Full wwPDB EM Validation Report ⓘ

Oct 21, 2024 – 08:08 PM JST

PDB ID	:	7W5B
EMDB ID	:	EMD-32321
Title	:	The cryo-EM structure of human C* complex
Authors	:	Zhan, X.; Lu, Y.; Shi, Y.
Deposited on	:	2021-11-29
Resolution	:	4.30 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:

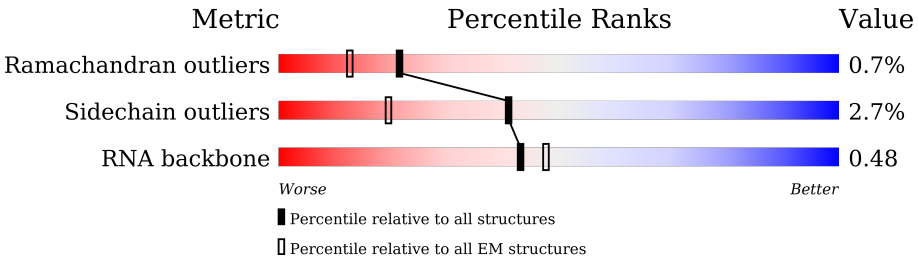
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 4.30 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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	A	2335	6% 92%
2	B	117	54% 16% 28%
3	C	972	86% 11%
4	D	2136	59% 80% 19%
5	E	357	83% 16%
6	F	107	46% 43% 9%
7	4	46	9% 15% 72%
8	G	174	10% 9% 30% 9% 53%

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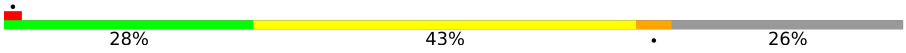
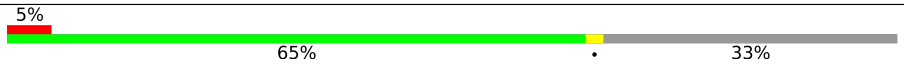
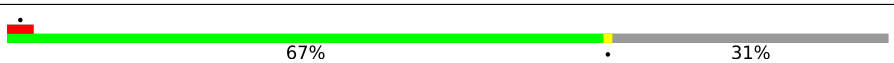
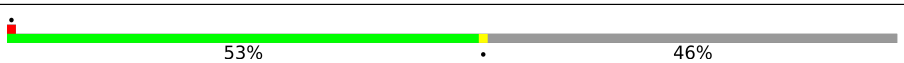
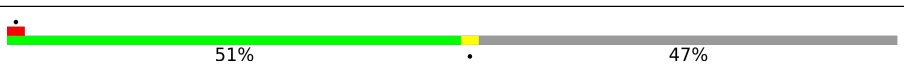
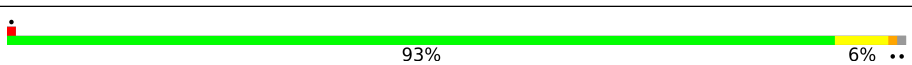
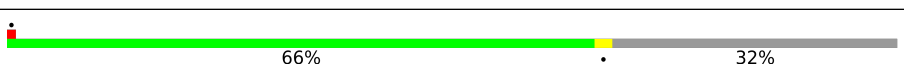
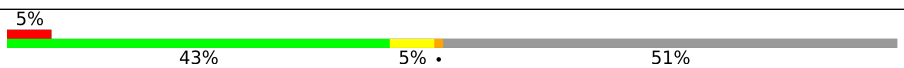
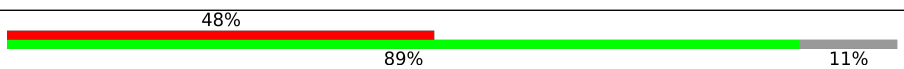
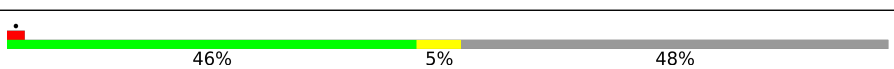
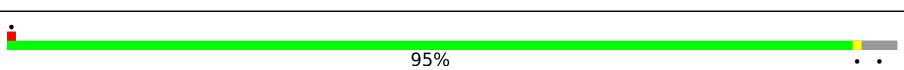
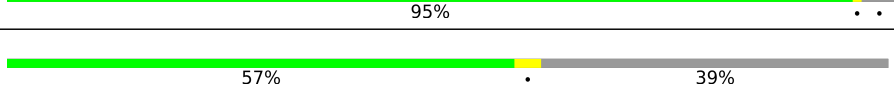
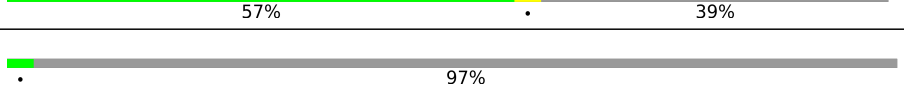
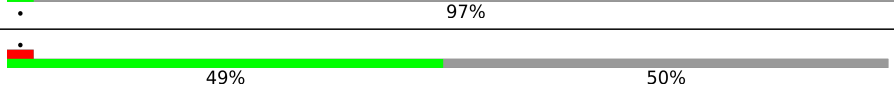
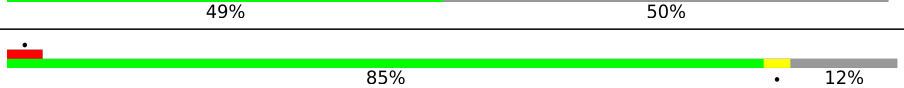
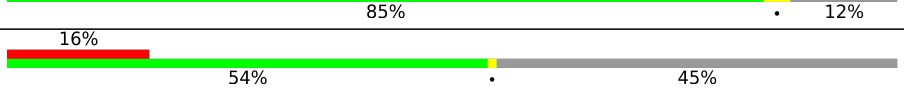
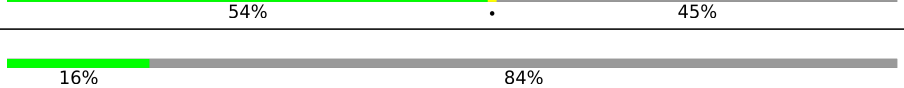
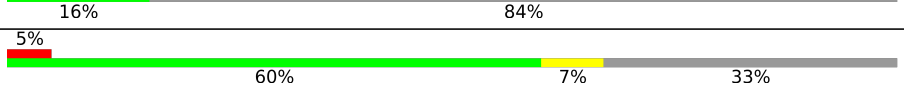
Mol	Chain	Length	Quality of chain
9	H	188	
10	I	855	
11	J	848	
12	K	225	
13	L	802	
14	M	243	
15	N	144	
16	O	420	
17	P	229	
18	Q	1485	
19	R	536	
20	S	166	
21	T	514	
22	U	2752	
23	V	908	
24	W	579	
25	Y	1220	
26	Z	758	
27	2	184	
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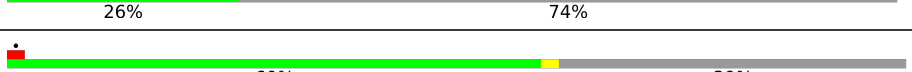
29	b	240	
29	i	240	
30	y	301	
31	a	126	
31	h	126	

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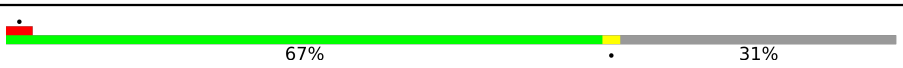
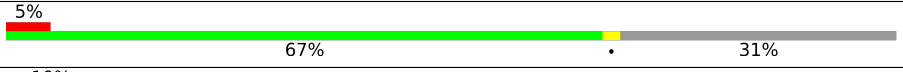
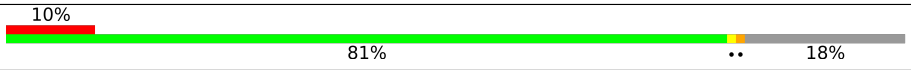
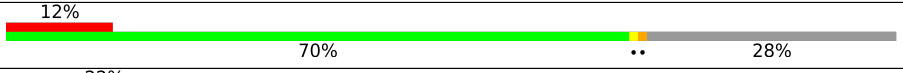
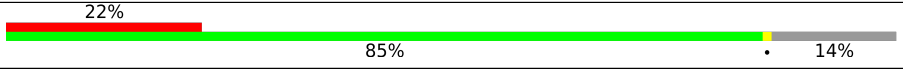
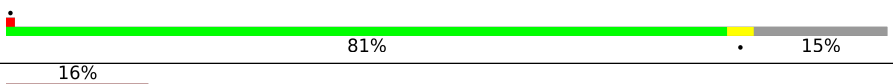
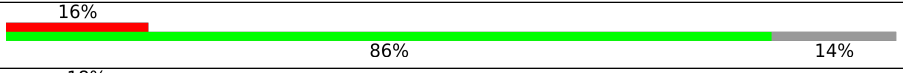
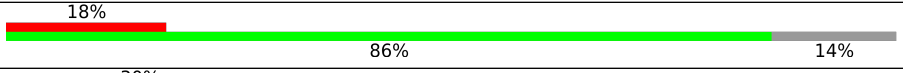
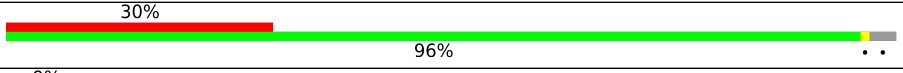
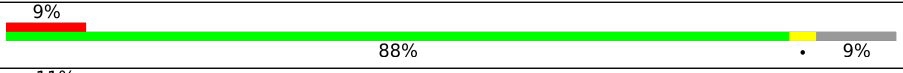
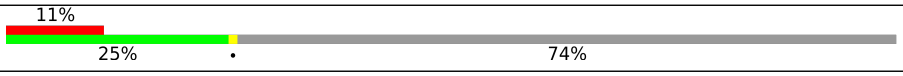
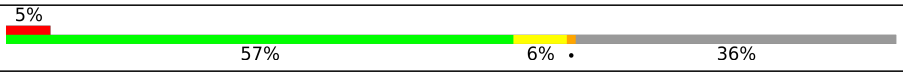
Mol	Chain	Length	Quality of chain
32	c	119	
32	j	119	
33	d	118	
33	k	118	
34	f	86	
34	m	86	
35	e	92	
35	l	92	
36	g	76	
36	n	76	
37	q	504	
37	r	504	
37	s	504	
37	t	504	
38	o	255	
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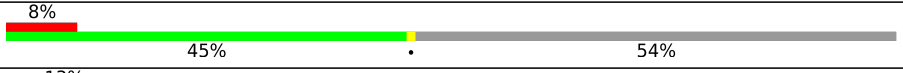
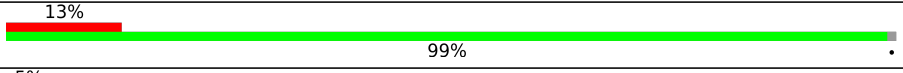
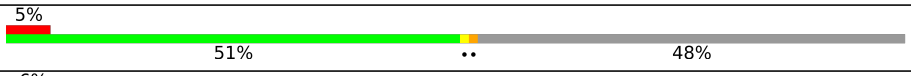
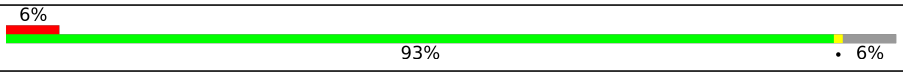
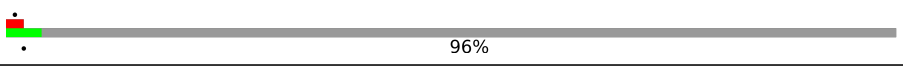
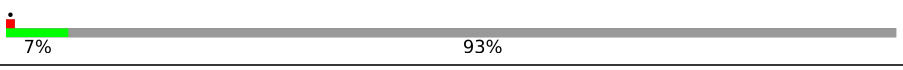
40	1	586	
41	v	146	
42	w	174	
43	u	411	
44	x	703	
45	3	415	

2 Entry composition

There are 50 unique types of molecules in this entry. The entry contains 106538 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 Pre-mRNA-processing-splicing factor 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	2253	17748	11367	3144	3167	70	0	0

- Molecule 2 is a RNA chain called U5 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	B	84	1768	792	295	597	84	0	0

- Molecule 3 is a protein called 116 kDa U5 small nuclear ribonucleoprotein component.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	862	6787	4339	1136	1281	31	0	0

- Molecule 4 is a protein called U5 small nuclear ribonucleoprotein 200 kDa helicase.

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

- Molecule 5 is a protein called U5 small nuclear ribonucleoprotein 40 kDa protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	299	2338	1470	410	445	13	0	0

- Molecule 6 is a RNA chain called U6 snRNA.

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

- Molecule 7 is a RNA chain called Pre-mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	4	13	Total	C	N	O	P	0	0
			276	123	50	90	13		

- Molecule 8 is a RNA chain called Pre-mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	G	82	Total	C	N	O	P	0	0
			1510	666	210	552	82		

- Molecule 9 is a RNA chain called U2 snRNA.

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

- Molecule 10 is a protein called Pre-mRNA-splicing factor SYF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	I	618	Total	C	N	O	S	0	0
			3857	2389	722	735	11		

- Molecule 11 is a protein called Crooked neck-like protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	J	569	Total	C	N	O	S	0	0
			3819	2379	718	716	6		

- Molecule 12 is a protein called Pre-mRNA-splicing factor SPF27.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	K	155	Total	C	N	O	0	0
			772	462	155	155		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	L	437	Total	C	N	O	S	0	0
			3015	1859	584	565	7		

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

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

- Molecule 15 is a protein called Protein BUD31 homolog.

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	P	113	Total	C	N	O	S	0	0
			953	583	189	179	2		

- Molecule 18 is a protein called RNA helicase aquarius.

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

- Molecule 19 is a protein called SNW domain-containing protein 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
19	R	280	Total	C	N	O	P	S	0	0
			2243	1401	411	416	2	13		

- Molecule 20 is a protein called Peptidyl-prolyl cis-trans isomerase-like 1.

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

- Molecule 21 is a protein called Pleiotropic regulator 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	T	312	Total	C	N	O	S	0	0
			2454	1550	446	450	8		

- Molecule 22 is a protein called Serine/arginine repetitive matrix protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	U	72	Total	C	N	O	S	0	0
			422	257	82	82	1		

- Molecule 23 is a protein called Pre-mRNA-splicing factor CWC22 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	V	452	Total	C	N	O	S	0	0
			2632	1639	492	495	6		

- Molecule 24 is a protein called Pre-mRNA-processing factor 17.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	W	509	Total	C	N	O	S	0	0
			4129	2628	715	762	24		

- Molecule 25 is a protein called ATP-dependent RNA helicase DHX8.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Y	667	Total	C	N	O	S	4	0
			3431	2057	680	693	1		

- Molecule 26 is a protein called Cactin.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Z	122	Total	C	N	O	S	0	0
			1084	712	197	173	2		

- Molecule 27 is a protein called PRKR-interacting protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	2	123	Total	C	N	O	S	0	0
			1013	635	193	180	5		

- Molecule 28 is a protein called Protein FAM32A.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	z	60	Total	C	N	O	S	0	0
			496	306	96	92	2		

- Molecule 29 is a protein called Small nuclear ribonucleoprotein-associated proteins B and B'.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	b	102	Total	C	N	O	S	0	0
			786	492	148	139	7		
29	i	86	Total	C	N	O	S	0	0
			690	434	126	123	7		

- Molecule 30 is a protein called Peptidyl-prolyl cis-trans isomerase E.

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

- Molecule 31 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	a	77	Total	C	N	O	S	0	0
			609	381	108	115	5		
31	h	81	Total	C	N	O	S	0	0
			633	397	112	118	6		

- Molecule 32 is a protein called Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	c	82	Total	C	N	O	S	0	0
			649	413	113	119	4		
32	j	82	Total	C	N	O	S	0	0
			649	413	113	119	4		

- Molecule 33 is a protein called Small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	d	97	Total	C	N	O	S	0	0
			776	488	143	140	5		
33	k	85	Total	C	N	O	S	0	0
			688	432	125	126	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
34	f	74	Total	C	N	O	S	0	0
			576	373	95	103	5		
34	m	73	Total	C	N	O	S	0	0
			566	367	93	101	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
35	e	79	Total	C	N	O	S	0	0
			652	412	116	119	5		
35	l	79	Total	C	N	O	S	0	0
			652	412	116	119	5		

- Molecule 36 is a protein called Small nuclear ribonucleoprotein G.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	g	74	Total	C	N	O	S	0	0
			577	364	104	103	6		
36	n	69	Total	C	N	O	S	0	0
			542	345	97	94	6		

- Molecule 37 is a protein called Pre-mRNA-processing factor 19.

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

- Molecule 38 is a protein called U2 small nuclear ribonucleoprotein A'.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	o	162	Total	C	N	O	S	0	0
			1282	820	219	240	3		

- Molecule 39 is a protein called U2 small nuclear ribonucleoprotein B".

Mol	Chain	Residues	Atoms					AltConf	Trace
39	p	94	Total	C	N	O	S	0	0
			760	488	135	132	5		

- Molecule 40 is a protein called Pre-mRNA-splicing factor SLU7.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	1	269	Total	C	N	O	S	0	0
			2209	1389	394	418	8		

- Molecule 41 is a protein called Protein mago nashi homolog.

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

- Molecule 42 is a protein called RNA-binding protein 8A.

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

- Molecule 43 is a protein called Eukaryotic initiation factor 4A-III.

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

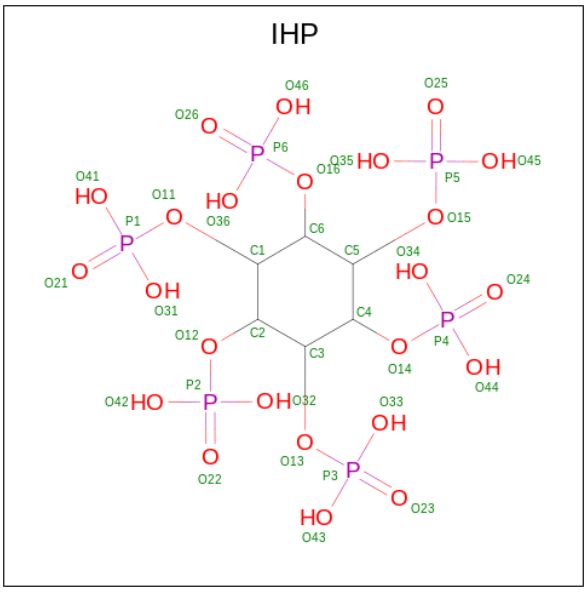
- Molecule 44 is a protein called Protein CASC3.

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

- Molecule 45 is a protein called NF-kappa-B-activating protein.

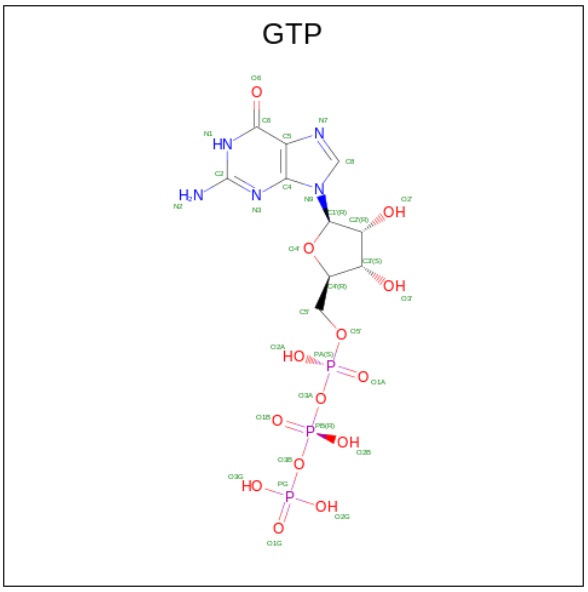
Mol	Chain	Residues	Atoms					AltConf	Trace
45	3	30	Total	C	N	O	S	0	0
			230	140	43	45	2		

- Molecule 46 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
			Total	C	O	P	
46	A	1	36	6	24	6	0

- Molecule 47 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$) (labeled as "Ligand of Interest" by depositor).



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

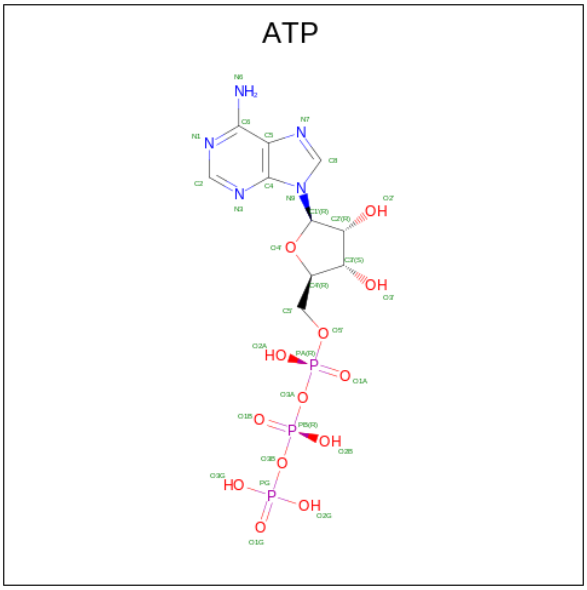
- Molecule 48 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 49 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	AltConf
49	N	3	Total Zn 3 3	0
49	O	3	Total Zn 3 3	0
49	1	1	Total Zn 1 1	0

- Molecule 50 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



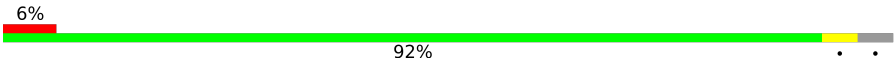
Mol	Chain	Residues	Atoms	AltConf
50	Q	1	Total C N O P 31 10 5 13 3	0

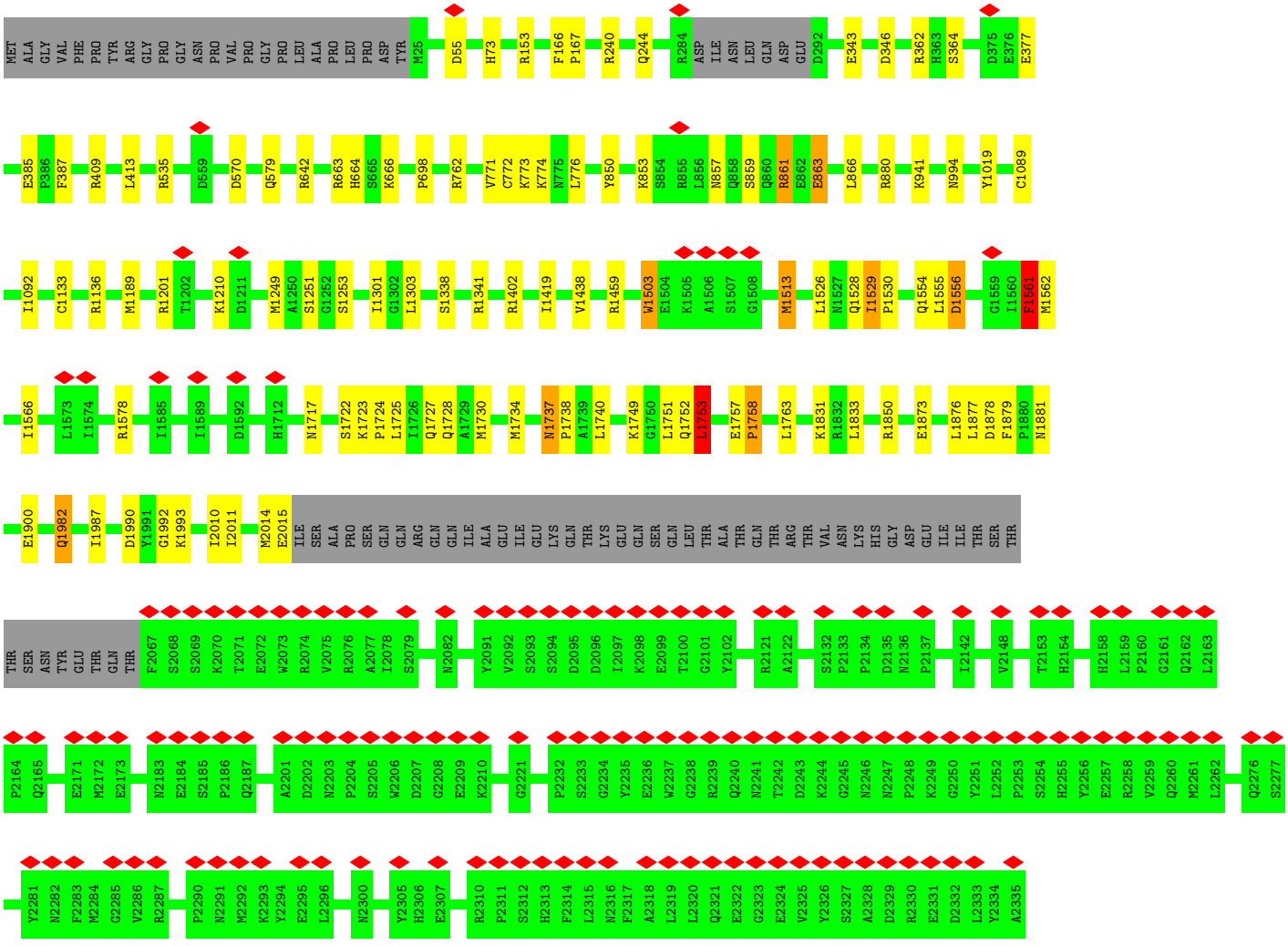
3 Residue-property plots (i)

