



Full wwPDB EM Validation Report ⓘ

Sep 23, 2026 – 05:12 pm BST

PDB ID : 9IF8 / pdb_00009if8
EMDB ID : EMD-52844
Title : Cryo-EM structure of the kinetoplastid post-catalytic trans-spliceosome (P complex)
Authors : Nadenoen, T.; Vanden Broeck, A.
Deposited on : 2025-02-17
Resolution : 2.80 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:

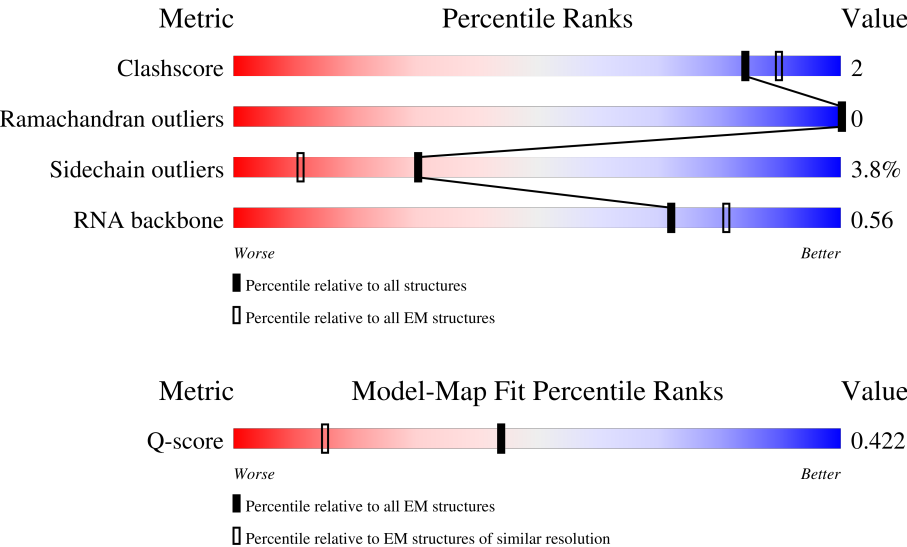
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	11806 (2.30 - 3.30)

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

Mol	Chain	Length	Quality of chain
1	LA	2427	14% 89% 8% .
2	LB	2367	86% 89% 10%
3	LC	1016	9% 81% 8% 10%

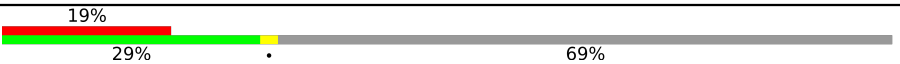
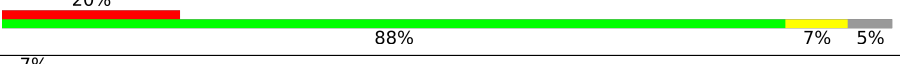
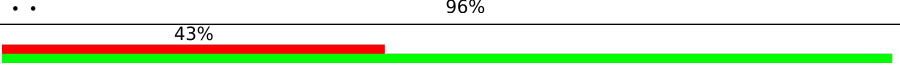
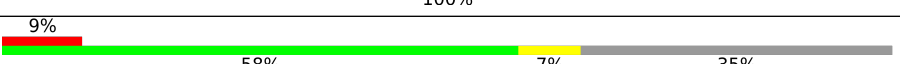
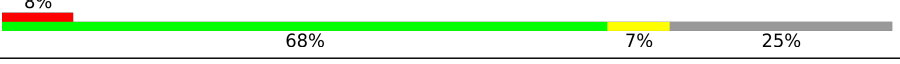
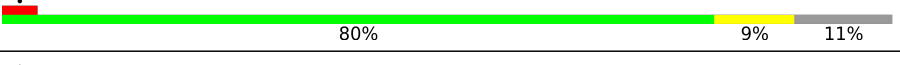
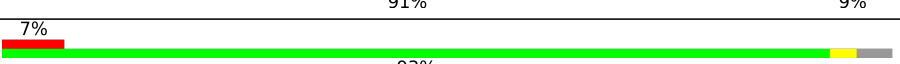
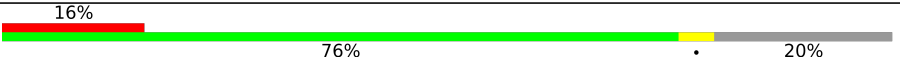
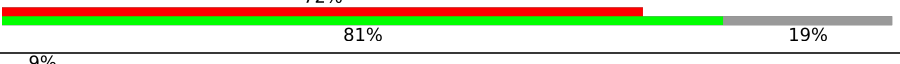
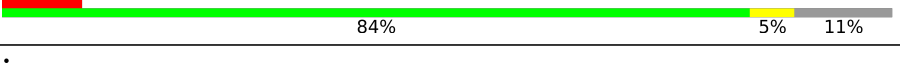
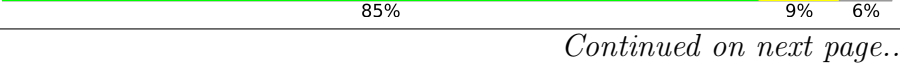
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Mol	Chain	Length	Quality of chain
4	LD	166	
5	LF	706	
6	LG	82	
7	LH	159	
8	LJ	509	
9	LL	326	
10	LN	322	
11	LP	207	
12	LQ	804	
13	LR	197	
14	LS	824	
15	LT	794	
16	LV	1087	
17	LW	307	
18	LY	114	
19	LZ	403	
20	SA	564	
21	SC	417	
22	SD	546	
23	SF	258	
24	SJ	414	
25	SK	175	
26	SL	544	
27	SN	192	
28	SO	621	

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Mol	Chain	Length	Quality of chain
29	SP	269	
30	SS	284	
31	ST	513	
31	SU	513	
31	SV	513	
31	SW	513	
32	TN	1181	
33	UX	21	
34	62	190	
35	63	134	
36	64	116	
37	65	151	
38	66	80	
39	67	91	
40	A	131	
41	RN	44	
42	24	102	
42	51	102	
42	U1	102	
43	25	103	
43	52	103	
43	U2	103	
44	2C	128	
45	2D	141	
46	2H	86	

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Mol	Chain	Length	Quality of chain
46	5E	86	
46	UE	86	
47	2I	76	
47	5F	76	
47	UF	76	
48	2J	81	
48	5G	81	
48	UG	81	
49	53	113	
49	U3	113	
50	5B	111	
50	UB	111	
51	LE	63	
52	LO	57	
53	N2	142	
54	N5	71	
55	N6	100	

2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 128394 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 Prp8 protein homologue, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	LA	2347	Total	C	N	O	S	2	0
			18216	11549	3257	3315	95		

- Molecule 2 is a protein called ATP-dependent RNA helicase, putative.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	LB	2128	Total	C	N	O	0	0
			10536	6280	2128	2128		

- Molecule 3 is a protein called Small nuclear ribonucleoprotein component-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	LC	911	Total	C	N	O	S	0	0
			7002	4420	1231	1323	28		

- Molecule 4 is a protein called PRKR-interacting protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	LD	125	Total	C	N	O	S	0	0
			1006	603	215	187	1		

- Molecule 5 is a protein called Splicing factor Cactin C-terminal domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	LF	408	Total	C	N	O	S	0	0
			3311	2102	598	594	17		

- Molecule 6 is a protein called RNA-binding motif protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	LG	80	Total	C	N	O	S	0	0
			592	372	101	115	4		

- Molecule 7 is a protein called Splicing regulator SDE2-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	LH	42	Total	C	N	O	S	0	0
			331	208	68	54	1		

- Molecule 8 is a protein called Guanine nucleotide-binding protein subunit beta-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	LJ	413	Total	C	N	O	S	0	0
			3196	2015	575	590	16		

- Molecule 9 is a protein called G10 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	LL	185	Total	C	N	O	S	1	0
			1455	910	275	254	16		

- Molecule 10 is a protein called Guanine nucleotide-binding protein subunit beta-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	LN	316	Total	C	N	O	S	0	0
			2314	1430	418	448	18		

- Molecule 11 is a protein called Spliceosome-associated CWC15-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	LP	72	Total	C	N	O	S	0	0
			589	370	114	103	2		

- Molecule 12 is a protein called Cell division control protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	LQ	551	Total	C	N	O	S	0	0
			4277	2620	824	817	16		

- Molecule 13 is a protein called CWF21 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	LR	107	Total	C	N	O	S	0	0
			798	482	156	156	4		

- Molecule 14 is a protein called Crooked neck-like protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	LS	755	Total	C	N	O	S	0	0
			6093	3800	1142	1129	22		

- Molecule 15 is a protein called Pre-mRNA-splicing factor SYF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	LT	794	Total	C	N	O	S	0	0
			6284	3978	1133	1142	31		

- Molecule 16 is a protein called RNA helicase.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	LV	973	Total	C	N	O	S	0	0
			7589	4749	1326	1465	49		

- Molecule 17 is a protein called U2 small nuclear ribonucleoprotein 40K, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	LW	188	Total	C	N	O	S	0	0
			1545	979	280	280	6		

- Molecule 18 is a protein called RRM domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	LY	107	Total	C	N	O	S	0	0
			876	558	163	151	4		

- Molecule 19 is a protein called NF-kappa-B-activating protein C-terminal domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	LZ	89	Total	C	N	O	S	0	0
			619	376	123	118	2		

- Molecule 20 is a protein called MI domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	SA	500	Total	C	N	O	S	0	0
			4143	2597	741	779	26		

- Molecule 21 is a protein called Pre-mRNA-splicing factor SLU7.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	SC	261	Total	C	N	O	S	0	0
			2108	1298	389	414	7		

- Molecule 22 is a protein called Pre-mRNA-splicing factor 18.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	SD	292	Total	C	N	O	S	0	0
			2339	1477	424	423	15		

- Molecule 23 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	SF	48	Total	C	N	O	0	0
			237	141	48	48		

- Molecule 24 is a protein called PRP19-related complex protein 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	SJ	273	Total	C	N	O	S	0	0
			2197	1359	412	417	9		

- Molecule 25 is a protein called Unspecified product.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	SK	87	Total	C	N	O	S	0	0
			699	452	118	125	4		

- Molecule 26 is a protein called SNW domain-containing protein 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
26	SL	221	Total	C	N	O	P	S	0	0
			1627	991	294	332	1	9		

- Molecule 27 is a protein called peptidylprolyl isomerase.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	SN	185	Total	C	N	O	S	0	0
			1396	885	239	264	8		

- Molecule 28 is a protein called Guanine nucleotide-binding protein subunit beta-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	SO	424	Total	C	N	O	S	0	0
			3334	2111	598	611	14		

- Molecule 29 is a protein called Pre-mRNA-splicing factor ISY1 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	SP	83	Total	C	N	O	S	0	0
			683	423	127	132	1		

- Molecule 30 is a protein called Pre-mRNA-splicing factor SPF27.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	SS	186	Total	C	N	O	S	0	0
			1504	936	279	282	7		

- Molecule 31 is a protein called Pre-mRNA-processing factor 19.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	ST	488	Total	C	N	O	S	0	0
			3606	2238	650	700	18		
31	SU	133	Total	C	N	O	S	0	0
			1022	637	184	195	6		
31	SV	133	Total	C	N	O	S	0	0
			1022	637	184	195	6		
31	SW	121	Total	C	N	O	S	0	0
			949	593	172	178	6		

- Molecule 32 is a protein called Probable RNA helicase.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	TN	44	Total	C	N	O	S	0	0
			351	227	59	63	2		

- Molecule 33 is a RNA chain called Unidentified protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
33	UX	21	Total	C	N	O	0	0
			105	63	21	21		

- Molecule 34 is a protein called LSM domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	62	124	Total	C	N	O	S	0	0
			937	578	177	175	7		

- Molecule 35 is a protein called Sm domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	63	79	Total	C	N	O	S	0	0
			602	377	102	119	4		

- Molecule 36 is a protein called U6 snRNA-associated Sm-like protein LSm4.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	64	83	Total	C	N	O	S	0	0
			640	390	123	121	6		

- Molecule 37 is a protein called LSM domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	65	114	Total	C	N	O	S	0	0
			876	547	151	172	6		

- Molecule 38 is a protein called Sm domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	66	71	Total	C	N	O	S	0	0
			541	338	94	106	3		

- Molecule 39 is a protein called Lsm7p protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	67	91	Total	C	N	O	S	0	0
			701	444	129	126	2		

- Molecule 40 is a protein called Sm domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	A	102	Total	C	N	O	S	0	0
			774	486	136	147	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	ACE	-	acetylation	UNP A0A640KIZ1

- Molecule 41 is a RNA chain called Y-branched pre-mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	RN	12	Total	C	N	O	P	0	0
			175	75	15	73	12		

- Molecule 42 is a protein called Small nuclear ribonucleoprotein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	24	102	Total	C	N	O	S	0	0
			783	489	132	157	5		
42	51	98	Total	C	N	O	S	0	0
			758	475	127	151	5		
42	U1	98	Total	C	N	O		0	0
			484	288	98	98			

- Molecule 43 is a protein called Small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	25	82	Total	C	N	O	S	0	0
			654	418	116	118	2		
43	52	89	Total	C	N	O	S	0	0
			715	457	128	128	2		
43	U2	83	Total	C	N	O		0	0
			411	245	83	83			

- Molecule 44 is a protein called Lsm5p, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	2C	114	Total	C	N	O	S	0	0
			881	535	174	168	4		

- Molecule 45 is a protein called Small nuclear ribonucleoprotein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	2D	99	Total	C	N	O	S	0	0
			792	502	140	148	2		

- Molecule 46 is a protein called Small nuclear ribonucleoprotein E.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	2H	81	Total	C	N	O	S	0	0
			657	409	124	120	4		
46	5E	78	Total	C	N	O	S	0	0
			629	393	117	116	3		
46	UE	79	Total	C	N	O		0	0
			388	230	79	79			

- Molecule 47 is a protein called Sm protein F.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	2I	76	Total	C	N	O	S	0	0
			598	377	104	113	4		
47	5F	76	Total	C	N	O	S	0	0
			598	377	104	113	4		
47	UF	76	Total	C	N	O		0	0
			375	223	76	76			

- Molecule 48 is a protein called Sm protein G.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	2J	77	Total	C	N	O	S	0	0
			583	361	107	112	3		
48	5G	77	Total	C	N	O	S	0	0
			583	361	107	112	3		
48	UG	77	Total	C	N	O		0	0
			379	225	77	77			

- Molecule 49 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	53	104	Total	C	N	O	S	0	0
			801	502	147	150	2		
49	U3	81	Total	C	N	O		0	0
			400	238	81	81			

- Molecule 50 is a protein called Sm protein B.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	5B	99	Total	C	N	O	S	0	0
			738	458	133	141	6		
50	UB	81	Total	C	N	O		0	0
			398	236	81	81			

- Molecule 51 is a RNA chain called SL-ligated pre-mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	LE	21	Total	C	N	O	P	0	0
			358	157	37	143	21		

- Molecule 52 is a RNA chain called SL RNA outtron.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	LO	47	Total	C	N	O	P	0	0
			1006	449	183	327	47		

- Molecule 53 is a RNA chain called U2 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	N2	76	Total	C	N	O	P	0	0
			1604	718	270	540	76		

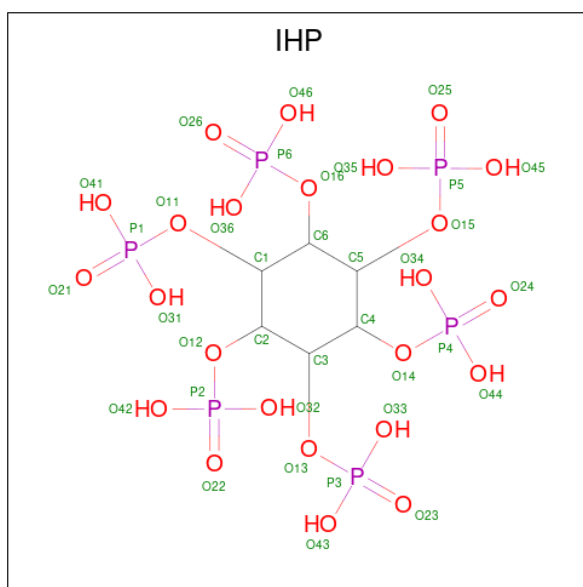
- Molecule 54 is a RNA chain called U5 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	N5	63	Total	C	N	O	P	0	0
			1328	595	230	440	63		

- Molecule 55 is a RNA chain called U6 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	N6	100	Total	C	N	O	P	0	0
			2127	952	381	694	100		

- Molecule 56 is INOSITOL HEXAKISPHOSPHATE (CCD ID: IHP) (formula: $C_6H_{18}O_{24}P_6$).

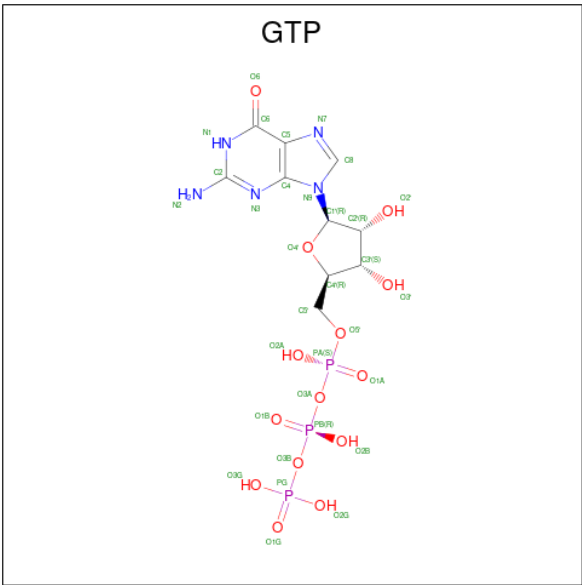


Mol	Chain	Residues	Atoms				AltConf
56	LA	1	Total	C	O	P	0
			36	6	24	6	

- Molecule 57 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
57	LA	1	Total	Mg	0
			1	1	
57	LC	1	Total	Mg	0
			1	1	
57	LE	1	Total	Mg	0
			1	1	
57	N2	1	Total	Mg	0
			1	1	
57	N5	1	Total	Mg	0
			1	1	
57	N6	7	Total	Mg	0
			7	7	

- Molecule 58 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).

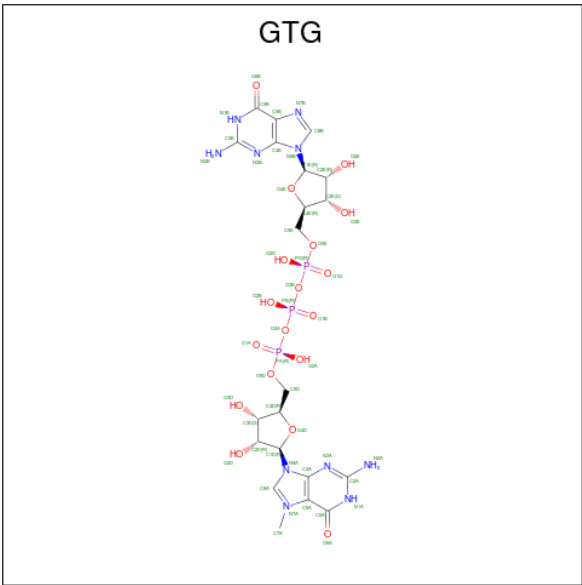


Mol	Chain	Residues	Atoms					AltConf
58	LC	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 59 is ZINC ION (CCD ID: ZN) (formula: Zn).

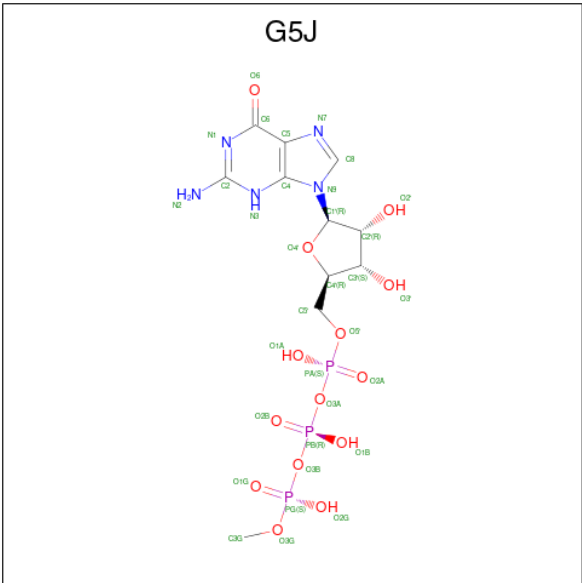
Mol	Chain	Residues	Atoms		AltConf
59	LL	3	Total	Zn	0
			3	3	
59	SC	1	Total	Zn	0
			1	1	

- Molecule 60 is 7-METHYL-GUANOSINE-5'-TRIPHOSPHATE-5'-GUANOSINE (CCD ID: GTG) (formula: C₂₁H₃₀N₁₀O₁₈P₃).



Mol	Chain	Residues	Atoms					AltConf
60	N5	1	Total	C	N	O	P	0
			52	21	10	18	3	

- Molecule 61 is 5'-O-[(S)-hydroxy{[(R)-hydroxy{[(S)-hydroxy(methoxy)phosphoryl]oxy}phosphoryl]oxy}phosphoryl]guanosine (CCD ID: G5J) (formula: C₁₁H₁₈N₅O₁₄P₃).

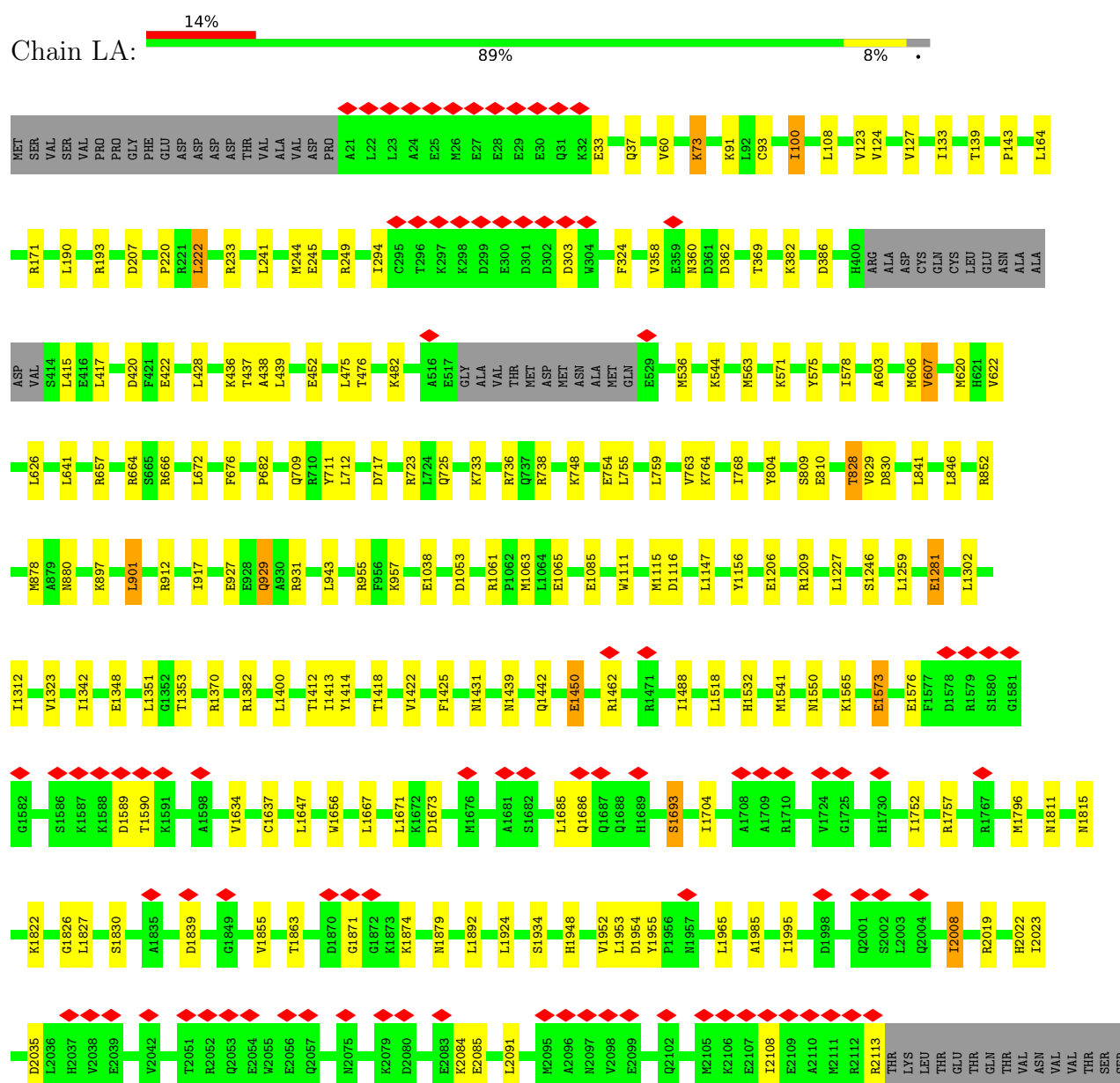


Mol	Chain	Residues	Atoms					AltConf
61	N6	1	Total	C	N	O	P	0
			33	11	5	14	3	

3 Residue-property plots [i](#)

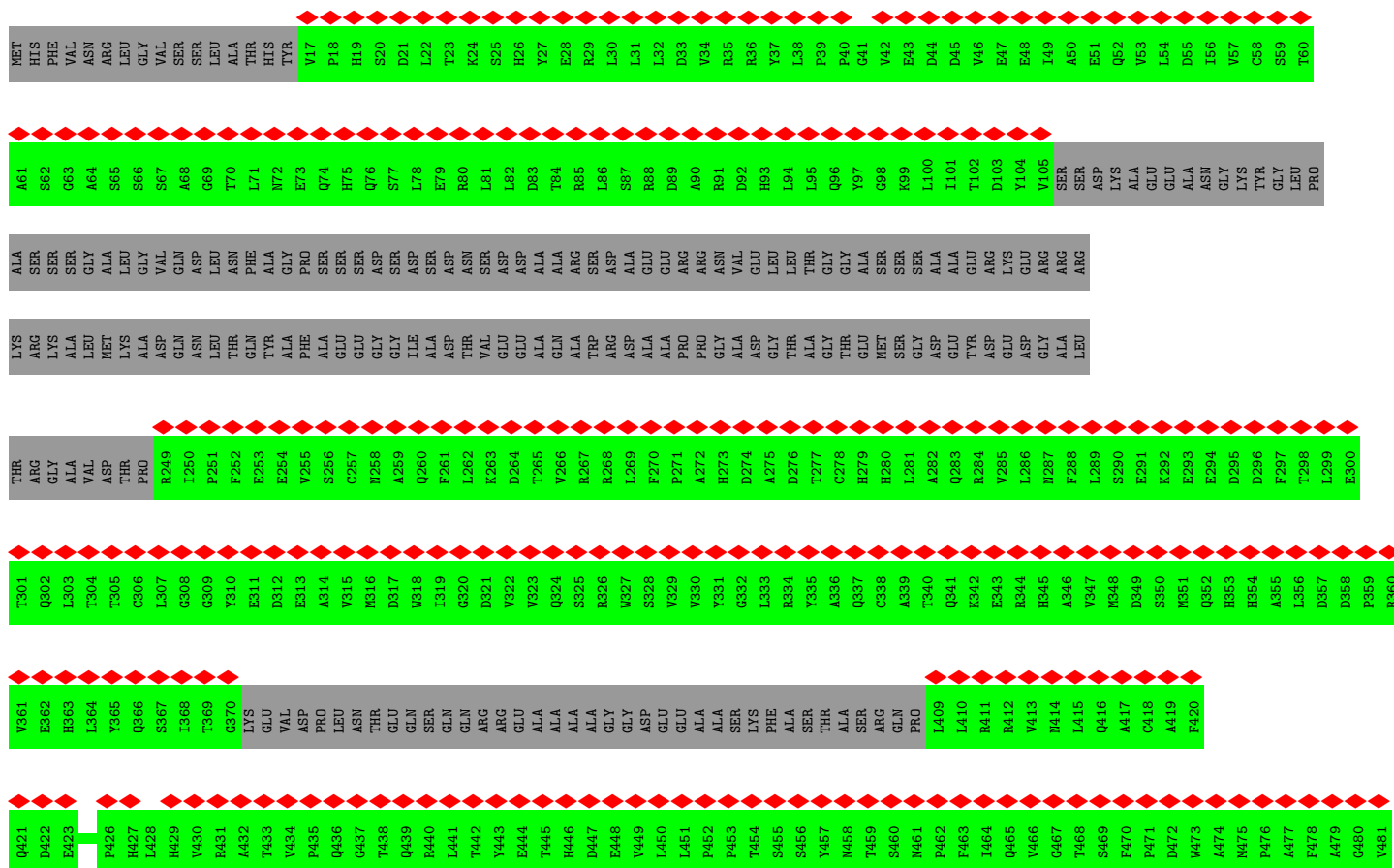
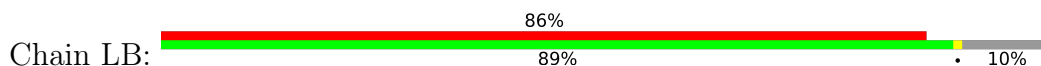
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Prp8 protein homologue, putative



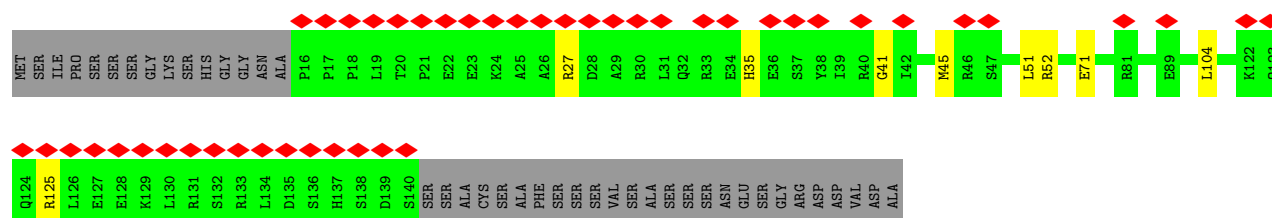
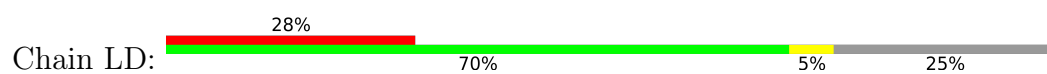


