
7:J:201:LEU:HD23	9:F:379:PHE:CZ	2.52	0.44
5:A:1125:LEU:CD2	5:A:1230:ILE:HG23	2.47	0.44
5:A:1458:TRP:CH2	5:A:1494:LEU:HD11	2.53	0.44
7:J:604:LEU:HB3	7:J:613:LEU:CD2	2.48	0.44
5:A:1461:TYR:CE1	5:A:1494:LEU:HD13	2.52	0.43
1:V:58:G:C4	1:V:59:C:C6	3.06	0.43
5:A:1385:PRO:HB2	5:A:1437:ILE:HD11	1.99	0.43
5:A:1601:ILE:N	5:A:1602:PRO:HD2	2.33	0.43
5:A:1961:LEU:HD12	5:A:2084:LEU:HD23	2.00	0.43
5:A:1320:LEU:HD23	5:A:1367:ILE:HD13	2.01	0.43
5:A:1837:SER:N	5:A:2084:LEU:HD21	2.34	0.43
8:D:39:CYS:SG	8:D:40:MET:N	2.91	0.43
5:A:1657:ILE:HA	5:A:1811:ALA:HB1	2.01	0.43
7:J:686:MET:O	7:J:690:THR:HG23	2.19	0.43
2:W:34:A:N6	2:W:47:A:C8	2.87	0.43
5:A:1028:TRP:NE1	5:A:1032:ILE:HD11	2.34	0.43
6:H:172:LEU:HD13	7:J:755:GLN:HG3	2.00	0.43
6:H:261:LEU:HB3	6:H:292:TRP:CZ3	2.53	0.43
7:J:737:VAL:HG22	7:J:767:PHE:CG	2.54	0.43
5:A:1047:ALA:HB3	5:A:1251:TYR:HB3	2.01	0.42
5:A:2011:LEU:HD23	5:A:2055:MET:HG3	2.01	0.42
6:H:125:ILE:HG22	6:H:337:ARG:CB	2.49	0.42
5:A:1070:LEU:HD21	5:A:1113:ILE:CD1	2.50	0.42
6:H:191:ALA:HB2	6:H:226:TRP:CZ2	2.54	0.42
7:J:207:LEU:HD12	9:F:382:SER:OG	2.19	0.42
7:J:846:PHE:CE1	7:J:859:LEU:HD13	2.55	0.42
8:D:120:ILE:HG22	8:D:131:VAL:CG1	2.50	0.42
2:W:34:A:C6	2:W:50:G:C6	3.07	0.42
7:J:565:VAL:HG11	7:J:599:PHE:CB	2.48	0.42
7:J:843:VAL:HG21	7:J:896:MET:HE2	2.01	0.42
8:D:97:THR:HG22	8:D:141:ARG:HA	2.00	0.42
1:V:33:A:H2'	1:V:34:G:O4'	2.18	0.42
5:A:943:ALA:O	5:A:947:PRO:HA	2.20	0.42
6:H:401:PHE:CE1	6:H:410:LEU:HG	2.55	0.42
7:J:207:LEU:HD13	9:F:430:SER:CB	2.50	0.42
7:J:485:VAL:O	7:J:489:LEU:HG	2.19	0.42
2:W:81:G:H2'	2:W:82:A:C8	2.54	0.42
5:A:2084:LEU:HD22	5:A:2086:GLN:CD	2.40	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:390:LEU:HD11	10:G:463:PHE:CD1	2.54	0.42
9:F:117:ILE:HD12	9:F:128:SER:CB	2.50	0.42
5:A:1601:ILE:HB	5:A:1602:PRO:HD3	2.01	0.42
9:F:114:ASN:HA	9:F:117:ILE:HG22	2.01	0.42
9:F:381:LEU:HD22	9:F:385:ARG:HB3	2.01	0.42
1:V:22:G:C4	1:V:23:C:C5	3.08	0.42
6:H:207:LEU:HD13	6:H:463:LEU:HD21	2.01	0.42
7:J:358:LEU:O	7:J:362:THR:HG23	2.19	0.42
7:J:653:ILE:HG21	7:J:677:ILE:HD13	2.02	0.42
8:D:49:ILE:HD12	8:D:114:ILE:HG13	2.02	0.42
10:G:272:VAL:HG22	10:G:300:GLN:NE2	2.35	0.42
5:A:1837:SER:HB3	5:A:2084:LEU:HD11	2.01	0.42
2:W:77:G:H4'	11:K:113:GLN:HG3	2.01	0.42
5:A:1085:LYS:HG3	5:A:1107:LEU:HD13	2.02	0.42
5:A:1811:ALA:HA	5:A:2101:LEU:HD13	2.02	0.42
5:A:1881:THR:HG21	5:A:1920:LEU:HD23	2.02	0.42
6:H:140:MET:HA	6:H:143:HIS:CD2	2.55	0.42
1:V:55:U:N3	7:J:200:ALA:O	2.53	0.42
2:W:65:U:H2'	2:W:66:C:C6	2.55	0.42
5:A:762:VAL:HG22	7:J:159:LEU:HD22	2.02	0.42
9:F:124:PHE:CE2	9:F:127:LEU:HD13	2.55	0.41
1:V:17:A:C2	1:V:18:A:C4	3.08	0.41
5:A:922:VAL:HG13	5:A:923:TYR:CD1	2.55	0.41
5:A:1948:MET:CE	5:A:1954:ILE:HD12	2.50	0.41
5:A:2083:ILE:HD11	10:G:287:ILE:HG12	2.02	0.41
6:H:290:ARG:NE	6:H:299:GLU:OE2	2.53	0.41
1:V:35:G:C2	1:V:36:A:C8	3.08	0.41
11:K:33:LEU:HD21	11:K:35:LYS:HG3	2.02	0.41
5:A:831:ARG:HH21	5:A:978:ILE:HG23	1.85	0.41
7:J:207:LEU:HD12	9:F:382:SER:HB2	2.03	0.41
7:J:392:ARG:HB3	7:J:397:GLN:HE22	1.84	0.41
9:F:369:GLY:O	9:F:370:ARG:C	2.58	0.41
2:W:45:A:C2'	2:W:46:U:OP1	2.69	0.41