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

• Molecule 1: Pre-mRNA-processing-splicing factor 8

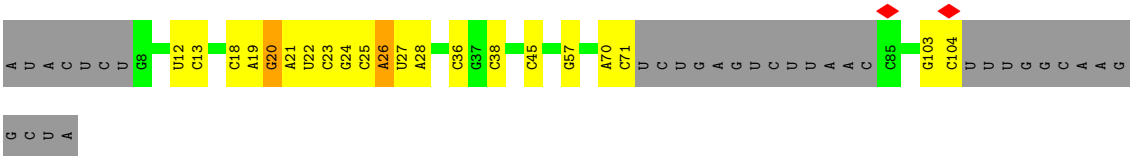
Chain A:



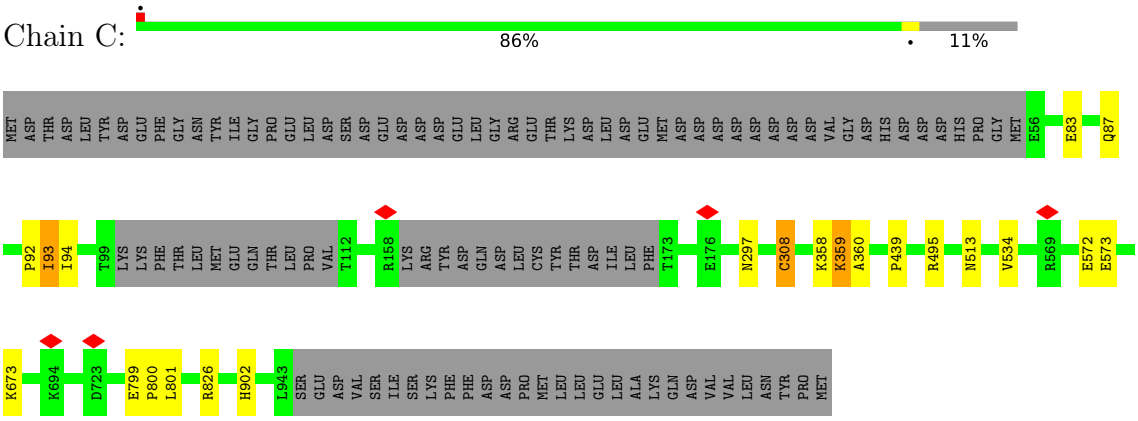


• Molecule 2: U5 snRNA

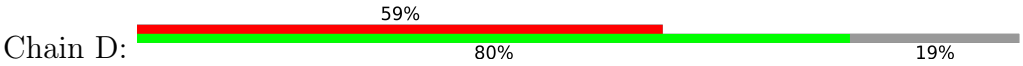
Chain B:

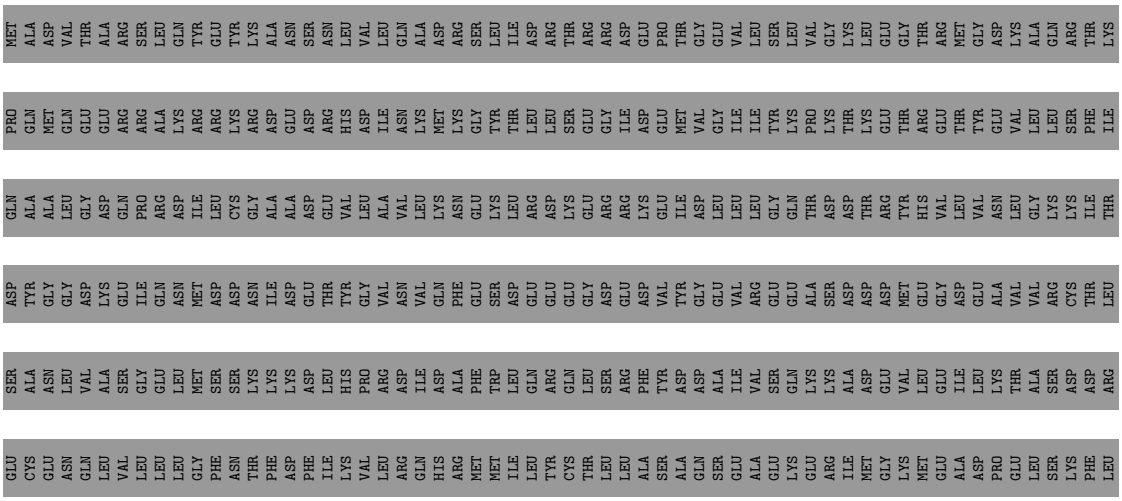


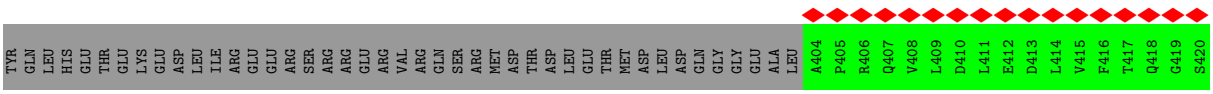
• Molecule 3: 116 kDa U5 small nuclear ribonucleoprotein component

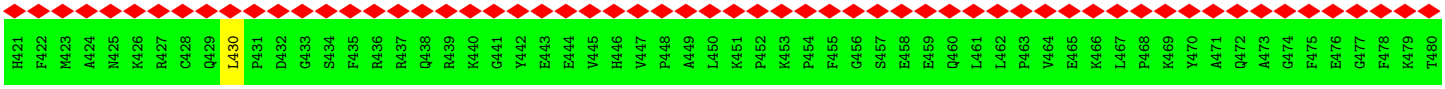


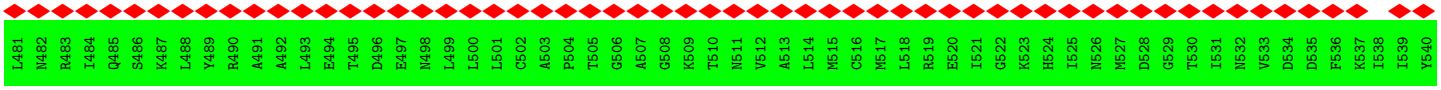
• Molecule 4: U5 small nuclear ribonucleoprotein 200 kDa helicase

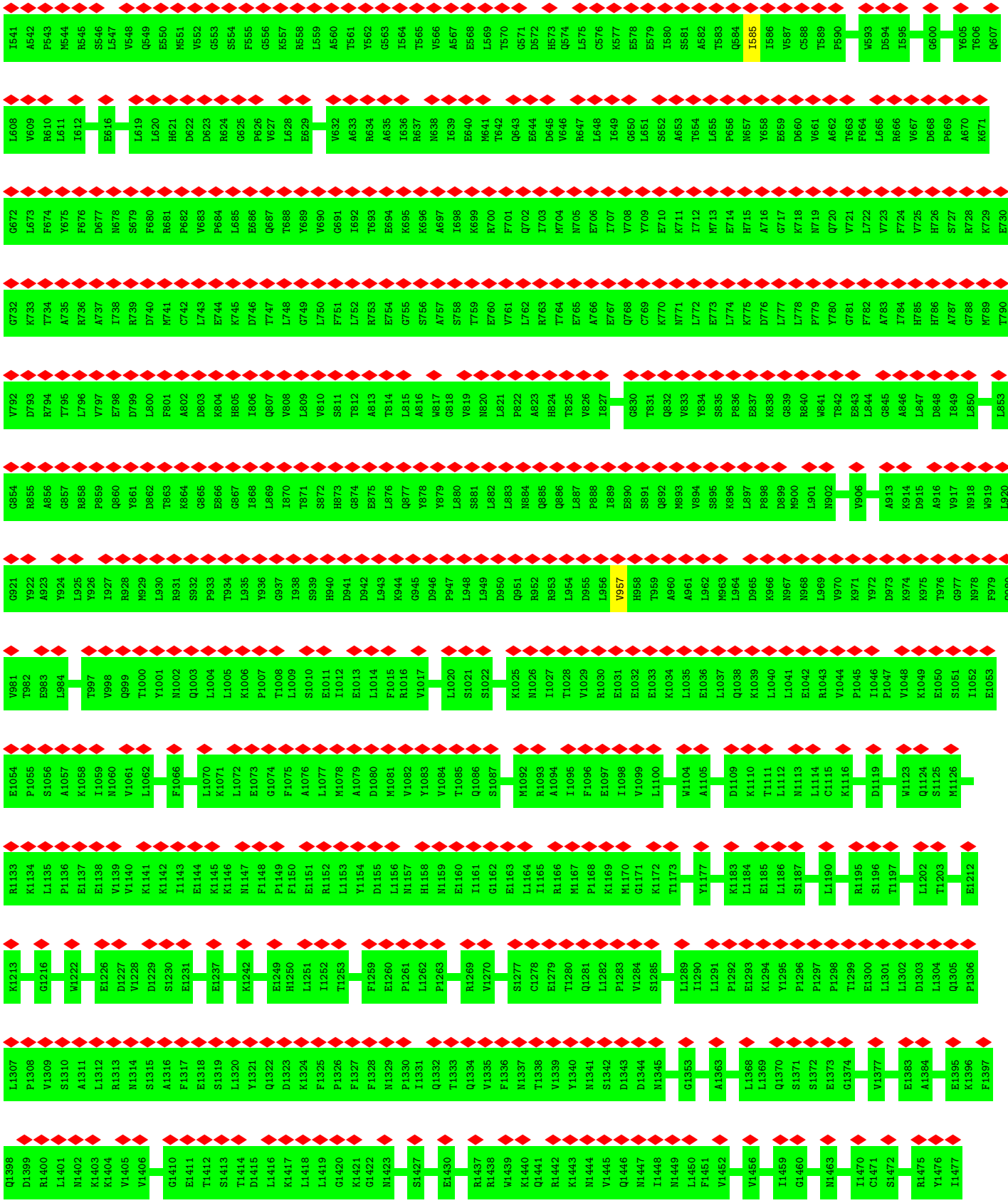


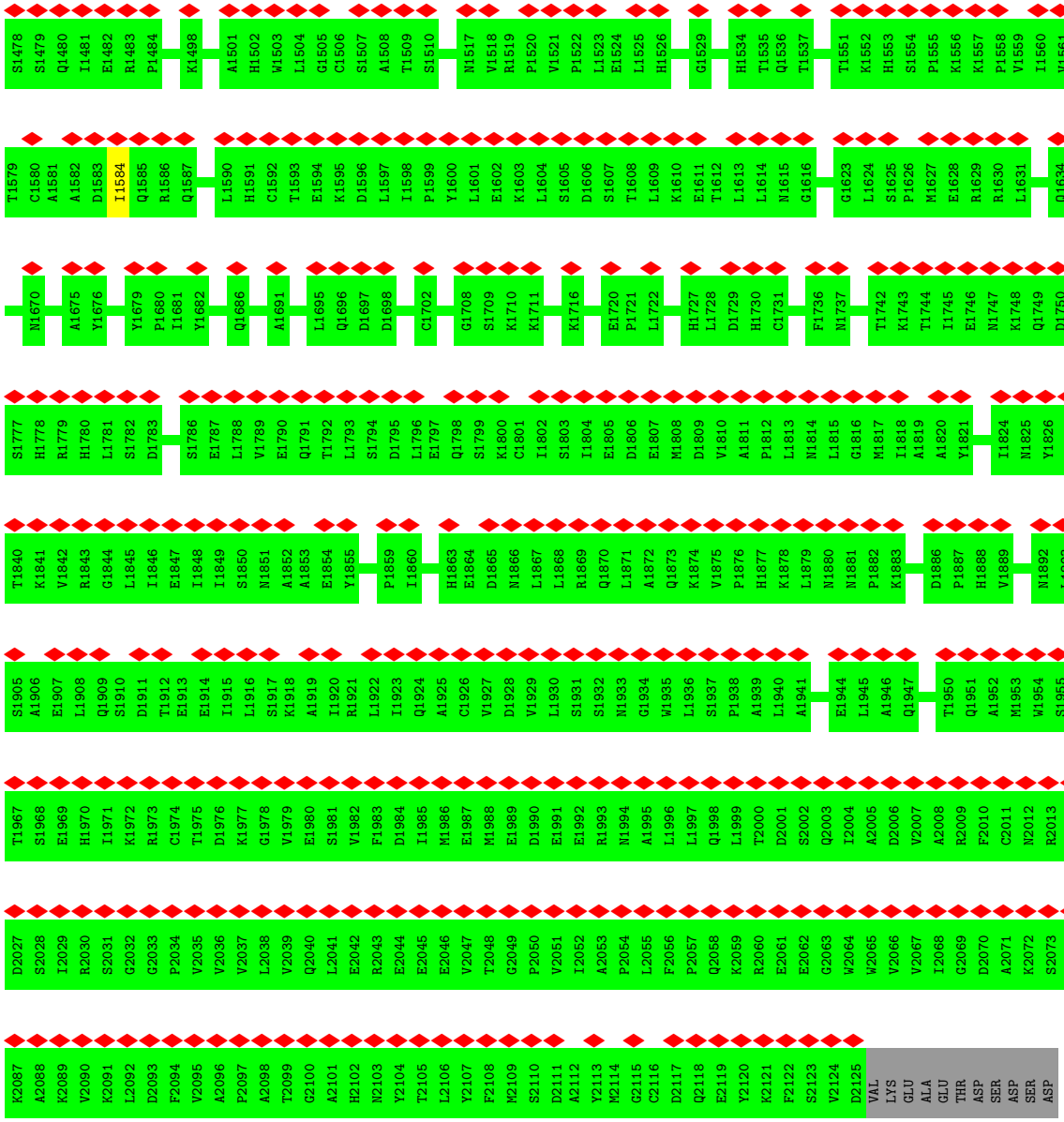









I541 A542 P543 M544 R545 S546 L547 V548 Q549 E550 M551 V552 G553 S554 F555 G556 K557 R558 L559 A560 T561 Y562 G563 I564 T565 V566 A567 E568 L569 T570 G571 D572 H573 Q574 L575 C576 K577 E578 E579 I580 S581 A582 T583 Q584 I585 I586 V587 C588 T589 P590 W593 D594 I595 Q600 Y605 T606 Q607
L608 V609 R610 L611 I612 E616 L619 L620 H621 D622 D623 R624 G625 P626 V627 L628 E629 V632 A633 R634 A635 I636 R637 N638 I639 E640 M641 T642 Q643 E644 D645 V646 R647 L648 I649 G650 L651 S652 A653 T654 L655 P656 N657 Y658 E659 D660 V661 A662 T663 F664 L665 R666 V667 D668 P669 A670 K671
G672 L673 F674 Y675 F676 D677 N678 S679 F680 R681 P682 V683 P684 L685 E686 Q687 T688 Y689 V690 G691 I692 T693 E694 K695 K696 A697 I698 K699 R700 F701 Q702 I703 M704 N705 E706 I707 V708 Y709 E710 K711 I712 M713 E714 H715 A716 G717 K718 N719 Q720 V721 L722 V723 F724 V725 H726 S727 R728 K729 E730 T731
G732 K733 T734 A735 R736 A737 I738 R739 D740 M741 C742 L743 E744 K745 D746 T747 L748 G749 L750 F751 L752 R753 E754 G755 S756 A757 S758 T759 E760 V761 L762 R763 T764 E765 A766 E767 Q768 C769 K770 N771 L772 E773 L774 K775 D776 L777 L778 P779 Y780 G781 F782 A783 I784 H785 H786 A787 G788 M789 T790 R791
V792 D793 R794 T795 L796 V797 E798 D799 L800 F801 A802 D803 K804 H805 I806 Q807 V808 L809 V810 S811 T812 A813 T814 L815 A816 W817 G818 V819 N820 L821 P822 A823 H824 T825 V826 I827 G830 T831 Q832 V833 Y834 S835 P836 E837 K838 G839 R840 W841 T842 E843 L844 G845 A846 L847 D848 I849 L850 L853
G854 R855 A856 G857 R858 P859 Q860 Y861 D862 T863 K864 G865 E866 G867 I868 L869 I870 T871 S872 H873 G874 E875 L876 Q877 Y878 Y879 L880 S881 L882 L883 N884 Q885 Q886 L887 P888 I889 E890 S891 Q892 M893 V894 S895 K896 L897 P898 D899 N900 L901 N902 Y906 A913 K914 D915 A916 V917 N918 W919 L920
G921 Y922 A923 Y924 L925 Y926 I927 R928 M929 L930 R931 S932 P933 T934 L935 Y936 G937 I938 S939 H940 D941 D942 L943 K944 G945 D946 P947 L948 L949 D950 Q951 R952 R953 L954 D955 L956 V957 H958 T959 A960 A961 L962 M963 L964 D965 K966 N967 N968 L969 V970 K971 Y972 D973 K974 K975 T976 G977 N978 F979 Q980
Y981 T982 E983 L984 T997 V998 Q999 T1000 Y1001 N1002 Q1003 L1004 L1005 K1006 P1007 T1008 L1009 S1010 E1011 I1012 E1013 L1014 F1015 R1016 V1017 L1020 S1021 S1022 K1025 N1026 I1027 T1028 V1029 R1030 E1031 E1032 E1033 K1034 L1035 E1036 L1037 Q1038 K1039 L1040 L1041 E1042 R1043 V1044 P1045 I1046 P1047 V1048 K1049 E1050 S1051 I1052 E1053
E1054 P1055 S1056 A1057 K1058 I1059 N1060 V1061 L1062 F1066 L1070 K1071 L1072 E1073 G1074 F1075 A1076 L1077 M1078 A1079 D1080 M1081 V1082 Y1083 V1084 T1085 Q1086 S1087 M1092 R1093 A1094 I1095 F1096 E1097 I1098 V1099 L1100 W1104 A1105 D1109 K1110 T1111 L1112 N1113 L1114 C1115 K1116 D1119 W1123 Q1124 S1125 M1126
R1133 K1134 L1135 P1136 E1137 E1138 V1139 V1140 K1141 K1142 I1143 E1144 K1145 K1146 N1147 F1148 P1149 F1150 E1151 R1152 L1153 Y1154 D1155 L1156 N1157 H1158 N1159 E1160 I1161 G1162 E1163 L1164 I1165 R1166 M1167 P1168 K1169 M1170 G1171 K1172 T1173 Y1177 K1183 L1184 E1185 L1186 S1187 L1190 R1195 S1196 T1197 L1202 T1203 E1212
K1213 G1216 W1222 E1226 D1227 V1228 D1229 S1230 E1231 E1237 K1242 E1249 H1250 L1251 I1252 T1253 F1259 E1260 P1261 L1262 P1263 R1269 V1270 S1277 C1278 E1279 T1280 Q1281 L1282 P1283 V1284 S1285 L1289 I1290 L1291 P1292 E1293 K1294 Y1295 P1296 P1297 P1298 T1299 E1300 L1301 L1302 D1303 L1304 Q1305 P1306
L1307 P1308 V1309 S1310 A1311 L1312 R1313 N1314 S1315 A1316 F1317 E1318 S1319 L1320 Y1321 Q1322 D1323 K1324 F1325 P1326 F1327 F1328 N1329 P1330 I1331 Q1332 T1333 Q1334 V1335 F1336 N1337 T1338 V1339 Y1340 N1341 S1342 D1343 D1344 N1345 G1353 A1363 L1368 L1369 Q1370 S1371 S1372 E1373 G1374 V1377 E1383 A1384 E1395 K1396 F1397
Q1398 D1399 R1400 L1401 N1402 K1403 K1404 V1405 V1406 G1410 E1411 T1412 S1413 T1414 D1415 L1416 K1417 L1418 L1419 G1420 K1421 G1422 N1423 S1427 E1430 R1437 R1438 W1439 K1440 Q1441 R1442 K1443 N1444 V1445 Q1446 N1447 I1448 N1449 L1450 F1451 V1452 V1456 I1459 G1460 N1463 I1470 C1471 S1472 R1475 Y1476 I1477

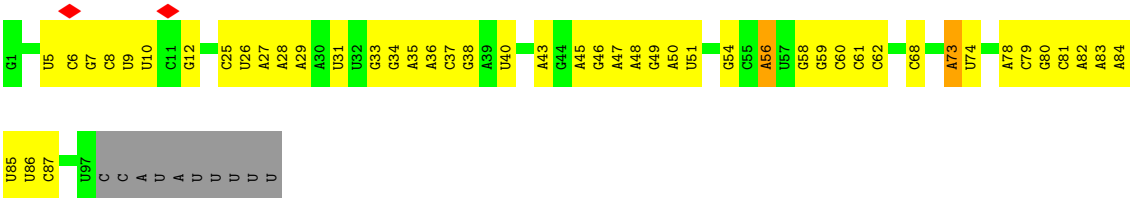


• Molecule 5: U5 small nuclear ribonucleoprotein 40 kDa protein

Chain E:

• Molecule 6: U6 snRNA

Chain F:

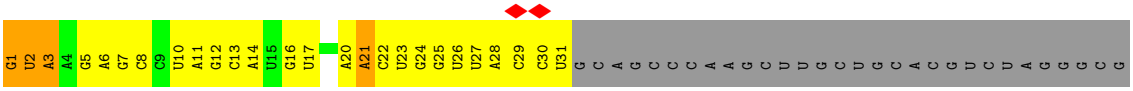


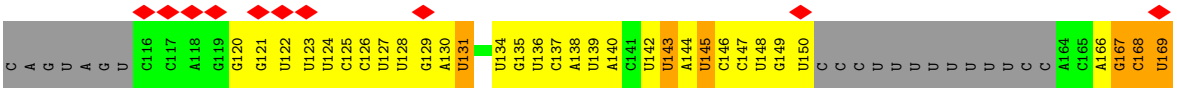
• Molecule 7: Pre-mRNA

Chain 4:

• Molecule 8: Pre-mRNA

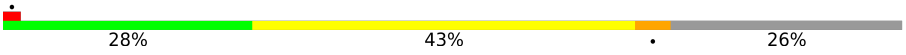
Chain G:

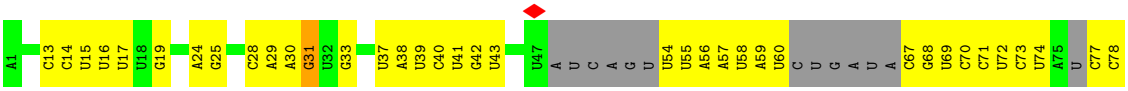


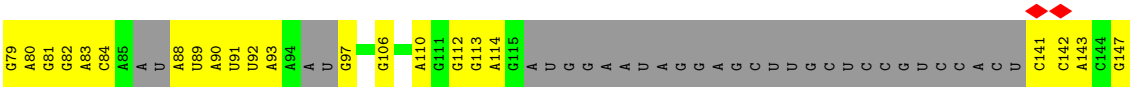


• Molecule 9: U2 snRNA

Chain H:

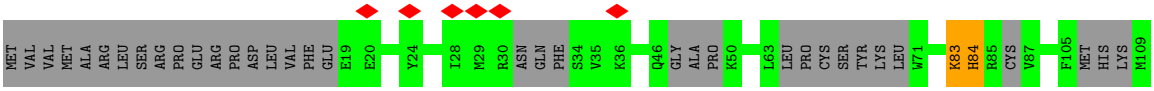


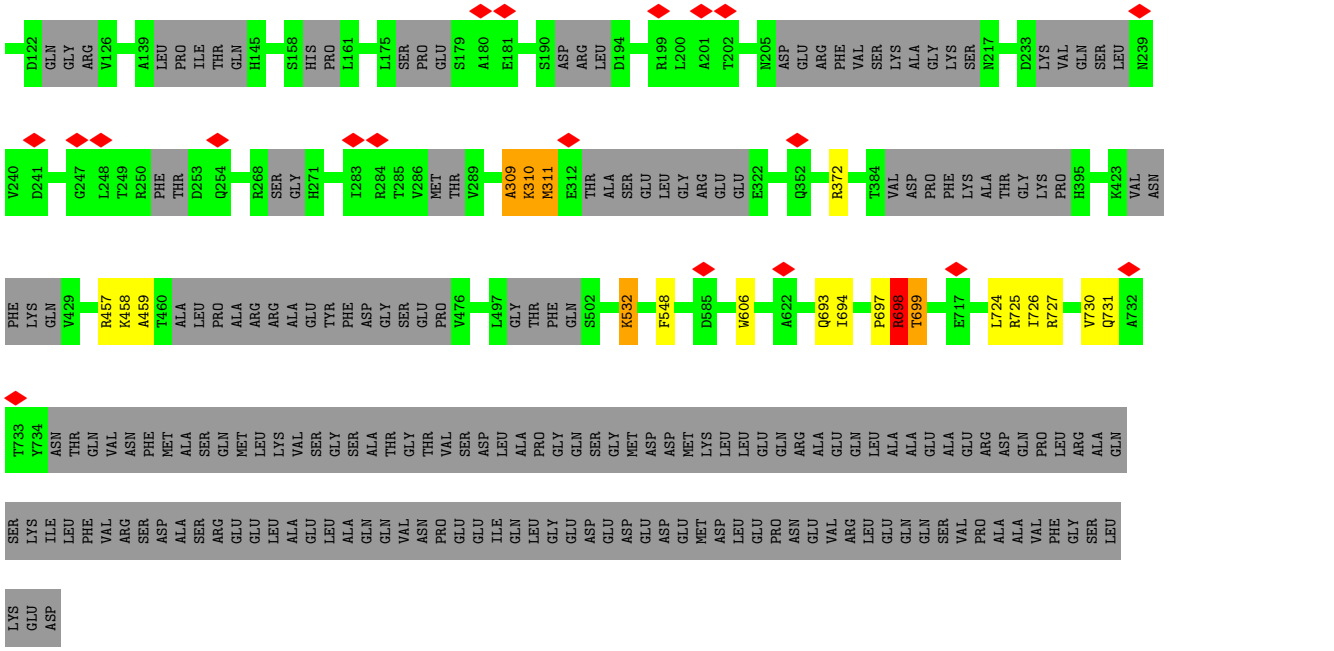




• Molecule 10: Pre-mRNA-splicing factor SYF1

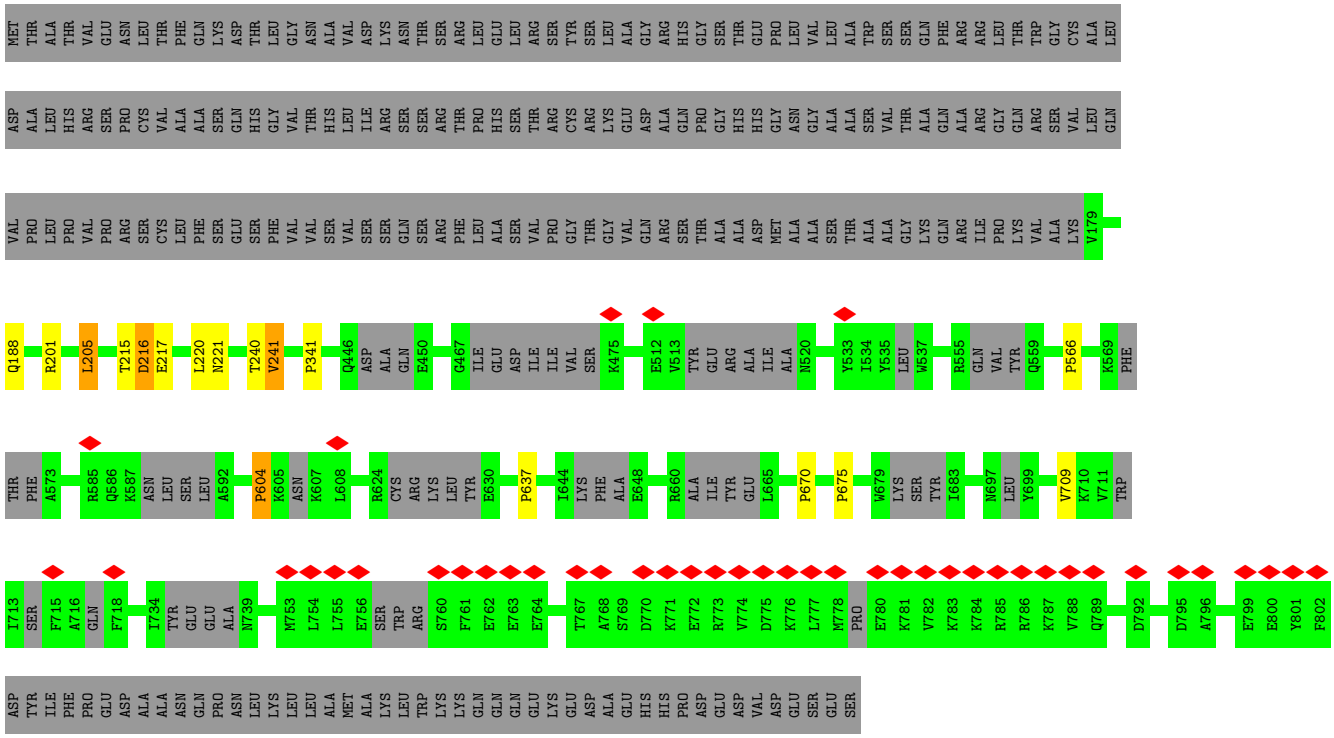
Chain I:





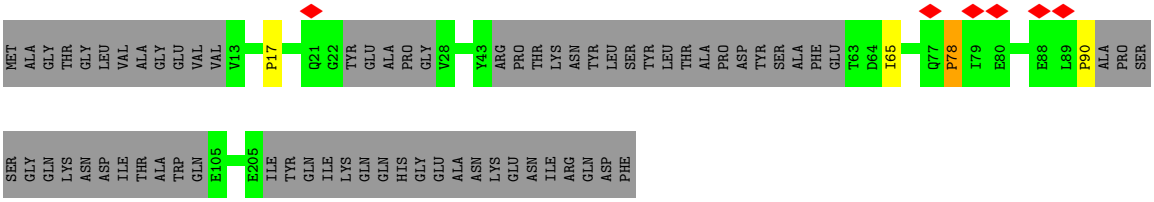
• Molecule 11: Crooked neck-like protein 1

Chain J:



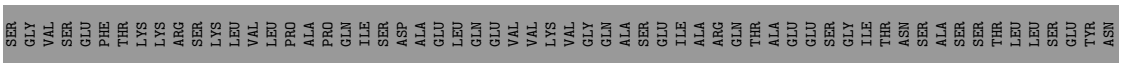
• Molecule 12: Pre-mRNA-splicing factor SPF27

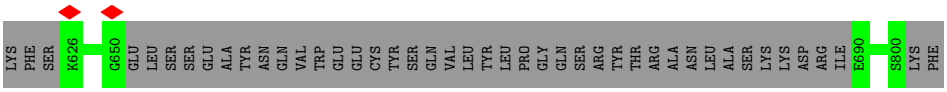
Chain K:



• Molecule 13: Cell division cycle 5-like protein

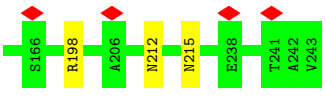
Chain L:





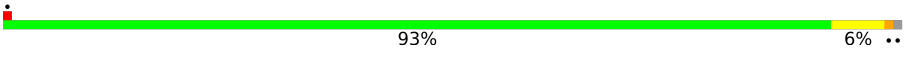
• Molecule 14: Pre-mRNA-splicing factor SYF2

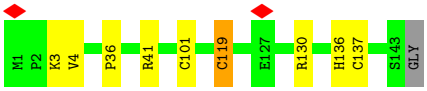
Chain M:



• Molecule 15: Protein BUD31 homolog

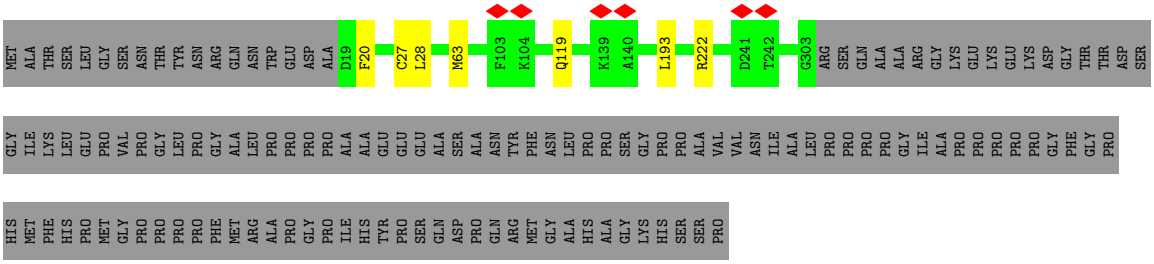
Chain N:





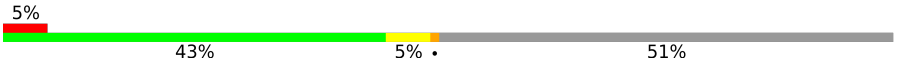
• Molecule 16: Pre-mRNA-splicing factor RBM22

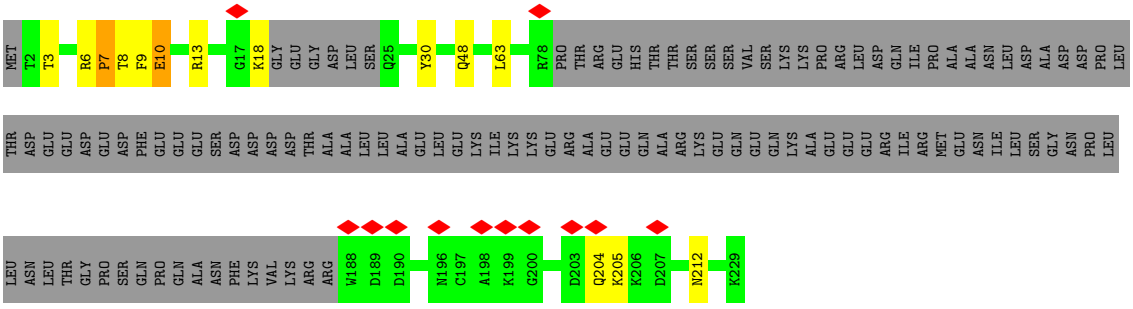
Chain O:



• Molecule 17: Spliceosome-associated protein CWC15 homolog

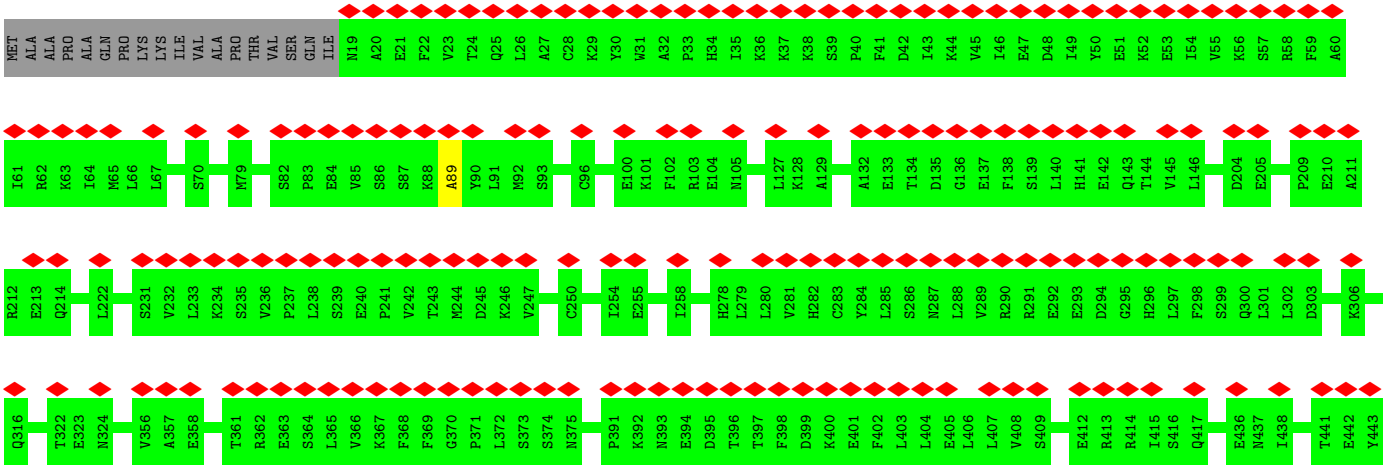
Chain P:

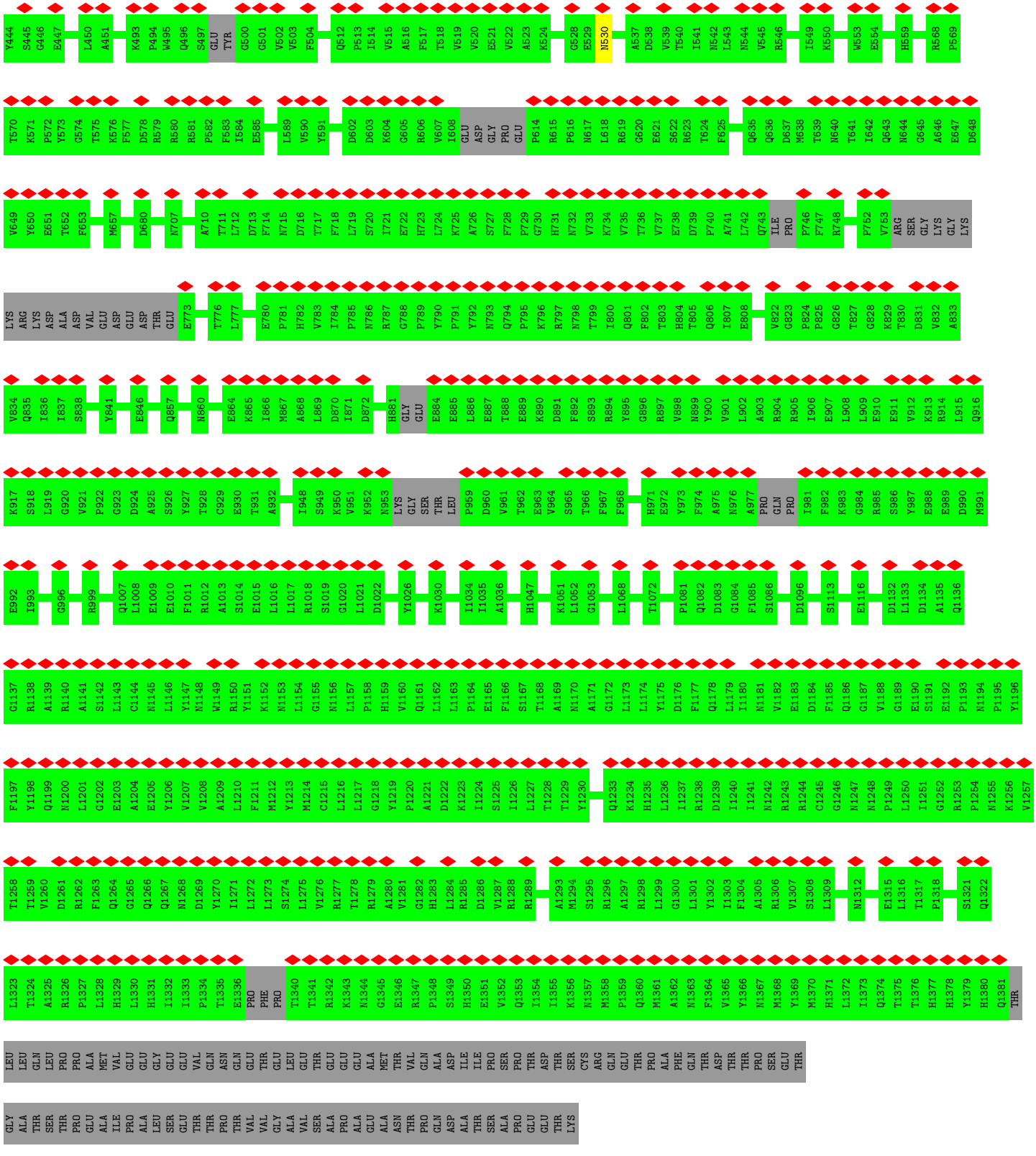




• Molecule 18: RNA helicase aquarius

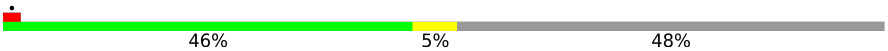
Chain Q:

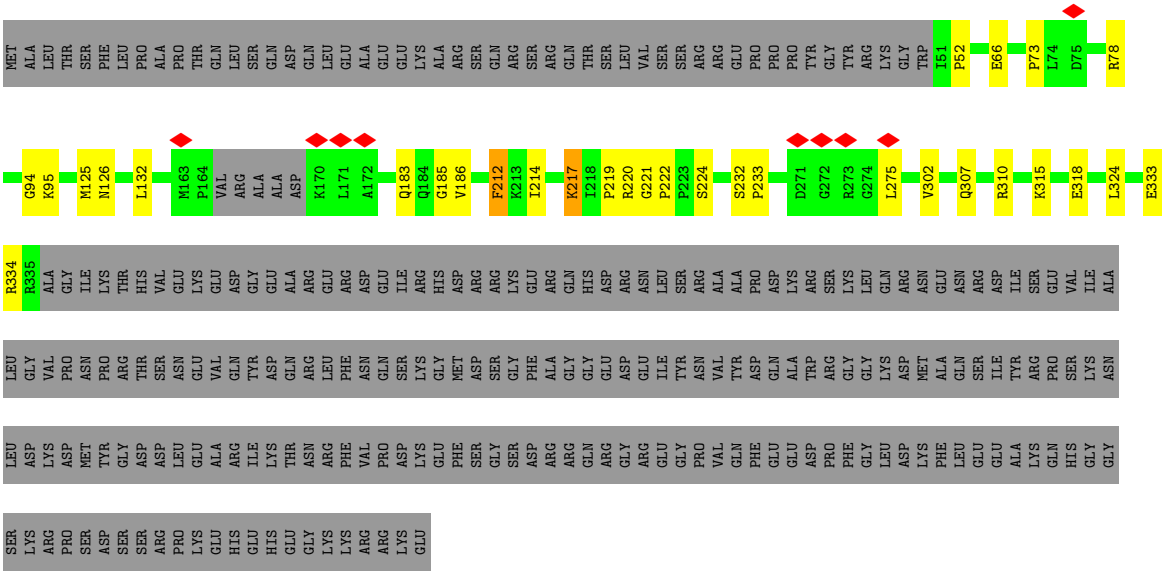




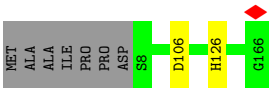
• Molecule 19: SNW domain-containing protein 1

Chain R:

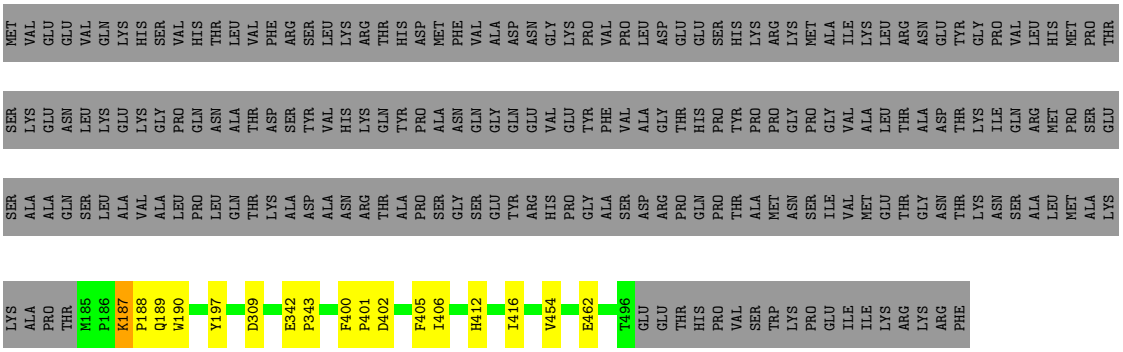




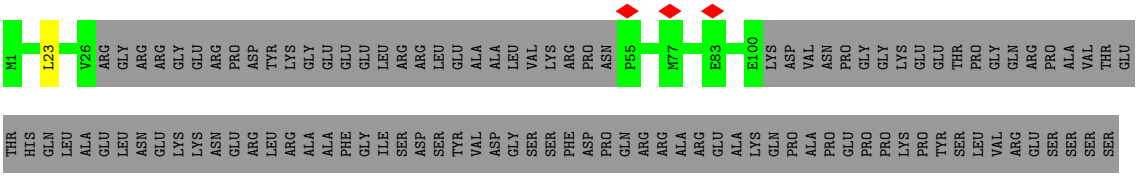
• Molecule 20: Peptidyl-prolyl cis-trans isomerase-like 1

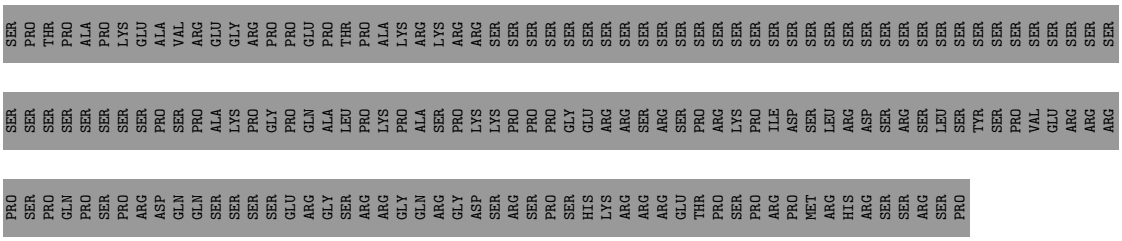


• Molecule 21: Pleiotropic regulator 1



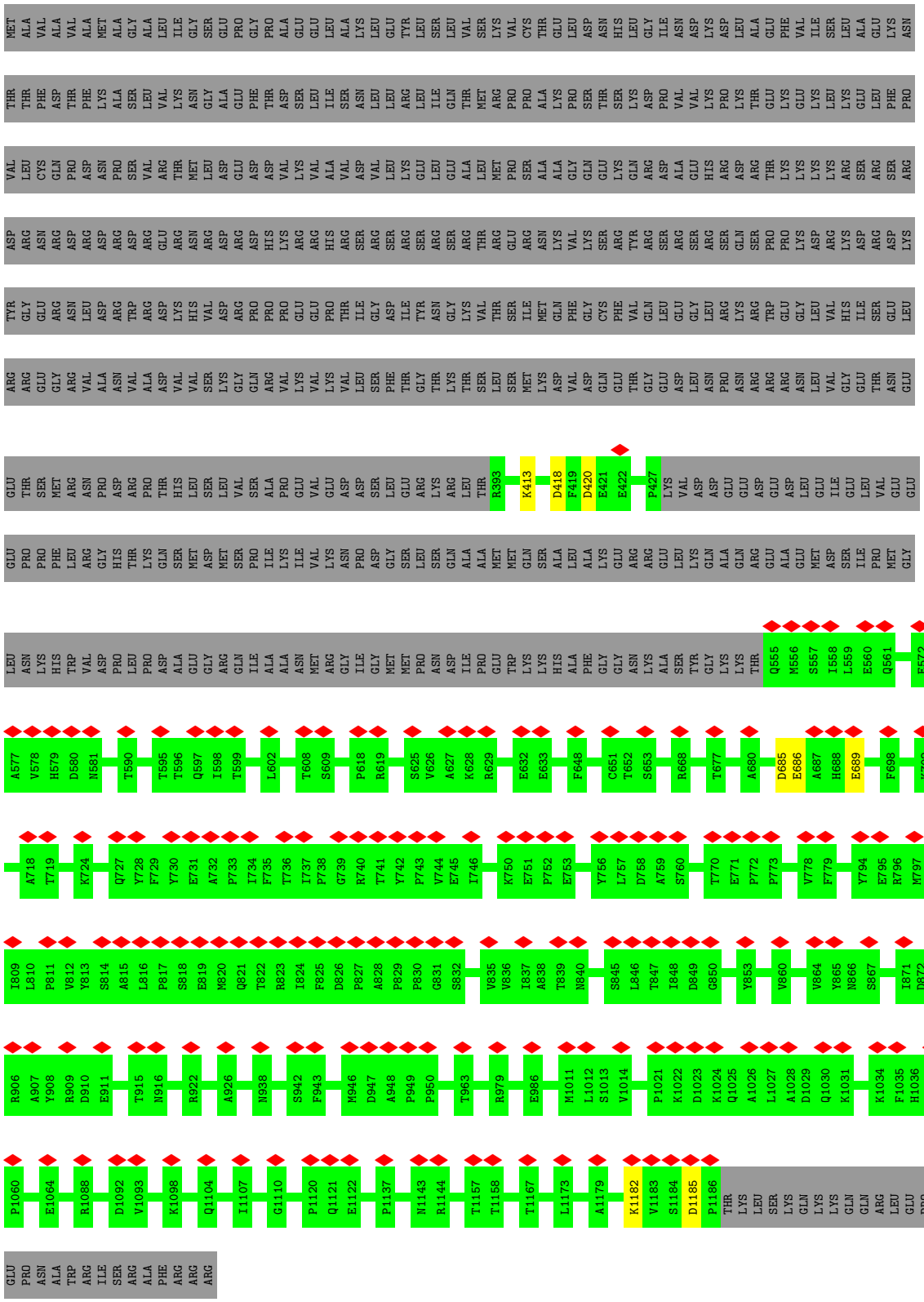
• Molecule 22: Serine/arginine repetitive matrix protein 2




SER PRO THR PRO ALA PRO LYS GLU ALA VAL ARG GLU GLY ARG PRO PRO GLU PRO THR PRO ALA LYS ARG LYS ARG ARG SER SER SER

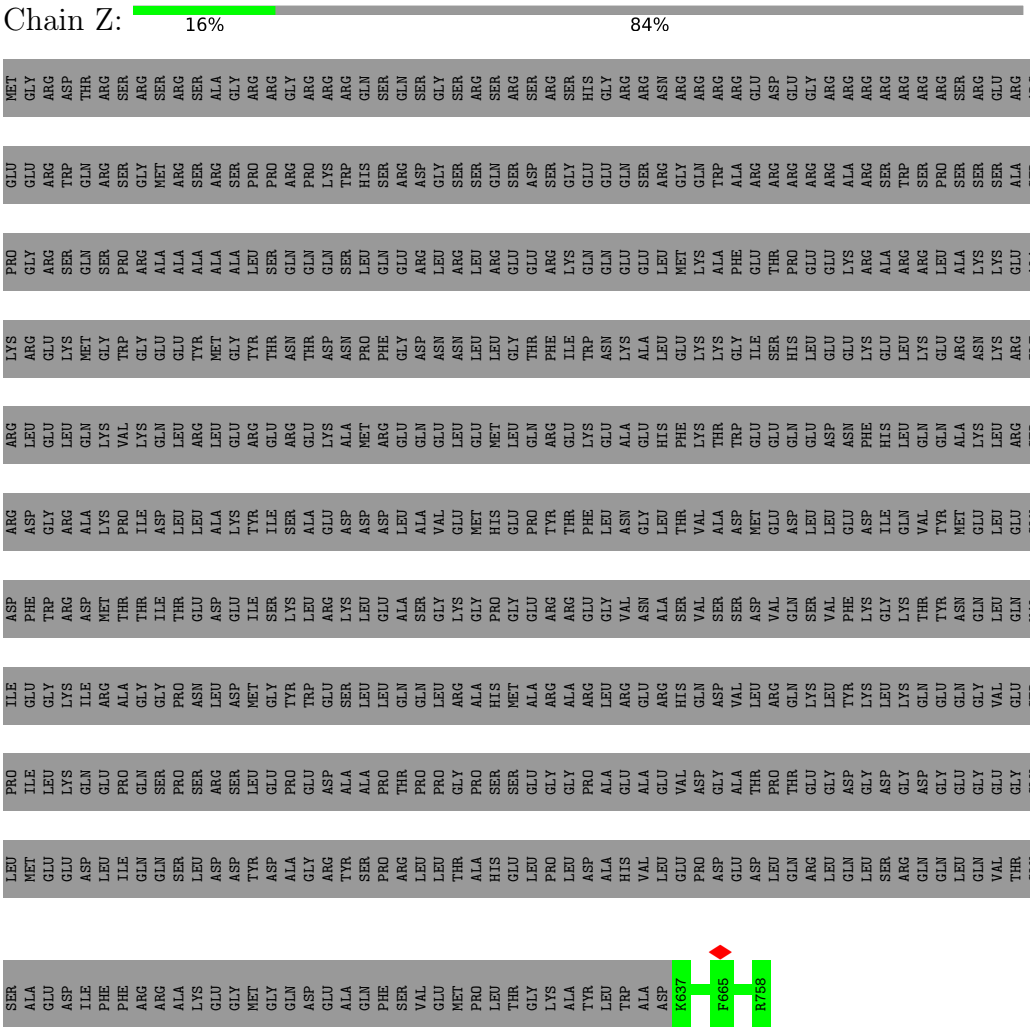
• Molecule 25: ATP-dependent RNA helicase DHX8

