



Full wwPDB EM Validation Report ⓘ

Dec 21, 2024 – 01:11 PM EST

PDB ID : 9DTR
EMDB ID : EMD-47157
Title : Structure of the yeast post-catalytic P complex spliceosome at 2.3 Angstrom resolution
Authors : Wilkinson, M.E.; Hoskins, A.A.
Deposited on : 2024-10-01
Resolution : 2.31 Å(reported)
Based on initial model : 6EXN

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

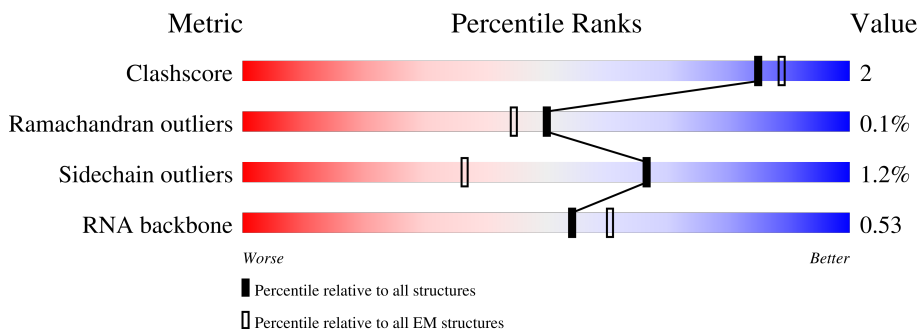
EMDB validation analysis : 0.0.1.dev113
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.40

1 Overall quality at a glance

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

The reported resolution of this entry is 2.31 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	2	1175	
2	5	214	
3	6	112	
4	A	2413	
5	C	1008	
6	D	173	
7	E	42	

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Mol	Chain	Length	Quality of chain
8	G	235	12% 12% 88%
9	H	577	58% 70% 9% 20%
10	I	95	23% 28% 17% 49%
11	J	451	15% 80% 5% 14%
12	K	379	12% 42% 55%
13	L	157	11% 99%
14	M	339	28% 72% 25%
15	N	364	45% 69% 27%
16	O	590	42% 69% 28%
17	P	175	10% 41% 58%
18	R	135	49% 61% 6% 33%
19	S	687	61% 79% 9% 12%
20	T	859	82% 74% 8% 18%
21	V	1145	64% 64% 33%
22	W	238	71% 67% 29%
23	Y	111	77% 73% 5% 23%
24	Z	140	38% 35% 62%
25	a	251	29% 68% 31%
26	b	196	46% 45% 54%
26	k	196	53% 53% 47%
27	c	382	30% 57% 42%
28	d	101	80% 80% 20%
28	n	101	79% 79% 21%
29	e	94	91% 85% 6% 9%
29	p	94	88% 88% 12%

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Mol	Chain	Length	Quality of chain
30	f	86	86% 83% 14%
30	q	86	86% 85% 14%
31	g	77	92% 91% 8%
31	r	77	91% 91% 9%
32	h	146	73% 73% 27%
32	l	146	73% 72% 27%
33	j	110	83% 83% 17%
33	m	110	83% 81% 17%
34	o	455	43% 76% 24%
35	s	175	100% 100%
36	t	503	26% 26% 74%
36	u	503	26% 26% 74%
36	v	503	26% 26% 74%
36	w	503	26% 26% 74%
37	y	215	37% 66% 34%

2 Entry composition

There are 43 unique types of molecules in this entry. The entry contains 91230 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called U2 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	2	132	2779	1242	456	949	132	0	0

- Molecule 2 is a RNA chain called U5 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	5	173	3671	1642	638	1218	173	0	0

- Molecule 3 is a RNA chain called U6 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	6	102	2170	972	386	710	102	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	A	1950	16079	10335	2766	2919	59	0	0

- Molecule 5 is a protein called Pre-mRNA-splicing factor SNU114.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	C	879	7040	4551	1173	1289	27	0	0

- Molecule 6 is a protein called Protein FYV6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	D	108	914	573	168	172	1	0	0

- Molecule 7 is a RNA chain called UBC4 mRNA spliced exons.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
7	E	33	703	315	126	229	33	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	21	G	C	conflict	GB NM_001178430
E	22	C	A	conflict	GB NM_001178430

- Molecule 8 is a protein called Pre-mRNA-splicing factor ISY1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
8	G	28	139	83	28	28	0	0

- Molecule 9 is a protein called Pre-mRNA-splicing factor CWC22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	H	460	3762	2415	622	707	18	0	0

- Molecule 10 is a RNA chain called UBC4 lariat-intron.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
10	I	48	1012	455	172	337	48	0	0

- Molecule 11 is a protein called Pre-mRNA-splicing factor PRP46.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	J	386	2990	1887	530	562	11	0	0

- Molecule 12 is a protein called Pre-mRNA-processing protein 45.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	K	170	1355	847	249	254	5	0	0

- Molecule 13 is a protein called Pre-mRNA-splicing factor BUD31.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	L	156	1283	803	239	231	10	0	0

- Molecule 14 is a protein called Pre-mRNA-splicing factor CWC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	M	255	2048	1297	362	378	11	0	0

- Molecule 15 is a protein called Pre-mRNA-splicing factor SLT11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	N	264	2092	1331	364	382	15	0	0

- Molecule 16 is a protein called Pre-mRNA-splicing factor CEF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	O	424	2918	1805	546	560	7	0	0

- Molecule 17 is a protein called Pre-mRNA-splicing factor CWC15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	P	74	607	382	120	104	1	0	0

- Molecule 18 is a protein called Pre-mRNA-splicing factor CWC21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	R	91	510	305	101	103	1	0	0

- Molecule 19 is a protein called Pre-mRNA-splicing factor CLF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	S	604	4683	2996	818	855	14	0	0

- Molecule 20 is a protein called Pre-mRNA-splicing factor SYF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	T	707	5543	3563	922	1038	20	0	0

- Molecule 21 is a protein called Pre-mRNA-splicing factor ATP-dependent RNA helicase PRP22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	V	764	6096	3860	1061	1145	30	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
V	635	ALA	SER	engineered mutation	UNP P24384

- Molecule 22 is a protein called U2 small nuclear ribonucleoprotein A'.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	W	170	1383	866	253	257	7	0	0

- Molecule 23 is a protein called U2 small nuclear ribonucleoprotein B'.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	Y	86	697	448	122	124	3	0	0

- Molecule 24 is a protein called Pre-mRNA-splicing factor NTC20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	Z	53	424	262	77	82	3	0	0

- Molecule 25 is a protein called Pre-mRNA-splicing factor 18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	a	172	1380	884	245	247	4	0	0

- Molecule 26 is a protein called Small nuclear ribonucleoprotein-associated protein B.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	b	90	Total	C	N	O	S	0	0
			725	461	131	130	3		
26	k	104	Total	C	N	O	S	0	0
			843	533	157	150	3		

- Molecule 27 is a protein called Pre-mRNA-splicing factor SLU7.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	c	223	Total	C	N	O	S	0	0
			1893	1183	344	358	8		

- Molecule 28 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	d	81	Total	C	N	O	S	0	0
			624	398	107	117	2		
28	n	80	Total	C	N	O	S	0	0
			615	392	105	116	2		

- Molecule 29 is a protein called Small nuclear ribonucleoprotein E.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	e	86	Total	C	N	O	S	0	0
			665	432	106	124	3		
29	p	83	Total	C	N	O	S	0	0
			646	420	102	121	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
30	f	74	Total	C	N	O	S	0	0
			592	381	103	107	1		
30	q	74	Total	C	N	O	S	0	0
			592	381	103	107	1		

- Molecule 31 is a protein called Small nuclear ribonucleoprotein G.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	g	71	Total	C	N	O	S	0	0
			551	348	96	105	2		
31	r	70	Total	C	N	O	S	0	0
			544	344	95	103	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
32	h	107	Total	C	N	O	S	0	0
			826	522	145	157	2		
32	l	107	Total	C	N	O	S	0	0
			826	522	145	157	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
33	j	91	Total	C	N	O	S	0	0
			747	478	135	130	4		
33	m	91	Total	C	N	O	S	0	0
			747	478	135	130	4		

- Molecule 34 is a protein called Pre-mRNA-processing factor 17.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	o	348	Total	C	N	O	S	0	0
			2821	1794	501	517	9		

- Molecule 35 is a protein called Pre-mRNA-splicing factor SNT309.

Mol	Chain	Residues	Atoms				AltConf	Trace
35	s	175	Total	C	N	O	0	0
			870	519	175	176		

- Molecule 36 is a protein called Pre-mRNA-processing factor 19.

Mol	Chain	Residues	Atoms				AltConf	Trace
36	t	132	Total	C	N	O	0	0
			658	394	132	132		
36	u	132	Total	C	N	O	0	0
			658	394	132	132		
36	v	132	Total	C	N	O	0	0
			658	394	132	132		
36	w	132	Total	C	N	O	0	0
			658	394	132	132		

- Molecule 37 is a protein called Pre-mRNA-splicing factor SYF2.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	y	141	Total	C	N	O	S	0	0
			1075	667	198	209	1		

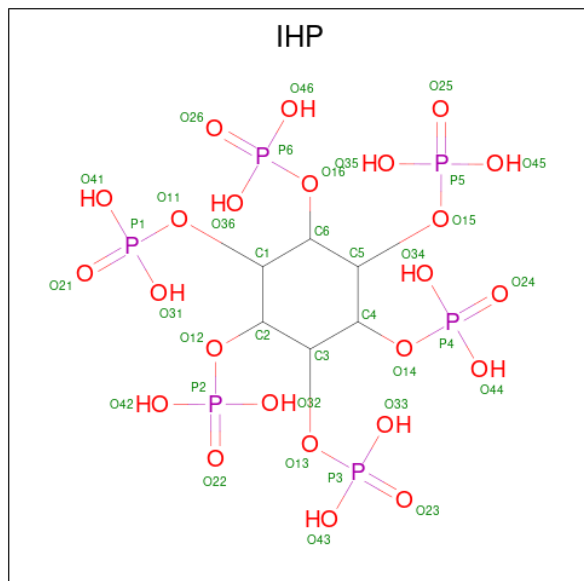
- Molecule 38 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
38	6	1	Total	Mg	0
			1	1	
38	C	1	Total	Mg	0
			1	1	

- Molecule 39 is POTASSIUM ION (three-letter code: K) (formula: K).

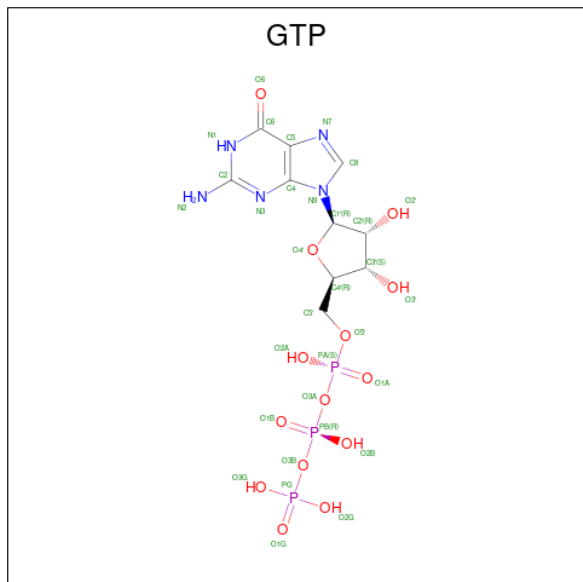
Mol	Chain	Residues	Atoms		AltConf
39	6	3	Total	K	0
			3	3	
39	E	1	Total	K	0
			1	1	

- Molecule 40 is INOSITOL HEXAKISPHOSPHATE (three-letter code: IHP) (formula: C₆H₁₈O₂₄P₆).



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

- Molecule 41 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



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

- Molecule 42 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
42	L	3	3	3	0
42	M	1	1	1	0
42	N	2	2	2	0
42	c	1	1	1	0

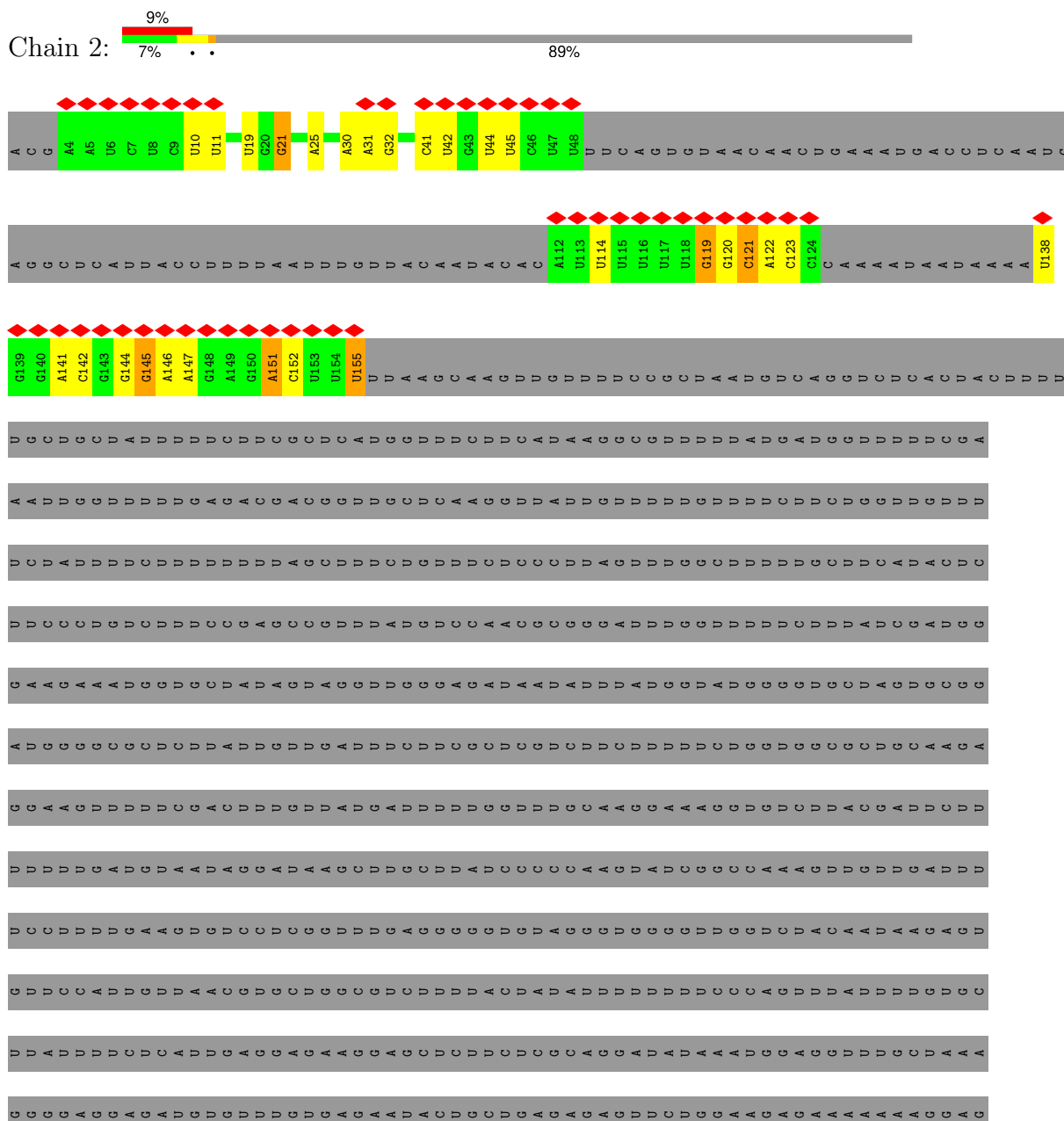
- Molecule 43 is water.

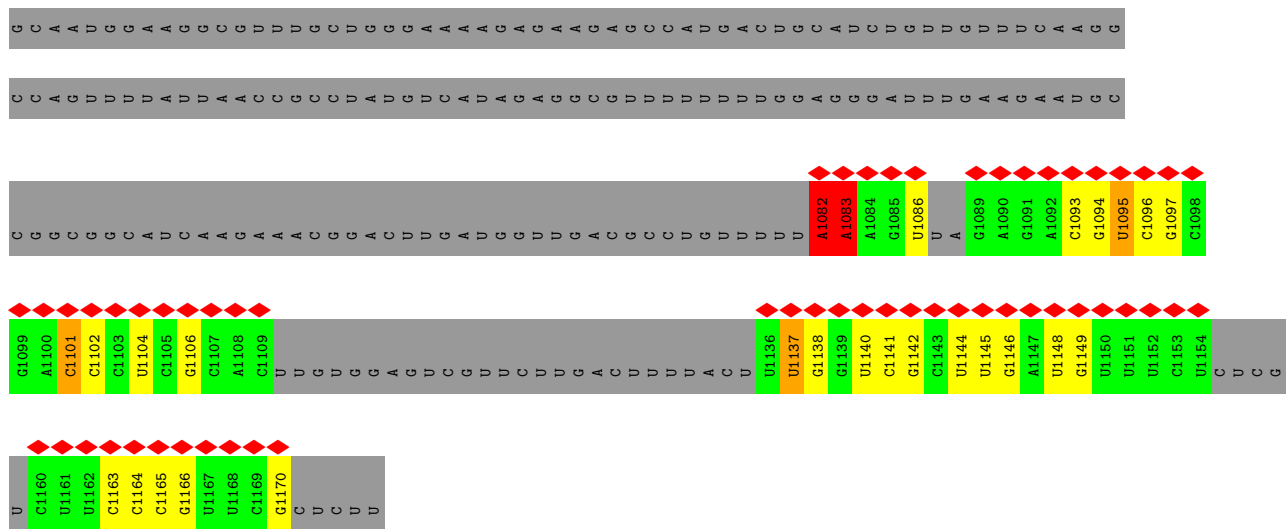
Mol	Chain	Residues	Atoms		AltConf
			Total	O	
43	6	1	1	1	0

3 Residue-property plots [i](#)

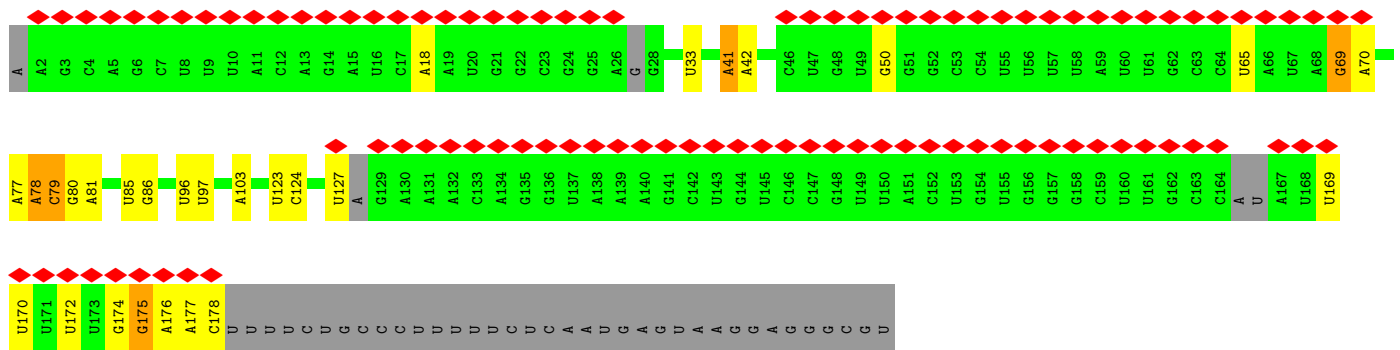
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: U2 snRNA

