Full wwPDB EM Validation Report ⓘ

May 25, 2024 – 09:17 am BST

PDB ID	:	8QPK
EMDB ID	:	EMD-18555
Title	:	Cryo-EM Structure of Pre-B+5'ss Complex (core part)
Authors	:	Zhang, Z.; Kumar, V.; Dybkov, O.; Will, C.L.; Zhong, J.; Ludwig, S.; Urlaub, H.; Kastner, B.; Stark, H.; Luehrmann, R.
Deposited on	:	2023-10-02
Resolution	:	4.20 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:

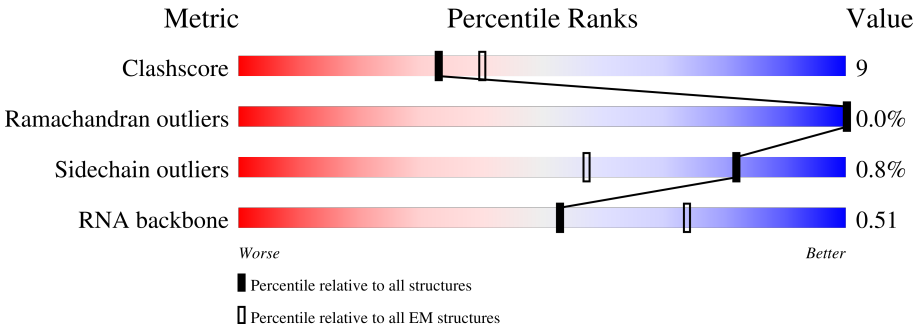
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance

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

The reported resolution of this entry is 4.20 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	G	820	11% · 88%
2	D	142	80% 19% ·
3	L	499	· 9% · 90%
4	A	2335	5% 68% 15% 17%
5	R	480	· 20% · 78%
6	U	565	· 74% 7% 19%
7	S	800	· 8% · 91%

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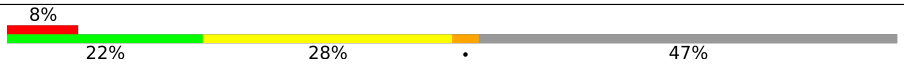
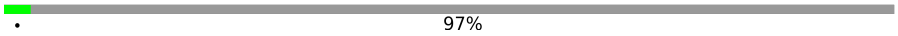
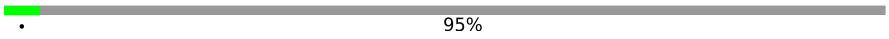
Mol	Chain	Length	Quality of chain
8	C	972	
9	5	117	
10	4	144	
11	X	155	
12	z	11	
13	6	106	
14	N	941	
15	B	2136	
16	7	793	

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 29527 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 Probable ATP-dependent RNA helicase DDX23.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	G	102	Total	C	N	O	0	0
			658	419	128	111		

- Molecule 2 is a protein called Thioredoxin-like protein 4A.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	141	Total	C	N	O	S	0	0
			1008	648	184	171	5		

- Molecule 3 is a protein called U4/U6 small nuclear ribonucleoprotein Prp31.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	L	50	Total	C	N	O	0	0
			251	151	50	50		

- Molecule 4 is a protein called Pre-mRNA-processing-splicing factor 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	1947	Total	C	N	O	S	0	0
			13055	8360	2412	2254	29		

- Molecule 5 is a protein called RNA-binding protein 42.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	R	106	Total	C	N	O	S	0	0
			659	412	124	121	2		

- Molecule 6 is a protein called Ubiquitin carboxyl-terminal hydrolase 39.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	U	456	Total	C	N	O	0	0
			2320	1404	459	457		

- Molecule 7 is a protein called U4/U6.U5 tri-snRNP-associated protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	S	73	Total	C	N	O	S	0	0
			446	274	90	81	1		

- Molecule 8 is a protein called 116 kDa U5 small nuclear ribonucleoprotein component.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	C	836	Total	C	N	O	S	0	0
			5163	3262	981	913	7		

- Molecule 9 is a RNA chain called U5 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	5	77	Total	C	N	O	P	0	0
			1620	726	271	546	77		

- Molecule 10 is a RNA chain called U4 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	4	76	Total	C	N	O	P	0	0
			1617	723	286	532	76		

- Molecule 11 is a protein called U4/U6.U5 small nuclear ribonucleoprotein 27 kDa protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	X	22	Total	C	N	O	0	0
			124	78	22	24		

- Molecule 12 is a RNA chain called 5'ss oligo.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	z	11	Total	C	N	O	P	0	0
			239	107	46	75	11		

- Molecule 13 is a RNA chain called U6 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	6	43	Total	C	N	O	P	0	0
			927	414	175	295	43		

- Molecule 14 is a protein called Pre-mRNA-processing factor 6.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	N	133	Total	C	N	O	0	0
			784	482	157	145		

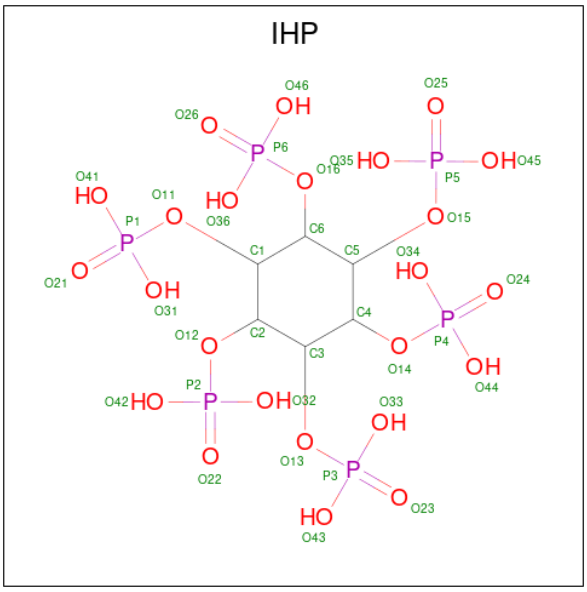
- Molecule 15 is a protein called U5 small nuclear ribonucleoprotein 200 kDa helicase.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	B	72	Total	C	N	O	0	0
			401	238	86	77		

- Molecule 16 is a protein called Splicing factor 3A subunit 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	7	36	Total	C	N	O	0	0
			219	136	43	40		

- Molecule 17 is INOSITOL HEXAKISPHOSPHATE (three-letter code: IHP) (formula: $C_6H_{18}O_{24}P_6$) (labeled as "Ligand of Interest" by depositor).



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

3 Residue-property plots (i)

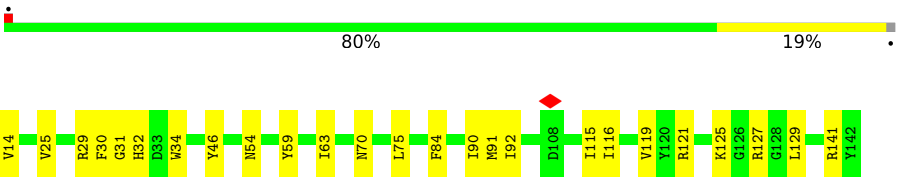
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Probable ATP-dependent RNA helicase DDX23

Chain G:

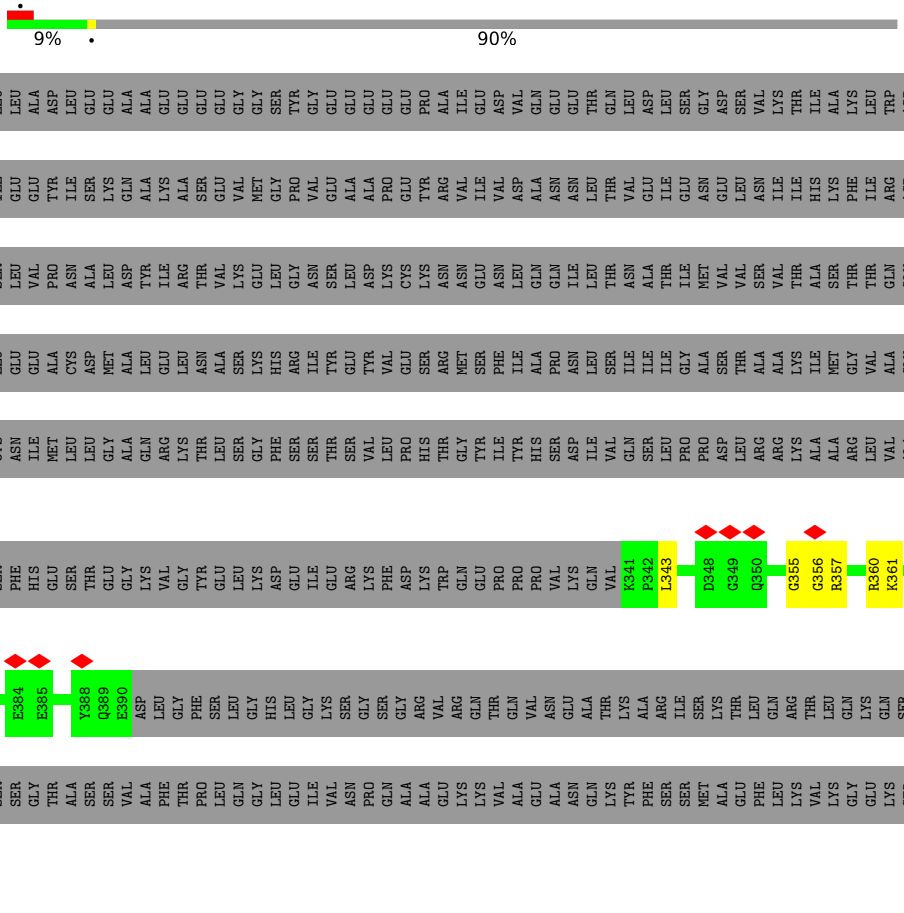
• Molecule 2: Thioredoxin-like protein 4A

Chain D:



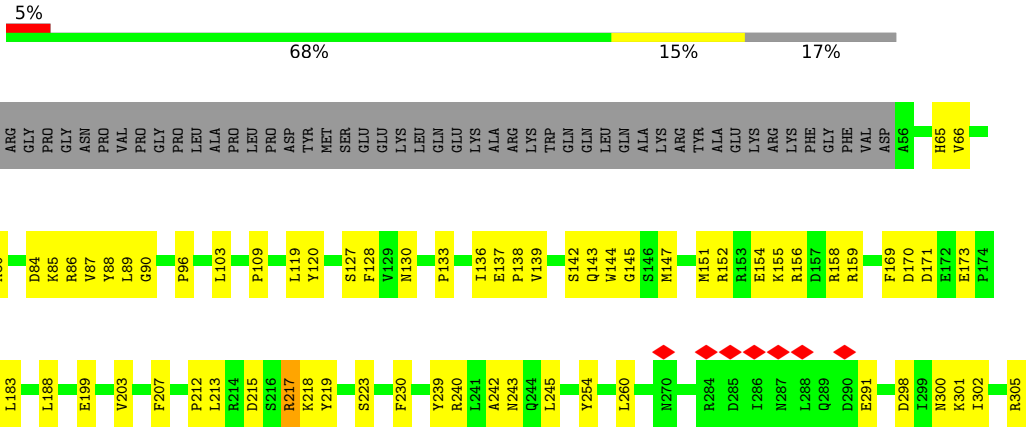
• Molecule 3: U4/U6 small nuclear ribonucleoprotein Prp31

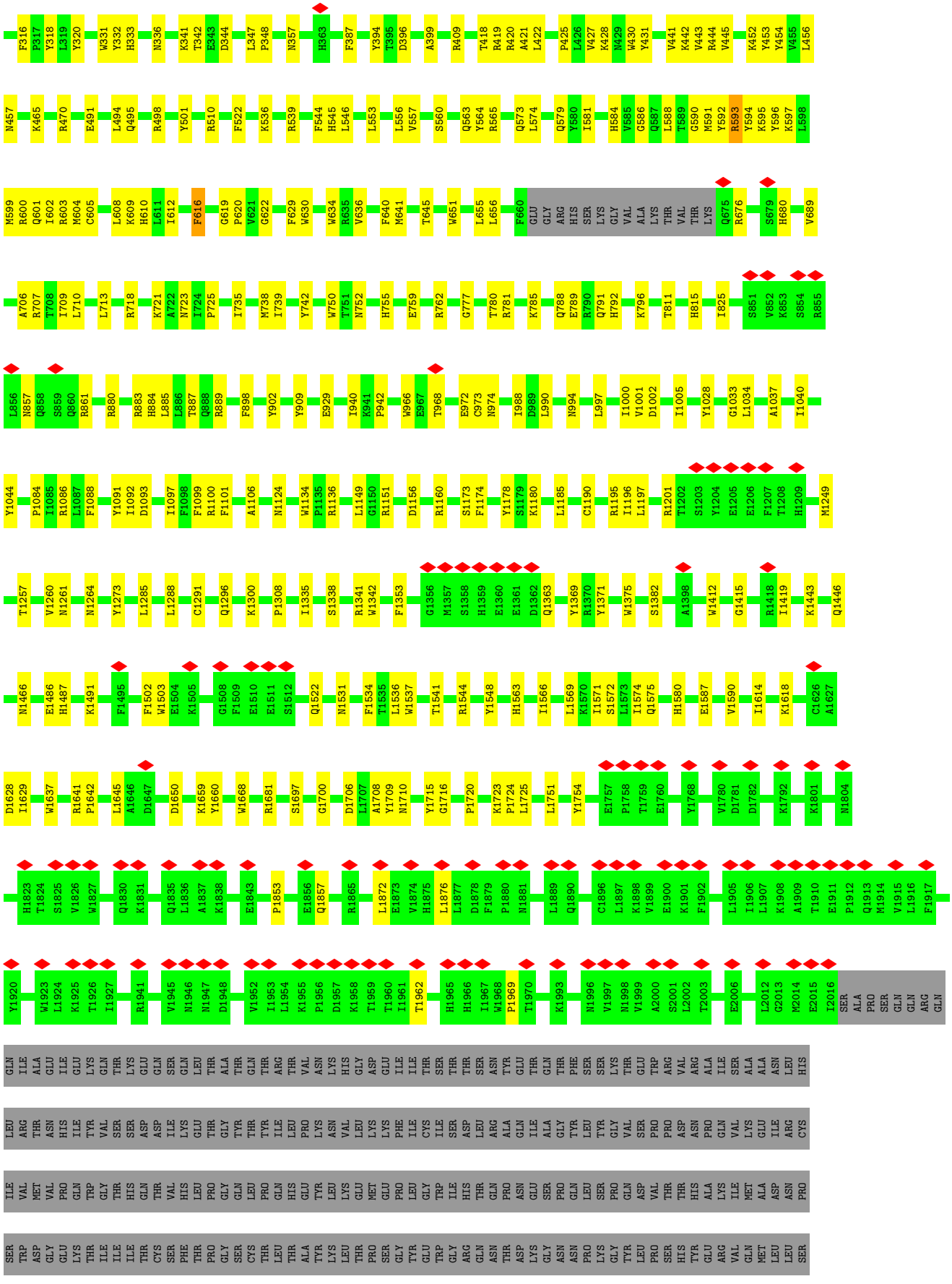
Chain L:



• Molecule 4: Pre-mRNA-processing-splicing factor 8

Chain A:

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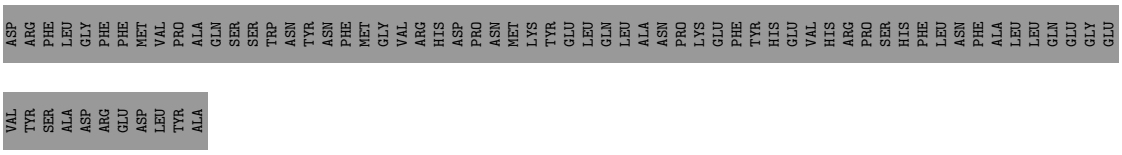
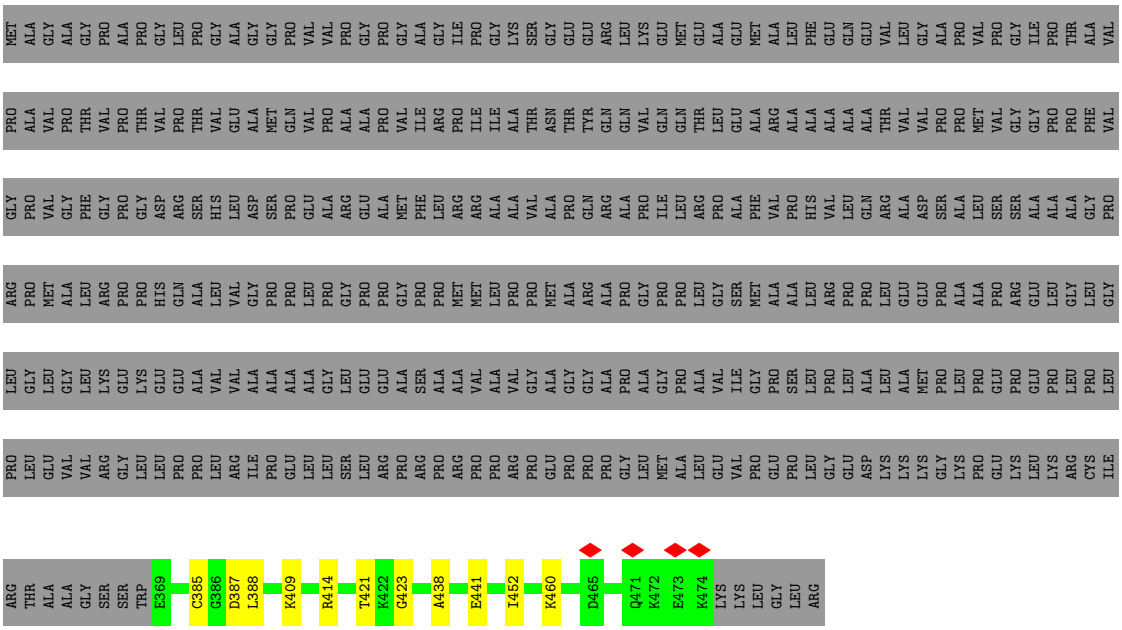
N457 K465 R470 E491 L494 Q495 R498 Y501 R510 F522 K536 R539 N357 F644 H545 L546 L553 L556 V557 S560 Q563 Y564 R565 Q573 L574 Q579 Y580 I581 H584 V585 G586 Q587 L588 T589 G590 M591 Y592 R593 Y594 K595 Y596 K597 L598
M599 R600 Q601 I602 R603 M604 C605 L608 K609 H610 L611 I612 F616 G619 P620 V621 G622 F629 W630 W634 R635 V636 F640 M641 T645 W651 L655 L656 F660 GLU GLY ARG HIS SER LYS GLY VAL ALA LYS THR VAL THR LYS Q675 R676 S679 H680 V689
A706 R707 T708 I709 L710 L713 R718 K721 A722 N723 K724 P725 I735 M738 I739 Y742 W750 T751 N752 H755 E759 R762 G777 T780 R781 K785 Q788 E789 R790 Q791 H792 K796 T811 H815 I825 S851 V852 K853 S854 R855
L856 N857 Q858 S859 Q860 R861 R880 R883 H884 L885 L886 T887 Q888 R889 F898 Y902 Y909 E929 I940 K941 P942 W966 E967 T968 E972 C973 N974 I988 D989 L990 N994 L997 I1000 V1001 D1002 I1005 Y1028 G1033 L1034 A1037 I1040
Y1044 P1084 I1085 R1086 L1087 F1088 Y1091 I1092 D1093 I1097 F1098 F1099 R1100 F1101 A1106 N1124 W1134 P1135 R1136 L1149 G1150 R1151 D1156 R1160 S1173 F1174 Y1178 S1179 K1180 L1185 C1190 R1195 I1196 L1197 R1201 T1202 S1203 Y1204 E1205 E1206 F1207 T1208 H1209 M1249
T1257 V1260 N1261 N1264 Y1273 L1285 L1288 C1291 Q1296 K1300 P1308 I1335 S1338 R1341 W1342 F1353 G1356 M1357 S1358 H1359 E1360 E1361 D1362 Q1363 Y1369 R1370 Y1371 W1375 S1382 A1398 W1412 G1415 R1418 I1419 K1443 Q1446
N1466 E1486 H1487 K1491 F1495 F1502 W1503 E1504 K1505 G1508 F1509 E1510 E1511 S1512 Q1522 N1531 F1534 T1535 L1536 W1537 T1541 R1544 Y1548 H1563 I1566 L1569 K1570 I1571 S1572 L1573 I1574 Q1575 H1580 E1587 V1590 I1614 K1618 C1626 A1627
D1628 I1629 W1637 R1641 P1642 L1645 A1646 D1647 D1650 K1659 Y1660 W1668 R1681 S1697 G1700 D1706 L1707 A1708 Y1709 N1710 Y1715 G1716 P1720 K1723 P1724 L1725 L1751 Y1754 E1757 P1758 T1759 E1760 Y1768 V1780 D1781 D1782 K1792 K1801 N1804
H1823 T1824 S1825 V1826 W1827 Q1830 K1831 Q1835 L1836 A1837 K1838 E1843 P1853 E1856 Q1857 R1865 L1872 E1873 V1874 H1875 L1876 L1877 D1878 F1879 P1880 N1881 L1869 Q1890 C1896 L1897 K1898 V1899 E1900 K1901 F1902 L1905 I1906 L1907 K1908 A1909 T1910 E1911 P1912 Q1913 M1914 V1915 L1916 F1917
Y1920 W1923 L1924 K1925 T1926 I1927 R1941 V1945 N1946 N1947 D1948 V1952 I1953 L1954 K1955 P1956 D1957 K1958 T1959 T1960 I1961 T1962 H1965 H1966 I1967 W1968 P1969 T1970 K1993 N1996 V1997 N1998 V1999 A2000 S2001 L2002 T2003 E2006 L2012 G2013 M2014 E2015 I2016 SER ALA PRO SER GLN GLN ARG GLN
GLN ILE ALA GLU ILE GLU LYS GLN THR LYS GLU GLN SER GLN LEU THR ALA THR GLN THR ARG THR VAL ASN LYS HIS GLY ASP GLU ILE THR SER THR THR SER ASN TYR GLU THR GLN THR PHE SER SER LYS THR GLU TRP ARG VAL ARG ALA ILE SER ASN LEU TYR GLY VAL SER PRO PRO ASP ASN PRO GLN VAL LYS GLU ILE ARG CYS
LEU ARG THR ASN HIS ILE TYR VAL SER SER ASP ASP ILE LYS GLU THR GLY TYR THR TYR ILE LEU PRO LYS ASN VAL LEU LYS LYS PHE ILE CYS ILE SER ASP LEU ARG ALA GLN ILE ALA GLY TYR LEU TYR GLY VAL SER PRO PRO ASP ASN PRO GLN VAL LYS GLU ILE ARG CYS
ILE VAL MET VAL PRO GLN TRP GLY THR HIS GLN THR VAL HIS LEU PRO GLY GLN LEU PRO GLN HIS GLU TYR LEU LYS GLU MET GLU PRO LEU GLY TRP ILE HIS THR GLN PRO ASN GLU SER PRO GLN LEU SER PRO GLN ASP VAL THR THR HIS ALA LYS ILE MET ALA ASP ASN PRO
SER TRP ASP GLY GLU LYS THR ILE ILE THR CYS SER PHE THR PRO GLY SER CYS THR LEU THR ALA TYR LYS LEU THR PRO SER GLY TYR GLU TRP GLY ARG GLN ASN THR ASP LYS GLY ASN ASN PRO LYS GLY TYR LEU PRO SER HIS TYR GLU ARG VAL GLN MET LEU SER



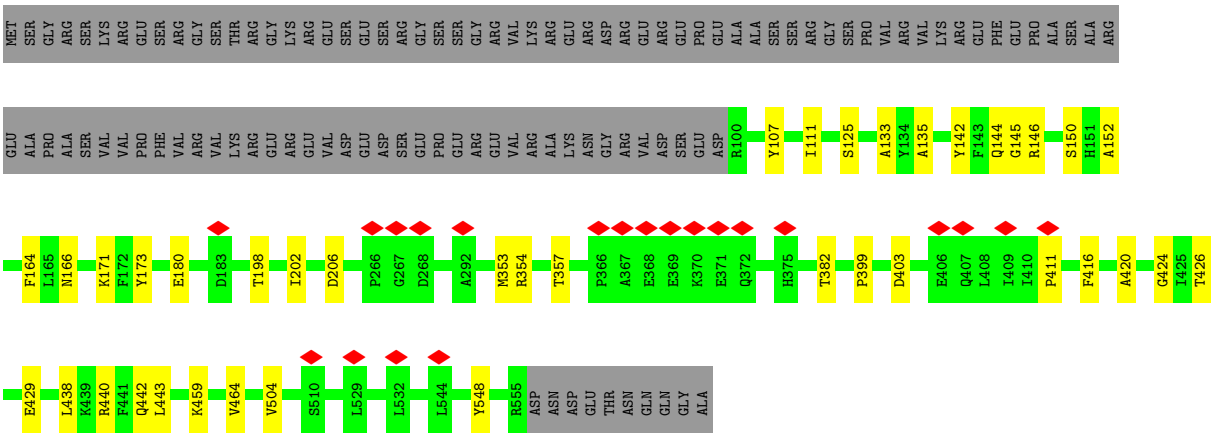
• Molecule 5: RNA-binding protein 42

Chain R:



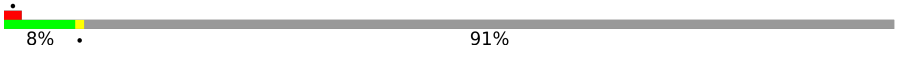
• Molecule 6: Ubiquitin carboxyl-terminal hydrolase 39

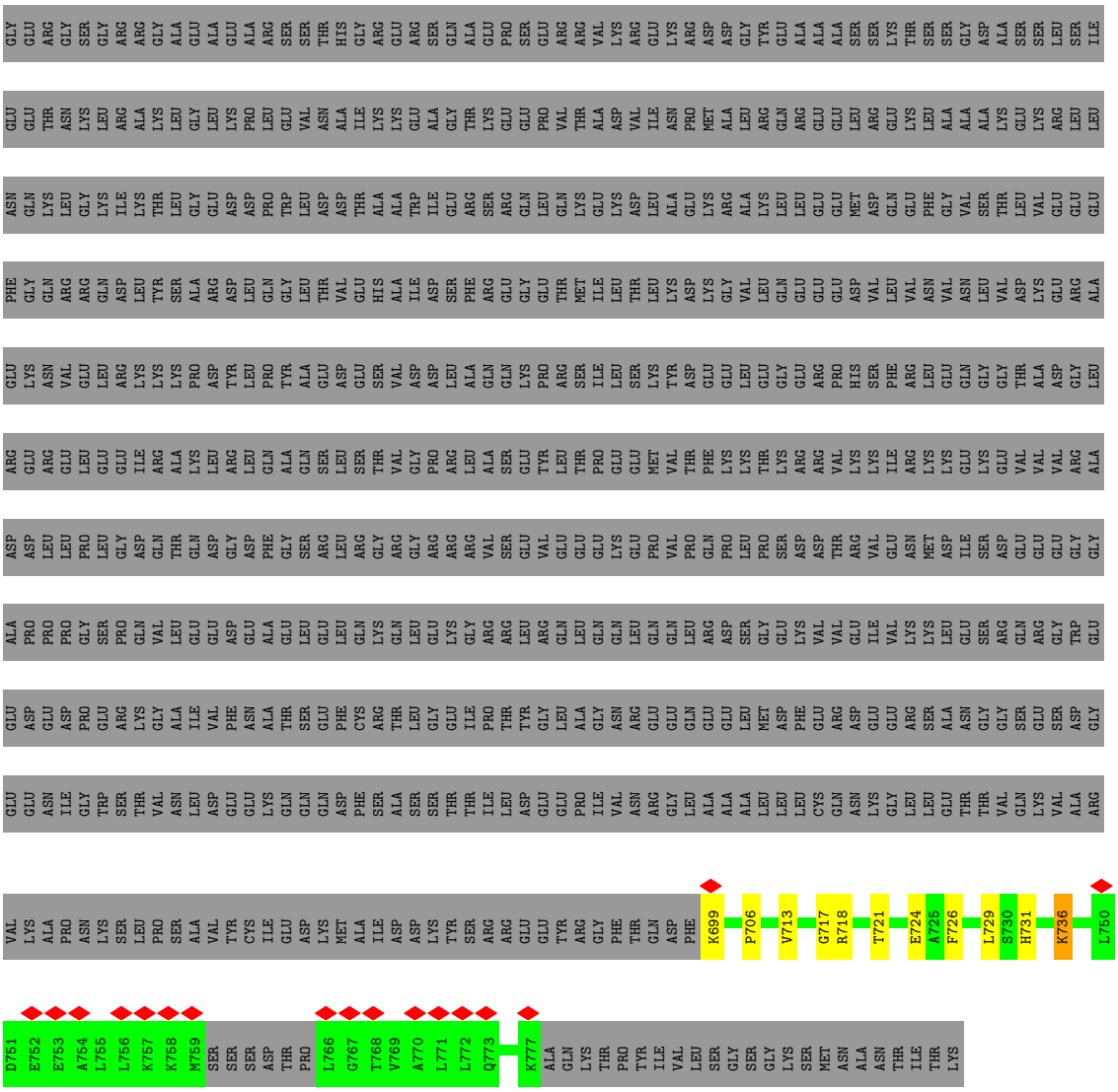
Chain U:



• Molecule 7: U4/U6.U5 tri-snRNP-associated protein 1

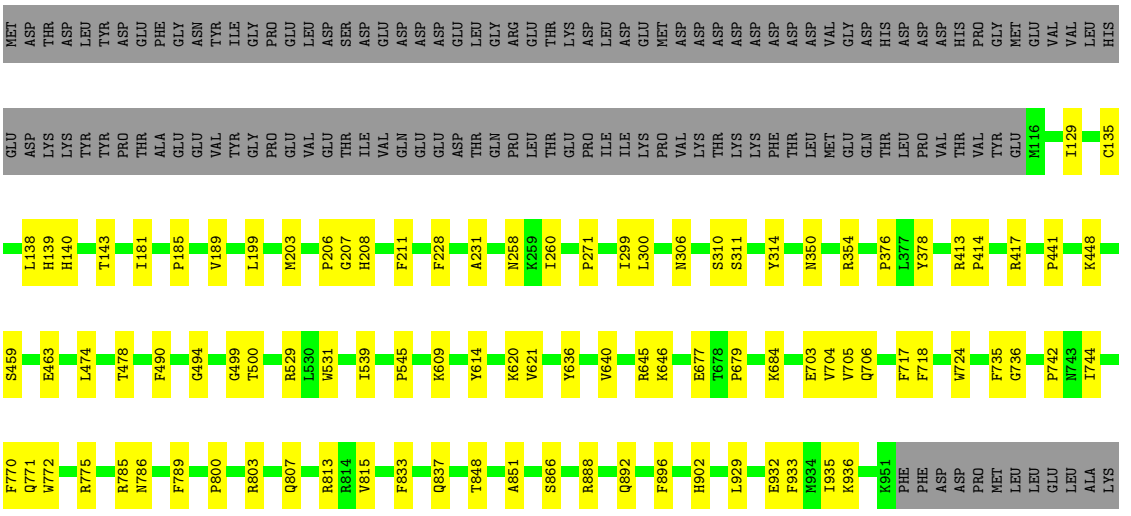
Chain S:

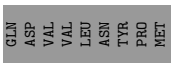




• Molecule 8: 116 kDa U5 small nuclear ribonucleoprotein component

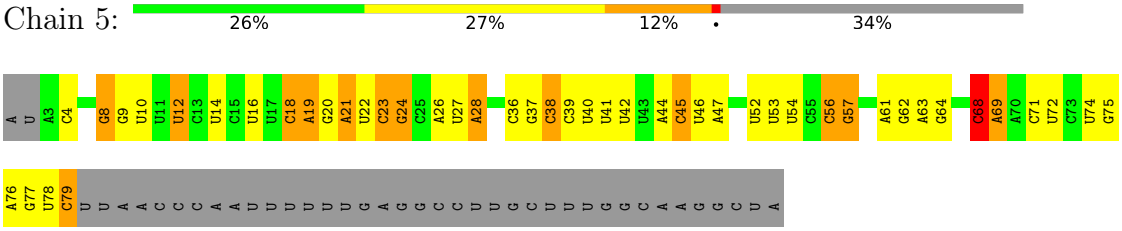
Chain C:





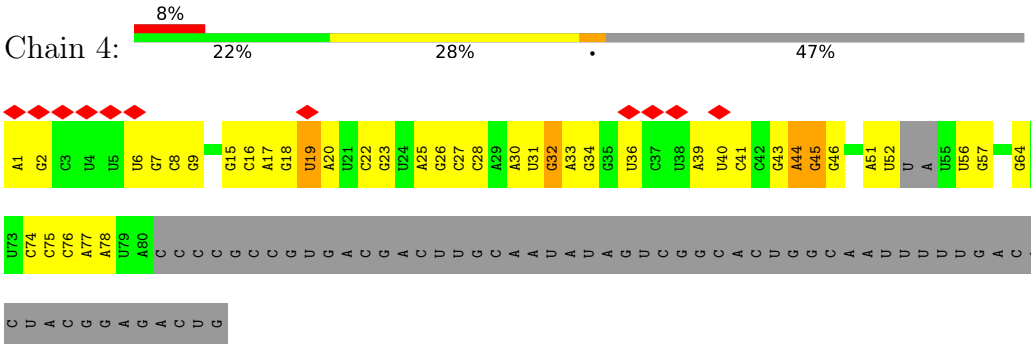
• Molecule 9: U5 snRNA

Chain 5:



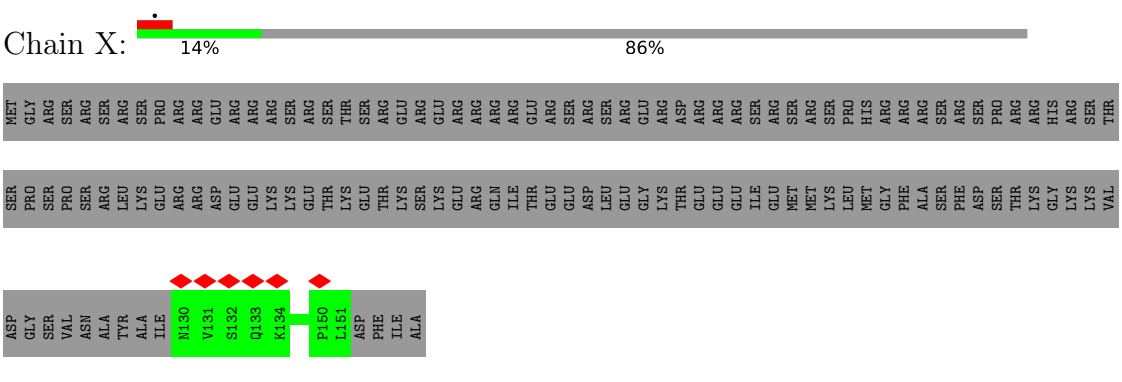
• Molecule 10: U4 snRNA

Chain 4:



• Molecule 11: U4/U6.U5 small nuclear ribonucleoprotein 27 kDa protein

Chain X:

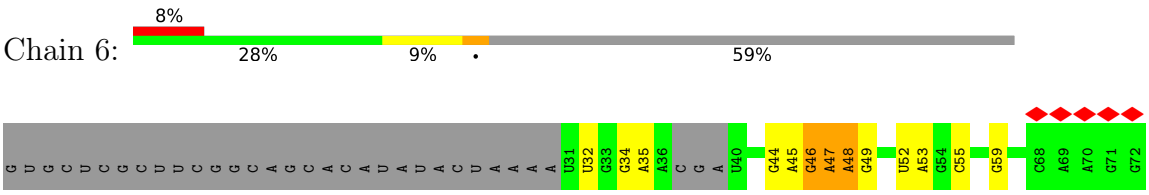


• Molecule 12: 5'ss oligo

Chain z:

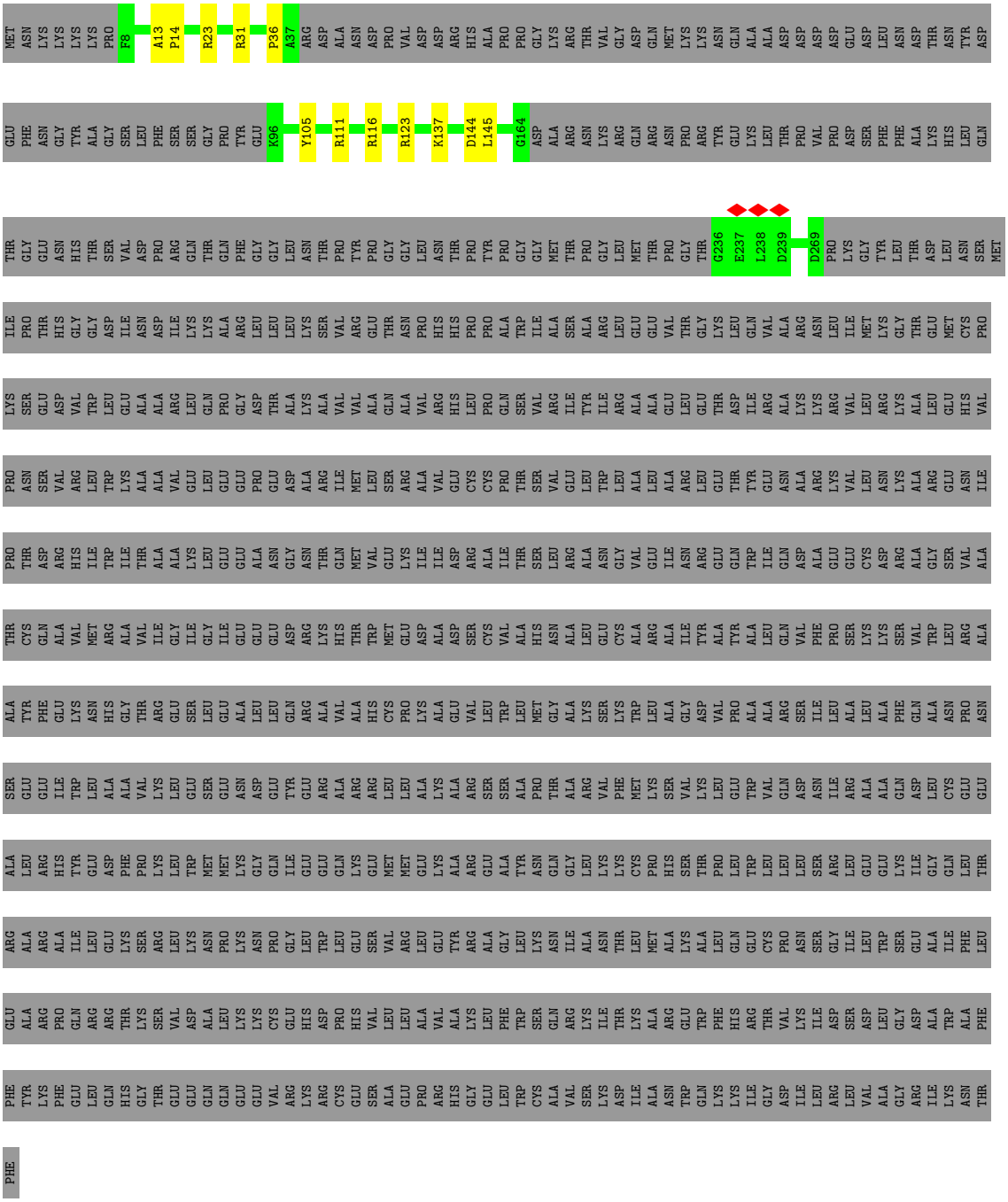
• Molecule 13: U6 snRNA

Chain 6:



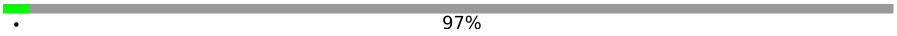
• Molecule 14: Pre-mRNA-processing factor 6

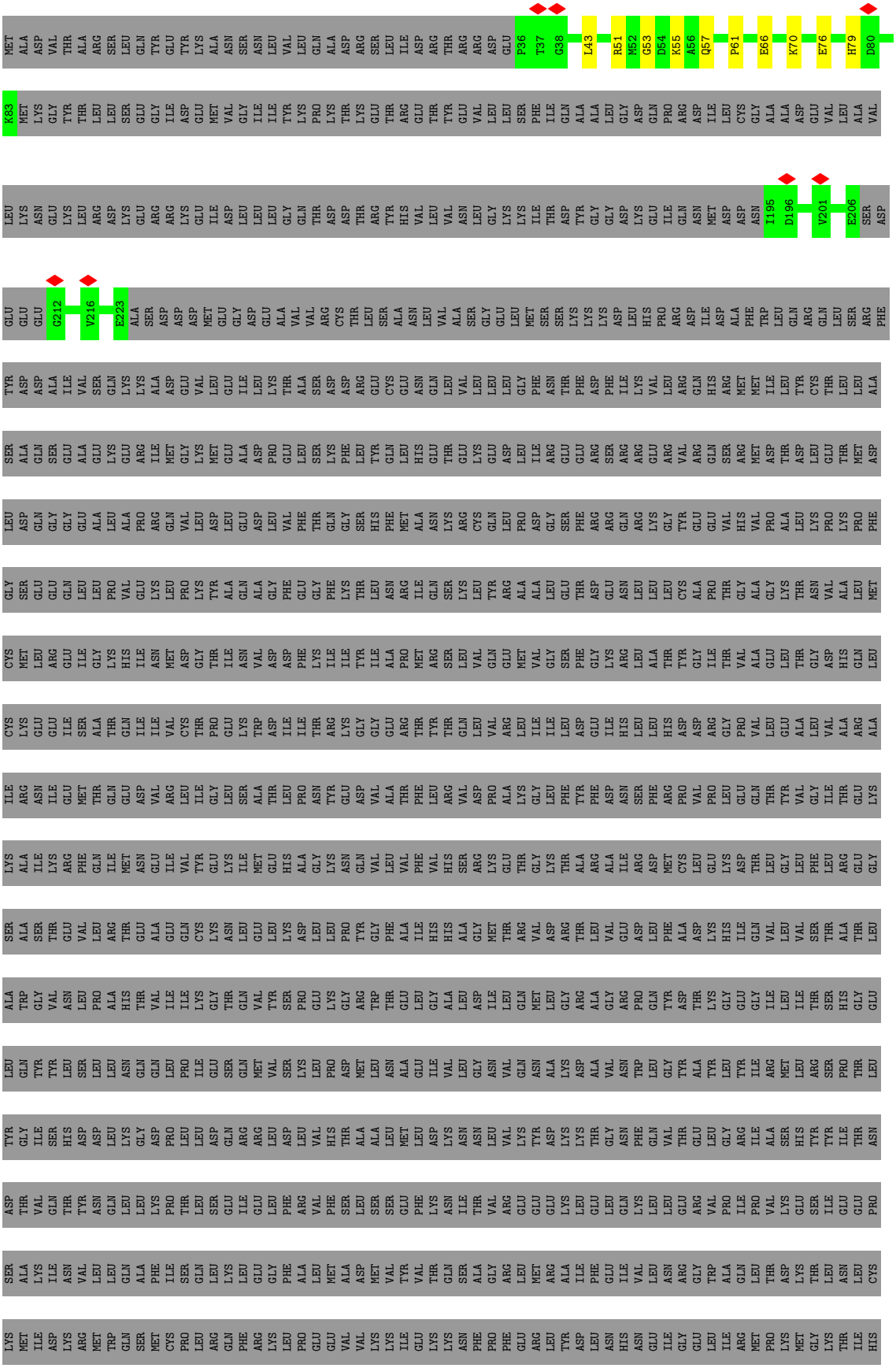
Chain N:

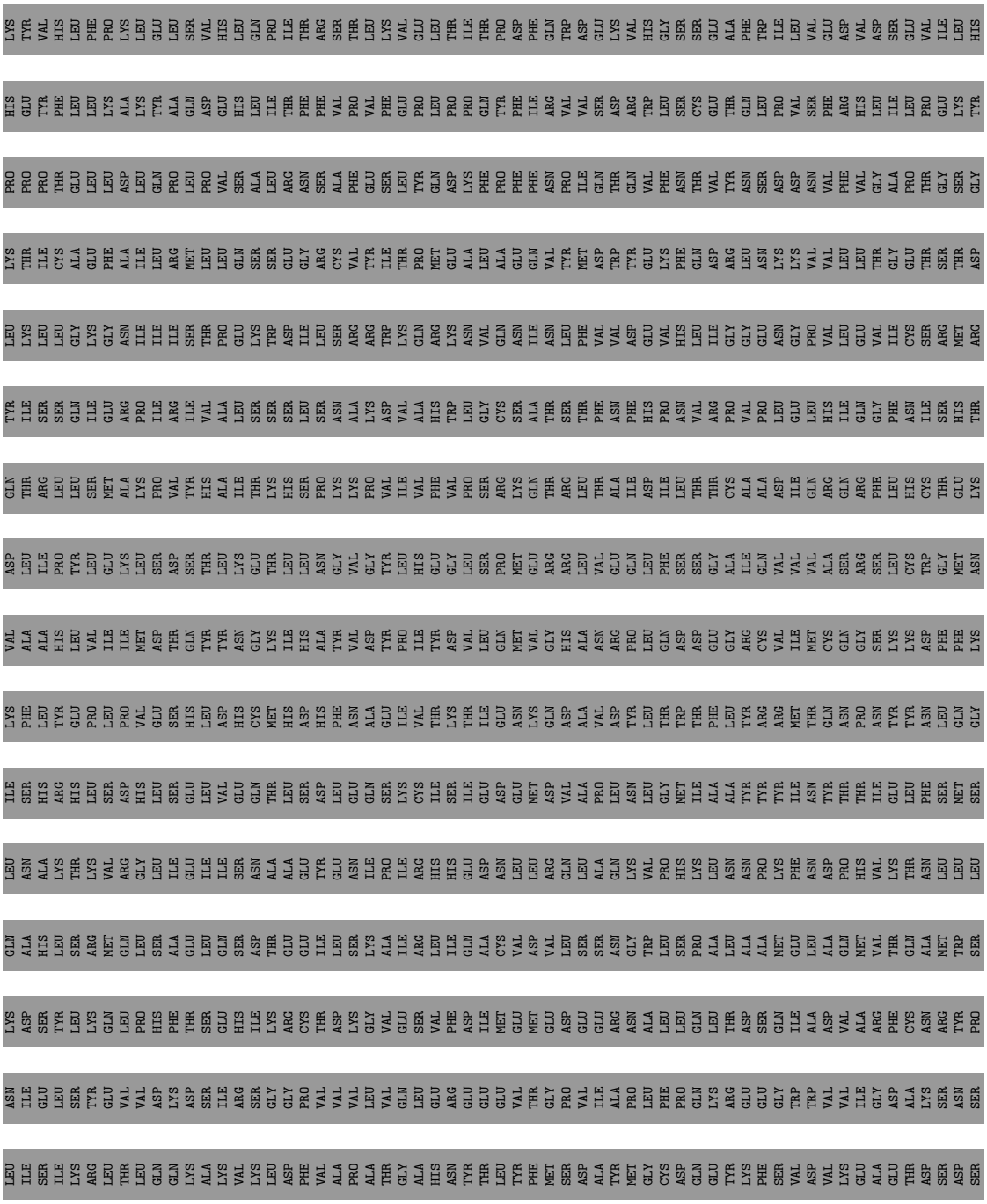


• Molecule 15: U5 small nuclear ribonucleoprotein 200 kDa helicase

Chain B:

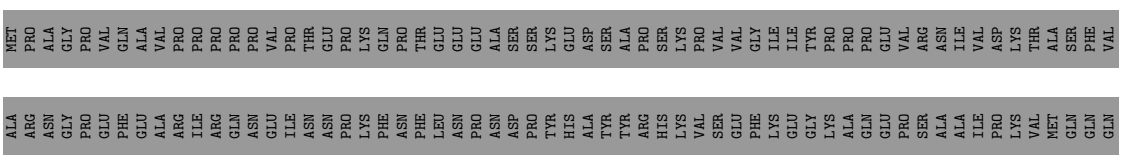


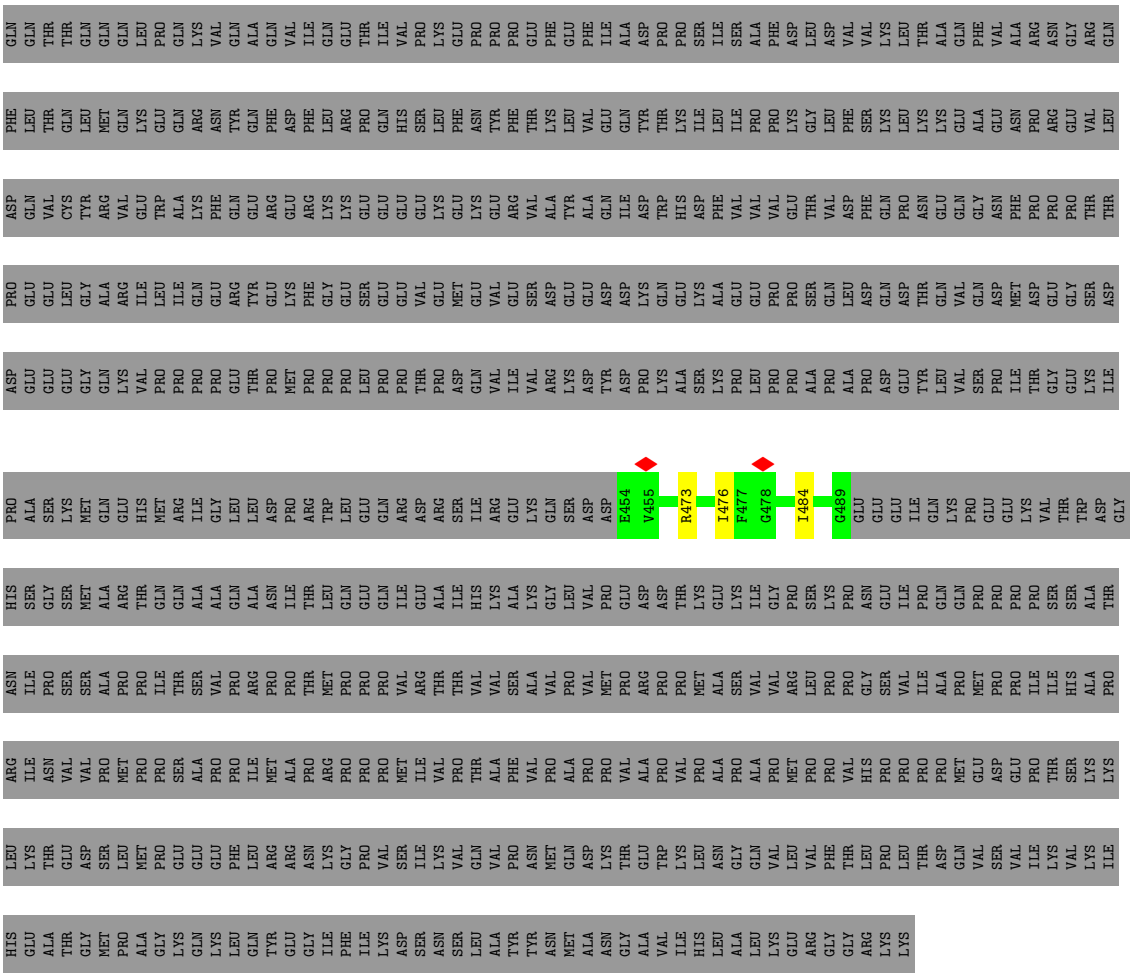

MET ALA ASP VAL THR ALA ARG SER LEU GLN TYR GLU TYR LYS ALA ASN SER ASN LEU VAL LEU GLN ALA ASP ARG SER LEU ILE ASP ARG ARG ARG ASP GLU P36 T37 G38 L43 R51 M52 G53 D54 K55 A56 Q57 P61 E66 K70 E76 H79 D80
K83 MET LYS GLY TYR THR LEU LEU SER GLU GLY ILE ASP GLU MET VAL GLY ILE ILE TYR LYS PRO LYS THR LYS GLU GLU THR TYR GLU VAL LEU LEU SER PHE ILE GLN ALA ALA LEU GLY ASP GLN PRO ARG ASP ILE LEU CYS GLY ALA ALA ASP GLU VAL LEU ALA VAL
LEU LYS ASN GLU LYS LEU ARG ASP LYS GLU ARG ARG LYS GLU ILE ASP LEU LEU LEU LEU GLY GLN THR ASP ASP THR ARG TYR HIS VAL LEU VAL ASN LEU GLY LYS LYS ILE THR ASP TYR GLY GLY ASP LYS GLU ILE GLN ASN MET ASP ASP ASN I195 D196 V201 E205 SER ASP
GLU GLU GLU G212 V216 E223 ALA SER ASP ASP MET GLU GLY ASP GLU ALA VAL ARG CYS THR LEU SER ALA ASN ASN LEU VAL ALA SER GLY GLU LEU MET SER SER LYS LYS LYS ASP LEU HIS PRO ARG ASP ILE ASP ALA PHE TRP LEU GLN ARG GLN LEU SER ARG PHE
TYR ASP ASP ALA ILE VAL SER GLN LYS LYS ALA ASP GLU VAL LEU GLU ILE LEU LYS THR ALA SER ASP ASP ARG GLU CYS GLU ASN GLN LEU VAL LEU LEU LEU GLY PHE ASN THR PHE ASP PHE ILE LYS VAL LEU ARG GLN HIS ARG MET MET ILE LEU TYR CYS THR LEU LEU ALA
SER ALA GLN SER GLU ALA GLU LYS GLU ARG ILE MET GLY LYS MET GLU ALA ASP PRO GLU GLU LEU SER LYS PHE LEU TYR GLN LEU HIS GLU THR GLU LYS GLU ASP LEU ILE ARG GLU GLU ARG SER ARG GLU ARG VAL ARG GLN SER ARG MET ASP THR ASP LEU GLU THR MET ASP
LEU ASP GLN GLY GLY GLU ALA LEU GLU ALA ASP LEU VAL LEU ASP LEU GLU GLU ALA ASP PRO ARG GLN VAL LEU ALA PRO ARG GLN VAL LEU ASP LEU GLU GLU ASP LEU VAL PHE THR GLN GLY SER HIS PHE MET ALA ASN LYS ARG CYS GLN LEU PRO ASP GLY SER PHE ARG ARG GLN ARG LYS GLY TYR GLU GLU VAL HIS VAL PRO ALA LEU LYS PRO LYS PRO PHE
GLY SER GLU GLU GLN LEU LEU PRO VAL GLU LYS LEU PRO LYS TYR ALA GLN ALA GLY PHE GLU GLY PHE LYS THR LEU ASN ARG ILE GLN SER LYS LEU TYR ARG ALA ALA LEU GLU THR ASP GLU ASN LEU LEU LEU CYS ALA PRO THR GLY ALA ALA GLY LYS THR ASN VAL ALA PRO MET
CYS MET LEU ARG GLU ILE GLY LYS HIS ILE ASN MET ASP GLY THR ILE ASN VAL ASP ASP PHE LYS ILE ILE TYR ILE ALA PRO MET ARG SER LEU VAL GLN GLU MET VAL GLY SER PHE GLY LYS ARG LEU ALA THR TYR GLY ILE THR VAL ALA GLU GLY LEU THR GLY ASP HIS GLN LEU
CYS LYS GLU GLU ILE SER ALA THR GLN ILE ILE VAL CYS THR PRO GLU LYS TRP ASP ILE ILE THR ARG LYS GLY GLY GLU ARG THR TYR THR GLN LEU VAL ARG LEU ILE ILE LEU LEU ASP GLU ILE HIS LEU LEU HIS ASP ASP ARG GLY PRO VAL LEU LEU GLU ALA LEU VAL ALA ARG ALA
ILE ARG ASN ILE GLU MET THR GLN GLU ASP VAL ARG LEU ILE THR LEU PRO ASN TYR GLU ASP VAL ALA THR PHE LEU ARG VAL ASP PRO ALA LYS GLY LEU PHE TYR PHE ASP ASN SER PHE ARG PRO VAL PRO LEU GLU GLU GLN THR TYR VAL GLY ILE THR GLU GLU LYS
LYS ALA ILE LYS ARG PHE GLN ILE MET ASN GLU ILE VAL TYR GLU LYS ILE MET GLU HIS ALA GLY LYS ASN GLN VAL LEU VAL PHE VAL HIS SER ARG LYS GLU THR GLY LYS THR ALA ARG ALA ILE ARG ASP MET CYS LEU GLU LYS ASP THR LEU GLU GLU GLY LEU PHE LEU ARG GLU GLY
SER ALA SER THR GLU VAL LEU LEU GLU ALA GLU GLN CYS LYS ASN LEU GLU LEU LYS ASP LEU PRO TYR GLY PHE ALA ILE HIS HIS ALA LEU GLY MET THR ARG VAL ASP ARG THR LEU VAL LEU GLU ASP LEU PHE ALA ALA ASP LYS HIS ILE GLN VAL LEU VAL SER THR ALA THR LEU
ALA TRP GLY VAL ASN LEU PRO ALA HIS THR VAL ILE ILE LYS GLY THR GLN VAL TYR SER PRO GLU LYS GLY ARG TRP THR GLU LEU GLY ALA LEU ASP ILE LEU GLN MET LEU GLY ARG ALA GLY ARG PRO GLN TYR ASP THR LYS GLY GLU GLY ILE LEU LEU ILE THR SER HIS GLY GLU
LEU GLN TYR TYR LEU SER GLN GLN LEU PRO ILE GLU SER GLN MET VAL SER LYS LEU PRO ASP MET LEU ASN ALA GLU ILE LEU VAL LEU GLN GLY ASN VAL GLN ASN ALA LYS ASP ALA VAL ASN TRP LEU GLY TYR ALA TYR LEU GLY TYR ILE ARG MET LEU ARG SER PRO THR LEU
TYR GLY ILE SER HIS ASP ASP LEU LYS GLY ASP PRO LEU LEU ASP GLN ARG ARG LEU ASP LEU ASP VAL HIS THR ALA ALA LEU MET LEU ASP LYS ASN ASN ILE VAL LEU GLY ASP PRO GLY LYS TYR ASP LYS LYS THR GLY ASN PHE GLN VAL THR GLU LEU GLY GLY ARG ILE ALA SER HIS TYR TYR ILE THR ASN
ASP THR VAL GLN LEU LEU LYS PRO THR LEU SER GLU ILE GLU LEU PHE ARG VAL PHE SER LEU SER SER GLU PHE LYS ASN ILE THR VAL ARG GLU GLU GLU LEU GLN LYS LYS LEU GLU GLU LEU GLN LYS VAL PRO ILE PRO VAL LYS GLU SER ILE GLU GLU PRO
SER ALA LYS ILE ASN VAL LEU LEU GLN ALA PHE ILE SER GLN LEU LYS LEU GLU GLY PHE ALA LEU MET ALA ASP MET VAL TYR VAL THR GLN SER ILE ALA GLY ARG LEU MET ARG GLU ASP ILE ALA ILE PHE GLU ILE ASN ARG GLY TRP ASP LYS SER THR LEU ASN LEU CYS
LYS MET ILE ASP LYS ARG MET TRP GLN PHE ARG LYS LEU PRO GLU VAL VAL LYS LYS ILE GLU LYS LYS ASN PHE PRO GLU ARG LEU TYR ASP LEU ASN HIS ASN GLU ILE GLY GLU LEU ILE ARG MET PRO LYS MET GLY LYS THR ILE HIS



• Molecule 16: Splicing factor 3A subunit 1

Chain 7: 95%




E454
V455
R473
I476
F477
G478
I484
G489

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	176879	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	45	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.096	Depositor
Minimum map value	-0.044	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0165	Depositor
Map size (Å)	580.0, 580.0, 580.0	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.16, 1.16, 1.16	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: IHP

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	G	0.25	0/667	0.45	0/906
2	D	0.25	0/1032	0.47	0/1409
3	L	0.23	0/253	0.35	0/352
4	A	0.25	0/13400	0.46	0/18475
5	R	0.24	0/668	0.44	0/913
6	U	0.23	0/2343	0.41	0/3285
7	S	0.24	0/450	0.46	0/610
8	C	0.25	0/5286	0.45	0/7297
9	5	0.15	0/1806	0.75	5/2807 (0.2%)
10	4	0.12	0/1805	0.66	0/2805
11	X	0.23	0/126	0.42	0/174
12	z	0.16	0/268	0.73	0/416
13	6	0.12	0/1038	0.65	0/1615
14	N	0.24	0/794	0.43	0/1086
15	B	0.23	0/401	0.49	0/544
16	7	0.23	0/220	0.47	0/300
All	All	0.23	0/30557	0.50	5/42994 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	5	68	C	N1-C2-O2	8.08	123.75	118.90
9	5	68	C	C2-N1-C1'	7.69	127.26	118.80
9	5	68	C	N3-C2-O2	-6.50	117.35	121.90
9	5	68	C	C6-N1-C1'	-5.26	114.49	120.80
9	5	68	C	C6-N1-C2	-5.22	118.21	120.30

There are no chirality outliers.

There are no planarity outliers.

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	G	658	0	505	11	0
2	D	1008	0	877	19	0
3	L	251	0	128	6	0
4	A	13055	0	10358	256	0
5	R	659	0	511	7	0
6	U	2320	0	1124	24	0
7	S	446	0	330	7	0
8	C	5163	0	3686	63	0
9	5	1620	0	822	30	0
10	4	1617	0	819	30	0
11	X	124	0	64	0	0
12	z	239	0	119	0	0
13	6	927	0	467	14	0
14	N	784	0	517	12	0
15	B	401	0	244	13	0
16	7	219	0	171	2	0
17	A	36	0	6	0	0
All	All	29527	0	20748	432	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 9.