2:W:45:A:C6	2:W:46:U:C4	3.08	0.41
3:U:93:G:C2	3:U:94:C:N3	2.89	0.41
5:A:2012:LEU:HA	5:A:2015:LEU:HD12	2.03	0.41
7:J:824:SER:O	7:J:828:LEU:HG	2.20	0.41
5:A:1048:VAL:HG22	5:A:1250:VAL:HG22	2.02	0.41
5:A:2014:ALA:HB1	5:A:2058:LEU:HD23	2.03	0.41
5:A:2029:ASP:HB3	5:A:2032:ILE:HD12	2.03	0.41
6:H:390:LEU:HD11	10:G:463:PHE:HD1	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:J:706:VAL:HG22	7:J:742:ALA:HB1	2.03	0.41
8:D:119:THR:HG22	8:D:131:VAL:HG21	2.01	0.41
10:G:341:VAL:HG22	10:G:428:TRP:CB	2.50	0.41
5:A:788:GLU:CB	7:J:181:LEU:HD23	2.51	0.41
5:A:1073:ILE:HD13	5:A:1116:TYR:CD1	2.55	0.41
5:A:1654:TRP:CZ3	5:A:1779:LEU:HD12	2.56	0.41
8:D:49:ILE:HG23	8:D:114:ILE:HG12	2.02	0.41
9:F:74:LEU:HD23	9:F:203:ILE:HB	2.03	0.41
10:G:257:GLU:HA	10:G:260:ILE:HG22	2.02	0.41
5:A:1026:TYR:O	5:A:1029:THR:OG1	2.33	0.41
5:A:1038:ILE:HG23	5:A:1039:TRP:CD2	2.55	0.41
5:A:1320:LEU:HD11	5:A:1366:ARG:HB3	2.02	0.41
5:A:1375:LEU:HD23	5:A:1375:LEU:HA	1.97	0.41
5:A:1999:ILE:HD13	5:A:2007:ARG:NH2	2.36	0.41
7:J:215:LEU:CD2	9:F:400:VAL:HG22	2.51	0.41
7:J:632:THR:HA	7:J:635:LEU:HD21	2.02	0.41
7:J:778:ILE:CG2	7:J:810:GLU:HG3	2.51	0.41
10:G:363:LEU:HD11	10:G:391:PHE:CD2	2.56	0.41
12:B:391:PHE:O	12:B:392:ARG:C	2.60	0.41
1:V:19:U:H4'	1:V:20:A:C8	2.56	0.41
5:A:1321:MET:O	5:A:1322:ALA:CB	2.69	0.41
6:H:353:TYR:CZ	11:K:126:ILE:HD11	2.56	0.41
6:H:364:VAL:HG12	6:H:365:ALA:N	2.36	0.41
10:G:341:VAL:HG12	10:G:381:ILE:HG23	2.02	0.41
11:K:12:ALA:HB1	11:K:16:LEU:HD23	2.03	0.41
5:A:1039:TRP:CD2	5:A:1271:PRO:HG3	2.55	0.40
7:J:764:LEU:HD23	7:J:764:LEU:HA	1.96	0.40
10:G:355:LYS:O	10:G:359:ASN:ND2	2.53	0.40
5:A:1913:THR:O	5:A:1917:VAL:HG23	2.21	0.40
5:A:2084:LEU:HB3	5:A:2086:GLN:HB3	2.02	0.40
5:A:1344:THR:HG21	5:A:1537:TRP:CD2	2.57	0.40
7:J:327:VAL:O	7:J:331:LEU:HG	2.21	0.40
9:F:119:LEU:CD1	9:F:197:ILE:HG22	2.50	0.40
10:G:339:CYS:SG	10:G:340:LYS:N	2.94	0.40
5:A:1216:ILE:HG13	5:A:1254:ASN:HB3	2.03	0.40
5:A:1458:TRP:CZ3	5:A:1494:LEU:HD11	2.56	0.40
6:H:183:LEU:HD21	6:H:453:VAL:HG21	2.03	0.40
6:H:410:LEU:HD23	6:H:410:LEU:HA	1.95	0.40
7:J:223:LEU:HD23	9:F:420:ALA:HB1	2.03	0.40
7:J:565:VAL:HG11	7:J:599:PHE:CG	2.56	0.40
7:J:617:PHE:CE2	7:J:644:ARG:HD3	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:816:ILE:HD12	5:A:817:LYS:N	2.36	0.40
6:H:399:VAL:CG1	6:H:410:LEU:HD22	2.51	0.40
6:H:453:VAL:HG22	6:H:463:LEU:HD22	2.04	0.40
7:J:344:ALA:HB3	7:J:357:MET:CE	2.52	0.40
8:D:112:GLU:CD	8:D:137:TYR:HH	2.25	0.40
9:F:200:ALA:HA	9:F:203:ILE:HG12	2.03	0.40
9:F:233:VAL:HG11	9:F:237:ILE:CG2	2.51	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	A	1343/2413 (56%)	1226 (91%)	104 (8%)	13 (1%)	15 55
6	H	355/465 (76%)	301 (85%)	48 (14%)	6 (2%)	9 45
7	J	719/899 (80%)	650 (90%)	56 (8%)	13 (2%)	8 43
8	D	138/143 (96%)	126 (91%)	11 (8%)	1 (1%)	22 61
9	F	413/494 (84%)	364 (88%)	38 (9%)	11 (3%)	5 35
10	G	316/469 (67%)	283 (90%)	32 (10%)	1 (0%)	41 75
11	K	122/126 (97%)	111 (91%)	9 (7%)	2 (2%)	9 46
12	B	69/2163 (3%)	57 (83%)	8 (12%)	4 (6%)	1 18
All	All	3475/7172 (48%)	3118 (90%)	306 (9%)	51 (2%)	14 47