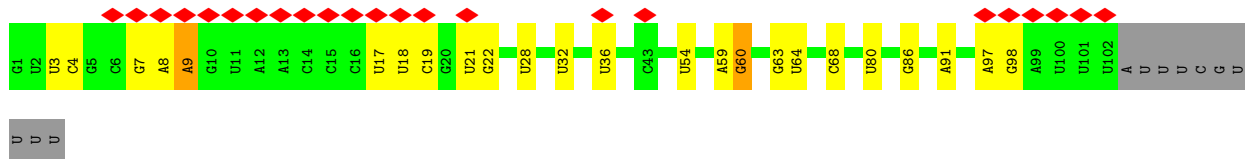




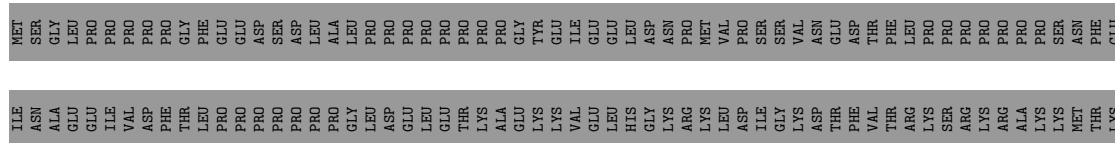
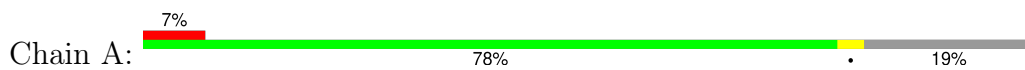
• Molecule 2: U5 snRNA

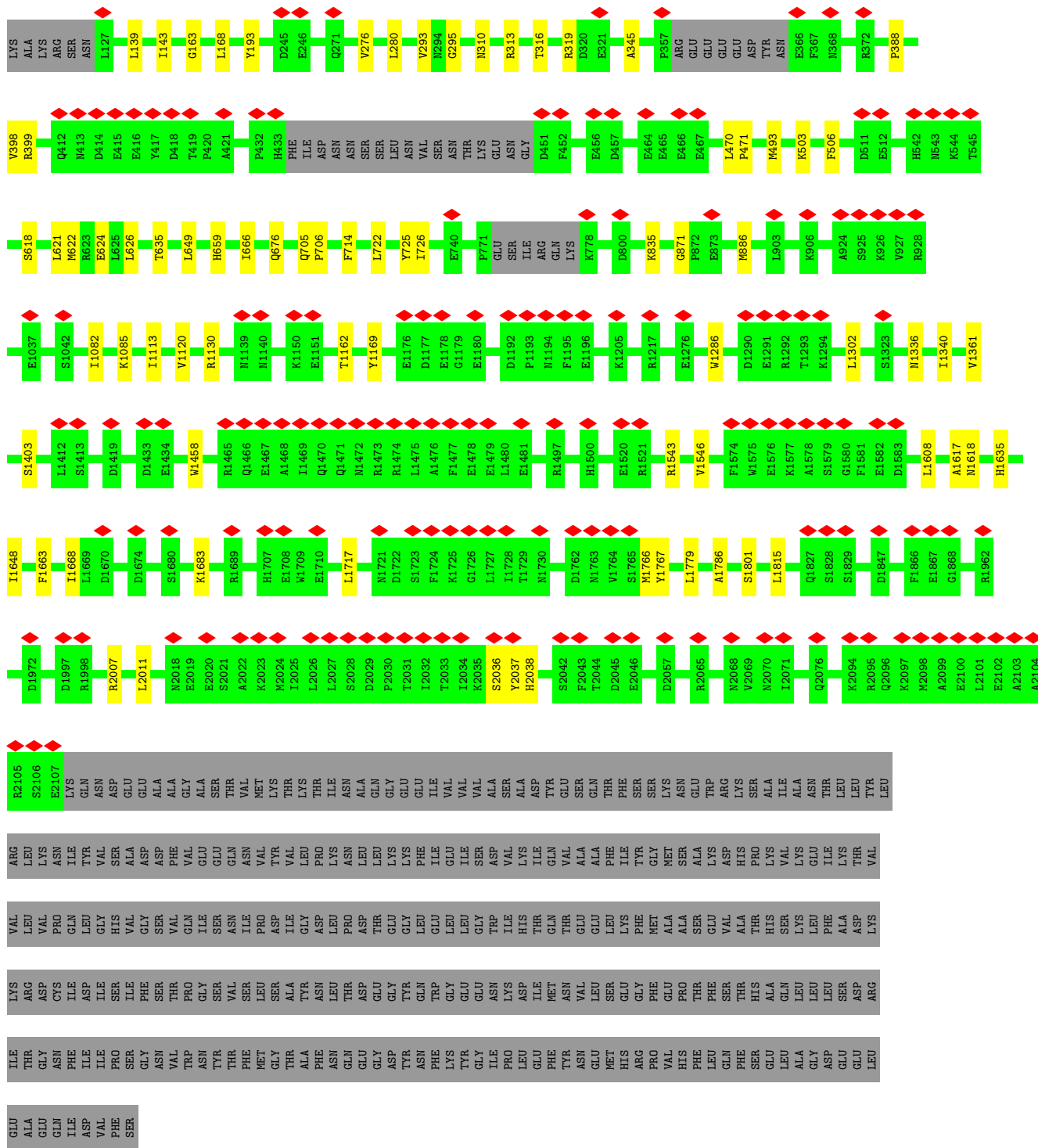


• Molecule 3: U6 snRNA

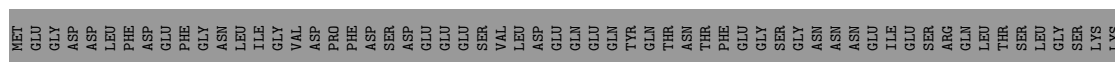
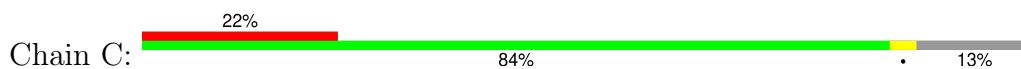


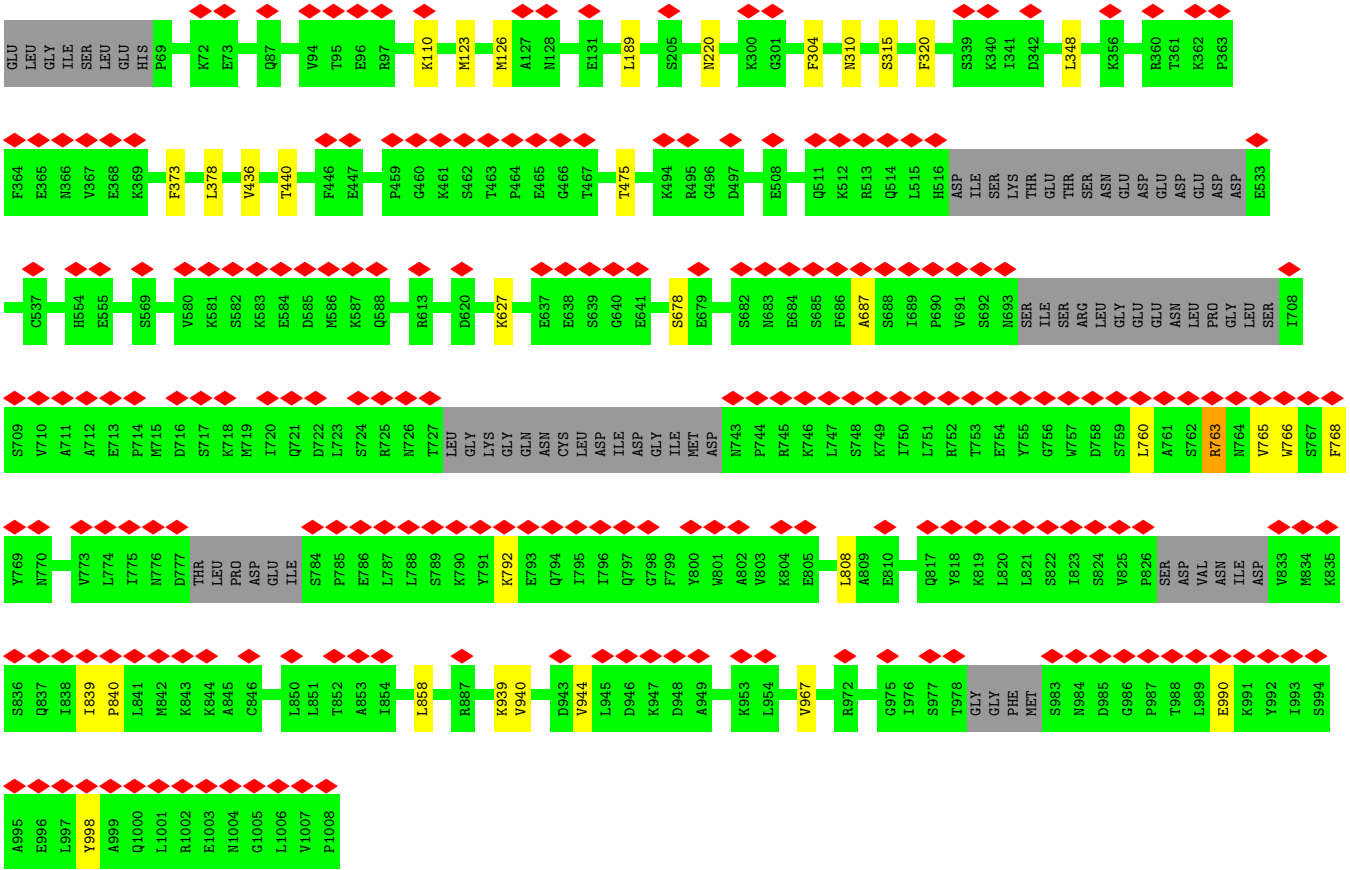
• Molecule 4: Pre-mRNA-splicing factor 8



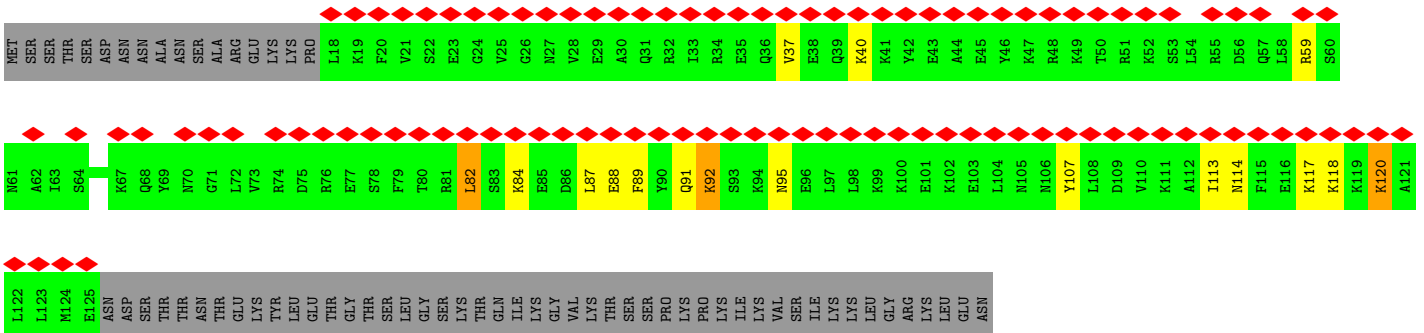


● Molecule 5: Pre-mRNA-splicing factor SNU114

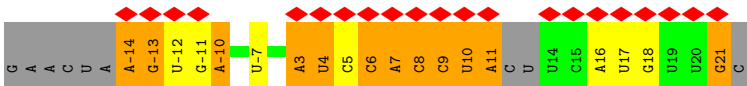
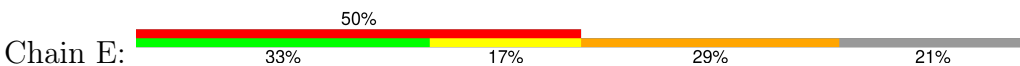




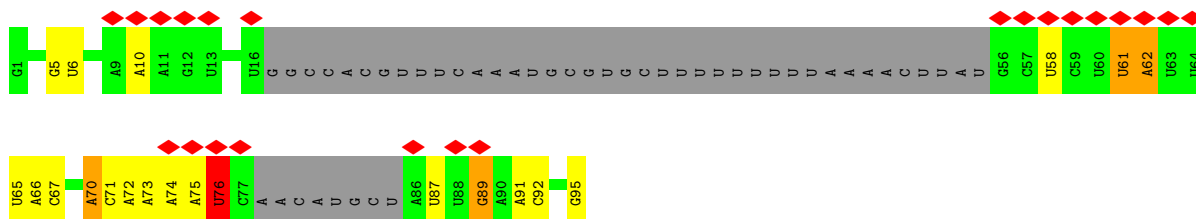
• Molecule 6: Protein FYV6



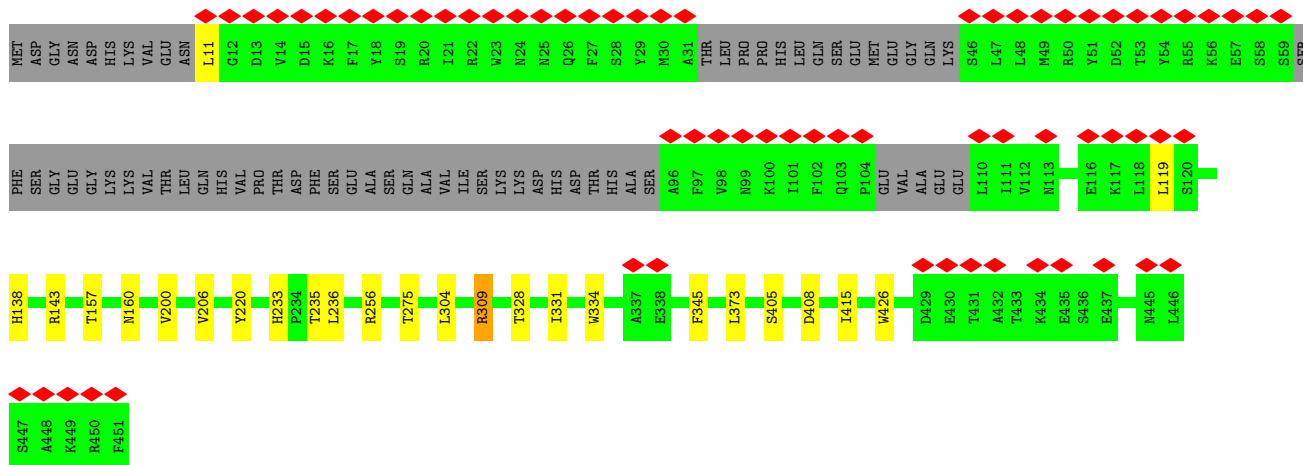
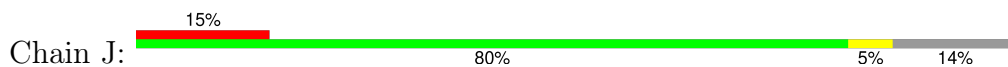
• Molecule 7: UBC4 mRNA spliced exons



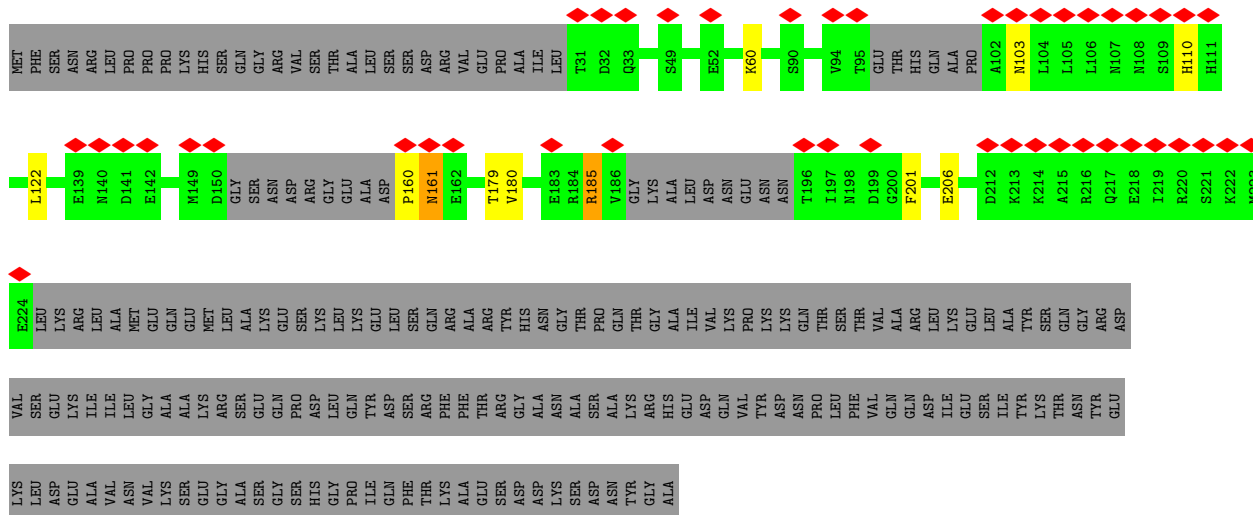
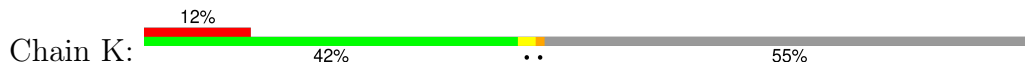
• Molecule 8: Pre-mRNA-splicing factor ISY1