All (432) 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)
6:U:164:PHE:H	6:U:173:TYR:H	1.29	0.81
4:A:1536:LEU:HD22	4:A:1572:SER:HB3	1.64	0.77
4:A:1571:ILE:HD12	4:A:1574:ILE:HD11	1.70	0.73
4:A:136:ILE:HG13	4:A:418:THR:HG22	1.69	0.73
4:A:596:TYR:HE1	9:5:46:U:H5'	1.54	0.73
4:A:545:HIS:CE1	4:A:593:ARG:HE	2.07	0.72
5:R:387:ASP:H	10:4:68:A:H61	1.38	0.71
8:C:478:THR:HA	8:C:494:GLY:HA3	1.73	0.70
7:S:731:HIS:HE1	10:4:66:A:H5'	1.56	0.70
1:G:301:ARG:HD3	4:A:341:LYS:HB3	1.72	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:443:VAL:N	4:A:610:HIS:HE1	1.90	0.69
4:A:604:MET:SD	4:A:636:VAL:HG11	2.32	0.69
5:R:385:CYS:HB3	5:R:452:ILE:HD11	1.74	0.68
4:A:545:HIS:HE1	4:A:593:ARG:HE	1.41	0.68
4:A:601:GLN:HB2	4:A:640:PHE:CE2	2.29	0.68
8:C:350:ASN:O	8:C:354:ARG:N	2.27	0.68
4:A:1706:ASP:O	4:A:1710:ASN:N	2.26	0.68
4:A:154:GLU:OE2	4:A:158:ARG:NH2	2.27	0.68
9:5:19:A:N3	9:5:21:A:N6	2.42	0.67
2:D:70:ASN:HA	2:D:75:LEU:HB2	1.76	0.67
4:A:1185:LEU:HB2	4:A:1196:ILE:HG22	1.78	0.66
4:A:84:ASP:HB3	4:A:88:TYR:HB2	1.78	0.66
4:A:305:ARG:HH22	8:C:929:LEU:HD22	1.60	0.66
8:C:208:HIS:HB3	8:C:211:PHE:HB2	1.76	0.66
9:5:16:U:OP1	14:N:111:ARG:NH1	2.30	0.65
4:A:155:LYS:HG2	4:A:622:GLY:H	1.61	0.65
4:A:89:LEU:HD21	4:A:656:LEU:HA	1.79	0.65
4:A:825:ILE:HD12	4:A:929:GLU:HB3	1.79	0.65
4:A:425:PRO:HB2	4:A:428:LYS:HB2	1.77	0.64
4:A:75:ASP:HA	4:A:498:ARG:HH21	1.62	0.64
9:5:23:C:O2'	9:5:57:G:N2	2.27	0.64
4:A:1614:ILE:HD11	4:A:1628:ASP:HA	1.78	0.64
7:S:713:VAL:HG13	7:S:717:GLY:HA2	1.78	0.64
4:A:199:GLU:OE1	4:A:240:ARG:NH1	2.30	0.63
5:R:438:ALA:HA	5:R:441:GLU:HB3	1.80	0.63
4:A:596:TYR:CE1	9:5:46:U:H5'	2.34	0.63
8:C:679:PRO:HD2	8:C:807:GLN:HB3	1.81	0.63
6:U:504:VAL:HA	6:U:548:TYR:H	1.64	0.62
4:A:136:ILE:HG22	4:A:138:PRO:HD2	1.82	0.62
4:A:723:ASN:ND2	4:A:788:GLN:OE1	2.32	0.62
4:A:706:ALA:O	4:A:709:ILE:HB	2.00	0.62
4:A:1273:TYR:O	4:A:1375:TRP:NE1	2.31	0.62
4:A:825:ILE:HB	4:A:1001:VAL:HG23	1.82	0.61
4:A:1124:ASN:O	4:A:1151:ARG:NH1	2.33	0.61
4:A:70:ILE:HG12	4:A:495:GLN:HE22	1.65	0.61
8:C:314:TYR:HB3	8:C:417:ARG:HA	1.81	0.61
4:A:940:ILE:HG22	4:A:942:PRO:HD2	1.82	0.61
8:C:704:VAL:HG12	8:C:705:VAL:HG23	1.83	0.60
4:A:1084:PRO:HB3	4:A:1101:PHE:HE1	1.66	0.60
6:U:173:TYR:HA	6:U:180:GLU:HA	1.82	0.60
4:A:1486:GLU:O	4:A:1491:LYS:NZ	2.33	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:54:ASN:ND2	3:L:343:LEU:O	2.35	0.60
4:A:1415:GLY:HA3	4:A:1419:ILE:HD12	1.83	0.60
9:5:77:G:OP2	9:5:79:C:N4	2.33	0.60
4:A:988:ILE:HD12	4:A:1044:TYR:HE2	1.67	0.59
4:A:1300:LYS:HD2	4:A:1308:PRO:HG2	1.84	0.59
4:A:1580:HIS:NE2	13:6:44:G:OP2	2.35	0.59
4:A:880:ARG:O	4:A:884:HIS:ND1	2.34	0.59
4:A:336:ASN:OD1	8:C:837:GLN:NE2	2.32	0.59
9:5:18:C:HO2'	9:5:19:A:H8	1.49	0.59
8:C:837:GLN:HE21	8:C:896:PHE:HB3	1.66	0.59
4:A:1534:PHE:HA	4:A:1537:TRP:HB3	1.84	0.59
4:A:239:TYR:O	4:A:243:ASN:ND2	2.36	0.59
4:A:178:TYR:HA	4:A:182:ILE:HD13	1.85	0.58
4:A:710:LEU:O	4:A:713:LEU:HB2	2.02	0.58
4:A:1338:SER:HA	4:A:1341:ARG:HH21	1.68	0.58
9:5:21:A:H2'	9:5:23:C:H5"	1.85	0.58
4:A:539:ARG:HB3	14:N:31:ARG:HG3	1.84	0.58
4:A:103:LEU:O	4:A:634:TRP:NE1	2.32	0.58
2:D:90:ILE:HD13	2:D:119:VAL:HG13	1.86	0.58
4:A:710:LEU:HA	4:A:713:LEU:HD12	1.84	0.58
2:D:125:LYS:HG2	2:D:127:ARG:HH21	1.69	0.58
4:A:219:TYR:HB3	4:A:230:PHE:HE1	1.69	0.57
4:A:564:TYR:CG	4:A:574:LEU:HD22	2.40	0.57
1:G:245:LYS:HA	1:G:248:HIS:CD2	2.40	0.57
4:A:909:TYR:HB2	4:A:1033:GLY:HA3	1.87	0.57
2:D:5:LEU:HD11	2:D:46:TYR:HB2	1.87	0.56
2:D:84:PHE:HE2	14:N:23:ARG:HD2	1.71	0.56
4:A:1260:VAL:O	4:A:1264:ASN:ND2	2.39	0.56
4:A:143:GLN:O	4:A:147:MET:HG2	2.06	0.56
4:A:1491:LYS:HG3	4:A:1709:TYR:HA	1.88	0.56
4:A:1382:SER:HA	4:A:1415:GLY:HA2	1.88	0.56
4:A:1531:ASN:HA	4:A:1534:PHE:CE1	2.41	0.56
4:A:557:VAL:HG22	4:A:581:ILE:HD12	1.88	0.55
8:C:185:PRO:HA	8:C:203:MET:HA	1.86	0.55
9:5:36:C:H2'	9:5:37:G:H8	1.71	0.55
10:4:64:G:H22	10:4:67:A:H5'	1.71	0.55
4:A:811:THR:O	4:A:815:HIS:ND1	2.39	0.55
4:A:1466:ASN:ND2	15:B:57:GLN:O	2.40	0.55
4:A:599:MET:SD	4:A:603:ARG:HD2	2.46	0.55
4:A:1725:LEU:HA	7:S:706:PRO:HG3	1.89	0.55
9:5:74:U:H2'	9:5:75:G:C8	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:4:74:C:N4	13:6:34:G:O6	2.39	0.55
4:A:342:THR:HG21	4:A:399:ALA:HB1	1.89	0.55
8:C:211:PHE:HE1	8:C:636:TYR:HA	1.71	0.55
4:A:357:ASN:ND2	8:C:866:SER:O	2.40	0.55
10:4:78:A:N6	13:6:32:U:O4	2.38	0.55
4:A:212:PRO:HB2	4:A:213:LEU:HD12	1.87	0.55
4:A:1190:CYS:O	4:A:1273:TYR:OH	2.24	0.55
4:A:223:SER:OG	9:5:12:U:O5'	2.24	0.55
4:A:156:ARG:HD2	4:A:620:PRO:HG2	1.89	0.54
4:A:966:TRP:O	4:A:1178:TYR:OH	2.22	0.54
4:A:441:VAL:HG13	4:A:444:ARG:HH21	1.71	0.54
1:G:245:LYS:HA	1:G:248:HIS:NE2	2.21	0.54
4:A:902:TYR:OH	4:A:1249:MET:SD	2.64	0.54
8:C:677:GLU:HA	8:C:684:LYS:HA	1.90	0.54
4:A:546:LEU:HD11	4:A:595:LYS:HB2	1.90	0.54
4:A:942:PRO:HD3	4:A:1091:TYR:HA	1.89	0.54
7:S:736:LYS:NZ	10:4:66:A:O2'	2.40	0.54
6:U:198:THR:O	6:U:202:ILE:N	2.39	0.54
3:L:355:GLY:O	13:6:55:C:N4	2.34	0.54
4:A:725:PRO:HB3	6:U:403:ASP:HA	1.90	0.54
4:A:1084:PRO:O	4:A:1086:ARG:NH1	2.41	0.54
4:A:1659:LYS:HB2	4:A:1697:SER:HB3	1.88	0.54
6:U:125:SER:N	6:U:142:TYR:O	2.41	0.54
4:A:318:TYR:O	8:C:645:ARG:NH1	2.41	0.53
4:A:605:CYS:O	4:A:608:LEU:HG	2.08	0.53
4:A:1566:ILE:HG21	4:A:1569:LEU:HD23	1.90	0.53
8:C:789:PHE:HZ	8:C:815:VAL:HG12	1.73	0.53
4:A:1308:PRO:HG3	4:A:1548:TYR:CZ	2.44	0.53
4:A:302:ILE:O	8:C:936:LYS:NZ	2.42	0.52
4:A:689:VAL:HG21	4:A:742:TYR:CD1	2.44	0.52
8:C:703:GLU:O	8:C:706:GLN:NE2	2.42	0.52
1:G:276:TRP:HA	4:A:603:ARG:HH21	1.74	0.52
4:A:601:GLN:O	4:A:604:MET:HG3	2.10	0.52
7:S:721:THR:HG23	7:S:724:GLU:H	1.75	0.52
4:A:453:TYR:HE1	4:A:600:ARG:CD	2.23	0.52
4:A:600:ARG:O	4:A:603:ARG:HG2	2.10	0.52
4:A:1502:PHE:O	4:A:1754:TYR:N	2.43	0.52
4:A:175:PRO:HG3	4:A:498:ARG:HD3	1.92	0.52
10:4:22:C:H2'	10:4:23:G:H8	1.76	0.52
4:A:457:ASN:ND2	9:5:28:A:OP2	2.43	0.51
4:A:1443:LYS:HA	4:A:1446:GLN:HB2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:C:620:LYS:NZ	8:C:621:VAL:O	2.44	0.51
15:B:66:GLU:O	15:B:70:LYS:HG2	2.11	0.51
4:A:84:ASP:CB	4:A:88:TYR:HB2	2.40	0.51
8:C:735:PHE:HA	8:C:744:ILE:HA	1.92	0.51
4:A:1371:TYR:HE1	15:B:55:LYS:HB2	1.74	0.51
8:C:833:PHE:HB2	8:C:902:HIS:HB2	1.93	0.51
4:A:1590:VAL:HG23	4:A:1629:ILE:HD11	1.93	0.51
8:C:636:TYR:O	8:C:640:VAL:HG23	2.11	0.51
10:4:19:U:H4'	10:4:20:A:C8	2.45	0.51
4:A:215:ASP:O	4:A:217:ARG:NH1	2.44	0.51
4:A:443:VAL:N	4:A:610:HIS:CE1	2.77	0.51
6:U:429:GLU:HA	6:U:438:LEU:HA	1.93	0.51
4:A:260:LEU:HD21	4:A:454:TYR:HE2	1.75	0.51
4:A:291:GLU:O	4:A:1136:ARG:NE	2.39	0.51
4:A:443:VAL:HA	4:A:610:HIS:CE1	2.46	0.50
4:A:752:ASN:HA	4:A:755:HIS:CD2	2.46	0.50
8:C:300:LEU:HA	8:C:306:ASN:HD22	1.76	0.50
2:D:125:LYS:HE2	2:D:125:LYS:HA	1.94	0.50
4:A:593:ARG:HG2	4:A:594:TYR:N	2.26	0.50
6:U:357:THR:N	6:U:382:THR:O	2.44	0.50
4:A:990:LEU:O	4:A:994:ASN:ND2	2.44	0.50
4:A:1487:HIS:HB3	4:A:1541:THR:HB	1.94	0.50
4:A:1001:VAL:HG22	4:A:1002:ASP:H	1.77	0.50
8:C:932:GLU:HA	8:C:935:ILE:HG22	1.93	0.50
4:A:428:LYS:HA	4:A:431:TYR:CZ	2.46	0.50
4:A:84:ASP:CG	4:A:88:TYR:HB2	2.32	0.50
4:A:443:VAL:HA	4:A:610:HIS:ND1	2.27	0.50
6:U:133:ALA:HA	6:U:144:GLN:HA	1.94	0.50
14:N:144:ASP:OD1	14:N:144:ASP:N	2.45	0.50
4:A:152:ARG:NH2	4:A:619:GLY:H	2.10	0.49
4:A:546:LEU:HD21	4:A:595:LYS:HB2	1.94	0.49
4:A:223:SER:N	9:5:12:U:OP1	2.45	0.49
8:C:350:ASN:O	8:C:354:ARG:CA	2.61	0.49
4:A:65:HIS:CE1	4:A:66:VAL:HG23	2.48	0.49
4:A:597:LYS:HG3	9:5:45:C:OP1	2.13	0.49
8:C:181:ILE:HA	8:C:211:PHE:CE2	2.47	0.49
8:C:474:LEU:HA	8:C:499:GLY:HA3	1.95	0.49
10:4:33:A:N3	10:4:45:G:O2'	2.46	0.49
10:4:6:U:H2'	10:4:7:G:C8	2.48	0.49
4:A:1645:LEU:HA	4:A:1723:LYS:HE3	1.94	0.49
8:C:139:HIS:NE2	8:C:143:THR:OG1	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:997:LEU:HA	4:A:1000:ILE:HG22	1.95	0.48
2:D:12:TRP:HB3	14:N:13:ALA:HB1	1.96	0.48
4:A:155:LYS:HG2	4:A:622:GLY:N	2.28	0.48
5:R:414:ARG:HA	5:R:421:THR:HA	1.96	0.48
4:A:169:PHE:HB2	4:A:173:GLU:HG2	1.96	0.48
4:A:84:ASP:OD1	4:A:87:VAL:HB	2.13	0.48
4:A:145:GLY:HA2	4:A:245:LEU:HG	1.95	0.48
6:U:135:ALA:HA	6:U:142:TYR:HA	1.94	0.48
6:U:353:MET:HA	6:U:443:LEU:HA	1.96	0.48
10:4:17:A:N3	13:6:59:G:N2	2.62	0.48
1:G:278:ALA:HA	4:A:445:VAL:HG21	1.96	0.48
4:A:254:TYR:HE1	8:C:892:GLN:HE21	1.62	0.48
4:A:544:PHE:N	4:A:651:TRP:HZ3	2.11	0.48
4:A:1335:ILE:N	4:A:1363:GLN:O	2.45	0.48
2:D:29:ARG:HH12	2:D:31:GLY:HA3	1.77	0.48
4:A:158:ARG:HH12	4:A:573:GLN:HE22	1.62	0.48
8:C:139:HIS:HB2	8:C:207:GLY:H	1.78	0.48
4:A:510:ARG:NH1	4:A:655:LEU:HD12	2.29	0.48
4:A:1537:TRP:HE3	4:A:1751:LEU:HD23	1.78	0.48
2:D:30:PHE:HB3	2:D:63:ILE:HD11	1.96	0.47
9:5:8:G:H21	9:5:71:C:H5	1.61	0.47
10:4:7:G:H2'	10:4:8:C:C6	2.49	0.47
4:A:1092:ILE:HG13	4:A:1093:ASP:N	2.29	0.47
5:R:387:ASP:N	10:4:68:A:H61	2.06	0.47
8:C:189:VAL:HA	8:C:199:LEU:HA	1.97	0.47
4:A:298:ASP:OD1	4:A:298:ASP:N	2.47	0.47
10:4:8:C:N4	10:4:9:G:O6	2.47	0.47
10:4:43:G:H4'	10:4:44:A:H5'	1.96	0.47
4:A:331:TRP:NE1	4:A:333:HIS:O	2.42	0.47
1:G:272:PHE:CD1	4:A:592:TYR:HB3	2.50	0.47
4:A:396:ASP:OD1	4:A:396:ASP:N	2.45	0.47
4:A:599:MET:O	4:A:602:ILE:HG12	2.15	0.47
8:C:500:THR:HG22	8:C:545:PRO:HA	1.96	0.47
4:A:465:LYS:C	9:5:23:C:H42	2.17	0.47
4:A:780:THR:HG22	4:A:898:PHE:HD2	1.80	0.47
13:6:34:G:H2'	13:6:35:A:C8	2.49	0.47
4:A:601:GLN:HG3	4:A:640:PHE:CG	2.50	0.47
4:A:1195:ARG:HH22	4:A:1197:LEU:HD22	1.80	0.47
4:A:1544:ARG:O	4:A:1563:HIS:ND1	2.48	0.47
4:A:1642:PRO:HB3	4:A:1716:GLY:HA2	1.96	0.47
4:A:136:ILE:HB	4:A:139:VAL:HG12	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:584:HIS:O	4:A:588:LEU:HD13	2.15	0.47
9:5:24:G:O6	9:5:56:C:N4	2.46	0.47
4:A:735:ILE:O	4:A:739:ILE:HG12	2.15	0.47
4:A:96:PRO:HB2	4:A:645:THR:HG22	1.97	0.47
4:A:442:LYS:C	4:A:610:HIS:HE1	2.18	0.47
8:C:718:PHE:HB3	8:C:724:TRP:HB2	1.96	0.47
9:5:71:C:H2'	9:5:72:U:H4'	1.97	0.47
4:A:90:GLY:HA3	14:N:105:TYR:CE2	2.50	0.46
3:L:356:GLY:O	3:L:360:ARG:N	2.41	0.46
4:A:109:PRO:HD3	4:A:630:TRP:HZ2	1.81	0.46
4:A:1285:LEU:HD22	15:B:43:LEU:HD13	1.96	0.46
8:C:614:TYR:HD2	8:C:640:VAL:HG22	1.81	0.46
10:4:67:A:H61	13:6:46:G:H1	1.63	0.46
10:4:76:C:H2'	10:4:77:A:C8	2.50	0.46
4:A:176:LEU:HD23	4:A:181:ASN:HD21	1.80	0.46
4:A:608:LEU:O	4:A:612:ILE:HG12	2.15	0.46
2:D:91:MET:HB2	2:D:129:LEU:HA	1.97	0.46
4:A:420:ARG:NH2	4:A:422:LEU:HD21	2.30	0.46
4:A:1156:ASP:OD2	4:A:1160:ARG:NH2	2.48	0.46
4:A:1371:TYR:CE1	15:B:55:LYS:HB2	2.50	0.46
13:6:47:A:H4'	13:6:48:A:H3'	1.97	0.46
4:A:137:GLU:OE2	4:A:419:ARG:NH1	2.48	0.46
4:A:332:TYR:O	8:C:888:ARG:NH1	2.33	0.46
6:U:399:PRO:HD3	6:U:411:PRO:HG3	1.98	0.46
4:A:909:TYR:HD2	4:A:1033:GLY:H	1.63	0.46
4:A:1185:LEU:HB2	4:A:1196:ILE:CG2	2.43	0.46
8:C:531:TRP:HA	8:C:539:ILE:HA	1.97	0.46
4:A:792:HIS:O	4:A:796:LYS:HG2	2.16	0.45
8:C:448:LYS:HB2	8:C:448:LYS:HE2	1.70	0.45
8:C:614:TYR:CD2	8:C:640:VAL:HG22	2.50	0.45
4:A:305:ARG:HH21	8:C:933:PHE:HZ	1.64	0.45
4:A:501:TYR:HA	4:A:522:PHE:HE1	1.80	0.45
10:4:57:G:H1	13:6:55:C:H42	1.63	0.45
10:4:56:U:H2'	10:4:57:G:C8	2.52	0.45
2:D:141:ARG:HA	2:D:141:ARG:HD3	1.86	0.45
4:A:1571:ILE:O	4:A:1575:GLN:HG2	2.16	0.45
10:4:27:C:N3	10:4:28:C:N4	2.65	0.45
2:D:121:ARG:NH1	4:A:1522:GLN:OE1	2.32	0.45
4:A:348:PRO:HA	4:A:394:TYR:CZ	2.52	0.45
10:4:67:A:N1	13:6:46:G:N2	2.58	0.45
4:A:1650:ASP:O	7:S:699:LYS:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:92:ILE:HD13	2:D:119:VAL:HG22	1.98	0.45
2:D:115:ILE:O	2:D:119:VAL:HG23	2.17	0.45
5:R:388:LEU:HB2	5:R:423:GLY:HA2	1.99	0.45
6:U:399:PRO:HG3	6:U:411:PRO:HD3	1.99	0.45
8:C:231:ALA:N	8:C:258:ASN:O	2.45	0.45
1:G:272:PHE:CE1	4:A:592:TYR:HB3	2.52	0.45
4:A:219:TYR:HB3	4:A:230:PHE:CE1	2.50	0.45
4:A:750:TRP:HH2	4:A:781:ARG:HB3	1.80	0.45
10:4:32:G:N2	10:4:43:G:O2'	2.49	0.45
4:A:442:LYS:C	4:A:610:HIS:CE1	2.91	0.45
4:A:470:ARG:NH2	9:5:16:U:OP2	2.50	0.45
9:5:37:G:H2'	9:5:38:C:H4'	1.99	0.45
4:A:791:GLN:HE22	4:A:1028:TYR:H	1.66	0.45
6:U:166:ASN:H	6:U:171:LYS:N	2.15	0.45
4:A:553:LEU:O	4:A:556:LEU:HG	2.18	0.44
4:A:968:THR:O	4:A:972:GLU:N	2.49	0.44
4:A:1106:ALA:HB1	4:A:1149:LEU:HD11	1.99	0.44
15:B:76:GLU:HA	15:B:79:HIS:ND1	2.31	0.44
2:D:32:HIS:HB3	2:D:34:TRP:NE1	2.32	0.44
4:A:152:ARG:HH21	4:A:619:GLY:H	1.65	0.44
4:A:1637:TRP:CZ2	4:A:1720:PRO:HD2	2.52	0.44
4:A:1681:ARG:HG3	4:A:1715:TYR:CZ	2.53	0.44
6:U:416:PHE:O	6:U:420:ALA:N	2.50	0.44
4:A:443:VAL:CA	4:A:610:HIS:CE1	3.01	0.44
4:A:316:PHE:HD2	4:A:320:TYR:HE2	1.65	0.44
4:A:1180:LYS:O	4:A:1201:ARG:NH2	2.50	0.44
6:U:354:ARG:N	6:U:442:GLN:O	2.50	0.44
8:C:459:SER:O	8:C:463:GLU:N	2.41	0.44
4:A:344:ASP:OD1	4:A:344:ASP:N	2.47	0.44
4:A:1587:GLU:HA	4:A:1590:VAL:HG12	2.00	0.44
6:U:426:THR:HA	6:U:440:ARG:HA	2.00	0.44
4:A:144:TRP:HZ3	4:A:629:PHE:HA	1.83	0.44
6:U:459:LYS:HA	6:U:464:VAL:HA	1.99	0.44
9:5:26:A:H2'	9:5:27:U:O4'	2.18	0.44
14:N:116:ARG:O	14:N:116:ARG:HG3	2.18	0.44
4:A:641:MET:O	4:A:645:THR:HG23	2.18	0.44
4:A:441:VAL:HG13	4:A:444:ARG:NH2	2.33	0.44
4:A:151:MET:HB2	4:A:616:PHE:CE1	2.53	0.43
4:A:156:ARG:HG2	4:A:620:PRO:HB2	1.99	0.43
4:A:590:GLY:O	4:A:593:ARG:HD3	2.18	0.43
4:A:1618:LYS:HA	4:A:1618:LYS:HD3	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1723:LYS:HB3	4:A:1724:PRO:HD3	1.99	0.43
4:A:780:THR:HG22	4:A:898:PHE:CD2	2.53	0.43
4:A:885:LEU:O	4:A:889:ARG:NH1	2.51	0.43
4:A:973:CYS:SG	4:A:974:ASN:N	2.91	0.43
8:C:314:TYR:HE1	8:C:413:ARG:HE	1.66	0.43
8:C:646:LYS:HA	8:C:646:LYS:HD3	1.82	0.43
9:5:52:U:O5'	14:N:123:ARG:NH2	2.51	0.43
9:5:68:C:H2'	9:5:69:A:C4	2.52	0.43
4:A:780:THR:HG22	4:A:898:PHE:HB2	2.01	0.43
3:L:357:ARG:O	3:L:361:LYS:N	2.47	0.43
4:A:1034:LEU:HB2	4:A:1037:ALA:HB2	1.99	0.43
4:A:1288:LEU:HA	4:A:1291:CYS:SG	2.58	0.43
4:A:498:ARG:HA	4:A:498:ARG:HD2	1.84	0.43
4:A:676:ARG:O	4:A:680:HIS:N	2.39	0.43
4:A:1872:LEU:O	4:A:1876:LEU:N	2.50	0.43
8:C:413:ARG:HB2	8:C:414:PRO:HD3	1.99	0.43
4:A:85:LYS:HG2	4:A:86:ARG:N	2.34	0.43
4:A:223:SER:HG	9:5:12:U:P	2.41	0.43
4:A:883:ARG:O	4:A:887:THR:OG1	2.27	0.43
4:A:1257:THR:HA	4:A:1260:VAL:HG12	2.01	0.43
4:A:1536:LEU:HG	4:A:1751:LEU:HD11	2.00	0.43
10:4:51:A:H2'	10:4:52:U:C6	2.53	0.43
4:A:136:ILE:HD12	4:A:136:ILE:H	1.83	0.43
4:A:857:ASN:O	4:A:861:ARG:N	2.44	0.43
8:C:138:LEU:HG	8:C:140:HIS:H	1.84	0.43
8:C:705:VAL:HG21	8:C:717:PHE:CE2	2.54	0.43
4:A:1261:ASN:HA	4:A:1264:ASN:HD22	1.83	0.43
1:G:309:LEU:HD12	1:G:309:LEU:H	1.83	0.43
1:G:331:GLU:O	1:G:335:GLN:HG2	2.19	0.43
4:A:718:ARG:HA	4:A:721:LYS:HD3	2.01	0.43
4:A:1342:TRP:CE2	4:A:1353:PHE:HB2	2.54	0.43
8:C:258:ASN:HA	8:C:310:SER:O	2.19	0.43
9:5:75:G:H2'	9:5:76:A:C8	2.54	0.43
8:C:350:ASN:O	8:C:354:ARG:HA	2.19	0.42
4:A:579:GLN:HE22	4:A:609:LYS:HG3	1.83	0.42
4:A:1097:ILE:HD12	4:A:1099:PHE:CZ	2.54	0.42
15:B:76:GLU:HA	15:B:79:HIS:CE1	2.54	0.42
2:D:12:TRP:NE1	14:N:14:PRO:HD2	2.34	0.42
4:A:510:ARG:NH2	14:N:36:PRO:O	2.51	0.42
4:A:785:LYS:O	4:A:789:GLU:OE1	2.36	0.42
4:A:1037:ALA:HA	4:A:1040:ILE:HG12	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1086:ARG:NH2	4:A:1100:ARG:O	2.51	0.42
4:A:601:GLN:NE2	4:A:605:CYS:SG	2.93	0.42
4:A:738:MET:HA	14:N:145:LEU:HD23	2.01	0.42
6:U:202:ILE:O	6:U:206:ASP:N	2.44	0.42
4:A:536:LYS:HA	4:A:536:LYS:HD2	1.82	0.42
6:U:146:ARG:H	6:U:150:SER:CB	2.33	0.42
8:C:742:PRO:HG2	8:C:785:ARG:NH1	2.35	0.42
8:C:848:THR:O	8:C:851:ALA:HB3	2.20	0.42
9:5:53:U:H2'	9:5:54:U:C6	2.54	0.42
4:A:119:LEU:O	4:A:128:PHE:N	2.38	0.42
4:A:427:VAL:HA	4:A:430:TRP:CD1	2.55	0.42
4:A:759:GLU:HA	4:A:762:ARG:HG2	2.02	0.42
8:C:135:CYS:O	8:C:228:PHE:HB2	2.20	0.42
9:5:61:A:H2'	9:5:62:G:C8	2.54	0.42
10:4:57:G:N2	13:6:55:C:N3	2.59	0.42
4:A:1185:LEU:O	4:A:1195:ARG:HA	2.19	0.42
8:C:260:ILE:H	8:C:311:SER:HA	1.85	0.42
8:C:772:TRP:CZ3	8:C:813:ARG:HD3	2.54	0.42
8:C:800:PRO:HA	8:C:803:ARG:HD2	2.02	0.42
3:L:356:GLY:HA2	13:6:55:C:H41	1.85	0.42
4:A:188:LEU:HD23	4:A:188:LEU:HA	1.93	0.42
9:5:63:A:H2'	9:5:64:G:C8	2.54	0.42
4:A:1285:LEU:HD13	15:B:43:LEU:HD22	2.01	0.42
4:A:1706:ASP:O	4:A:1710:ASN:CA	2.68	0.42
7:S:726:PHE:HA	7:S:729:LEU:HD12	2.01	0.42
1:G:348:ALA:O	1:G:351:ARG:HG3	2.20	0.42
4:A:218:LYS:HA	4:A:218:LYS:HD3	1.82	0.42
4:A:885:LEU:HD11	4:A:1005:ILE:HA	2.02	0.42
9:5:4:C:N4	9:5:77:G:O6	2.52	0.42
10:4:44:A:O3'	10:4:45:G:H4'	2.20	0.42
4:A:109:PRO:HD3	4:A:630:TRP:CZ2	2.55	0.41
4:A:1369:TYR:O	15:B:53:GLY:N	2.39	0.41
6:U:420:ALA:O	6:U:424:GLY:N	2.51	0.41
8:C:181:ILE:HA	8:C:211:PHE:HE2	1.85	0.41
16:7:473:ARG:HH12	16:7:484:ILE:HG12	1.85	0.41
4:A:133:PRO:HB2	4:A:421:ALA:HB3	2.02	0.41
4:A:142:SER:HA	4:A:242:ALA:HB2	2.02	0.41
4:A:591:MET:O	4:A:592:TYR:C	2.58	0.41
6:U:145:GLY:HA3	6:U:152:ALA:H	1.85	0.41
8:C:129:ILE:O	8:C:441:PRO:HD3	2.19	0.41
4:A:428:LYS:HA	4:A:431:TYR:CE1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:608:LEU:HD12	4:A:609:LYS:N	2.35	0.41
4:A:1668:TRP:CE2	4:A:1708:ALA:HB2	2.56	0.41
4:A:120:TYR:HA	4:A:127:SER:HA	2.01	0.41
4:A:453:TYR:HE1	4:A:600:ARG:HD2	1.85	0.41
4:A:560:SER:O	4:A:563:GLN:HG3	2.20	0.41
2:D:25:VAL:HG11	2:D:116:ILE:HD11	2.02	0.41
4:A:182:ILE:HA	4:A:565:ARG:CZ	2.50	0.41
4:A:1134:TRP:CH2	4:A:1195:ARG:HG2	2.55	0.41
8:C:490:PHE:CZ	8:C:609:LYS:HD2	2.55	0.41
8:C:742:PRO:HB2	8:C:786:ASN:H	1.85	0.41
4:A:452:LYS:O	4:A:456:LEU:HD23	2.20	0.41
4:A:203:VAL:O	4:A:207:PHE:HB2	2.21	0.41
8:C:736:GLY:H	8:C:770:PHE:HE2	1.67	0.41
1:G:311:GLN:O	1:G:315:GLU:N	2.42	0.41
3:L:378:MET:N	4:A:1503:TRP:O	2.51	0.41
4:A:347:LEU:HG	4:A:348:PRO:HD2	2.03	0.41
4:A:586:GLY:O	4:A:590:GLY:HA2	2.21	0.41
4:A:1097:ILE:HD12	4:A:1099:PHE:CE1	2.56	0.41
4:A:1173:SER:OG	4:A:1174:PHE:N	2.54	0.41
4:A:1296:GLN:O	4:A:1300:LYS:HG3	2.21	0.41
4:A:1412:TRP:CD2	15:B:61:PRO:HG3	2.56	0.41
8:C:299:ILE:O	8:C:306:ASN:ND2	2.53	0.41
10:4:15:G:H2'	10:4:16:C:C6	2.56	0.41
4:A:752:ASN:HA	4:A:755:HIS:NE2	2.36	0.41
4:A:1853:PRO:O	4:A:1857:GLN:N	2.52	0.41
8:C:771:GLN:O	8:C:775:ARG:HG3	2.21	0.41
10:4:16:C:H2'	10:4:17:A:O4'	2.21	0.41
15:B:51:ARG:HB3	15:B:51:ARG:HH11	1.86	0.41
4:A:119:LEU:HD23	4:A:130:ASN:HB3	2.03	0.40
4:A:387:PHE:HD2	8:C:376:PRO:HG2	1.86	0.40
4:A:1369:TYR:CE1	15:B:43:LEU:HD11	2.55	0.40
8:C:139:HIS:ND1	8:C:206:PRO:HA	2.36	0.40
10:4:8:C:H2'	10:4:9:G:C8	2.56	0.40
4:A:1088:PHE:HD1	4:A:1097:ILE:HG22	1.86	0.40
4:A:1660:TYR:CZ	4:A:1700:GLY:HA2	2.56	0.40
6:U:107:TYR:O	6:U:111:ILE:N	2.55	0.40
10:4:75:C:H1'	13:6:35:A:N1	2.37	0.40
4:A:147:MET:O	4:A:151:MET:HG2	2.21	0.40
4:A:170:ASP:OD1	4:A:171:ASP:N	2.54	0.40
13:6:52:U:H2'	13:6:53:A:H8	1.87	0.40
4:A:183:LEU:HD23	4:A:183:LEU:HA	1.92	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:300:ASN:C	4:A:301:LYS:HE2	2.41	0.40
4:A:777:GLY:O	4:A:780:THR:OG1	2.35	0.40
5:R:409:LYS:HD2	5:R:409:LYS:HA	1.90	0.40
8:C:271:PRO:HG3	8:C:378:TYR:CD2	2.57	0.40
10:4:34:G:H4'	10:4:46:G:O2'	2.21	0.40
2:D:14:VAL:HA	2:D:59:TYR:HE2	1.86	0.40
4:A:491:GLU:O	4:A:494:LEU:HG	2.21	0.40
4:A:1962:THR:HA	4:A:1969:PRO:HA	2.03	0.40
6:U:166:ASN:H	6:U:171:LYS:H	1.70	0.40
9:5:37:G:H1	9:5:45:C:N4	2.20	0.40
14:N:137:LYS:HB3	16:7:476:ILE:HA	2.03	0.40
15:B:51:ARG:HB3	15:B:51:ARG:NH1	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	98/820 (12%)	96 (98%)	2 (2%)	0	100	100
2	D	139/142 (98%)	136 (98%)	3 (2%)	0	100	100
3	L	48/499 (10%)	48 (100%)	0	0	100	100
4	A	1943/2335 (83%)	1861 (96%)	81 (4%)	1 (0%)	51	85
5	R	104/480 (22%)	101 (97%)	3 (3%)	0	100	100
6	U	454/565 (80%)	441 (97%)	13 (3%)	0	100	100
7	S	69/800 (9%)	68 (99%)	1 (1%)	0	100	100
8	C	834/972 (86%)	814 (98%)	20 (2%)	0	100	100
11	X	20/155 (13%)	20 (100%)	0	0	100	100
14	N	127/941 (14%)	125 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	B	66/2136 (3%)	66 (100%)	0	0	100	100
16	7	34/793 (4%)	34 (100%)	0	0	100	100
All	All	3936/10638 (37%)	3810 (97%)	125 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	80	LYS