- Molecule 2: ATP-dependent RNA helicase, putative

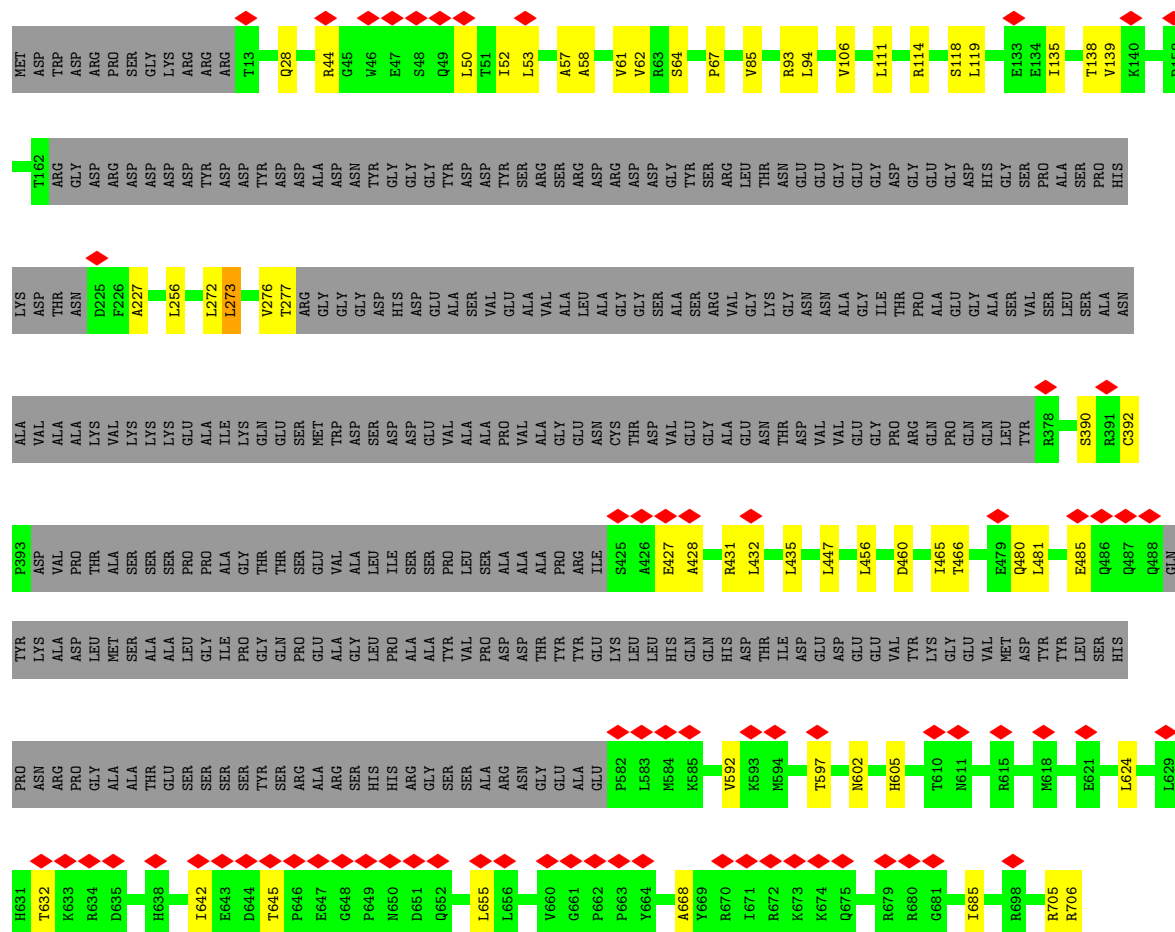


V1260	L1261	E1262	K1263	A1264	A1267	C1268	P1269	P1270	V1271	V1272	V1273	P1274	M1275	V1276	K1277	P1278	A1279	P1280	T1281	H1282	L1283	F1284	V1285	L1286	V1287	V1288	S1289	P1290	H1291	W1292	L1293	A1294	A1295	T1296	A1297	F1298	S1300	V1301	C1302	L1303	L1304	N1305	T1306	L1307	L1308	P1309	P1310	V1311	A1312	A1313	P1314	L1315	L1316	E1317	V1318	D1319	Q1320				
V1200	D1201	A1202	A1203	V1204	R1205	P1206	L1207	T1208	R1209	G1210	M1211	L1212	Y1213	V1214	D1215	I1216	I1217	E1218	P1219	P1220	D1221	F1222	D1223	Y1224	V1225	E1226	S1227	L1228	H1229	G1230	R1231	S1232	V1233	C1234	E1235	V1236	V1237	L1238	S1239	I1240	E1241	H1242	L1243	N1244	G1245	R1246	L1247	L1248	H1249	V1250	E1251	S1252	L1253	Q1254	L1255	P1256	L1257	A1258	N1259		
Q1140	V1141	R1142	S1143	Y1144	L1145	P1146	S1147	K1148	H1149	F1150	D1151	A1152	I1153	L1154	P1155	A1156	L1157	E1158	R1159	V1160	R1161	V1162	P1163	W1164	E1165	E1166	V1167	R1168	L1169	W1170	S1171	V1172	E1173	D1174	L1175	A1176	E1177	K1178	L1179	S1180	D1181	D1182	R1183	L1184	A1185	Q1186	S1187	A1188	Y1189	E1190	L1191	I1192	H1193	A1194	V1195	P1196	H1197	Y1198	A1199		
C1074	Y1075	I1076	S1077	Q1078	K1079	G1080	L1081	E1082	G1083	L1084	P1085	L1086	M1087	S1088	E1089	M1090	V1091	Y1092	R1099	I1100	L1101	R1102	A1103	L1104	Y1105	E1106	V1107	C1108	L1109	V1110	R1111	E1112	Y1113	G1114	R1115	T1116	A1117	R1118	Q1119	F1120	L1121	E1122	L1123	Y1124	L1125	M1126	H1129	R1130	Q1131	W1132	A1133	V1134	Q1135	S1136	P1137	L1138	R1139				
C995	I996	A997	S998	Y999	C1000	Y1001	I1002	V943	P944	T1003	Y1004	T1005	S1006	M1007	A1008	T1009	Y1010	L1011	S952	A953	S954	D955	P956	L957	L958	L959	H960	H961	L962	A963	N964	V965	H967	T968	A969	C970	E971	E972	L973	K974	E975	S976	K977	M978	V979	D980	Y981	D982	A983	R984	S985	R986	K987	V988	A989	G990	T991	N992	Y993	G994	
L936	Y937	V938	R939	M940	R941	Q942	V943	P944	E945	V946	Y947	G948	I949	R950	P951	S952	A953	S954	D955	P956	L957	L958	L959	H960	H961	L962	A963	N964	V965	H967	T968	A969	C970	E971	E972	L973	K974	E975	S976	K977	M978	V979	D980	Y981	D982	A983	R984	S985	R986	K987	V988	A989	G990	T991	N992	Y993	G994				
G870	Y871	G872	A873	A874	V875	C876	R877	A878	T879	I880	P884	L887	H888	Y889	Y890	S952	A953	S954	D955	P956	L957	L958	L959	H960	H961	L962	A963	N964	V965	H967	T968	A969	C970	E971	E972	L973	K974	E975	S976	K977	M978	V979	D980	Y981	D982	A983	R984	S985	R986	K987	V988	A989	G990	T991	N992	Y993	G994				
G793	I794	H795	L799	S800	R801	D802	E803	R804	N805	T806	E807	E808	Q809	L810	F811	D812	G814	H815	I816	K817	V818	L819	V820	C821	T822	S823	T824	L825	M827	G828	V829	N830	L831	P832	A833	N834	R835	V836	I837	I838	S855	A856	L857	D858	V859	L860	Q861	M862	F863	G864	R865	A866	G867	R868	A869						
F730	F735	E736	T737	E738	H739	T740	A741	R742	Y743	L744	Q745	R746	R747	L748	A749	E750	F751	R752	R753	G754	Y755	Y756	F757	V758	R759	P760	D761	S762	D763	H765	T766	V767	L768	L769	E770	A771	S772	S773	G774	T775	G776	G777	A778	V779	L780	R781	R782	S783	L784	Q785	Q786	L787	L788	P789	D790	G791	F792				
G671	H672	N673	R674	Q675	R676	G677	L678	F679	V680	L612	L613	K614	L615	L616	I617	R618	P619	E620	G614	H622	L623	L624	H625	N626	L566	G567	L568	T569	V570	C571	L641	Q642	Q643	Q644	L645	R646	A647	E648	M649	G650	L651	R652	L653	V654	G655	L656	H657	L658	I659	T659	L660	P661	N662	H663	A664	D665	W666	D667	L668	T669	I670
R602	K603	S604	E605	E606	L607	G608	V609	A610	S611	L612	L613	K614	L615	L616	I617	R618	D619	E620	V621	H622	L623	L624	H625	N626	L566	G567	L568	T569	V570	C571	L641	Q642	Q643	Q644	L645	R646	A647	E648	M649	G650	L651	R652	L653	V654	G655	L656	H657	L658	I659	T659	L660	P661	N662	H663	A664	D665	W666	D667	L668	T669	I670
M542	V543	Y544	V545	A546	P547	G548	K549	A550	L551	V552	H553	E554	V555	V556	R557	T558	F559	S560	K561	R562	L563	E564	S565	L566	G567	L568	T569	V570	C571	L641	Q642	Q643	Q644	L645	R646	A647	E648	M649	G650	L651	R652	L653	V654	G655	L656	H657	L658	I659	T659	L660	P661	N662	H663	A664	D665	W666	D667	L668	T669	I670	
E482	E483	L484	N485	A486	M487	S488	K489	K490	V491	Y492	D493	C494	A495	F496	H497	S498	D499	E500	N501	M502	L503	V504	S505	A506	P507	T508	G509	A510	C511	K512	L513	N514	V515	A516	M517	L518	A519	M520	L521	R522	T523	I524	A525	A526	S527	R528	N529	P530	K531	T532	G533	V534	I535	G537	H538	N539	L540	K541			

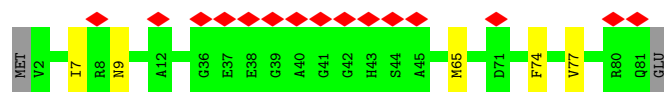




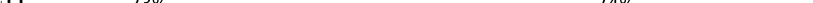
• Molecule 5: Splicing factor Cactin C-terminal domain-containing protein

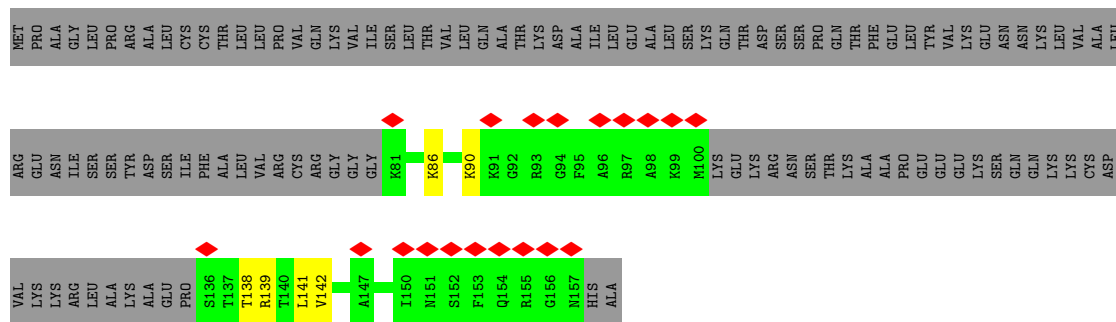


• Molecule 6: RNA-binding motif protein

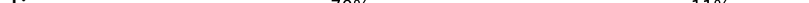


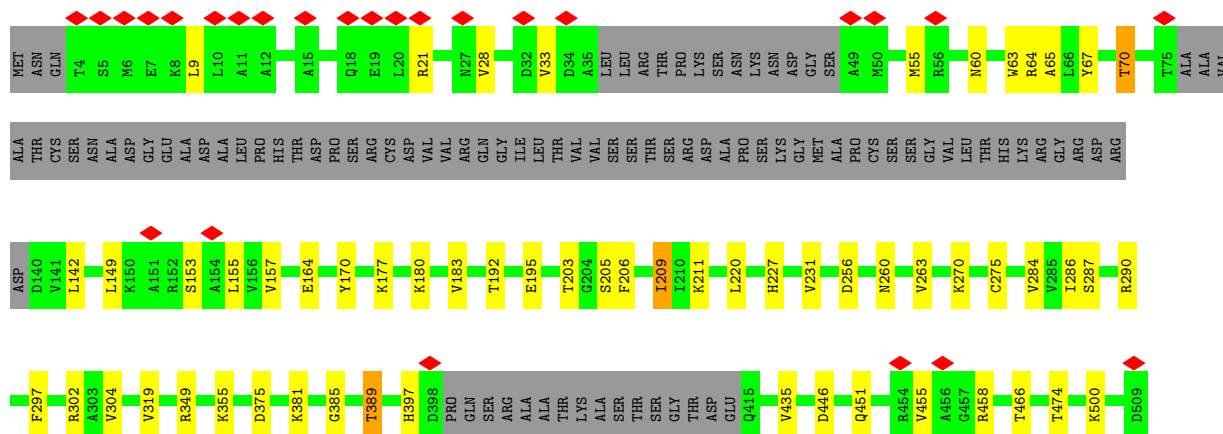
• Molecule 7: Splicing regulator SDE2-like protein

Chain LH: 

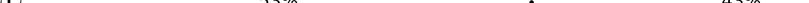


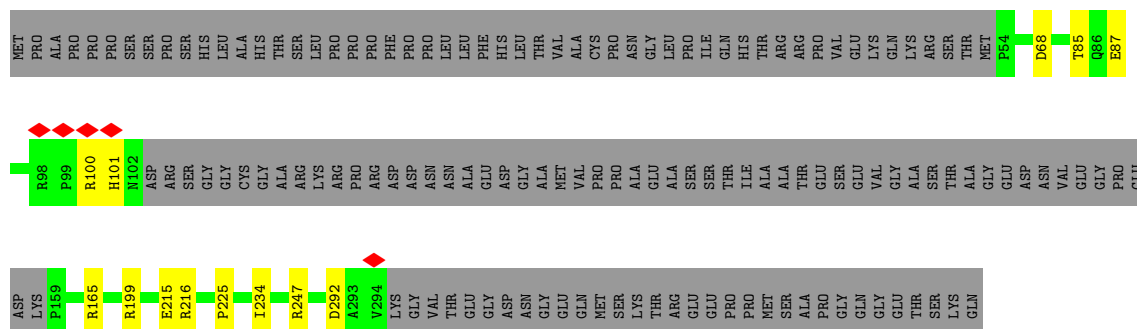
- Molecule 8: Guanine nucleotide-binding protein subunit beta-like protein

Chain LJ: 

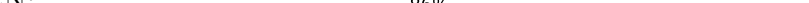


- Molecule 9: G10 protein

Chain LL: 

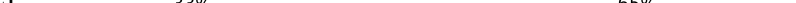


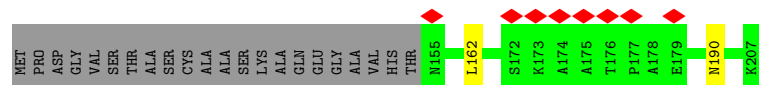
- Molecule 10: Guanine nucleotide-binding protein subunit beta-like protein

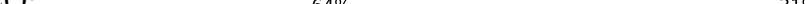
Chain LN: 

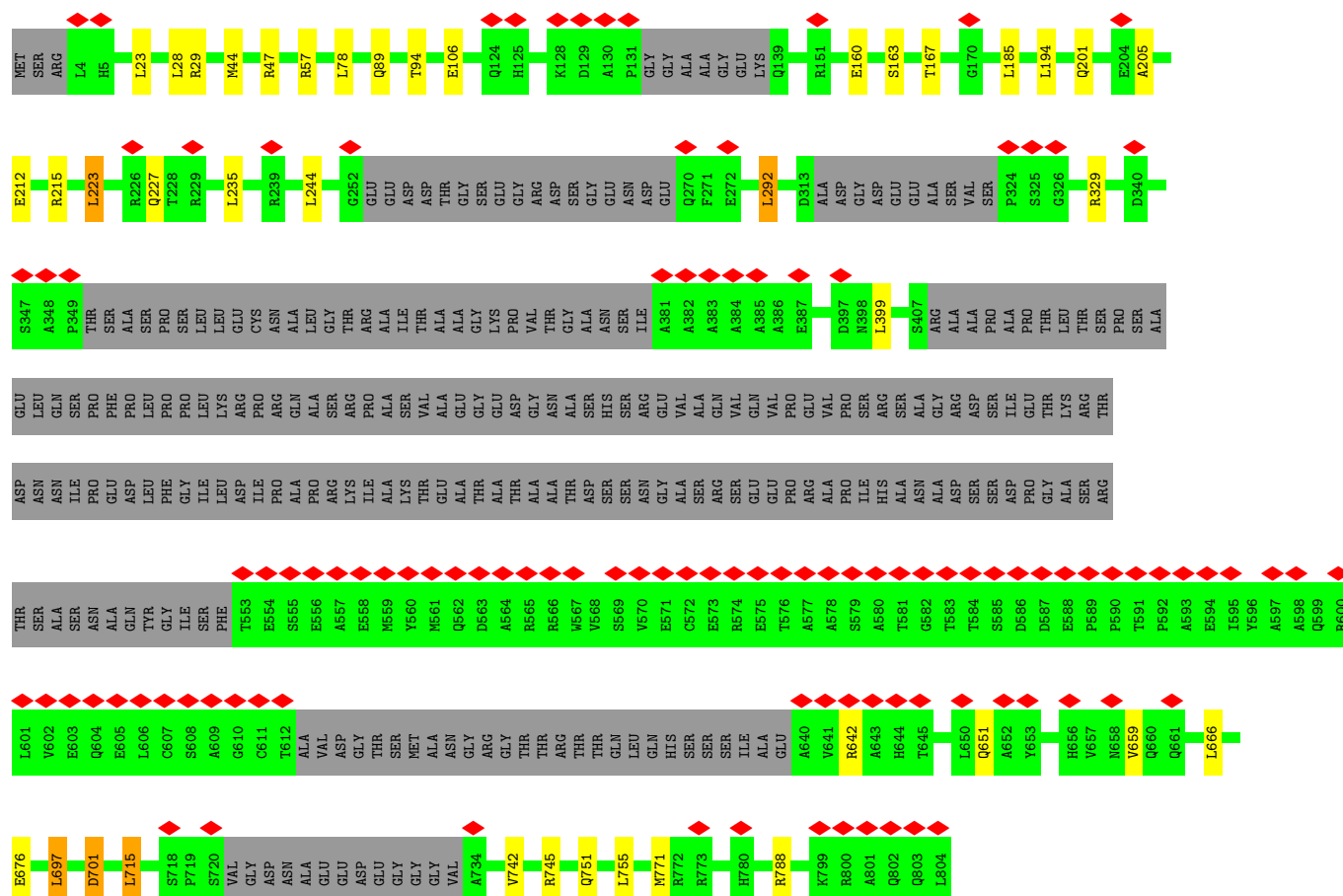




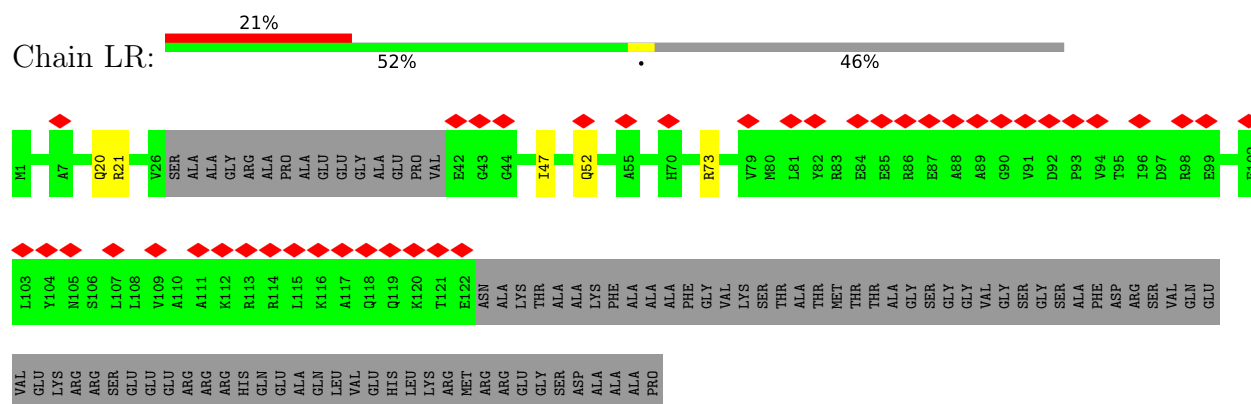
- Chain LP: 



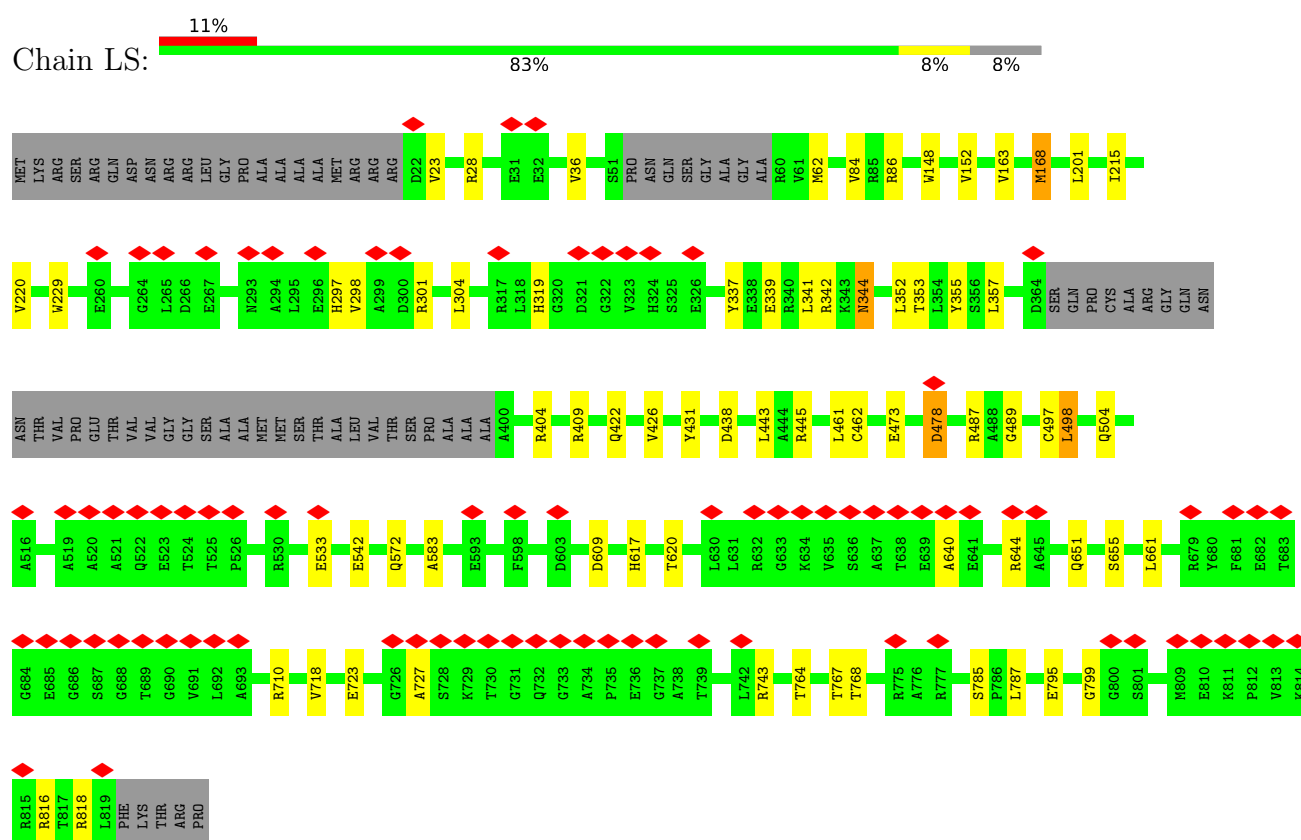
- Chain LQ: 



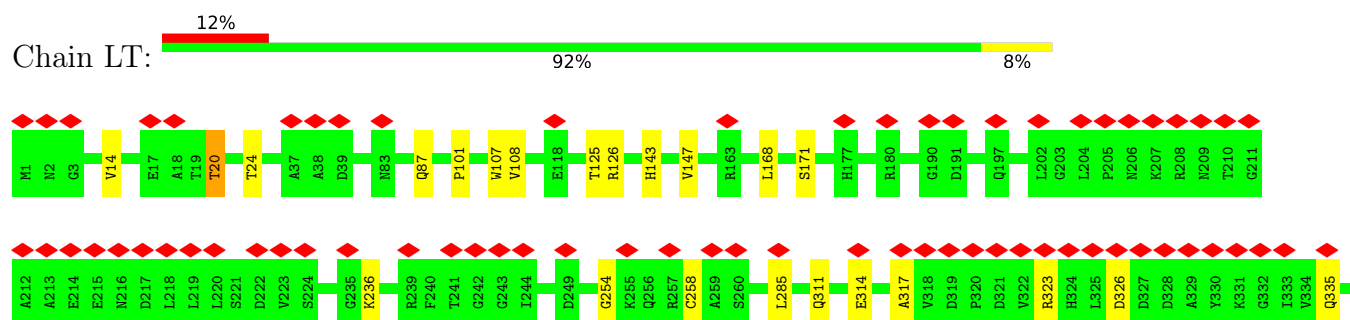
- Molecule 13: CWF21 domain-containing protein

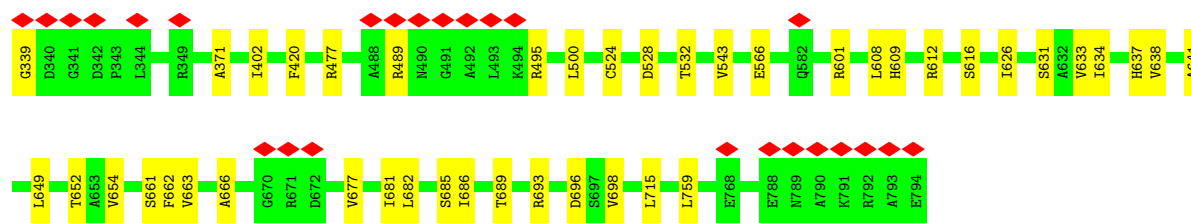


- Molecule 14: Crooked neck-like protein 1

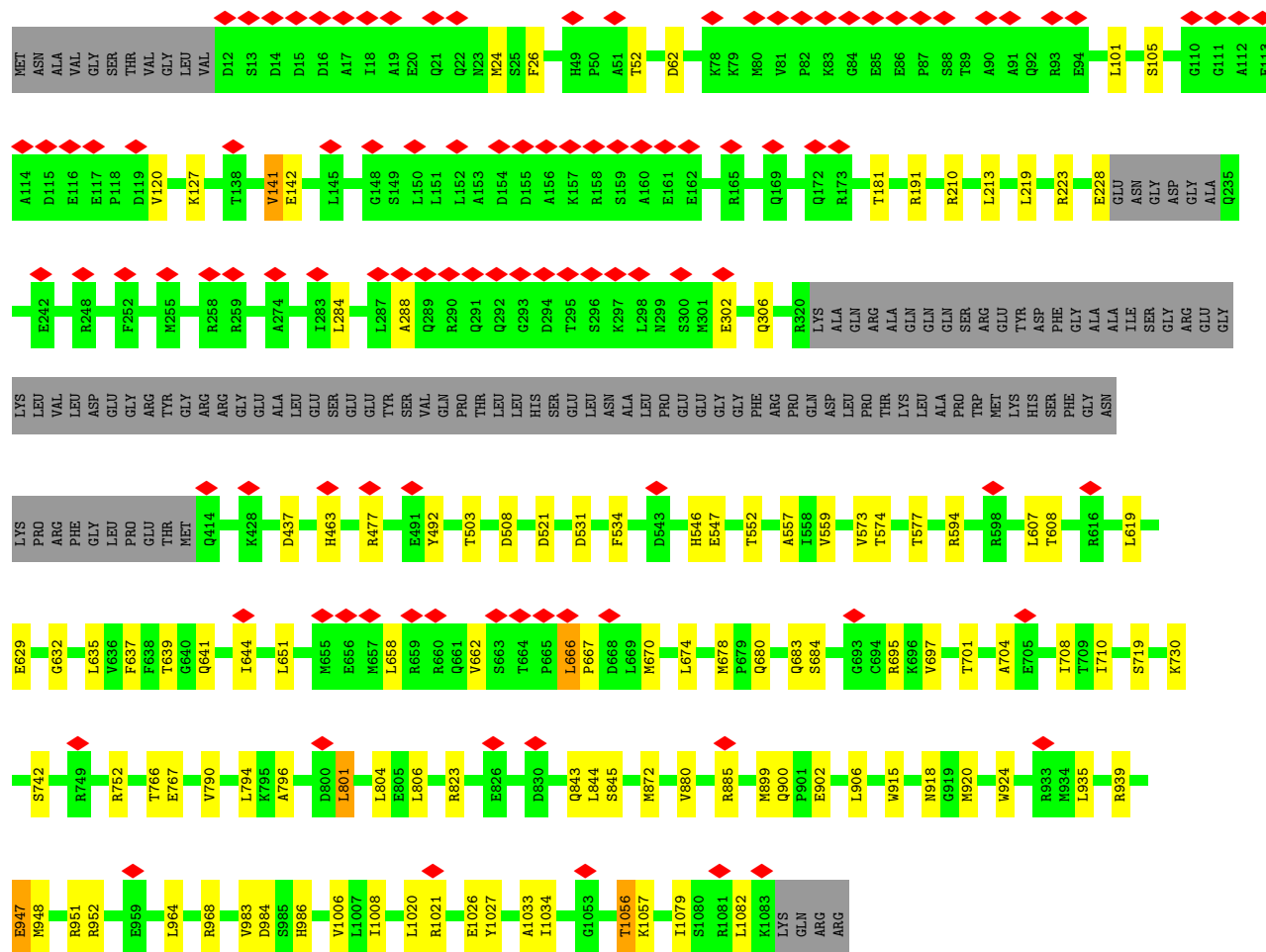
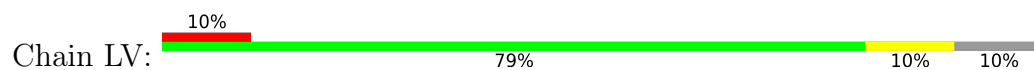