• Molecule 11: Pre-mRNA-splicing factor PRP46

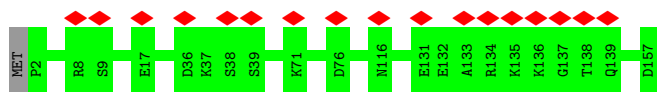


• Molecule 12: Pre-mRNA-processing protein 45

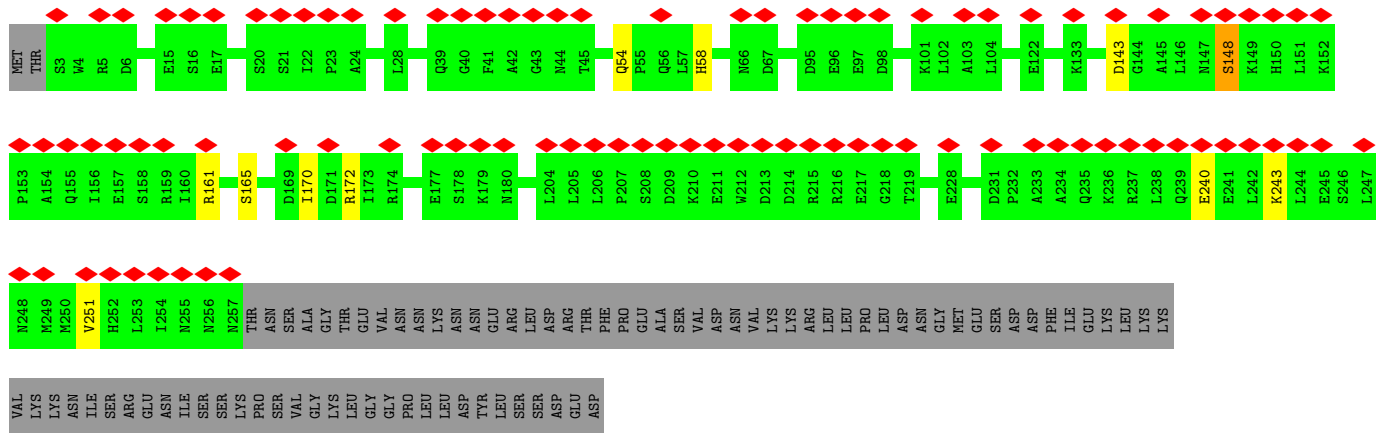


• Molecule 13: Pre-mRNA-splicing factor BUD31

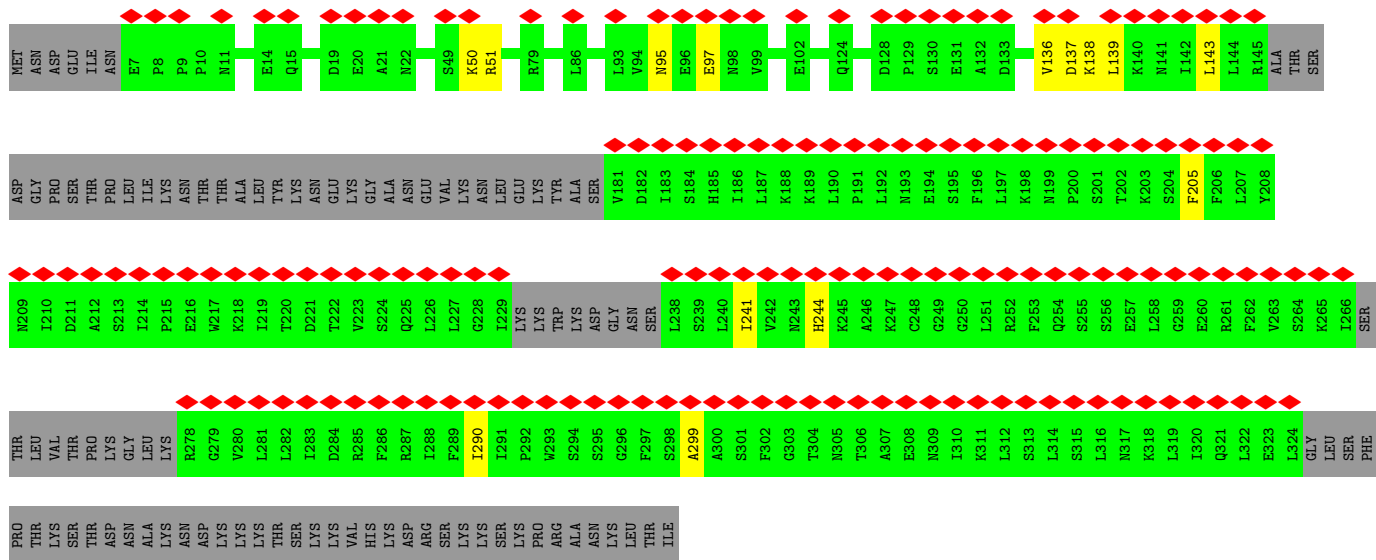
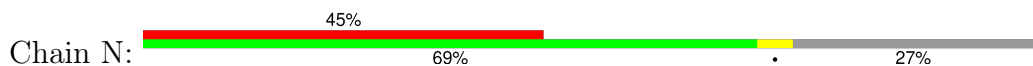




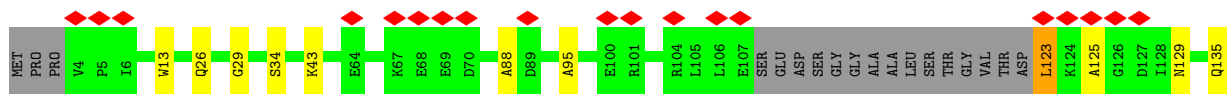
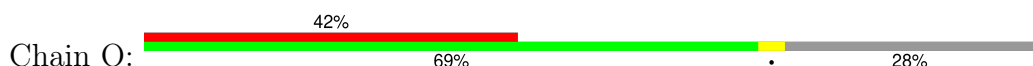
• Molecule 14: Pre-mRNA-splicing factor CWC2

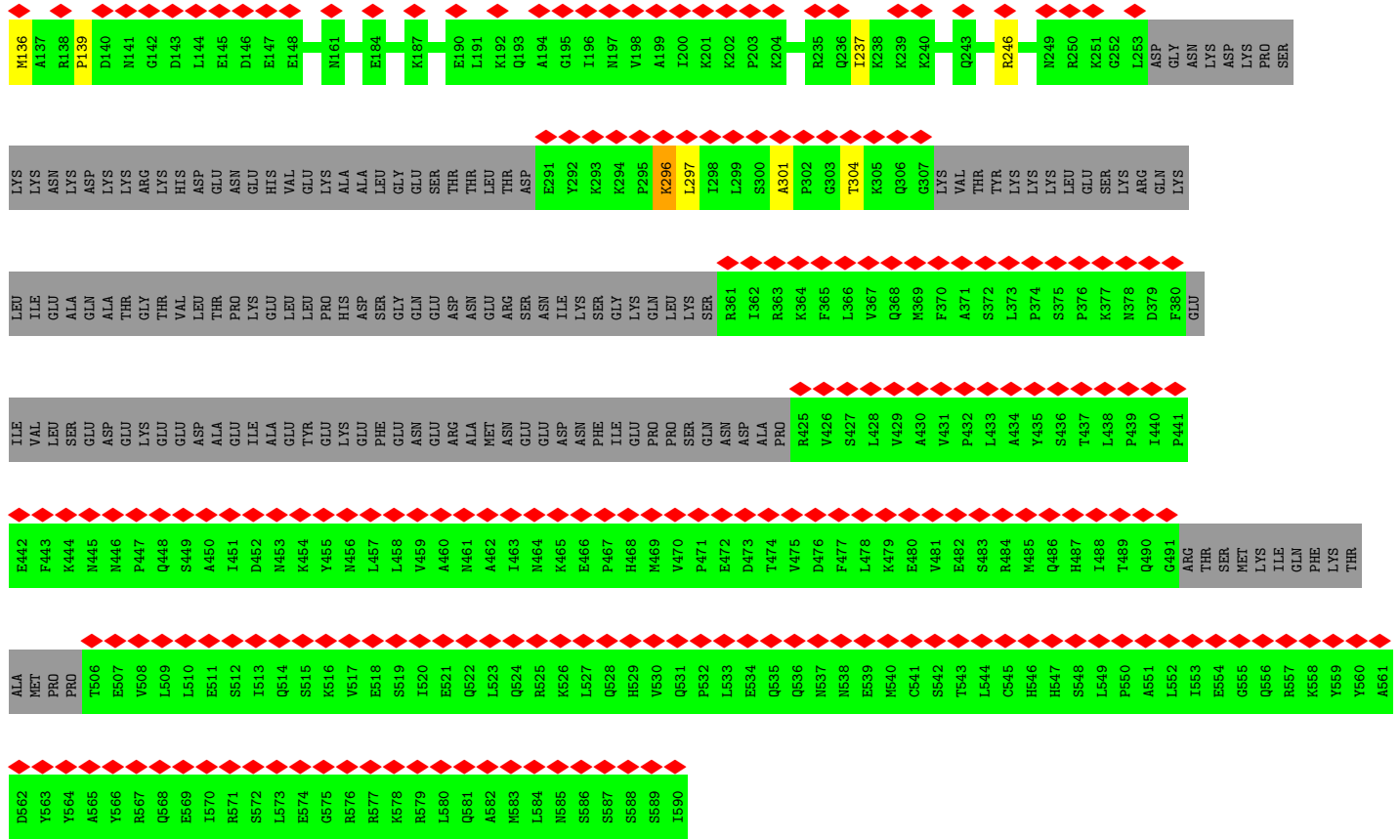


• Molecule 15: Pre-mRNA-splicing factor SLT11

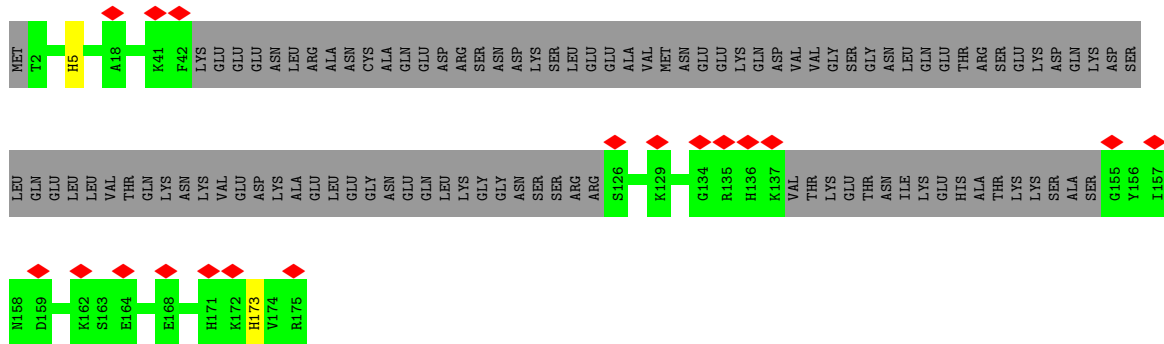


• Molecule 16: Pre-mRNA-splicing factor CEF1



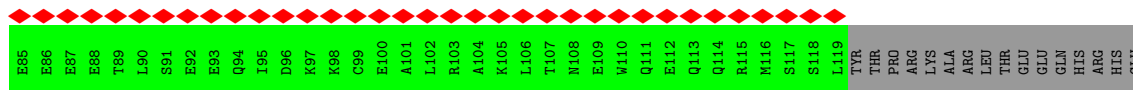


● Molecule 17: Pre-mRNA-splicing factor CWC15

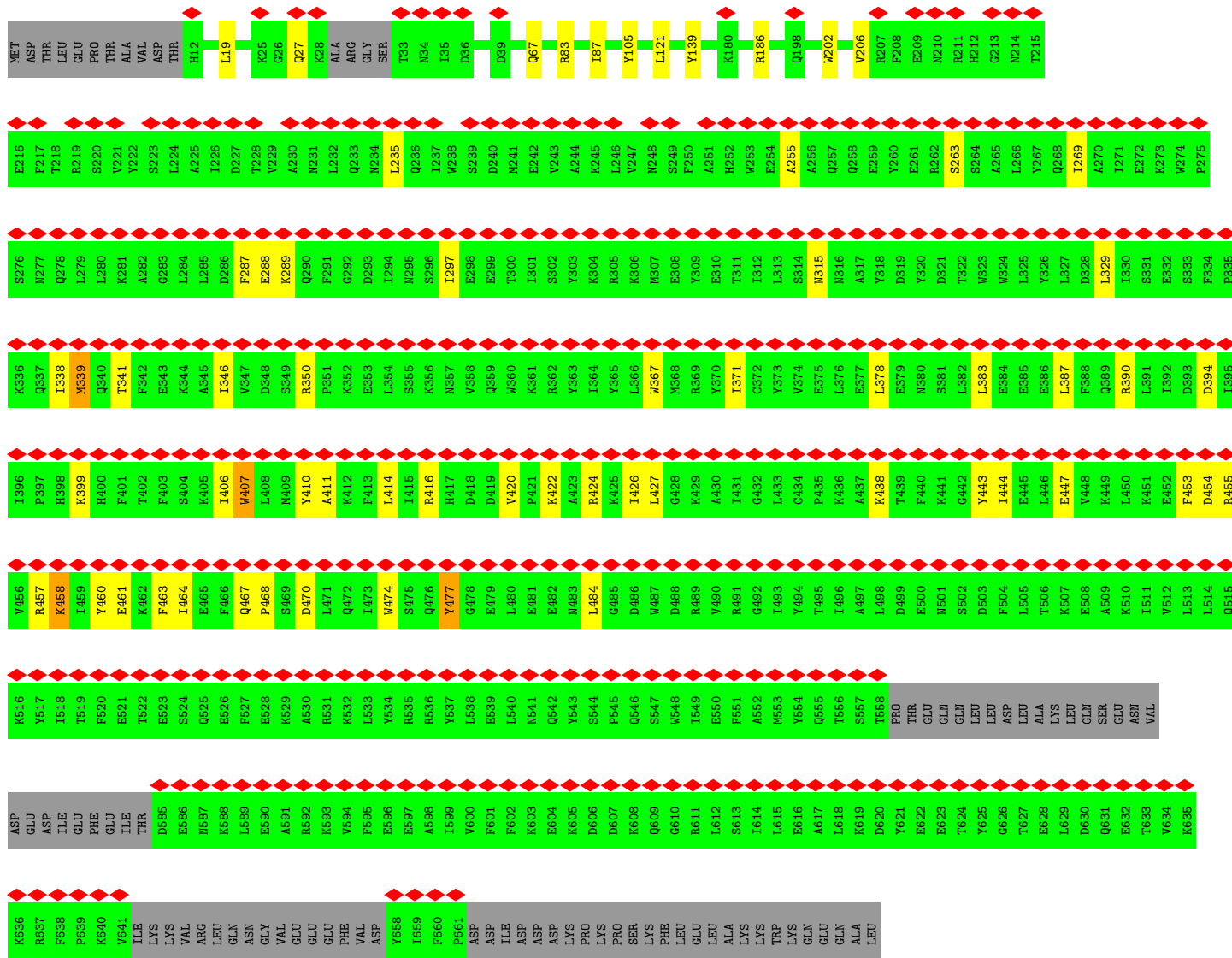
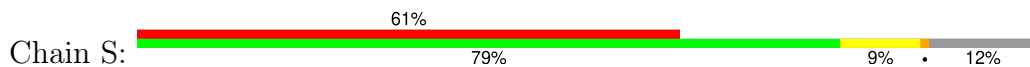


● Molecule 18: Pre-mRNA-splicing factor CWC21

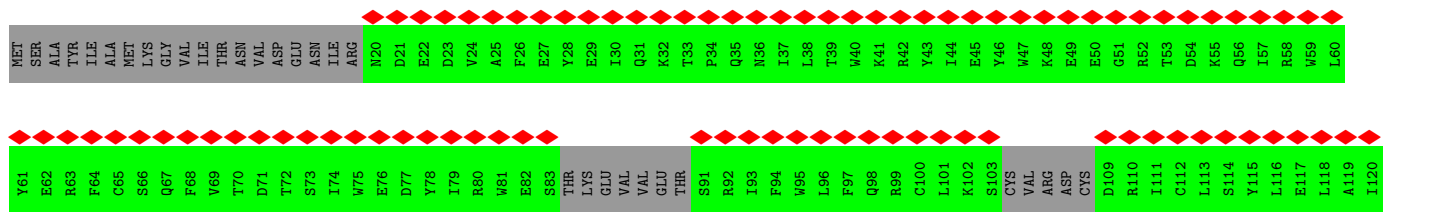
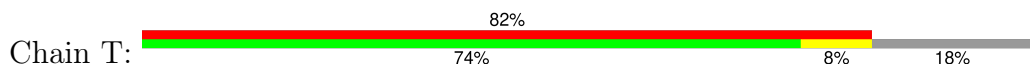




• Molecule 19: Pre-mRNA-splicing factor CLF1



• Molecule 20: Pre-mRNA-splicing factor SYF1

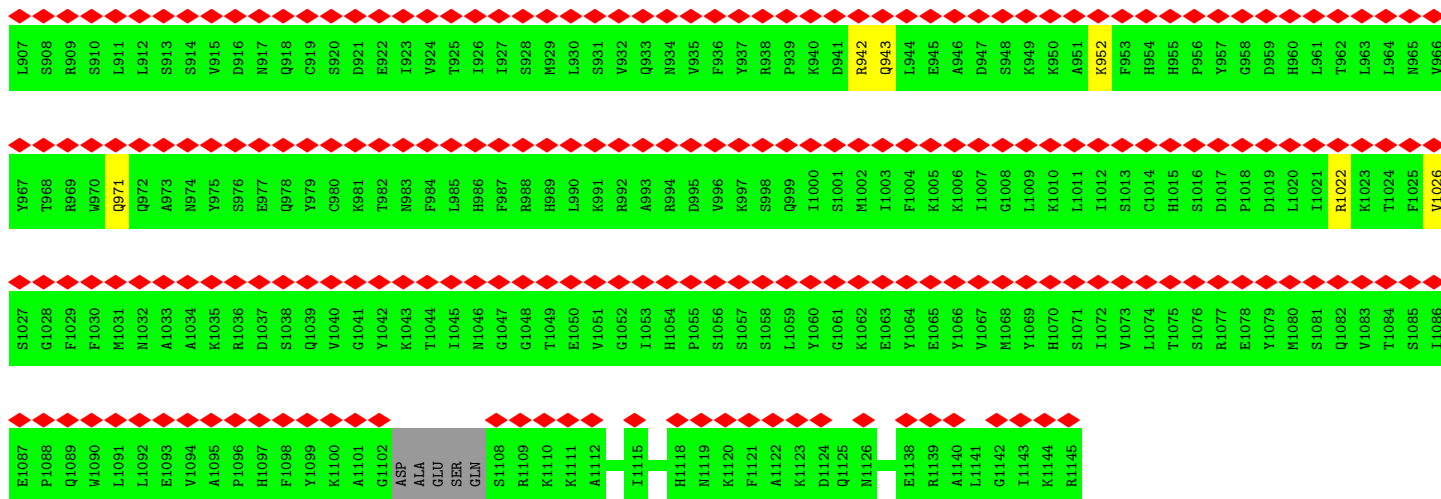


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L181	I182	N183	V184	L185	L186	V187	K188	G189	F190	T191	LYS	GLY	GLY	PHE	ILE	SER	GLU	GLU	SER	GLY	ASN	GLY	SER	ARG	ASP	I209	W210	S211	S212	H213	L214	E216	R217	Y218	L219	K220	V221	A222	P223	Q224	Q225	R226	R227	E228	E229	S230	L231	A232	T233	L234	A235	L236	T237	R238	D239	N240			
I241	T242	I243	K244	S245	V246	Y247	E248	K249	TYR	LEU	PRO	GLN	ASP	GLU	ASN	SER	GLY	LYS	TYR	LEU	PRO	SER	SER	LEU	P267	F268	E269	N270	L271	F272	N273	Y274	L275	A276	S277	L278	E279	K280	L281	G282	L283	D284	N285	Q286	Y287	E288	E289	F290	M291	R292	Q293	M294	N295	G296	I297	Y298	P299	D300	
K301	W302	L303	F304	L305	I306	L307	S308	L309	A310	K311	Y312	Y313	I314	S315	R316	G317	R318	L319	D320	S321	C322	G323	D324	L325	L326	K327	K328	S329	L330	Q331	Q332	T333	L334	R335	Y336	D337	S338	F339	D340	R341	I342	Y343	N344	F345	Y346	L347	L348	F349	Q350	Q351	E352	C353	S354	Q355	F356	I357	L358	G359	K360
LEU	LYS	GLU	ASN	ASP	SER	LYS	PHE	ASN	GLN	LYS	ASP	W374	T375	E376	K377	L378	Q379	A380	H381	M382	A383	T384	E386	S387	L388	I389	N390	L391	Y392	D393	I394	Y395	L396	N397	D398	V399	A400	L401	R402	Q403	D404	S405	M406	L407	V408	E409	T410	W411	M412	K413	R414	V415	S416	L417	Q418	K419	S420		
A421	A422	E423	K424	C425	M426	V427	Y428	S429	E430	A431	I432	L433	K434	I435	D436	P437	R438	K439	V440	G441	T442	P443	G444	S445	F446	G447	R448	L449	M450	C451	S452	Y453	G454	D455	L456	Y457	M458	R459	S460	M461	A462	I463	S464	T465	A466	R467	E468	L469	W470	T471	Q472	S473	L474	K475	V476	Y477	P479	Y480	
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S541	L542	R543	I544	W545	S546	K547	Y548	I549	D550	Y551	L552	E553	A554	Y555	C556	P557	K558	D559	A560	M561	S562	S563	D564	R565	I566	F567	N568	K569	T570	K571	M572	A573	Y574	M575	T576	V577	L578	D579	L580	R581	L582	I583	T584	P585	A586	M587	A588	E589	K590	F591	A592	L593	F594	L595	Q596	N597	H598	Y599	E600
W601	M602	E603	S604	F605	Q606	V607	Y608	E609	K610	T611	L612	P613	L614	F615	P616	P617	E618	I619	Q620	Y621	E622	L623	M624	I625	Y626	Y627	L628	E629	V630	A631	T632	S633	H634	Q635	L636	S637	S638	L639	S640	P641	E642	H643	T644	R645	F646	L647	F648	E649	K650	A651	L652	K653	M654	L655	C656	S657	N658	G659	I660
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G721	P722	S723	V724	T725	R726	E727	L728	Y729	Q730	E731	G732	I733	Q734	I735	L736	F737	N738	S739	K740	A741	V742	E743	F744	V745	I746	K747	F748	S749	D750	F751	E752	S753	S754	I755	G756	E757	T758	I759	R760	A761	R762	E763	L764	L765	A766	Y767	G768	A769	K770	L771	L772	P773	P774	S775	R776	N777	T778	E779	L780
W781	D782	S783	F784	E785	I786	F787	E788	L789	K790	H791	G792	D793	K794	E795	T796	Y797	K798	D799	M800	L801	K802	M803	K804	K805	V806	L807	E808	S809	ASN	MET	LEU	ILE	ASP	SER	ALA	VAL	SER	HIS	GLU	GLY	ASN	ASN	PHE	VAL	ALA	ALA	ALA	THR	SER	HIS	SER	PRO	ASN	SER	HIS	THR			
LEU	THR	GLN	SER	SER	SER	TYR	SER	ILE	ASN	PRO	ASP	GLU	ILE	GLU	LEU	ASP	ILE																																										