All (51) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	A	1093	LYS
5	A	1278	VAL
5	A	2088	ILE

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Mol	Chain	Res	Type
6	H	362	TYR
7	J	479	GLU
7	J	592	HIS
7	J	683	ASN
9	F	74	LEU
9	F	363	PRO
9	F	407	GLU
11	K	106	ASP
12	B	388	GLN
12	B	393	GLU
5	A	979	SER
6	H	361	GLY
7	J	200	ALA
8	D	127	ASN
9	F	59	LEU
9	F	79	ASP
9	F	148	ASN
9	F	165	ALA
9	F	435	ALA
12	B	424	PRO
5	A	980	PRO
5	A	1322	ALA
5	A	1623	PHE
5	A	1768	PRO
6	H	216	SER
6	H	435	GLY
7	J	867	GLU
9	F	58	ALA
9	F	146	ASN
9	F	365	LYS
5	A	1324	GLY
5	A	1535	LYS
5	A	2068	ASN
6	H	429	LYS
7	J	237	ASP
7	J	819	ALA
10	G	266	PRO
12	B	392	ARG
5	A	1386	ALA
6	H	230	SER
7	J	206	ASP
7	J	287	SER

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Mol	Chain	Res	Type
7	J	399	PRO
5	A	1638	ILE
7	J	558	PRO
11	K	82	PRO
7	J	241	PRO
7	J	887	THR

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	1216/2182 (56%)	1194 (98%)	22 (2%)	59 81
6	H	305/410 (74%)	290 (95%)	15 (5%)	25 59
7	J	627/813 (77%)	600 (96%)	27 (4%)	29 63
8	D	129/132 (98%)	121 (94%)	8 (6%)	18 53
9	F	346/445 (78%)	324 (94%)	22 (6%)	17 52
10	G	289/436 (66%)	283 (98%)	6 (2%)	53 78
11	K	102/104 (98%)	90 (88%)	12 (12%)	5 28
12	B	56/1955 (3%)	52 (93%)	4 (7%)	14 48
All	All	3070/6477 (47%)	2954 (96%)	116 (4%)	36 66

All (116) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	A	753	TYR
5	A	755	ASP
5	A	757	GLU
5	A	758	LEU
5	A	765	ASP
5	A	831	ARG
5	A	852	LEU
5	A	950	THR
5	A	971	MET

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Mol	Chain	Res	Type
5	A	972	MET
5	A	1004	ASP
5	A	1103	LEU
5	A	1268	ARG
5	A	1276	GLU
5	A	1277	GLU
5	A	1282	ASP
5	A	1512	ARG
5	A	1749	SER
5	A	1827	GLN
5	A	1942	ASP
5	A	1991	ILE
5	A	2048	TRP
6	H	111	THR
6	H	136	LEU
6	H	144	GLN
6	H	146	PHE
6	H	199	LEU
6	H	225	ASP
6	H	232	ASN
6	H	271	VAL
6	H	286	ASP
6	H	300	LEU
6	H	302	LEU
6	H	331	SER
6	H	389	ILE
6	H	422	TYR
6	H	454	SER
7	J	194	PRO
7	J	237	ASP
7	J	239	THR
7	J	255	ARG
7	J	270	GLU
7	J	291	TYR
7	J	328	ARG
7	J	347	PHE
7	J	357	MET
7	J	421	LEU
7	J	459	LEU
7	J	460	THR
7	J	508	TRP
7	J	512	ASP

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Mol	Chain	Res	Type
7	J	554	ARG
7	J	588	ASP
7	J	589	PHE
7	J	635	LEU
7	J	636	TYR
7	J	644	ARG
7	J	657	ASN
7	J	661	LEU
7	J	708	LEU
7	J	715	ASP
7	J	767	PHE
7	J	772	LEU
7	J	874	TRP
8	D	39	CYS
8	D	43	ASP
8	D	48	SER
8	D	71	ASP
8	D	76	LEU
8	D	80	MET
8	D	118	GLU
8	D	139	HIS
9	F	57	LEU
9	F	59	LEU
9	F	63	ASP
9	F	67	LEU
9	F	74	LEU
9	F	81	LYS
9	F	82	ARG
9	F	84	LEU
9	F	85	GLN
9	F	120	TYR
9	F	153	GLU
9	F	154	SER
9	F	156	GLU
9	F	221	LYS
9	F	305	MET
9	F	327	THR
9	F	364	LYS
9	F	376	LYS
9	F	378	LYS
9	F	401	LEU
9	F	410	LEU

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Mol	Chain	Res	Type
9	F	419	GLN
10	G	189	THR
10	G	199	ASP
10	G	278	MET
10	G	285	GLN
10	G	329	MET
10	G	395	LEU
11	K	11	LEU
11	K	21	LEU
11	K	32	GLN
11	K	33	LEU
11	K	34	LYS
11	K	46	ARG
11	K	64	LEU
11	K	69	LEU
11	K	79	VAL
11	K	93	VAL
11	K	113	GLN
11	K	119	ASP
12	B	387	GLU
12	B	390	LYS
12	B	396	HIS
12	B	403	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
5	A	1030	GLN
5	A	1087	ASN
5	A	1190	ASN
5	A	1273	GLN
5	A	1281	ASN
5	A	1368	GLN
5	A	1695	ASN
5	A	1737	GLN
5	A	1831	GLN
5	A	1856	ASN
5	A	1869	ASN
5	A	2018	ASN
6	H	303	GLN
6	H	306	HIS
7	J	397	GLN

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Mol	Chain	Res	Type
7	J	498	GLN
7	J	537	GLN
7	J	578	GLN
7	J	673	GLN
7	J	733	ASN
9	F	148	ASN
9	F	320	GLN
9	F	331	HIS
10	G	276	ASN
10	G	300	GLN
11	K	38	ASN
11	K	45	ASN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	V	66/67 (98%)	29 (43%)	6 (9%)
2	W	54/112 (48%)	20 (37%)	9 (16%)
3	U	19/214 (8%)	8 (42%)	1 (5%)
All	All	139/393 (35%)	57 (41%)	16 (11%)

All (57) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	V	2	U
1	V	11	A
1	V	18	A
1	V	19	U
1	V	20	A
1	V	22	G
1	V	25	U
1	V	26	A
1	V	29	A
1	V	31	U
1	V	32	G
1	V	33	A
1	V	34	G
1	V	35	G
1	V	36	A
1	V	37	U
1	V	39	C

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Mol	Chain	Res	Type
1	V	40	G
1	V	41	U
1	V	45	A
1	V	46	G
1	V	55	U
1	V	56	U
1	V	57	U
1	V	59	C
1	V	64	U
1	V	65	G
1	V	66	A
1	V	67	A
2	W	28	U
2	W	29	U
2	W	31	G
2	W	32	U
2	W	33	C
2	W	38	U
2	W	45	A
2	W	46	U
2	W	47	A
2	W	49	A
2	W	50	G
2	W	56	A
2	W	61	C
2	W	75	A
2	W	76	A
2	W	83	A
2	W	84	C
2	W	85	C
2	W	86	G
2	W	87	U
3	U	93	G
3	U	94	C
3	U	95	C
3	U	96	U
3	U	97	U
3	U	99	U
3	U	101	C
3	U	103	A