- Molecule 15: Pre-mRNA-splicing factor SYF1

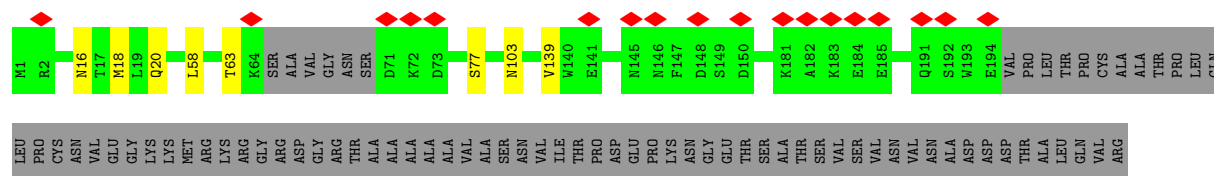




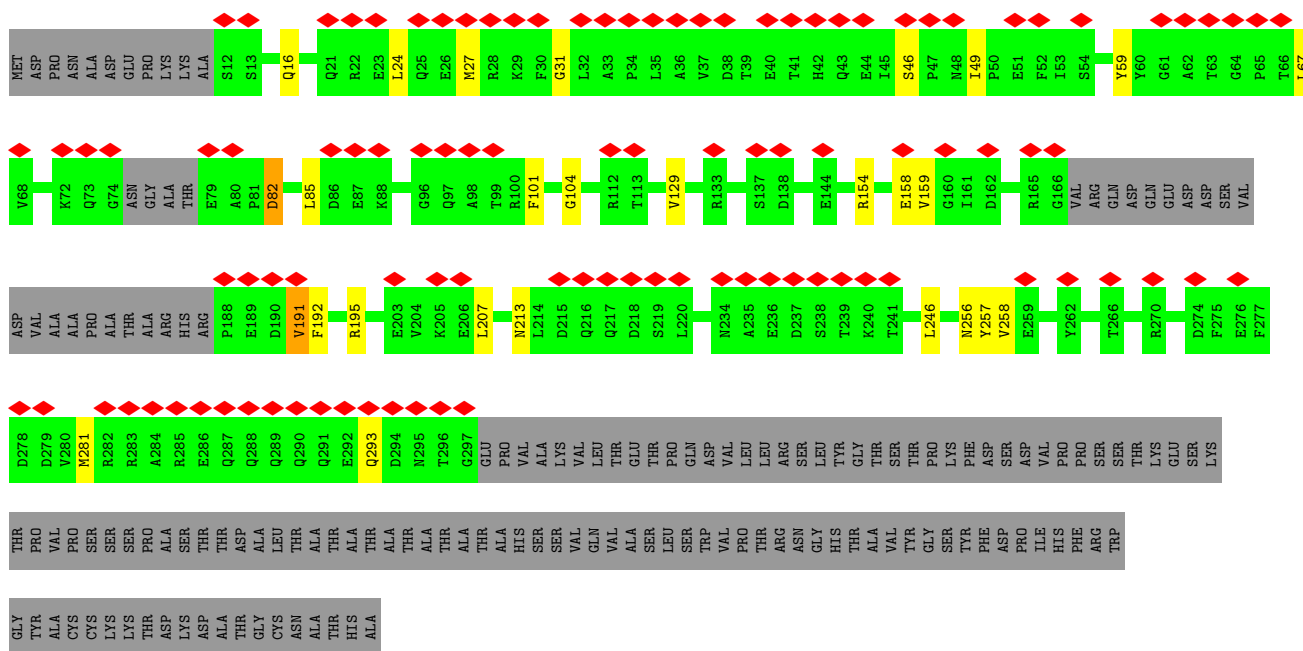
• Molecule 16: RNA helicase



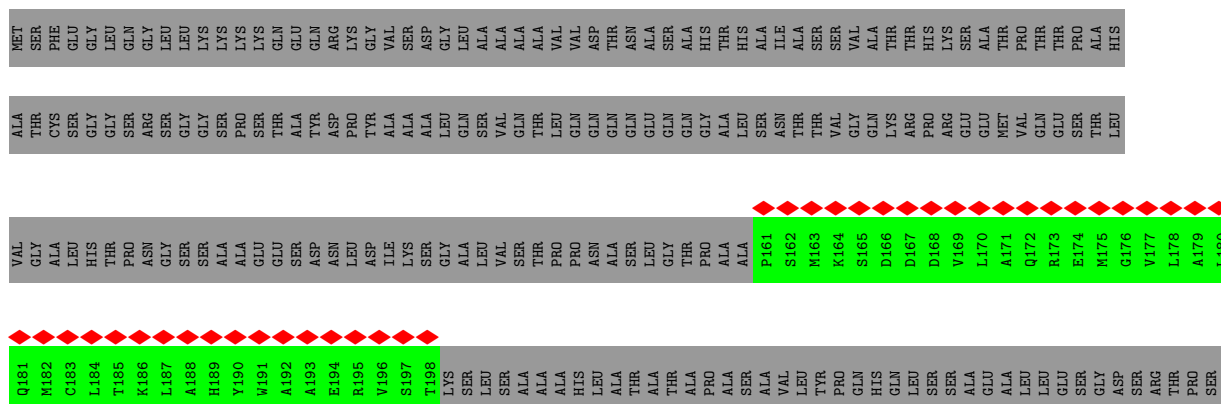
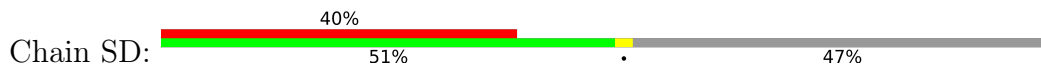
• Molecule 17: U2 small nuclear ribonucleoprotein 40K, putative

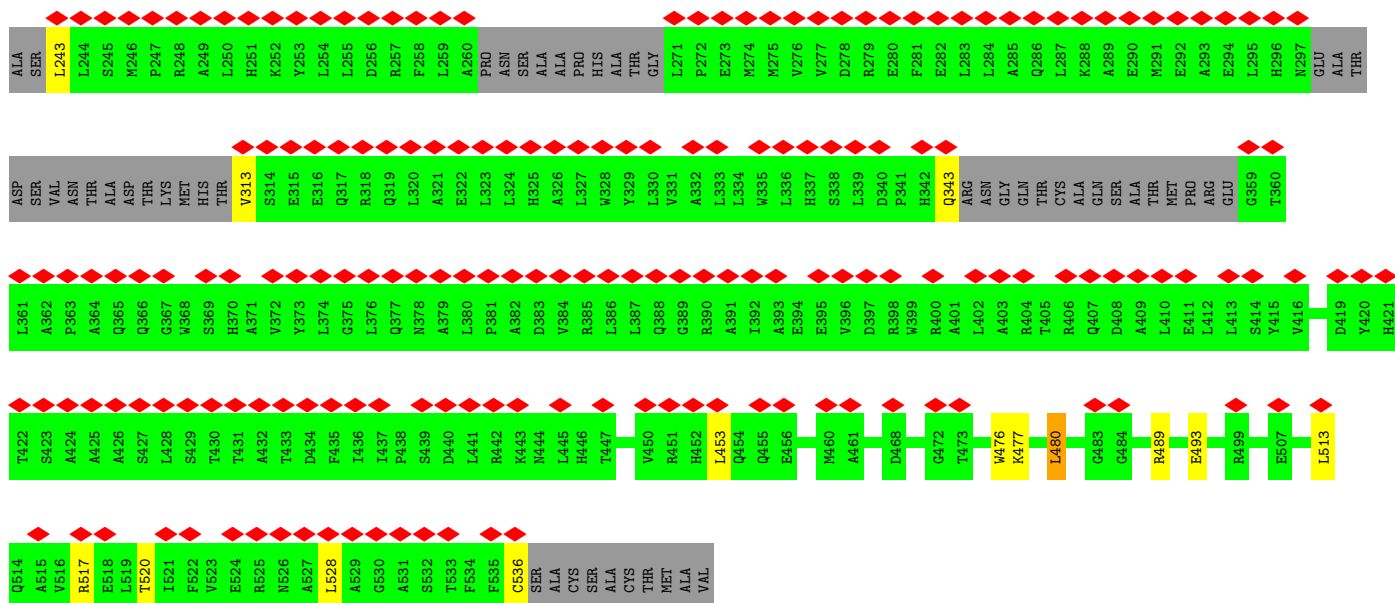


- Molecule 21: Pre-mRNA-splicing factor SLU7

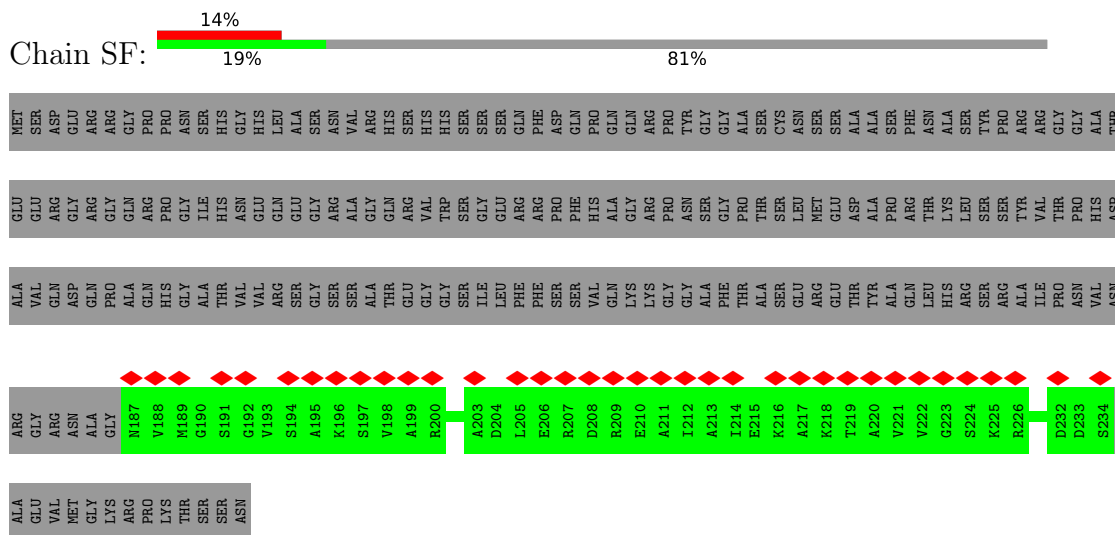


- Molecule 22: Pre-mRNA-splicing factor 18

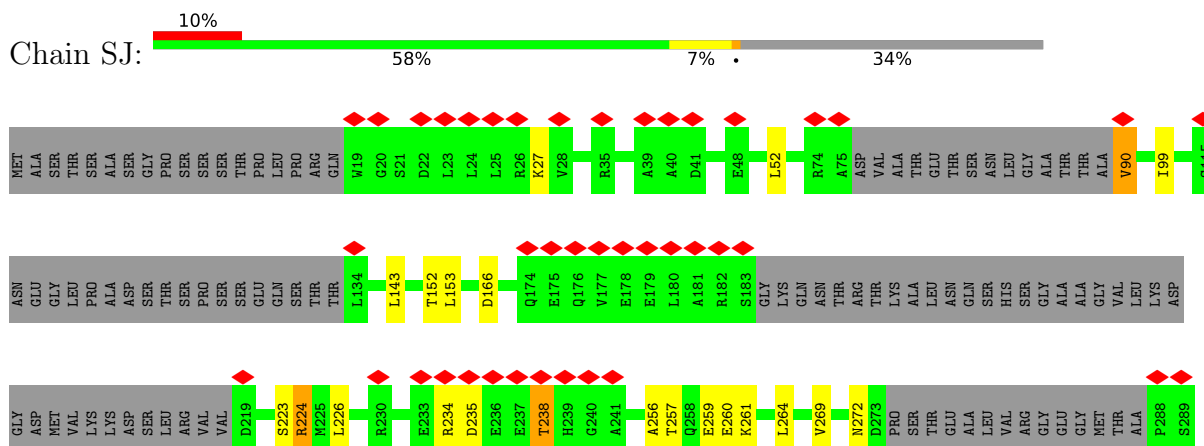


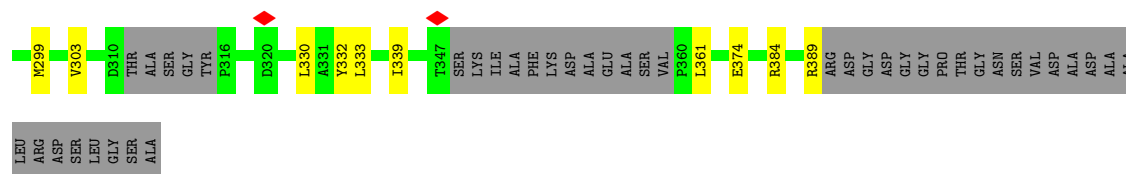


- Molecule 23: Uncharacterized protein

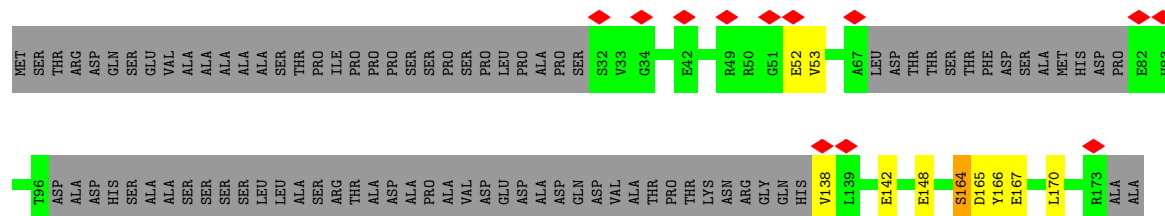


- Molecule 24: PRP19-related complex protein 3

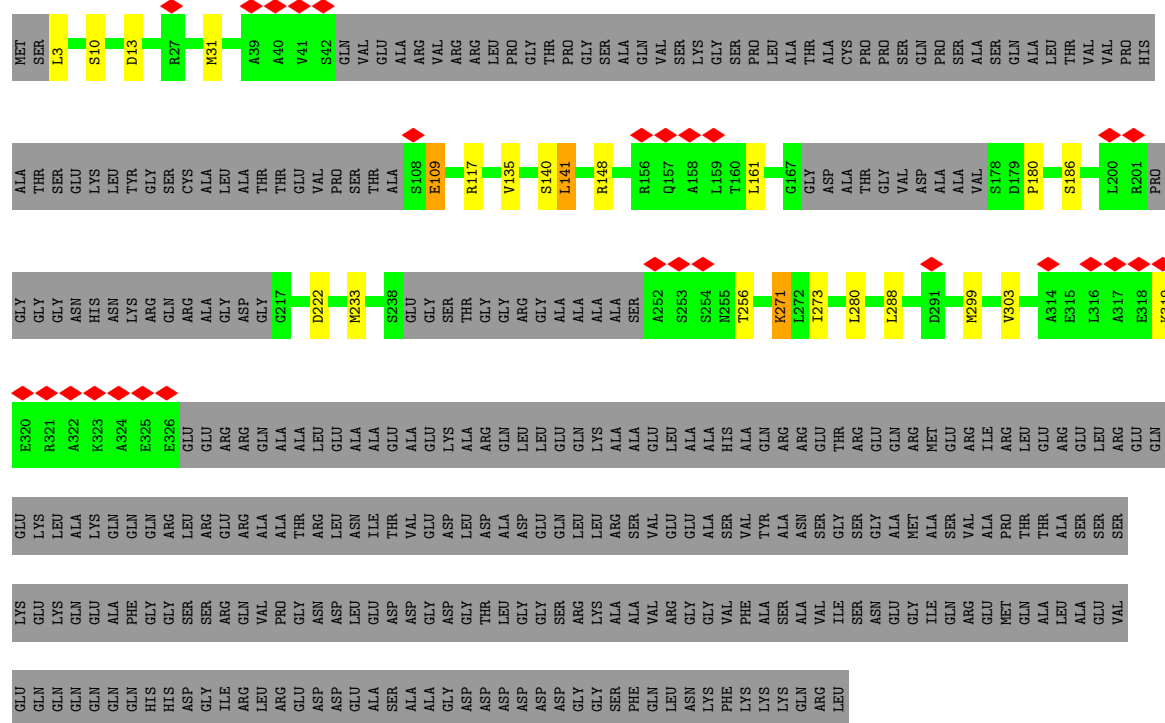




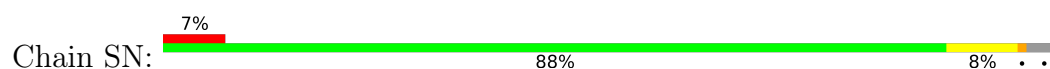
- Molecule 25: Unspecified product



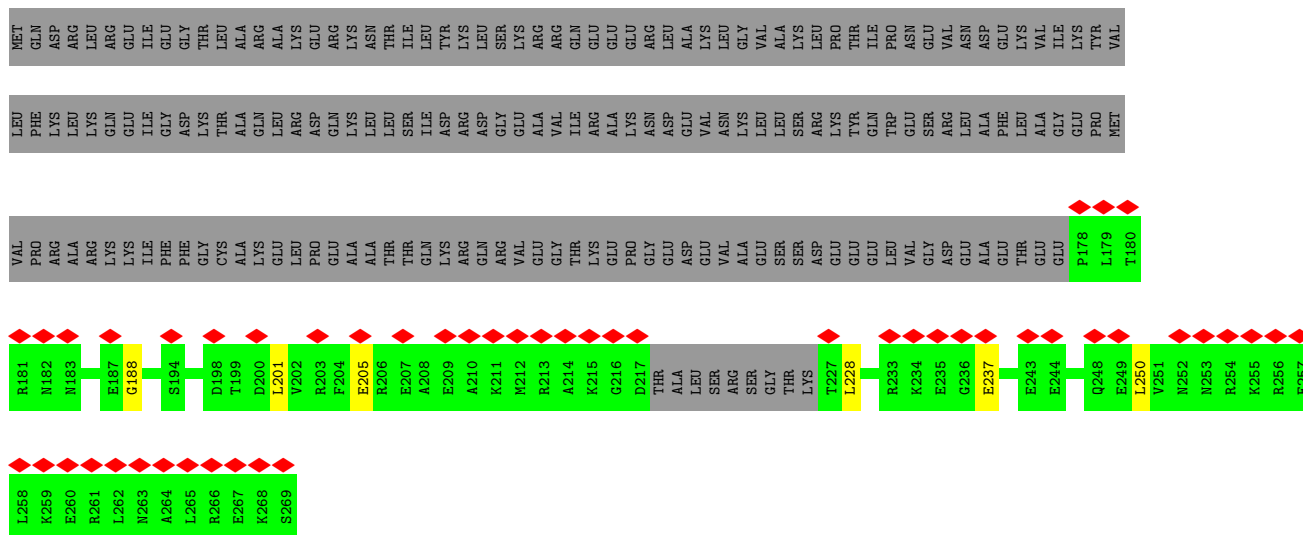
- Molecule 26: SNW domain-containing protein 1



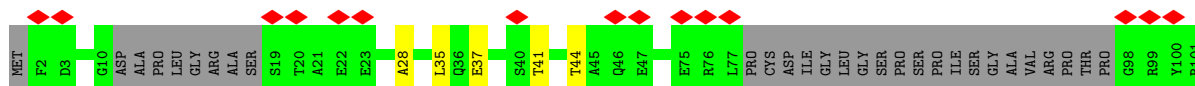
- Molecule 27: peptidylprolyl isomerase

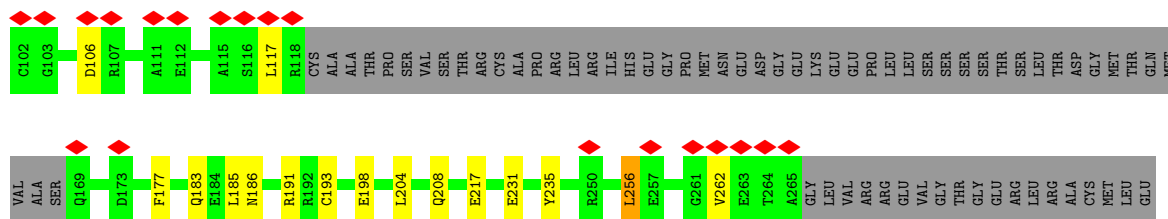


Chain SO:

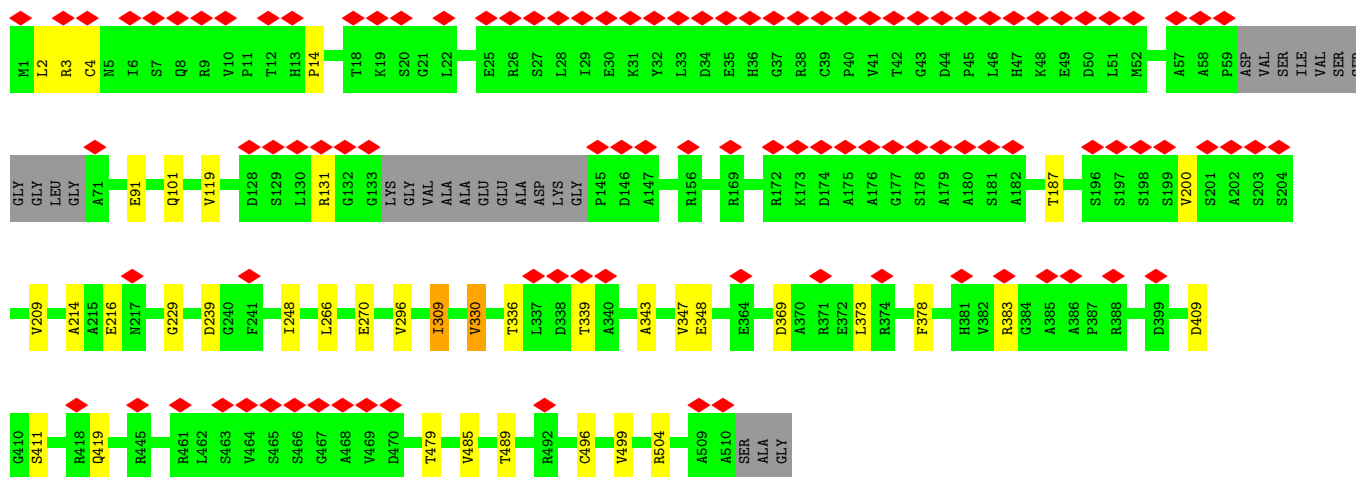
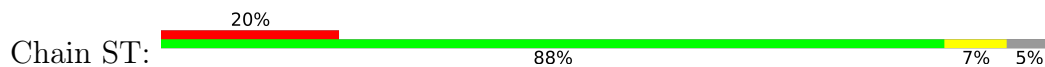


Chain SS:

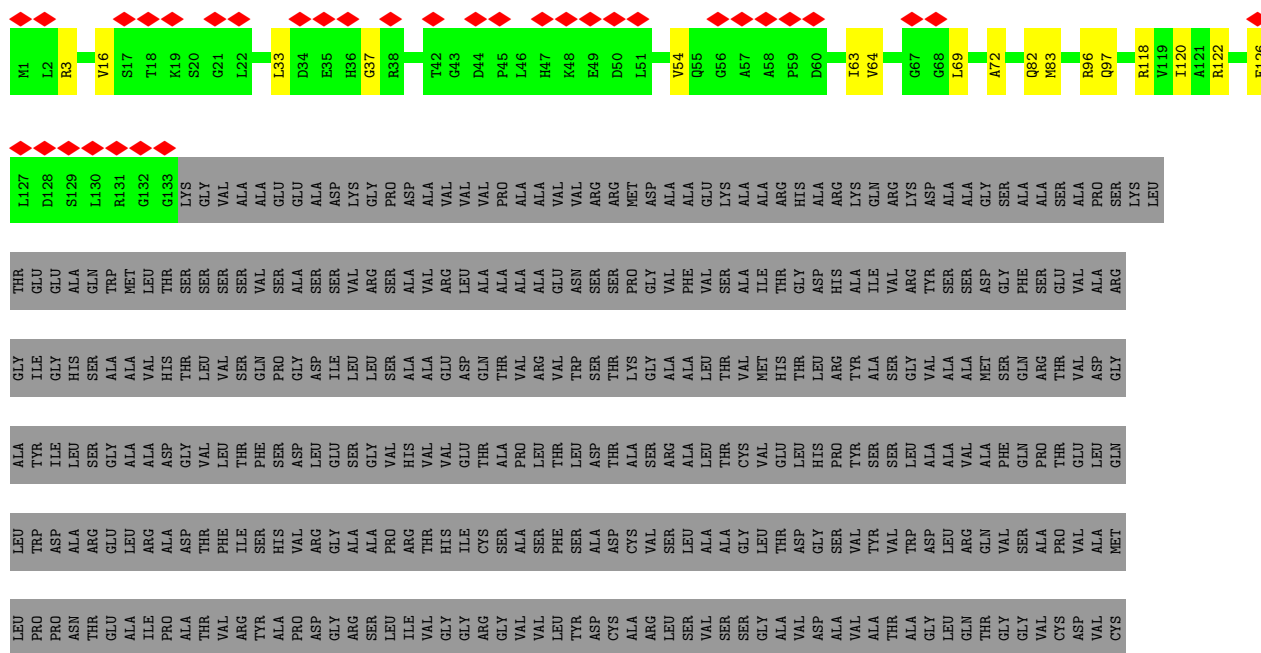




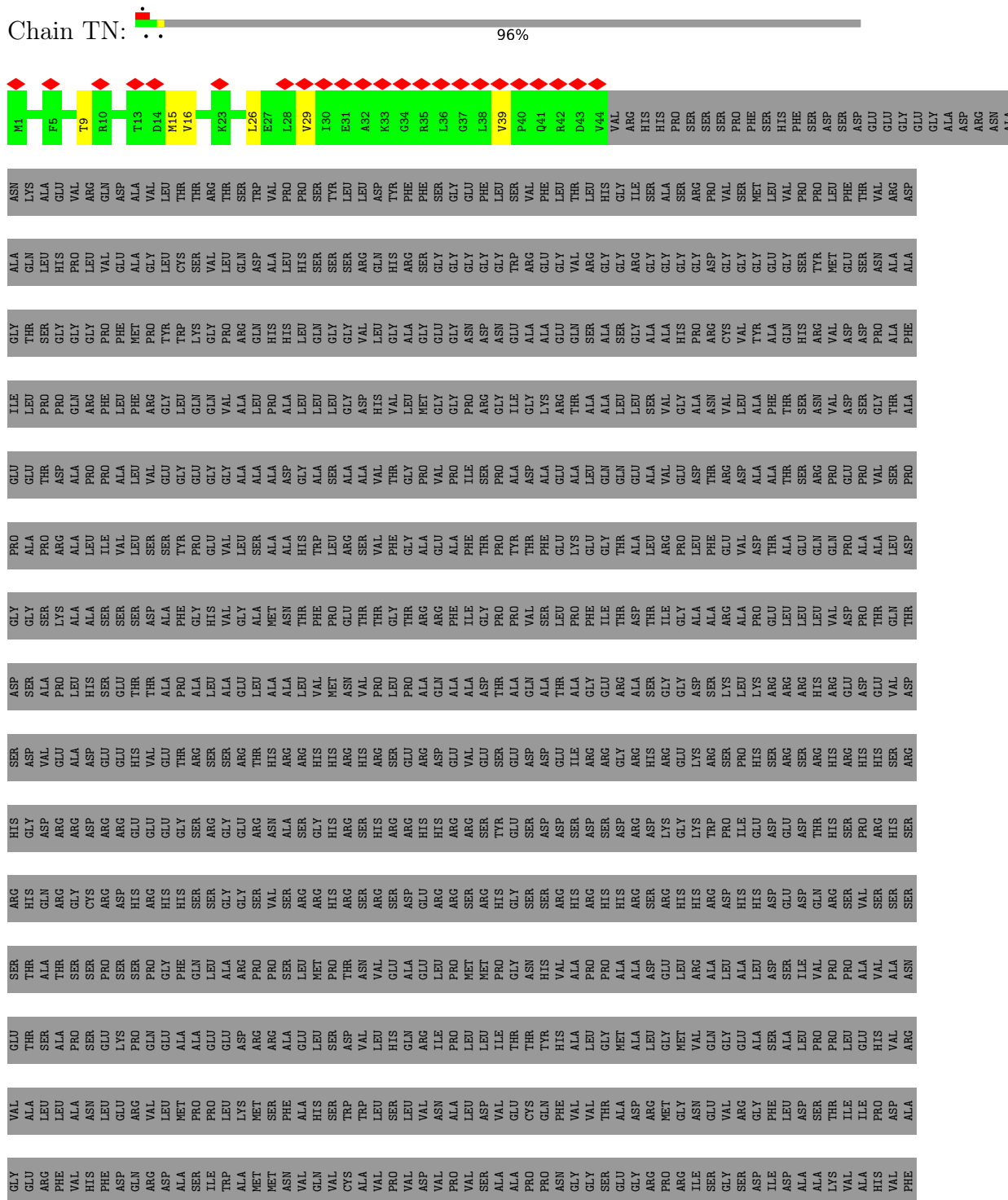
• Molecule 31: Pre-mRNA-processing factor 19

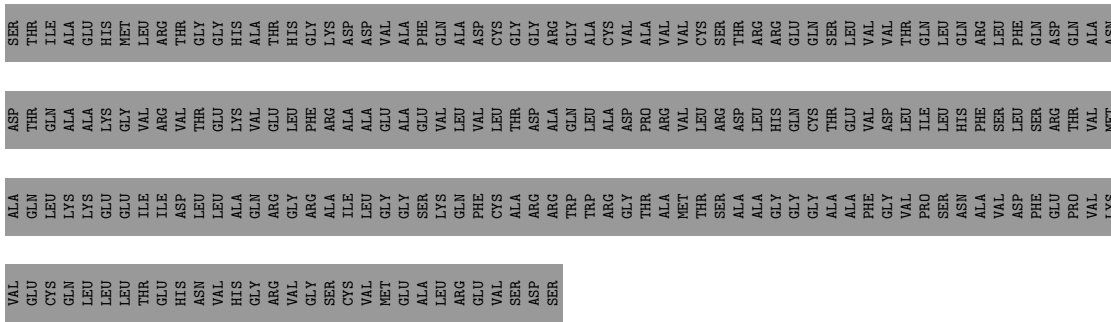


• Molecule 31: Pre-mRNA-processing factor 19

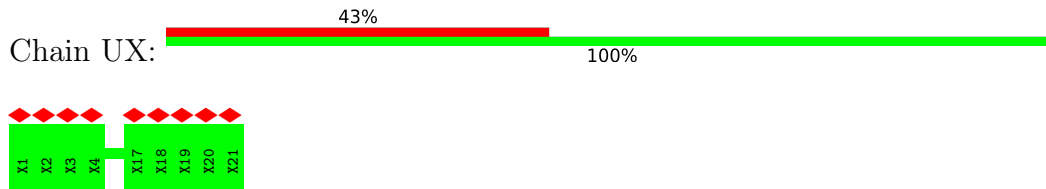


- Molecule 32: Probable RNA helicase

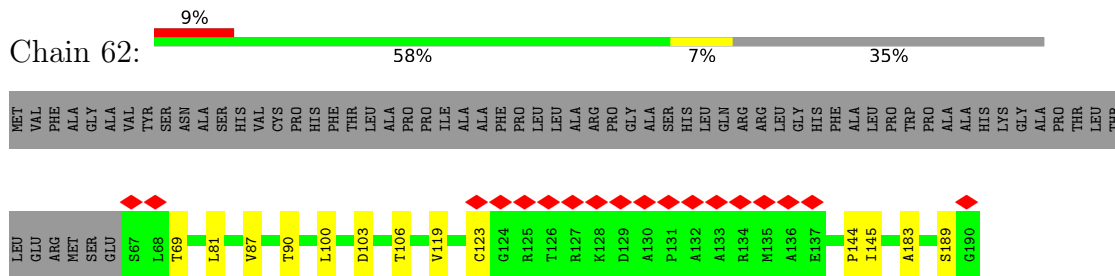




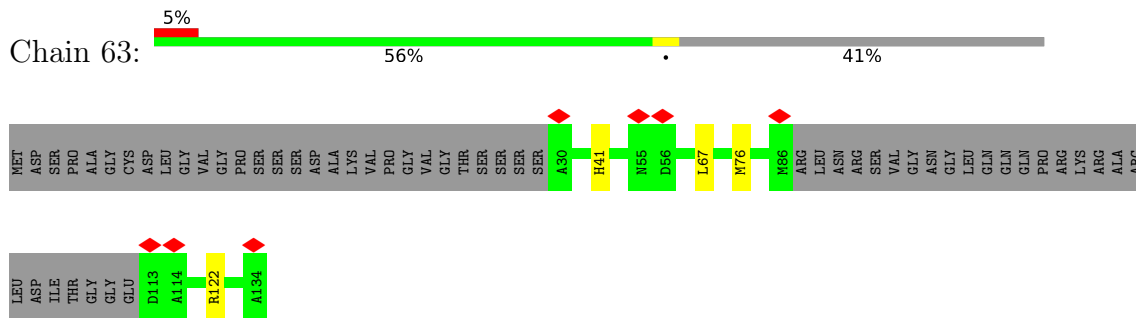
- Molecule 33: Unidentified protein



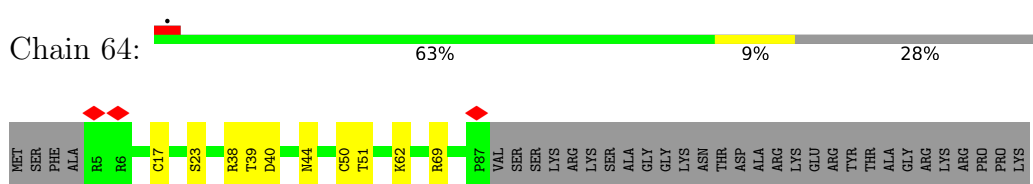
- Molecule 34: LSM domain-containing protein