Chain Y:



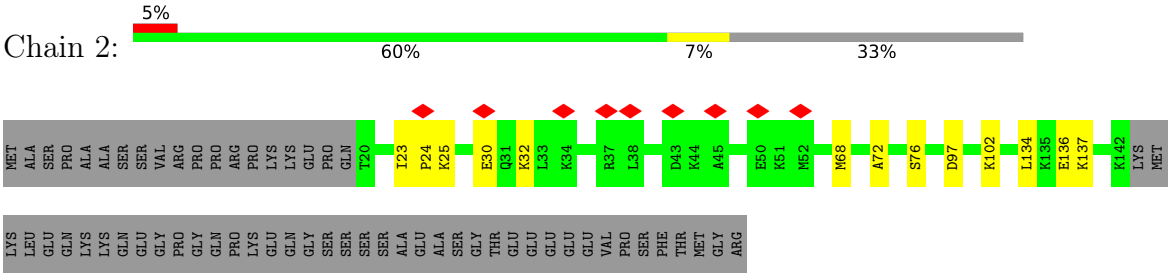
• Molecule 26: Cactin

Chain Z:



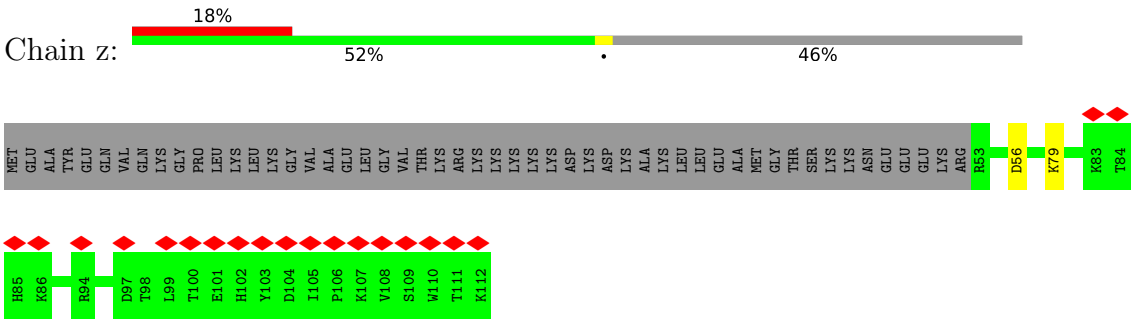
• Molecule 27: PRKR-interacting protein 1

Chain 2:



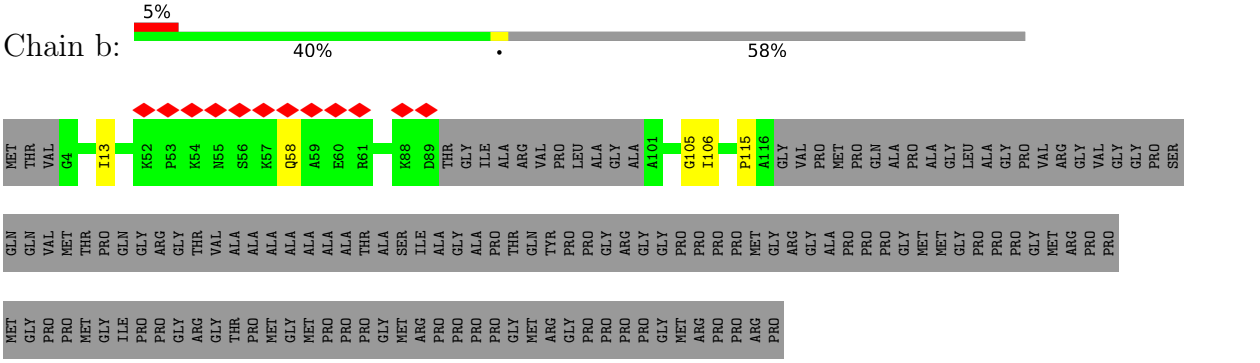
• Molecule 28: Protein FAM32A

Chain z:



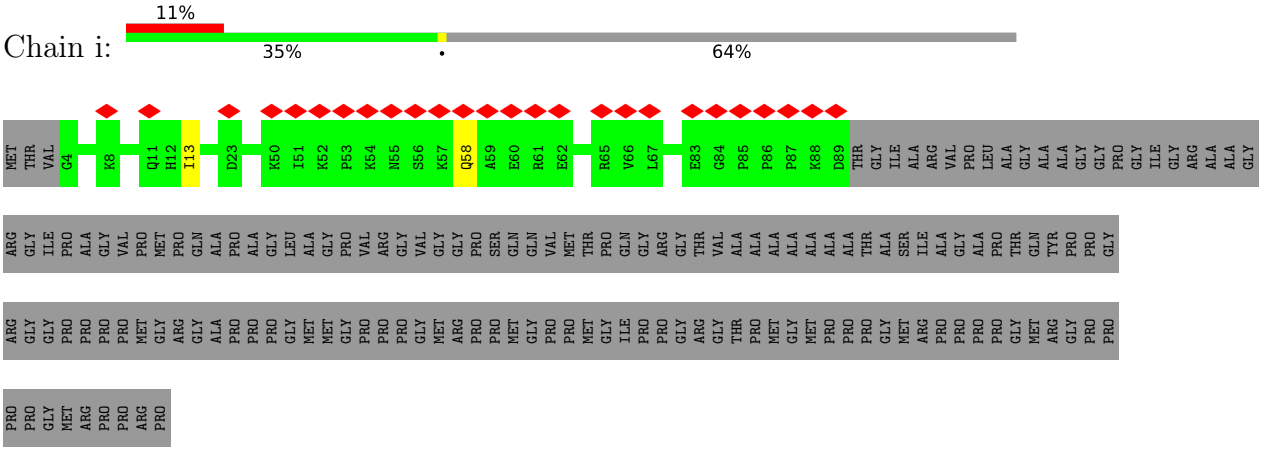
• Molecule 29: Small nuclear ribonucleoprotein-associated proteins B and B'

Chain b:



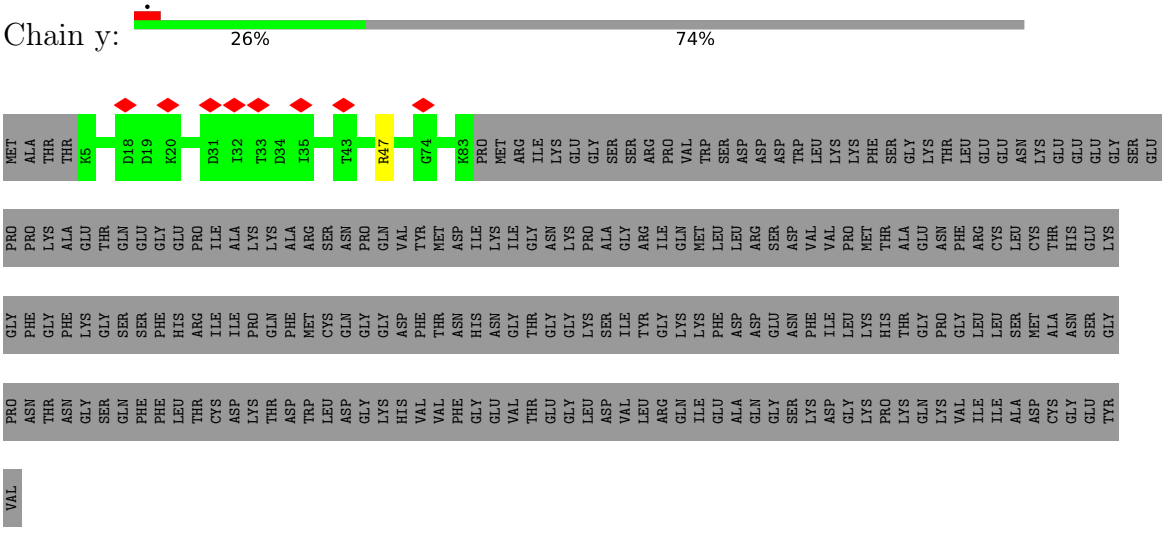
• Molecule 29: Small nuclear ribonucleoprotein-associated proteins B and B'

Chain i:



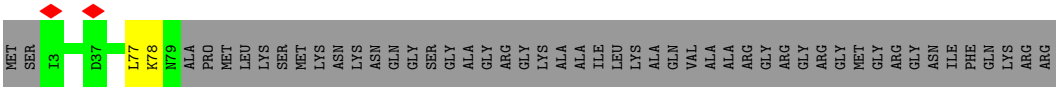
• Molecule 30: Peptidyl-prolyl cis-trans isomerase E

Chain y:



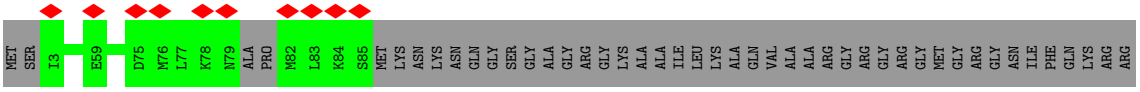
• Molecule 31: Small nuclear ribonucleoprotein Sm D3

Chain a:



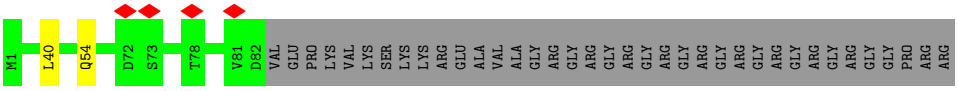
• Molecule 31: Small nuclear ribonucleoprotein Sm D3

Chain h:



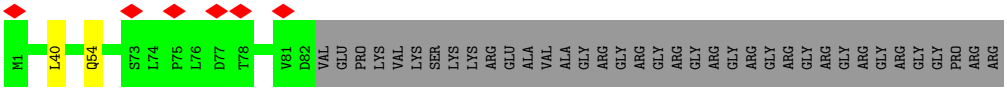
• Molecule 32: Small nuclear ribonucleoprotein Sm D1

Chain c:



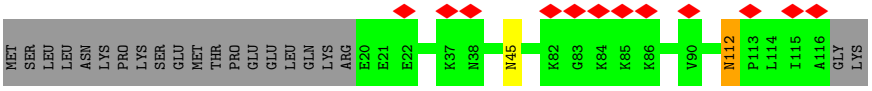
• Molecule 32: Small nuclear ribonucleoprotein Sm D1

Chain j:



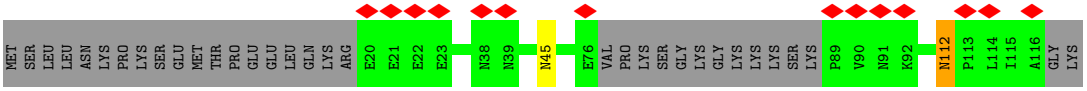
• Molecule 33: Small nuclear ribonucleoprotein Sm D2

Chain d:



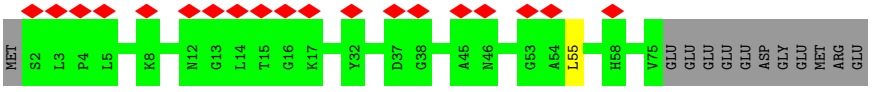
• Molecule 33: Small nuclear ribonucleoprotein Sm D2

Chain k:



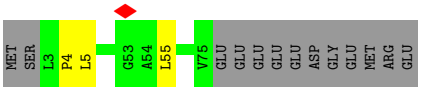
• Molecule 34: Small nuclear ribonucleoprotein F

Chain f:



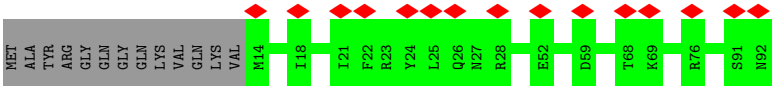
• Molecule 34: Small nuclear ribonucleoprotein F

Chain m:



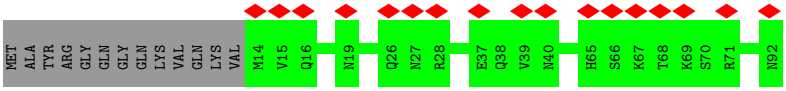
• Molecule 35: Small nuclear ribonucleoprotein E

Chain e:



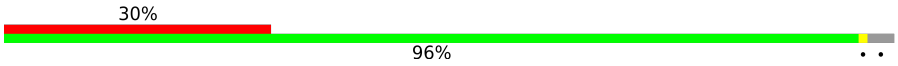
• Molecule 35: Small nuclear ribonucleoprotein E

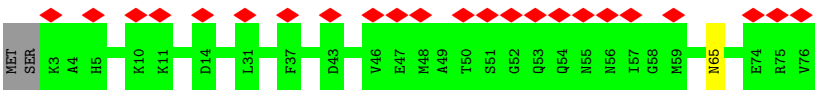
Chain l:



• Molecule 36: Small nuclear ribonucleoprotein G

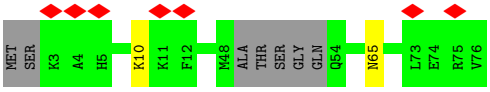
Chain g:





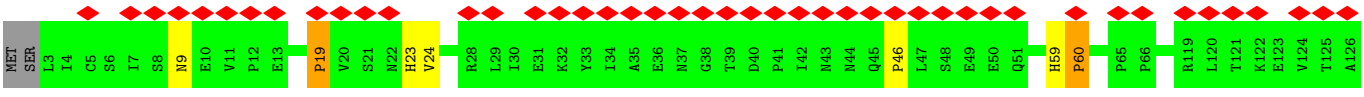
• Molecule 36: Small nuclear ribonucleoprotein G

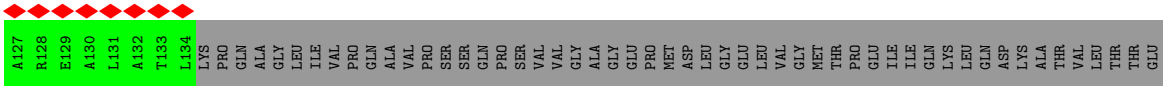
Chain n:

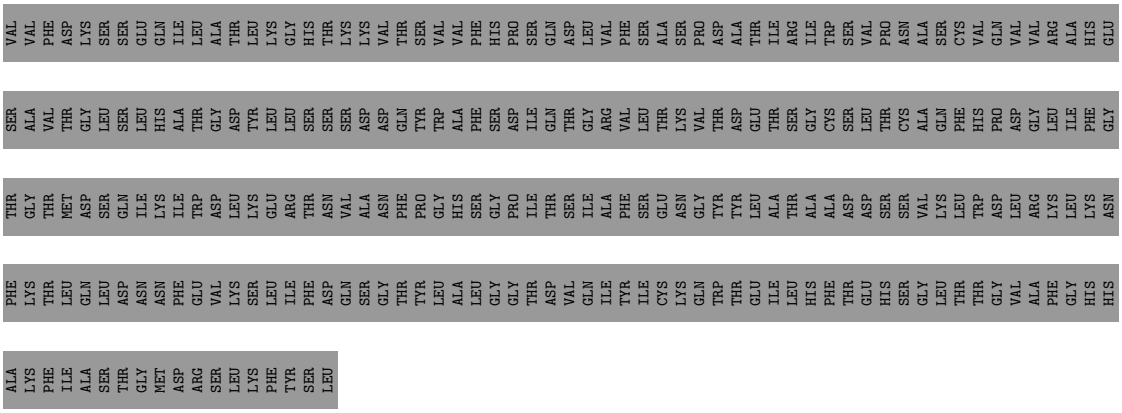


• Molecule 37: Pre-mRNA-processing factor 19

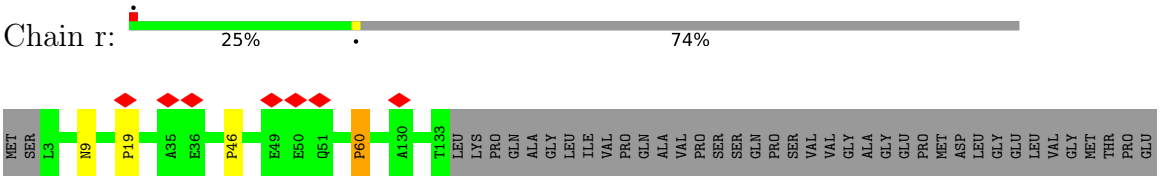
Chain q:



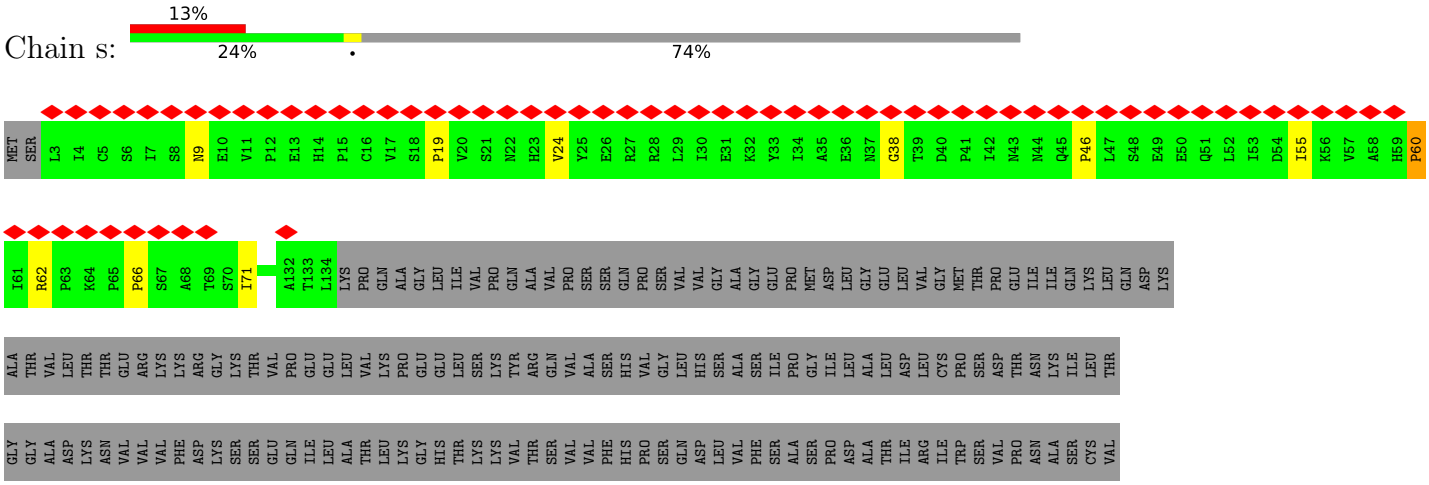


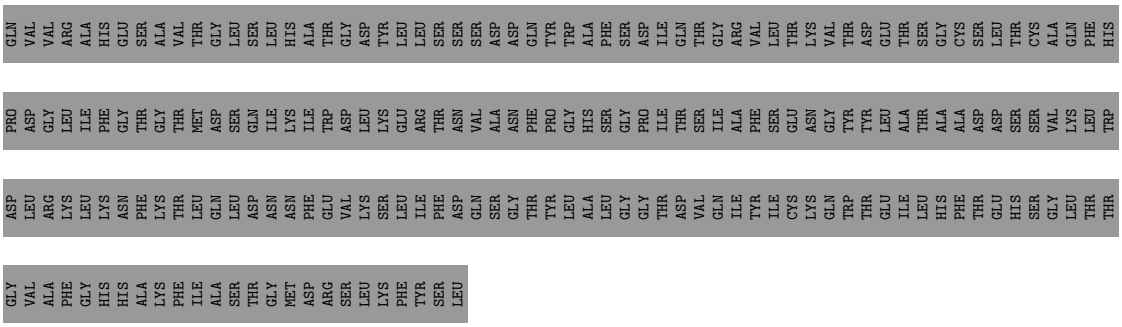


• Molecule 37: Pre-mRNA-processing factor 19



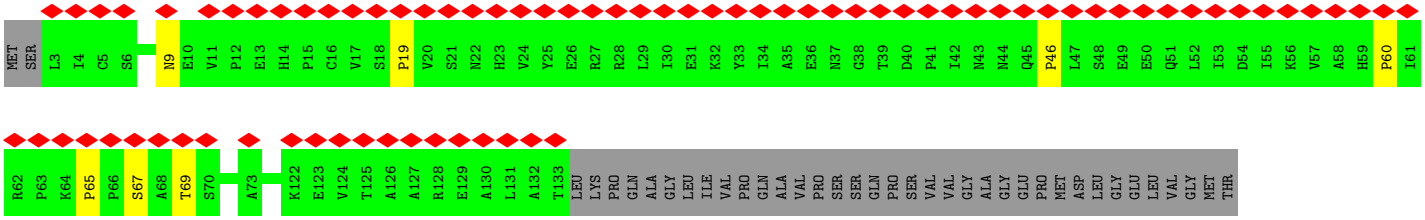
• Molecule 37: Pre-mRNA-processing factor 19





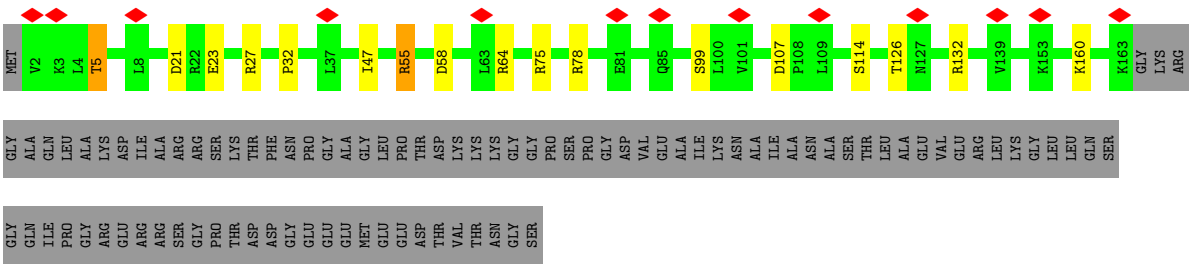
• Molecule 37: Pre-mRNA-processing factor 19

Chain t:



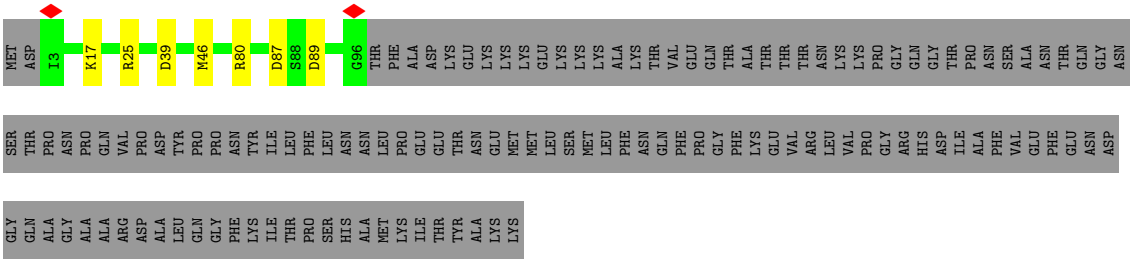
• Molecule 38: U2 small nuclear ribonucleoprotein A'

Chain o:



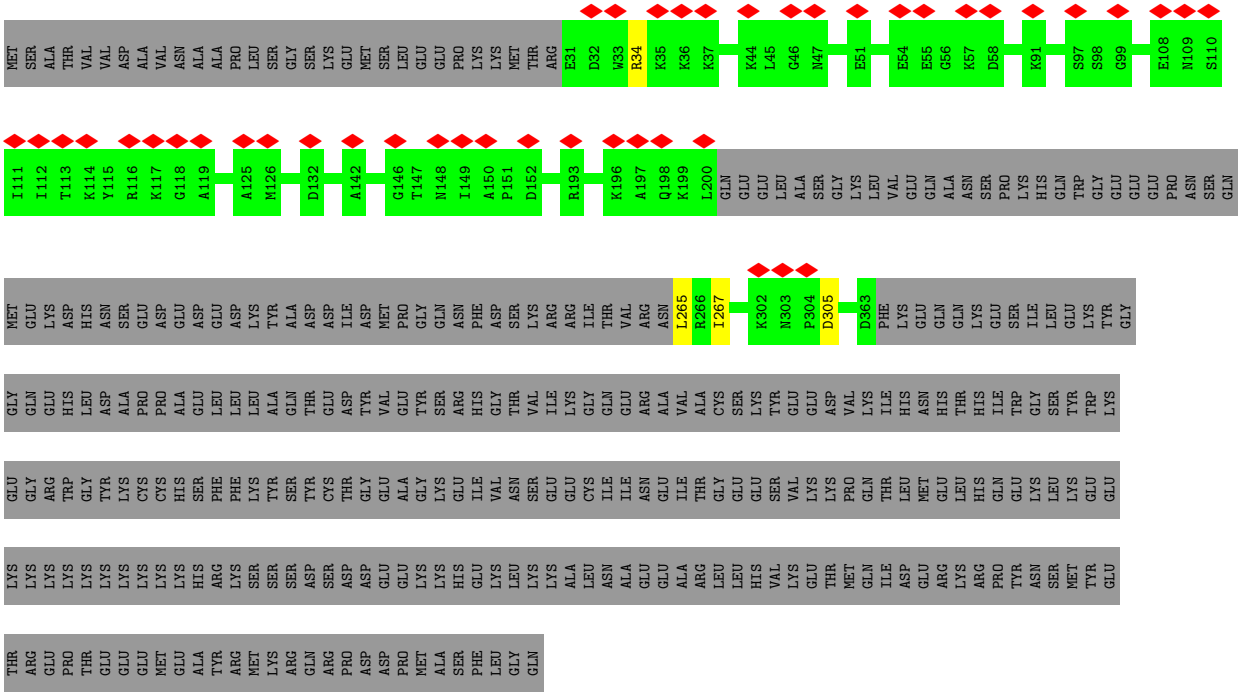
• Molecule 39: U2 small nuclear ribonucleoprotein B"