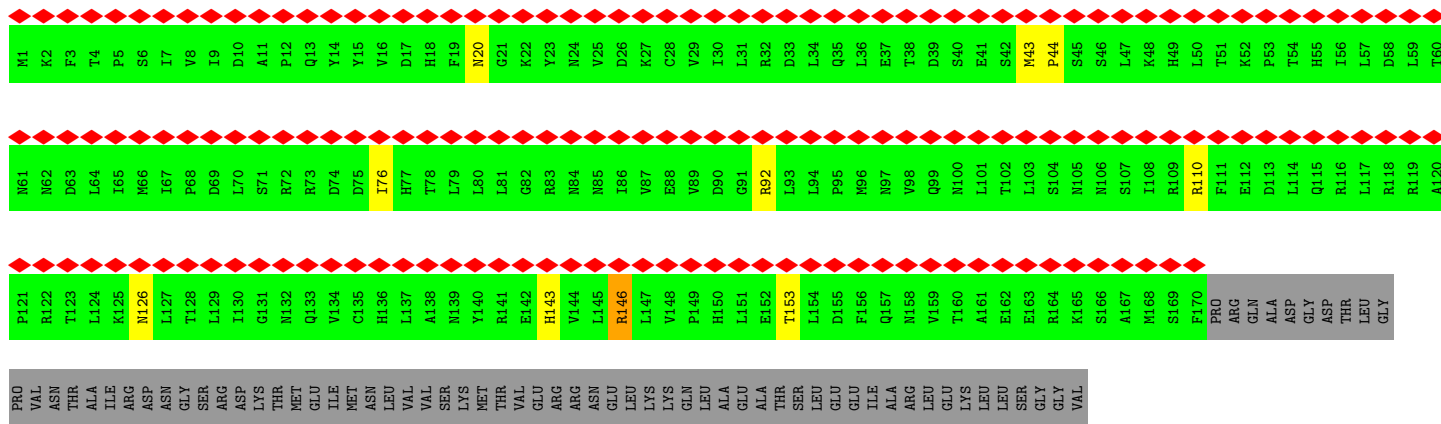
• Molecule 21: Pre-mRNA-splicing factor ATP-dependent RNA helicase PRP22



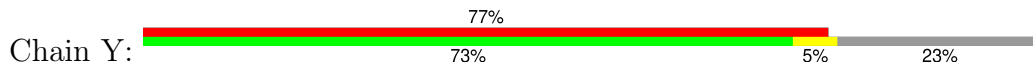
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M849	I789	P729	T669	T609	A549	R489	Q429	P369	A309	LYS	LYS	LYS	GLY	GLN	ASP
L850	E790	V730	P670	V610	E550	S490	S430	K370	I310	ILE	ILE	VAL	ASN	GLY	ILE
K851	Q791	S731	M671	A611	E551	E491	F431	F371	D311	SER	ARG	ARG	ASN	GLY	LYS
A852	L792	S732	M672	T612	G552	L492	D432	L372	D312	LEU	LEU	ILE	THR	VAL	ILE
M853	I793	A733	D673	D613	G553	I493	D433	K373	Y313	MET	THR	THR	PHE	ASN	ALA
G854	V794	L734	Y674	V614	C554	Q494	P434	D374	P314	LYS	ASN	PHE	LYS	LYS	ILE
I855	S795	P735	L675	L615	K555	A495	T435	Q375	E315	ILE	ILE	GLY	ILE	VAL	VAL
N856	P796	S736	E676	F616	V656	V496	K436	Q376	L316	ASP	GLN	CYS	TYR	GLY	GLY
D857	I797	E737	A677	A617	G557	R497	ASN	VAL	K317	VAL	ILE	PHE	GLN	SER	SER
L858	S798	I738	A678	L618	H558	D498	LYS	LYS	ASP	GLY	GLY	VAL	ALA	SER	ASP
L859	Q799	S739	L619	L619	D559	N499	ASP	ALA	ILE	GLY	GLY	VAL	ALA	PRO	ASP
K860	A800	S740	D680	K620	V660	Q500	SER	LYS	PRO	GLY	GLY	PHE	SER	VAL	PRO
F861	Q801	K741	C681	K621	G561	F501	ASN	TYR	ILE	ILE	ILE	GLY	PRO	VAL	ILE
D862	A802	I742	V682	A622	Y562	L502	GLU	GLU	THR	LYS	LYS	ARG	VAL	ILE	ILE
F863	N803	F743	T563	I503	T563	V503	ILE	GLN	THR	TYR	TYR	ARG	GLN	PHE	GLU
M864	Q804	E744	I664	I504	I664	I504	GLN	GLN	SER	GLN	SER	ARG	LYS	VAL	VAL
D865	R805	P745	R665	V505	R665	V505	MET	LEU	LEU	GLY	GLY	VAL	VAL	VAL	VAL
P866	K806	T746	H686	G506	F666	G506	LYS	ALA	ALA	THR	SER	VAL	VAL	VAL	VAL
P867	G807	P747	E687	E507	E687	E507	ASN	T389	I388	VAL	VAL	VAL	VAL	VAL	VAL
K868	A808	K748	N688	T508	D688	T508	GLN	K390	LYS	GLY	GLY	LEU	LEU	LEU	LEU
A809	A809	G749	E689	G509	V669	G509	ILE	V391	ASP	ASP	ASP	VAL	VAL	VAL	VAL
G810	G810	S750	T570	S510	T570	S510	VAL	P392	ARG	ARG	ARG	THR	THR	THR	THR
R811	R811	K751	G571	G511	G571	G511	THR	R393	GLY	GLY	GLY	LEU	LEU	LEU	LEU
T812	T812	R752	P572	K512	P572	K512	GLU	R394	SER	ARG	ARG	GLY	GLY	GLY	GLY
L873	G813	V753	D573	T513	D573	T513	TRP	G394	ILE	ILE	ILE	LEU	LEU	LEU	LEU
N874	P814	V754	I694	T514	T574	T514	GLY	F395	VAL	VAL	VAL	ALA	ALA	ALA	ALA
A875	G815	F755	R695	Q515	R695	Q515	LYS	M396	GLY	GLY	GLY	LYS	LYS	LYS	LYS
L876	K816	A756	L696	I516	I576	I516	ASN	N397	ASN	ASN	ASN	ILE	ILE	ILE	ILE
T877	C817	T757	F697	T517	K577	T517	MET	R398	THR	THR	THR	GLY	GLY	GLY	GLY
E878	Y818	N758	L698	Q518	Y578	Q518	ASN	S399	ARG	ARG	ARG	ALA	ALA	ALA	ALA
L879	R819	I759	N699	L438	M579	L438	SER	A400	VAL	VAL	VAL	ILE	ILE	ILE	ILE
L880	L820	A760	S840	E520	D881	E520	ILE	I401	ASP	ASP	ASP	GLY	GLY	GLY	GLY
H881	Y821	E761	A641	D521	D881	D521	TYR	N402	SER	SER	SER	GLY	GLY	GLY	GLY
L882	T822	T762	K642	E522	G582	E522	GLY	G403	LYS	LYS	LYS	GLN	GLN	GLN	GLN
Q883	E823	S763	F643	E523	M583	E523	LYS	S404	GLU	GLU	GLU	VAL	VAL	VAL	VAL
S884	S824	I764	L584	G524	L584	G524	THR	M405	GLN	GLN	GLN	ARG	ARG	ARG	ARG
A825	A825	T765	E645	F525	Q585	F525	SER	I407	ARG	ARG	ARG	GLN	GLN	GLN	GLN
F826	F826	I766	Y646	S526	R586	S526	LEU	R408	ASP	ASP	ASP	HIS	HIS	HIS	HIS
D887	Y827	D767	F647	N527	E587	N527	PRO	D409	GLU	GLU	GLU	ILE	ILE	ILE	ILE
E888	N828	G768	L648	E528	A888	E528	ILE	H410	THR	THR	THR	PHE	PHE	PHE	PHE
G889	E829	I769	M649	G529	L589	G529	SER	R411	ASP	ASP	ASP	VAL	VAL	VAL	VAL
K890	M830	Y770	C650	M530	A478	M530	GLU	Q479	GLU	GLU	GLU	VAL	VAL	VAL	VAL
L891	L831	Y771	L711	I531	Q479	I531	LYS	E412	ILE	ILE	ILE	VAL	VAL	VAL	VAL
T892	E832	T772	L712	I532	R480	I532	GLU	E413	GLU	GLU	GLU	ARG	ARG	ARG	ARG
N893	N833	V773	D713	G533	Q481	G533	ARG	K414	SER	SER	SER	GLN	GLN	GLN	GLN
L894	T834	D774	L594	C533	T482	C533	THR	L415	GLN	GLN	GLN	GLY	GLY	GLY	GLY
G895	V835	P775	V715	T535	L483	T535	SER	R416	ARG	ARG	ARG	GLY	GLY	GLY	GLY
K896	P836	G776	K716	Q535	P484	Q535	LEU	K417	ASP	ASP	ASP	HIS	HIS	HIS	HIS
E897	E837	F777	T717	R537	V485	R537	PRO	R419	THR	THR	THR	ILE	ILE	ILE	ILE
M898	I838	A778	L718	R538	Y486	R538	ILE	E420	ASP	ASP	ASP	VAL	VAL	VAL	VAL
S899	Q839	K779	G719	E539	Y486	E539	SER	I421	GLU	GLU	GLU	PHE	PHE	PHE	PHE
L900	R840	I780	F719	V539	F599	V539	THR	E422	THR	THR	THR	GLY	GLY	GLY	GLY
F901	Q841	N781	F620	A540	I600	A540	ASP	E423	GLU	GLU	GLU	ILE	ILE	ILE	ILE
P902	N842	I782	V621	A541	M601	A541	LYS	Q424	VAL	VAL	VAL	LYS	LYS	LYS	LYS
M903	L843	G783	E623	S543	D603	S543	GLY	I425	VAL	VAL	VAL	ILE	ILE	ILE	ILE
A904	S844	E724	V644	E604	E604	E604	SER	R426	GLN	GLN	GLN	VAL	VAL	VAL	VAL
P905	H845	A785	L665	A545	A605	A545	ASN								
T906	T846	R786	Y666	K546	H606	K546	LEU								



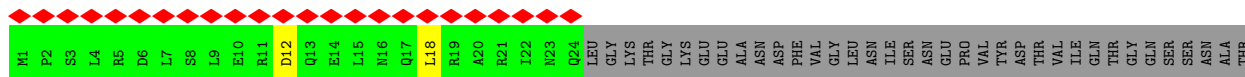
● Molecule 22: U2 small nuclear ribonucleoprotein A'

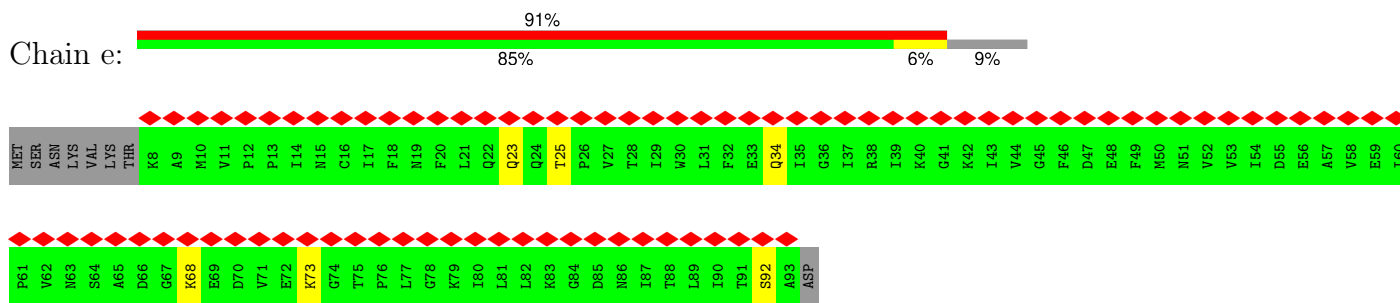


● Molecule 23: U2 small nuclear ribonucleoprotein B''

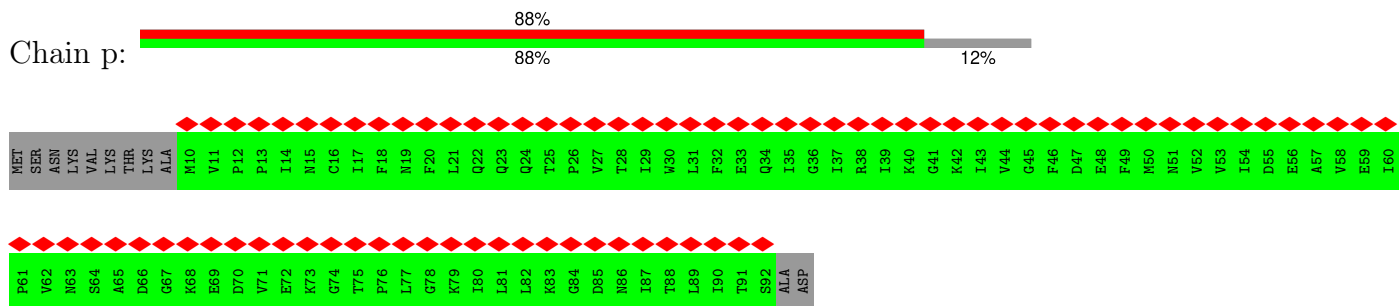


● Molecule 24: Pre-mRNA-splicing factor NTC20

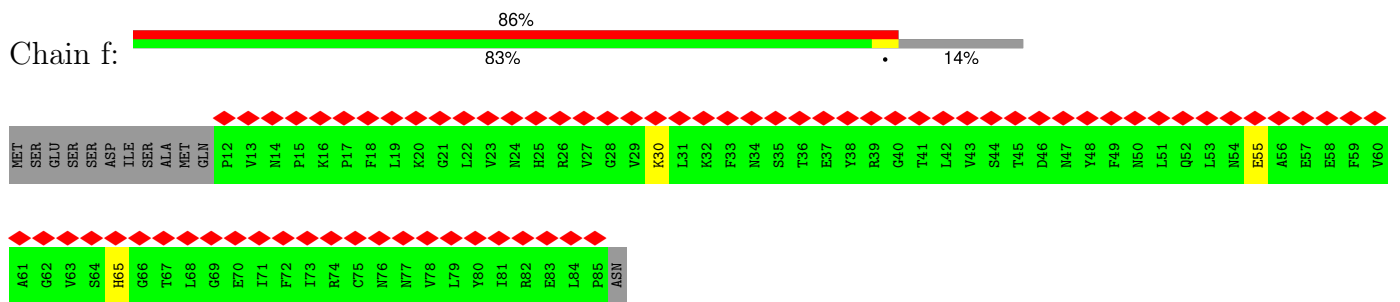




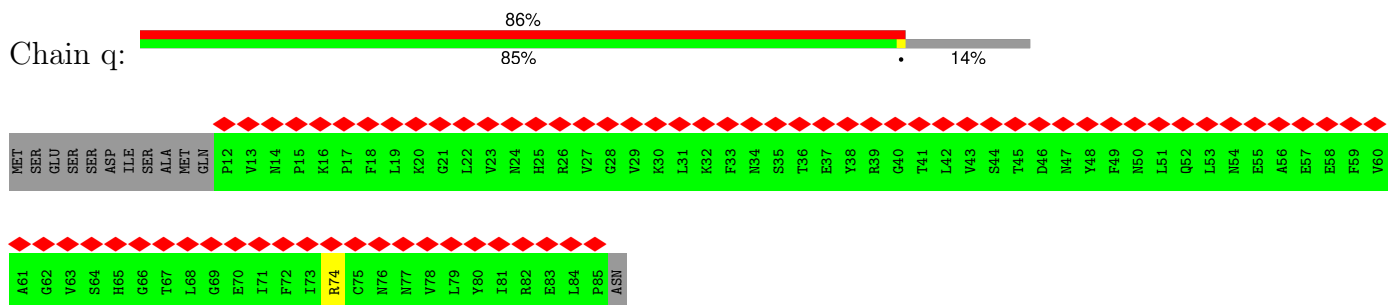
• Molecule 29: Small nuclear ribonucleoprotein E



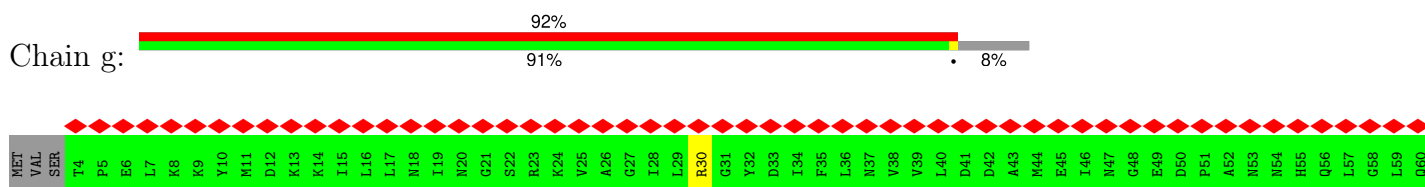
• Molecule 30: Small nuclear ribonucleoprotein F

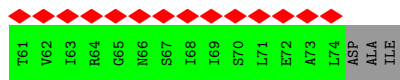


• Molecule 30: Small nuclear ribonucleoprotein F

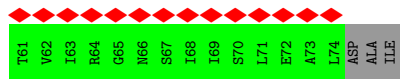
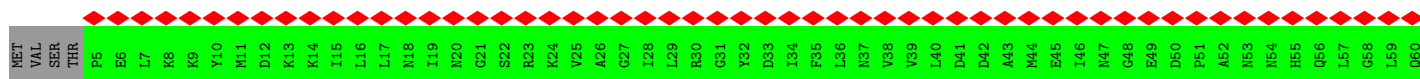
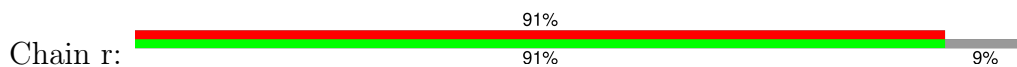


• Molecule 31: Small nuclear ribonucleoprotein G

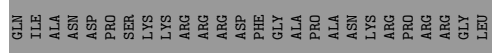
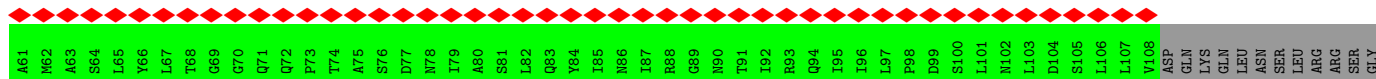
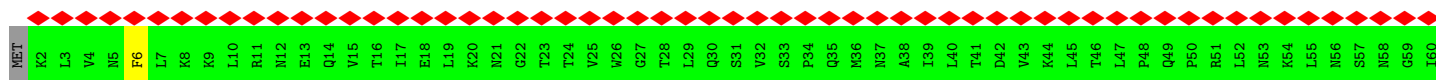