- Molecule 35: Sm domain-containing protein

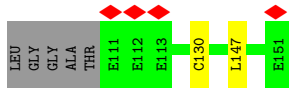


- Molecule 36: U6 snRNA-associated Sm-like protein LSm4



- Molecule 37: LSM domain-containing protein





-

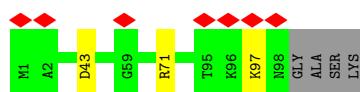
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| E4 | 8 | Red | Yes |
| A5 | 7 | Red | Yes |
| A6 | 6 | Green | No |
| H7 | 5 | Red | Yes |
| V8 | 4 | Green | No |
| K12 | 3 | Yellow | No |
| E13 | 3 | Yellow | No |
| L18 | 2 | Green | No |
| V35 | 2 | Green | No |
| V46 | 2 | Green | No |
| D52 | 2 | Green | No |
| I65 | 2 | Green | No |
| G72 | 2 | Green | No |
| I86 | 2 | Green | No |
| I91 | 1 | Red | Yes |

-
- ACE1 V16 L21 D29 N33 D50 A75 R76 R77 L92 R93 D115 V116 V124 T125 A126 VAL GLY LYS TERP

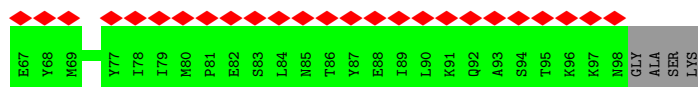
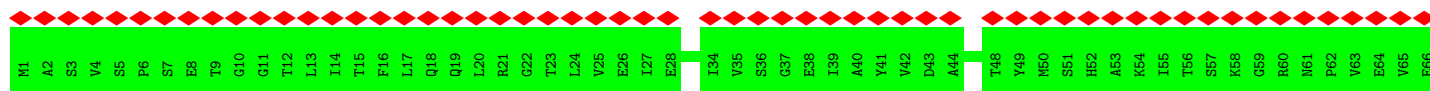
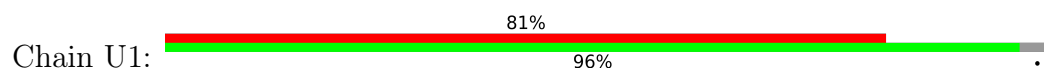
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| A4 | 100 |
| A5 | 100 |
| A6 | 100 |
| A7 | 100 |
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| A10 | 100 |
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| A12 | 100 |
| A13 | 100 |
| A14 | 100 |
| A15 | 100 |
| A16 | 100 |
| A17 | 100 |
| A18 | 100 |
| A19 | 100 |
| A20 | 100 |
| A21 | 100 |
| A22 | 100 |
| A23 | 100 |
| A24 | 100 |
| A25 | 100 |
| A26 | 100 |
| A27 | 100 |
| A28 | 100 |
| A29 | 100 |
| A30 | 100 |
| A31 | 100 |
| A32 | 100 |
| A33 | 100 |
| A34 | 100 |
| A35 | 100 |
| A36 | 100 |
| A37 | 100 |
| A38 | 100 |
| A39 | 100 |
| A40 | 100 |
| G44 | 100 |

-

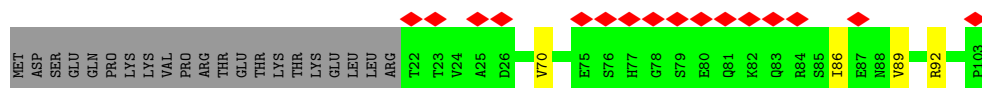
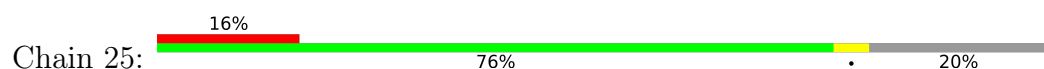
- 



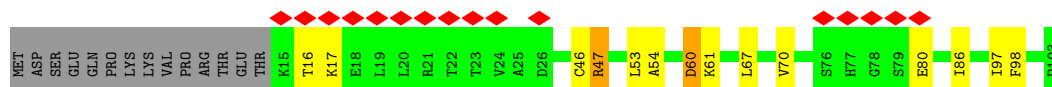
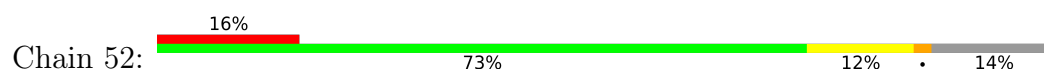
- Molecule 42: Small nuclear ribonucleoprotein, putative



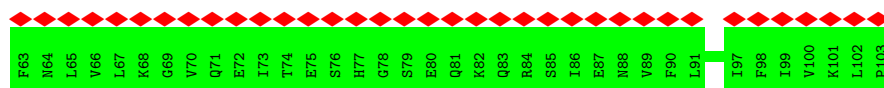
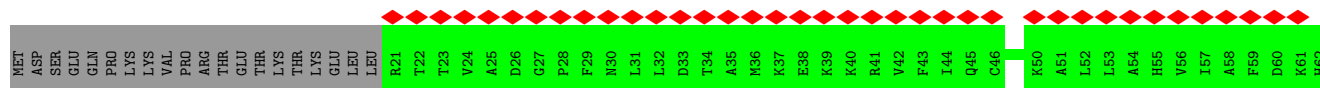
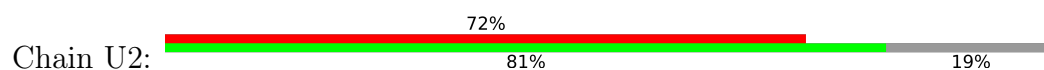
- Molecule 43: Small nuclear ribonucleoprotein Sm D2



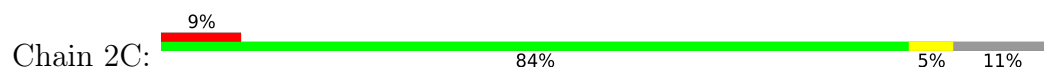
- Molecule 43: Small nuclear ribonucleoprotein Sm D2



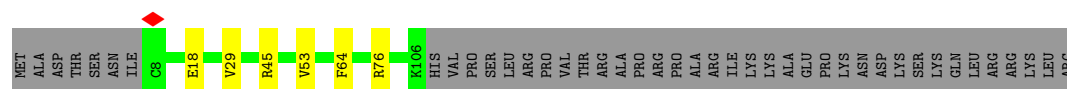
- Molecule 43: Small nuclear ribonucleoprotein Sm D2



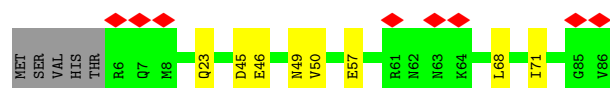
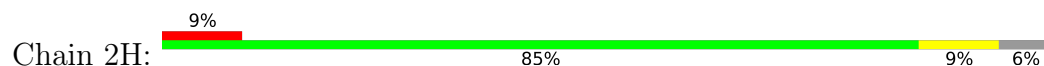
- Molecule 44: Lsm5p, putative



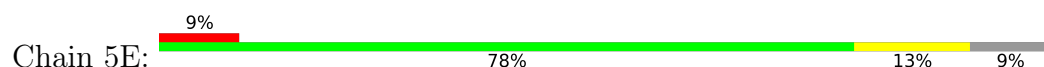
- Molecule 45: Small nuclear ribonucleoprotein, putative



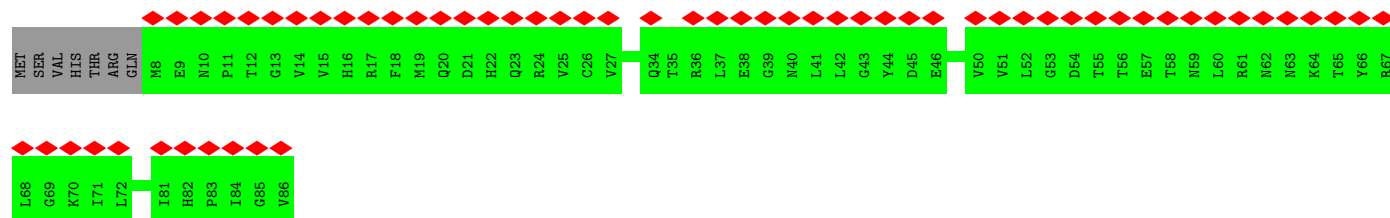
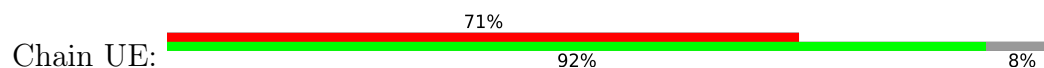
- Molecule 46: Small nuclear ribonucleoprotein E



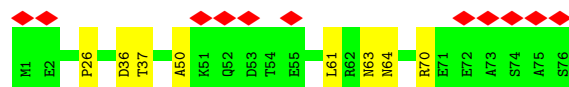
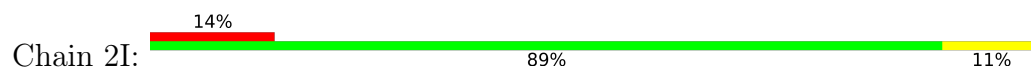
- Molecule 46: Small nuclear ribonucleoprotein E



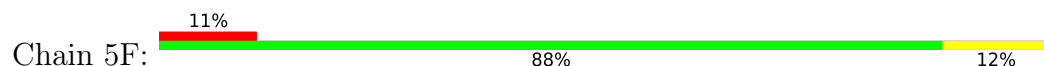
- Molecule 46: Small nuclear ribonucleoprotein E



- Molecule 47: Sm protein F

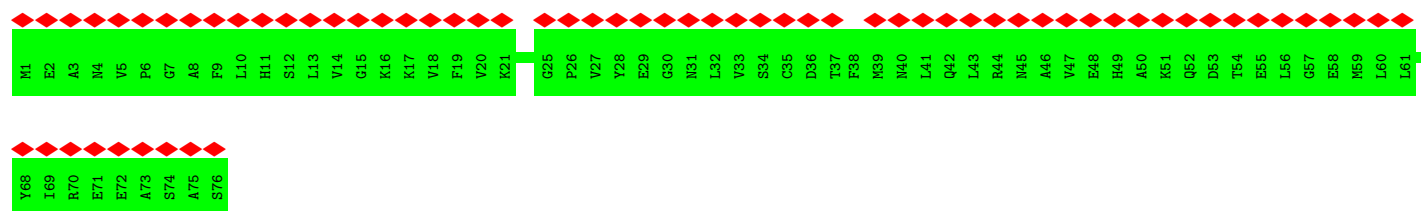


- Molecule 47: Sm protein F

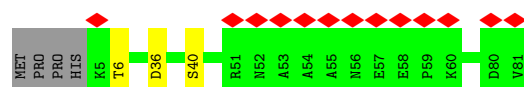
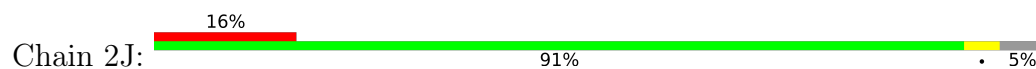


- Molecule 47: Sm protein F

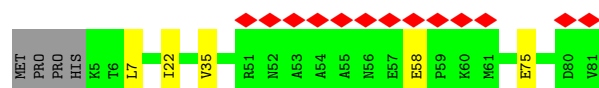




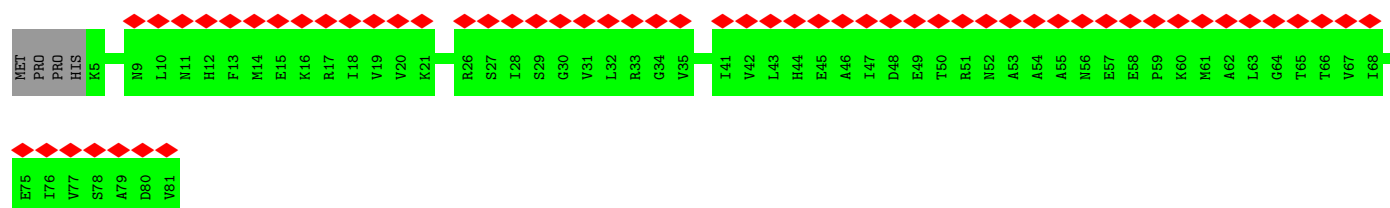
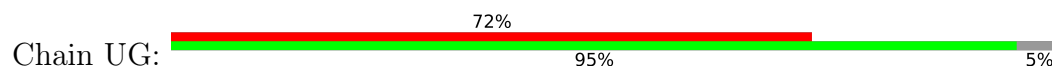
• Molecule 48: Sm protein G



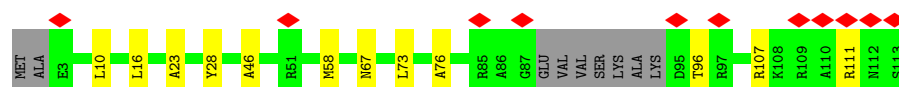
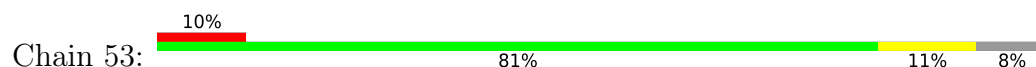
• Molecule 48: Sm protein G



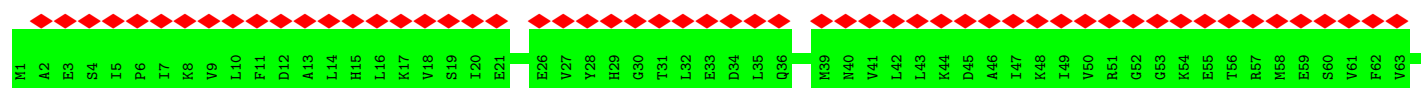
• Molecule 48: Sm protein G

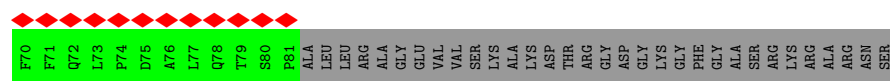


• Molecule 49: Small nuclear ribonucleoprotein Sm D3

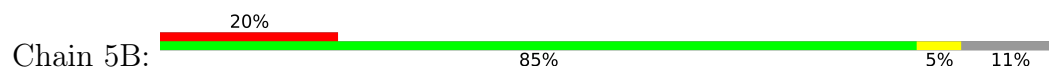


• Molecule 49: Small nuclear ribonucleoprotein Sm D3

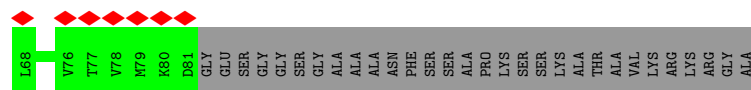
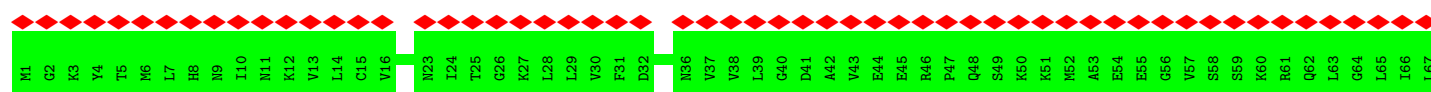
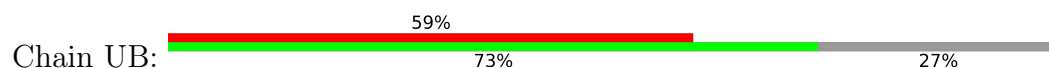




• Molecule 50: Sm protein B



• Molecule 50: Sm protein B



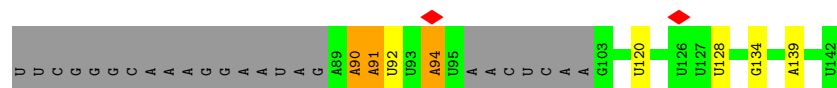
• Molecule 51: SL-ligated pre-mRNA



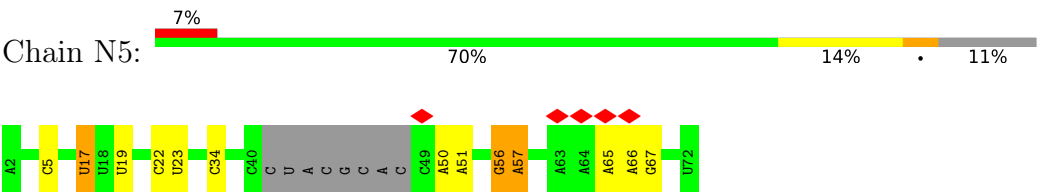
• Molecule 52: SL RNA outtron



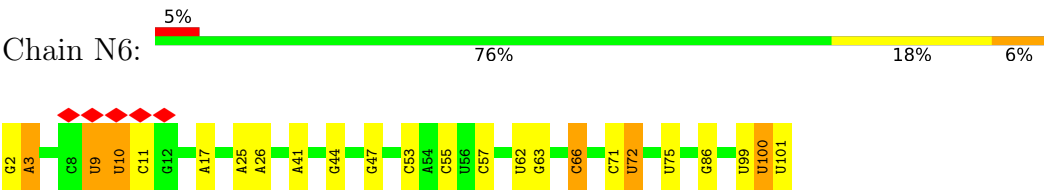
• Molecule 53: U2 snRNA



• Molecule 54: U5 snRNA



• Molecule 55: U6 snRNA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	141035	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	64000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	10.252	Depositor
Minimum map value	0.000	Depositor
Average map value	0.115	Depositor
Map value standard deviation	0.195	Depositor
Recommended contour level	0.8	Depositor
Map size (Å)	426.00003, 426.00003, 426.00003	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.065, 1.065, 1.065	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PSU, IHP, GTP, MG, ZN, G5J, GTG, SEP, ACE

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	LA	0.34	0/18638	0.43	0/25264
2	LB	0.13	0/10532	0.31	0/14676
3	LC	0.32	0/7137	0.40	0/9693
4	LD	0.17	0/1015	0.33	0/1351
5	LF	0.23	0/3385	0.38	0/4582
6	LG	0.19	0/600	0.32	0/810
7	LH	0.16	0/333	0.35	0/435
8	LJ	0.37	0/3268	0.43	0/4432
9	LL	0.29	0/1488	0.37	0/2008
10	LN	0.25	0/2358	0.36	0/3205
11	LP	0.31	0/604	0.40	0/808
12	LQ	0.25	0/4328	0.34	0/5818
13	LR	0.24	0/804	0.37	0/1083
14	LS	0.28	0/6216	0.36	0/8406
15	LT	0.28	0/6427	0.36	0/8731
16	LV	0.27	0/7721	0.39	0/10452
17	LW	0.26	0/1569	0.37	0/2119
18	LY	0.31	0/895	0.34	0/1201
19	LZ	0.14	0/625	0.31	0/843
20	SA	0.20	0/4211	0.33	0/5669
21	SC	0.17	0/2147	0.32	0/2887
22	SD	0.14	0/2381	0.29	0/3219
23	SF	0.12	0/236	0.26	0/327
24	SJ	0.25	0/2240	0.34	0/3029
25	SK	0.29	0/721	0.40	0/982
26	SL	0.28	0/1631	0.37	0/2202
27	SN	0.31	0/1424	0.37	0/1940
28	SO	0.28	0/3423	0.40	0/4651
29	SP	0.15	0/690	0.28	0/918
30	SS	0.21	0/1526	0.31	0/2057
31	ST	0.23	0/3666	0.35	0/4992
31	SU	0.22	0/1037	0.37	0/1403

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
31	SV	0.20	0/1037	0.34	0/1403
31	SW	0.23	0/963	0.35	0/1301
32	TN	0.23	0/359	0.38	0/486
34	62	0.27	0/947	0.37	0/1282
35	63	0.29	0/611	0.32	0/831
36	64	0.29	0/646	0.35	0/869
37	65	0.29	0/888	0.37	0/1198
38	66	0.28	0/551	0.38	0/745
39	67	0.30	0/712	0.38	0/962
40	A	0.35	1/781 (0.1%)	0.37	0/1063
41	RN	0.18	0/74	0.22	0/111
42	24	0.23	0/792	0.31	0/1066
42	51	0.30	0/767	0.38	0/1035
42	U1	0.13	0/483	0.28	0/671
43	25	0.22	0/664	0.33	0/890
43	52	0.32	0/725	0.41	0/970
43	U2	0.09	0/410	0.29	0/570
44	2C	0.25	0/887	0.36	0/1192
45	2D	0.26	0/806	0.34	0/1086
46	2H	0.21	0/669	0.35	0/905
46	5E	0.23	0/641	0.42	0/869
46	UE	0.11	0/387	0.31	0/536
47	2I	0.21	0/608	0.35	0/818
47	5F	0.27	0/608	0.43	0/818
47	UF	0.16	0/374	0.33	0/519
48	2J	0.22	0/588	0.36	0/791
48	5G	0.23	0/588	0.32	0/791
48	UG	0.10	0/378	0.30	0/524
49	53	0.31	0/810	0.39	0/1085
49	U3	0.14	0/399	0.32	0/554
50	5B	0.30	0/745	0.42	0/997
50	UB	0.13	0/397	0.27	0/550
51	LE	0.38	0/256	0.37	0/398
52	LO	0.17	0/1124	0.26	0/1748
53	N2	0.34	0/1787	0.37	0/2774
54	N5	0.38	0/1480	0.31	0/2298
55	N6	0.36	0/2378	0.35	0/3702
All	All	0.27	1/130596 (0.0%)	0.37	0/178601

All (1) bond length outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	A	1	ACE	C-N	6.24	1.45	1.33