Chain p:



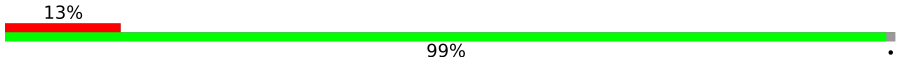
• Molecule 40: Pre-mRNA-splicing factor SLU7

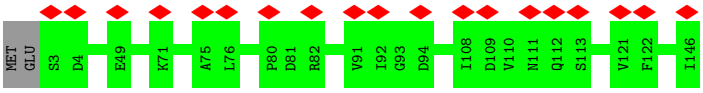
Chain 1:



• Molecule 41: Protein mago nashi homolog

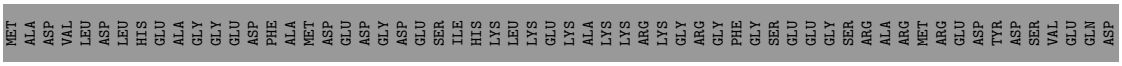
Chain v:

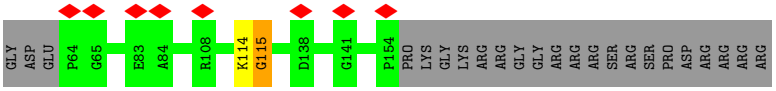




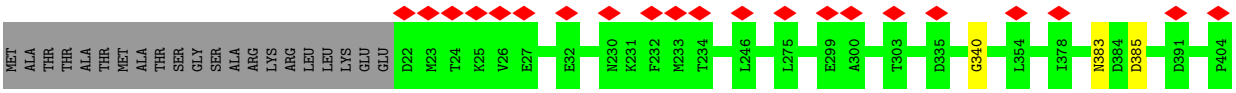
• Molecule 42: RNA-binding protein 8A

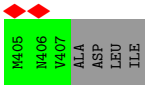
Chain w:



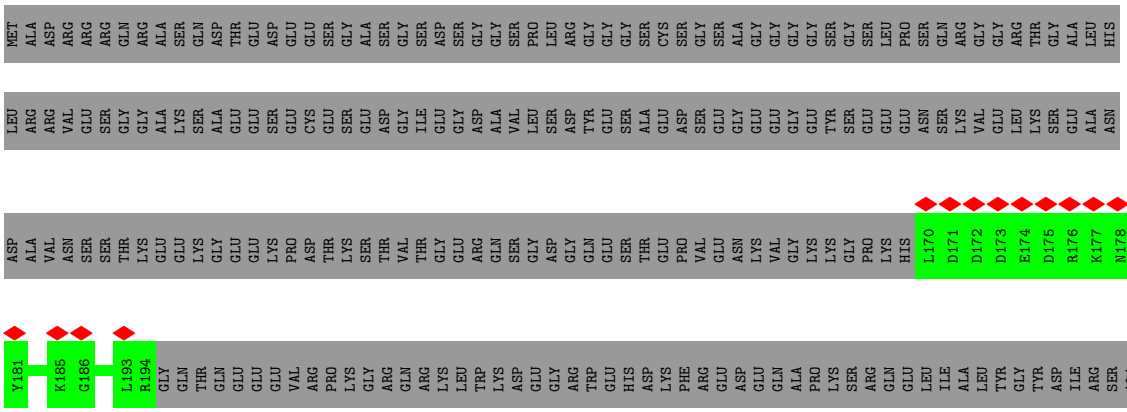


• Molecule 43: Eukaryotic initiation factor 4A-III



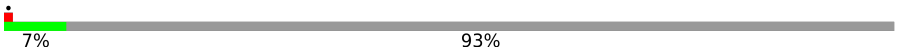


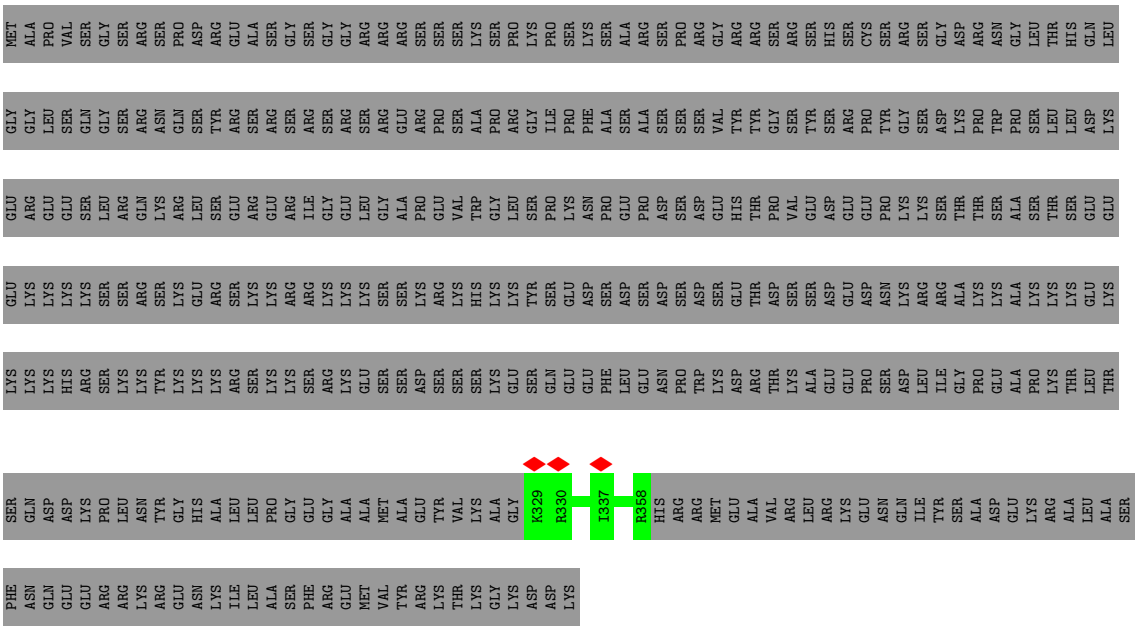
• Molecule 44: Protein CASC3



• Molecule 45: NF-kappa-B-activating protein

Chain 3:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	58374	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	2.144	Depositor
Minimum map value	-1.098	Depositor
Average map value	0.014	Depositor
Map value standard deviation	0.086	Depositor
Recommended contour level	0.37	Depositor
Map size (Å)	535.2, 535.2, 535.2	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.338, 1.338, 1.338	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: GTP, IHP, ATP, ZN, SEP, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.73	8/18191 (0.0%)	0.78	17/24720 (0.1%)
2	B	0.61	1/1970 (0.1%)	0.84	4/3060 (0.1%)
3	C	0.57	0/6938	0.71	3/9428 (0.0%)
4	D	0.33	0/8529	0.59	0/11891
5	E	0.56	0/2392	0.66	0/3242
6	F	0.49	0/2323	0.78	2/3619 (0.1%)
7	4	1.34	0/307	1.53	7/476 (1.5%)
8	G	0.63	4/1674 (0.2%)	1.24	19/2594 (0.7%)
9	H	0.95	26/3305 (0.8%)	1.63	112/5130 (2.2%)
10	I	0.43	0/3884	0.86	10/5301 (0.2%)
11	J	0.56	0/3861	0.60	6/5241 (0.1%)
12	K	0.44	0/768	0.55	2/1067 (0.2%)
13	L	0.48	0/3046	0.63	2/4115 (0.0%)
14	M	0.54	0/1119	0.70	1/1497 (0.1%)
15	N	0.77	3/1210 (0.2%)	0.69	0/1622
16	O	0.60	1/2344 (0.0%)	0.70	4/3163 (0.1%)
17	P	0.66	0/967	0.87	3/1285 (0.2%)
18	Q	0.24	0/6565	0.45	0/9143
19	R	0.69	3/2262 (0.1%)	0.84	6/3031 (0.2%)
20	S	0.52	0/1268	0.64	1/1714 (0.1%)
21	T	0.81	0/2519	0.82	5/3433 (0.1%)
22	U	0.49	0/424	0.59	0/582
23	V	0.34	0/2642	0.56	1/3602 (0.0%)
24	W	0.45	0/4237	0.72	4/5723 (0.1%)
25	Y	0.52	0/3436	0.75	3/4774 (0.1%)
26	Z	0.32	0/1129	0.53	0/1525
27	2	0.47	0/1030	0.75	1/1371 (0.1%)
28	z	0.27	0/505	0.55	1/672 (0.1%)
29	b	0.55	0/797	0.81	0/1062
29	i	0.53	0/700	0.82	0/933
30	y	0.36	0/389	0.72	1/540 (0.2%)
31	a	0.47	0/616	0.72	1/830 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
31	h	0.47	0/639	0.68	0/857
32	c	0.56	0/657	0.77	0/888
32	j	0.56	0/657	0.77	0/888
33	d	0.69	0/786	0.86	0/1053
33	k	0.69	0/696	0.86	0/935
34	f	0.82	0/588	0.84	0/795
34	m	0.83	0/578	0.88	0/783
35	e	0.62	0/660	0.83	0/886
35	l	0.61	0/660	0.84	0/886
36	g	0.53	0/584	0.78	0/779
36	n	0.53	0/548	0.83	0/729
37	q	0.35	0/658	0.63	3/919 (0.3%)
37	r	0.32	0/653	0.59	3/912 (0.3%)
37	s	0.34	0/658	0.65	3/919 (0.3%)
37	t	0.35	0/653	0.59	3/912 (0.3%)
38	o	0.59	0/1299	1.63	17/1761 (1.0%)
39	p	0.56	0/774	1.35	6/1035 (0.6%)
40	1	0.38	0/2262	0.56	0/3045
41	v	0.30	0/710	0.65	0/987
42	w	0.30	0/444	0.78	2/614 (0.3%)
43	u	0.32	0/1906	0.69	0/2653
44	x	0.34	0/123	0.70	0/170
45	3	0.32	0/232	0.48	0/307
All	All	0.57	46/108772 (0.0%)	0.80	253/150099 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	19
3	C	0	9
4	D	0	1
5	E	0	1
10	I	0	6
11	J	0	5
15	N	0	4
16	O	0	1
17	P	0	3
19	R	0	7
21	T	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
24	W	0	2
33	d	0	1
33	k	0	1
All	All	0	63

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1724	PRO	N-CA	12.46	1.68	1.47
19	R	222	PRO	N-CA	12.17	1.68	1.47
8	G	21	A	O3'-P	-8.36	1.51	1.61
1	A	1529	ILE	C-N	7.75	1.49	1.34
9	H	142	C	C1'-N1	7.48	1.59	1.48
9	H	77	C	C1'-N1	7.46	1.59	1.48
8	G	145	U	O3'-P	-7.29	1.52	1.61
9	H	72	U	C1'-N1	7.01	1.59	1.48
9	H	55	U	C1'-N1	7.00	1.59	1.48
2	B	103	G	C1'-N9	-6.98	1.37	1.46
9	H	74	U	C1'-N1	6.95	1.59	1.48
9	H	54	U	C1'-N1	6.94	1.59	1.48
9	H	89	U	C1'-N1	6.93	1.59	1.48
9	H	92	U	C1'-N1	6.93	1.59	1.48
9	H	69	U	C1'-N1	6.92	1.59	1.48
9	H	60	U	C1'-N1	6.90	1.59	1.48
15	N	101	CYS	CB-SG	-6.88	1.70	1.82
9	H	58	U	C1'-N1	6.87	1.59	1.48
9	H	91	U	C1'-N1	6.85	1.59	1.48
9	H	150	U	C1'-N1	6.78	1.58	1.48
9	H	182	U	C1'-N1	6.75	1.58	1.48
9	H	73	C	C1'-N1	6.46	1.58	1.48
9	H	151	C	C1'-N1	6.46	1.58	1.48
9	H	67	C	C1'-N1	6.44	1.58	1.48
9	H	141	C	C1'-N1	6.43	1.58	1.48
9	H	184	C	C1'-N1	6.39	1.58	1.48
9	H	97	G	C1'-N9	-6.34	1.38	1.46
9	H	71	C	C1'-N1	6.33	1.58	1.48
9	H	70	C	C1'-N1	6.32	1.58	1.48
9	H	148	C	C1'-N1	6.32	1.58	1.48
9	H	84	C	C1'-N1	6.26	1.58	1.48
9	H	78	C	C1'-N1	6.26	1.58	1.48
8	G	168	C	O3'-P	6.16	1.68	1.61
1	A	863	GLU	CD-OE1	-6.04	1.19	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	776	LEU	C-O	-5.95	1.12	1.23
19	R	219	PRO	C-O	-5.86	1.11	1.23
1	A	863	GLU	CD-OE2	-5.85	1.19	1.25
8	G	3	A	O3'-P	-5.84	1.54	1.61
16	O	27	CYS	CB-SG	-5.65	1.72	1.81
1	A	771	VAL	C-O	-5.46	1.12	1.23
15	N	137	CYS	CB-SG	-5.39	1.73	1.81
15	N	119	CYS	CB-SG	-5.31	1.73	1.81
19	R	221	GLY	C-N	5.30	1.44	1.34
1	A	859	SER	CA-CB	-5.21	1.45	1.52
9	H	110	A	C1'-N9	-5.11	1.39	1.46
1	A	1438	VAL	CB-CG1	-5.10	1.42	1.52

All (253) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	o	55	ARG	NE-CZ-NH1	15.12	127.86	120.30
1	A	535	ARG	CB-CA-C	14.48	139.35	110.40
1	A	772	CYS	CA-CB-SG	-13.84	89.09	114.00
38	o	55	ARG	CD-NE-CZ	13.75	142.85	123.60
8	G	167	G	O4'-C1'-N9	-12.96	97.83	108.20
9	H	167	U	C5-C4-O4	11.87	133.02	125.90
8	G	177	G	N9-C1'-C2'	-11.45	99.12	114.00
38	o	55	ARG	NE-CZ-NH2	-11.38	114.61	120.30
38	o	75	ARG	NE-CZ-NH1	-11.23	114.68	120.30
7	4	-12	G	N9-C1'-C2'	-11.05	99.64	114.00
9	H	164	C	N1-C2-O2	-10.13	112.82	118.90
9	H	31	G	N9-C1'-C2'	-9.81	101.21	112.00
8	G	177	G	C4'-C3'-O3'	9.44	131.87	113.00
8	G	1	G	N9-C1'-C2'	-9.24	101.83	112.00
39	p	25	ARG	NE-CZ-NH1	9.17	124.88	120.30
6	F	56	A	O5'-P-OP1	-8.93	97.67	105.70
9	H	162	U	N3-C2-O2	-8.92	115.96	122.20
39	p	80	ARG	CD-NE-CZ	8.87	136.02	123.60
1	A	1561	PHE	CB-CA-C	-8.63	93.14	110.40
7	4	-6	C	C2-N1-C1'	8.50	128.15	118.80
2	B	20	G	N9-C1'-C2'	8.50	125.05	114.00
9	H	164	C	C5'-C4'-O4'	-8.34	99.09	109.10
8	G	3	A	N9-C1'-C2'	-8.32	102.85	112.00
9	H	169	C	P-O3'-C3'	8.22	129.57	119.70
1	A	861	ARG	CG-CD-NE	-8.20	94.59	111.80
10	I	84	HIS	O-C-N	-8.15	109.65	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	I	83	LYS	O-C-N	-8.15	109.66	122.70
10	I	311	MET	O-C-N	-8.13	109.69	122.70
10	I	310	LYS	O-C-N	-8.11	109.72	122.70
9	H	167	U	N3-C4-O4	-8.07	113.75	119.40
10	I	309	ALA	O-C-N	-8.04	109.84	122.70
9	H	166	G	O4'-C1'-N9	7.99	114.59	108.20
16	O	193	LEU	CA-CB-CG	7.88	133.43	115.30
8	G	1	G	C1'-C2'-O2'	-7.87	87.00	110.60
8	G	172	C	P-O3'-C3'	7.83	129.10	119.70
21	T	402	ASP	CB-CG-OD1	7.70	125.23	118.30
38	o	107	ASP	CB-CG-OD1	7.62	125.16	118.30
1	A	1850	ARG	N-CA-CB	7.60	124.28	110.60
9	H	164	C	P-O3'-C3'	7.52	128.73	119.70
9	H	167	U	N1-C2-O2	7.52	128.06	122.80
38	o	27	ARG	NE-CZ-NH2	-7.50	116.55	120.30
9	H	164	C	N3-C2-O2	7.49	127.14	121.90
1	A	663	ARG	CG-CD-NE	-7.38	96.29	111.80
1	A	1724	PRO	N-CA-C	-7.36	92.97	112.10
19	R	222	PRO	CA-N-CD	-7.32	101.25	111.50
9	H	69	U	OP2-P-O3'	7.29	121.25	105.20
9	H	114	A	OP2-P-O3'	7.27	121.19	105.20
8	G	169	U	N1-C1'-C2'	-7.26	104.01	112.00
9	H	148	C	OP2-P-O3'	7.24	121.13	105.20
9	H	73	C	OP2-P-O3'	7.24	121.13	105.20
9	H	70	C	OP2-P-O3'	7.23	121.11	105.20
9	H	59	A	OP2-P-O3'	7.23	121.11	105.20
9	H	113	G	OP2-P-O3'	7.23	121.10	105.20
9	H	183	G	OP2-P-O3'	7.23	121.10	105.20
9	H	77	C	OP2-P-O3'	7.22	121.09	105.20
9	H	88	A	OP2-P-O3'	7.21	121.07	105.20
9	H	57	A	OP2-P-O3'	7.21	121.06	105.20
9	H	55	U	OP2-P-O3'	7.21	121.05	105.20
9	H	82	G	OP2-P-O3'	7.21	121.05	105.20
9	H	141	C	OP2-P-O3'	7.21	121.05	105.20
9	H	72	U	OP2-P-O3'	7.21	121.05	105.20
9	H	71	C	OP2-P-O3'	7.20	121.05	105.20
9	H	149	A	OP2-P-O3'	7.20	121.05	105.20
9	H	91	U	OP2-P-O3'	7.20	121.04	105.20
9	H	181	G	OP2-P-O3'	7.20	121.04	105.20
9	H	182	U	OP2-P-O3'	7.20	121.04	105.20
9	H	92	U	OP2-P-O3'	7.20	121.03	105.20
9	H	54	U	OP2-P-O3'	7.20	121.03	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	H	68	G	OP2-P-O3'	7.20	121.03	105.20
9	H	81	G	OP2-P-O3'	7.20	121.03	105.20
9	H	78	C	OP2-P-O3'	7.19	121.02	105.20
9	H	180	G	OP2-P-O3'	7.19	121.01	105.20
9	H	79	G	OP2-P-O3'	7.18	121.00	105.20
9	H	58	U	OP2-P-O3'	7.18	120.99	105.20
9	H	84	C	OP2-P-O3'	7.17	120.98	105.20
9	H	89	U	OP2-P-O3'	7.17	120.98	105.20
9	H	90	A	OP2-P-O3'	7.17	120.98	105.20
9	H	74	U	OP2-P-O3'	7.17	120.97	105.20
9	H	150	U	OP2-P-O3'	7.17	120.96	105.20
9	H	67	C	OP2-P-O3'	7.16	120.96	105.20
9	H	93	A	OP2-P-O3'	7.16	120.95	105.20
9	H	56	A	OP2-P-O3'	7.15	120.93	105.20
9	H	83	A	OP2-P-O3'	7.14	120.90	105.20
9	H	168	A	P-O5'-C5'	-7.14	109.48	120.90
9	H	80	A	OP2-P-O3'	7.13	120.89	105.20
37	s	60	PRO	N-CA-CB	7.09	111.81	103.30
9	H	167	U	N3-C2-O2	-7.06	117.26	122.20
21	T	187	LYS	C-N-CD	-7.02	105.16	120.60
8	G	174	G	C4'-C3'-O3'	6.96	126.92	113.00
16	O	119	GLN	CB-CA-C	6.88	124.17	110.40
9	H	82	G	O3'-P-O5'	-6.86	90.97	104.00
9	H	183	G	O3'-P-O5'	-6.85	90.99	104.00
9	H	77	C	O3'-P-O5'	-6.82	91.03	104.00
9	H	68	G	O3'-P-O5'	-6.81	91.05	104.00
9	H	78	C	O3'-P-O5'	-6.81	91.05	104.00
9	H	141	C	O3'-P-O5'	-6.81	91.06	104.00
9	H	56	A	O3'-P-O5'	-6.81	91.06	104.00
9	H	113	G	O3'-P-O5'	-6.81	91.06	104.00
9	H	148	C	O3'-P-O5'	-6.81	91.07	104.00
9	H	59	A	O3'-P-O5'	-6.80	91.07	104.00
9	H	54	U	O3'-P-O5'	-6.80	91.09	104.00
9	H	180	G	O3'-P-O5'	-6.80	91.09	104.00
9	H	57	A	O3'-P-O5'	-6.79	91.10	104.00
9	H	182	U	O3'-P-O5'	-6.79	91.10	104.00
19	R	132	LEU	CA-CB-CG	6.79	130.91	115.30
9	H	72	U	O3'-P-O5'	-6.79	91.11	104.00
9	H	74	U	O3'-P-O5'	-6.79	91.11	104.00
9	H	73	C	O3'-P-O5'	-6.78	91.11	104.00
2	B	104	C	C2'-C3'-O3'	-6.78	94.58	109.50
9	H	91	U	O3'-P-O5'	-6.78	91.12	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	H	93	A	O3'-P-O5'	-6.78	91.12	104.00
9	H	150	U	O3'-P-O5'	-6.78	91.12	104.00
9	H	149	A	O3'-P-O5'	-6.78	91.13	104.00
9	H	81	G	O3'-P-O5'	-6.77	91.14	104.00
9	H	90	A	O3'-P-O5'	-6.77	91.14	104.00
9	H	181	G	O3'-P-O5'	-6.77	91.14	104.00
9	H	79	G	O3'-P-O5'	-6.77	91.14	104.00
9	H	55	U	O3'-P-O5'	-6.76	91.15	104.00
9	H	80	A	O3'-P-O5'	-6.76	91.15	104.00
9	H	84	C	O3'-P-O5'	-6.76	91.15	104.00
9	H	155	C	P-O3'-C3'	6.76	127.81	119.70
9	H	89	U	O3'-P-O5'	-6.76	91.16	104.00
9	H	92	U	O3'-P-O5'	-6.76	91.16	104.00
9	H	67	C	O3'-P-O5'	-6.75	91.19	104.00
9	H	69	U	O3'-P-O5'	-6.75	91.18	104.00
9	H	71	C	O3'-P-O5'	-6.74	91.19	104.00
9	H	58	U	O3'-P-O5'	-6.74	91.19	104.00
9	H	114	A	O3'-P-O5'	-6.74	91.19	104.00
38	o	23	GLU	OE1-CD-OE2	-6.74	115.21	123.30
9	H	83	A	O3'-P-O5'	-6.73	91.20	104.00
9	H	88	A	O3'-P-O5'	-6.73	91.21	104.00
9	H	70	C	O3'-P-O5'	-6.72	91.23	104.00
9	H	166	G	C8-N9-C4	-6.71	103.72	106.40
37	t	60	PRO	N-CA-CB	6.68	111.32	103.30
39	p	89	ASP	CB-CG-OD1	6.67	124.30	118.30
23	V	467	LEU	CA-CB-CG	6.64	130.58	115.30
8	G	174	G	N9-C1'-C2'	-6.63	104.70	112.00
37	q	46	PRO	N-CA-CB	6.60	111.22	103.30
37	s	46	PRO	N-CA-CB	6.58	111.19	103.30
1	A	343	GLU	N-CA-CB	-6.57	98.78	110.60
37	r	46	PRO	N-CA-CB	6.51	111.12	103.30
12	K	90	PRO	N-CA-CB	6.47	111.06	103.30
37	q	60	PRO	N-CA-CB	6.46	111.05	103.30
42	w	114	LYS	N-CA-C	-6.42	93.67	111.00
13	L	159	LEU	CA-CB-CG	6.40	130.02	115.30
9	H	165	A	O4'-C1'-N9	-6.37	103.11	108.20
8	G	131	U	C2'-C3'-O3'	-6.36	95.51	109.50
38	o	5	THR	N-CA-CB	-6.34	98.25	110.30
8	G	171	G	C2'-C3'-O3'	6.34	123.84	113.70
27	2	97	ASP	CA-C-N	-6.32	103.31	117.20
12	K	78	PRO	N-CA-CB	6.28	110.83	103.30
3	C	308	CYS	CA-CB-SG	6.26	125.27	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	H	166	G	N9-C4-C5	6.25	107.90	105.40
13	L	9	GLY	C-N-CA	6.24	137.29	121.70
8	G	21	A	O3'-P-O5'	6.13	115.66	104.00
7	4	-6	C	C6-N1-C1'	-6.11	113.46	120.80
38	o	78	ARG	NE-CZ-NH2	-6.10	117.25	120.30
9	H	166	G	N3-C4-C5	-6.04	125.58	128.60
38	o	132	ARG	CD-NE-CZ	6.01	132.02	123.60
16	O	193	LEU	CB-CG-CD2	-6.00	100.80	111.00
38	o	21	ASP	CB-CG-OD1	6.00	123.70	118.30
9	H	162	U	N1-C2-O2	6.00	127.00	122.80
11	J	220	LEU	CA-CB-CG	5.97	129.03	115.30
11	J	670	PRO	N-CA-CB	5.96	110.45	103.30
1	A	663	ARG	CB-CA-C	-5.96	98.49	110.40
21	T	401	PRO	C-N-CA	5.95	136.58	121.70
37	t	46	PRO	N-CA-CB	5.95	110.44	103.30
17	P	7	PRO	C-N-CA	5.94	136.55	121.70
11	J	637	PRO	N-CA-CB	5.92	110.40	103.30
39	p	25	ARG	CD-NE-CZ	5.91	131.88	123.60
9	H	172	C	P-O3'-C3'	5.89	126.77	119.70
10	I	458	LYS	O-C-N	5.88	132.11	122.70
38	o	27	ARG	CB-CA-C	-5.88	98.65	110.40
11	J	675	PRO	N-CA-CB	5.87	110.34	103.30
38	o	64	ARG	NE-CZ-NH1	5.87	123.23	120.30
9	H	168	A	C5'-C4'-C3'	-5.86	106.62	116.00
2	B	26	A	P-O5'-C5'	-5.85	111.53	120.90
11	J	604	PRO	N-CA-CB	5.85	110.33	103.30
10	I	459	ALA	O-C-N	5.84	132.05	122.70
8	G	21	A	P-O3'-C3'	-5.84	112.69	119.70
9	H	164	C	C5-C4-N4	-5.84	116.11	120.20
37	r	19	PRO	N-CA-CB	5.83	110.30	103.30
37	q	19	PRO	N-CA-CB	5.80	110.26	103.30
10	I	457	ARG	O-C-N	5.78	131.94	122.70
19	R	222	PRO	N-CA-C	-5.76	97.12	112.10
11	J	566	PRO	N-CA-CB	5.76	110.21	103.30
9	H	167	U	O3'-P-O5'	-5.73	93.12	104.00
19	R	217	LYS	CB-CA-C	-5.72	98.97	110.40
24	W	139	LEU	CA-CB-CG	5.69	128.38	115.30
9	H	156	U	P-O3'-C3'	-5.68	112.88	119.70
19	R	214	ILE	CG1-CB-CG2	-5.68	98.91	111.40
37	t	19	PRO	N-CA-CB	5.66	110.10	103.30
7	4	-12	G	C4'-C3'-O3'	5.64	124.28	113.00
17	P	10	GLU	CB-CA-C	5.64	121.67	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	o	75	ARG	NH1-CZ-NH2	5.62	125.59	119.40
1	A	1737	ASN	CB-CA-C	5.61	121.61	110.40
9	H	166	G	C6-N1-C2	-5.55	121.77	125.10
37	s	19	PRO	N-CA-CB	5.55	109.95	103.30
38	o	58	ASP	N-CA-CB	-5.55	100.61	110.60
8	G	2	U	N1-C1'-C2'	-5.54	105.91	112.00
24	W	532	LEU	CB-CG-CD1	-5.49	101.67	111.00
6	F	73	A	P-O3'-C3'	5.49	126.28	119.70
8	G	168	C	O5'-P-OP2	-5.46	100.78	105.70
37	r	60	PRO	N-CA-CB	5.45	109.84	103.30
2	B	20	G	O4'-C1'-N9	5.41	112.53	108.20
9	H	106	G	O5'-P-OP1	5.41	117.19	110.70
1	A	1556	ASP	CB-CA-C	-5.36	99.69	110.40
9	H	162	U	C2-N3-C4	-5.35	123.79	127.00
9	H	156	U	OP2-P-O3'	5.35	116.97	105.20
38	o	47	ILE	N-CA-CB	5.34	123.08	110.80
19	R	275	LEU	CA-CB-CG	5.32	127.53	115.30
20	S	106	ASP	CB-CG-OD1	5.31	123.08	118.30
9	H	157	G	O4'-C1'-N9	-5.30	103.96	108.20
30	y	47	ARG	CB-CA-C	-5.29	99.81	110.40
24	W	82	ASN	C-N-CD	-5.27	109.00	120.60
39	p	39	ASP	CB-CG-OD2	-5.26	113.56	118.30
21	T	309	ASP	O-C-N	5.26	131.12	122.70
1	A	1301	ILE	CG1-CB-CG2	-5.26	99.83	111.40
21	T	309	ASP	CB-CG-OD1	5.25	123.03	118.30
1	A	1982	GLN	CB-CA-C	-5.25	99.91	110.40
1	A	1459	ARG	NE-CZ-NH1	-5.24	117.68	120.30
1	A	1753	LEU	N-CA-CB	-5.24	99.92	110.40
7	4	-6	C	O4'-C1'-N1	5.24	112.39	108.20
9	H	157	G	P-O5'-C5'	-5.23	112.53	120.90
28	z	56	ASP	CB-CG-OD2	5.22	123.00	118.30
1	A	863	GLU	CB-CG-CD	-5.22	100.11	114.20
7	4	-6	C	N1-C2-O2	5.22	122.03	118.90
25	Y	685	ASP	C-N-CA	5.22	134.74	121.70
9	H	156	U	C4'-C3'-C2'	5.21	107.81	102.60
16	O	28	LEU	CB-CG-CD2	-5.20	102.16	111.00
42	w	115	GLY	N-CA-C	5.19	126.08	113.10
24	W	243	VAL	CG1-CB-CG2	-5.17	102.63	110.90
39	p	39	ASP	CB-CG-OD1	5.17	122.95	118.30
8	G	143	U	N1-C1'-C2'	-5.16	106.32	112.00
8	G	2	U	C3'-C2'-C1'	5.16	105.63	101.50
31	a	78	LYS	N-CA-CB	5.13	119.84	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1303	LEU	CA-CB-CG	-5.13	103.49	115.30
25	Y	686	GLU	C-N-CA	5.12	134.49	121.70
9	H	160	A	P-O5'-C5'	-5.11	112.72	120.90
9	H	176	G	OP1-P-OP2	-5.11	111.94	119.60
10	I	697	PRO	C-N-CA	5.10	134.45	121.70
3	C	93	ILE	CG1-CB-CG2	-5.10	100.19	111.40
25	Y	689	GLU	N-CA-C	-5.08	97.28	111.00
9	H	170	C	N3-C4-C5	-5.08	119.87	121.90
8	G	173	G	O5'-P-OP2	-5.07	101.14	105.70
9	H	160	A	C4'-C3'-C2'	-5.06	97.54	102.60
10	I	698	ARG	N-CA-CB	5.06	119.71	110.60
9	H	170	C	O4'-C1'-C2'	-5.04	100.76	105.80
38	o	99	SER	N-CA-CB	-5.04	102.94	110.50
14	M	120	PRO	CB-CA-C	-5.03	99.41	112.00
3	C	359	LYS	CA-CB-CG	5.01	124.42	113.40
17	P	63	LEU	CB-CG-CD1	-5.01	102.49	111.00
7	4	-6	C	N3-C2-O2	-5.00	118.40	121.90