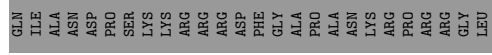
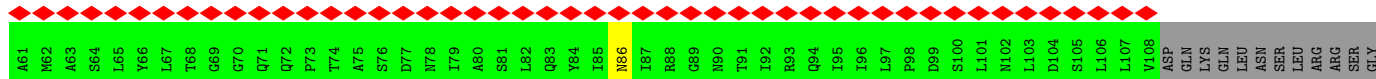
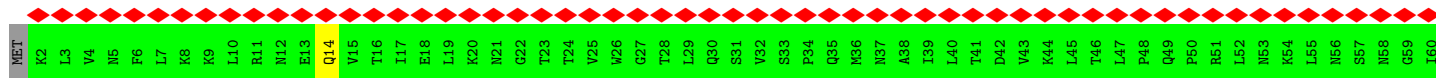
• Molecule 31: Small nuclear ribonucleoprotein G



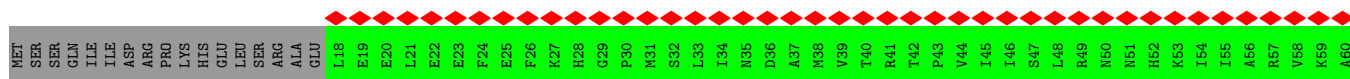
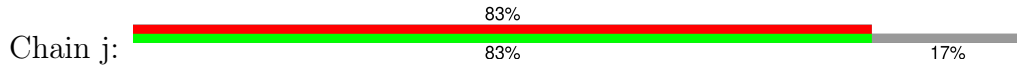
• Molecule 32: Small nuclear ribonucleoprotein Sm D1

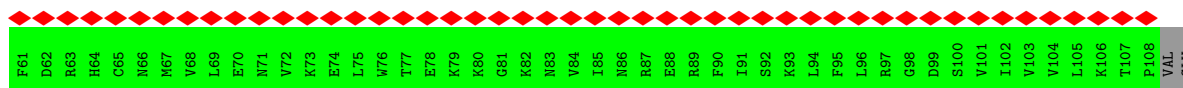


• Molecule 32: Small nuclear ribonucleoprotein Sm D1

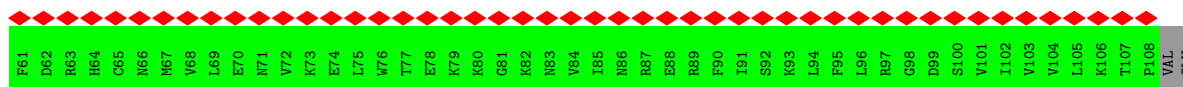
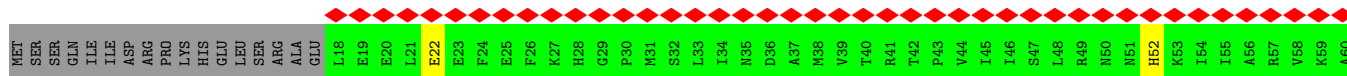
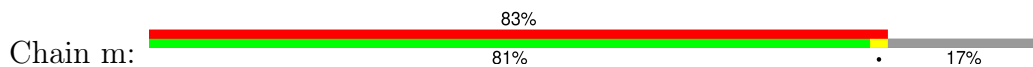


• Molecule 33: Small nuclear ribonucleoprotein Sm D2

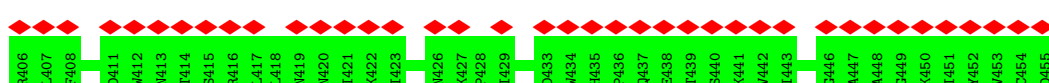
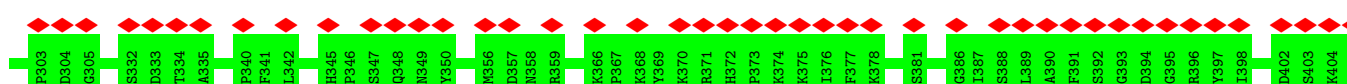
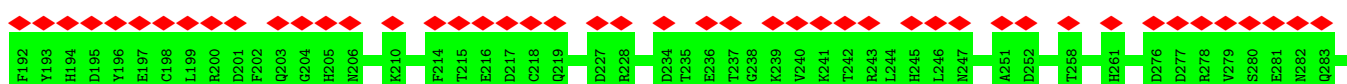
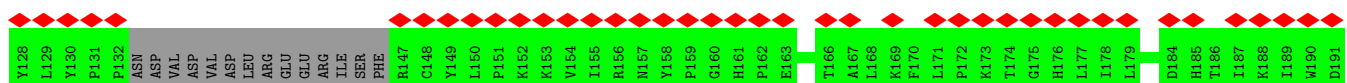
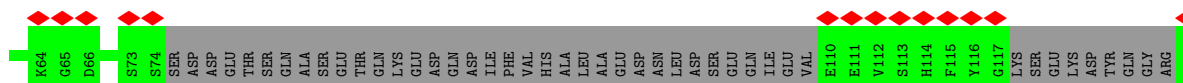
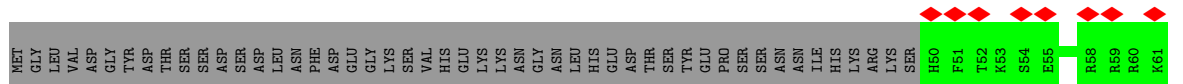
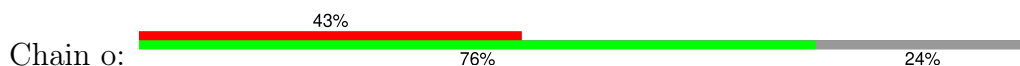




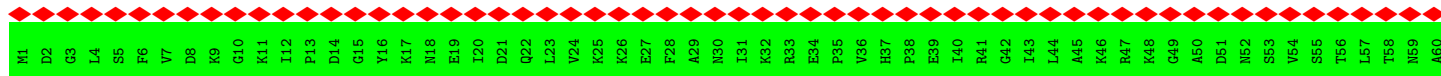
• Molecule 33: Small nuclear ribonucleoprotein Sm D2

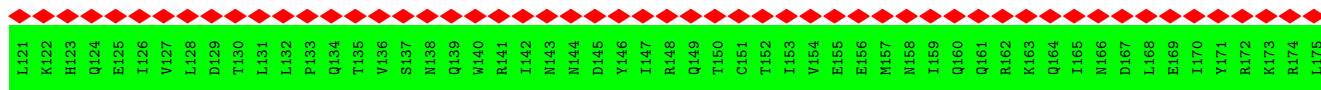


• Molecule 34: Pre-mRNA-processing factor 17

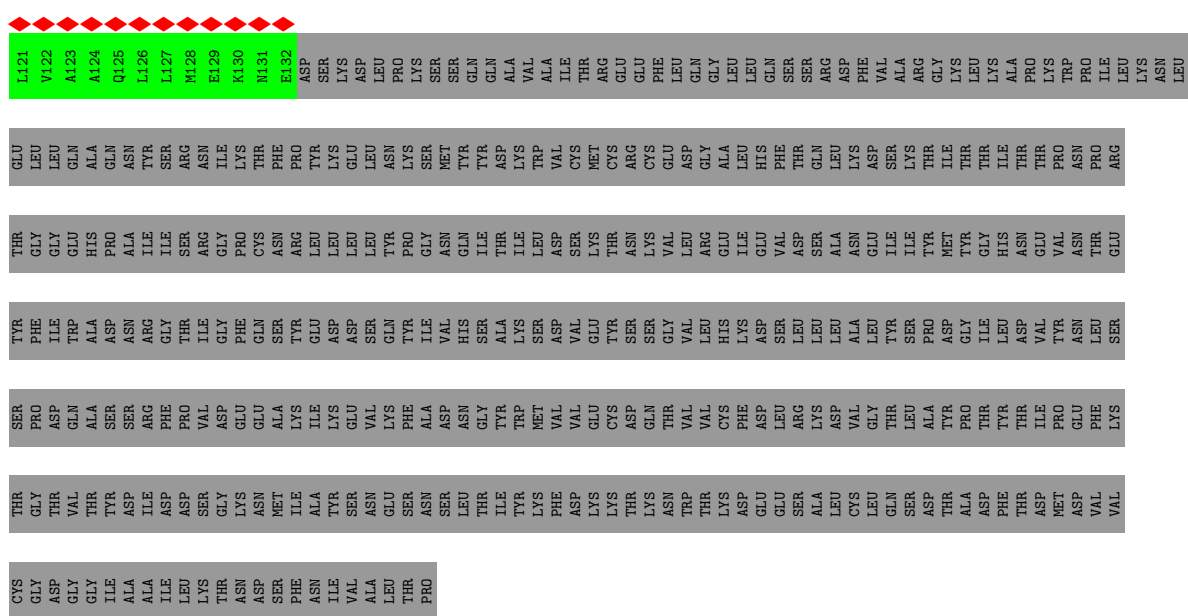


• Molecule 35: Pre-mRNA-splicing factor SNT309

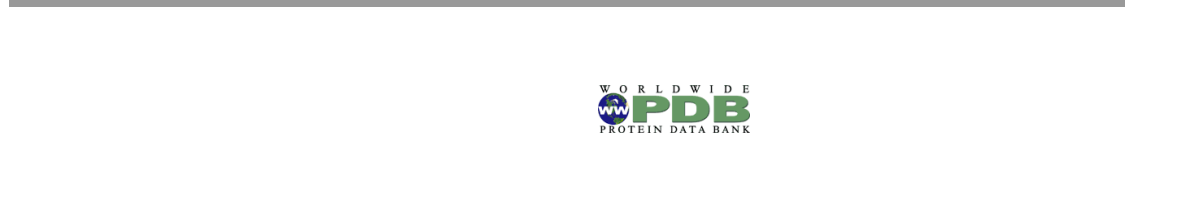
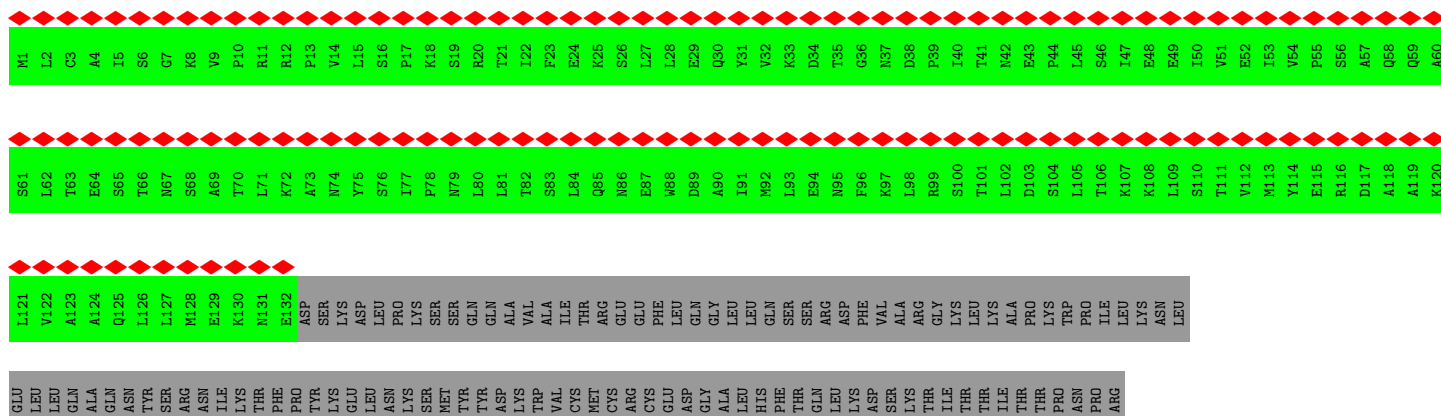




● Molecule 36: Pre-mRNA-processing factor 19



● Molecule 36: Pre-mRNA-processing factor 19



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	209005	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 ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1300	Depositor
Maximum defocus (nm)	3100	Depositor
Magnification	130000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.138	Depositor
Minimum map value	-0.054	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.02	Depositor
Map size (\AA)	464.63998, 464.63998, 464.63998	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.968, 0.968, 0.968	Depositor

5 Model quality

5.1 Standard geometry

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

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	2	0.59	0/3090	1.14	10/4792 (0.2%)
2	5	0.73	0/4098	1.05	6/6373 (0.1%)
3	6	0.82	0/2405	0.98	0/3744
4	A	0.38	0/16489	0.59	0/22348
5	C	0.47	0/7189	0.62	0/9728
6	D	0.35	0/922	0.63	0/1220
7	E	0.68	0/785	1.39	17/1218 (1.4%)
8	G	0.24	0/137	0.52	0/188
9	H	0.46	0/3824	0.58	0/5154
10	I	0.66	0/1128	1.13	7/1747 (0.4%)
11	J	0.37	0/3052	0.64	0/4143
12	K	0.34	0/1375	0.60	0/1854
13	L	0.37	0/1307	0.60	0/1748
14	M	0.34	0/2094	0.61	0/2815
15	N	0.30	0/2124	0.57	0/2860
16	O	0.33	0/2945	0.54	0/3992
17	P	0.35	0/623	0.66	0/832
18	R	0.31	0/510	0.50	0/698
19	S	0.36	0/4780	0.54	0/6483
20	T	0.36	0/5658	0.52	0/7669
21	V	0.43	0/6210	0.61	0/8377
22	W	0.31	0/1406	0.62	0/1905
23	Y	0.31	0/706	0.62	0/941
24	Z	0.31	0/424	0.58	0/564
25	a	0.31	0/1409	0.57	0/1911
26	b	0.36	0/731	0.63	0/983
26	k	0.33	0/849	0.63	0/1138
27	c	0.37	0/1925	0.63	0/2565
28	d	0.40	0/633	0.61	0/857
28	n	0.33	0/624	0.57	0/846
29	e	0.36	0/676	0.59	0/916
29	p	0.32	0/657	0.60	0/891

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
30	f	0.37	0/605	0.60	0/819
30	q	0.35	0/605	0.60	0/819
31	g	0.35	0/556	0.60	0/749
31	r	0.32	0/549	0.62	0/738
32	h	0.33	0/835	0.59	0/1135
32	l	0.31	0/835	0.59	0/1135
33	j	0.36	0/759	0.62	0/1019
33	m	0.31	0/759	0.60	0/1019
34	o	0.31	0/2903	0.62	0/3921
35	s	0.25	0/869	0.40	0/1210
36	t	0.25	0/657	0.43	0/917
36	u	0.25	0/657	0.41	0/917
36	v	0.25	0/657	0.40	0/917
36	w	0.25	0/657	0.40	0/917
37	y	0.33	0/1085	0.52	0/1453
All	All	0.43	0/93773	0.68	40/129185 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
11	J	0	1
12	K	0	1
19	S	0	1
21	V	0	1
22	W	0	1
27	c	0	1
All	All	0	6

There are no bond length outliers.

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1082	A	N1-C2-N3	9.71	134.15	129.30
7	E	6	C	OP1-P-OP2	-9.25	105.73	119.60
1	2	1082	A	C2-N3-C4	-8.11	106.54	110.60
7	E	3	A	OP1-P-O3'	8.05	122.92	105.20
1	2	155	U	N1-C2-O2	-7.95	117.23	122.80
7	E	4	U	OP1-P-OP2	-7.91	107.73	119.60
10	I	76	U	N3-C2-O2	-7.85	116.70	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	I	76	U	N1-C2-O2	7.24	127.86	122.80
7	E	5	C	OP1-P-OP2	-7.11	108.94	119.60
7	E	9	C	OP1-P-O3'	6.94	120.47	105.20
7	E	5	C	OP1-P-O3'	6.73	120.01	105.20
7	E	10	U	OP1-P-OP2	-6.71	109.54	119.60
1	2	1082	A	C8-N9-C4	-6.68	103.13	105.80
7	E	7	A	OP1-P-OP2	-6.65	109.63	119.60
1	2	138	U	OP1-P-OP2	-6.65	109.63	119.60
7	E	5	C	O4'-C4'-C3'	6.49	111.29	106.10
1	2	1082	A	N7-C8-N9	6.42	117.01	113.80
10	I	95	G	OP1-P-OP2	-6.23	110.25	119.60
2	5	79	C	C6-N1-C2	-6.21	117.82	120.30
2	5	69	G	P-O3'-C3'	6.21	127.15	119.70
7	E	3	A	OP1-P-OP2	-6.18	110.32	119.60
1	2	151	A	N1-C2-N3	6.14	132.37	129.30
1	2	1083	A	N1-C2-N3	6.10	132.35	129.30
10	I	76	U	C2-N1-C1'	5.82	124.69	117.70
1	2	1086	U	N1-C2-N3	5.74	118.34	114.90
7	E	11	A	OP1-P-OP2	-5.73	111.00	119.60
2	5	172	U	O4'-C1'-N1	5.71	112.77	108.20
10	I	70	A	OP1-P-OP2	-5.61	111.18	119.60
7	E	-14	A	P-O3'-C3'	5.48	126.28	119.70
7	E	-13	G	O4'-C1'-N9	5.48	112.58	108.20
7	E	-12	U	P-O3'-C3'	5.47	126.27	119.70
7	E	9	C	OP1-P-OP2	-5.46	111.41	119.60
1	2	1101	C	C6-N1-C2	-5.44	118.12	120.30
2	5	41	A	P-O3'-C3'	5.39	126.17	119.70
10	I	70	A	P-O3'-C3'	5.32	126.08	119.70
10	I	89	G	O4'-C1'-N9	5.29	112.43	108.20
7	E	8	C	OP1-P-OP2	-5.28	111.68	119.60
2	5	79	C	O4'-C1'-N1	5.17	112.33	108.20
7	E	9	C	O4'-C1'-N1	5.14	112.31	108.20
2	5	103	A	O4'-C1'-N9	5.08	112.27	108.20

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
11	J	309	ARG	Sidechain
12	K	185	ARG	Sidechain
19	S	186	ARG	Sidechain
21	V	840	ARG	Sidechain