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	35/721 (5%)	35 (100%)	0	100	100
2	D	82/130 (63%)	82 (100%)	0	100	100
3	L	3/424 (1%)	3 (100%)	0	100	100
4	A	877/2108 (42%)	870 (99%)	7 (1%)	81	89
5	R	40/369 (11%)	39 (98%)	1 (2%)	47	68
6	U	26/511 (5%)	26 (100%)	0	100	100
7	S	23/681 (3%)	21 (91%)	2 (9%)	10	34
8	C	266/866 (31%)	265 (100%)	1 (0%)	91	94
11	X	3/144 (2%)	3 (100%)	0	100	100
14	N	29/792 (4%)	29 (100%)	0	100	100
15	B	12/1908 (1%)	12 (100%)	0	100	100
16	7	11/709 (2%)	11 (100%)	0	100	100
All	All	1407/9363 (15%)	1396 (99%)	11 (1%)	82	89

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	159	ARG

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Mol	Chain	Res	Type
4	A	217	ARG
4	A	409	ARG
4	A	593	ARG
4	A	616	PHE
4	A	707	ARG
4	A	1641	ARG
5	R	460	LYS
7	S	718	ARG
7	S	736	LYS
8	C	529	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
4	A	243	ASN
4	A	357	ASN
4	A	495	GLN
4	A	545	HIS
4	A	610	HIS
4	A	723	ASN
7	S	731	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
10	4	74/144 (51%)	16 (21%)	2 (2%)
12	z	10/11 (90%)	5 (50%)	0
13	6	41/106 (38%)	5 (12%)	0
9	5	76/117 (64%)	27 (35%)	1 (1%)
All	All	201/378 (53%)	53 (26%)	3 (1%)

All (53) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
9	5	8	G
9	5	9	G
9	5	10	U
9	5	12	U
9	5	14	U
9	5	18	C

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Mol	Chain	Res	Type
9	5	19	A
9	5	20	G
9	5	21	A
9	5	22	U
9	5	23	C
9	5	24	G
9	5	28	A
9	5	38	C
9	5	39	C
9	5	40	U
9	5	41	U
9	5	42	U
9	5	44	A
9	5	45	C
9	5	47	A
9	5	56	C
9	5	57	G
9	5	68	C
9	5	69	A
9	5	78	U
9	5	79	C
10	4	2	G
10	4	18	G
10	4	19	U
10	4	25	A
10	4	26	G
10	4	30	A
10	4	31	U
10	4	32	G
10	4	36	U
10	4	39	A
10	4	40	U
10	4	41	C
10	4	44	A
10	4	45	G
10	4	68	A
10	4	69	C
12	z	-2	A
12	z	1	G
12	z	2	U
12	z	3	A
12	z	7	A

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Mol	Chain	Res	Type
13	6	45	A
13	6	46	G
13	6	47	A
13	6	48	A
13	6	49	G

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
9	5	19	A
10	4	1	A
10	4	68	A

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

1 ligand is 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	$\#\|Z\| > 2$
17	IHP	A	2401	-	36,36,36	1.20	4 (11%)	54,60,60	1.64	6 (11%)

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
17	IHP	A	2401	-	-	1/30/54/54	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	2401	IHP	P5-O15	2.60	1.64	1.59
17	A	2401	IHP	P1-O11	2.26	1.63	1.59
17	A	2401	IHP	C4-C3	2.19	1.56	1.52
17	A	2401	IHP	C5-C4	2.17	1.56	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	A	2401	IHP	C5-C6-C1	5.05	121.47	110.41
17	A	2401	IHP	C3-C2-C1	4.61	120.50	110.41
17	A	2401	IHP	C5-C4-C3	4.38	120.01	110.41
17	A	2401	IHP	C4-C3-C2	3.47	118.00	110.41
17	A	2401	IHP	O15-C5-C4	2.42	114.40	108.69
17	A	2401	IHP	C6-C1-C2	2.20	115.23	110.41

There are no chirality outliers.

All (1) torsion outliers are listed below:

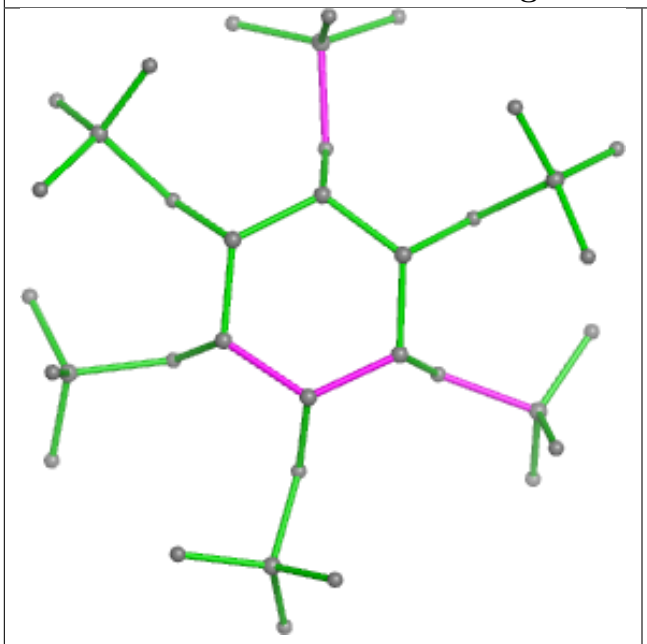
Mol	Chain	Res	Type	Atoms
17	A	2401	IHP	C5-O15-P5-O25

There are no ring outliers.

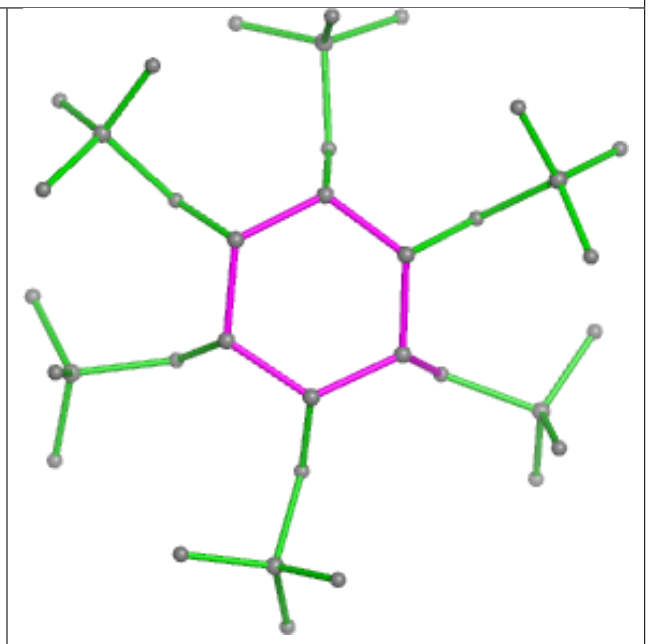
No monomer is involved in short contacts.

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 then 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.

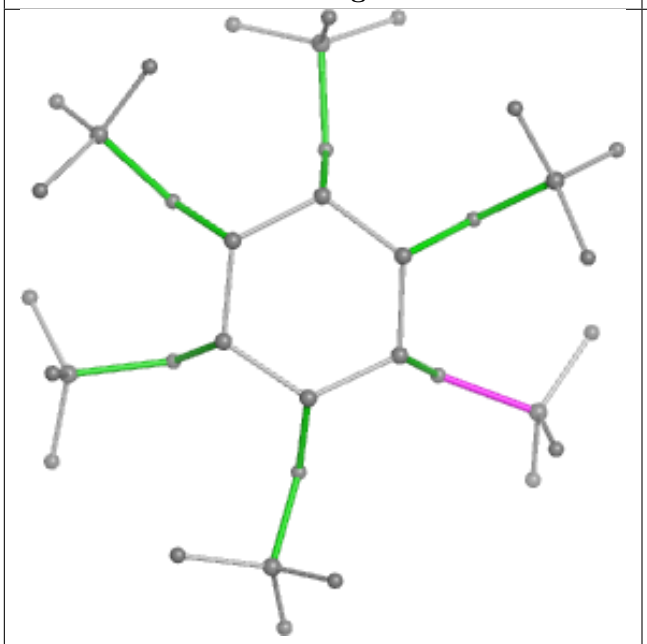
Ligand IHP A 2401



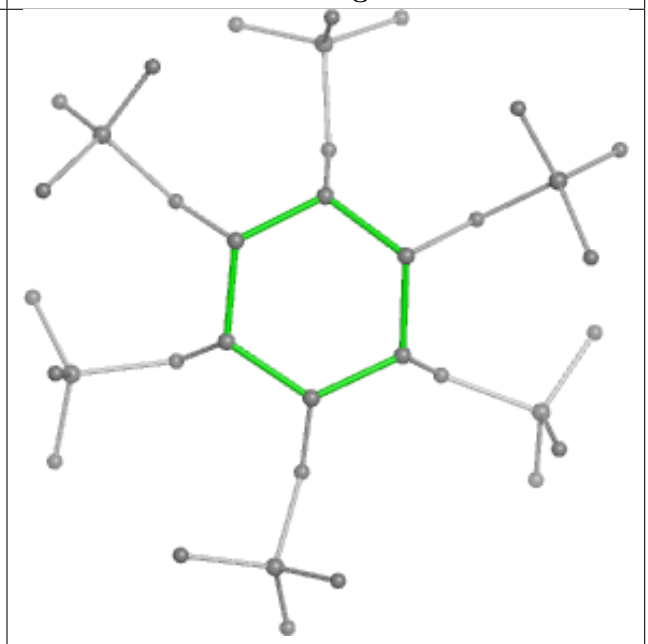
Bond lengths



Bond angles



Torsions



Rings

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.

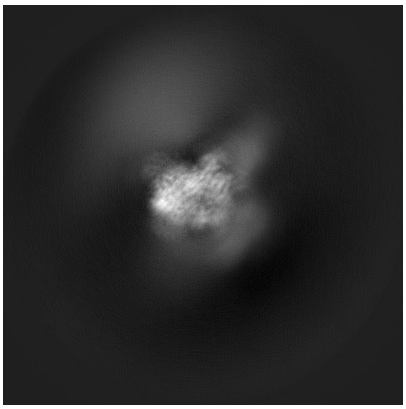
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-18555. These allow visual inspection of the internal detail of the map and identification of artifacts.