All (16) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	V	17	A
1	V	19	U
1	V	31	U
1	V	39	C
1	V	44	G
1	V	45	A
2	W	31	G
2	W	32	U
2	W	45	A
2	W	48	C
2	W	49	A
2	W	55	G
2	W	75	A
2	W	83	A
2	W	84	C
3	U	95	C

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)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
4	x	1
5	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	x	62:UNK	C	101:UNK	N	54.04
1	A	1860:VAL	C	1861:THR	N	4.50

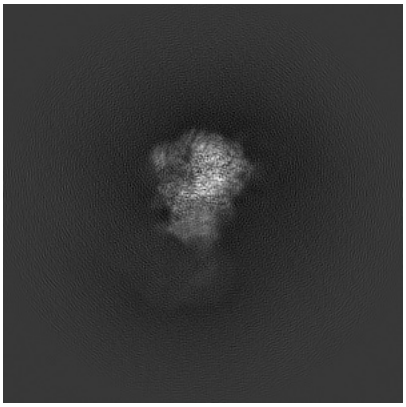
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-8014. These allow visual inspection of the internal detail of the map and identification of artifacts.

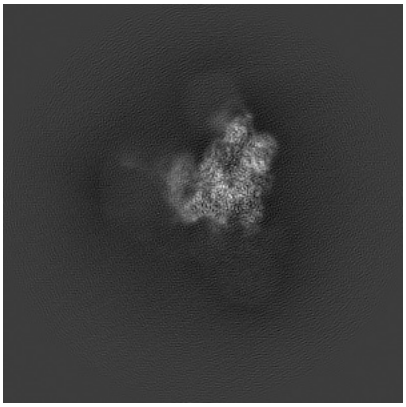
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

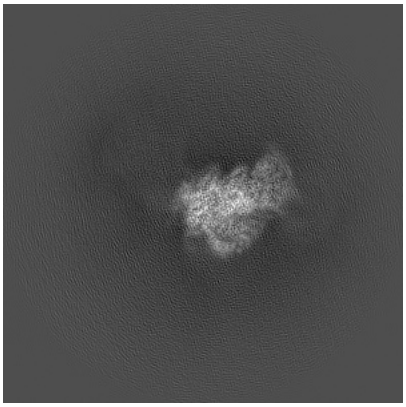
6.1.1 Primary map



X



Y

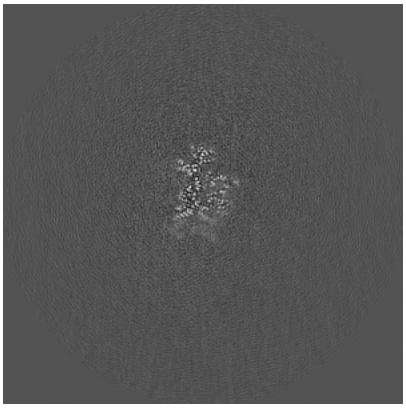


Z

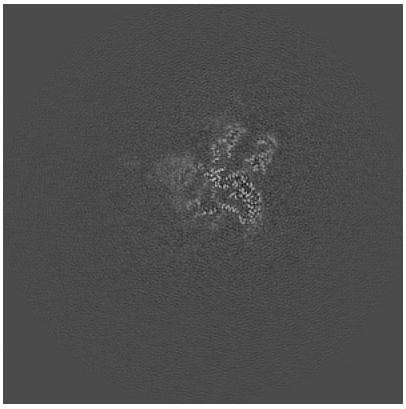
The images above show the map projected in three orthogonal directions.

6.2 Central slices

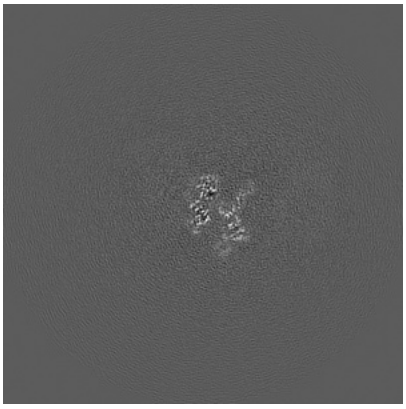
6.2.1 Primary map



X Index: 190



Y Index: 190

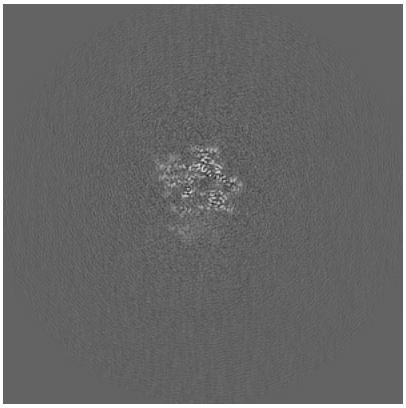


Z Index: 190

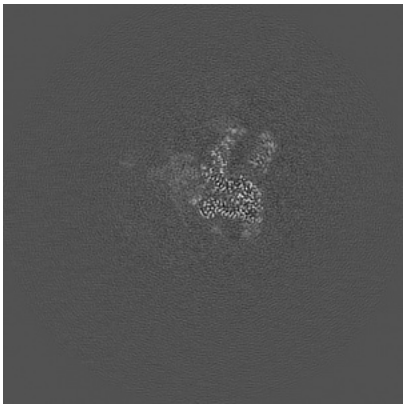
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

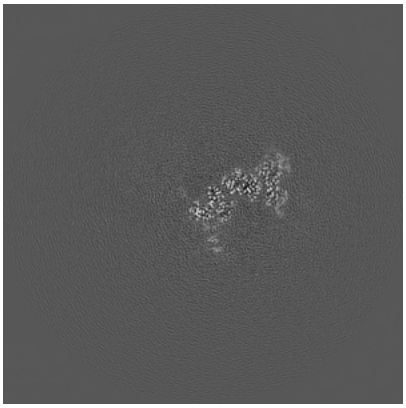
6.3.1 Primary map



X Index: 197



Y Index: 186

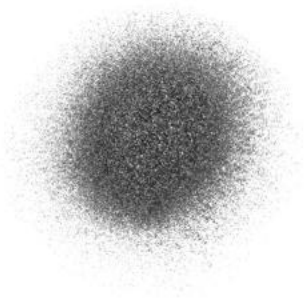


Z Index: 221

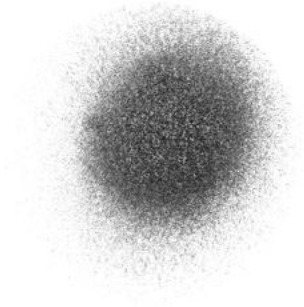
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