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Mol	Chain	Res	Type	Group
22	W	92	ARG	Sidechain
27	c	77	ARG	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2	2779	0	1411	24	0
2	5	3671	0	1856	6	0
3	6	2170	0	1095	14	0
4	A	16079	0	16079	43	0
5	C	7040	0	7241	21	0
6	D	914	0	953	19	0
7	E	703	0	356	2	0
8	G	139	0	67	0	0
9	H	3762	0	3825	38	0
10	I	1012	0	510	5	0
11	J	2990	0	2906	12	0
12	K	1355	0	1383	7	0
13	L	1283	0	1301	0	0
14	M	2048	0	2011	9	0
15	N	2092	0	2162	9	0
16	O	2918	0	2467	15	0
17	P	607	0	596	2	0
18	R	510	0	327	6	0
19	S	4683	0	4267	39	0
20	T	5543	0	5182	41	0
21	V	6096	0	6158	10	0
22	W	1383	0	1407	2	0
23	Y	697	0	733	2	0
24	Z	424	0	455	2	0
25	a	1380	0	1425	0	0
26	b	725	0	778	0	0
26	k	843	0	917	0	0
27	c	1893	0	1849	0	0
28	d	624	0	647	0	0
28	n	615	0	634	0	0
29	e	665	0	690	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	p	646	0	667	0	0
30	f	592	0	594	0	0
30	q	592	0	594	0	0
31	g	551	0	572	0	0
31	r	544	0	566	0	0
32	h	826	0	874	0	0
32	l	826	0	874	0	0
33	j	747	0	784	0	0
33	m	747	0	784	0	0
34	o	2821	0	2743	0	0
35	s	870	0	363	0	0
36	t	658	0	291	0	0
36	u	658	0	291	0	0
36	v	658	0	291	0	0
36	w	658	0	291	0	0
37	y	1075	0	1004	0	0
38	6	1	0	0	0	0
38	C	1	0	0	0	0
39	6	3	0	0	0	0
39	E	1	0	0	0	0
40	A	36	0	6	1	0
40	S	36	0	6	1	0
41	C	32	0	12	0	0
42	L	3	0	0	0	0
42	M	1	0	0	0	0
42	N	2	0	0	0	0
42	c	1	0	0	0	0
43	6	1	0	0	0	0
All	All	91230	0	83295	296	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 (296) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:84:LYS:HA	6:D:87:LEU:HD12	1.50	0.92
14:M:161:ARG:HH21	15:N:299:ALA:HB2	1.40	0.86
1:2:1141:C:H2'	1:2:1142:G:C8	2.20	0.76
11:J:143:ARG:HH11	11:J:160:ASN:HD21	1.35	0.74
5:C:763:ARG:HH22	18:R:82:ASP:CB	2.01	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:467:GLN:HE22	19:S:470:ASP:HB2	1.54	0.73
4:A:345:ALA:HB2	18:R:1:MET:HB2	1.72	0.71
1:2:1141:C:H2'	1:2:1142:G:H8	1.55	0.71
1:2:1137:U:H2'	1:2:1138:G:H8	1.56	0.69
3:6:8:A:H2'	3:6:9:A:C8	2.28	0.68
20:T:290:PHE:O	20:T:294:MET:HG2	1.95	0.67
9:H:85:SER:HB2	9:H:221:THR:H	1.59	0.66
9:H:50:LEU:HD11	9:H:258:LEU:HD22	1.77	0.66
19:S:414:LEU:HD13	19:S:422:LYS:HG3	1.78	0.66
14:M:161:ARG:NH1	15:N:241:ILE:HG12	2.11	0.65
14:M:161:ARG:NH2	15:N:299:ALA:HB2	2.09	0.65
1:2:1137:U:H2'	1:2:1138:G:C8	2.31	0.65
4:A:313:ARG:O	4:A:316:THR:HG23	1.97	0.65
2:5:175:G:H4'	2:5:176:A:H5'	1.79	0.65
20:T:393:ASP:HB3	20:T:417:LEU:HD13	1.78	0.65
20:T:344:ASN:O	20:T:348:LEU:HG	1.97	0.64
6:D:120:LYS:HE2	6:D:120:LYS:HA	1.80	0.63
9:H:466:THR:HG22	9:H:471:GLY:HA3	1.81	0.63
19:S:438:LYS:HD2	40:S:701:IHP:H5	1.82	0.62
20:T:745:VAL:HG11	20:T:768:GLY:HA3	1.83	0.61
3:6:86:G:H22	19:S:67:GLN:HE22	1.49	0.61
1:2:10:U:H2'	1:2:11:U:C6	2.36	0.60
19:S:420:VAL:HG12	19:S:424:ARG:HH21	1.67	0.59
16:O:301:ALA:O	16:O:304:THR:HG23	2.03	0.59
5:C:944:VAL:HG13	5:C:967:VAL:HG21	1.84	0.59
20:T:333:THR:HG21	20:T:339:PHE:HB2	1.85	0.58
5:C:304:PHE:CD1	5:C:310:ASN:HB3	2.39	0.58
9:H:38:GLN:O	9:H:42:ARG:HG2	2.03	0.58
20:T:378:LEU:O	20:T:382:MET:HG3	2.03	0.58
4:A:1286:TRP:CE2	4:A:1302:LEU:HD11	2.38	0.58
4:A:293:VAL:HG12	4:A:295:GLY:H	1.69	0.58
5:C:304:PHE:HD1	5:C:310:ASN:HB3	1.68	0.58
5:C:760:LEU:HG	18:R:75:VAL:HA	1.85	0.57
20:T:481:ILE:HD11	20:T:538:LEU:HA	1.84	0.57
4:A:399:ARG:HH11	4:A:399:ARG:HG2	1.70	0.57
6:D:114:ASN:HB3	6:D:118:LYS:HE2	1.85	0.57
9:H:48:ASN:HD21	9:H:252:THR:HA	1.69	0.57
4:A:659:HIS:HE1	40:A:2500:IHP:O33	1.88	0.57
1:2:41:C:H2'	1:2:42:U:C6	2.40	0.56
4:A:168:LEU:HD21	4:A:626:LEU:HD21	1.87	0.56
1:2:44:U:H2'	1:2:45:U:C6	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:6:18:U:H2'	3:6:19:C:C6	2.40	0.56
4:A:635:THR:HG22	4:A:649:LEU:HD12	1.88	0.56
6:D:117:LYS:HD3	6:D:117:LYS:N	2.21	0.56
15:N:205:PHE:HB3	15:N:290:ILE:HD11	1.87	0.56
1:2:30:A:H61	16:O:34:SER:HB2	1.70	0.55
20:T:484:LEU:HD11	20:T:535:GLN:OE1	2.06	0.55
3:6:8:A:H2'	3:6:9:A:H8	1.70	0.55
9:H:60:VAL:HG13	9:H:76:LEU:HD21	1.88	0.55
9:H:18:TRP:CE2	9:H:55:ILE:HD11	2.42	0.54
21:V:555:LYS:H	21:V:555:LYS:HD3	1.72	0.54
19:S:455:ARG:HA	19:S:458:LYS:HG3	1.90	0.54
19:S:474:TRP:HA	19:S:477:TYR:HE1	1.73	0.54
20:T:552:LEU:HD21	20:T:569:LYS:HD2	1.89	0.53
20:T:742:VAL:O	20:T:746:ILE:HG13	2.08	0.53
6:D:107:TYR:HE2	20:T:801:LEU:HD12	1.73	0.53
16:O:123:LEU:N	16:O:123:LEU:HD22	2.24	0.53
10:I:65:U:H2'	10:I:66:A:C8	2.43	0.53
20:T:801:LEU:O	20:T:805:LYS:HG2	2.08	0.53
11:J:233:HIS:HD1	11:J:235:THR:H	1.57	0.53
1:2:1148:U:H2'	1:2:1149:G:C8	2.44	0.52
14:M:165:SER:HA	14:M:170:ILE:HD13	1.92	0.52
4:A:1162:THR:HG22	4:A:1169:TYR:HB2	1.92	0.52
6:D:87:LEU:HD23	16:O:123:LEU:HD23	1.91	0.52
11:J:119:LEU:HD12	19:S:235:LEU:HD22	1.90	0.52
2:5:50:G:H1	2:5:65:U:H3	1.56	0.52
4:A:1361:VAL:HG22	4:A:1403:SER:HB2	1.92	0.52
6:D:59:ARG:HB2	10:I:76:U:C5	2.44	0.52
9:H:34:MET:HG2	9:H:75:ALA:HB2	1.91	0.52
9:H:148:LEU:HD11	9:H:180:ILE:HD13	1.90	0.52
9:H:51:ILE:HG13	9:H:251:LEU:HD23	1.92	0.51
6:D:82:LEU:HD21	16:O:129:ASN:HB2	1.91	0.51
15:N:136:VAL:HA	15:N:139:LEU:HG	1.91	0.51
5:C:315:SER:HB3	5:C:320:PHE:CE2	2.46	0.51
19:S:383:LEU:O	19:S:387:LEU:HG	2.11	0.51
9:H:433:LEU:HD21	9:H:472:LEU:HB2	1.92	0.51
23:Y:34:GLN:HB3	23:Y:97:LYS:HE3	1.94	0.50
9:H:26:SER:HA	9:H:59:ASN:ND2	2.26	0.50
1:2:155:U:O2	1:2:1082:A:H2	1.94	0.50
19:S:399:LYS:HD3	19:S:399:LYS:N	2.26	0.50
20:T:288:GLU:O	20:T:292:ARG:HG3	2.11	0.50
1:2:141:A:H2'	1:2:142:C:C6	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:151:A:H2'	1:2:152:C:C6	2.47	0.50
9:H:18:TRP:HZ3	9:H:51:ILE:HG22	1.77	0.50
10:I:61:U:H2'	10:I:62:A:C8	2.47	0.50
19:S:420:VAL:HG12	19:S:424:ARG:NH2	2.27	0.50
19:S:416:ARG:HH12	24:Z:112:LEU:HD12	1.76	0.50
21:V:411:ARG:HH22	21:V:702:GLU:HB3	1.76	0.50
14:M:240:GLU:O	14:M:243:LYS:HG2	2.12	0.50
6:D:87:LEU:CD2	16:O:123:LEU:HD23	2.42	0.49
9:H:382:ARG:HA	9:H:422:PHE:CD2	2.46	0.49
20:T:302:TRP:HZ2	20:T:329:SER:HG	1.60	0.49
3:6:8:A:H2	3:6:18:U:H3	1.59	0.49
9:H:433:LEU:HD21	9:H:472:LEU:CB	2.43	0.49
20:T:275:LEU:HD12	20:T:294:MET:SD	2.53	0.49
20:T:621:TYR:CZ	20:T:625:ILE:HD11	2.48	0.49
5:C:687:ALA:HB1	18:R:60:VAL:CB	2.43	0.49
9:H:346:LEU:O	9:H:350:MET:HG2	2.13	0.49
4:A:1663:PHE:CE2	4:A:1683:LYS:HE3	2.47	0.49
19:S:411:ALA:HB2	19:S:427:LEU:HD21	1.93	0.49
3:6:3:U:H2'	3:6:4:C:C6	2.48	0.49
3:6:17:U:H2'	3:6:18:U:C6	2.48	0.48
21:V:740:SER:HA	21:V:743:PHE:CZ	2.48	0.48
1:2:1095:U:H2'	1:2:1096:C:C6	2.48	0.48
10:I:66:A:H2'	10:I:67:C:C6	2.49	0.48
19:S:443:TYR:O	19:S:447:GLU:HG2	2.13	0.48
6:D:37:VAL:HA	6:D:40:LYS:HE3	1.96	0.48
1:2:1148:U:H2'	1:2:1149:G:H8	1.79	0.47
7:E:-10:A:C8	7:E:-10:A:H5'	2.49	0.47
20:T:584:THR:HG22	20:T:587:MET:HB2	1.96	0.47
4:A:835:LYS:HD2	17:P:173:HIS:CD2	2.49	0.47
20:T:335:ARG:HD2	20:T:336:TYR:H	1.78	0.47
14:M:54:GLN:H	14:M:58:HIS:CD2	2.33	0.47
20:T:302:TRP:O	20:T:306:ILE:HG22	2.14	0.47
21:V:617:ALA:HB3	21:V:861:PHE:CZ	2.50	0.47
1:2:144:G:H3'	1:2:145:G:O4'	2.15	0.47
6:D:114:ASN:HB3	6:D:118:LYS:CE	2.45	0.47
19:S:407:TRP:HE1	19:S:426:ILE:HD11	1.80	0.47
1:2:30:A:N6	16:O:34:SER:HB2	2.30	0.47
14:M:172:ARG:HB2	15:N:244:HIS:CD2	2.50	0.47
19:S:453:PHE:HB3	19:S:484:LEU:HD11	1.97	0.47
1:2:119:G:C2	1:2:121:C:H5''	2.50	0.47
4:A:316:THR:HG22	4:A:319:ARG:NH1	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:V:562:TYR:HA	21:V:578:TYR:O	2.15	0.47
20:T:352:GLU:O	20:T:355:GLN:HG3	2.15	0.46
5:C:475:THR:HG21	5:C:627:LYS:HB3	1.98	0.46
9:H:466:THR:HG22	9:H:471:GLY:CA	2.44	0.46
11:J:373:LEU:HD11	11:J:426:TRP:CE2	2.51	0.46
20:T:334:LEU:O	20:T:334:LEU:HD12	2.16	0.46
20:T:564:ASP:OD1	20:T:566:ILE:HD12	2.16	0.46
4:A:621:LEU:HD23	4:A:722:LEU:HD21	1.98	0.46
12:K:179:THR:HG21	19:S:19:LEU:HD13	1.97	0.46
1:2:10:U:H2'	1:2:11:U:H6	1.81	0.45
11:J:233:HIS:HD1	11:J:236:LEU:H	1.62	0.45
20:T:536:THR:HG23	20:T:537:VAL:HG13	1.98	0.45
20:T:600:GLU:HB3	20:T:603:GLU:OE1	2.15	0.45
12:K:185:ARG:HD2	16:O:29:GLY:HA2	1.98	0.45
9:H:25:VAL:O	9:H:29:ILE:HG12	2.15	0.45
4:A:2036:SER:O	4:A:2037:TYR:CG	2.70	0.45
9:H:465:PHE:O	9:H:470:LEU:N	2.44	0.45
1:2:1163:C:H2'	1:2:1164:C:C6	2.52	0.45
5:C:765:VAL:HG11	5:C:768:PHE:CE1	2.52	0.45
9:H:253:MET:O	9:H:257:THR:HG23	2.17	0.45
19:S:339:MET:HE1	19:S:378:LEU:HD11	1.99	0.45
4:A:1543:ARG:O	4:A:1546:VAL:HG12	2.17	0.45
19:S:329:LEU:HD13	20:T:642:GLU:HG3	1.98	0.45
5:C:939:LYS:HE2	5:C:940:VAL:O	2.17	0.45
21:V:1022:ARG:O	21:V:1026:VAL:HG23	2.17	0.45
4:A:722:LEU:HD23	4:A:722:LEU:HA	1.86	0.44
20:T:503:ARG:HG2	20:T:503:ARG:HH11	1.82	0.44
4:A:676:GLN:HG2	4:A:714:PHE:HB2	1.98	0.44
6:D:114:ASN:HB3	6:D:118:LYS:NZ	2.33	0.44
20:T:301:LYS:HB2	20:T:301:LYS:HE3	1.68	0.44
9:H:22:ARG:HA	9:H:55:ILE:HG21	1.99	0.44
15:N:95:ASN:C	15:N:97:GLU:H	2.21	0.44
4:A:1336:ASN:O	4:A:1340:ILE:HD13	2.17	0.44
9:H:145:LYS:O	9:H:145:LYS:HD3	2.18	0.44
9:H:228:ILE:HD12	9:H:228:ILE:N	2.33	0.44
9:H:459:ARG:O	9:H:462:ILE:HG13	2.18	0.44
19:S:410:TYR:CD2	19:S:426:ILE:HG12	2.53	0.44
6:D:113:ILE:O	6:D:117:LYS:HE3	2.17	0.44
20:T:622:GLU:O	20:T:626:GLU:HG2	2.17	0.44
5:C:808:LEU:HD22	5:C:944:VAL:HG11	2.00	0.44
11:J:309:ARG:HG3	11:J:328:THR:HG22	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:367:TRP:O	19:S:371:ILE:HG12	2.17	0.44
19:S:390:ARG:O	19:S:394:ASP:HB3	2.18	0.44
19:S:464:ILE:HD12	19:S:468:PRO:HA	1.99	0.44
1:2:155:U:O2	1:2:1082:A:C2	2.70	0.44
9:H:421:LYS:HE3	9:H:422:PHE:CE1	2.53	0.44
20:T:505:PHE:HE1	20:T:551:TYR:HB3	1.83	0.44
1:2:21:G:N7	17:P:5:HIS:HB3	2.33	0.44
3:6:18:U:H2'	3:6:19:C:H6	1.82	0.44
3:6:63:G:H2'	3:6:64:U:C6	2.52	0.44
4:A:622:MET:HE2	4:A:726:ILE:HG13	2.00	0.44
19:S:414:LEU:HD23	19:S:414:LEU:HA	1.81	0.44
16:O:13:TRP:CZ2	16:O:43:LYS:HG2	2.53	0.43
16:O:296:LYS:HD2	16:O:297:LEU:H	1.83	0.43
24:Z:18:LEU:HD12	24:Z:18:LEU:HA	1.66	0.43
4:A:886:MET:SD	4:A:1120:VAL:HG22	2.59	0.43
6:D:88:GLU:O	6:D:92:LYS:HG2	2.18	0.43
6:D:89:PHE:CZ	16:O:139:PRO:HD3	2.52	0.43
4:A:139:LEU:HD13	4:A:193:TYR:CG	2.54	0.43
11:J:405:SER:HA	11:J:415:ILE:O	2.19	0.43
23:Y:61:VAL:HG22	23:Y:74:ILE:HD12	2.00	0.43
4:A:503:LYS:HA	4:A:506:PHE:CE2	2.54	0.43
20:T:584:THR:HG23	20:T:587:MET:H	1.82	0.43
19:S:255:ALA:HB2	19:S:287:PHE:HE2	1.83	0.43
20:T:430:GLU:O	20:T:434:LYS:HG2	2.18	0.43
6:D:91:GLN:HG2	6:D:95:ASN:OD1	2.19	0.43
9:H:11:ILE:HD11	9:H:244:LYS:HE3	2.01	0.43
19:S:289:LYS:HG3	19:S:297:ILE:HG12	2.01	0.43
20:T:185:LEU:HD22	20:T:315:SER:HB3	2.01	0.43
4:A:139:LEU:HD13	4:A:193:TYR:CD2	2.53	0.43
4:A:163:GLY:HA3	12:K:122:LEU:O	2.18	0.43
9:H:18:TRP:NE1	9:H:55:ILE:HD11	2.33	0.43
9:H:203:LYS:HE2	9:H:203:LYS:HB3	1.71	0.43
11:J:220:TYR:CE2	11:J:256:ARG:HA	2.54	0.43
12:K:160:PRO:C	12:K:161:ASN:HD22	2.21	0.43
19:S:410:TYR:CE2	19:S:426:ILE:HG12	2.54	0.43
4:A:1082:ILE:HG23	4:A:1113:ILE:HD11	2.01	0.43
3:6:21:U:H2'	3:6:22:G:H8	1.84	0.42
7:E:21:G:C8	7:E:21:G:H5''	2.54	0.42
10:I:5:G:H2'	10:I:6:U:C6	2.54	0.42
19:S:444:ILE:HD13	19:S:460:TYR:CZ	2.54	0.42
20:T:641:PRO:HB3	20:T:676:ILE:HG12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1130:ARG:HD2	4:A:1130:ARG:HA	1.87	0.42
9:H:454:ASP:HB2	9:H:457:HIS:CD2	2.54	0.42
20:T:484:LEU:HD13	20:T:538:LEU:HD22	2.00	0.42
4:A:1668:ILE:HD13	4:A:1801:SER:HB2	2.01	0.42
4:A:2007:ARG:O	4:A:2011:LEU:HG	2.20	0.42
11:J:304:LEU:HD13	11:J:334:TRP:CD2	2.54	0.42
22:W:143:HIS:O	22:W:146:ARG:HD2	2.19	0.42
1:2:1140:U:H2'	1:2:1141:C:C6	2.55	0.42
5:C:760:LEU:HD23	18:R:78:SER:CB	2.49	0.42
9:H:148:LEU:HD11	9:H:180:ILE:HG21	2.01	0.42
14:M:143:ASP:OD1	14:M:148:SER:HA	2.19	0.42
20:T:713:ILE:HG21	20:T:729:TYR:CZ	2.55	0.42
5:C:123:MET:HA	5:C:126:MET:HG2	2.02	0.42
1:2:1082:A:H2'	1:2:1083:A:C8	2.55	0.42
1:2:1165:C:H2'	1:2:1166:G:H8	1.85	0.42
4:A:705:GLN:HB3	4:A:706:PRO:HD3	2.02	0.42
5:C:678:SER:OG	5:C:858:LEU:HB2	2.20	0.42
2:5:85:U:H2'	2:5:86:G:H8	1.85	0.42
19:S:461:GLU:HA	19:S:464:ILE:HG22	2.01	0.42
20:T:512:LEU:HD11	20:T:544:ILE:HG22	2.00	0.42
21:V:503:VAL:HG23	21:V:650:CYS:SG	2.59	0.42
4:A:871:GLY:HA2	12:K:201:PHE:CE2	2.55	0.42
9:H:93:THR:O	9:H:97:GLU:HG2	2.20	0.42
22:W:43:MET:HB3	22:W:44:PRO:HD3	2.02	0.42
4:A:618:SER:HB3	4:A:725:TYR:HB3	2.02	0.42
9:H:48:ASN:ND2	9:H:252:THR:HA	2.34	0.42
21:V:783:TYR:CE2	21:V:785:ALA:HA	2.55	0.42
4:A:1617:ALA:HA	4:A:1635:HIS:CE1	2.55	0.41
14:M:251:VAL:HG12	15:N:143:LEU:HD21	2.01	0.41
4:A:139:LEU:O	4:A:143:ILE:HG12	2.19	0.41
5:C:373:PHE:CE2	5:C:378:LEU:HG	2.55	0.41
5:C:436:VAL:O	5:C:440:THR:HG23	2.20	0.41
5:C:348:LEU:HD23	5:C:348:LEU:HA	1.88	0.41
9:H:145:LYS:HD2	9:H:147:SER:HB2	2.01	0.41
9:H:362:ASN:HD22	9:H:397:LEU:HD12	1.84	0.41
18:R:58:LEU:O	18:R:60:VAL:N	2.53	0.41
19:S:424:ARG:HB2	19:S:424:ARG:NH1	2.36	0.41
19:S:454:ASP:HA	19:S:457:ARG:NH1	2.35	0.41
3:6:17:U:H2'	3:6:18:U:H6	1.85	0.41
3:6:97:A:H2'	3:6:98:G:C8	2.56	0.41
4:A:470:LEU:HB3	4:A:471:PRO:HD2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:J:331:ILE:HB	11:J:345:PHE:HB2	2.03	0.41
19:S:202:TRP:O	19:S:206:VAL:HG13	2.21	0.41
6:D:89:PHE:HA	6:D:92:LYS:NZ	2.34	0.41
12:K:179:THR:HG23	16:O:26:GLN:HB3	2.02	0.41
15:N:137:ASP:OD1	15:N:138:LYS:N	2.53	0.41
19:S:338:ILE:O	19:S:341:THR:HG22	2.20	0.41
20:T:485:GLU:OE1	20:T:543:ARG:HD3	2.20	0.41
2:5:123:U:H2'	2:5:124:C:C6	2.56	0.41
6:D:107:TYR:CE2	20:T:805:LYS:HD3	2.55	0.41
20:T:679:LEU:HD23	20:T:679:LEU:HA	1.92	0.41
2:5:96:U:HO2'	2:5:97:U:H5	1.68	0.41
3:6:59:A:H3'	3:6:60:G:H5''	2.03	0.41
4:A:1608:LEU:HD21	4:A:1648:ILE:HD11	2.03	0.41
4:A:1717:LEU:HB2	4:A:1786:ALA:HB3	2.03	0.41
5:C:110:LYS:HE2	5:C:110:LYS:HB3	1.88	0.41
19:S:105:TYR:CG	19:S:121:LEU:HD21	2.56	0.41
19:S:406:ILE:HD13	19:S:406:ILE:HA	1.90	0.41
20:T:508:LEU:HD22	20:T:544:ILE:HG23	2.03	0.41
5:C:766:TRP:CD1	5:C:792:LYS:HE3	2.55	0.41
9:H:49:ILE:HD13	9:H:49:ILE:HA	1.85	0.41
19:S:269:ILE:HD12	19:S:269:ILE:HA	1.95	0.41
4:A:1458:TRP:CG	21:V:305:SER:HB2	2.56	0.41
9:H:49:ILE:HD12	9:H:56:ILE:HD11	2.02	0.41
9:H:470:LEU:O	9:H:473:LEU:HB2	2.21	0.41
12:K:180:VAL:CG2	12:K:185:ARG:HG2	2.51	0.41
20:T:643:HIS:O	20:T:647:LEU:HG	2.21	0.41
3:6:21:U:H2'	3:6:22:G:C8	2.56	0.40
11:J:200:VAL:HG12	11:J:206:VAL:HG22	2.02	0.40
19:S:346:ILE:HG23	19:S:367:TRP:NE1	2.35	0.40
21:V:785:ALA:HB2	21:V:871:LEU:HD23	2.03	0.40
2:5:78:A:OP2	2:5:78:A:H8	2.04	0.40
4:A:276:VAL:HG12	4:A:280:LEU:HB2	2.04	0.40
4:A:1779:LEU:HB3	4:A:1815:LEU:HD21	2.03	0.40
5:C:839:ILE:HB	5:C:840:PRO:HD3	2.02	0.40
11:J:138:HIS:HE1	11:J:157:THR:OG1	2.04	0.40
16:O:88:ALA:HB2	16:O:95:ALA:HA	2.03	0.40
16:O:237:ILE:HD13	16:O:237:ILE:HA	1.94	0.40
4:A:1766:MET:HG3	4:A:1767:TYR:H	1.87	0.40
5:C:990:GLU:HB2	5:C:998:TYR:CD2	2.57	0.40
9:H:11:ILE:O	9:H:15:ARG:HG2	2.22	0.40
4:A:624:GLU:HG3	4:A:666:ILE:HA	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:82:LEU:O	16:O:125:ALA:HA	2.21	0.40
4:A:388:PRO:HB2	4:A:398:VAL:HG11	2.03	0.40
19:S:83:ARG:O	19:S:87:ILE:HG12	2.22	0.40
19:S:414:LEU:CD1	19:S:422:LYS:HG3	2.50	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	A	1942/2413 (80%)	1888 (97%)	54 (3%)	0	100	100
5	C	865/1008 (86%)	833 (96%)	32 (4%)	0	100	100
6	D	106/173 (61%)	106 (100%)	0	0	100	100
8	G	24/235 (10%)	24 (100%)	0	0	100	100
9	H	456/577 (79%)	449 (98%)	7 (2%)	0	100	100
11	J	378/451 (84%)	360 (95%)	18 (5%)	0	100	100
12	K	162/379 (43%)	157 (97%)	5 (3%)	0	100	100
13	L	154/157 (98%)	152 (99%)	2 (1%)	0	100	100
14	M	253/339 (75%)	248 (98%)	5 (2%)	0	100	100
15	N	256/364 (70%)	247 (96%)	9 (4%)	0	100	100
16	O	412/590 (70%)	407 (99%)	5 (1%)	0	100	100
17	P	68/175 (39%)	67 (98%)	1 (2%)	0	100	100
18	R	87/135 (64%)	82 (94%)	3 (3%)	2 (2%)	5	4
19	S	596/687 (87%)	586 (98%)	10 (2%)	0	100	100
20	T	689/859 (80%)	671 (97%)	18 (3%)	0	100	100
21	V	754/1145 (66%)	722 (96%)	31 (4%)	1 (0%)	48	60