There are no chirality outliers.

All (63) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1019	TYR	Peptide
1	A	1201	ARG	Peptide
1	A	1210	LYS	Peptide
1	A	1338	SER	Peptide
1	A	1503	TRP	Peptide
1	A	1513	MET	Mainchain
1	A	1561	PHE	Mainchain
1	A	166	PHE	Peptide
1	A	1717	ASN	Mainchain
1	A	1749	LYS	Mainchain
1	A	1753	LEU	Mainchain
1	A	2010	ILE	Mainchain
1	A	346	ASP	Peptide
1	A	377	GLU	Peptide
1	A	385	GLU	Peptide
1	A	55	ASP	Peptide
1	A	698	PRO	Peptide
1	A	73	HIS	Peptide
1	A	941	LYS	Peptide
3	C	308	CYS	Peptide

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Mol	Chain	Res	Type	Group
3	C	358	LYS	Peptide
3	C	360	ALA	Peptide
3	C	534	VAL	Peptide
3	C	799	GLU	Peptide
3	C	800	PRO	Peptide
3	C	902	HIS	Peptide
3	C	92	PRO	Peptide
3	C	93	ILE	Peptide
4	D	430	LEU	Peptide
5	E	192	ASN	Peptide
10	I	309	ALA	Mainchain
10	I	310	LYS	Mainchain
10	I	311	MET	Mainchain
10	I	693	GLN	Mainchain
10	I	83	LYS	Mainchain
10	I	84	HIS	Mainchain
11	J	205	LEU	Peptide
11	J	215	THR	Peptide
11	J	216	ASP	Peptide
11	J	240	THR	Peptide
11	J	241	VAL	Peptide
15	N	136	HIS	Peptide
15	N	3	LYS	Peptide
15	N	36	PRO	Peptide
15	N	4	VAL	Peptide
16	O	63	MET	Peptide
17	P	204	GLN	Peptide
17	P	30	TYR	Peptide
17	P	48	GLN	Peptide
19	R	125	MET	Peptide
19	R	126	ASN	Peptide
19	R	183	GLN	Peptide
19	R	185	GLY	Peptide
19	R	212	PHE	Peptide
19	R	66	GLU	Peptide
19	R	94	GLY	Peptide
21	T	342	GLU	Peptide
21	T	400	PHE	Peptide
21	T	405	PHE	Peptide
24	W	257	ILE	Peptide
24	W	518	PRO	Peptide
33	d	112	ASN	Peptide

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Mol	Chain	Res	Type	Group
33	k	112	ASN	Peptide

5.2 Too-close contacts (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	2247/2335 (96%)	2044 (91%)	191 (8%)	12 (0%)	25 63
3	C	856/972 (88%)	781 (91%)	71 (8%)	4 (0%)	25 63
4	D	1720/2136 (80%)	1632 (95%)	85 (5%)	3 (0%)	44 78
5	E	297/357 (83%)	275 (93%)	22 (7%)	0	100 100
10	I	576/855 (67%)	558 (97%)	14 (2%)	4 (1%)	19 56
11	J	530/848 (62%)	489 (92%)	33 (6%)	8 (2%)	8 39
12	K	147/225 (65%)	136 (92%)	8 (5%)	3 (2%)	6 32
13	L	425/802 (53%)	408 (96%)	15 (4%)	2 (0%)	25 63
14	M	128/243 (53%)	117 (91%)	11 (9%)	0	100 100
15	N	141/144 (98%)	124 (88%)	16 (11%)	1 (1%)	19 56
16	O	283/420 (67%)	259 (92%)	23 (8%)	1 (0%)	30 67
17	P	107/229 (47%)	89 (83%)	15 (14%)	3 (3%)	4 25
18	Q	1308/1485 (88%)	1280 (98%)	26 (2%)	2 (0%)	44 78
19	R	274/536 (51%)	247 (90%)	23 (8%)	4 (2%)	8 39
20	S	157/166 (95%)	148 (94%)	9 (6%)	0	100 100
21	T	310/514 (60%)	275 (89%)	29 (9%)	6 (2%)	6 33
22	U	68/2752 (2%)	60 (88%)	8 (12%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
23	V	444/908 (49%)	431 (97%)	12 (3%)	1 (0%)	44 78
24	W	507/579 (88%)	432 (85%)	69 (14%)	6 (1%)	11 43
25	Y	667/1220 (55%)	642 (96%)	23 (3%)	2 (0%)	37 72
26	Z	120/758 (16%)	107 (89%)	13 (11%)	0	100 100
27	2	121/184 (66%)	110 (91%)	7 (6%)	4 (3%)	3 22
28	z	58/112 (52%)	56 (97%)	2 (3%)	0	100 100
29	b	98/240 (41%)	93 (95%)	2 (2%)	3 (3%)	3 23
29	i	84/240 (35%)	82 (98%)	2 (2%)	0	100 100
30	y	77/301 (26%)	75 (97%)	2 (3%)	0	100 100
31	a	75/126 (60%)	74 (99%)	1 (1%)	0	100 100
31	h	77/126 (61%)	76 (99%)	1 (1%)	0	100 100
32	c	80/119 (67%)	77 (96%)	3 (4%)	0	100 100
32	j	80/119 (67%)	77 (96%)	3 (4%)	0	100 100
33	d	95/118 (80%)	91 (96%)	4 (4%)	0	100 100
33	k	81/118 (69%)	78 (96%)	3 (4%)	0	100 100
34	f	72/86 (84%)	68 (94%)	4 (6%)	0	100 100
34	m	71/86 (83%)	67 (94%)	3 (4%)	1 (1%)	9 40
35	e	77/92 (84%)	76 (99%)	1 (1%)	0	100 100
35	l	77/92 (84%)	76 (99%)	1 (1%)	0	100 100
36	g	72/76 (95%)	70 (97%)	2 (3%)	0	100 100
36	n	65/76 (86%)	63 (97%)	2 (3%)	0	100 100
37	q	130/504 (26%)	117 (90%)	7 (5%)	6 (5%)	2 18
37	r	129/504 (26%)	118 (92%)	9 (7%)	2 (2%)	8 37
37	s	130/504 (26%)	116 (89%)	6 (5%)	8 (6%)	1 14
37	t	129/504 (26%)	116 (90%)	9 (7%)	4 (3%)	3 23
38	o	160/255 (63%)	146 (91%)	12 (8%)	2 (1%)	10 42
39	p	92/225 (41%)	90 (98%)	2 (2%)	0	100 100
40	1	265/586 (45%)	246 (93%)	19 (7%)	0	100 100
41	v	142/146 (97%)	138 (97%)	4 (3%)	0	100 100
42	w	89/174 (51%)	87 (98%)	1 (1%)	1 (1%)	12 46
43	u	384/411 (93%)	372 (97%)	9 (2%)	3 (1%)	16 53

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
44	x	23/703 (3%)	22 (96%)	1 (4%)	0	100 100
45	3	28/415 (7%)	27 (96%)	1 (4%)	0	100 100
All	All	14373/25726 (56%)	13438 (94%)	839 (6%)	96 (1%)	21 56

All (96) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1092	ILE
1	A	1831	LYS
1	A	1881	ASN
3	C	801	LEU
4	D	957	VAL
4	D	1584	ILE
10	I	698	ARG
11	J	217	GLU
11	J	241	VAL
12	K	78	PRO
13	L	10	VAL
13	L	125	PRO
17	P	8	THR
19	R	233	PRO
21	T	187	LYS
21	T	188	PRO
21	T	190	TRP
24	W	73	ASP
24	W	74	PRO
24	W	82	ASN
24	W	83	PRO
27	2	24	PRO
27	2	76	SER
37	q	24	VAL
37	q	59	HIS
37	q	60	PRO
37	s	9	ASN
37	s	55	ILE
37	s	60	PRO
37	s	66	PRO
37	s	71	ILE
37	t	9	ASN
37	t	69	THR
34	m	4	PRO

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Mol	Chain	Res	Type
43	u	383	ASN
1	A	1992	GLY
3	C	94	ILE
3	C	439	PRO
10	I	532	LYS
11	J	709	VAL
18	Q	530	ASN
21	T	406	ILE
25	Y	1185	ASP
37	q	9	ASN
37	q	19	PRO
38	o	160	LYS
42	w	115	GLY
43	u	340	GLY
43	u	385	ASP
1	A	167	PRO
1	A	1503	TRP
1	A	1513	MET
10	I	699	THR
11	J	188	GLN
11	J	205	LEU
17	P	6	ARG
19	R	52	PRO
23	V	597	PRO
24	W	258	PRO
27	2	32	LYS
27	2	72	ALA
37	q	23	HIS
37	r	9	ASN
37	s	24	VAL
37	t	67	SER
1	A	570	ASP
3	C	83	GLU
11	J	341	PRO
11	J	604	PRO
12	K	65	ILE
15	N	41	ARG
17	P	205	LYS
19	R	73	PRO
19	R	186	VAL
25	Y	1182	LYS
37	t	65	PRO

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Mol	Chain	Res	Type
38	o	32	PRO
1	A	364	SER
1	A	1530	PRO
18	Q	89	ALA
21	T	343	PRO
21	T	462	GLU
29	b	105	GLY
29	b	106	ILE
37	s	62	ARG
1	A	1758	PRO
10	I	372	ARG
11	J	216	ASP
16	O	20	PHE
29	b	115	PRO
1	A	1419	ILE
12	K	17	PRO
24	W	271	PRO
37	s	38	GLY
4	D	585	ILE
37	r	60	PRO

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	A	1775/2108 (84%)	1704 (96%)	71 (4%)	27 49
3	C	758/866 (88%)	749 (99%)	9 (1%)	67 79
5	E	256/300 (85%)	256 (100%)	0	100 100
10	I	199/749 (27%)	187 (94%)	12 (6%)	16 38
11	J	241/751 (32%)	239 (99%)	2 (1%)	79 85
13	L	218/709 (31%)	209 (96%)	9 (4%)	26 49
14	M	117/209 (56%)	112 (96%)	5 (4%)	25 48
15	N	130/130 (100%)	128 (98%)	2 (2%)	60 75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
16	O	255/361 (71%)	254 (100%)	1 (0%)	89 91
17	P	101/203 (50%)	94 (93%)	7 (7%)	13 34
19	R	236/457 (52%)	223 (94%)	13 (6%)	18 41
20	S	129/134 (96%)	128 (99%)	1 (1%)	79 85
21	T	268/441 (61%)	263 (98%)	5 (2%)	52 70
22	U	21/2432 (1%)	20 (95%)	1 (5%)	21 44
23	V	98/838 (12%)	95 (97%)	3 (3%)	35 56
24	W	448/502 (89%)	439 (98%)	9 (2%)	50 69
25	Y	32/1085 (3%)	29 (91%)	3 (9%)	7 23
26	Z	110/655 (17%)	110 (100%)	0	100 100
27	2	106/157 (68%)	98 (92%)	8 (8%)	11 31
28	z	51/99 (52%)	50 (98%)	1 (2%)	50 69
29	b	83/177 (47%)	81 (98%)	2 (2%)	44 64
29	i	77/177 (44%)	75 (97%)	2 (3%)	41 61
31	a	68/101 (67%)	67 (98%)	1 (2%)	60 75
31	h	70/101 (69%)	70 (100%)	0	100 100
32	c	77/101 (76%)	75 (97%)	2 (3%)	41 61
32	j	77/101 (76%)	75 (97%)	2 (3%)	41 61
33	d	90/110 (82%)	88 (98%)	2 (2%)	47 66
33	k	80/110 (73%)	78 (98%)	2 (2%)	42 63
34	f	63/74 (85%)	62 (98%)	1 (2%)	58 74
34	m	61/74 (82%)	59 (97%)	2 (3%)	33 55
35	e	74/84 (88%)	74 (100%)	0	100 100
35	l	74/84 (88%)	74 (100%)	0	100 100
36	g	64/66 (97%)	63 (98%)	1 (2%)	58 74
36	n	60/66 (91%)	58 (97%)	2 (3%)	33 55
38	o	139/218 (64%)	135 (97%)	4 (3%)	37 58
39	p	82/195 (42%)	79 (96%)	3 (4%)	29 51
40	1	235/520 (45%)	231 (98%)	4 (2%)	56 73
45	3	25/366 (7%)	25 (100%)	0	100 100
All	All	7048/15911 (44%)	6856 (97%)	192 (3%)	41 60

All (192) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	153	ARG
1	A	240	ARG
1	A	244	GLN
1	A	362	ARG
1	A	387	PHE
1	A	409	ARG
1	A	413	LEU
1	A	579	GLN
1	A	642	ARG
1	A	664	HIS
1	A	666	LYS
1	A	762	ARG
1	A	773	LYS
1	A	774	LYS
1	A	850	TYR
1	A	853	LYS
1	A	857	ASN
1	A	861	ARG
1	A	863	GLU
1	A	866	LEU
1	A	880	ARG
1	A	994	ASN
1	A	1089	CYS
1	A	1133	CYS
1	A	1136	ARG
1	A	1189	MET
1	A	1249	MET
1	A	1251	SER
1	A	1253	SER
1	A	1341	ARG
1	A	1402	ARG
1	A	1526	LEU
1	A	1528	GLN
1	A	1529	ILE
1	A	1554	GLN
1	A	1555	LEU
1	A	1556	ASP
1	A	1561	PHE
1	A	1562	MET
1	A	1566	ILE
1	A	1578	ARG
1	A	1722	SER

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Mol	Chain	Res	Type
1	A	1723	LYS
1	A	1725	LEU
1	A	1727	GLN
1	A	1728	GLN
1	A	1730	MET
1	A	1734	MET
1	A	1737	ASN
1	A	1738	PRO
1	A	1740	LEU
1	A	1751	LEU
1	A	1752	GLN
1	A	1753	LEU
1	A	1757	GLU
1	A	1758	PRO
1	A	1763	LEU
1	A	1833	LEU
1	A	1873	GLU
1	A	1876	LEU
1	A	1877	LEU
1	A	1878	ASP
1	A	1879	PHE
1	A	1900	GLU
1	A	1982	GLN
1	A	1987	ILE
1	A	1990	ASP
1	A	1993	LYS
1	A	2011	ILE
1	A	2014	MET
1	A	2015	GLU
3	C	87	GLN
3	C	297	ASN
3	C	359	LYS
3	C	495	ARG
3	C	513	ASN
3	C	572	GLU
3	C	573	GLU
3	C	673	LYS
3	C	826	ARG
10	I	532	LYS
10	I	548	PHE
10	I	606	TRP
10	I	694	ILE

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Mol	Chain	Res	Type
10	I	698	ARG
10	I	699	THR
10	I	724	LEU
10	I	725	ARG
10	I	726	ILE
10	I	727	ARG
10	I	730	VAL
10	I	731	GLN
11	J	201	ARG
11	J	221	ASN
13	L	4	ILE
13	L	5	MET
13	L	6	ILE
13	L	7	LYS
13	L	10	VAL
13	L	123	LEU
13	L	133	GLU
13	L	181	ARG
13	L	240	ARG
14	M	118	LYS
14	M	152	LEU
14	M	198	ARG
14	M	212	ASN
14	M	215	ASN
15	N	119	CYS
15	N	130	ARG
16	O	222	ARG
17	P	3	THR
17	P	7	PRO
17	P	9	PHE
17	P	10	GLU
17	P	13	ARG
17	P	18	LYS
17	P	212	ASN
19	R	78	ARG
19	R	95	LYS
19	R	212	PHE
19	R	217	LYS
19	R	220	ARG
19	R	302	VAL
19	R	307	GLN
19	R	310	ARG

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Mol	Chain	Res	Type
19	R	315	LYS
19	R	318	GLU
19	R	324	LEU
19	R	333	GLU
19	R	334	ARG
20	S	126	HIS
21	T	189	GLN
21	T	197	TYR
21	T	412	HIS
21	T	416	ILE
21	T	454	VAL
22	U	23	LEU
23	V	458	THR
23	V	535	THR
23	V	597	PRO
24	W	129	ARG
24	W	182	LYS
24	W	200	VAL
24	W	243	VAL
24	W	322	ARG
24	W	492	ASN
24	W	495	ARG
24	W	500	LYS
24	W	529	ASN
25	Y	413	LYS
25	Y	418	ASP
25	Y	420	ASP
27	2	23	ILE
27	2	25	LYS
27	2	30	GLU
27	2	68	MET
27	2	102	LYS
27	2	134	LEU
27	2	136	GLU
27	2	137	LYS
28	z	79	LYS
29	b	13	ILE
29	b	58	GLN
31	a	77	LEU
32	c	40	LEU
32	c	54	GLN
33	d	45	ASN

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Mol	Chain	Res	Type
33	d	112	ASN
34	f	55	LEU
36	g	65	ASN
29	i	13	ILE
29	i	58	GLN
32	j	40	LEU
32	j	54	GLN
33	k	45	ASN
33	k	112	ASN
34	m	5	LEU
34	m	55	LEU
36	n	10	LYS
36	n	65	ASN
38	o	5	THR
38	o	55	ARG
38	o	114	SER
38	o	126	THR
39	p	17	LYS
39	p	46	MET
39	p	87	ASP
40	1	34	ARG
40	1	265	LEU
40	1	267	ILE
40	1	305	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (102) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	GLN
1	A	78	ASN
1	A	105	ASN
1	A	181	ASN
1	A	361	HIS
1	A	457	ASN
1	A	467	GLN
1	A	495	GLN
1	A	584	HIS
1	A	703	GLN
1	A	704	ASN
1	A	711	GLN
1	A	792	HIS
1	A	793	ASN

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Mol	Chain	Res	Type
1	A	834	HIS
1	A	994	ASN
1	A	1014	ASN
1	A	1124	ASN
1	A	1130	ASN
1	A	1148	ASN
1	A	1359	HIS
1	A	1460	HIS
1	A	1476	GLN
1	A	1487	HIS
1	A	1531	ASN
1	A	1599	GLN
1	A	1615	HIS
1	A	1717	ASN
1	A	1727	GLN
1	A	1766	GLN
1	A	1775	GLN
1	A	1816	GLN
1	A	1881	ASN
1	A	1944	HIS
1	A	1995	ASN
1	A	2004	GLN
3	C	60	HIS
3	C	137	HIS
3	C	208	HIS
3	C	210	ASN
3	C	245	HIS
3	C	297	ASN
3	C	451	HIS
3	C	513	ASN
5	E	101	ASN
5	E	253	ASN
10	I	601	GLN
11	J	212	GLN
11	J	221	ASN
11	J	331	GLN
11	J	347	HIS
13	L	186	GLN
13	L	266	HIS
14	M	212	ASN
15	N	37	HIS
15	N	54	HIS