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	LA	18216	0	17438	113	0
2	LB	10536	0	4965	6	0
3	LC	7002	0	6999	42	0
4	LD	1006	0	1048	9	0
5	LF	3311	0	3287	21	0
6	LG	592	0	578	3	0
7	LH	331	0	354	4	0
8	LJ	3196	0	3166	33	0
9	LL	1455	0	1471	8	0
10	LN	2314	0	2243	11	0
11	LP	589	0	578	2	0
12	LQ	4277	0	4111	27	0
13	LR	798	0	754	3	0
14	LS	6093	0	5956	44	0
15	LT	6284	0	6228	39	0
16	LV	7589	0	7426	62	0
17	LW	1545	0	1586	3	0
18	LY	876	0	888	3	0
19	LZ	619	0	531	3	0
20	SA	4143	0	4117	24	0
21	SC	2108	0	2017	17	0
22	SD	2339	0	2337	3	0
23	SF	237	0	122	0	0
24	SJ	2197	0	2133	19	0
25	SK	699	0	675	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	SL	1627	0	1617	17	0
27	SN	1396	0	1400	6	0
28	SO	3334	0	3286	19	0
29	SP	683	0	691	2	0
30	SS	1504	0	1485	12	0
31	ST	3606	0	3602	20	0
31	SU	1022	0	1039	14	0
31	SV	1022	0	1039	9	0
31	SW	949	0	965	11	0
32	TN	351	0	361	6	0
33	UX	105	0	23	0	0
34	62	937	0	973	7	0
35	63	602	0	598	3	0
36	64	640	0	656	5	0
37	65	876	0	864	5	0
38	66	541	0	522	2	0
39	67	701	0	730	6	0
40	A	774	0	795	5	0
41	RN	175	0	104	1	0
42	24	783	0	803	7	0
42	51	758	0	777	0	0
42	U1	484	0	219	0	0
43	25	654	0	678	3	0
43	52	715	0	752	8	0
43	U2	411	0	182	0	0
44	2C	881	0	911	4	0
45	2D	792	0	807	4	0
46	2H	657	0	651	5	0
46	5E	629	0	621	9	0
46	UE	388	0	161	0	0
47	2I	598	0	597	5	0
47	5F	598	0	597	11	0
47	UF	375	0	175	0	0
48	2J	583	0	603	2	0
48	5G	583	0	603	1	0
48	UG	379	0	178	0	0
49	53	801	0	822	10	0
49	U3	400	0	181	0	0
50	5B	738	0	765	1	0
50	UB	398	0	176	0	0
51	LE	358	0	199	2	0
52	LO	1006	0	509	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
53	N2	1604	0	813	9	0
54	N5	1328	0	680	8	0
55	N6	2127	0	1078	18	0
56	LA	36	0	6	1	0
57	LA	1	0	0	0	0
57	LC	1	0	0	0	0
57	LE	1	0	0	0	0
57	N2	1	0	0	0	0
57	N5	1	0	0	0	0
57	N6	7	0	0	0	0
58	LC	32	0	12	2	0
59	LL	3	0	0	0	0
59	SC	1	0	0	0	0
60	N5	52	0	25	0	0
61	N6	33	0	0	1	0
All	All	128394	0	116339	555	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (555) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:SA:389:ARG:HG3	20:SA:426:PHE:HE1	1.37	0.89
20:SA:389:ARG:CG	20:SA:426:PHE:HE1	1.89	0.85
16:LV:1021:ARG:NH2	51:LE:58:N:OP1	2.09	0.84
55:N6:53:C:OP2	55:N6:72:U:O2'	1.96	0.83
20:SA:389:ARG:CG	20:SA:426:PHE:CE1	2.65	0.79
20:SA:232:GLU:O	21:SC:104:GLY:N	2.16	0.78
20:SA:389:ARG:HG3	20:SA:426:PHE:CE1	2.16	0.78
28:SO:475:THR:HG22	28:SO:481:LEU:HD12	1.64	0.78
4:LD:125:ARG:NH1	53:N2:134:G:OP1	2.17	0.77
31:SU:3:ARG:NH2	31:SV:69:LEU:O	2.18	0.76
12:LQ:676:GLU:OE1	30:SS:191:ARG:NH1	2.19	0.76
1:LA:171:ARG:NH2	21:SC:158:GLU:O	2.20	0.75
3:LC:186:ARG:NH2	3:LC:188:ASP:OD2	2.20	0.74
16:LV:843:GLN:OE1	16:LV:952:ARG:NH1	2.19	0.74
31:ST:248:ILE:O	31:SU:97:GLN:NE2	2.21	0.74
31:ST:214:ALA:O	31:ST:489:THR:OG1	2.05	0.74
1:LA:723:ARG:NH2	55:N6:62:U:OP2	2.21	0.73
4:LD:104:LEU:HD11	45:2D:64:PHE:CD1	2.23	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:LL:87:GLU:OE2	9:LL:165:ARG:NH1	2.22	0.73
8:LJ:21:ARG:NH2	31:SW:111:GLN:OE1	2.22	0.73
15:LT:543:VAL:O	24:SJ:272:ASN:ND2	2.21	0.73
16:LV:708:ILE:O	16:LV:752:ARG:NH1	2.21	0.72
1:LA:91:LYS:NZ	52:LO:54:C:OP1	2.20	0.72
52:LO:59:C:O2'	55:N6:25:A:N3	2.22	0.72
31:ST:479:THR:OG1	31:ST:504:ARG:NH2	2.23	0.72
3:LC:165:SER:O	3:LC:170:LYS:NZ	2.23	0.71
24:SJ:256:ALA:O	24:SJ:261:LYS:NZ	2.23	0.71
31:ST:91:GLU:OE2	31:SU:96:ARG:NH2	2.23	0.71
28:SO:417:GLN:NE2	28:SO:461:PHE:O	2.23	0.71
14:LS:337:TYR:OH	15:LT:612:ARG:NH1	2.23	0.70
16:LV:302:GLU:O	16:LV:306:GLN:N	2.25	0.70
15:LT:495:ARG:NH2	34:62:189:SER:OG	2.25	0.70
15:LT:637:HIS:O	15:LT:641:ALA:N	2.25	0.70
24:SJ:166:ASP:OD1	24:SJ:224:ARG:NH2	2.25	0.69
18:LY:46:ASN:O	53:N2:120:U:O2'	2.06	0.69
28:SO:451:ARG:NH1	28:SO:486:TYR:O	2.25	0.69
14:LS:743:ARG:NH2	14:LS:795:GLU:OE1	2.24	0.69
1:LA:880:ASN:OD1	26:SL:319:LYS:NZ	2.26	0.69
1:LA:1573:GLU:HG2	21:SC:49:ILE:HD11	1.75	0.68
30:SS:37:GLU:OE1	31:SU:122:ARG:NH2	2.26	0.68
42:24:46:MET:SD	43:25:92:ARG:NH1	2.65	0.68
15:LT:477:ARG:NH1	15:LT:528:ASP:OD2	2.26	0.68
8:LJ:64:ARG:NH2	31:SW:35:GLU:OE1	2.27	0.68
14:LS:768:THR:OG1	16:LV:127:LYS:NZ	2.27	0.68
15:LT:566:GLU:OE1	15:LT:601:ARG:NE	2.26	0.68
1:LA:1281:GLU:O	20:SA:415:ARG:NH2	2.26	0.67
1:LA:717:ASP:OD1	26:SL:148:ARG:NH1	2.27	0.67
35:63:122:ARG:NH2	55:N6:100:U:O2'	2.26	0.67
14:LS:426:VAL:HG11	25:SK:166:TYR:HB3	1.75	0.67
1:LA:1871:GLY:O	7:LH:86:LYS:NZ	2.23	0.67
1:LA:1634:VAL:HG11	1:LA:1647:LEU:HD13	1.75	0.67
31:ST:2:LEU:HD23	31:SW:2:LEU:HD22	1.75	0.66
5:LF:58:ALA:O	5:LF:62:VAL:HG23	1.95	0.66
14:LS:297:HIS:O	14:LS:301:ARG:NH2	2.28	0.66
15:LT:677:VAL:O	15:LT:681:ILE:HG22	1.95	0.66
1:LA:2085:GLU:OE2	5:LF:605:HIS:NE2	2.29	0.66
1:LA:1439:ASN:CG	20:SA:370:ILE:HD11	2.21	0.66
16:LV:666:LEU:HD13	16:LV:667:PRO:HD2	1.77	0.66
30:SS:198:GLU:OE2	31:SV:9:ARG:NH1	2.27	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:SA:389:ARG:HG2	20:SA:426:PHE:CE1	2.30	0.66
46:5E:74:ARG:NH1	47:5F:39:MET:SD	2.69	0.66
36:64:38:ARG:NH2	39:67:13:GLU:O	2.30	0.65
9:LL:216:ARG:NH1	9:LL:292:ASP:O	2.30	0.65
1:LA:1874:LYS:NZ	55:N6:41:A:OP2	2.26	0.65
3:LC:110:LEU:HD22	3:LC:199:HIS:CE1	2.31	0.65
12:LQ:329:ARG:NH2	26:SL:288:LEU:O	2.29	0.64
8:LJ:63:TRP:NE1	30:SS:193:CYS:SG	2.71	0.64
5:LF:114:ARG:NH2	5:LF:460:ASP:OD1	2.31	0.64
5:LF:427:GLU:OE1	5:LF:431:ARG:NH1	2.31	0.64
48:2J:36:ASP:OD1	48:2J:40:SER:N	2.30	0.64
31:SV:86:GLU:OE1	31:SW:31:LYS:NZ	2.18	0.64
1:LA:897:LYS:NZ	16:LV:228:GLU:OE2	2.30	0.64
8:LJ:63:TRP:NE1	8:LJ:70:THR:O	2.31	0.63
19:LZ:395:GLN:O	19:LZ:399:SER:N	2.29	0.63
1:LA:657:ARG:NH1	54:N5:23:U:OP2	2.31	0.63
14:LS:86:ARG:NH1	55:N6:75:U:O2'	2.32	0.63
16:LV:191:ARG:NH1	16:LV:902:GLU:OE1	2.31	0.63
1:LA:362:ASP:O	1:LA:436:LYS:NZ	2.31	0.63
43:52:97:ILE:O	47:5F:65:ASN:ND2	2.32	0.62
1:LA:1965:LEU:HD13	1:LA:2091:LEU:O	1.99	0.62
5:LF:57:ALA:O	5:LF:61:VAL:HG23	1.99	0.62
8:LJ:55:MET:SD	30:SS:185:LEU:HD11	2.39	0.62
20:SA:29:GLN:OE1	20:SA:272:ASP:N	2.31	0.62
2:LB:606:GLU:O	2:LB:610:ALA:N	2.32	0.62
28:SO:541:GLU:O	28:SO:582:LYS:NZ	2.32	0.62
1:LA:2035:ASP:OD2	4:LD:27:ARG:NE	2.33	0.62
1:LA:2019:ARG:NH2	5:LF:706:ARG:OXT	2.33	0.62
1:LA:1830:SER:OG	19:LZ:347:SER:O	2.15	0.62
16:LV:902:GLU:HB2	16:LV:906:LEU:HD12	1.82	0.62
36:64:69:ARG:NH1	39:67:72:GLY:O	2.33	0.61
3:LC:447:LEU:HD23	3:LC:448:PRO:HD2	1.82	0.61
8:LJ:65:ALA:HB1	31:SV:83:MET:SD	2.40	0.61
14:LS:352:LEU:HD23	15:LT:649:LEU:HD11	1.82	0.61
43:52:54:ALA:HB2	43:52:70:VAL:HA	1.81	0.61
1:LA:917:ILE:CG2	16:LV:1082:LEU:HD11	2.31	0.61
1:LA:1550:ASN:ND2	21:SC:59:TYR:OH	2.34	0.61
28:SO:595:LEU:HD11	28:SO:610:THR:HB	1.83	0.61
3:LC:71:GLU:OE1	8:LJ:180:LYS:NZ	2.32	0.61
3:LC:160:VAL:HG13	3:LC:447:LEU:HD21	1.82	0.61
3:LC:756:PHE:CZ	3:LC:760:ILE:HD11	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:LA:736:ARG:NH2	54:N5:19:U:OP1	2.34	0.61
1:LA:1752:ILE:HG22	21:SC:82:ASP:O	2.01	0.61
20:SA:389:ARG:HG2	20:SA:426:PHE:CD1	2.36	0.61
24:SJ:339:ILE:HD11	24:SJ:374:GLU:HG3	1.81	0.60
27:SN:134:MET:HE2	27:SN:149:VAL:HG11	1.83	0.60
55:N6:9:U:O2'	55:N6:10:U:O5'	2.15	0.60
12:LQ:205:ALA:HB3	28:SO:479:ARG:HD3	1.82	0.60
15:LT:631:SER:OG	24:SJ:259:GLU:OE1	2.16	0.60
16:LV:674:LEU:O	16:LV:701:THR:OG1	2.18	0.60
47:5F:62:ARG:NH2	54:N5:56:G:OP2	2.34	0.60
34:62:183:ALA:HB2	35:63:76:MET:HE3	1.82	0.60
1:LA:73:LYS:NZ	9:LL:85:THR:O	2.26	0.60
12:LQ:212:GLU:OE2	28:SO:521:LEU:HD21	2.01	0.60
1:LA:810:GLU:OE1	8:LJ:500:LYS:NZ	2.32	0.60
8:LJ:157:VAL:HG22	8:LJ:455:VAL:HG11	1.83	0.60
7:LH:139:ARG:O	15:LT:311:GLN:NE2	2.35	0.60
10:LN:191:GLU:OE2	10:LN:236:ARG:NE	2.35	0.60
42:24:29:LEU:O	42:24:76:ARG:NH2	2.35	0.60
55:N6:3:A:H61	55:N6:17:A:H61	1.48	0.59
31:ST:229:GLY:O	31:SV:65:SER:OG	2.19	0.59
16:LV:641:GLN:O	16:LV:885:ARG:NH2	2.36	0.59
14:LS:352:LEU:HD13	25:SK:170:LEU:HD21	1.84	0.59
9:LL:215:GLU:HG2	61:N6:201:G5J:C5'	2.32	0.59
20:SA:149:TYR:CE1	20:SA:192:ILE:HD11	2.37	0.59
42:24:43:ASP:OD1	42:24:47:ASN:N	2.33	0.59
1:LA:1671:LEU:HD21	1:LA:1796:MET:HE1	1.84	0.59
1:LA:901:LEU:HD22	1:LA:943:LEU:HD22	1.83	0.58
5:LF:632:THR:O	14:LS:28:ARG:NH1	2.36	0.58
40:A:29:ASP:OD1	40:A:33:ASN:N	2.36	0.58
1:LA:755:LEU:HD23	1:LA:768:ILE:HG23	1.85	0.58
16:LV:191:ARG:NH2	16:LV:900:GLN:OE1	2.36	0.58
1:LA:955:ARG:NH1	12:LQ:106:GLU:OE1	2.35	0.58
16:LV:823:ARG:O	16:LV:823:ARG:NH1	2.35	0.58
37:65:12:GLN:NE2	39:67:52:ASP:OD1	2.37	0.58
42:24:67:GLU:OE1	44:2C:21:TYR:OH	2.16	0.58
15:LT:693:ARG:NH1	26:SL:222:ASP:O	2.36	0.58
1:LA:1227:LEU:HD11	1:LA:1246:SER:HB2	1.85	0.58
20:SA:73:ARG:NH2	20:SA:267:ASP:O	2.36	0.58
20:SA:46:ARG:O	20:SA:51:ASN:ND2	2.35	0.57
1:LA:193:ARG:NH2	1:LA:626:LEU:O	2.38	0.57
31:ST:200:VAL:HG21	31:SU:83:MET:HG2	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:LA:1422:VAL:HG21	1:LA:1425:PHE:CZ	2.40	0.57
1:LA:620:MET:HE1	1:LA:641:LEU:HB2	1.87	0.57
3:LC:75:GLY:O	8:LJ:220:LEU:HD22	2.05	0.57
12:LQ:751:GLN:NE2	31:SV:60:ASP:OD1	2.36	0.57
16:LV:521:ASP:OD2	16:LV:552:THR:OG1	2.23	0.57
12:LQ:215:ARG:NH2	14:LS:62:MET:O	2.37	0.57
16:LV:24:MET:HE1	16:LV:141:VAL:HG13	1.86	0.57
47:5F:37:THR:O	54:N5:50:A:N6	2.29	0.57
1:LA:1085:GLU:OE1	12:LQ:47:ARG:NH1	2.38	0.57
5:LF:276:VAL:HG21	16:LV:26:PHE:CE1	2.40	0.57
46:5E:71:ILE:HG22	47:5F:70:ARG:CB	2.35	0.57
16:LV:947:GLU:OE1	16:LV:948:MET:N	2.38	0.56
3:LC:498:ALA:HB2	3:LC:514:VAL:HG22	1.87	0.56
10:LN:229:PHE:CD2	30:SS:256:LEU:HD13	2.40	0.56
26:SL:31:MET:SD	26:SL:31:MET:N	2.78	0.56
1:LA:852:ARG:NH2	1:LA:1053:ASP:O	2.38	0.56
3:LC:110:LEU:HD23	3:LC:186:ARG:CG	2.36	0.56
26:SL:10:SER:OG	27:SN:87:ALA:O	2.17	0.56
14:LS:404:ARG:NH1	14:LS:438:ASP:OD2	2.38	0.56
14:LS:816:ARG:NH1	16:LV:120:VAL:HG13	2.20	0.56
1:LA:1412:THR:O	1:LA:1414:TYR:N	2.38	0.56
31:ST:119:VAL:HG12	31:SU:120:ILE:HD12	1.88	0.56
5:LF:28:GLN:NE2	16:LV:796:ALA:O	2.37	0.56
8:LJ:170:TYR:OH	8:LJ:446:ASP:OD2	2.21	0.56
14:LS:489:GLY:O	14:LS:498:LEU:HD23	2.06	0.55
1:LA:143:PRO:HG2	1:LA:244:MET:HE1	1.87	0.55
14:LS:723:GLU:O	14:LS:727:ALA:N	2.39	0.55
5:LF:685:ILE:HD12	14:LS:23:VAL:HG12	1.88	0.55
1:LA:2023:ILE:HG22	4:LD:51:LEU:CD1	2.36	0.55
24:SJ:389:ARG:NH2	53:N2:12:G:N7	2.52	0.55
1:LA:759:LEU:HD13	1:LA:763:VAL:HG21	1.89	0.55
20:SA:287:LYS:O	20:SA:291:GLY:N	2.40	0.55
31:SV:33:LEU:O	31:SV:37:GLY:N	2.39	0.55
31:ST:339:THR:O	31:ST:343:ALA:HB2	2.07	0.55
1:LA:1589:ASP:OD1	1:LA:1590:THR:HG23	2.07	0.55
14:LS:201:LEU:HD22	24:SJ:303:VAL:HG11	1.88	0.55
1:LA:415:LEU:HD22	3:LC:357:ALA:HB1	1.88	0.54
3:LC:976:PRO:O	3:LC:996:ARG:NH1	2.40	0.54
46:2H:71:ILE:HG22	47:2I:70:ARG:HB3	1.90	0.54
14:LS:422:GLN:NE2	14:LS:461:LEU:O	2.40	0.54
15:LT:634:ILE:O	15:LT:638:VAL:N	2.34	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:LA:207:ASP:O	1:LA:249:ARG:NH2	2.40	0.54
1:LA:164:LEU:HD22	1:LA:682:PRO:HG3	1.89	0.54
1:LA:1822:LYS:O	1:LA:1826:GLY:N	2.41	0.54
14:LS:341:LEU:HD13	14:LS:409:ARG:NH2	2.22	0.54
46:5E:15:VAL:HG21	46:5E:48:MET:HE1	1.89	0.54
14:LS:533:GLU:OE2	14:LS:572:GLN:NE2	2.40	0.54
15:LT:254:GLY:O	15:LT:258:CYS:N	2.40	0.54
16:LV:503:THR:HG23	16:LV:508:ASP:CG	2.32	0.54
4:LD:41:GLY:O	4:LD:45:MET:N	2.41	0.54
1:LA:1879:ASN:ND2	1:LA:1985:ALA:O	2.41	0.53
27:SN:174:PRO:O	31:ST:383:ARG:NH2	2.38	0.53
6:LG:65:MET:HB3	6:LG:77:VAL:HG21	1.90	0.53
8:LJ:21:ARG:HB3	31:SW:104:LEU:HD11	1.88	0.53
1:LA:220:PRO:HB2	1:LA:222:LEU:HD13	1.90	0.53
1:LA:666:ARG:NH1	56:LA:2501:IHP:O44	2.42	0.53
5:LF:273:LEU:O	5:LF:277:THR:N	2.41	0.53
8:LJ:192:THR:HG22	8:LJ:203:THR:HG22	1.91	0.53
20:SA:64:LEU:O	20:SA:68:ARG:N	2.42	0.53
30:SS:186:ASN:ND2	31:SU:72:ALA:O	2.40	0.53
20:SA:200:LEU:O	20:SA:202:MET:HE2	2.09	0.53
31:SW:92:GLN:OE1	31:SW:96:ARG:NH1	2.42	0.53
16:LV:902:GLU:CB	16:LV:906:LEU:HD12	2.39	0.53
36:64:62:LYS:HB2	39:67:86:ILE:HD13	1.91	0.53
17:LW:18:MET:HE2	18:LY:24:ARG:HB2	1.90	0.53
14:LS:357:LEU:HD21	15:LT:609:HIS:CD2	2.44	0.52
20:SA:43:VAL:HG11	20:SA:59:LEU:HG	1.91	0.52
27:SN:41:ARG:NH2	27:SN:59:SER:O	2.42	0.52
31:ST:3:ARG:NH2	31:SW:58:ALA:O	2.42	0.52
1:LA:764:LYS:NZ	53:N2:16:U:OP1	2.43	0.52
1:LA:571:LYS:NZ	55:N6:63:G:OP2	2.41	0.52
5:LF:428:ALA:O	5:LF:432:LEU:N	2.43	0.52
15:LT:108:VAL:HG21	15:LT:143:HIS:HB3	1.91	0.52
16:LV:844:LEU:O	16:LV:845:SER:OG	2.20	0.52
30:SS:44:THR:HG21	31:SU:118:ARG:HH12	1.75	0.52
31:SU:33:LEU:O	31:SU:37:GLY:N	2.41	0.52
26:SL:109:GLU:OE2	26:SL:117:ARG:NH1	2.43	0.52
36:64:40:ASP:OD1	36:64:44:ASN:N	2.43	0.52
3:LC:382:ARG:NH1	3:LC:391:GLU:OE2	2.39	0.52
10:LN:257:GLY:N	10:LN:262:THR:O	2.40	0.52
1:LA:748:LYS:NZ	53:N2:20:G:O2'	2.41	0.52
1:LA:2022:HIS:NE2	4:LD:52:ARG:O	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:LV:794:LEU:HD12	16:LV:801:LEU:HG	1.91	0.52
20:SA:383:MET:HE1	20:SA:388:GLU:HG3	1.90	0.52
12:LQ:23:LEU:HD22	12:LQ:28:LEU:HD23	1.92	0.51
14:LS:352:LEU:HD23	15:LT:649:LEU:HD21	1.92	0.51
1:LA:100:ILE:HD13	1:LA:563:MET:SD	2.50	0.51
16:LV:968:ARG:NH1	16:LV:1033:ALA:O	2.44	0.51
3:LC:795:ASP:OD1	13:LR:73:ARG:NH2	2.43	0.51
8:LJ:349:ARG:NH2	26:SL:180:PRO:O	2.44	0.51
12:LQ:399:LEU:HD13	14:LS:583:ALA:HB1	1.92	0.51
3:LC:183:TYR:OH	3:LC:221:ASP:OD2	2.20	0.51
12:LQ:205:ALA:HB3	28:SO:479:ARG:CD	2.40	0.51
16:LV:608:THR:HG22	32:TN:9:THR:CG2	2.41	0.51
1:LA:1400:LEU:HD21	1:LA:1541:MET:HE1	1.93	0.51
16:LV:670:MET:O	16:LV:697:VAL:N	2.41	0.51
52:LO:42:A:O2'	55:N6:71:C:OP2	2.16	0.51
1:LA:607:VAL:HG21	1:LA:712:LEU:HD11	1.93	0.51
49:53:10:LEU:HD23	49:53:73:LEU:HD21	1.92	0.51
1:LA:1532:HIS:O	16:LV:210:ARG:NH2	2.43	0.50
14:LS:298:VAL:HG13	14:LS:304:LEU:HB3	1.93	0.50
15:LT:654:VAL:HG13	15:LT:689:THR:HG22	1.93	0.50
15:LT:500:LEU:HD21	37:65:72:ASP:C	2.37	0.50
8:LJ:142:LEU:HD22	8:LJ:149:LEU:HD11	1.93	0.50
1:LA:1209:ARG:NH1	1:LA:1413:ILE:HG23	2.26	0.50
24:SJ:339:ILE:HD11	24:SJ:374:GLU:CG	2.41	0.50
34:62:119:VAL:HG23	34:62:144:PRO:HG3	1.93	0.50
46:5E:71:ILE:HG22	47:5F:70:ARG:HB3	1.92	0.50
5:LF:465:ILE:HD12	5:LF:466:THR:O	2.11	0.50
1:LA:830:ASP:CG	54:N5:17:U:HO2'	2.20	0.50
1:LA:927:GLU:OE2	1:LA:931:ARG:NE	2.44	0.50
8:LJ:270:LYS:NZ	55:N6:57:C:OP2	2.43	0.50
16:LV:608:THR:HG22	32:TN:9:THR:HG23	1.93	0.50
1:LA:1116:ASP:OD1	1:LA:1156:TYR:OH	2.28	0.50
3:LC:477:ALA:HB3	3:LC:486:ALA:HB2	1.94	0.50
14:LS:431:TYR:CE2	14:LS:443:LEU:HD11	2.46	0.50
21:SC:191:VAL:HG13	21:SC:192:PHE:CD1	2.47	0.50
1:LA:754:GLU:OE1	1:LA:804:TYR:OH	2.15	0.50
12:LQ:78:LEU:HD21	26:SL:303:VAL:HG22	1.94	0.50
12:LQ:215:ARG:NH1	28:SO:551:GLY:O	2.45	0.50
12:LQ:697:LEU:HD13	12:LQ:742:VAL:HG13	1.93	0.50
45:2D:45:ARG:NH2	48:2J:6:THR:O	2.40	0.50
5:LF:597:THR:O	5:LF:602:ASN:ND2	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:SO:479:ARG:NH1	28:SO:498:ALA:O	2.45	0.49
1:LA:1351:LEU:HD22	20:SA:370:ILE:CG2	2.42	0.49
2:LB:1436:THR:O	2:LB:1496:GLY:N	2.45	0.49
12:LQ:771:MET:HE3	30:SS:235:TYR:CB	2.43	0.49
20:SA:262:THR:OG1	20:SA:264:ASP:OD1	2.24	0.49
28:SO:420:HIS:ND1	28:SO:425:GLU:O	2.41	0.49
43:52:98:PHE:CG	47:5F:59:MET:HE2	2.47	0.49
1:LA:2008:ILE:HD12	21:SC:257:TYR:HA	1.95	0.49
2:LB:1412:GLN:O	2:LB:1416:GLU:N	2.45	0.49
14:LS:487:ARG:NH2	14:LS:542:GLU:OE1	2.45	0.49
47:2I:37:THR:O	53:N2:90:A:N6	2.45	0.49
1:LA:1209:ARG:HH11	1:LA:1413:ILE:HG23	1.78	0.49
21:SC:101:PHE:CZ	21:SC:129:VAL:HG22	2.48	0.49
8:LJ:67:TYR:CZ	31:SU:64:VAL:HG21	2.48	0.49
14:LS:640:ALA:O	14:LS:644:ARG:N	2.42	0.49
15:LT:500:LEU:HD21	37:65:72:ASP:O	2.12	0.49
32:TN:29:VAL:HG22	32:TN:39:VAL:HG21	1.95	0.49
1:LA:428:LEU:O	3:LC:395:LYS:NZ	2.43	0.49
15:LT:662:PHE:O	15:LT:666:ALA:N	2.36	0.49
15:LT:371:ALA:HB3	24:SJ:99:ILE:HG23	1.95	0.49
16:LV:477:ARG:NH2	16:LV:547:GLU:OE1	2.46	0.48
42:24:69:MET:HE1	44:2C:18:LEU:HD11	1.94	0.48
46:2H:45:ASP:OD1	46:2H:49:ASN:N	2.46	0.48
1:LA:382:LYS:NZ	20:SA:205:GLU:OE2	2.36	0.48
1:LA:1370:ARG:NH2	54:N5:17:U:OP2	2.46	0.48
3:LC:443:ILE:HG22	3:LC:447:LEU:HD12	1.95	0.48
14:LS:795:GLU:O	14:LS:799:GLY:N	2.46	0.48
15:LT:682:LEU:O	15:LT:685:SER:OG	2.22	0.48
16:LV:619:LEU:HD22	16:LV:651:LEU:HG	1.94	0.48
16:LV:632:GLY:O	16:LV:695:ARG:NH1	2.46	0.48
31:ST:2:LEU:HD23	31:SW:2:LEU:CD2	2.42	0.48
1:LA:1450:GLU:HG2	1:LA:1488:ILE:HD11	1.96	0.48
1:LA:1686:GLN:CD	1:LA:1704:ILE:HD12	2.39	0.48
8:LJ:355:LYS:N	8:LJ:375:ASP:OD2	2.45	0.48
3:LC:560:TYR:OH	3:LC:617:ASP:OD2	2.27	0.48
1:LA:133:ILE:HD12	1:LA:536:MET:HE1	1.96	0.48
1:LA:878:MET:HB2	1:LA:1063:MET:HE1	1.96	0.48
49:53:23:ALA:N	49:53:67:ASN:O	2.47	0.48
3:LC:847:LEU:O	3:LC:1003:ARG:NH1	2.41	0.48
14:LS:352:LEU:CD2	15:LT:649:LEU:HD11	2.43	0.48
27:SN:182:LEU:HD11	31:ST:378:PHE:HE2	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:52:47:ARG:NH2	54:N5:57:A:OP2	2.46	0.48
1:LA:1811:ASN:O	1:LA:1815:ASN:ND2	2.42	0.48
8:LJ:256:ASP:HB2	8:LJ:263:VAL:HG21	1.96	0.48
1:LA:1111:TRP:NE1	1:LA:1115:MET:HE3	2.29	0.47
14:LS:609:ASP:OD1	14:LS:710:ARG:NH2	2.47	0.47
14:LS:617:HIS:HA	14:LS:620:THR:HG22	1.96	0.47
15:LT:108:VAL:HG13	15:LT:147:VAL:HG21	1.96	0.47
1:LA:60:VAL:HG13	9:LL:225:PRO:HD2	1.96	0.47
26:SL:135:VAL:HG11	26:SL:141:LEU:HG	1.95	0.47
46:2H:71:ILE:HG22	47:2I:70:ARG:CB	2.43	0.47
4:LD:71:GLU:OE2	28:SO:471:LYS:NZ	2.48	0.47
8:LJ:60:ASN:ND2	31:SW:35:GLU:OE2	2.43	0.47
18:LY:6:GLN:OE1	18:LY:90:VAL:HG11	2.15	0.47
34:62:183:ALA:CB	35:63:76:MET:HE3	2.45	0.47
1:LA:2108:ILE:HG13	21:SC:258:VAL:HG13	1.97	0.47
8:LJ:381:LYS:O	8:LJ:385:GLY:N	2.44	0.47
16:LV:658:LEU:O	16:LV:662:VAL:HG12	2.15	0.47
16:LV:678:MET:O	16:LV:683:GLN:NE2	2.48	0.47
46:5E:19:MET:HE3	47:5F:1:MET:HE3	1.96	0.47
1:LA:828:THR:OG1	1:LA:829:VAL:N	2.47	0.47
3:LC:756:PHE:CE2	3:LC:760:ILE:HD11	2.49	0.47
8:LJ:205:SER:OG	8:LJ:206:PHE:N	2.47	0.47
8:LJ:209:ILE:HD11	8:LJ:211:LYS:HE2	1.95	0.47
10:LN:3:LEU:HD23	10:LN:24:GLY:HA3	1.97	0.47
43:52:54:ALA:HB3	43:52:67:LEU:HD22	1.96	0.47
48:5G:7:LEU:HD11	48:5G:35:VAL:HG13	1.96	0.47
1:LA:127:VAL:HG12	9:LL:234:ILE:HD11	1.97	0.47
5:LF:655:LEU:HD22	5:LF:668:ALA:HB1	1.97	0.47
13:LR:47:ILE:HD13	13:LR:52:GLN:OE1	2.15	0.47
16:LV:680:GLN:O	16:LV:684:SER:N	2.46	0.47
30:SS:28:ALA:HB2	31:ST:330:VAL:HG13	1.96	0.47
39:67:8:VAL:HG13	39:67:12:LYS:O	2.15	0.47
1:LA:190:LEU:HD21	1:LA:622:VAL:HG13	1.97	0.47
1:LA:917:ILE:HG23	16:LV:1082:LEU:HD11	1.96	0.47
1:LA:1673:ASP:OD2	21:SC:207:LEU:HD22	2.15	0.47
20:SA:66:ARG:NH1	20:SA:279:GLU:OE2	2.48	0.47
47:2I:63:ASN:OD1	47:2I:64:ASN:N	2.48	0.47
14:LS:651:GLN:O	14:LS:655:SER:N	2.42	0.46
53:N2:94:A:H5"	53:N2:94:A:N3	2.30	0.46
1:LA:124:VAL:HG22	1:LA:544:LYS:HG2	1.97	0.46
1:LA:955:ARG:NH2	12:LQ:160:GLU:OE1	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:LF:85:VAL:CG1	5:LF:227:ALA:HB1	2.46	0.46
16:LV:918:ASN:OD1	16:LV:924:TRP:NE1	2.49	0.46
1:LA:1462:ARG:HB2	16:LV:213:LEU:HD13	1.97	0.46
3:LC:149:ILE:HD13	49:53:76:ALA:CB	2.46	0.46
20:SA:149:TYR:CD1	20:SA:192:ILE:HD11	2.51	0.46
1:LA:957:LYS:HD3	12:LQ:44:MET:HE3	1.98	0.46
1:LA:1656:TRP:NE1	1:LA:1693:SER:O	2.41	0.46
26:SL:299:MET:O	26:SL:303:VAL:HG23	2.16	0.46
1:LA:1061:ARG:NH1	1:LA:1065:GLU:OE2	2.49	0.46
15:LT:335:GLN:O	15:LT:339:GLY:N	2.49	0.46
1:LA:420:ASP:O	49:53:107:ARG:NH2	2.49	0.46
1:LA:1822:LYS:O	1:LA:1827:LEU:N	2.49	0.46
16:LV:920:MET:SD	16:LV:939:ARG:NH1	2.87	0.46
19:LZ:342:LEU:O	21:SC:246:LEU:HD13	2.16	0.46
10:LN:3:LEU:HD23	10:LN:24:GLY:CA	2.45	0.46
12:LQ:201:GLN:O	28:SO:479:ARG:NH1	2.49	0.46
15:LT:168:LEU:HD13	29:SP:188:GLY:HA3	1.98	0.46
24:SJ:235:ASP:O	24:SJ:238:THR:OG1	2.33	0.46
28:SO:595:LEU:HD12	28:SO:611:ALA:O	2.15	0.46
3:LC:461:TYR:OH	3:LC:601:HIS:NE2	2.42	0.45
16:LV:667:PRO:HD3	32:TN:26:LEU:HD13	1.97	0.45
34:62:103:ASP:OD2	34:62:106:THR:OG1	2.33	0.45
8:LJ:290:ARG:NH2	55:N6:55:C:O2'	2.44	0.45
10:LN:201:THR:HG22	10:LN:217:MET:HE2	1.98	0.45
21:SC:256:ASN:ND2	21:SC:281:MET:HE3	2.32	0.45
16:LV:629:GLU:O	16:LV:695:ARG:NH2	2.49	0.45
45:2D:29:VAL:O	45:2D:76:ARG:NH2	2.50	0.45
3:LC:482:GLU:HB3	3:LC:485:ALA:HB3	1.98	0.45
7:LH:138:THR:O	7:LH:142:VAL:HG23	2.16	0.45
16:LV:1020:LEU:HD23	16:LV:1027:TYR:O	2.16	0.45
34:62:145:ILE:HG23	40:A:116:TRP:CE3	2.51	0.45
46:5E:40:ASN:ND2	46:5E:53:GLY:O	2.49	0.45
15:LT:634:ILE:O	15:LT:638:VAL:HG23	2.16	0.45
31:ST:369:ASP:O	31:ST:373:LEU:N	2.47	0.45
37:65:74:LEU:CD2	38:66:3:VAL:HG21	2.47	0.45
1:LA:917:ILE:HD11	1:LA:929:GLN:HG2	1.98	0.45
8:LJ:302:ARG:NH1	11:LP:11:GLU:O	2.48	0.45
10:LN:189:GLU:OE1	10:LN:192:ARG:NE	2.49	0.45
12:LQ:771:MET:HE1	30:SS:231:GLU:HB3	1.99	0.45
31:ST:14:PRO:HG3	31:SW:2:LEU:HD11	1.99	0.45
15:LT:317:ALA:O	15:LT:323:ARG:NH2	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:SD:476:TRP:HZ3	22:SD:480:LEU:HD13	1.82	0.45
43:52:98:PHE:CD1	47:5F:59:MET:HE2	2.52	0.45
1:LA:1382:ARG:NH2	1:LA:1637:CYS:O	2.49	0.45
2:LB:1805:ASN:O	2:LB:1809:ALA:N	2.49	0.45
46:5E:57:GLU:HB2	46:5E:68:LEU:HD11	1.99	0.45
1:LA:1589:ASP:OD1	1:LA:1590:THR:N	2.50	0.44
12:LQ:185:LEU:O	26:SL:271:LYS:NZ	2.51	0.44
40:A:93:ARG:NH1	55:N6:99:U:O4'	2.50	0.44
1:LA:324:PHE:O	3:LC:951:GLN:NE2	2.51	0.44
3:LC:171:THR:OG1	58:LC:1500:GTP:O2B	2.36	0.44
12:LQ:701:ASP:OD2	12:LQ:745:ARG:NH1	2.50	0.44
24:SJ:384:ARG:NH2	55:N6:86:G:N7	2.64	0.44
1:LA:672:LEU:O	1:LA:676:PHE:N	2.44	0.44
3:LC:925:GLU:HB3	3:LC:934:ILE:HD11	1.99	0.44
1:LA:438:ALA:HB1	3:LC:401:VAL:HG12	1.98	0.44
17:LW:16:ASN:N	17:LW:20:GLN:O	2.46	0.44
24:SJ:330:LEU:HD12	24:SJ:333:LEU:HD12	2.00	0.44
3:LC:609:ALA:O	3:LC:613:VAL:HG23	2.17	0.44
14:LS:339:GLU:O	14:LS:342:ARG:N	2.50	0.44
15:LT:686:ILE:O	15:LT:689:THR:OG1	2.32	0.44
28:SO:462:ASN:OD1	28:SO:464:THR:OG1	2.34	0.44
1:LA:1757:ARG:CZ	21:SC:85:LEU:HD22	2.48	0.44
3:LC:201:LEU:HD23	3:LC:573:VAL:HG22	1.99	0.44
5:LF:52:ILE:HG23	5:LF:481:LEU:HD21	2.00	0.44
15:LT:626:ILE:HA	15:LT:633:VAL:HG21	2.00	0.44
20:SA:29:GLN:NE2	20:SA:272:ASP:O	2.45	0.44
31:SU:63:ILE:HD12	31:SV:83:MET:CE	2.47	0.44
2:LB:1449:TRP:O	2:LB:1453:PHE:N	2.49	0.44
12:LQ:223:LEU:HD22	12:LQ:227:GLN:HB2	1.99	0.44
3:LC:192:ARG:NH1	3:LC:699:ASP:OD2	2.50	0.44
22:SD:476:TRP:CZ3	22:SD:480:LEU:HD13	2.53	0.44
1:LA:241:LEU:HD11	1:LA:438:ALA:HA	2.00	0.44
1:LA:245:GLU:HG3	1:LA:437:THR:HG23	1.99	0.44
1:LA:386:ASP:N	1:LA:386:ASP:OD1	2.49	0.44
37:65:33:MET:HE1	39:67:6:ALA:HB2	1.99	0.44
16:LV:794:LEU:HD13	16:LV:804:LEU:HD12	1.99	0.43
25:SK:164:SER:O	25:SK:167:GLU:N	2.51	0.43
44:2C:62:ARG:NH2	53:N2:139:A:N7	2.66	0.43
5:LF:67:PRO:HB2	5:LF:138:THR:HG21	1.99	0.43
26:SL:135:VAL:HG13	26:SL:140:SER:HB2	1.99	0.43
28:SO:497:ASP:OD1	28:SO:498:ALA:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:62:90:THR:OG1	40:A:124:VAL:HG13	2.18	0.43
5:LF:119:LEU:HD21	5:LF:456:LEU:HD11	2.00	0.43
8:LJ:142:LEU:HD21	14:LS:229:TRP:CH2	2.53	0.43
15:LT:101:PRO:O	15:LT:107:TRP:NE1	2.43	0.43
46:2H:46:GLU:O	53:N2:91:A:N6	2.51	0.43
1:LA:33:GLU:OE2	1:LA:37:GLN:NE2	2.52	0.43
3:LC:207:GLY:N	3:LC:211:GLN:O	2.52	0.43
10:LN:243:LEU:HD22	10:LN:273:VAL:HG21	2.01	0.43
12:LQ:292:LEU:HD22	26:SL:273:ILE:HD12	2.00	0.43
13:LR:21:ARG:NH2	51:LE:29:G:OP1	2.52	0.43
1:LA:1757:ARG:NH2	21:SC:85:LEU:HD22	2.33	0.43
6:LG:7:ILE:HG23	6:LG:77:VAL:HG22	2.01	0.43
27:SN:84:HIS:ND1	27:SN:115:ASP:OD1	2.51	0.43
28:SO:253:TYR:OH	45:2D:18:GLU:OE1	2.36	0.43
1:LA:422:GLU:OE1	49:53:107:ARG:NH1	2.45	0.43
1:LA:929:GLN:HB3	16:LV:1079:ILE:HD11	2.01	0.43
3:LC:922:MET:HE1	3:LC:936:ALA:HB1	2.01	0.43
8:LJ:474:THR:HG22	11:LP:190:ASN:ND2	2.33	0.43
9:LL:68:ASP:N	9:LL:68:ASP:OD1	2.49	0.43
14:LS:86:ARG:NH2	55:N6:57:C:N3	2.57	0.43
16:LV:62:ASP:OD1	16:LV:62:ASP:N	2.48	0.43
16:LV:531:ASP:OD2	16:LV:534:PHE:N	2.51	0.43
25:SK:165:ASP:OD1	25:SK:166:TYR:N	2.52	0.43
1:LA:2023:ILE:HG22	4:LD:51:LEU:HD13	2.00	0.43
8:LJ:389:THR:HG21	8:LJ:458:ARG:O	2.19	0.43
14:LS:478:ASP:OD1	14:LS:478:ASP:N	2.49	0.43
40:A:21:LEU:HD12	40:A:92:LEU:HD11	2.01	0.43
3:LC:146:TYR:CD1	3:LC:149:ILE:HD11	2.53	0.43
3:LC:331:ALA:N	58:LC:1500:GTP:O6	2.52	0.43
24:SJ:90:VAL:HG13	24:SJ:234:ARG:HH22	1.83	0.43
12:LQ:57:ARG:CZ	26:SL:280:LEU:HD22	2.48	0.42
21:SC:27:MET:O	21:SC:31:GLY:N	2.52	0.42
46:5E:71:ILE:HG22	47:5F:70:ARG:HB2	2.00	0.42
1:LA:438:ALA:CB	3:LC:401:VAL:HG12	2.49	0.42
3:LC:188:ASP:OD1	3:LC:189:GLU:N	2.52	0.42
6:LG:9:ASN:ND2	6:LG:74:PHE:O	2.52	0.42
9:LL:247:ARG:NH1	52:LO:56:G:OP2	2.52	0.42
14:LS:661:LEU:HD23	14:LS:718:VAL:HG22	2.01	0.42
16:LV:101:LEU:O	16:LV:105:SER:N	2.44	0.42
28:SO:397:ASP:O	28:SO:401:GLY:N	2.52	0.42
1:LA:1839:ASP:OD1	1:LA:1839:ASP:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:LN:308:VAL:HG21	10:LN:322:TRP:HD1	1.84	0.42
12:LQ:666:LEU:HD22	30:SS:177:PHE:CE1	2.55	0.42
24:SJ:52:LEU:HG	24:SJ:99:ILE:HD11	2.02	0.42
31:SU:63:ILE:HD12	31:SV:83:MET:SD	2.59	0.42
8:LJ:227:HIS:CD2	8:LJ:231:VAL:HG22	2.55	0.42
10:LN:101:ARG:CZ	10:LN:104:ILE:HD11	2.50	0.42
49:53:28:TYR:HD1	49:53:58:MET:HE1	1.84	0.42
3:LC:915:LEU:O	3:LC:920:GLY:N	2.50	0.42
16:LV:546:HIS:HB3	16:LV:577:THR:HG23	2.01	0.42
43:25:70:VAL:HG21	43:25:89:VAL:HB	2.00	0.42
49:53:46:ALA:HB3	49:53:58:MET:HE3	2.01	0.42
50:5B:16:VAL:HG11	50:5B:68:LEU:HD23	2.02	0.42
1:LA:1565:LYS:NZ	21:SC:82:ASP:OD2	2.52	0.42
4:LD:52:ARG:NH2	41:RN:4:N:O4'	2.53	0.42
14:LS:163:VAL:CG1	24:SJ:332:TYR:HB2	2.49	0.42
15:LT:20:THR:HG22	15:LT:24:THR:HB	2.01	0.42
15:LT:663:VAL:HG21	26:SL:233:MET:HG2	2.01	0.42
49:53:107:ARG:O	49:53:111:ARG:N	2.40	0.42
1:LA:723:ARG:NH1	55:N6:63:G:N7	2.67	0.42
1:LA:733:LYS:NZ	55:N6:66:C:O2	2.41	0.42
31:SU:16:VAL:HG23	31:SU:54:VAL:HG21	2.02	0.42
1:LA:723:ARG:O	1:LA:725:GLN:NE2	2.53	0.42
2:LB:620:GLU:N	2:LB:656:LEU:O	2.53	0.42
17:LW:77:SER:O	17:LW:103:ASN:ND2	2.53	0.42
31:ST:266:LEU:HD13	31:ST:309:ILE:HG21	2.02	0.42
43:52:60:ASP:OD1	43:52:61:LYS:N	2.53	0.42
5:LF:135:ILE:O	5:LF:139:VAL:HG23	2.20	0.41
16:LV:1056:THR:OG1	16:LV:1057:LYS:N	2.52	0.41
24:SJ:257:THR:HG22	24:SJ:260:GLU:OE2	2.19	0.41
31:ST:131:ARG:NH1	31:SU:126:GLU:OE2	2.53	0.41
49:53:96:THR:O	49:53:96:THR:OG1	2.38	0.41
15:LT:402:ILE:HG23	15:LT:420:PHE:CZ	2.55	0.41
16:LV:906:LEU:HD13	16:LV:964:LEU:HD22	2.03	0.41
32:TN:15:MET:SD	32:TN:16:VAL:N	2.89	0.41
1:LA:439:LEU:HD22	3:LC:283:ILE:HG23	2.03	0.41
1:LA:1312:ILE:HG23	1:LA:1342:ILE:HD13	2.02	0.41
1:LA:1673:ASP:OD2	21:SC:207:LEU:HD13	2.20	0.41
14:LS:344:ASN:OD1	14:LS:344:ASN:N	2.52	0.41
16:LV:637:PHE:O	16:LV:719:SER:OG	2.25	0.41
16:LV:947:GLU:OE2	16:LV:951:ARG:NH2	2.46	0.41
38:66:61:GLU:OE1	55:N6:101:U:O3'	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:LS:163:VAL:HG13	24:SJ:332:TYR:HB2	2.02	0.41
16:LV:557:ALA:HB1	16:LV:804:LEU:HD22	2.02	0.41
3:LC:443:ILE:HG22	3:LC:447:LEU:CD1	2.51	0.41
5:LF:44:ARG:HG3	5:LF:61:VAL:HG22	2.03	0.41
12:LQ:244:LEU:HD12	26:SL:161:LEU:HB2	2.02	0.41
42:24:69:MET:HE2	44:2C:18:LEU:HG	2.01	0.41
43:52:16:THR:HG23	47:5F:7:GLY:CA	2.50	0.41
7:LH:141:LEU:HD21	15:LT:236:LYS:HG3	2.01	0.41
14:LS:352:LEU:O	14:LS:355:TYR:N	2.53	0.41
14:LS:201:LEU:HA	24:SJ:299:MET:HG2	2.03	0.41
16:LV:437:ASP:OD2	16:LV:463:HIS:NE2	2.54	0.41
16:LV:915:TRP:CG	16:LV:935:LEU:HD13	2.56	0.41
31:SW:5:ASN:HD22	31:SW:41:VAL:HG21	1.85	0.41
32:TN:15:MET:HE3	32:TN:16:VAL:HB	2.02	0.41
10:LN:43:ASP:OD1	10:LN:47:ALA:N	2.53	0.41
15:LT:612:ARG:O	15:LT:616:SER:N	2.44	0.41
31:ST:409:ASP:OD2	31:ST:411:SER:OG	2.32	0.41
3:LC:75:GLY:N	8:LJ:183:VAL:O	2.50	0.41
8:LJ:153:SER:O	8:LJ:157:VAL:HG23	2.20	0.41
8:LJ:256:ASP:O	8:LJ:260:ASN:N	2.46	0.41
12:LQ:715:LEU:HD12	31:ST:499:VAL:HG11	2.02	0.41
14:LS:445:ARG:NH2	14:LS:478:ASP:OD2	2.53	0.41
16:LV:24:MET:HE2	16:LV:142:GLU:HG2	2.01	0.41
16:LV:557:ALA:HB2	16:LV:806:LEU:HD23	2.02	0.41
16:LV:635:LEU:HD21	16:LV:704:ALA:HB1	2.03	0.41
16:LV:666:LEU:HD13	16:LV:667:PRO:CD	2.48	0.41
8:LJ:297:PHE:CE1	8:LJ:304:VAL:HG22	2.56	0.41
42:24:79:ILE:HG23	43:25:86:ILE:CG2	2.51	0.41
14:LS:148:TRP:CD1	14:LS:168:MET:HE3	2.56	0.40
16:LV:872:MET:HE1	16:LV:880:VAL:HG21	2.03	0.40
22:SD:453:LEU:HD22	22:SD:520:THR:HG22	2.04	0.40
28:SO:111:ALA:HB1	28:SO:115:ARG:HH21	1.86	0.40
1:LA:603:ALA:HB2	1:LA:711:TYR:HB3	2.02	0.40
16:LV:284:LEU:O	16:LV:288:ALA:HB3	2.21	0.40
15:LT:126:ARG:NH1	29:SP:205:GLU:OE2	2.55	0.40
15:LT:314:GLU:OE2	24:SJ:27:LYS:NZ	2.53	0.40
15:LT:759:LEU:HD21	25:SK:148:GLU:HG2	2.02	0.40
47:2I:26:PRO:HA	47:2I:50:ALA:HB2	2.02	0.40
3:LC:149:ILE:HD12	49:53:16:LEU:CD1	2.52	0.40
16:LV:899:MET:HG2	16:LV:1006:VAL:HG22	2.04	0.40
36:64:50:CYS:SG	36:64:51:THR:N	2.94	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:LA:1892:LEU:HD22	1:LA:1995:ILE:HG21	2.02	0.40
14:LS:445:ARG:NE	14:LS:473:GLU:OE2	2.54	0.40
46:2H:57:GLU:HB2	46:2H:68:LEU:HD11	2.04	0.40
46:5E:46:GLU:O	54:N5:51:A:N6	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	LA	2341/2427 (96%)	2293 (98%)	48 (2%)	0	100	100
2	LB	2120/2367 (90%)	2098 (99%)	22 (1%)	0	100	100
3	LC	901/1016 (89%)	886 (98%)	15 (2%)	0	100	100
4	LD	123/166 (74%)	123 (100%)	0	0	100	100
5	LF	398/706 (56%)	394 (99%)	4 (1%)	0	100	100
6	LG	78/82 (95%)	78 (100%)	0	0	100	100
7	LH	38/159 (24%)	38 (100%)	0	0	100	100
8	LJ	405/509 (80%)	398 (98%)	7 (2%)	0	100	100
9	LL	182/326 (56%)	179 (98%)	3 (2%)	0	100	100
10	LN	312/322 (97%)	303 (97%)	9 (3%)	0	100	100
11	LP	68/207 (33%)	66 (97%)	2 (3%)	0	100	100
12	LQ	535/804 (66%)	525 (98%)	10 (2%)	0	100	100
13	LR	103/197 (52%)	101 (98%)	2 (2%)	0	100	100
14	LS	749/824 (91%)	738 (98%)	11 (2%)	0	100	100
15	LT	792/794 (100%)	786 (99%)	6 (1%)	0	100	100
16	LV	967/1087 (89%)	950 (98%)	17 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	LW	184/307 (60%)	182 (99%)	2 (1%)	0	100	100
18	LY	105/114 (92%)	105 (100%)	0	0	100	100
19	LZ	87/403 (22%)	87 (100%)	0	0	100	100
20	SA	496/564 (88%)	490 (99%)	6 (1%)	0	100	100
21	SC	255/417 (61%)	253 (99%)	2 (1%)	0	100	100
22	SD	282/546 (52%)	280 (99%)	2 (1%)	0	100	100
23	SF	46/258 (18%)	45 (98%)	1 (2%)	0	100	100
24	SJ	259/414 (63%)	256 (99%)	3 (1%)	0	100	100
25	SK	81/175 (46%)	79 (98%)	2 (2%)	0	100	100
26	SL	210/544 (39%)	206 (98%)	4 (2%)	0	100	100
27	SN	181/192 (94%)	177 (98%)	4 (2%)	0	100	100
28	SO	416/621 (67%)	405 (97%)	11 (3%)	0	100	100
29	SP	79/269 (29%)	79 (100%)	0	0	100	100
30	SS	178/284 (63%)	177 (99%)	1 (1%)	0	100	100
31	ST	482/513 (94%)	470 (98%)	12 (2%)	0	100	100
31	SU	131/513 (26%)	128 (98%)	3 (2%)	0	100	100
31	SV	131/513 (26%)	130 (99%)	1 (1%)	0	100	100
31	SW	117/513 (23%)	116 (99%)	1 (1%)	0	100	100
32	TN	42/1181 (4%)	40 (95%)	2 (5%)	0	100	100
34	62	122/190 (64%)	121 (99%)	1 (1%)	0	100	100
35	63	75/134 (56%)	74 (99%)	1 (1%)	0	100	100
36	64	81/116 (70%)	81 (100%)	0	0	100	100
37	65	108/151 (72%)	105 (97%)	3 (3%)	0	100	100
38	66	69/80 (86%)	69 (100%)	0	0	100	100
39	67	89/91 (98%)	86 (97%)	3 (3%)	0	100	100
40	A	98/131 (75%)	98 (100%)	0	0	100	100
42	24	100/102 (98%)	99 (99%)	1 (1%)	0	100	100
42	51	96/102 (94%)	95 (99%)	1 (1%)	0	100	100
42	U1	96/102 (94%)	95 (99%)	1 (1%)	0	100	100
43	25	80/103 (78%)	78 (98%)	2 (2%)	0	100	100
43	52	87/103 (84%)	85 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
43	U2	81/103 (79%)	81 (100%)	0	0	100	100
44	2C	112/128 (88%)	112 (100%)	0	0	100	100
45	2D	97/141 (69%)	96 (99%)	1 (1%)	0	100	100
46	2H	79/86 (92%)	78 (99%)	1 (1%)	0	100	100
46	5E	76/86 (88%)	72 (95%)	4 (5%)	0	100	100
46	UE	77/86 (90%)	76 (99%)	1 (1%)	0	100	100
47	2I	74/76 (97%)	71 (96%)	3 (4%)	0	100	100
47	5F	74/76 (97%)	72 (97%)	2 (3%)	0	100	100
47	UF	74/76 (97%)	72 (97%)	2 (3%)	0	100	100
48	2J	75/81 (93%)	75 (100%)	0	0	100	100
48	5G	75/81 (93%)	75 (100%)	0	0	100	100
48	UG	75/81 (93%)	75 (100%)	0	0	100	100
49	53	100/113 (88%)	99 (99%)	1 (1%)	0	100	100
49	U3	79/113 (70%)	78 (99%)	1 (1%)	0	100	100
50	5B	97/111 (87%)	94 (97%)	3 (3%)	0	100	100
50	UB	79/111 (71%)	77 (98%)	2 (2%)	0	100	100
All	All	16299/23288 (70%)	16050 (98%)	249 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	LA	1824/2116 (86%)	1760 (96%)	64 (4%)	32	67
3	LC	751/831 (90%)	721 (96%)	30 (4%)	28	63
4	LD	104/136 (76%)	103 (99%)	1 (1%)	68	88
5	LF	353/584 (60%)	331 (94%)	22 (6%)	16	45
6	LG	59/61 (97%)	59 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	LH	33/133 (25%)	32 (97%)	1 (3%)	36	72
8	LJ	336/414 (81%)	317 (94%)	19 (6%)	18	49
9	LL	154/268 (58%)	151 (98%)	3 (2%)	50	81
10	LN	240/243 (99%)	220 (92%)	20 (8%)	10	32
11	LP	62/171 (36%)	59 (95%)	3 (5%)	23	56
12	LQ	416/657 (63%)	399 (96%)	17 (4%)	27	62
13	LR	75/149 (50%)	74 (99%)	1 (1%)	61	86
14	LS	615/665 (92%)	596 (97%)	19 (3%)	35	70
15	LT	661/661 (100%)	645 (98%)	16 (2%)	43	77
16	LV	808/940 (86%)	779 (96%)	29 (4%)	31	66
17	LW	175/273 (64%)	172 (98%)	3 (2%)	53	83
18	LY	90/97 (93%)	86 (96%)	4 (4%)	25	59
19	LZ	47/321 (15%)	46 (98%)	1 (2%)	47	79
20	SA	448/496 (90%)	434 (97%)	14 (3%)	35	70
21	SC	228/356 (64%)	217 (95%)	11 (5%)	23	56
22	SD	247/439 (56%)	236 (96%)	11 (4%)	24	58
24	SJ	234/341 (69%)	223 (95%)	11 (5%)	23	57
25	SK	76/145 (52%)	71 (93%)	5 (7%)	15	43
26	SL	170/413 (41%)	164 (96%)	6 (4%)	32	67
27	SN	156/160 (98%)	148 (95%)	8 (5%)	21	54
28	SO	360/511 (70%)	342 (95%)	18 (5%)	22	54
29	SP	73/233 (31%)	69 (94%)	4 (6%)	19	51
30	SS	158/238 (66%)	148 (94%)	10 (6%)	16	45
31	ST	383/398 (96%)	367 (96%)	16 (4%)	26	61
31	SU	113/398 (28%)	111 (98%)	2 (2%)	51	82
31	SV	113/398 (28%)	108 (96%)	5 (4%)	25	59
31	SW	105/398 (26%)	101 (96%)	4 (4%)	29	64
32	TN	40/953 (4%)	40 (100%)	0	100	100
34	62	101/151 (67%)	96 (95%)	5 (5%)	22	54
35	63	70/113 (62%)	68 (97%)	2 (3%)	37	73
36	64	72/98 (74%)	69 (96%)	3 (4%)	26	61