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
22	W	168/238 (71%)	152 (90%)	15 (9%)	1 (1%)	22	26
23	Y	84/111 (76%)	81 (96%)	3 (4%)	0	100	100
24	Z	49/140 (35%)	48 (98%)	1 (2%)	0	100	100
25	a	170/251 (68%)	165 (97%)	5 (3%)	0	100	100
26	b	86/196 (44%)	85 (99%)	1 (1%)	0	100	100
26	k	100/196 (51%)	97 (97%)	3 (3%)	0	100	100
27	c	207/382 (54%)	196 (95%)	11 (5%)	0	100	100
28	d	79/101 (78%)	78 (99%)	1 (1%)	0	100	100
28	n	78/101 (77%)	77 (99%)	1 (1%)	0	100	100
29	e	84/94 (89%)	81 (96%)	3 (4%)	0	100	100
29	p	81/94 (86%)	80 (99%)	1 (1%)	0	100	100
30	f	72/86 (84%)	70 (97%)	2 (3%)	0	100	100
30	q	72/86 (84%)	70 (97%)	2 (3%)	0	100	100
31	g	69/77 (90%)	65 (94%)	4 (6%)	0	100	100
31	r	68/77 (88%)	66 (97%)	2 (3%)	0	100	100
32	h	105/146 (72%)	104 (99%)	1 (1%)	0	100	100
32	l	105/146 (72%)	102 (97%)	3 (3%)	0	100	100
33	j	89/110 (81%)	88 (99%)	1 (1%)	0	100	100
33	m	89/110 (81%)	88 (99%)	1 (1%)	0	100	100
34	o	340/455 (75%)	323 (95%)	17 (5%)	0	100	100
35	s	173/175 (99%)	166 (96%)	7 (4%)	0	100	100
36	t	130/503 (26%)	127 (98%)	2 (2%)	1 (1%)	16	20
36	u	130/503 (26%)	129 (99%)	1 (1%)	0	100	100
36	v	130/503 (26%)	129 (99%)	1 (1%)	0	100	100
36	w	130/503 (26%)	124 (95%)	5 (4%)	1 (1%)	16	20
37	y	133/215 (62%)	132 (99%)	1 (1%)	0	100	100
All	All	10223/15286 (67%)	9922 (97%)	295 (3%)	6 (0%)	50	60

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
18	R	59	ALA
21	V	943	GLN

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Mol	Chain	Res	Type
18	R	57	PRO
36	t	74	ASN
36	w	74	ASN
22	W	76	ILE

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
4	A	1770/2182 (81%)	1765 (100%)	5 (0%)	91 95
5	C	795/910 (87%)	792 (100%)	3 (0%)	89 94
6	D	100/159 (63%)	97 (97%)	3 (3%)	36 51
9	H	429/538 (80%)	421 (98%)	8 (2%)	52 68
11	J	318/397 (80%)	315 (99%)	3 (1%)	75 86
12	K	152/328 (46%)	147 (97%)	5 (3%)	33 47
13	L	140/141 (99%)	140 (100%)	0	100 100
14	M	219/296 (74%)	218 (100%)	1 (0%)	86 93
15	N	243/332 (73%)	241 (99%)	2 (1%)	79 88
16	O	219/525 (42%)	214 (98%)	5 (2%)	45 62
17	P	61/151 (40%)	61 (100%)	0	100 100
18	R	21/121 (17%)	21 (100%)	0	100 100
19	S	433/633 (68%)	422 (98%)	11 (2%)	42 59
20	T	551/786 (70%)	541 (98%)	10 (2%)	54 70
21	V	675/1028 (66%)	666 (99%)	9 (1%)	65 78
22	W	161/219 (74%)	156 (97%)	5 (3%)	35 50
23	Y	77/100 (77%)	76 (99%)	1 (1%)	65 78
24	Z	49/128 (38%)	47 (96%)	2 (4%)	26 38
25	a	152/225 (68%)	150 (99%)	2 (1%)	65 78
26	b	83/176 (47%)	81 (98%)	2 (2%)	44 60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
26	k	97/176 (55%)	97 (100%)	0	100	100
27	c	204/346 (59%)	200 (98%)	4 (2%)	50	67
28	d	70/89 (79%)	70 (100%)	0	100	100
28	n	69/89 (78%)	69 (100%)	0	100	100
29	e	75/83 (90%)	69 (92%)	6 (8%)	10	12
29	p	74/83 (89%)	74 (100%)	0	100	100
30	f	66/77 (86%)	63 (96%)	3 (4%)	23	34
30	q	66/77 (86%)	65 (98%)	1 (2%)	60	75
31	g	61/66 (92%)	60 (98%)	1 (2%)	58	73
31	r	60/66 (91%)	60 (100%)	0	100	100
32	h	96/129 (74%)	95 (99%)	1 (1%)	73	84
32	l	96/129 (74%)	94 (98%)	2 (2%)	48	65
33	j	85/103 (82%)	85 (100%)	0	100	100
33	m	85/103 (82%)	83 (98%)	2 (2%)	44	60
34	o	314/413 (76%)	314 (100%)	0	100	100
37	y	102/193 (53%)	102 (100%)	0	100	100
All	All	8268/11597 (71%)	8171 (99%)	97 (1%)	66	80

All (97) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	310	ASN
4	A	493	MET
4	A	1085	LYS
4	A	1618	ASN
4	A	2038	HIS
5	C	189	LEU
5	C	220	ASN
5	C	763	ARG
6	D	82	LEU
6	D	92	LYS
6	D	120	LYS
9	H	85	SER
9	H	108	ARG
9	H	132	GLU
9	H	205	TYR

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Mol	Chain	Res	Type
9	H	249	ASN
9	H	470	LEU
9	H	472	LEU
9	H	473	LEU
11	J	11	LEU
11	J	275	THR
11	J	408	ASP
12	K	60	LYS
12	K	103	ASN
12	K	110	HIS
12	K	161	ASN
12	K	206	GLU
14	M	148	SER
15	N	50	LYS
15	N	51	ARG
16	O	123	LEU
16	O	135	GLN
16	O	136	MET
16	O	246	ARG
16	O	296	LYS
19	S	27	GLN
19	S	139	TYR
19	S	263	SER
19	S	288	GLU
19	S	315	ASN
19	S	339	MET
19	S	350	ARG
19	S	407	TRP
19	S	458	LYS
19	S	463	PHE
19	S	477	TYR
20	T	290	PHE
20	T	292	ARG
20	T	294	MET
20	T	346	TYR
20	T	349	PHE
20	T	442	THR
20	T	448	ARG
20	T	451	CYS
20	T	484	LEU
20	T	784	PHE
21	V	315	GLU

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Mol	Chain	Res	Type
21	V	388	ILE
21	V	555	LYS
21	V	575	ARG
21	V	770	TYR
21	V	886	ASP
21	V	942	ARG
21	V	952	LYS
21	V	971	GLN
22	W	20	ASN
22	W	110	ARG
22	W	126	ASN
22	W	146	ARG
22	W	153	THR
23	Y	69	ARG
24	Z	12	ASP
24	Z	102	LYS
25	a	114	ASN
25	a	177	ASN
26	b	26	ASP
26	b	33	GLN
27	c	79	LYS
27	c	159	LEU
27	c	286	LYS
27	c	298	LYS
29	e	23	GLN
29	e	25	THR
29	e	34	GLN
29	e	68	LYS
29	e	73	LYS
29	e	92	SER
30	f	30	LYS
30	f	55	GLU
30	f	65	HIS
31	g	30	ARG
32	h	6	PHE
32	l	14	GLN
32	l	86	ASN
33	m	22	GLU
33	m	52	HIS
30	q	74	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (60) such sidechains are listed below:

Mol	Chain	Res	Type
4	A	146	HIS
4	A	178	ASN
4	A	181	HIS
4	A	405	ASN
4	A	487	ASN
4	A	559	GLN
4	A	659	HIS
4	A	676	GLN
4	A	848	ASN
4	A	1404	HIS
4	A	1522	ASN
4	A	1902	GLN
4	A	1929	GLN
5	C	103	HIS
5	C	108	GLN
5	C	158	HIS
5	C	355	HIS
5	C	471	HIS
5	C	1004	ASN
9	H	354	HIS
9	H	362	ASN
9	H	429	ASN
9	H	457	HIS
11	J	138	HIS
11	J	160	ASN
11	J	181	HIS
11	J	271	GLN
11	J	280	GLN
11	J	306	HIS
12	K	103	ASN
12	K	148	HIS
14	M	44	ASN
14	M	58	HIS
15	N	72	GLN
16	O	47	GLN
16	O	82	ASN
17	P	34	HIS
19	S	67	GLN
19	S	79	HIS
19	S	467	GLN
21	V	402	ASN
21	V	781	ASN
21	V	841	GLN

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Mol	Chain	Res	Type
22	W	106	ASN
22	W	115	GLN
22	W	143	HIS
23	Y	64	ASN
25	a	177	ASN
25	a	203	HIS
25	a	208	HIS
25	a	212	GLN
27	c	89	ASN
27	c	124	ASN
32	h	86	ASN
32	l	78	ASN
32	l	86	ASN
34	o	185	HIS
30	q	77	ASN
37	y	185	ASN
37	y	200	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	126/1175 (10%)	26 (20%)	5 (3%)
10	I	45/95 (47%)	13 (28%)	6 (13%)
2	5	169/214 (78%)	16 (9%)	4 (2%)
3	6	101/112 (90%)	9 (8%)	0
7	E	32/42 (76%)	14 (43%)	6 (18%)
All	All	473/1638 (28%)	78 (16%)	21 (4%)

All (78) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	19	U
1	2	21	G
1	2	25	A
1	2	31	A
1	2	32	G
1	2	114	U
1	2	119	G
1	2	120	G
1	2	121	C
1	2	122	A

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Mol	Chain	Res	Type
1	2	123	C
1	2	145	G
1	2	147	A
1	2	1083	A
1	2	1094	G
1	2	1095	U
1	2	1097	G
1	2	1101	C
1	2	1102	C
1	2	1104	U
1	2	1106	G
1	2	1137	U
1	2	1144	U
1	2	1145	U
1	2	1146	G
1	2	1170	G
2	5	18	A
2	5	33	U
2	5	42	A
2	5	70	A
2	5	77	A
2	5	78	A
2	5	79	C
2	5	80	G
2	5	81	A
2	5	127	U
2	5	169	U
2	5	170	U
2	5	174	G
2	5	175	G
2	5	177	A
2	5	178	C
3	6	7	G
3	6	9	A
3	6	32	U
3	6	36	U
3	6	54	U
3	6	60	G
3	6	68	C
3	6	80	U
3	6	91	A
7	E	-13	G

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Mol	Chain	Res	Type
7	E	-11	G
7	E	-10	A
7	E	3	A
7	E	4	U
7	E	6	C
7	E	7	A
7	E	8	C
7	E	9	C
7	E	10	U
7	E	11	A
7	E	17	U
7	E	18	G
7	E	21	G
10	I	10	A
10	I	62	A
10	I	70	A
10	I	71	C
10	I	72	A
10	I	73	A
10	I	74	A
10	I	75	A
10	I	76	U
10	I	87	U
10	I	89	G
10	I	91	A
10	I	92	C

All (21) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	31	A
1	2	146	A
1	2	1082	A
1	2	1093	C
1	2	1145	U
2	5	41	A
2	5	69	G
2	5	70	A
2	5	80	G
7	E	-14	A
7	E	-11	G
7	E	-7	U

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Mol	Chain	Res	Type
7	E	3	A
7	E	9	C
7	E	16	A
10	I	58	U
10	I	61	U
10	I	70	A
10	I	71	C
10	I	75	A
10	I	91	A

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PSU	6	28	3	18,21,22	1.06	1 (5%)	21,30,33	2.08	5 (23%)

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
3	PSU	6	28	3	-	1/7/25/26	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	6	28	PSU	C6-C5	3.01	1.38	1.35

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	6	28	PSU	N1-C2-N3	5.26	120.72	115.17
3	6	28	PSU	C4-N3-C2	-5.09	119.36	126.37
3	6	28	PSU	C6-C5-C4	3.07	120.25	118.17
3	6	28	PSU	O2-C2-N1	-2.79	119.91	122.79
3	6	28	PSU	C6-N1-C2	-2.56	120.32	122.69

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	6	28	PSU	O4'-C1'-C5-C4

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 16 ligands modelled in this entry, 13 are monoatomic - leaving 3 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
41	GTP	C	2501	38	29,34,34	1.28	2 (6%)	35,54,54	1.44	5 (14%)
40	IHP	S	701	-	36,36,36	0.69	0	60,60,60	0.85	2 (3%)
40	IHP	A	2500	-	36,36,36	0.82	0	60,60,60	0.60	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
41	GTP	C	2501	38	-	2/18/38/38	0/3/3/3
40	IHP	S	701	-	-	2/30/54/54	0/1/1/1
40	IHP	A	2500	-	-	1/30/54/54	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	C	2501	GTP	C5-C6	-4.53	1.38	1.47
41	C	2501	GTP	C5-C4	-2.17	1.37	1.43