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Mol	Chain	Res	Type
16	O	113	ASN
16	O	196	GLN
16	O	294	ASN
19	R	189	ASN
19	R	279	HIS
20	S	87	HIS
20	S	111	GLN
20	S	126	HIS
21	T	189	GLN
21	T	278	ASN
21	T	407	GLN
21	T	437	HIS
21	T	455	GLN
23	V	474	HIS
23	V	499	GLN
24	W	71	HIS
24	W	82	ASN
24	W	242	HIS
24	W	472	ASN
24	W	492	ASN
24	W	529	ASN
24	W	549	HIS
27	2	93	GLN
28	z	62	GLN
28	z	95	HIS
28	z	102	HIS
29	b	22	GLN
29	b	76	ASN
31	a	60	GLN
32	c	64	ASN
33	d	69	ASN
34	f	58	HIS
36	g	65	ASN
31	h	60	GLN
29	i	22	GLN
29	i	76	ASN
32	j	64	ASN
33	k	69	ASN
34	m	12	ASN
34	m	58	HIS
36	n	65	ASN
38	o	130	HIS

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Mol	Chain	Res	Type
39	p	7	HIS
40	1	85	GLN
40	1	154	HIS
40	1	156	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	82/117 (70%)	17 (20%)	4 (4%)
6	F	96/107 (89%)	45 (46%)	16 (16%)
7	4	13/46 (28%)	8 (61%)	3 (23%)
8	G	80/174 (45%)	63 (78%)	20 (25%)
9	H	133/188 (70%)	34 (25%)	10 (7%)
All	All	404/632 (63%)	167 (41%)	53 (13%)

All (167) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	12	U
2	B	13	C
2	B	19	A
2	B	20	G
2	B	21	A
2	B	22	U
2	B	23	C
2	B	24	G
2	B	25	C
2	B	26	A
2	B	28	A
2	B	36	C
2	B	38	C
2	B	45	C
2	B	57	G
2	B	70	A
2	B	71	C
6	F	6	C
6	F	7	G
6	F	8	C
6	F	9	U
6	F	10	U
6	F	12	G

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Mol	Chain	Res	Type
6	F	25	C
6	F	26	U
6	F	27	A
6	F	28	A
6	F	29	A
6	F	31	U
6	F	33	G
6	F	34	G
6	F	35	A
6	F	36	A
6	F	37	C
6	F	38	G
6	F	40	U
6	F	43	A
6	F	45	A
6	F	46	G
6	F	47	A
6	F	48	A
6	F	49	G
6	F	51	U
6	F	54	G
6	F	56	A
6	F	59	G
6	F	60	C
6	F	61	C
6	F	62	C
6	F	68	C
6	F	73	A
6	F	74	U
6	F	78	A
6	F	79	C
6	F	80	G
6	F	81	C
6	F	82	A
6	F	83	A
6	F	84	A
6	F	85	U
6	F	86	U
6	F	87	C
7	4	-12	G
7	4	-11	G
7	4	-10	C

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Mol	Chain	Res	Type
7	4	-9	C
7	4	-7	C
7	4	-6	C
7	4	-4	A
7	4	-1	G
8	G	2	U
8	G	3	A
8	G	5	G
8	G	6	A
8	G	7	G
8	G	8	C
8	G	10	U
8	G	11	A
8	G	12	G
8	G	13	C
8	G	14	A
8	G	17	U
8	G	21	A
8	G	22	C
8	G	23	U
8	G	24	G
8	G	25	G
8	G	26	U
8	G	27	U
8	G	28	A
8	G	29	C
8	G	30	C
8	G	31	U
8	G	120	G
8	G	121	G
8	G	122	U
8	G	123	U
8	G	124	U
8	G	125	C
8	G	126	C
8	G	127	U
8	G	128	U
8	G	129	G
8	G	130	A
8	G	131	U
8	G	134	U
8	G	135	G

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Mol	Chain	Res	Type
8	G	136	U
8	G	137	C
8	G	138	A
8	G	139	U
8	G	140	A
8	G	143	U
8	G	144	A
8	G	145	U
8	G	146	C
8	G	147	C
8	G	148	U
8	G	149	G
8	G	150	U
8	G	166	A
8	G	167	G
8	G	168	C
8	G	169	U
8	G	170	C
8	G	171	G
8	G	172	C
8	G	173	G
8	G	174	G
8	G	175	U
8	G	176	U
8	G	177	G
8	G	179	G
9	H	13	C
9	H	14	C
9	H	15	U
9	H	16	U
9	H	17	U
9	H	19	G
9	H	24	A
9	H	25	G
9	H	28	C
9	H	29	A
9	H	30	A
9	H	31	G
9	H	33	G
9	H	37	U
9	H	39	U
9	H	40	C

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Mol	Chain	Res	Type
9	H	41	U
9	H	42	G
9	H	43	U
9	H	112	G
9	H	143	A
9	H	147	G
9	H	152	G
9	H	153	A
9	H	154	C
9	H	156	U
9	H	157	G
9	H	164	C
9	H	165	A
9	H	168	A
9	H	169	C
9	H	177	A
9	H	178	A
9	H	179	C

All (53) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	B	18	C
2	B	19	A
2	B	20	G
2	B	27	U
6	F	5	U
6	F	7	G
6	F	25	C
6	F	26	U
6	F	33	G
6	F	34	G
6	F	35	A
6	F	36	A
6	F	45	A
6	F	50	A
6	F	58	G
6	F	59	G
6	F	73	A
6	F	81	C
6	F	84	A
6	F	86	U

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Mol	Chain	Res	Type
7	4	-13	C
7	4	-12	G
7	4	-11	G
8	G	1	G
8	G	16	G
8	G	20	A
8	G	21	A
8	G	22	C
8	G	23	U
8	G	137	C
8	G	142	U
8	G	143	U
8	G	144	A
8	G	145	U
8	G	147	C
8	G	166	A
8	G	167	G
8	G	168	C
8	G	171	G
8	G	172	C
8	G	173	G
8	G	175	U
8	G	176	U
9	H	15	U
9	H	28	C
9	H	29	A
9	H	30	A
9	H	38	A
9	H	39	U
9	H	40	C
9	H	156	U
9	H	164	C
9	H	168	A

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
19	SEP	R	232	19	8,9,10	1.56	1 (12%)	8,12,14	1.71	2 (25%)
19	SEP	R	224	19	8,9,10	1.00	0	8,12,14	1.53	1 (12%)

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
19	SEP	R	232	19	-	1/5/8/10	-
19	SEP	R	224	19	-	0/5/8/10	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	R	232	SEP	P-O1P	3.40	1.61	1.50

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	R	232	SEP	P-OG-CB	-4.04	107.16	118.30
19	R	224	SEP	OG-CB-CA	-2.66	105.55	108.14
19	R	232	SEP	OG-CB-CA	2.37	110.45	108.14

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	R	232	SEP	N-CA-CB-OG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
47	GTP	C	1500	48	26,34,34	1.50	3 (11%)	32,54,54	1.95	7 (21%)
50	ATP	Q	1501	48	26,33,33	1.72	8 (30%)	31,52,52	1.85	10 (32%)
46	IHP	A	3000	-	36,36,36	0.72	0	54,60,60	1.05	0

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
47	GTP	C	1500	48	-	1/18/38/38	0/3/3/3
50	ATP	Q	1501	48	-	4/18/38/38	0/3/3/3
46	IHP	A	3000	-	-	3/30/54/54	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	C	1500	GTP	C5-C6	-4.83	1.37	1.47
50	Q	1501	ATP	C2'-C1'	-3.59	1.48	1.53
50	Q	1501	ATP	C4-N3	3.40	1.40	1.35
50	Q	1501	ATP	C6-N6	3.34	1.46	1.34
50	Q	1501	ATP	C2'-C3'	-2.74	1.45	1.53
47	C	1500	GTP	C5-C4	-2.42	1.36	1.43
50	Q	1501	ATP	O2'-C2'	-2.25	1.37	1.43
47	C	1500	GTP	O4'-C4'	-2.25	1.40	1.45
50	Q	1501	ATP	C2-N3	2.18	1.35	1.32
50	Q	1501	ATP	C3'-C4'	-2.18	1.47	1.53
50	Q	1501	ATP	O3'-C3'	-2.16	1.37	1.43

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	C	1500	GTP	PA-O3A-PB	-5.64	113.48	132.83
50	Q	1501	ATP	PB-O3B-PG	-5.47	114.07	132.83
47	C	1500	GTP	PB-O3B-PG	-4.37	117.84	132.83
50	Q	1501	ATP	N3-C2-N1	-4.18	122.14	128.68
47	C	1500	GTP	C5-C6-N1	3.72	120.52	113.95
47	C	1500	GTP	C2-N1-C6	-3.47	118.71	125.10
47	C	1500	GTP	C3'-C2'-C1'	3.21	105.81	100.98
47	C	1500	GTP	C8-N7-C5	2.82	108.36	102.99
50	Q	1501	ATP	PA-O3A-PB	-2.62	123.85	132.83
50	Q	1501	ATP	C1'-N9-C4	-2.50	122.25	126.64
50	Q	1501	ATP	O2G-PG-O1G	-2.41	101.23	110.68
50	Q	1501	ATP	O2A-PA-O1A	-2.35	100.65	112.24
50	Q	1501	ATP	O2G-PG-O3B	2.25	112.17	104.64
47	C	1500	GTP	O6-C6-C5	-2.22	120.04	124.37
50	Q	1501	ATP	O2B-PB-O1B	-2.08	101.97	112.24
50	Q	1501	ATP	O5'-C5'-C4'	2.07	116.12	108.99
50	Q	1501	ATP	O3G-PG-O3B	2.05	111.50	104.64

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
46	A	3000	IHP	C3-O13-P3-O43
47	C	1500	GTP	O4'-C4'-C5'-O5'
50	Q	1501	ATP	C5'-O5'-PA-O1A
50	Q	1501	ATP	C5'-O5'-PA-O2A
46	A	3000	IHP	C3-C4-O14-P4
50	Q	1501	ATP	PB-O3A-PA-O2A
46	A	3000	IHP	C4-O14-P4-O44
50	Q	1501	ATP	C5'-O5'-PA-O3A

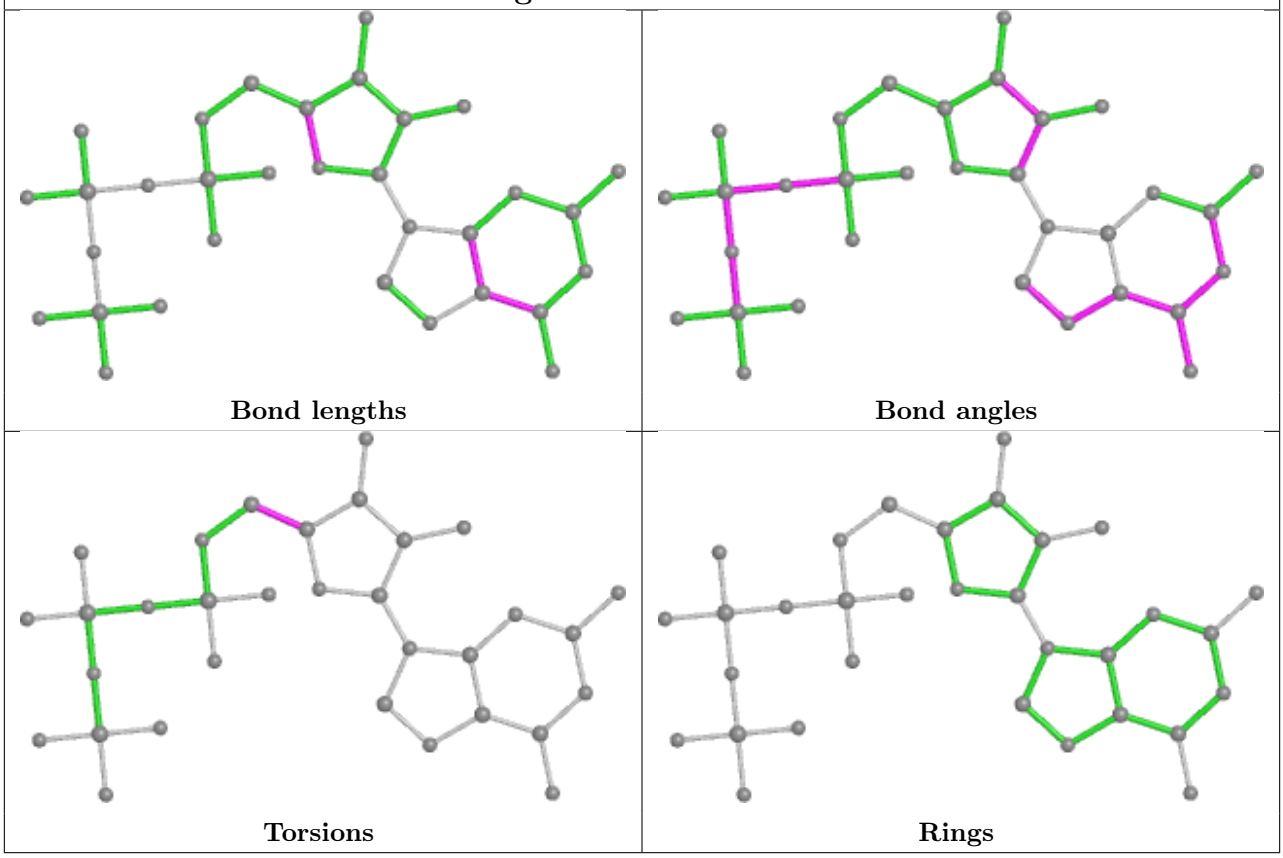
There are no ring outliers.

No monomer is involved in short contacts.

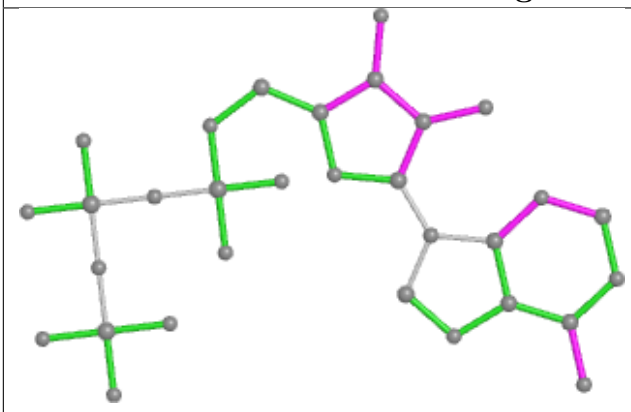
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

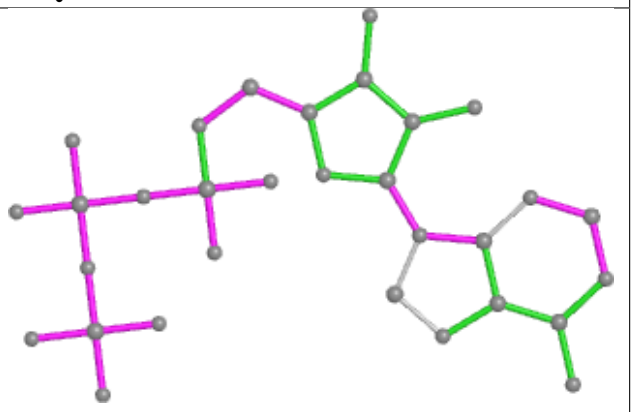
Ligand GTP C 1500



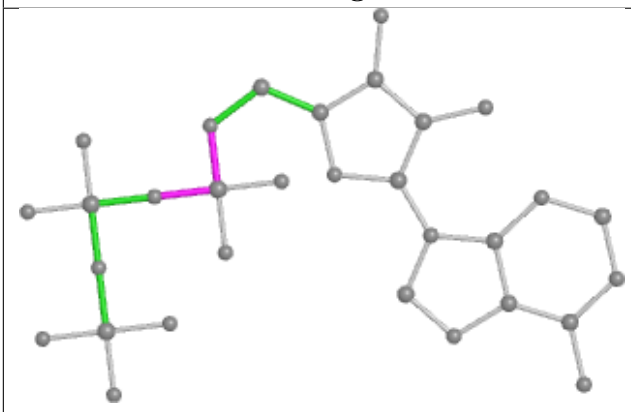
Ligand ATP Q 1501



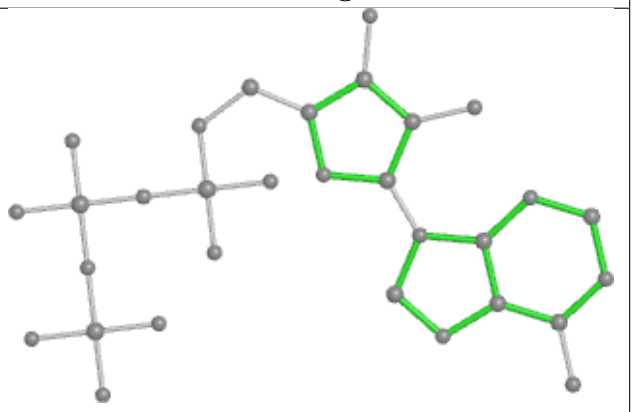
Bond lengths



Bond angles

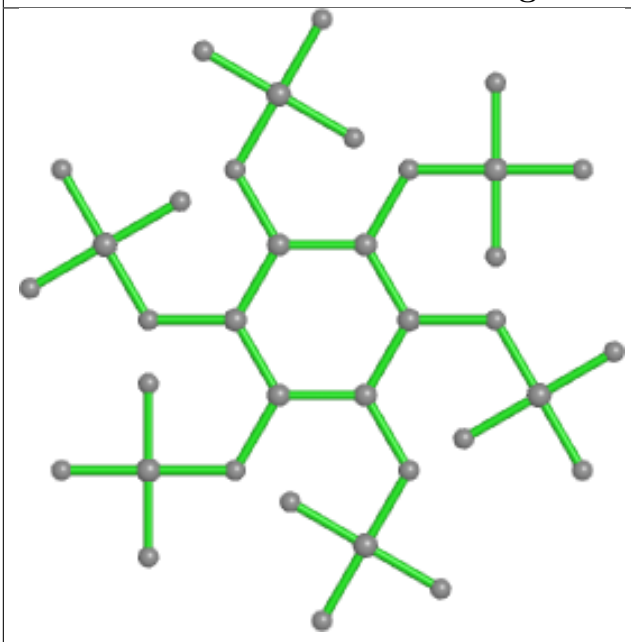


Torsions

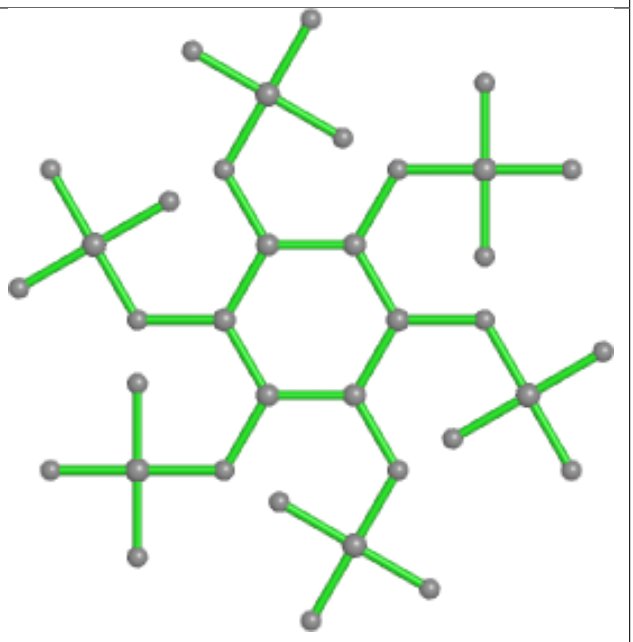


Rings

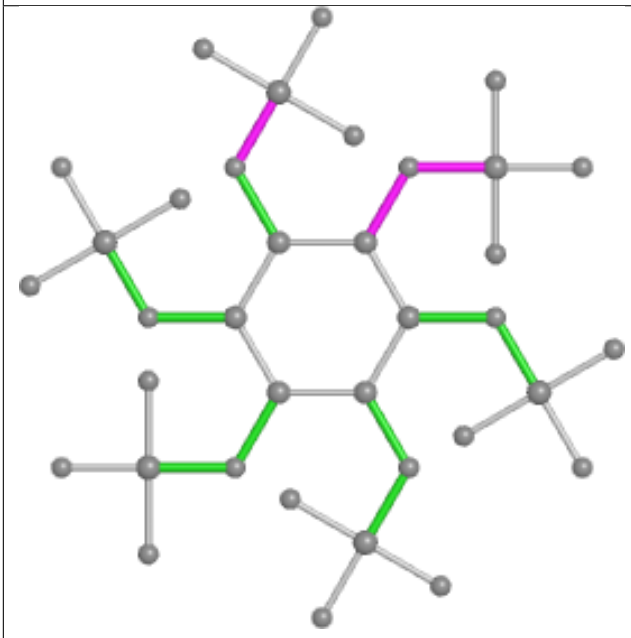
Ligand IHP A 3000



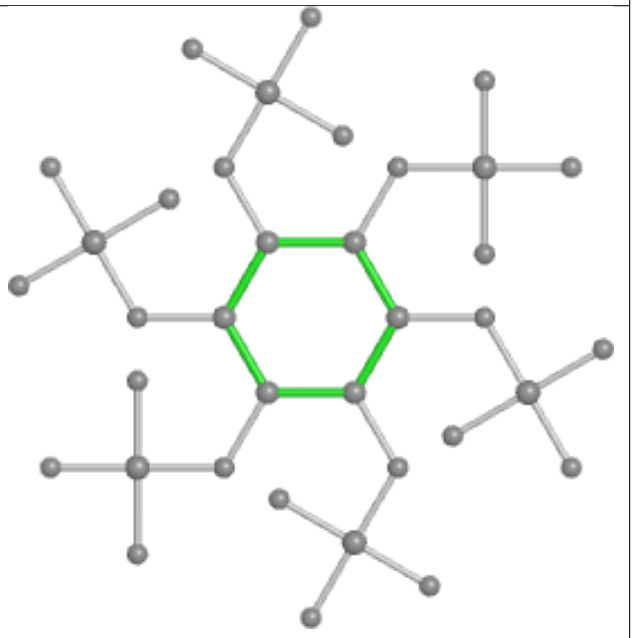
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

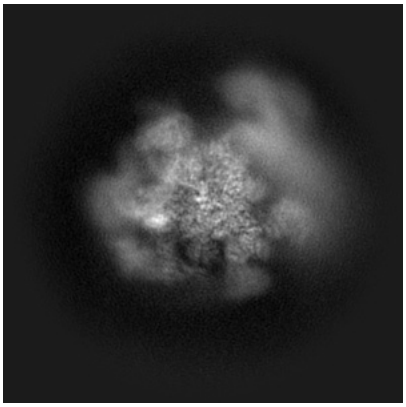
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-32321. These allow visual inspection of the internal detail of the map and identification of artifacts.

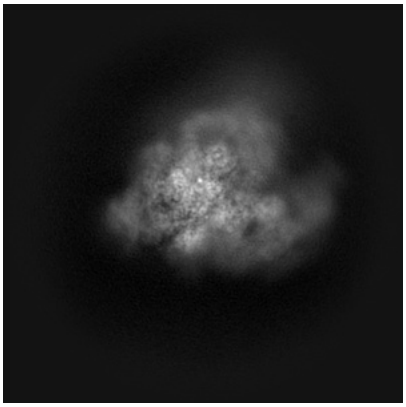
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

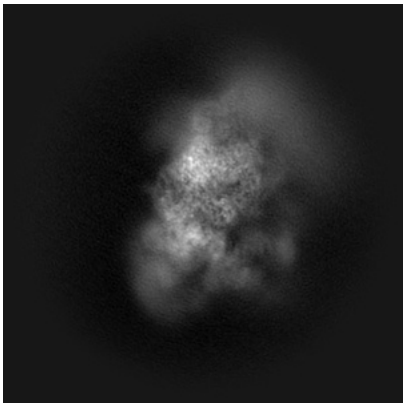
6.1.1 Primary map



X



Y

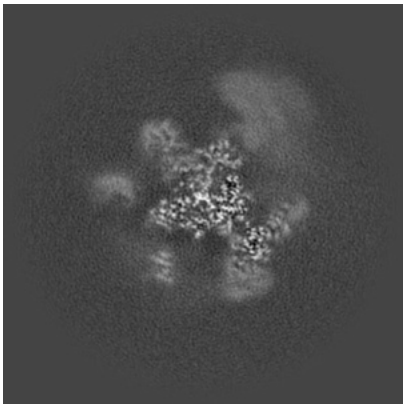


Z

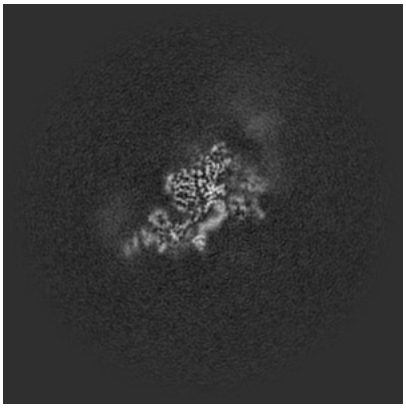
The images above show the map projected in three orthogonal directions.