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
37	65	98/122 (80%)	91 (93%)	7 (7%)	13	39
38	66	59/64 (92%)	54 (92%)	5 (8%)	10	31
39	67	77/77 (100%)	71 (92%)	6 (8%)	11	35
40	A	86/109 (79%)	85 (99%)	1 (1%)	63	87
42	24	88/88 (100%)	87 (99%)	1 (1%)	65	87
42	51	86/88 (98%)	83 (96%)	3 (4%)	32	67
43	25	73/94 (78%)	73 (100%)	0	100	100
43	52	80/94 (85%)	73 (91%)	7 (9%)	9	29
44	2C	100/108 (93%)	96 (96%)	4 (4%)	28	63
45	2D	88/126 (70%)	87 (99%)	1 (1%)	65	87
46	2H	74/79 (94%)	72 (97%)	2 (3%)	39	74
46	5E	71/79 (90%)	70 (99%)	1 (1%)	59	85
47	2I	65/65 (100%)	63 (97%)	2 (3%)	35	70
47	5F	65/65 (100%)	64 (98%)	1 (2%)	57	84
48	2J	64/68 (94%)	64 (100%)	0	100	100
48	5G	64/68 (94%)	61 (95%)	3 (5%)	23	57
49	53	86/93 (92%)	86 (100%)	0	100	100
50	5B	82/90 (91%)	79 (96%)	3 (4%)	30	65
All	All	11356/16536 (69%)	10921 (96%)	435 (4%)	30	64

All (435) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	LA	73	LYS
1	LA	93	CYS
1	LA	100	ILE
1	LA	108	LEU
1	LA	123	VAL
1	LA	139	THR
1	LA	222	LEU
1	LA	233	ARG
1	LA	294	ILE
1	LA	303	ASP
1	LA	358	VAL
1	LA	360	ASN
1	LA	369	THR

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Mol	Chain	Res	Type
1	LA	417	LEU
1	LA	452	GLU
1	LA	475	LEU
1	LA	476	THR
1	LA	482	LYS
1	LA	575	TYR
1	LA	578	ILE
1	LA	606[A]	MET
1	LA	606[B]	MET
1	LA	607	VAL
1	LA	664	ARG
1	LA	709	GLN
1	LA	738	ARG
1	LA	809	SER
1	LA	828	THR
1	LA	841	LEU
1	LA	846	LEU
1	LA	901	LEU
1	LA	912	ARG
1	LA	929	GLN
1	LA	1038	GLU
1	LA	1147	LEU
1	LA	1206	GLU
1	LA	1259	LEU
1	LA	1281	GLU
1	LA	1302	LEU
1	LA	1323	VAL
1	LA	1348	GLU
1	LA	1353	THR
1	LA	1418	THR
1	LA	1431	ASN
1	LA	1442	GLN
1	LA	1450	GLU
1	LA	1518	LEU
1	LA	1573	GLU
1	LA	1576	GLU
1	LA	1667	LEU
1	LA	1685	LEU
1	LA	1693	SER
1	LA	1855	VAL
1	LA	1863	THR
1	LA	1924	LEU

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Mol	Chain	Res	Type
1	LA	1934	SER
1	LA	1948	HIS
1	LA	1952	VAL
1	LA	1953	LEU
1	LA	1954	ASP
1	LA	1955	TYR
1	LA	2008	ILE
1	LA	2084	LYS
1	LA	2113	ARG
3	LC	105	GLU
3	LC	160	VAL
3	LC	213	THR
3	LC	217	VAL
3	LC	246	VAL
3	LC	252	LEU
3	LC	256	SER
3	LC	264	ILE
3	LC	313	THR
3	LC	384	THR
3	LC	447	LEU
3	LC	545	LEU
3	LC	588	THR
3	LC	594	LEU
3	LC	597	ARG
3	LC	605	VAL
3	LC	639	VAL
3	LC	651	VAL
3	LC	672	LEU
3	LC	678	LEU
3	LC	691	SER
3	LC	705	LEU
3	LC	743	ASN
3	LC	745	VAL
3	LC	768	PHE
3	LC	779	ARG
3	LC	808	LYS
3	LC	900	GLU
3	LC	903	CYS
3	LC	934	ILE
4	LD	35	HIS
5	LF	50	LEU
5	LF	53	LEU

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Mol	Chain	Res	Type
5	LF	64	SER
5	LF	93	ARG
5	LF	94	LEU
5	LF	106	VAL
5	LF	111	LEU
5	LF	118	SER
5	LF	256	LEU
5	LF	272	LEU
5	LF	273	LEU
5	LF	390	SER
5	LF	392	CYS
5	LF	435	LEU
5	LF	447	LEU
5	LF	480	GLN
5	LF	485	GLU
5	LF	592	VAL
5	LF	624	LEU
5	LF	642	ILE
5	LF	645	THR
5	LF	705	ARG
7	LH	90	LYS
8	LJ	9	LEU
8	LJ	28	VAL
8	LJ	33	VAL
8	LJ	70	THR
8	LJ	155	LEU
8	LJ	164	GLU
8	LJ	177	LYS
8	LJ	195	GLU
8	LJ	209	ILE
8	LJ	275	CYS
8	LJ	284	VAL
8	LJ	286	ILE
8	LJ	287	SER
8	LJ	319	VAL
8	LJ	389	THR
8	LJ	397	HIS
8	LJ	435	VAL
8	LJ	451	GLN
8	LJ	466	THR
9	LL	100	ARG
9	LL	101	HIS

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Mol	Chain	Res	Type
9	LL	199	ARG
10	LN	49	LEU
10	LN	61	VAL
10	LN	62	CYS
10	LN	107	ARG
10	LN	110	VAL
10	LN	113	ARG
10	LN	125	THR
10	LN	131	VAL
10	LN	143	ASP
10	LN	149	VAL
10	LN	157	VAL
10	LN	163	THR
10	LN	178	LEU
10	LN	195	CYS
10	LN	241	ARG
10	LN	262	THR
10	LN	264	VAL
10	LN	285	THR
10	LN	287	THR
10	LN	317	VAL
11	LP	11	GLU
11	LP	16	GLN
11	LP	162	LEU
12	LQ	29	ARG
12	LQ	89	GLN
12	LQ	94	THR
12	LQ	163	SER
12	LQ	167	THR
12	LQ	194	LEU
12	LQ	223	LEU
12	LQ	235	LEU
12	LQ	292	LEU
12	LQ	642	ARG
12	LQ	651	GLN
12	LQ	659	VAL
12	LQ	697	LEU
12	LQ	701	ASP
12	LQ	715	LEU
12	LQ	755	LEU
12	LQ	788	ARG
13	LR	20	GLN

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Mol	Chain	Res	Type
14	LS	36	VAL
14	LS	84	VAL
14	LS	152	VAL
14	LS	168	MET
14	LS	215	ILE
14	LS	220	VAL
14	LS	319	HIS
14	LS	344	ASN
14	LS	353	THR
14	LS	462	CYS
14	LS	478	ASP
14	LS	497	CYS
14	LS	498	LEU
14	LS	504	GLN
14	LS	764	THR
14	LS	767	THR
14	LS	785	SER
14	LS	787	LEU
14	LS	818	ARG
15	LT	14	VAL
15	LT	20	THR
15	LT	87	GLN
15	LT	125	THR
15	LT	171	SER
15	LT	285	LEU
15	LT	326	ASP
15	LT	489	ARG
15	LT	524	CYS
15	LT	532	THR
15	LT	608	LEU
15	LT	652	THR
15	LT	661	SER
15	LT	696	ASP
15	LT	698	VAL
15	LT	715	LEU
16	LV	52	THR
16	LV	141	VAL
16	LV	181	THR
16	LV	219	LEU
16	LV	223	ARG
16	LV	492	TYR
16	LV	559	VAL

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Mol	Chain	Res	Type
16	LV	573	VAL
16	LV	574	THR
16	LV	594	ARG
16	LV	607	LEU
16	LV	639	THR
16	LV	644	ILE
16	LV	666	LEU
16	LV	710	ILE
16	LV	730	LYS
16	LV	742	SER
16	LV	766	THR
16	LV	767	GLU
16	LV	790	VAL
16	LV	801	LEU
16	LV	947	GLU
16	LV	983	VAL
16	LV	984	ASP
16	LV	986	HIS
16	LV	1008	ILE
16	LV	1026	GLU
16	LV	1034	ILE
16	LV	1056	THR
17	LW	58	LEU
17	LW	63	THR
17	LW	139	VAL
18	LY	18	SER
18	LY	23	ARG
18	LY	31	THR
18	LY	98	ARG
19	LZ	366	HIS
20	SA	52	LEU
20	SA	125	ARG
20	SA	145	VAL
20	SA	159	GLU
20	SA	186	ARG
20	SA	193	LEU
20	SA	217	LEU
20	SA	221	LEU
20	SA	267	ASP
20	SA	351	ILE
20	SA	360	ARG
20	SA	443	LEU

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Mol	Chain	Res	Type
20	SA	462	VAL
20	SA	533	LEU
21	SC	16	GLN
21	SC	24	LEU
21	SC	46	SER
21	SC	67	LEU
21	SC	82	ASP
21	SC	154	ARG
21	SC	159	VAL
21	SC	191	VAL
21	SC	195	ARG
21	SC	213	ASN
21	SC	293	GLN
22	SD	243	LEU
22	SD	313	VAL
22	SD	343	GLN
22	SD	477	LYS
22	SD	480	LEU
22	SD	489	ARG
22	SD	493	GLU
22	SD	513	LEU
22	SD	517	ARG
22	SD	528	LEU
22	SD	536	CYS
24	SJ	90	VAL
24	SJ	143	LEU
24	SJ	152	THR
24	SJ	153	LEU
24	SJ	223	SER
24	SJ	224	ARG
24	SJ	226	LEU
24	SJ	238	THR
24	SJ	264	LEU
24	SJ	269	VAL
24	SJ	361	LEU
25	SK	52	GLU
25	SK	53	VAL
25	SK	138	VAL
25	SK	142	GLU
25	SK	164	SER
26	SL	3	LEU
26	SL	13	ASP

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Mol	Chain	Res	Type
26	SL	109	GLU
26	SL	141	LEU
26	SL	256	THR
26	SL	271	LYS
27	SN	41	ARG
27	SN	42	LEU
27	SN	53	LEU
27	SN	60	VAL
27	SN	80	VAL
27	SN	91	SER
27	SN	106	ILE
27	SN	173	VAL
28	SO	115	ARG
28	SO	152	LEU
28	SO	289	VAL
28	SO	294	GLU
28	SO	376	GLU
28	SO	409	ASN
28	SO	411	GLU
28	SO	416	VAL
28	SO	417	GLN
28	SO	419	LEU
28	SO	442	VAL
28	SO	449	TYR
28	SO	466	LEU
28	SO	481	LEU
28	SO	488	SER
28	SO	490	VAL
28	SO	521	LEU
28	SO	583	LYS
29	SP	201	LEU
29	SP	228	LEU
29	SP	237	GLU
29	SP	250	LEU
30	SS	35	LEU
30	SS	41	THR
30	SS	106	ASP
30	SS	117	LEU
30	SS	183	GLN
30	SS	204	LEU
30	SS	208	GLN
30	SS	217	GLU