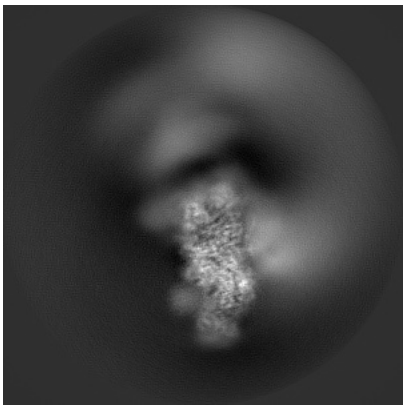
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

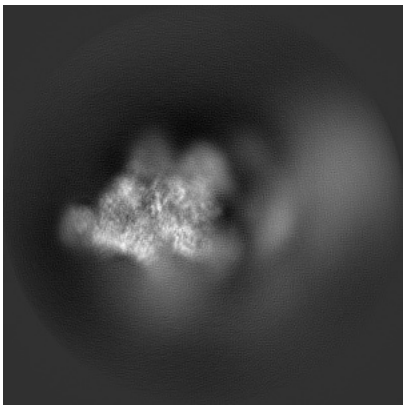
6.1.1 Primary map



X

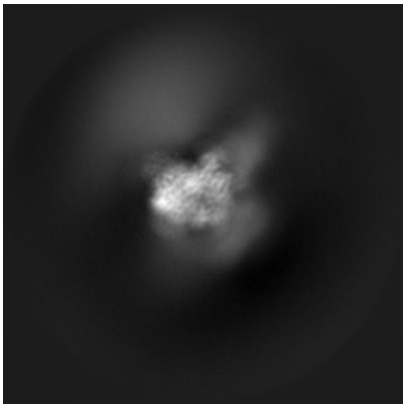


Y

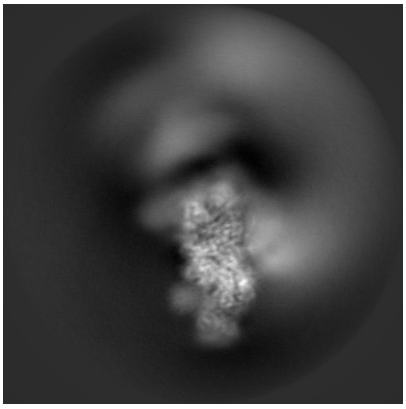


Z

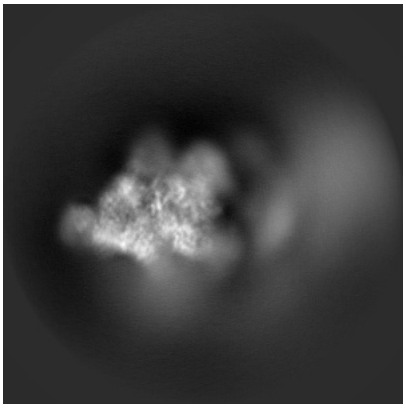
6.1.2 Raw map



X



Y

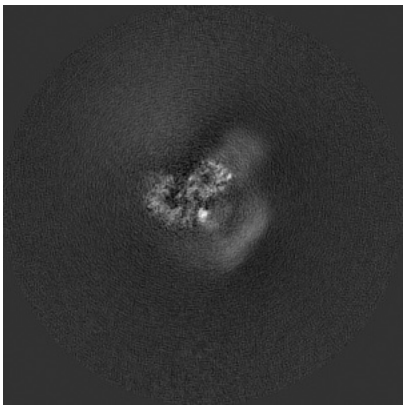


Z

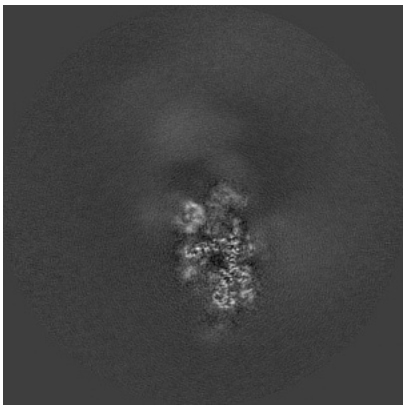
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

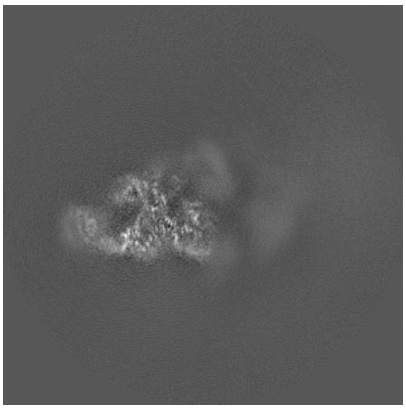
6.2.1 Primary map



X Index: 250

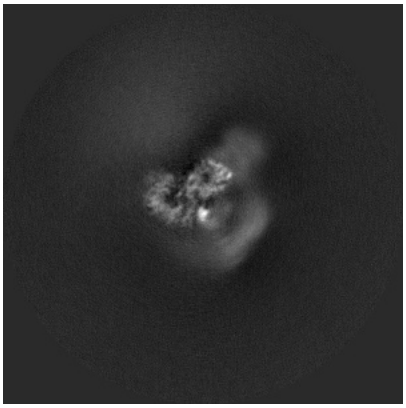


Y Index: 250

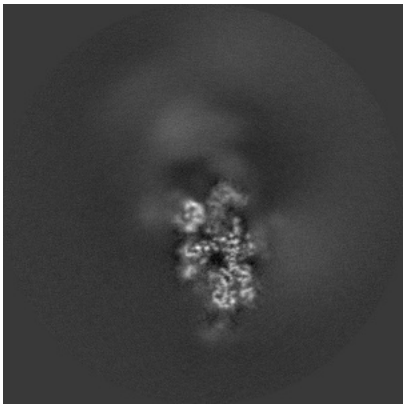


Z Index: 250

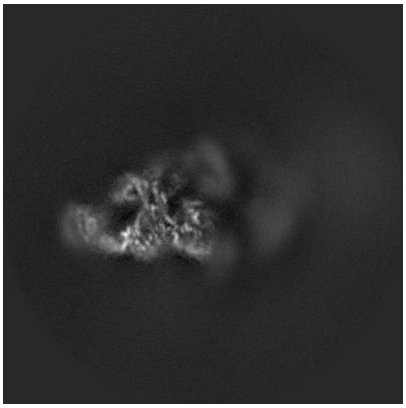
6.2.2 Raw map



X Index: 250



Y Index: 250

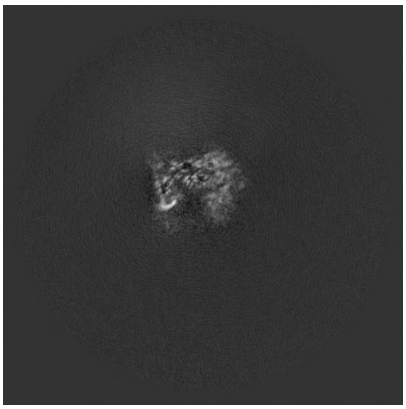


Z Index: 250

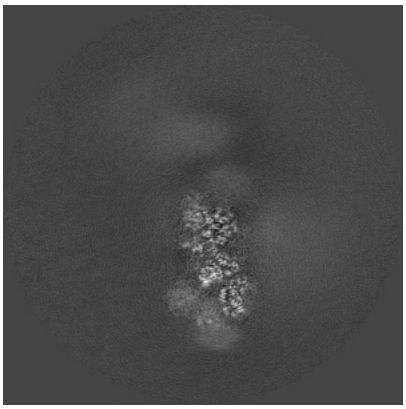
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

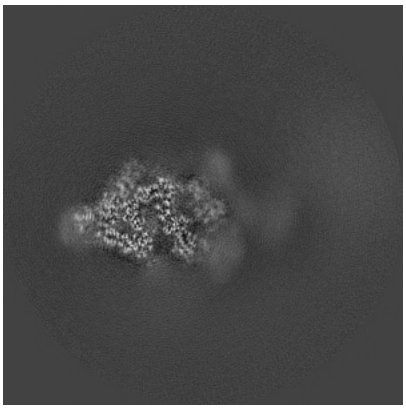
6.3.1 Primary map



X Index: 153

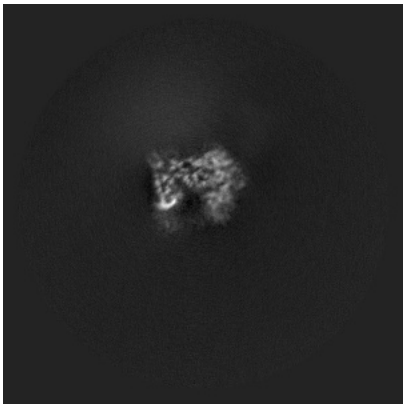


Y Index: 214

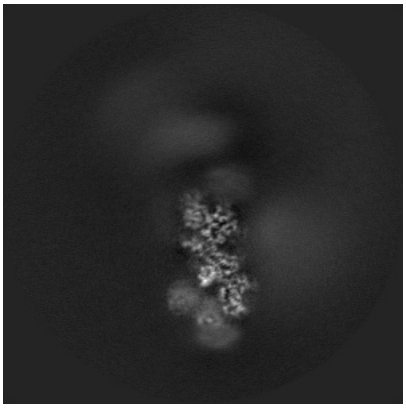


Z Index: 276

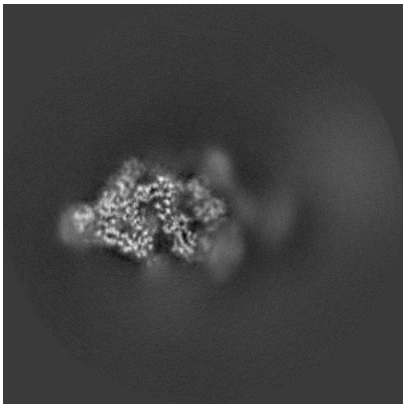
6.3.2 Raw map



X Index: 153



Y Index: 213

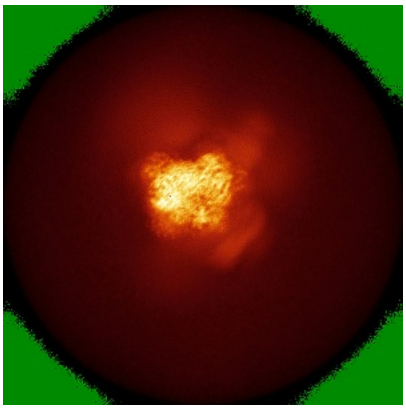


Z Index: 276

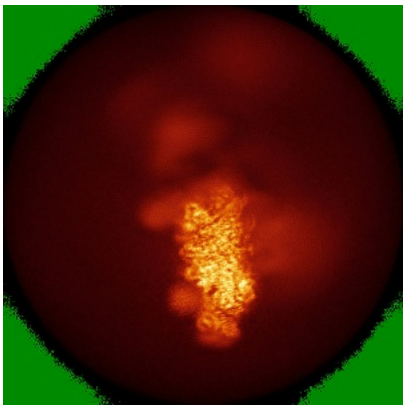
The images above show the largest variance slices of the map in three orthogonal directions.

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

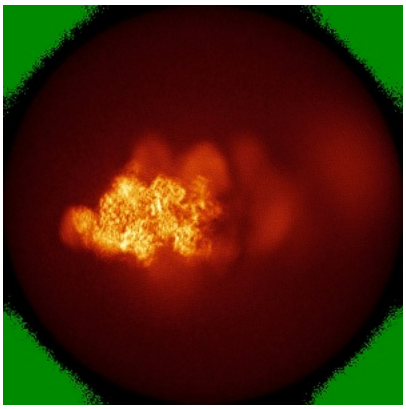
6.4.1 Primary map



X

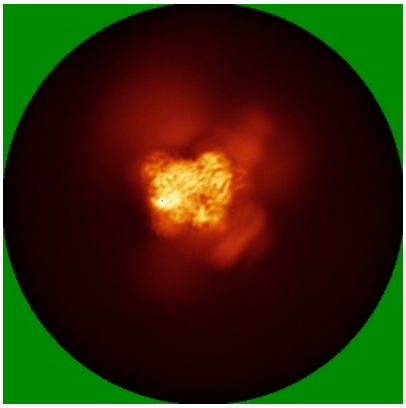


Y

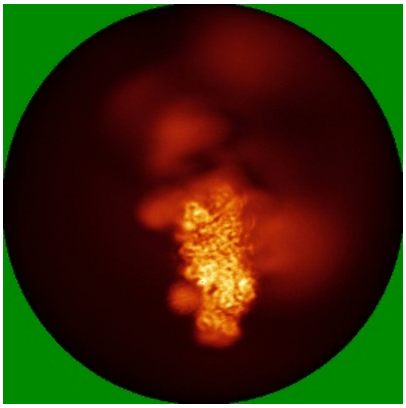


Z

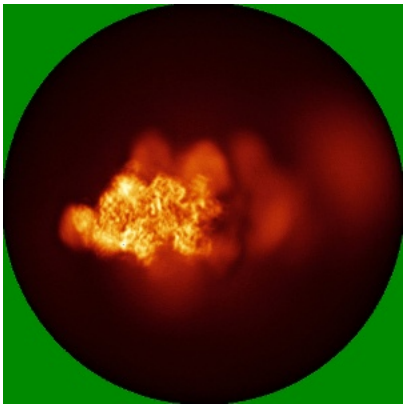
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X

Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.0165. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X

Y

Z

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

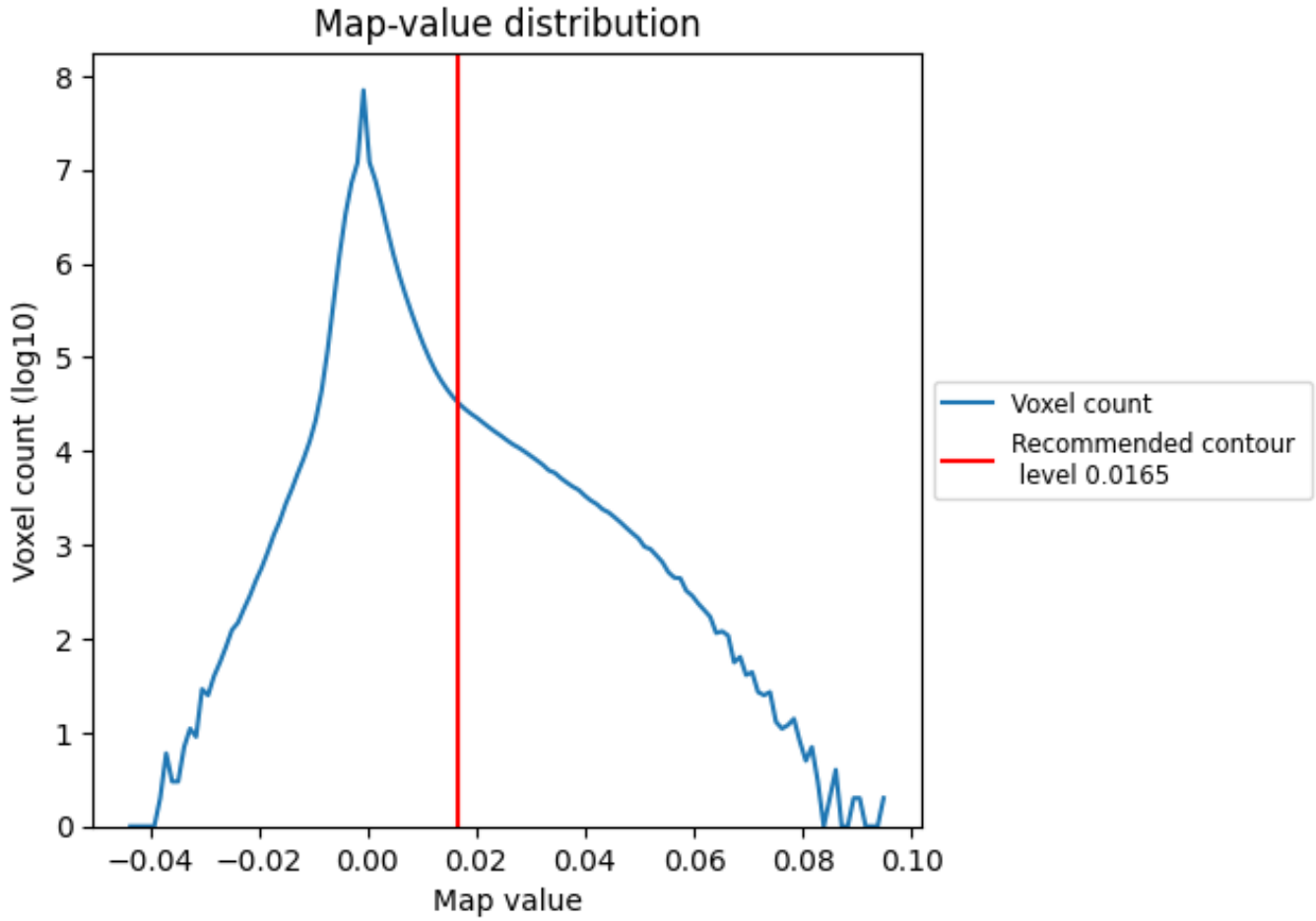
6.6 Mask visualisation (i)

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

7 Map analysis

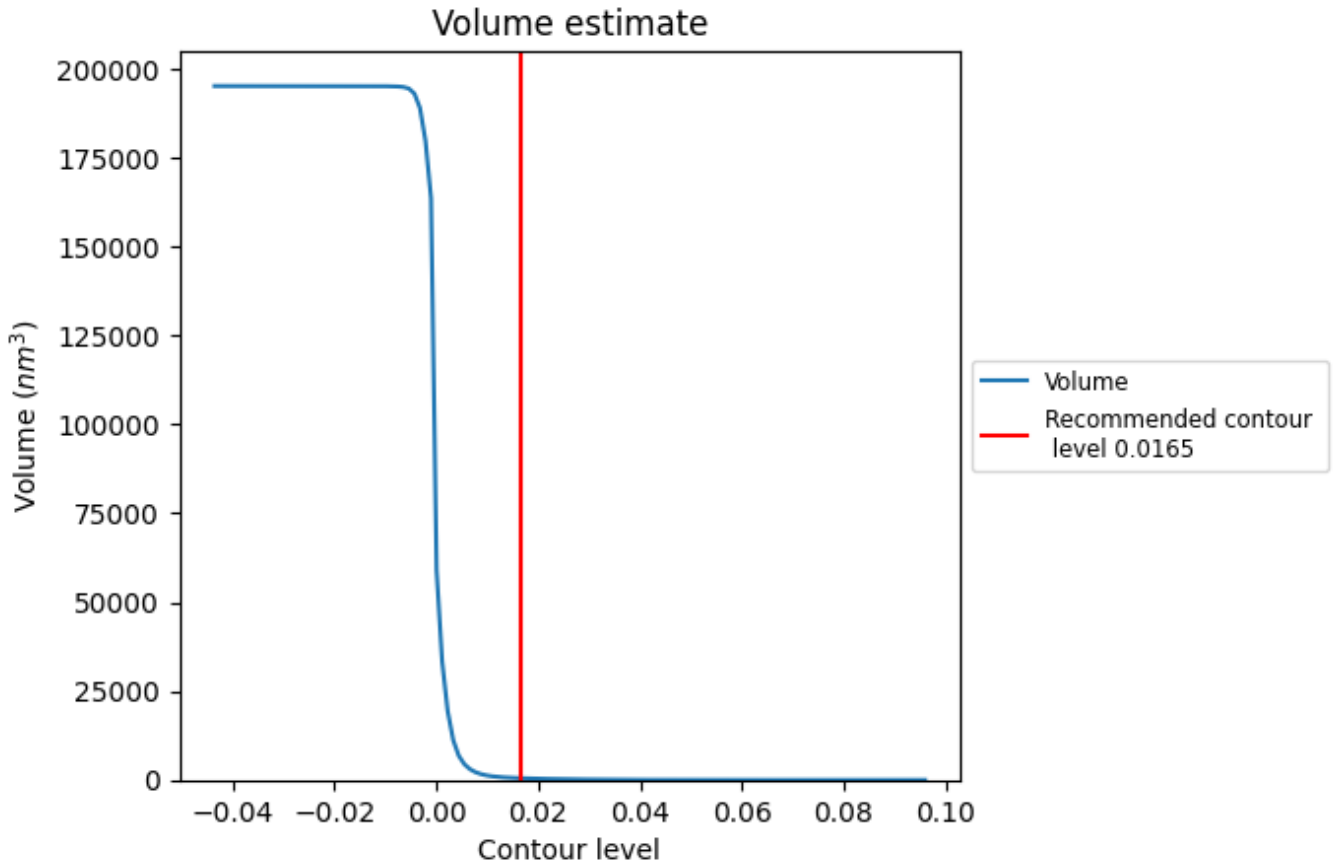
This section contains the results of statistical analysis of the map.