6.2 Central slices

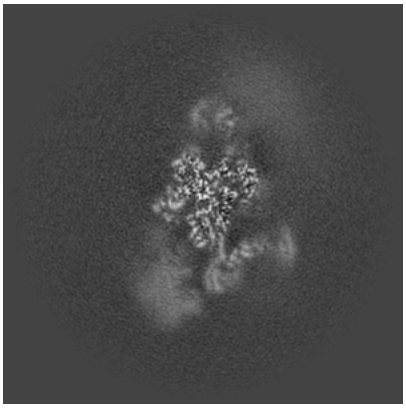
6.2.1 Primary map



X Index: 200



Y Index: 200

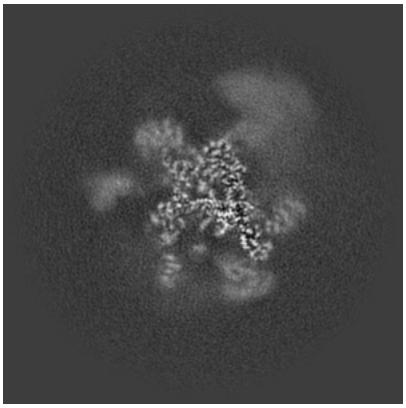


Z Index: 200

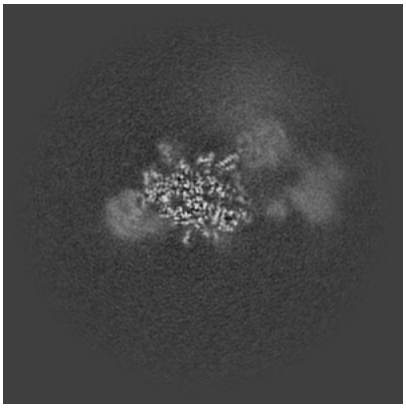
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

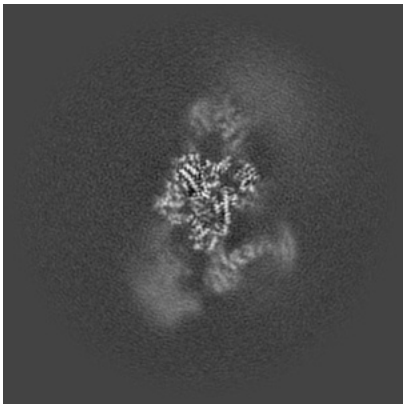
6.3.1 Primary map



X Index: 194



Y Index: 238

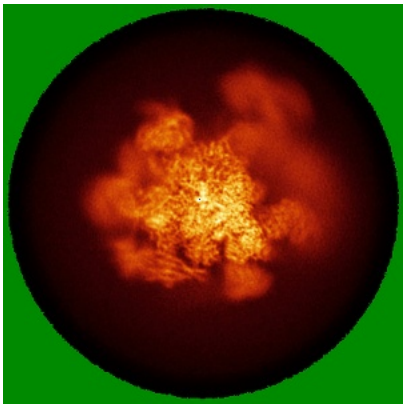


Z Index: 197

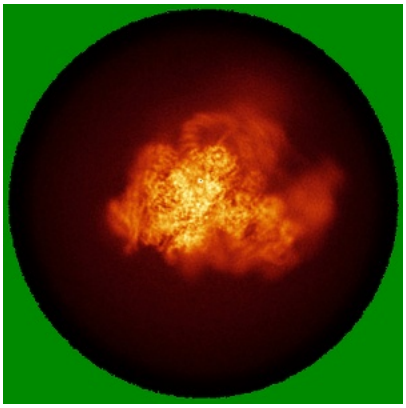
The images above show the largest variance slices of the map in three orthogonal directions.

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

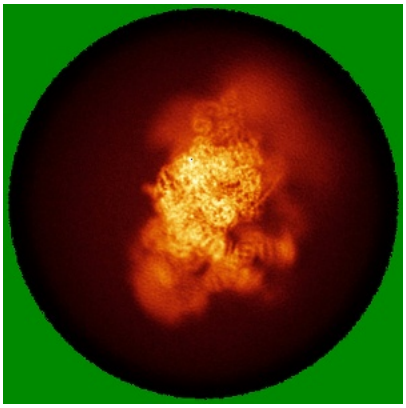
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.37. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

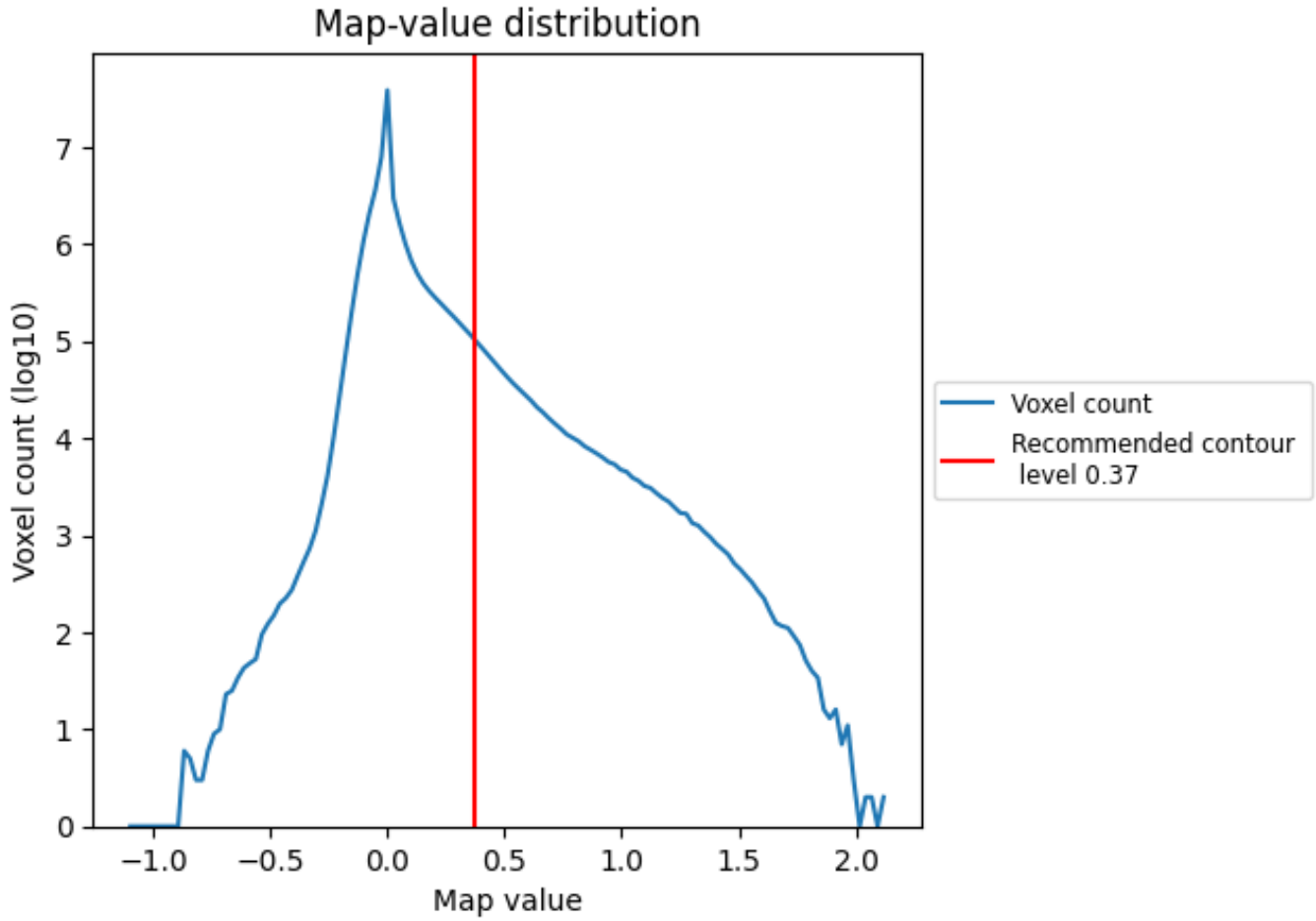
6.6 Mask visualisation (i)

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

7 Map analysis

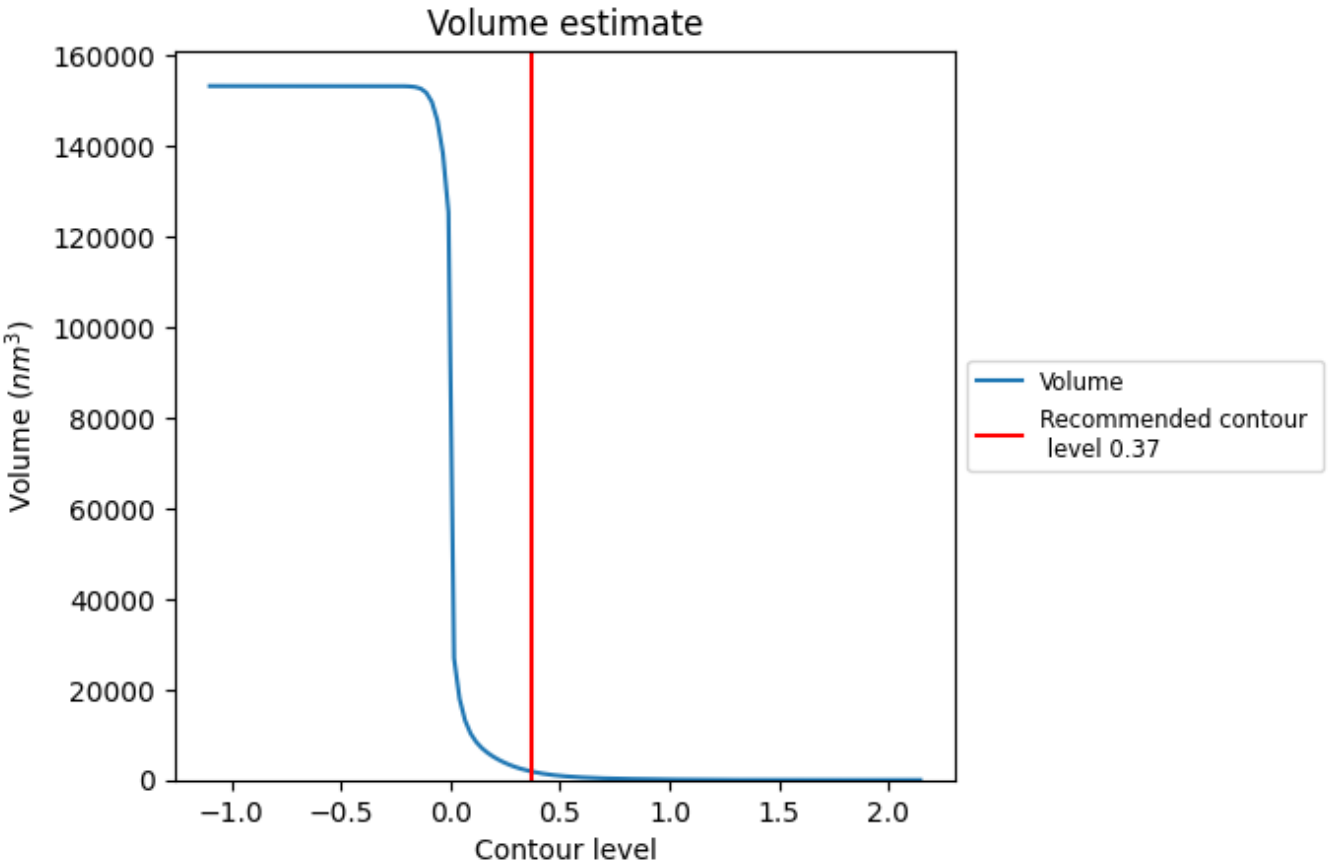
This section contains the results of statistical analysis of the map.

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.

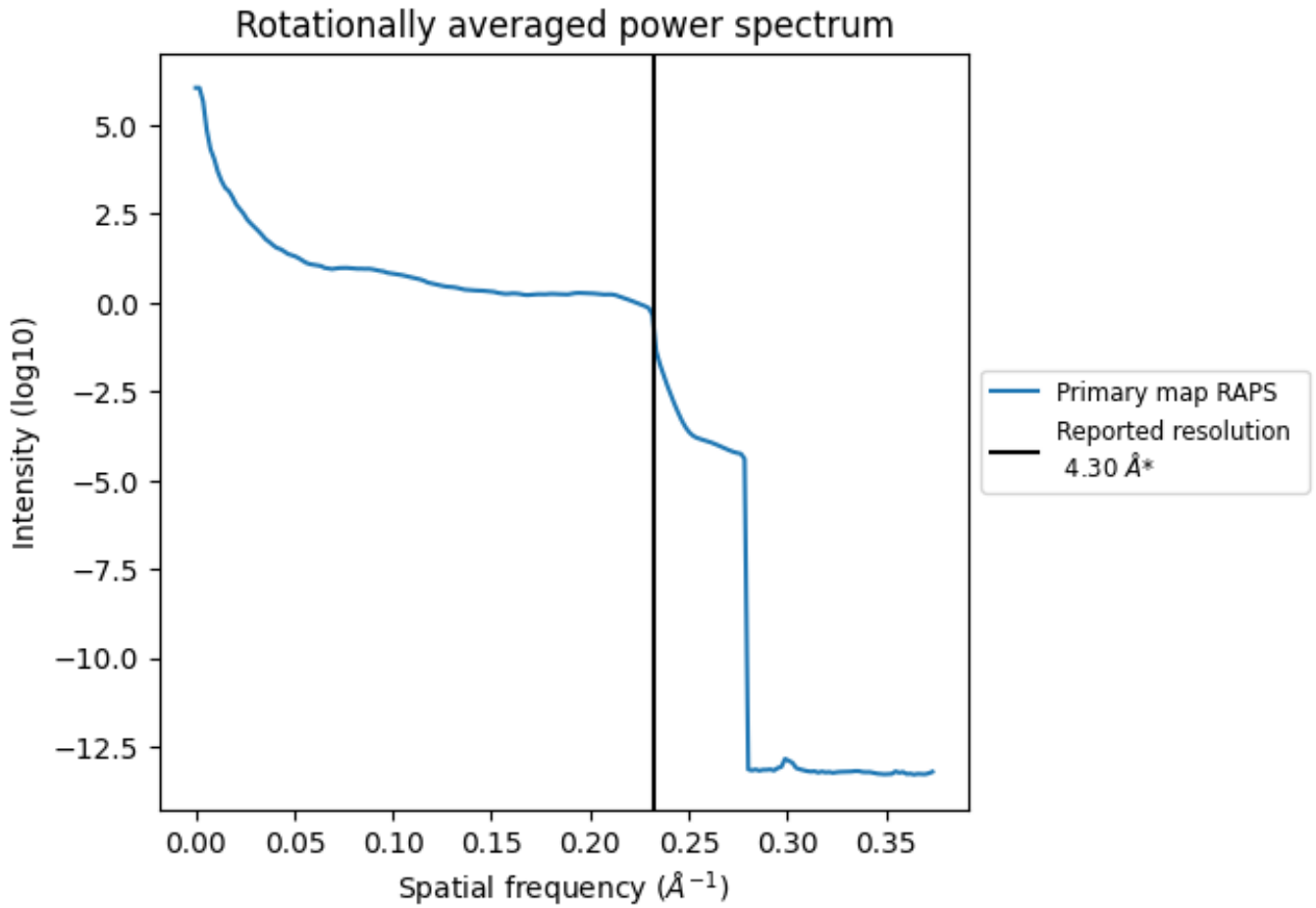
7.2 Volume estimate



The volume at the recommended contour level is 1869 nm^3; this corresponds to an approximate mass of 1688 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 0.233 $Å^{-1}$

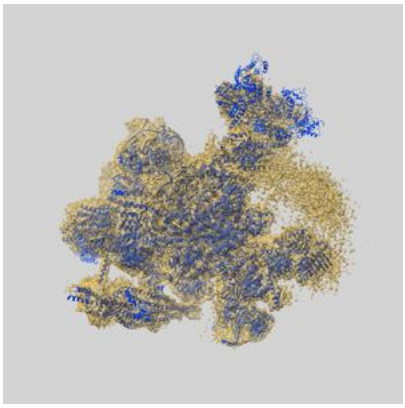
8 Fourier-Shell correlation (i)

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

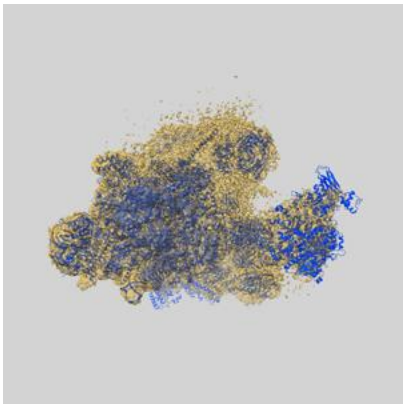
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-32321 and PDB model 7W5B. Per-residue inclusion information can be found in section 3 on page 14.

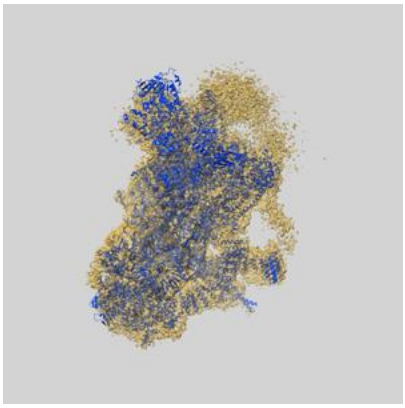
9.1 Map-model overlay



X



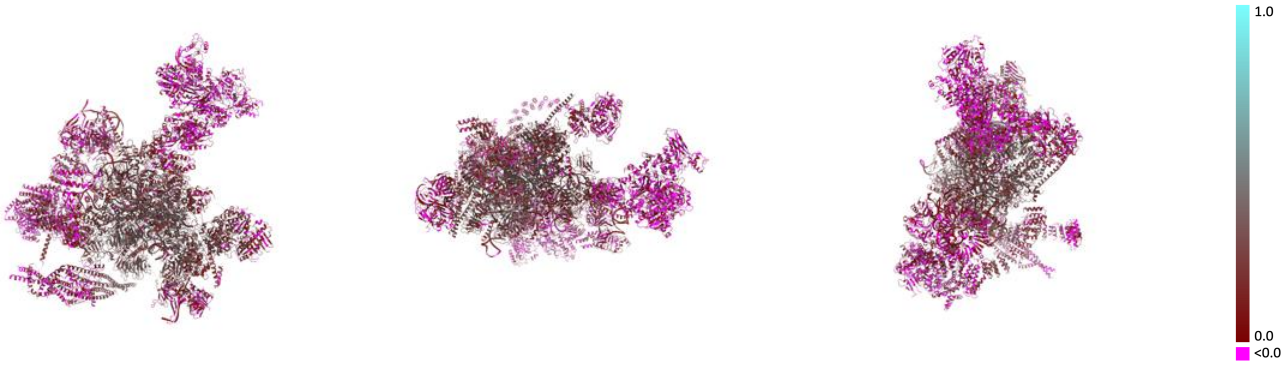
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.37 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.

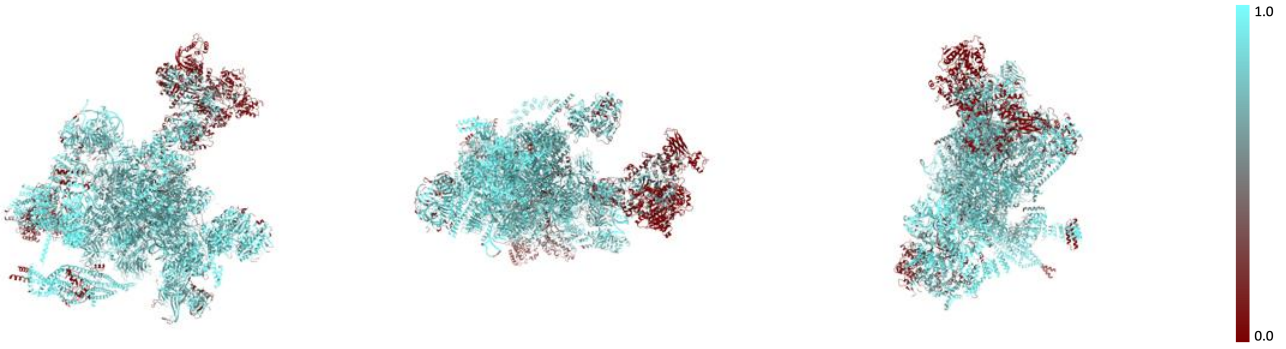
9.2 Q-score mapped to coordinate model



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.

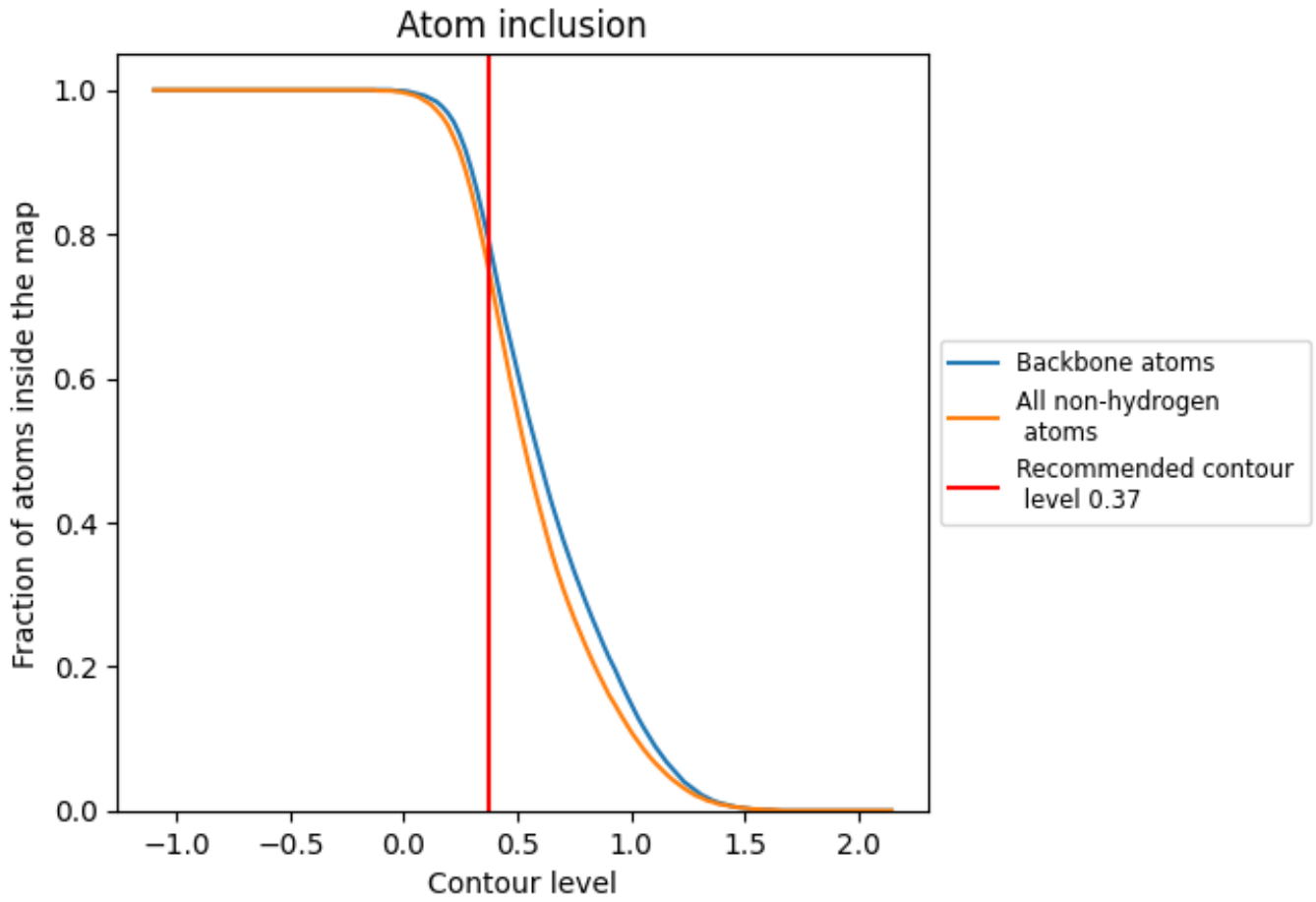
9.3 Atom inclusion mapped to coordinate model



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 (0.37).

9.4 Atom inclusion (i)



At the recommended contour level, 80% of all backbone atoms, 76% 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 (0.37) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7550	0.1920
1	0.6780	0.2120
2	0.7950	0.1810
3	0.6740	0.2640
4	0.9860	0.3870
A	0.8190	0.2900
B	0.9440	0.2580
C	0.8620	0.2950
D	0.2740	0.0240
E	0.9100	0.2900
F	0.9610	0.3000
G	0.7620	0.1640
H	0.9120	0.1490
I	0.8920	0.1500
J	0.8430	0.1950
K	0.9520	0.2010
L	0.8500	0.2470
M	0.8040	0.2660
N	0.8740	0.3000
O	0.8590	0.2530
P	0.7430	0.2680
Q	0.4580	0.0290
R	0.8280	0.3040
S	0.8900	0.2590
T	0.9120	0.3710
U	0.9180	0.2580
V	0.8400	0.2200
W	0.8180	0.2180
Y	0.6650	0.0970
Z	0.8400	0.2360
a	0.7800	0.1570
b	0.7990	0.1220
c	0.8970	0.0790
d	0.7990	0.0610
e	0.7010	0.0590

Continued on next page...

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Chain	Atom inclusion	Q-score
f	0.7170	0.0680
g	0.5610	0.0740
h	0.7390	0.0730
i	0.6150	0.0230
j	0.8330	0.0500
k	0.7490	0.0550
l	0.6900	0.0660
m	0.9190	0.1090
n	0.7640	0.0740
o	0.8050	0.0720
p	0.8980	0.0790
q	0.6060	0.0700
r	0.9400	0.1470
s	0.4960	0.1050
t	0.4110	0.0150
u	0.9030	0.2540
v	0.7860	0.1330
w	0.8720	0.1370
x	0.4110	0.0800
y	0.8210	0.0850
z	0.5410	0.1300