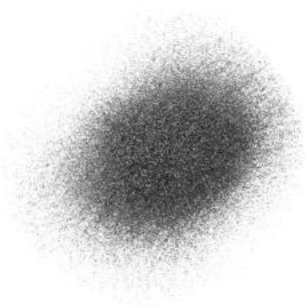
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

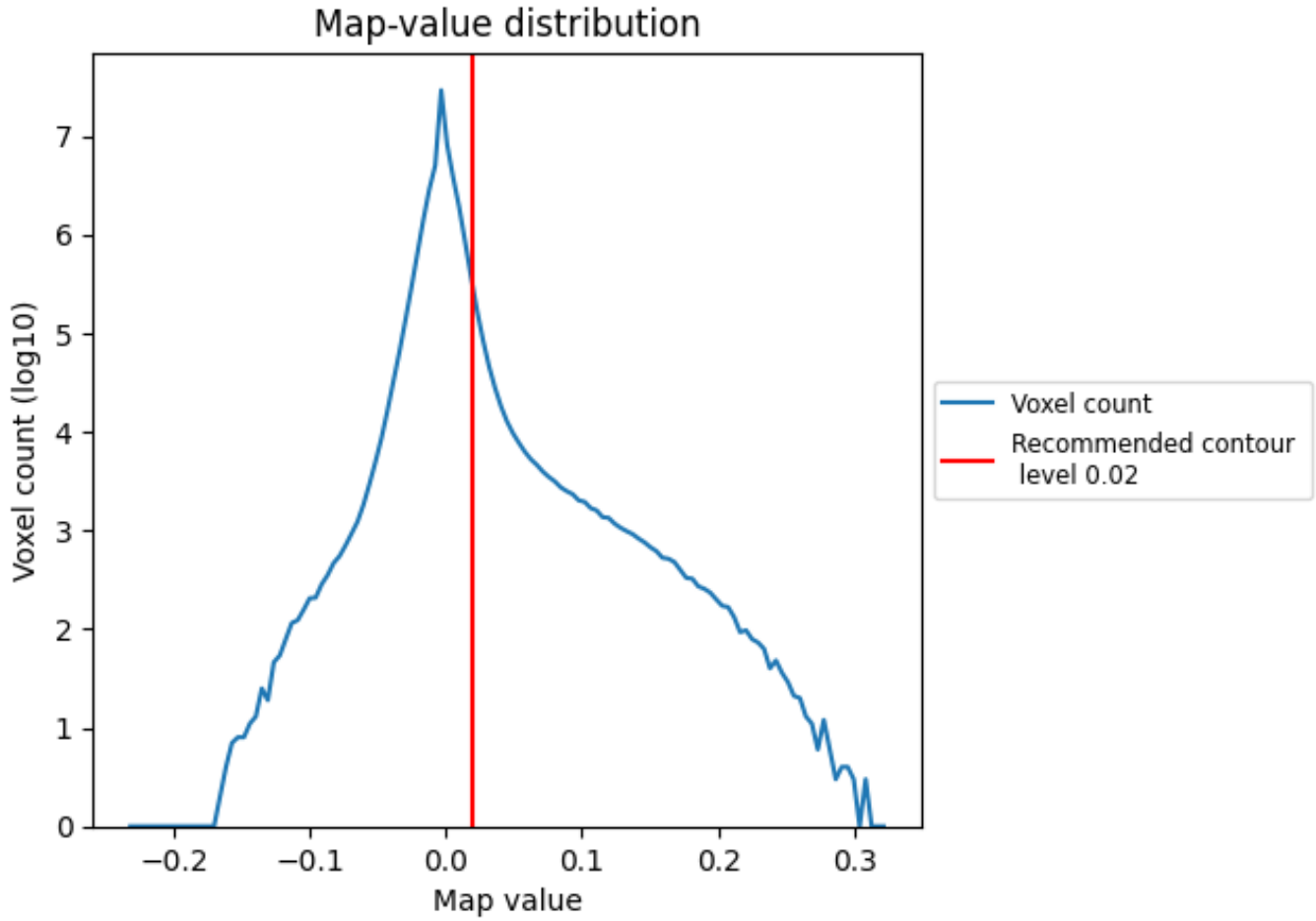
6.5 Mask visualisation (i)

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

7 Map analysis

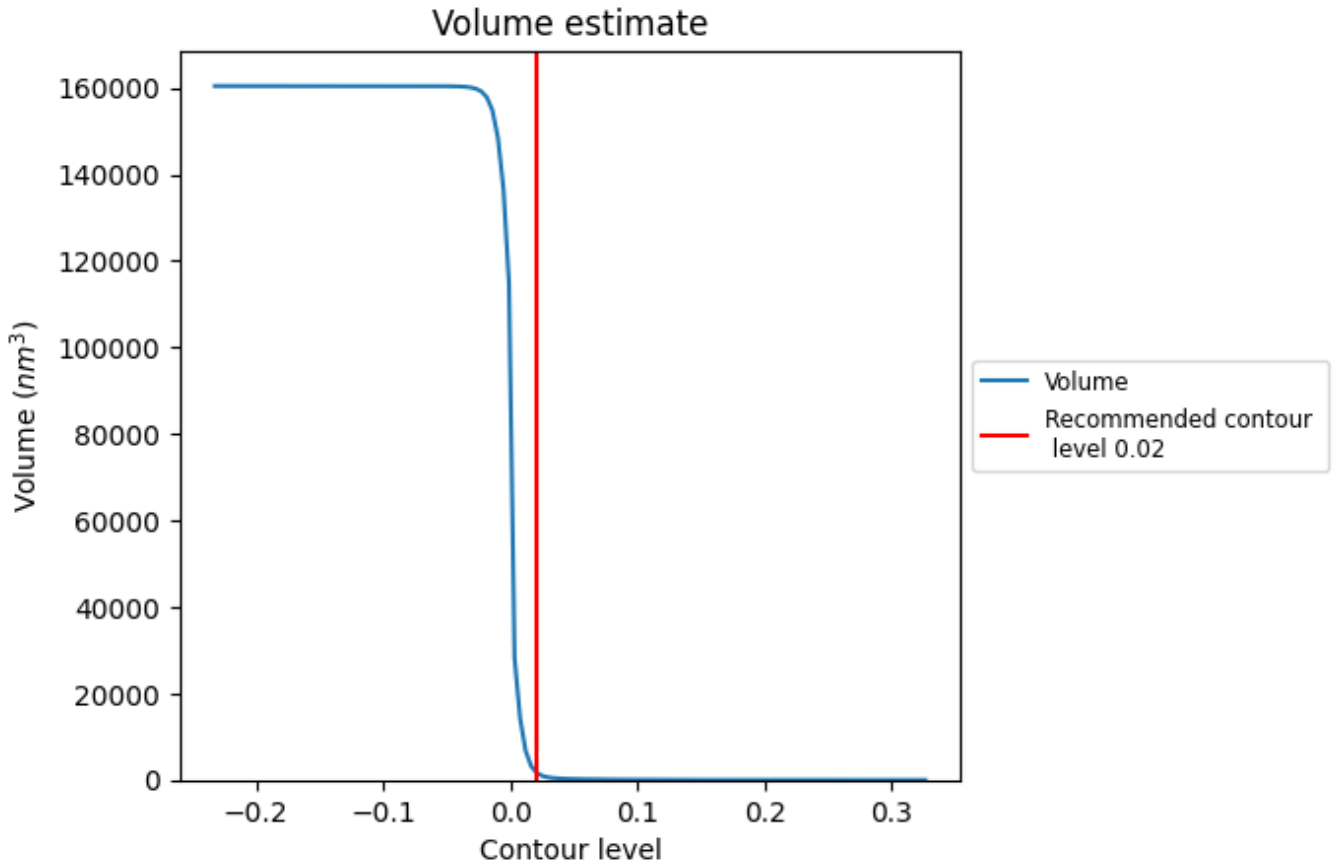
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