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Mol	Chain	Res	Type
30	SS	256	LEU
30	SS	262	VAL
31	ST	4	CYS
31	ST	101	GLN
31	ST	187	THR
31	ST	209	VAL
31	ST	216	GLU
31	ST	239	ASP
31	ST	270	GLU
31	ST	296	VAL
31	ST	309	ILE
31	ST	330	VAL
31	ST	336	THR
31	ST	347	VAL
31	ST	348	GLU
31	ST	419	GLN
31	ST	485	VAL
31	ST	496	CYS
31	SU	69	LEU
31	SU	82	GLN
31	SV	74	VAL
31	SV	76	THR
31	SV	77	LEU
31	SV	84	GLU
31	SV	106	LEU
31	SW	53	THR
31	SW	81	LEU
31	SW	102	LEU
31	SW	106	LEU
34	62	69	THR
34	62	81	LEU
34	62	87	VAL
34	62	100	LEU
34	62	123	CYS
35	63	41	HIS
35	63	67	LEU
36	64	17	CYS
36	64	23	SER
36	64	39	THR
37	65	34	ILE
37	65	46	ARG
37	65	58	GLU

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Mol	Chain	Res	Type
37	65	78	VAL
37	65	82	THR
37	65	130	CYS
37	65	147	LEU
38	66	5	LEU
38	66	13	VAL
38	66	21	GLU
38	66	36	VAL
38	66	62	ASN
39	67	8	VAL
39	67	18	LEU
39	67	35	VAL
39	67	46	VAL
39	67	65	ILE
39	67	91	ILE
40	A	16	VAL
42	24	23	THR
44	2C	46	CYS
44	2C	54	VAL
44	2C	84	ARG
44	2C	99	THR
45	2D	53	VAL
46	2H	23	GLN
46	2H	50	VAL
47	2I	36	ASP
47	2I	61	LEU
42	51	43	ASP
42	51	71	ARG
42	51	97	LYS
43	52	17	LYS
43	52	46	CYS
43	52	47	ARG
43	52	53	LEU
43	52	60	ASP
43	52	80	GLU
43	52	86	ILE
50	5B	43	VAL
50	5B	66	ILE
50	5B	77	THR
46	5E	50	VAL
47	5F	5	VAL
48	5G	22	ILE

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Mol	Chain	Res	Type
48	5G	58	GLU
48	5G	75	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (79) such sidechains are listed below:

Mol	Chain	Res	Type
1	LA	621	HIS
1	LA	915	HIS
1	LA	1092	HIS
1	LA	1242	ASN
1	LA	1303	GLN
1	LA	1365	HIS
1	LA	1404	HIS
1	LA	1689	HIS
1	LA	1731	ASN
1	LA	1786	HIS
3	LC	184	HIS
3	LC	798	HIS
3	LC	823	HIS
3	LC	910	GLN
3	LC	957	HIS
3	LC	967	HIS
5	LF	457	HIS
8	LJ	306	HIS
9	LL	101	HIS
10	LN	209	HIS
11	LP	159	HIS
12	LQ	658	ASN
12	LQ	700	GLN
13	LR	3	ASN
13	LR	25	ASN
14	LS	64	HIS
14	LS	297	HIS
14	LS	335	GLN
15	LT	74	HIS
15	LT	177	HIS
15	LT	193	ASN
15	LT	509	HIS
15	LT	515	HIS
15	LT	558	HIS
16	LV	102	HIS
16	LV	475	GLN

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Mol	Chain	Res	Type
16	LV	953	ASN
17	LW	106	HIS
17	LW	143	ASN
18	LY	32	GLN
18	LY	79	GLN
20	SA	155	HIS
20	SA	191	GLN
21	SC	132	ASN
21	SC	199	HIS
24	SJ	33	GLN
24	SJ	342	GLN
26	SL	21	HIS
26	SL	144	GLN
27	SN	38	GLN
28	SO	330	GLN
28	SO	427	HIS
28	SO	555	GLN
30	SS	183	GLN
31	ST	167	HIS
31	ST	231	HIS
31	ST	288	HIS
31	ST	419	GLN
31	SU	36	HIS
31	SU	92	GLN
31	SU	97	GLN
31	SU	98	GLN
31	SV	36	HIS
34	62	167	HIS
35	63	43	HIS
36	64	33	ASN
37	65	32	HIS
37	65	62	ASN
37	65	64	GLN
37	65	132	GLN
39	67	36	HIS
43	25	62	HIS
46	2H	10	ASN
46	2H	22	HIS
46	2H	23	GLN
46	2H	31	HIS
48	2J	44	HIS
50	5B	23	ASN

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Mol	Chain	Res	Type
46	5E	82	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
33	UX	0/21	-	-
41	RN	1/44 (2%)	1 (100%)	0
51	LE	11/63 (17%)	1 (9%)	0
52	LO	45/57 (78%)	5 (11%)	1 (2%)
53	N2	73/142 (51%)	13 (17%)	1 (1%)
54	N5	61/71 (85%)	9 (14%)	0
55	N6	100/100 (100%)	9 (9%)	2 (2%)
All	All	291/498 (58%)	38 (13%)	4 (1%)

All (38) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
41	RN	44	G
51	LE	29	G
52	LO	73	A
52	LO	74	G
52	LO	80	G
52	LO	81	G
52	LO	82	A
53	N2	7	U
53	N2	13	C
53	N2	15	A
53	N2	16	U
53	N2	17	U
53	N2	18	U
53	N2	20	G
53	N2	24	A
53	N2	90	A
53	N2	91	A
53	N2	92	U
53	N2	94	A
53	N2	128	U
54	N5	5	C
54	N5	17	U
54	N5	22	C
54	N5	34	C

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Mol	Chain	Res	Type
54	N5	56	G
54	N5	57	A
54	N5	65	A
54	N5	66	A
54	N5	67	G
55	N6	3	A
55	N6	10	U
55	N6	11	C
55	N6	26	A
55	N6	44	G
55	N6	47	G
55	N6	66	C
55	N6	72	U
55	N6	100	U

All (4) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
52	LO	81	G
53	N2	90	A
55	N6	2	G
55	N6	9	U

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
51	PSU	LE	28	51	18,21,22	1.09	1 (5%)	22,30,33	1.73	4 (18%)
26	SEP	SL	186	26	8,9,10	1.37	1 (12%)	8,12,14	1.06	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
51	PSU	LE	28	51	-	3/7/25/26	0/2/2/2
26	SEP	SL	186	26	-	0/5/8/10	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	LE	28	PSU	C6-C5	3.58	1.39	1.35
26	SL	186	SEP	P-O1P	2.95	1.60	1.50

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	LE	28	PSU	C4-N3-C2	-4.57	119.75	126.34
51	LE	28	PSU	N1-C2-N3	4.57	120.31	115.13
51	LE	28	PSU	O2-C2-N1	-2.96	119.53	122.79
51	LE	28	PSU	C6-N1-C2	-2.45	120.17	122.68
26	SL	186	SEP	P-OG-CB	-2.12	112.47	118.30

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
51	LE	28	PSU	O4'-C1'-C5-C4
51	LE	28	PSU	O4'-C1'-C5-C6
51	LE	28	PSU	O4'-C4'-C5'-O5'

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 20 ligands modelled in this entry, 16 are monoatomic - leaving 4 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
60	GTG	N5	101	54	53,57,57	3.41	19 (35%)	79,90,90	2.87	34 (43%)
61	G5J	N6	201	55,57	31,35,35	0.75	1 (3%)	38,55,55	0.80	0
56	IHP	LA	2501	-	36,36,36	1.48	6 (16%)	54,60,60	1.02	4 (7%)
58	GTP	LC	1500	57	30,34,34	3.01	14 (46%)	46,54,54	2.05	16 (34%)

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
60	GTG	N5	101	54	-	8/32/64/64	0/6/6/6
61	G5J	N6	201	55,57	-	5/25/41/41	0/3/3/3
56	IHP	LA	2501	-	-	4/30/54/54	0/1/1/1
58	GTP	LC	1500	57	-	3/22/38/38	0/3/3/3

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
60	N5	101	GTG	O3D-C3D	-10.18	1.19	1.43
58	LC	1500	GTP	O6-C6	8.63	1.40	1.23
60	N5	101	GTG	O6B-C6B	8.57	1.39	1.23
60	N5	101	GTG	O6A-C6A	8.47	1.39	1.23
60	N5	101	GTG	C5A-N7A	7.78	1.48	1.39
58	LC	1500	GTP	C5-N7	6.70	1.52	1.39
60	N5	101	GTG	C5B-N7B	6.67	1.52	1.39
60	N5	101	GTG	C5A-C4A	6.28	1.54	1.38
58	LC	1500	GTP	C2-N2	4.64	1.45	1.34
60	N5	101	GTG	C2A-N2A	4.57	1.45	1.34
60	N5	101	GTG	C2B-N2B	4.47	1.44	1.34
58	LC	1500	GTP	C8-N9	-4.44	1.27	1.37
58	LC	1500	GTP	C2-N1	4.39	1.48	1.37
60	N5	101	GTG	O4E-C1E	4.29	1.52	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
60	N5	101	GTG	C4B-N9B	-4.23	1.27	1.38
60	N5	101	GTG	C8B-N9B	-4.03	1.28	1.37
58	LC	1500	GTP	C2-N3	3.99	1.42	1.33
58	LC	1500	GTP	C4-N9	-3.88	1.28	1.38
60	N5	101	GTG	C4A-N9A	3.71	1.47	1.38
56	LA	2501	IHP	P5-O15	3.44	1.65	1.59
60	N5	101	GTG	C2E-C3E	-3.31	1.44	1.53
56	LA	2501	IHP	P6-O16	3.20	1.65	1.59
60	N5	101	GTG	C2A-N1A	3.06	1.45	1.37
56	LA	2501	IHP	P2-O12	3.06	1.65	1.59
56	LA	2501	IHP	P4-O14	2.97	1.64	1.59
60	N5	101	GTG	O4E-C4E	2.96	1.51	1.45
60	N5	101	GTG	C2D-C3D	-2.88	1.45	1.53
56	LA	2501	IHP	P3-O13	2.72	1.64	1.59
56	LA	2501	IHP	P1-O11	2.65	1.64	1.59
61	N6	201	G5J	C6-C5	-2.64	1.37	1.45
58	LC	1500	GTP	PG-O3G	-2.63	1.44	1.54
58	LC	1500	GTP	PG-O2G	-2.54	1.45	1.54
58	LC	1500	GTP	C2'-C3'	-2.52	1.46	1.53
58	LC	1500	GTP	PA-O2A	-2.20	1.45	1.55
60	N5	101	GTG	C4B-N3B	2.16	1.39	1.34
60	N5	101	GTG	C5B-C4B	2.12	1.44	1.38
58	LC	1500	GTP	O4'-C1'	2.12	1.47	1.42
58	LC	1500	GTP	PB-O2B	-2.10	1.45	1.55
58	LC	1500	GTP	C4-N3	2.10	1.39	1.34
60	N5	101	GTG	C2A-N3A	2.09	1.38	1.33

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
60	N5	101	GTG	C8A-N7A-C5A	8.84	118.84	107.78
60	N5	101	GTG	C6A-C5A-N7A	8.32	142.31	132.25
60	N5	101	GTG	C8B-N9B-C4B	7.72	120.75	106.05
60	N5	101	GTG	N9A-C4A-N3A	7.27	140.54	125.94
58	LC	1500	GTP	C8-N9-C4	7.00	119.38	106.05
60	N5	101	GTG	N9B-C4B-N3B	5.22	136.42	125.94
60	N5	101	GTG	C5B-C4B-N3B	-5.04	120.29	128.46
60	N5	101	GTG	C7X-N7A-C5A	-5.01	120.54	126.77
60	N5	101	GTG	C2A-N3A-C4A	4.79	120.83	112.30
60	N5	101	GTG	C4A-C5A-N7A	-4.78	99.85	107.67
60	N5	101	GTG	C5A-C4A-N3A	-4.76	119.02	128.15
60	N5	101	GTG	C8A-N9A-C4A	4.61	118.82	107.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	LC	1500	GTP	PB-O3B-PG	-4.54	117.26	132.83
60	N5	101	GTG	C2B-N3B-C4B	4.14	119.68	112.30
60	N5	101	GTG	N9A-C8A-N7A	-4.10	102.06	112.21
60	N5	101	GTG	C6B-C5B-N7B	3.72	137.17	130.25
60	N5	101	GTG	C5A-C6A-N1A	3.70	119.53	111.79
60	N5	101	GTG	C4B-C5B-N7B	-3.54	105.12	110.72
56	LA	2501	IHP	C6-C1-C2	3.40	117.86	110.41
60	N5	101	GTG	O6A-C6A-C5A	-3.39	120.41	128.06
58	LC	1500	GTP	C2-N1-C6	-3.38	118.93	125.10
60	N5	101	GTG	N9B-C8B-N7B	-3.21	107.35	113.39
58	LC	1500	GTP	O3G-PG-O3B	3.10	115.02	104.64
58	LC	1500	GTP	PA-O3A-PB	-3.09	122.21	132.83
60	N5	101	GTG	PB-O3A-PA	-3.05	122.34	132.83
60	N5	101	GTG	C2B-N1B-C6B	-2.95	119.72	125.10
60	N5	101	GTG	C7X-N7A-C8A	-2.73	120.62	124.84
60	N5	101	GTG	C4E-O4E-C1E	-2.73	103.45	109.47
58	LC	1500	GTP	C2'-C3'-C4'	2.69	107.88	102.64
58	LC	1500	GTP	C5-C6-N1	2.66	119.95	113.19
58	LC	1500	GTP	C3'-C2'-C1'	2.62	106.41	101.43
60	N5	101	GTG	C2A-N1A-C6A	-2.60	120.37	125.10
56	LA	2501	IHP	C3-C2-C1	2.59	116.09	110.41
60	N5	101	GTG	C5B-C6B-N1B	2.57	119.70	113.19
60	N5	101	GTG	PG-O3B-PB	-2.56	124.05	132.83
56	LA	2501	IHP	C6-C5-C4	-2.56	104.81	110.41
60	N5	101	GTG	O6B-C6B-C5B	-2.52	119.92	126.60
60	N5	101	GTG	C1E-N9B-C8B	-2.50	119.59	126.70
60	N5	101	GTG	C5A-C4A-N9A	-2.49	100.43	105.89
60	N5	101	GTG	C3D-C2D-C1D	2.44	106.07	101.43
58	LC	1500	GTP	O6-C6-C5	-2.44	120.12	126.60
58	LC	1500	GTP	C1'-N9-C8	-2.44	119.76	126.70
58	LC	1500	GTP	N9-C4-N3	2.43	130.83	125.94
60	N5	101	GTG	C1E-N9B-C4B	-2.30	119.66	126.50
58	LC	1500	GTP	O2G-PG-O3B	2.24	112.14	104.64
60	N5	101	GTG	O2G-PG-O1G	-2.17	101.53	112.24
58	LC	1500	GTP	C8-N7-C5	-2.14	100.37	104.24
58	LC	1500	GTP	C5-C4-N9	-2.13	101.77	105.63
60	N5	101	GTG	O2A-PA-O1A	-2.11	101.79	112.24
60	N5	101	GTG	O2B-PB-O1B	-2.08	101.93	112.24
56	LA	2501	IHP	C5-C4-C3	-2.08	105.86	110.41
60	N5	101	GTG	C1D-N9A-C8A	-2.07	119.74	126.74
58	LC	1500	GTP	O2B-PB-O1B	-2.01	102.31	112.24
58	LC	1500	GTP	O2A-PA-O1A	-2.00	102.35	112.24

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
56	LA	2501	IHP	C1-O11-P1-O31
56	LA	2501	IHP	C4-O14-P4-O34
56	LA	2501	IHP	C5-O15-P5-O45
58	LC	1500	GTP	C5'-O5'-PA-O1A
60	N5	101	GTG	PB-O3B-PG-O5E
60	N5	101	GTG	O4E-C4E-C5E-O5E
60	N5	101	GTG	C3E-C4E-C5E-O5E
61	N6	201	G5J	C5'-O5'-PA-O2A
61	N6	201	G5J	O4'-C1'-N9-C4
58	LC	1500	GTP	C5'-O5'-PA-O3A
60	N5	101	GTG	C5D-O5D-PA-O3A
61	N6	201	G5J	C5'-O5'-PA-O3A
60	N5	101	GTG	PB-O3A-PA-O1A
61	N6	201	G5J	O4'-C1'-N9-C8
61	N6	201	G5J	C5'-O5'-PA-O1A
60	N5	101	GTG	C4E-C5E-O5E-PG
56	LA	2501	IHP	C4-O14-P4-O44
60	N5	101	GTG	O4D-C4D-C5D-O5D
58	LC	1500	GTP	PB-O3A-PA-O2A
60	N5	101	GTG	C5E-O5E-PG-O1G

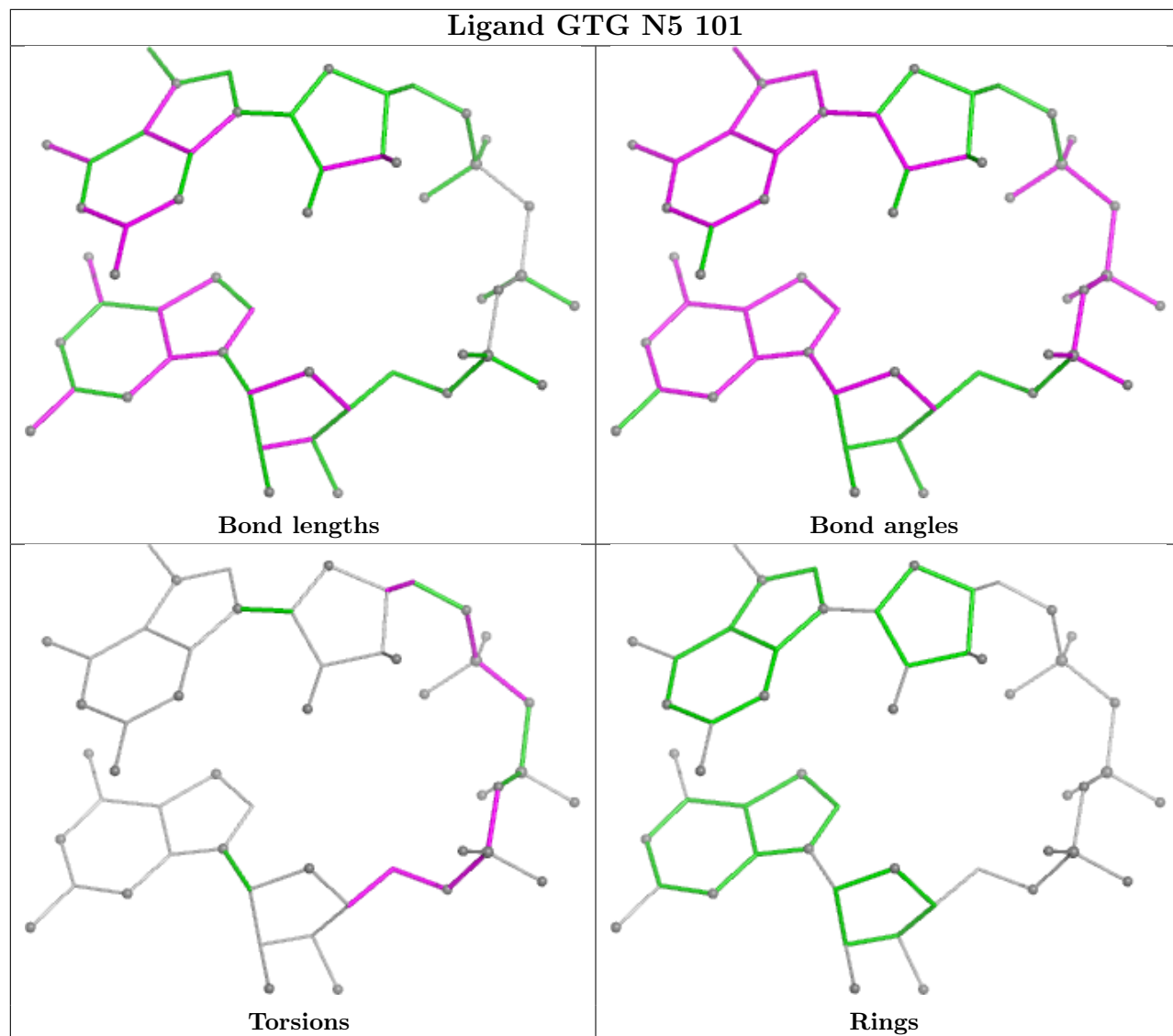
There are no ring outliers.

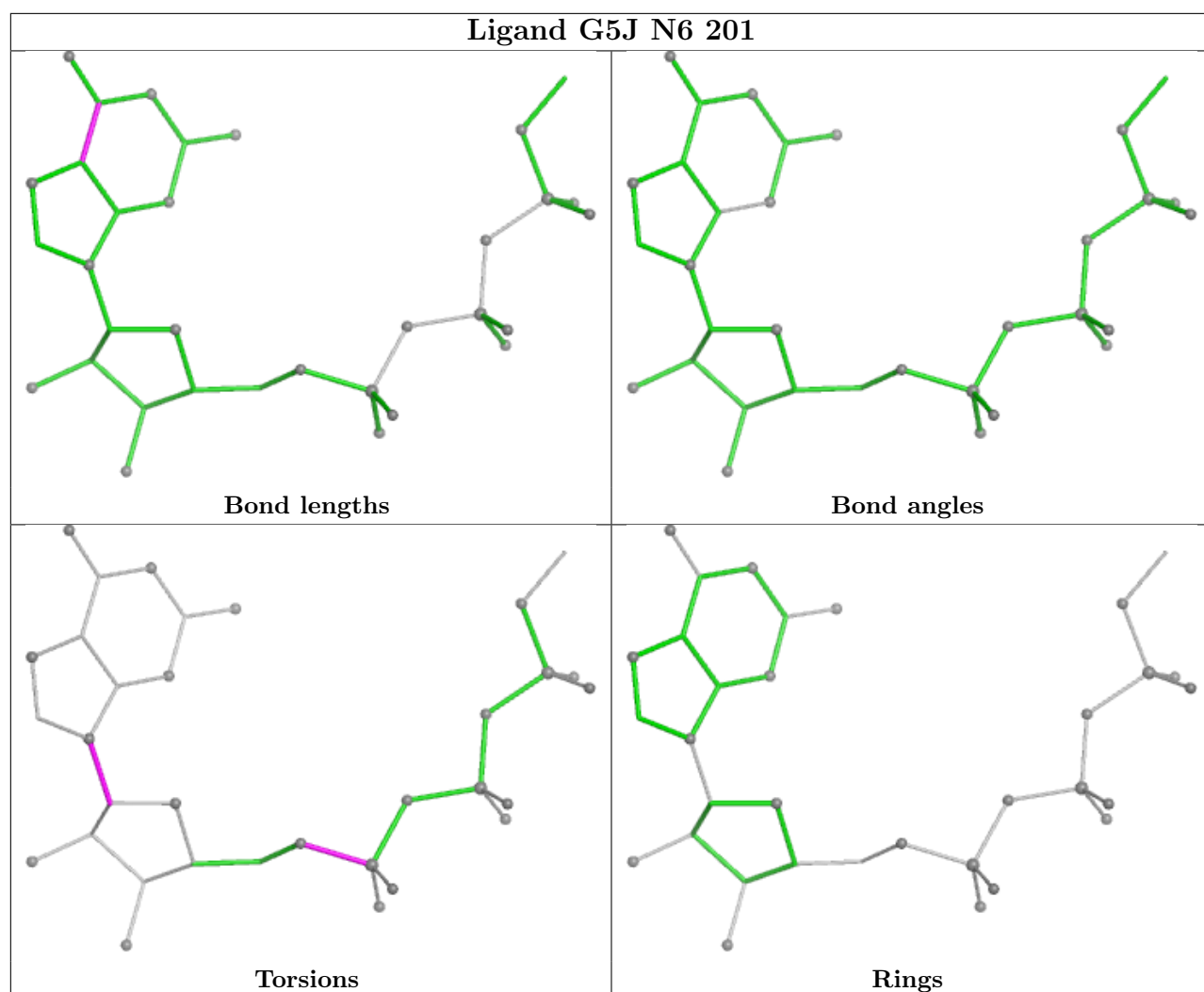
3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
61	N6	201	G5J	1	0
56	LA	2501	IHP	1	0
58	LC	1500	GTP	2	0

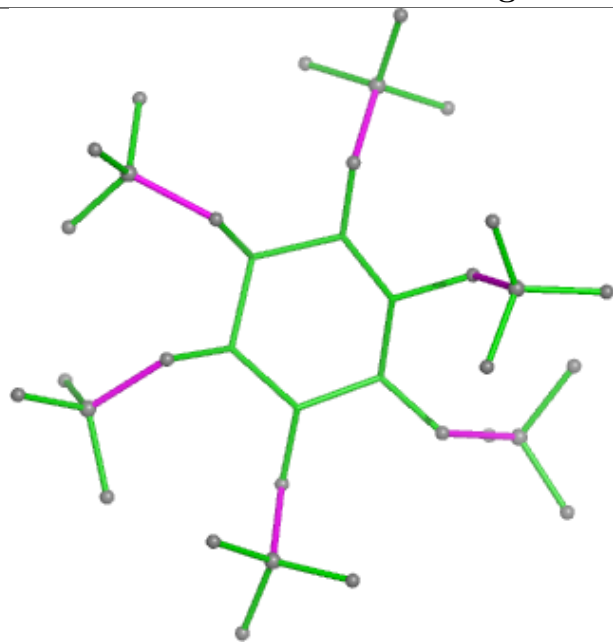
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

equivalents in the CSD to analyse the geometry.

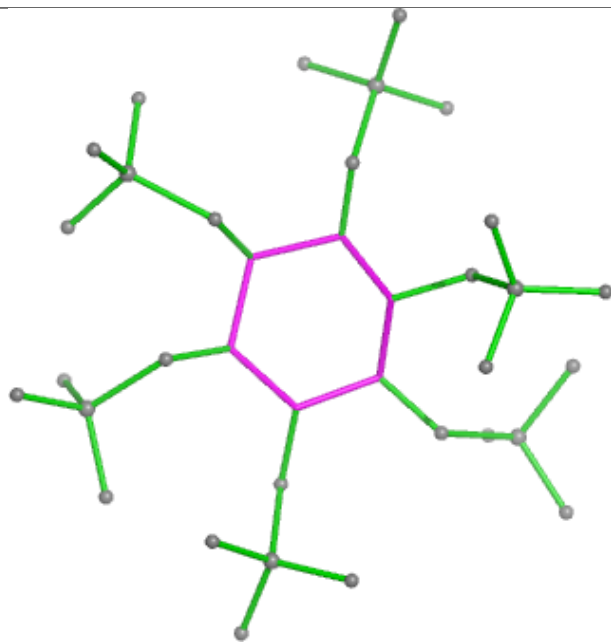




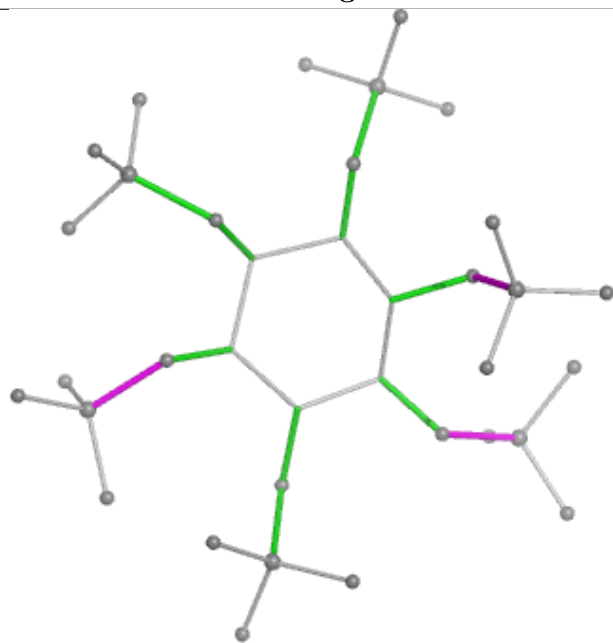
Ligand IHP LA 2501



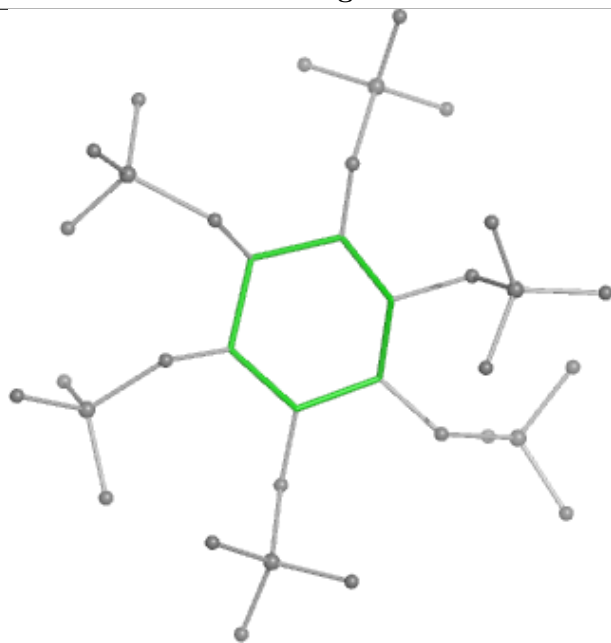
Bond lengths



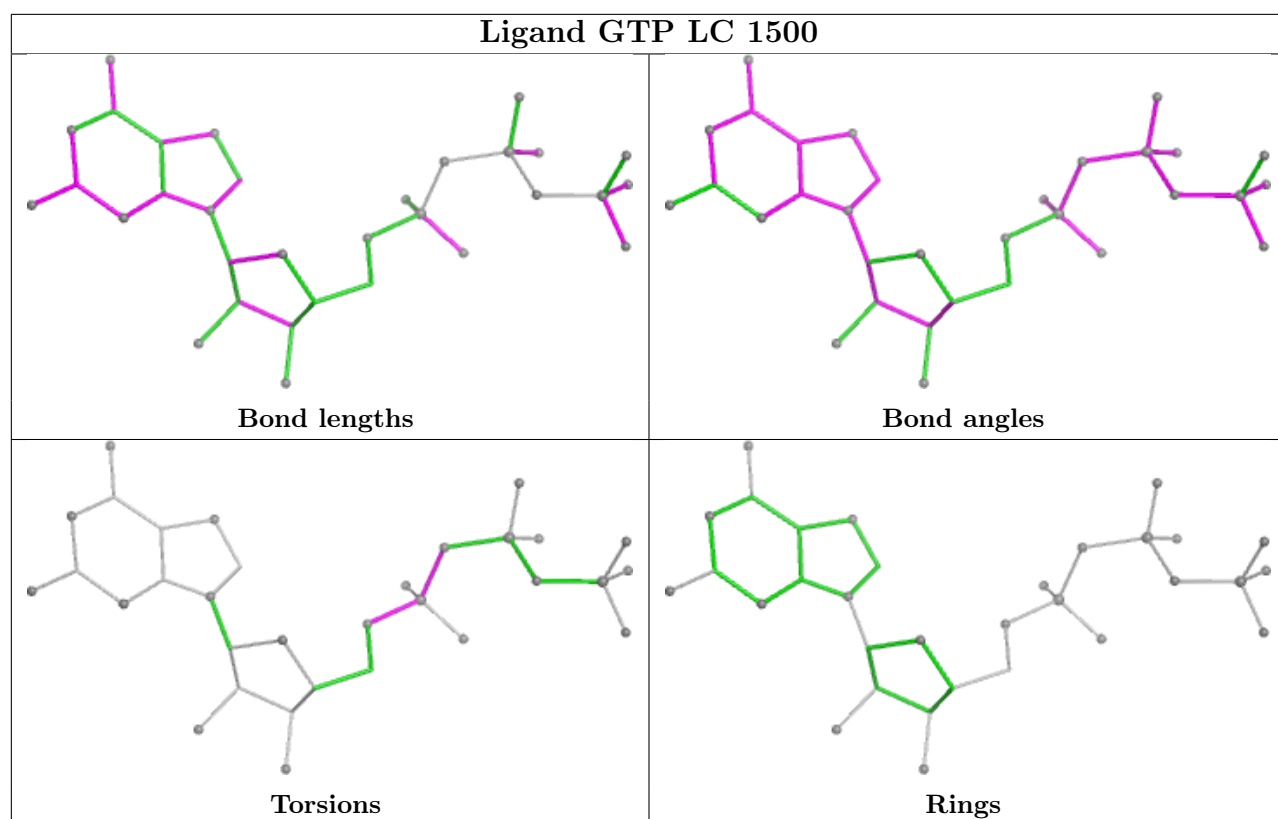
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

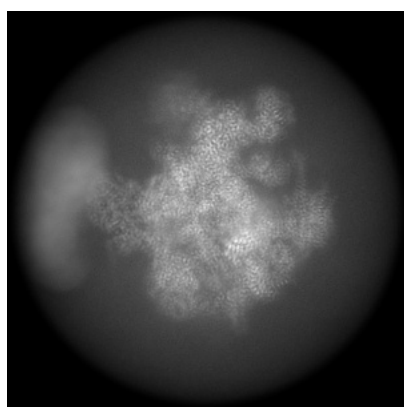
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-52844. These allow visual inspection of the internal detail of the map and identification of artifacts.