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.

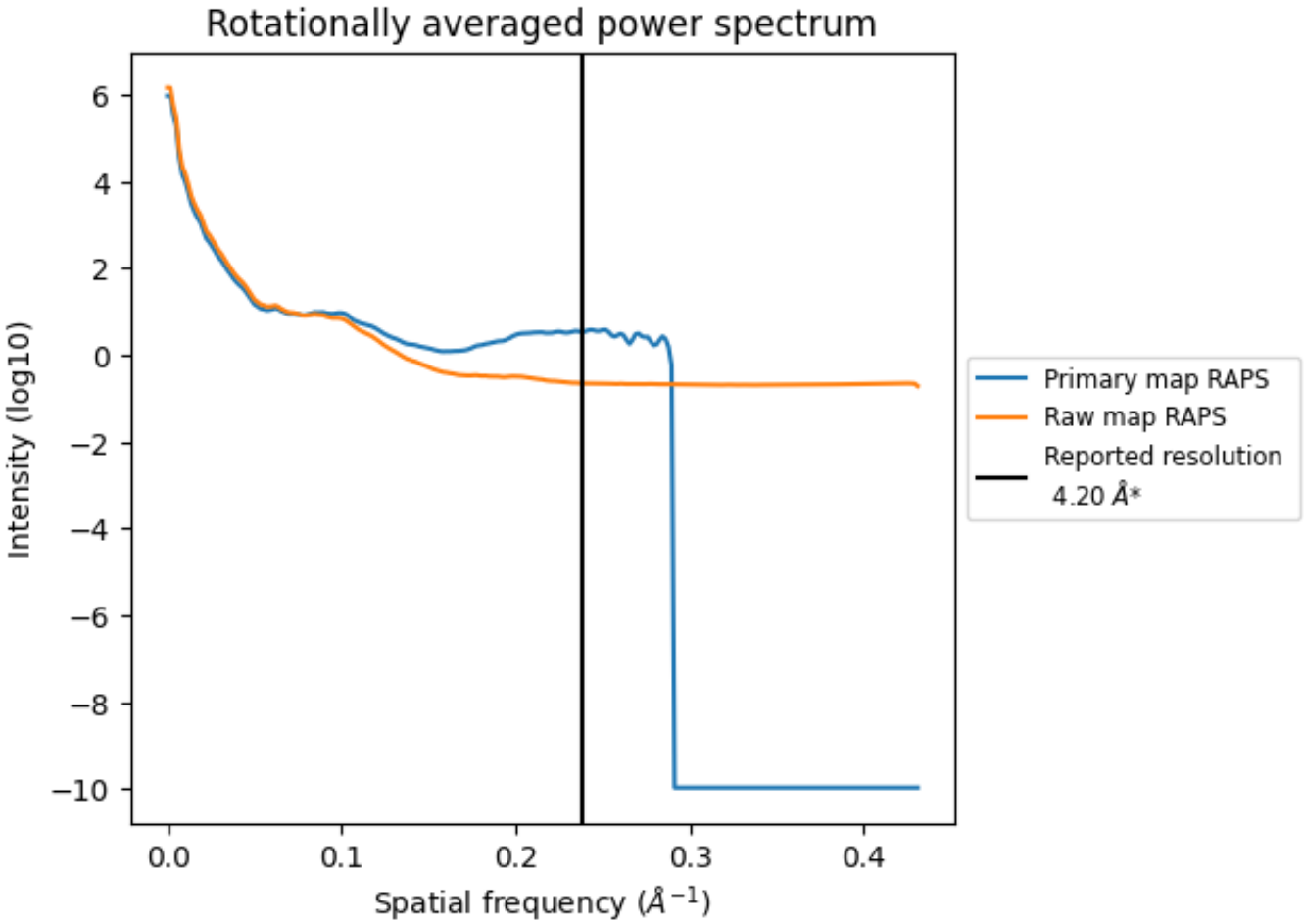
7.2 Volume estimate



The volume at the recommended contour level is 494 nm^3; this corresponds to an approximate mass of 446 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)

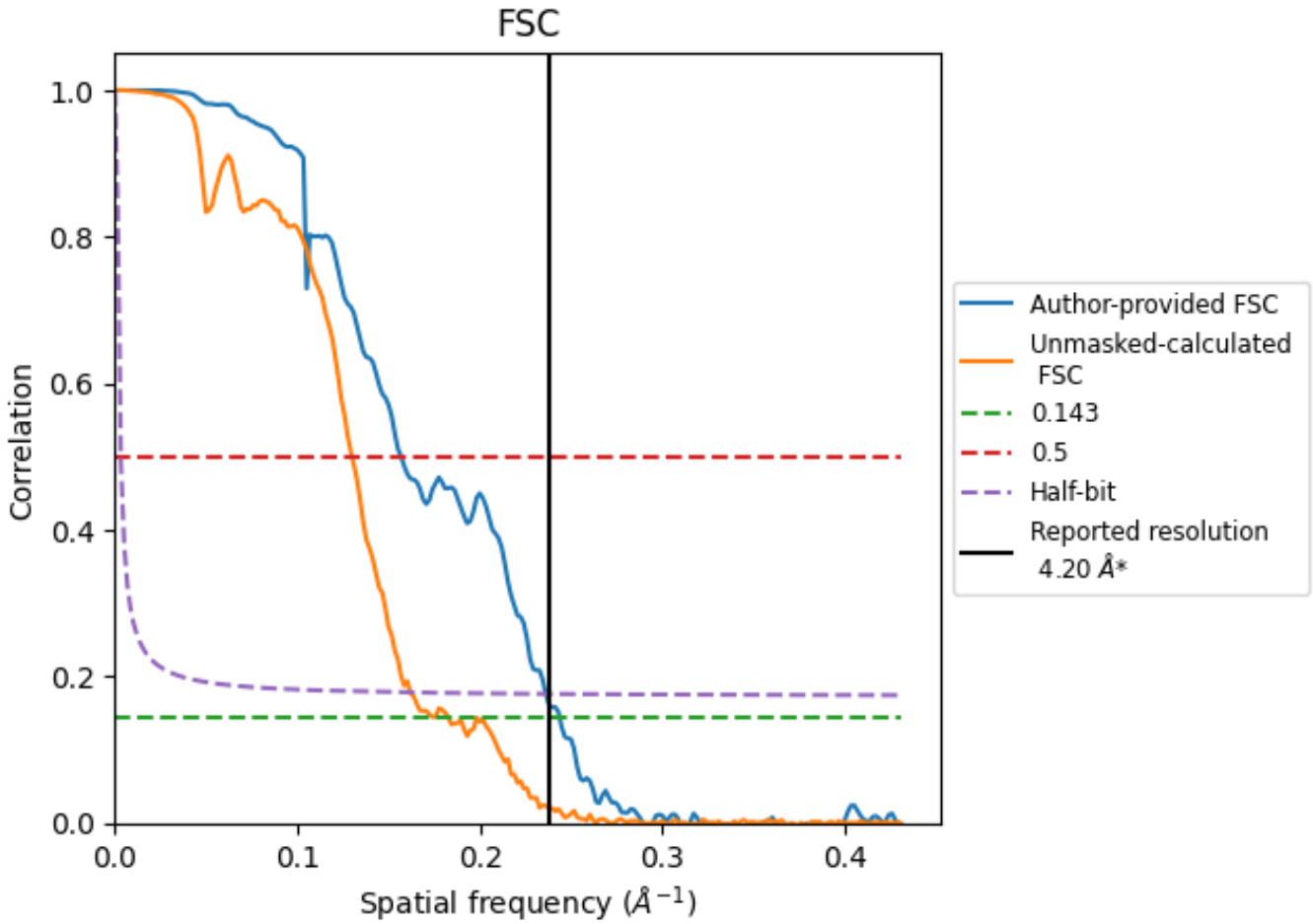


*Reported resolution corresponds to spatial frequency of 0.238 Å^{-1}

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 0.238 Å^{-1}

8.2 Resolution estimates (i)

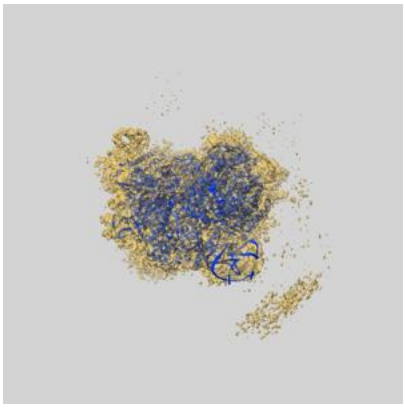
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.20	-	-
Author-provided FSC curve	4.10	6.37	4.23
Unmasked-calculated*	5.46	7.69	6.18

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 5.46 differs from the reported value 4.2 by more than 10 %

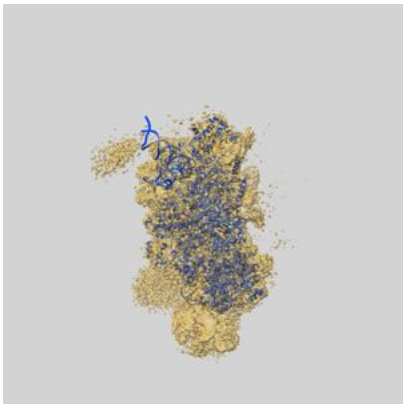
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-18555 and PDB model 8QPK. Per-residue inclusion information can be found in section 3 on page 7.

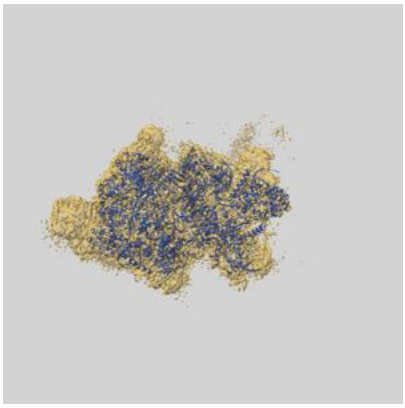
9.1 Map-model overlay



X



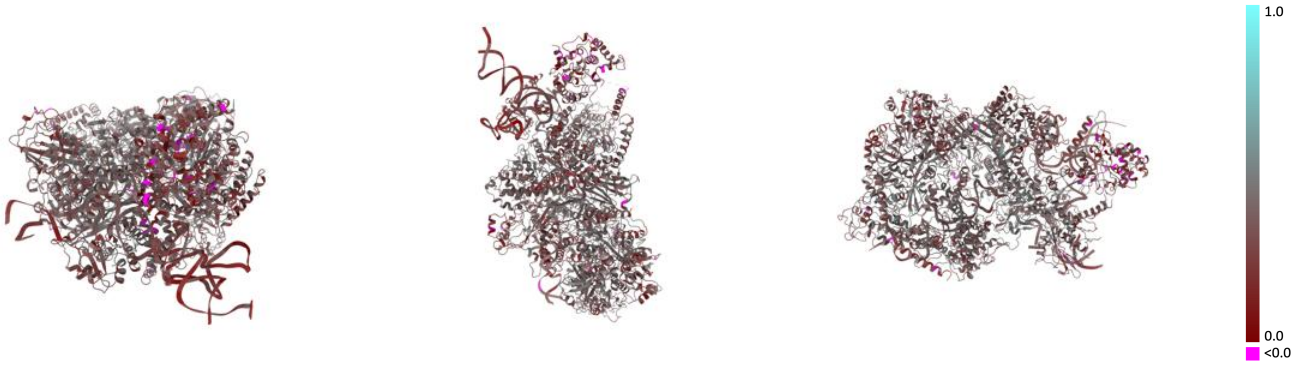
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0165 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.

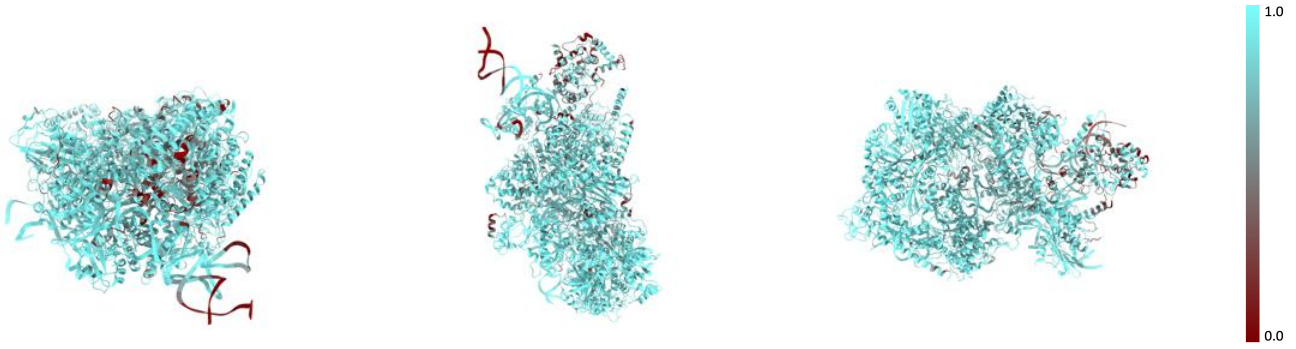
9.2 Q-score mapped to coordinate model



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.

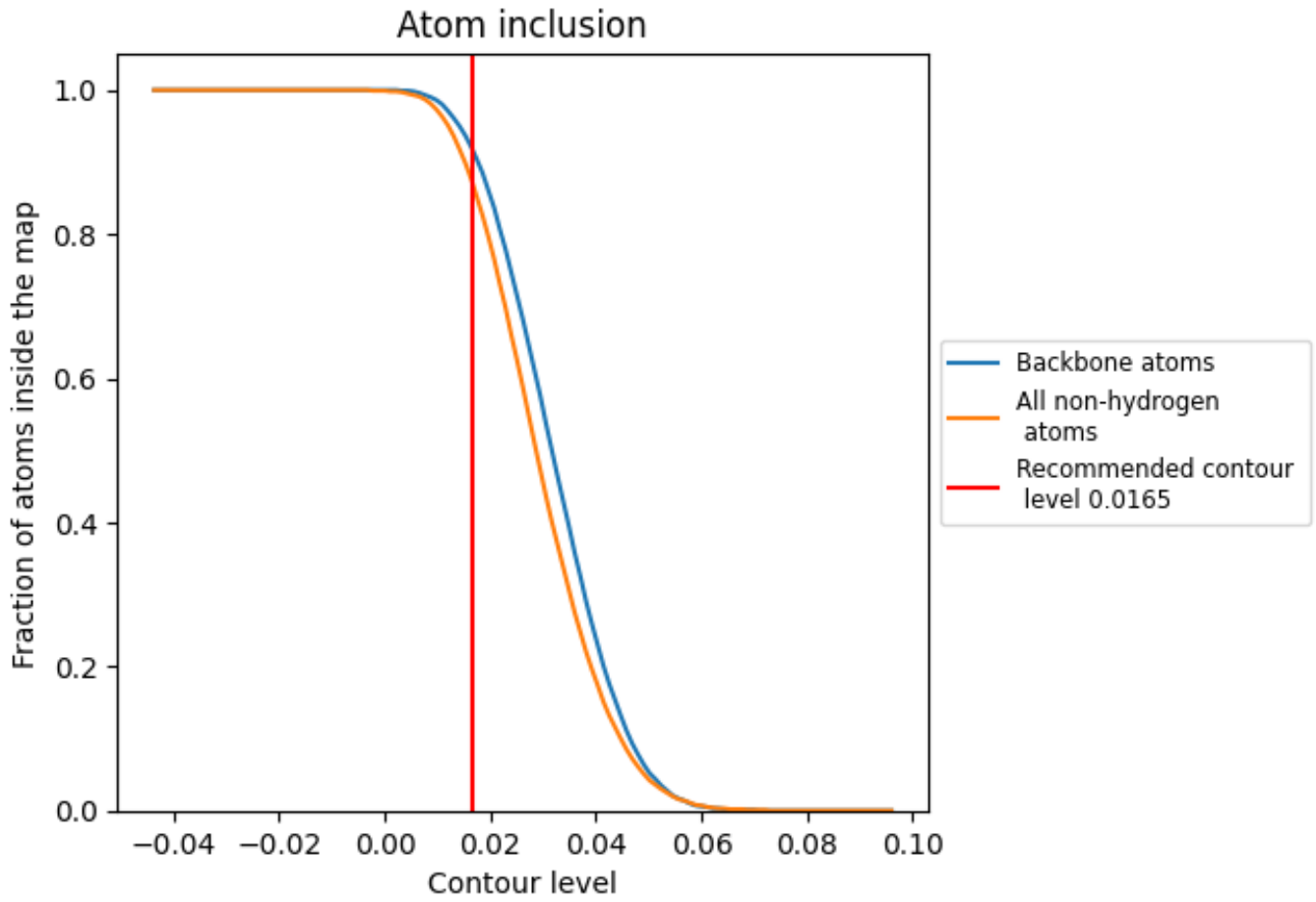
9.3 Atom inclusion mapped to coordinate model



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 (0.0165).

9.4 Atom inclusion (i)



At the recommended contour level, 92% of all backbone atoms, 88% 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 (0.0165) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8750	0.3650
4	0.7590	0.2470
5	0.9560	0.3240
6	0.7370	0.2920
7	0.8780	0.4000
A	0.8620	0.3820
B	0.7770	0.3570
C	0.9500	0.3930
D	0.8950	0.4320
G	0.8130	0.3570
L	0.6570	0.3490
N	0.9380	0.3830
R	0.9110	0.3380
S	0.7060	0.3240
U	0.9150	0.3240
X	0.7540	0.4020
z	0.9620	0.3970