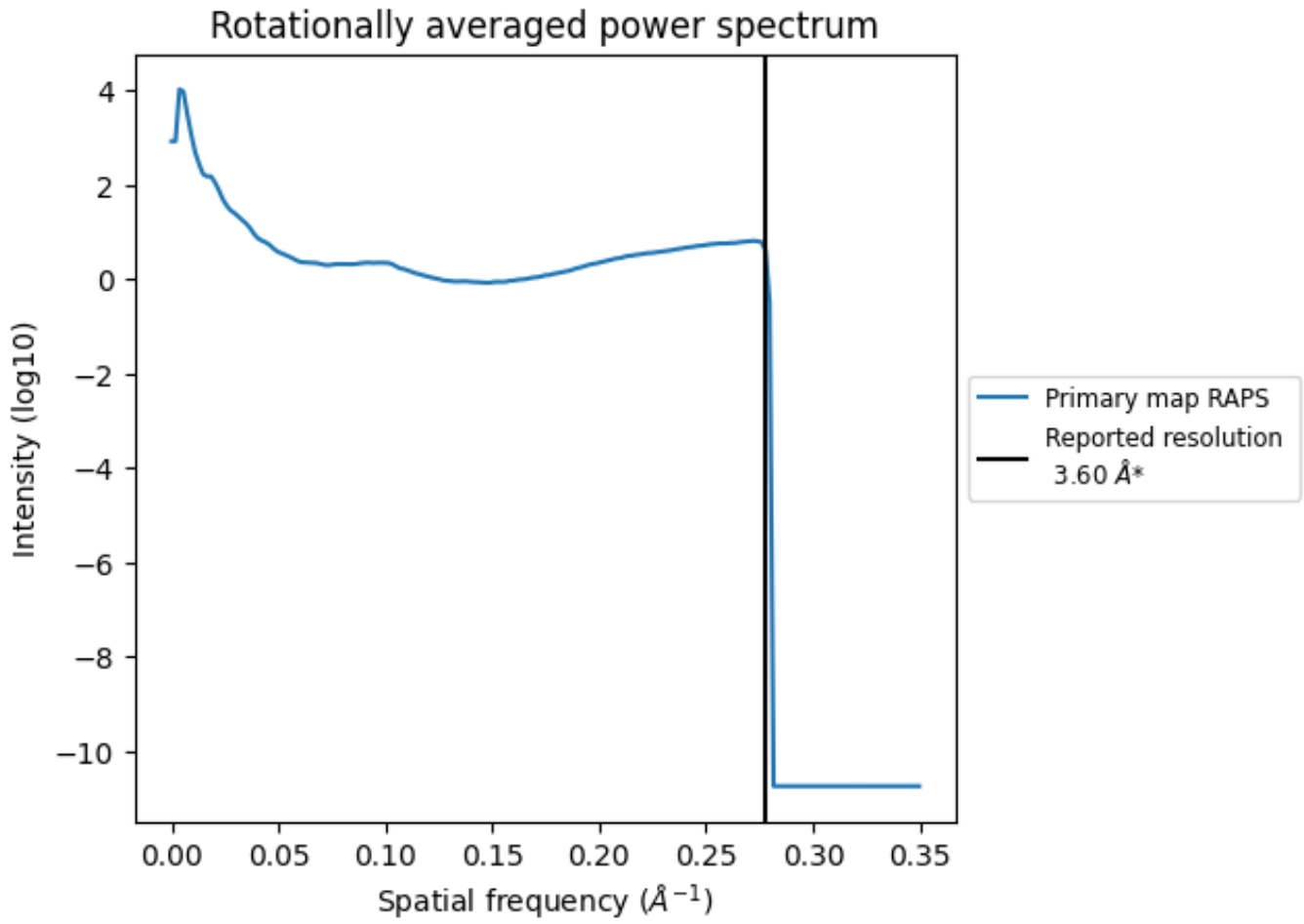
7.2 Volume estimate



The volume at the recommended contour level is 1921 nm^3; this corresponds to an approximate mass of 1735 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)