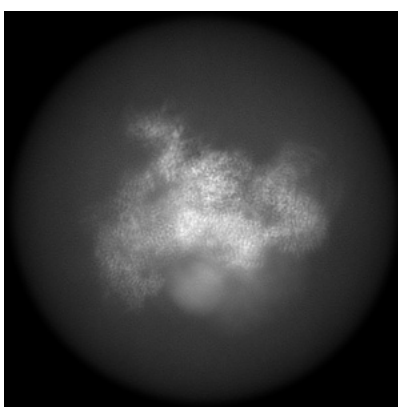
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

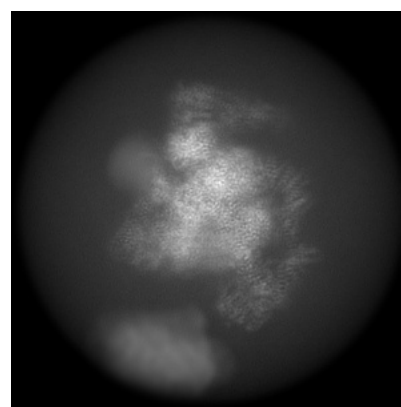
6.1.1 Primary map



X



Y

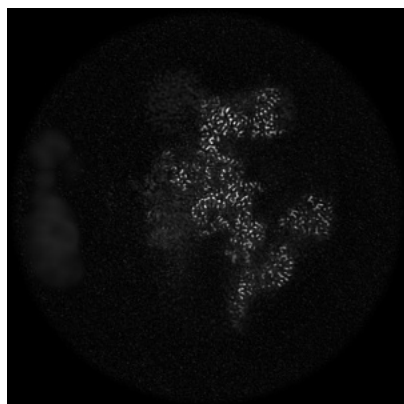


Z

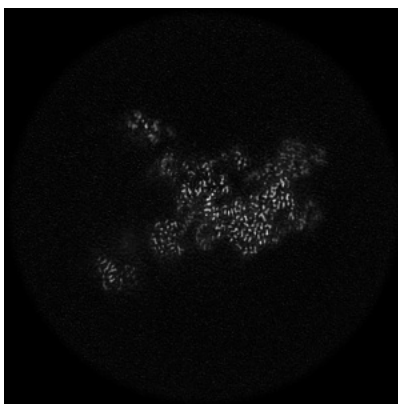
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

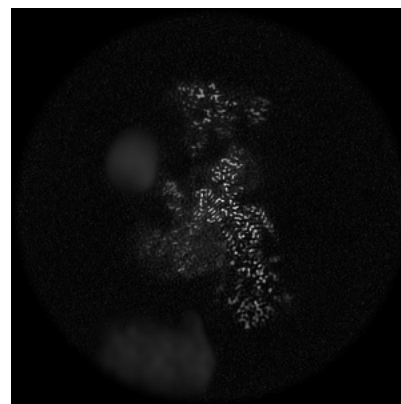
6.2.1 Primary map



X Index: 200



Y Index: 200

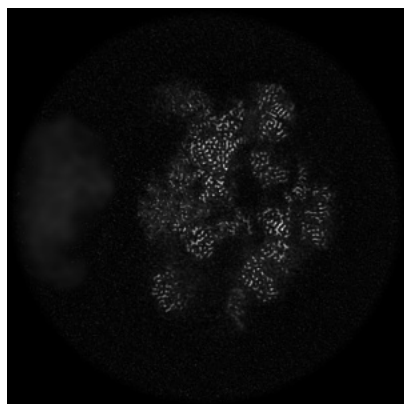


Z Index: 200

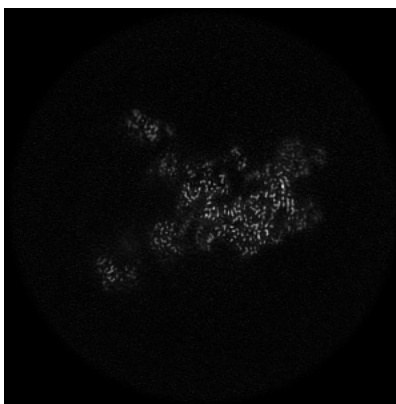
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

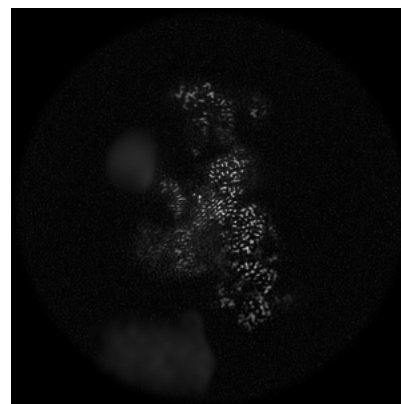
6.3.1 Primary map



X Index: 180



Y Index: 201

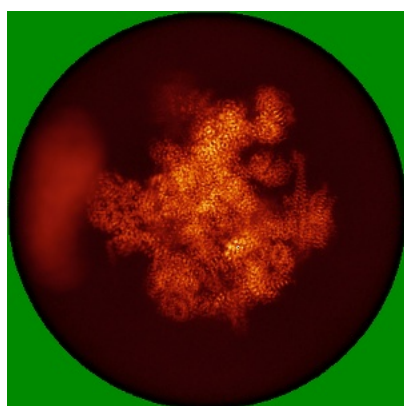


Z Index: 203

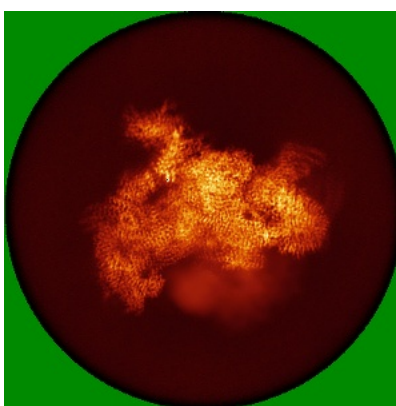
The images above show the largest variance slices of the map in three orthogonal directions.

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

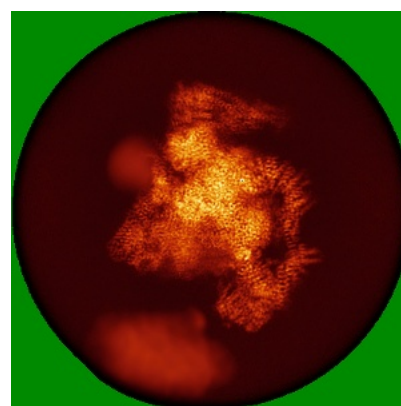
6.4.1 Primary map



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 0.8. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

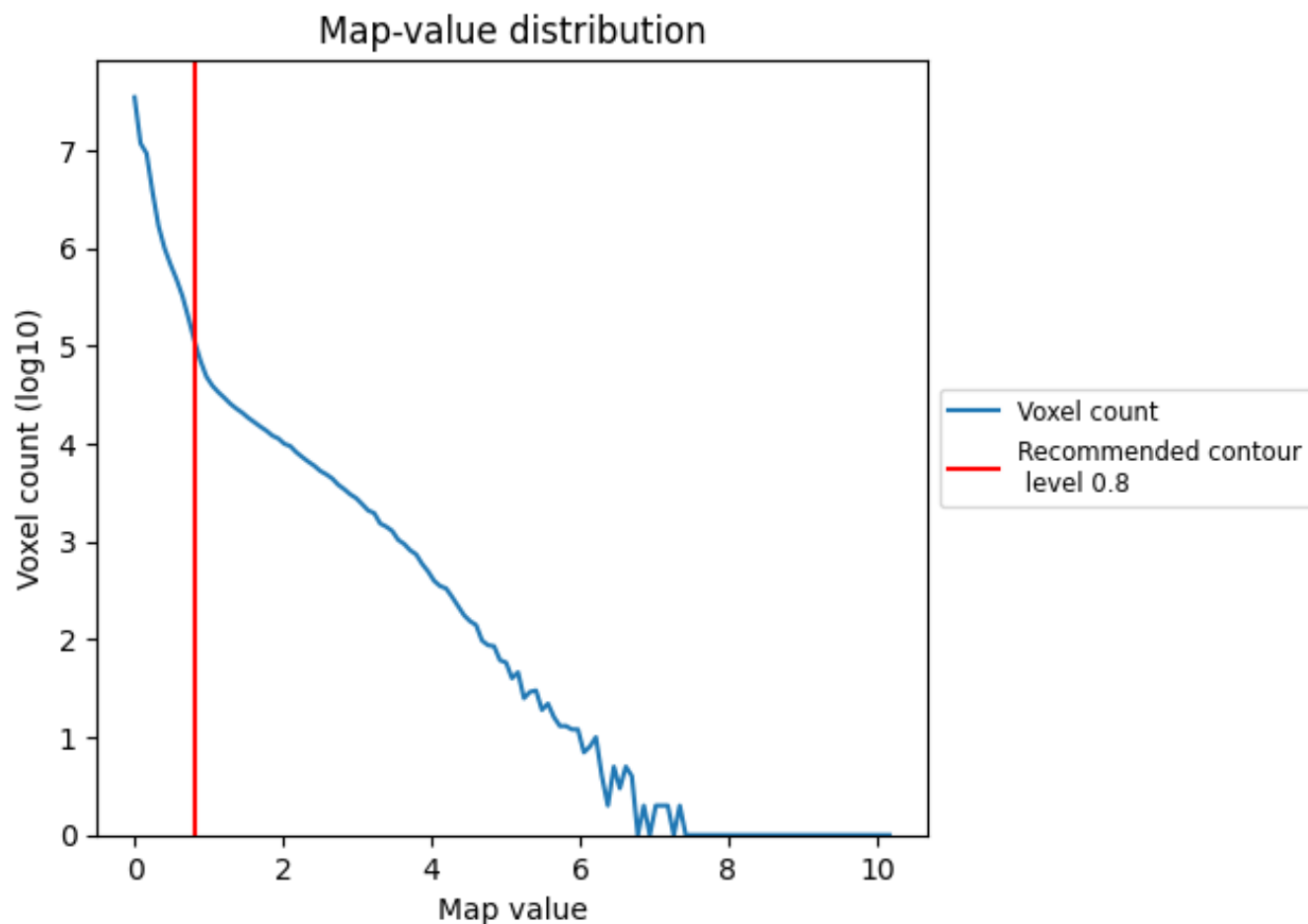
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

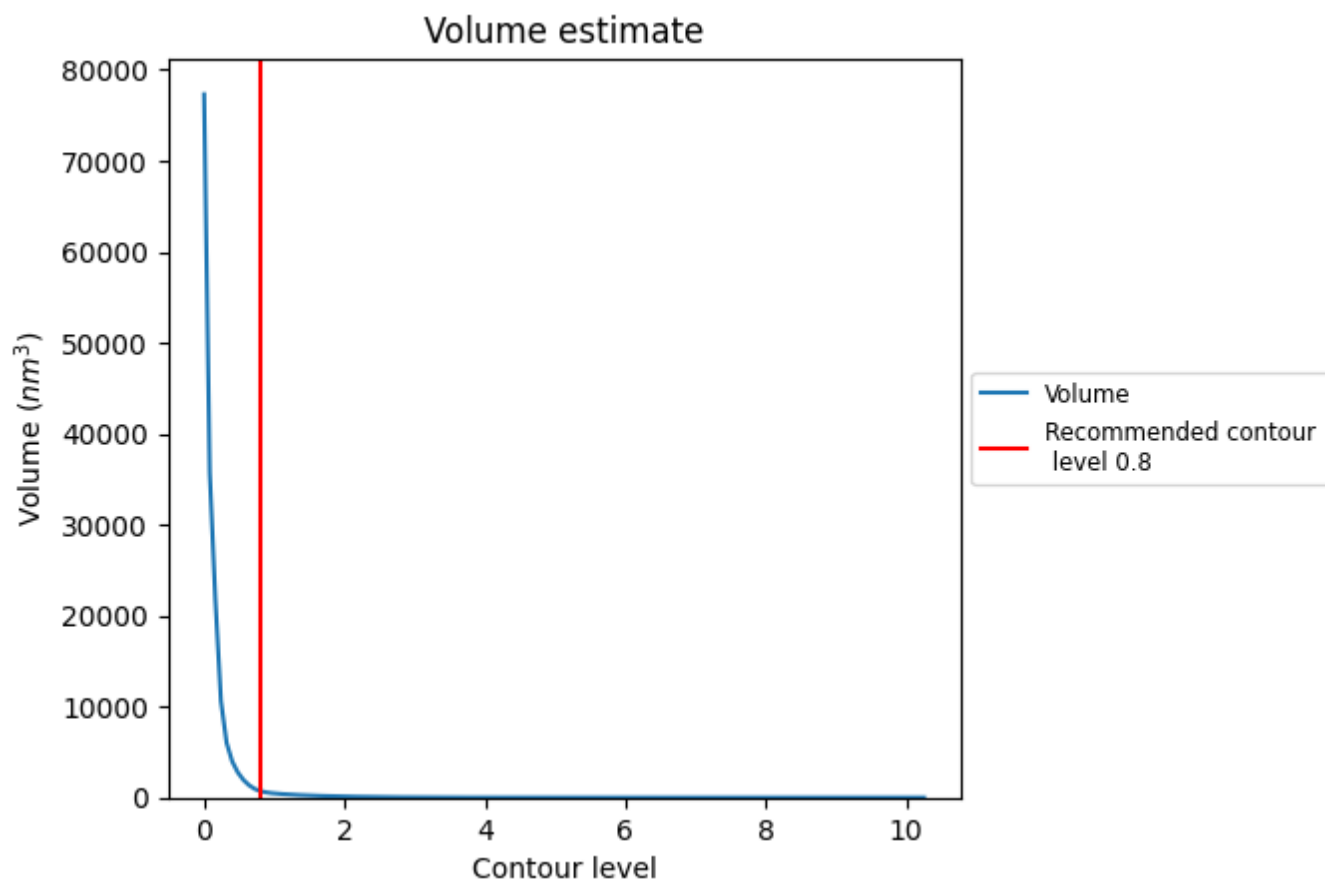
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

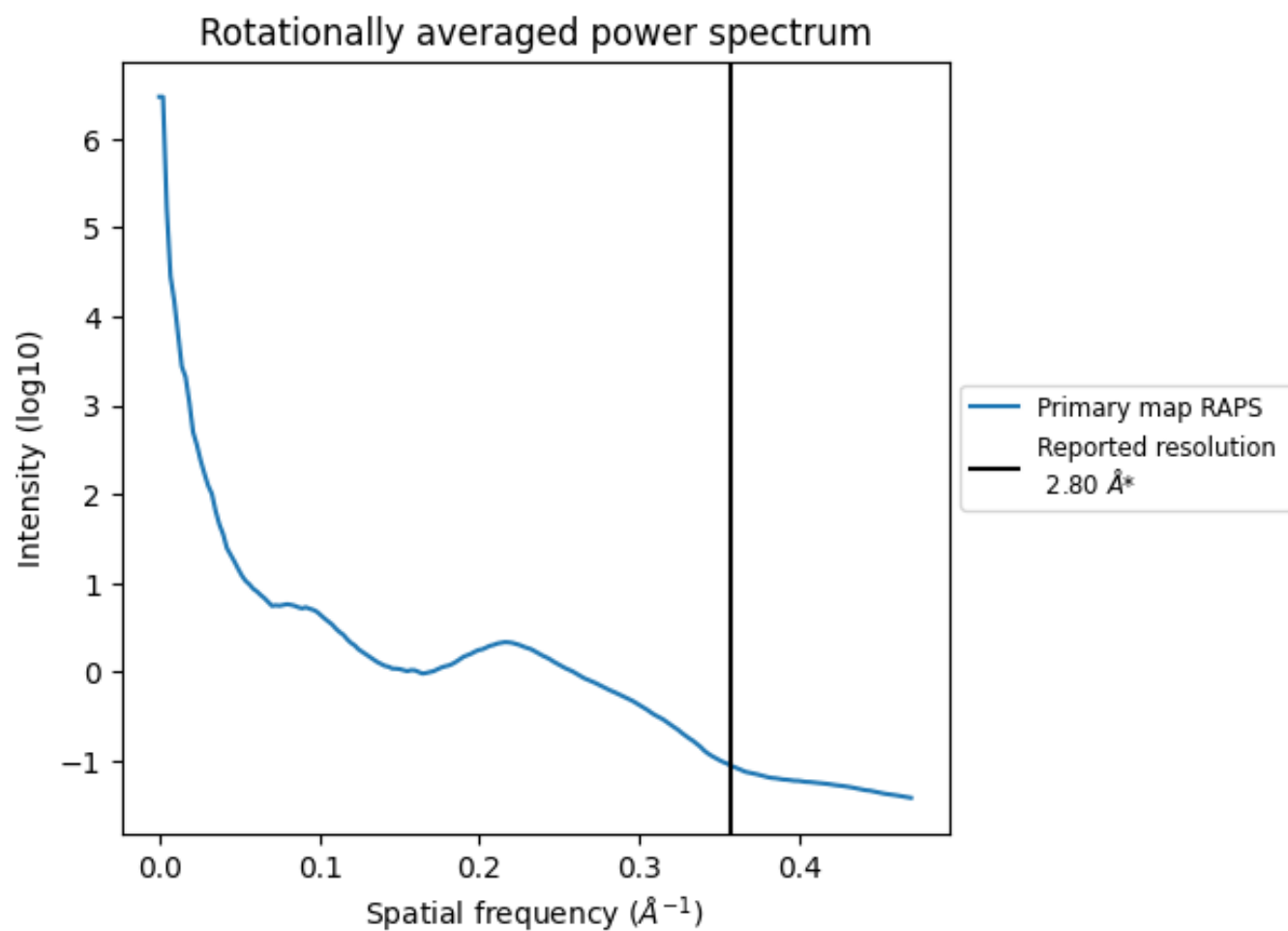
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 717 nm³; this corresponds to an approximate mass of 648 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 ⓘ



*Reported resolution corresponds to spatial frequency of 0.357 Å⁻¹

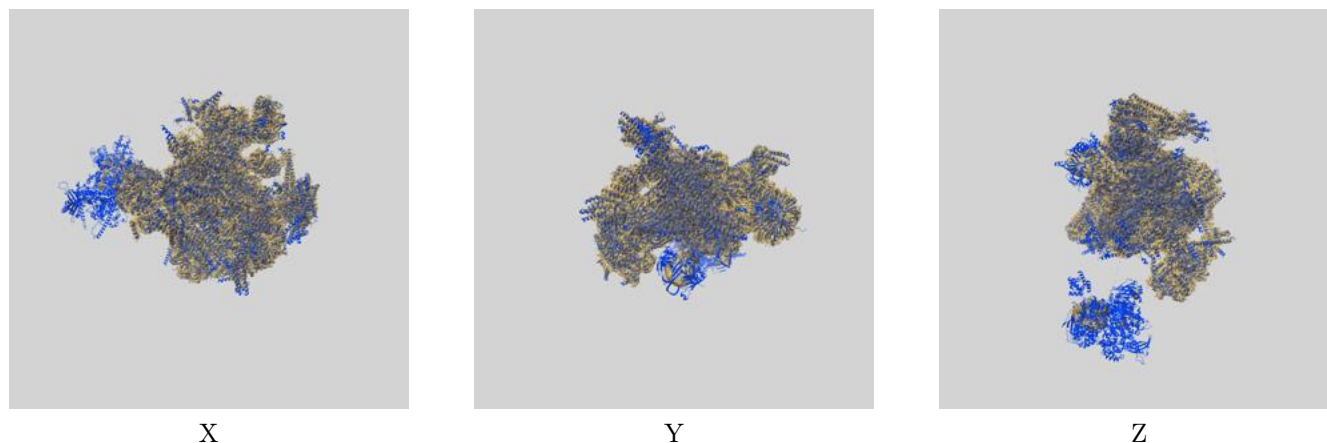
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

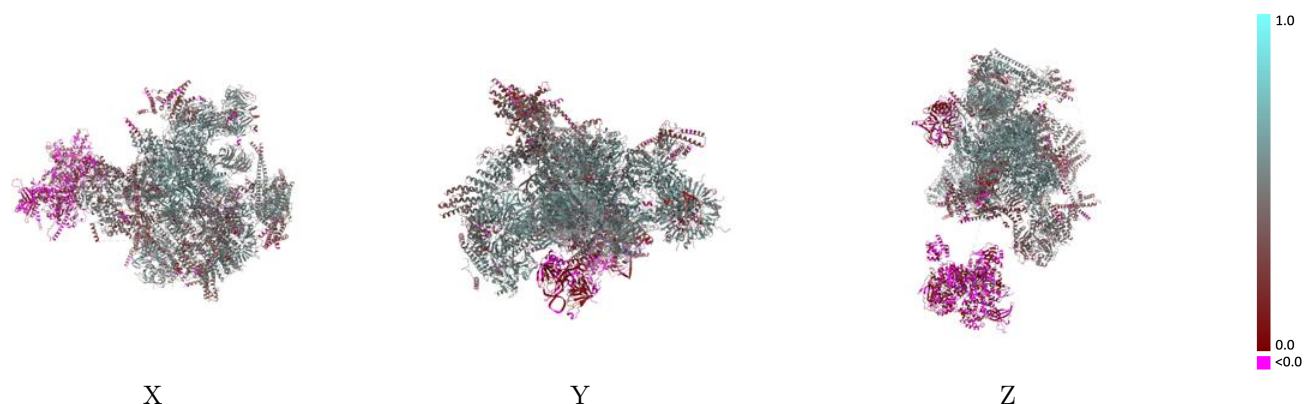
This section contains information regarding the fit between EMDB map EMD-52844 and PDB model 9IF8. Per-residue inclusion information can be found in section 3 on page 18.

9.1 Map-model overlay [i](#)



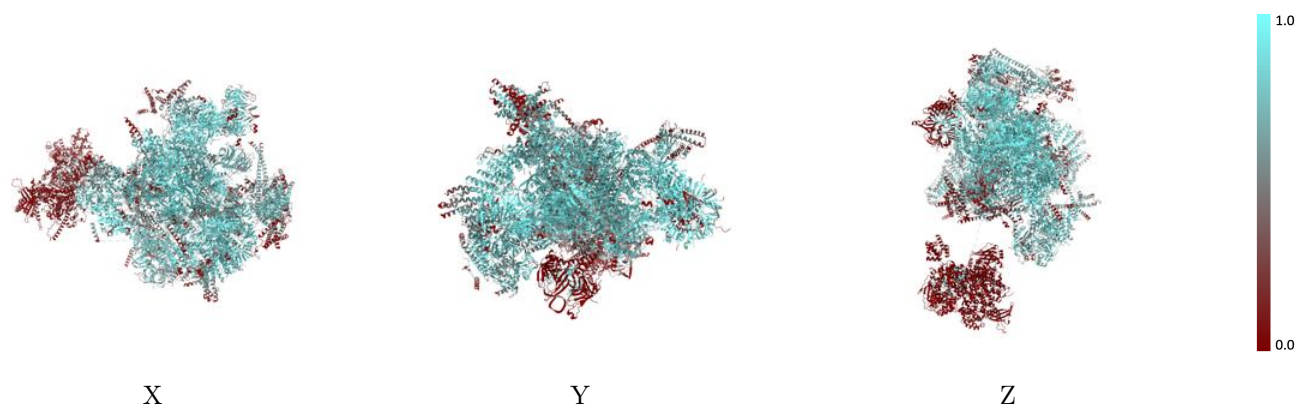
The images above show the 3D surface view of the map at the recommended contour level 0.8 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



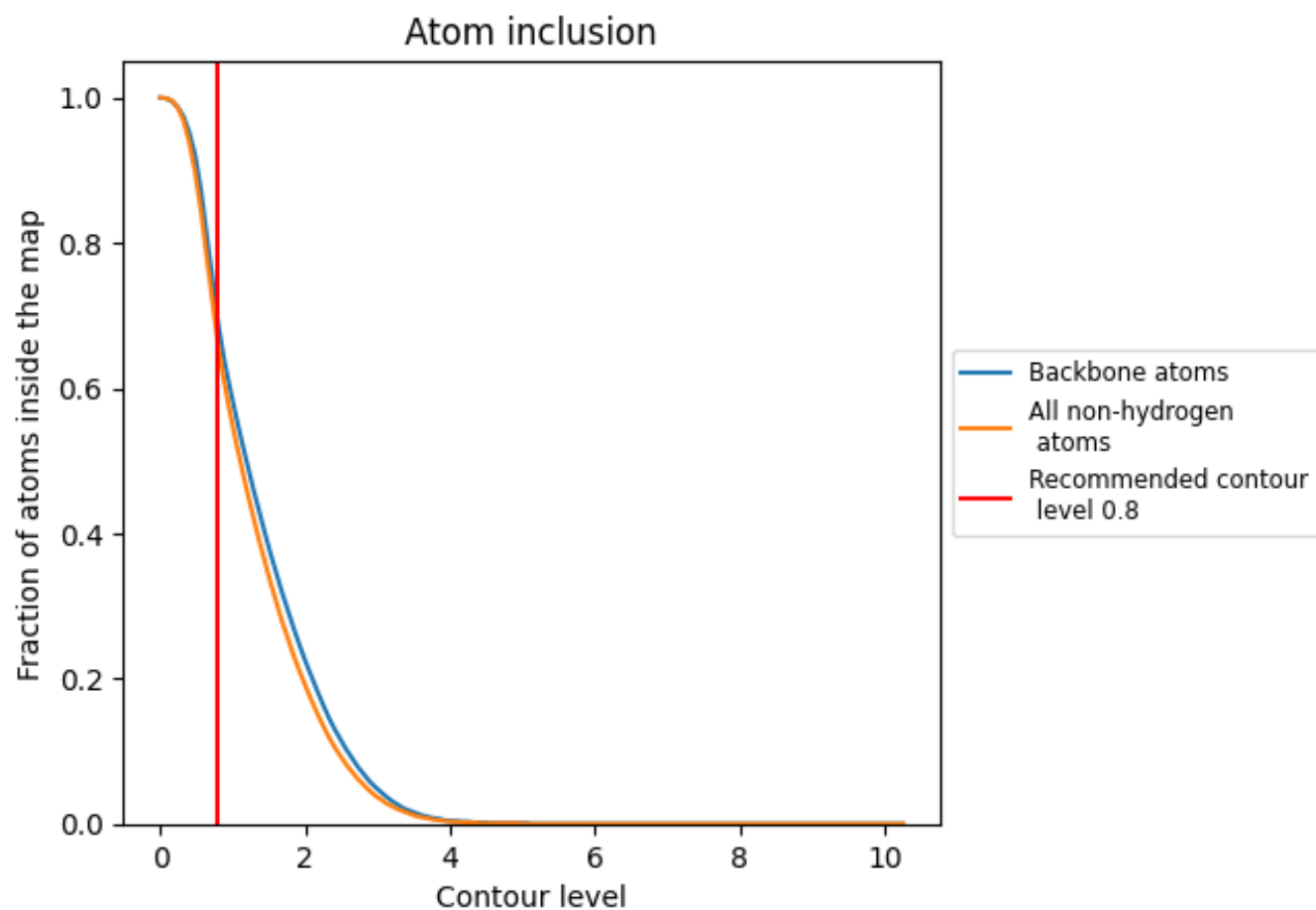
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.8).

9.4 Atom inclusion [i](#)



At the recommended contour level, 69% of all backbone atoms, 66% 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 (0.8) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6580	 0.4220
24	 0.6900	 0.4910
25	 0.6210	 0.4950
2C	 0.7890	 0.5300
2D	 0.8330	 0.5530
2H	 0.7250	 0.5120
2I	 0.6860	 0.4960
2J	 0.6880	 0.5030
51	 0.8080	 0.5000
52	 0.7250	 0.4710
53	 0.8020	 0.5020
5B	 0.6800	 0.4440
5E	 0.7440	 0.4900
5F	 0.7400	 0.5070
5G	 0.7140	 0.4660
62	 0.7770	 0.5080
63	 0.8280	 0.5410
64	 0.8480	 0.5430
65	 0.8280	 0.5410
66	 0.8400	 0.5610
67	 0.8550	 0.5500
A	 0.8330	 0.5500
LA	 0.8110	 0.5070
LB	 0.0440	 0.0120
LC	 0.8340	 0.4960
LD	 0.4750	 0.3610
LE	 0.8610	 0.5200
LF	 0.6600	 0.3540
LG	 0.5870	 0.4800
LH	 0.4050	 0.3260
LJ	 0.8730	 0.5810
LL	 0.8640	 0.5370
LN	 0.7430	 0.4800
LO	 0.6930	 0.2820
LP	 0.7910	 0.5380



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Chain	Atom inclusion	Q-score
LQ	 0.6840	 0.4730
LR	 0.5380	 0.3220
LS	 0.7600	 0.4290
LT	 0.7600	 0.4650
LV	 0.7020	 0.3980
LW	 0.7560	 0.5480
LY	 0.8040	 0.5680
LZ	 0.3480	 0.2910
N2	 0.8540	 0.5510
N5	 0.8740	 0.5390
N6	 0.8860	 0.5400
RN	 0.7540	 0.4370
SA	 0.5310	 0.3640
SC	 0.4950	 0.3840
SD	 0.2580	 0.2880
SF	 0.2570	 0.3750
SJ	 0.7310	 0.4570
SK	 0.7440	 0.4130
SL	 0.7670	 0.5090
SN	 0.8370	 0.5640
SO	 0.8030	 0.5430
SP	 0.3560	 0.3270
SS	 0.6240	 0.4690
ST	 0.6550	 0.4940
SU	 0.5910	 0.4710
SV	 0.3710	 0.3440
SW	 0.5750	 0.4460
TN	 0.3950	 0.2660
U1	 0.1610	 0.0450
U2	 0.1020	 0.0050
U3	 0.1550	 0.0230
UB	 0.2060	 0.0450
UE	 0.2270	 0.0300
UF	 0.1410	 0.0020
UG	 0.2640	 0.0300
UX	 0.5520	 0.3630