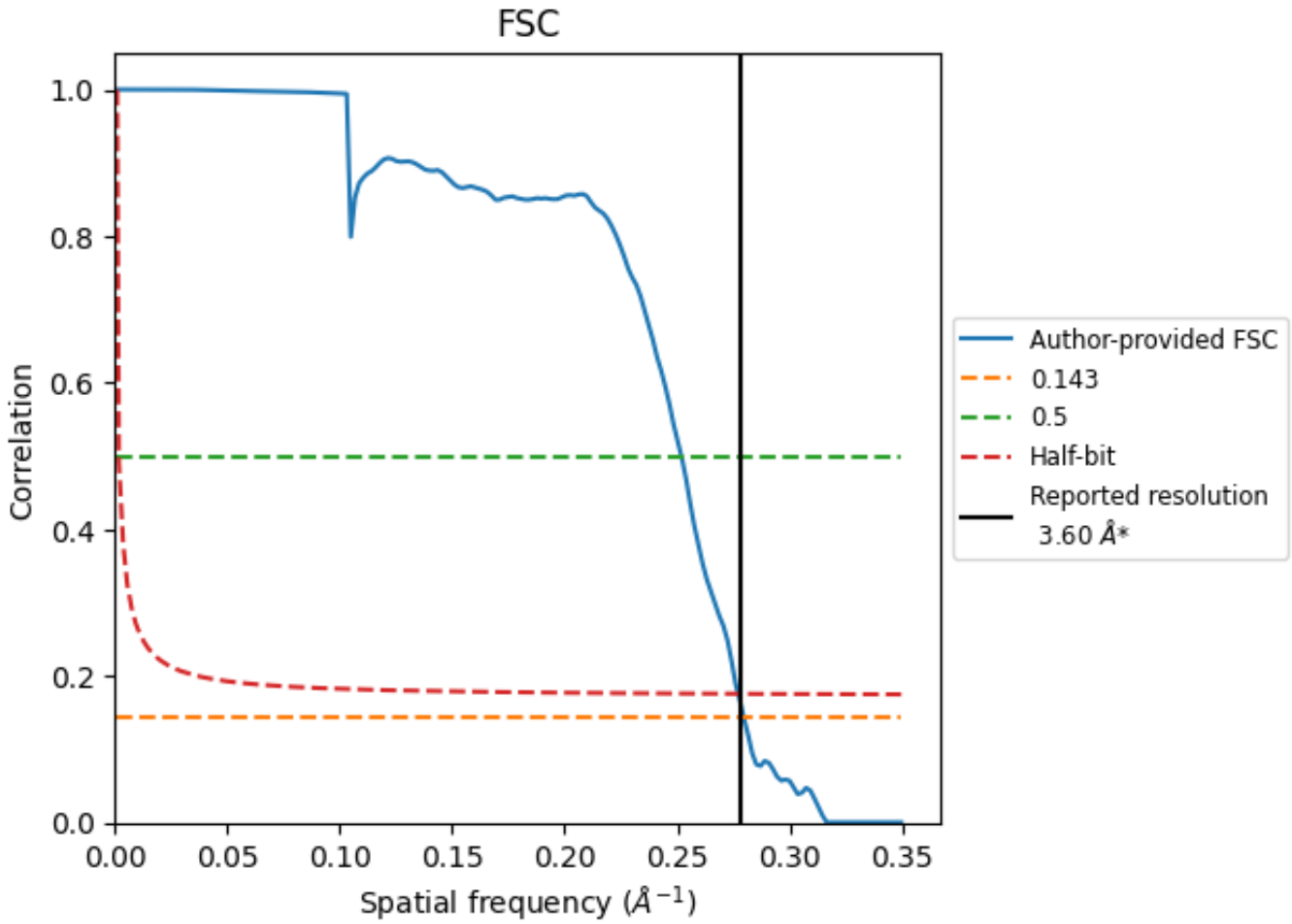


*Reported resolution corresponds to spatial frequency of 0.278 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.278 Å^{-1}

8.2 Resolution estimates (i)

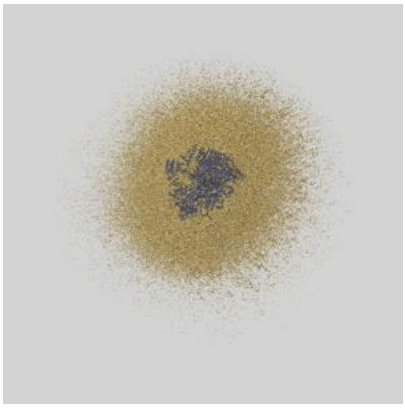
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.58	3.97	3.61
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

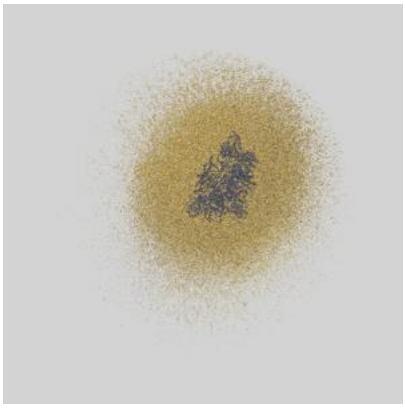
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-8014 and PDB model 5GAP. Per-residue inclusion information can be found in section 3 on page 6.

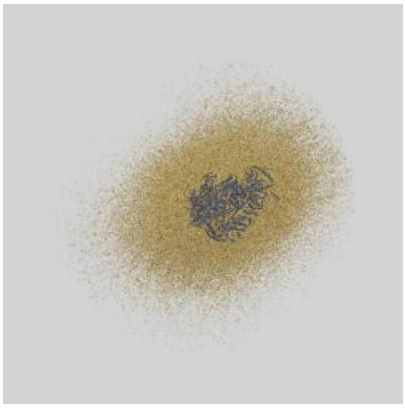
9.1 Map-model overlay



X



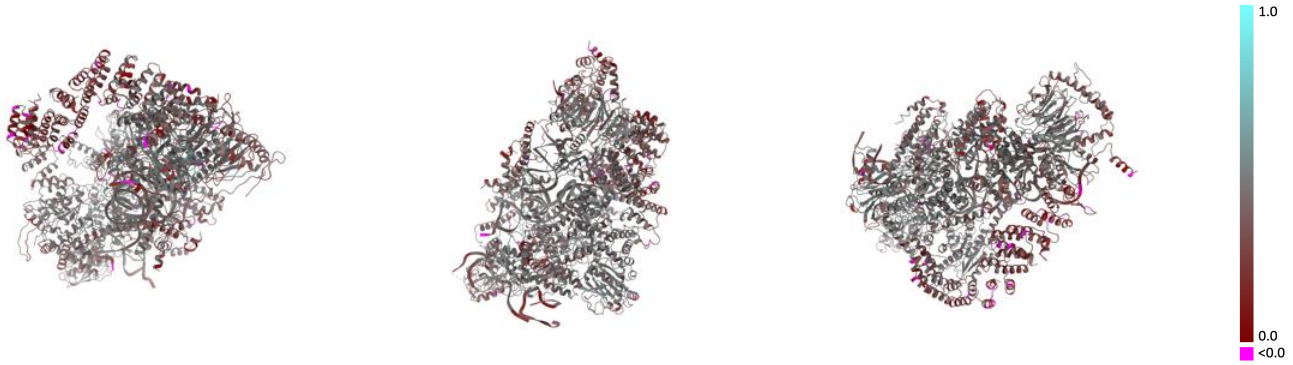
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.02 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.

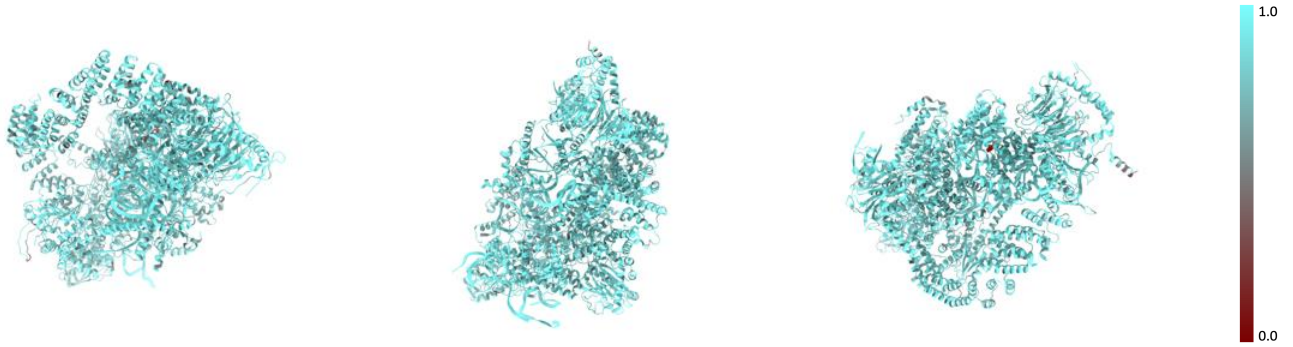
9.2 Q-score mapped to coordinate model



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.

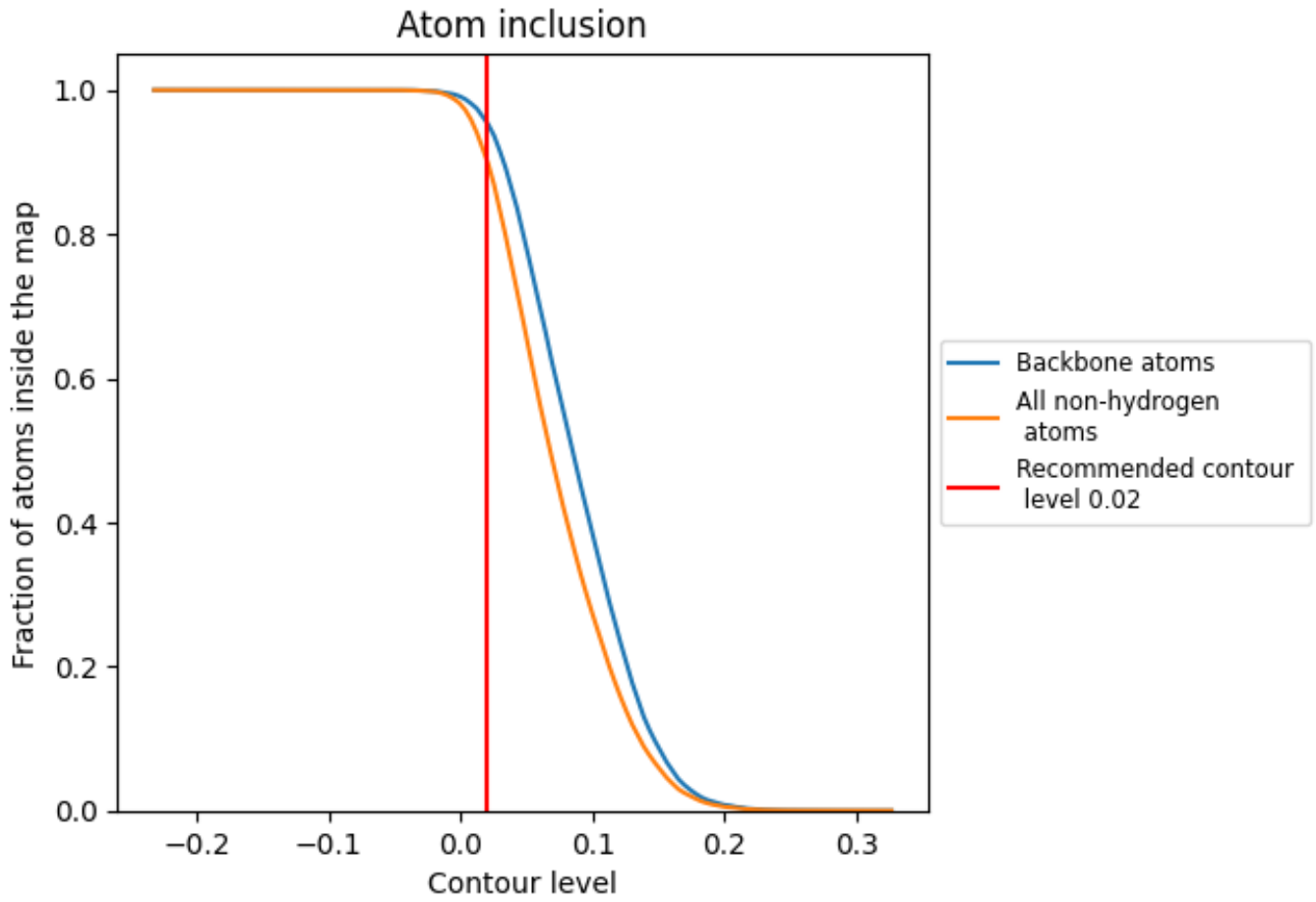
9.3 Atom inclusion mapped to coordinate model



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 (0.02).

9.4 Atom inclusion (i)



At the recommended contour level, 95% of all backbone atoms, 90% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9015	0.3970
A	0.9039	0.4340
B	0.8192	0.3180
D	0.8951	0.4260
F	0.8993	0.4110
G	0.8874	0.3770
H	0.8954	0.4080
J	0.8807	0.3130
K	0.9134	0.4670
U	0.9251	0.2810
V	0.9670	0.4390
W	0.9639	0.3760
x	0.9390	0.4020