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	C	2501	GTP	C8-N7-C5	3.84	109.09	102.55
41	C	2501	GTP	C5-C6-N1	3.10	119.99	114.07
41	C	2501	GTP	C2-N1-C6	-2.94	119.73	125.11
41	C	2501	GTP	O2B-PB-O3A	2.81	114.88	107.27
40	S	701	IHP	C6-C1-C2	2.78	116.53	110.43
41	C	2501	GTP	O4'-C1'-N9	2.66	112.27	108.75
40	S	701	IHP	P2-O12-C2	-2.03	118.02	123.43

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
40	S	701	IHP	C1-O11-P1-O21
40	A	2500	IHP	C3-O13-P3-O43
40	S	701	IHP	C4-O14-P4-O34
41	C	2501	GTP	PA-O3A-PB-O1B
41	C	2501	GTP	PB-O3B-PG-O3G

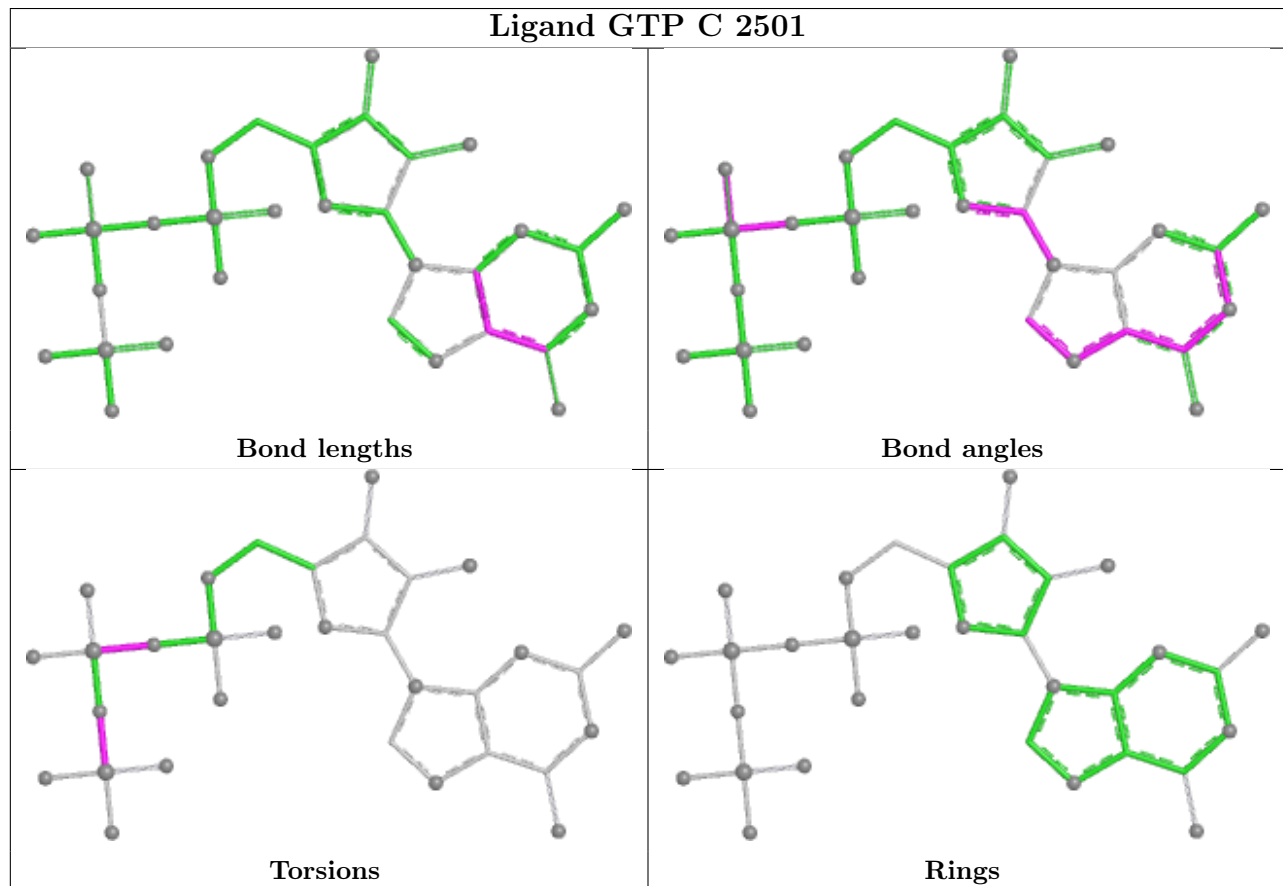
There are no ring outliers.

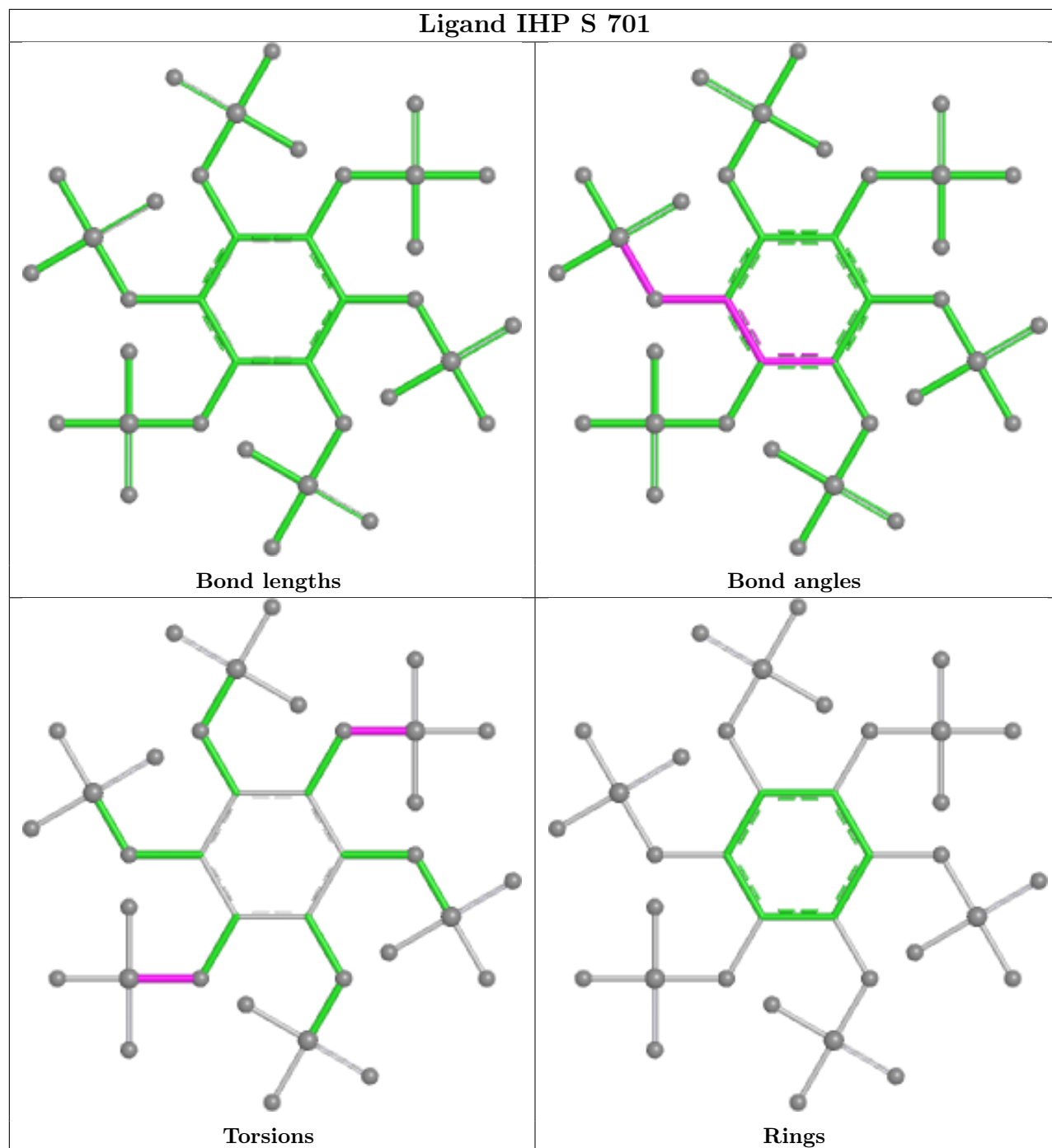
2 monomers are involved in 2 short contacts:

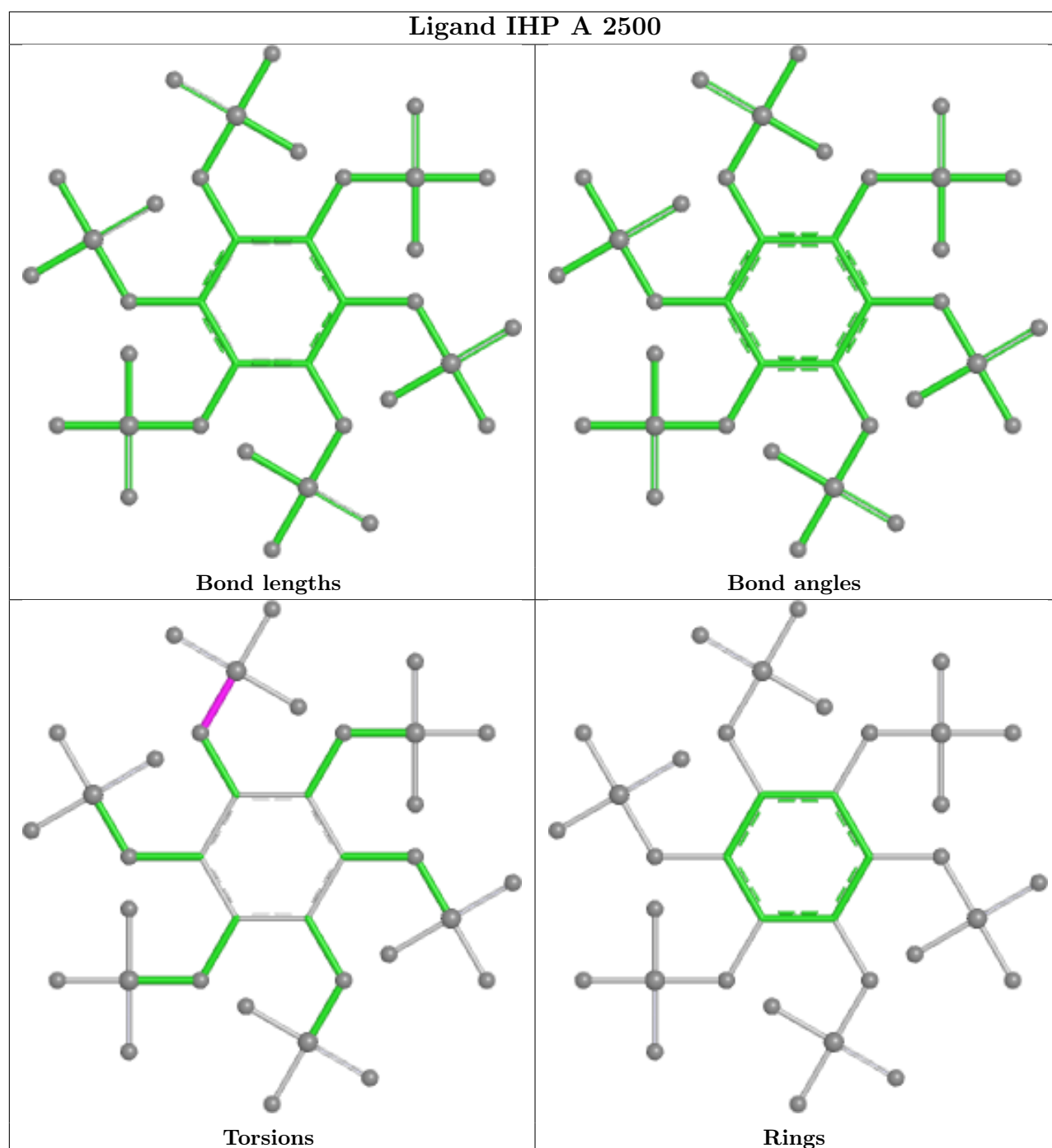
Mol	Chain	Res	Type	Clashes	Symm-Clashes
40	S	701	IHP	1	0
40	A	2500	IHP	1	0

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

also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

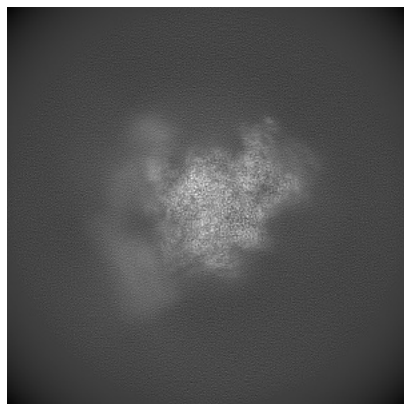
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-47157. These allow visual inspection of the internal detail of the map and identification of artifacts.

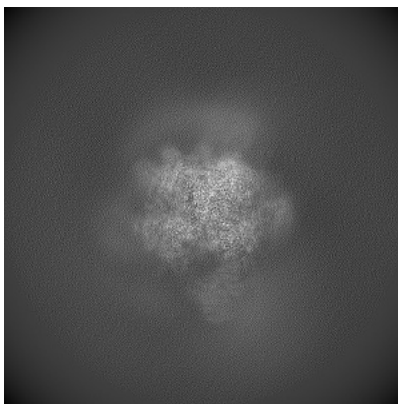
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

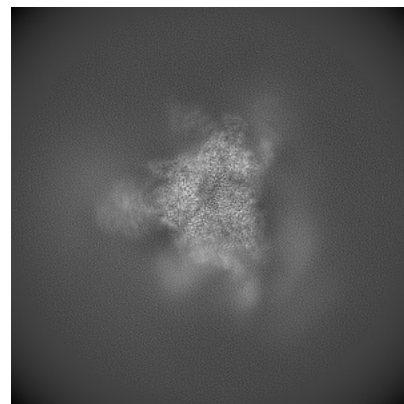
6.1.1 Primary map



X

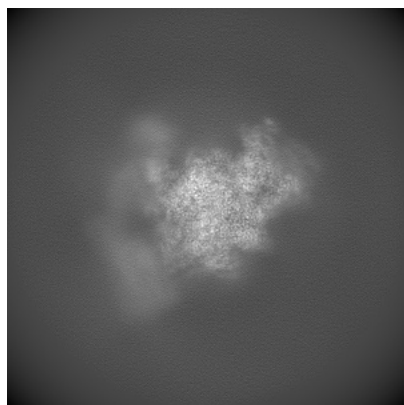


Y

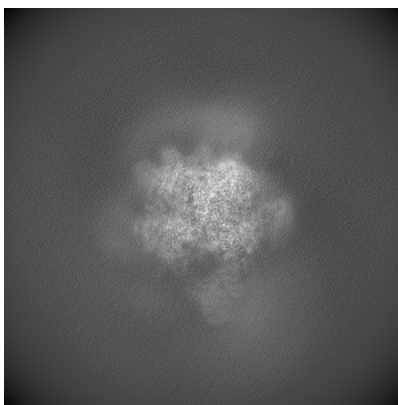


Z

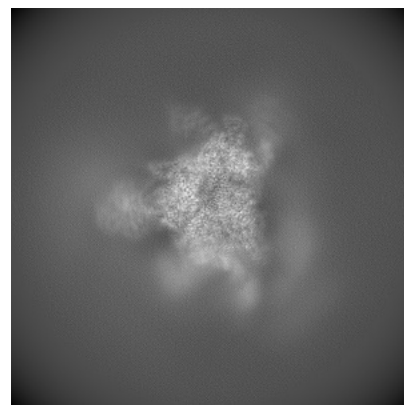
6.1.2 Raw map



X



Y

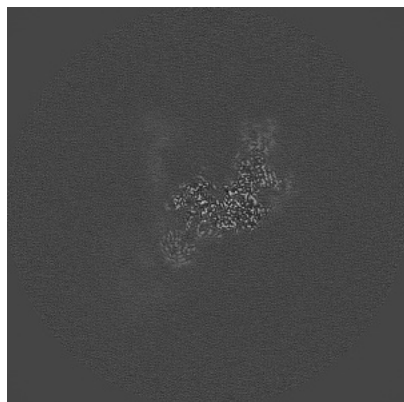


Z

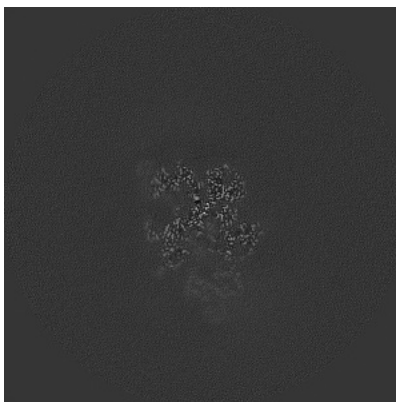
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

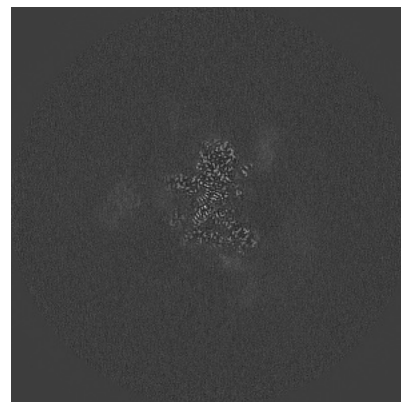
6.2.1 Primary map



X Index: 240

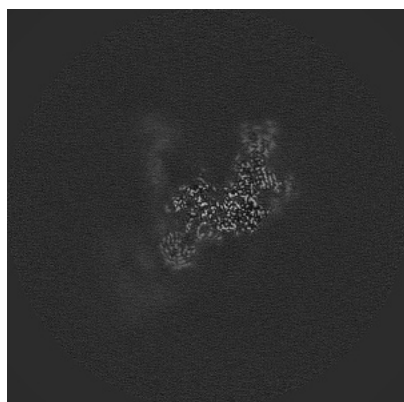


Y Index: 240

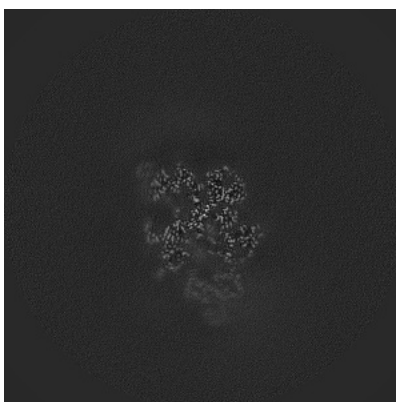


Z Index: 240

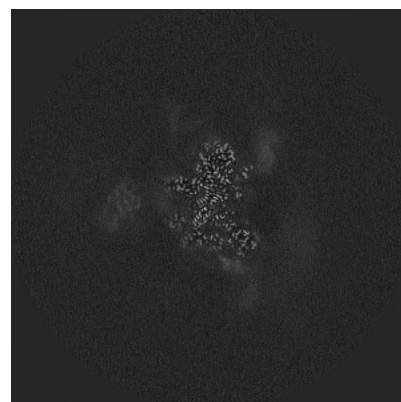
6.2.2 Raw map



X Index: 240



Y Index: 240

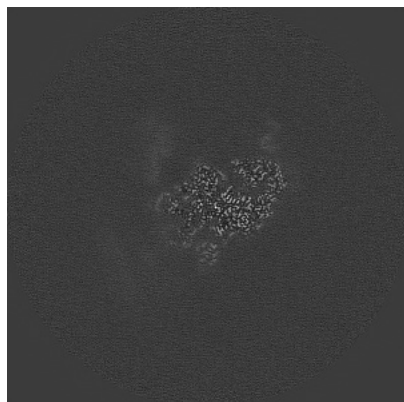


Z Index: 240

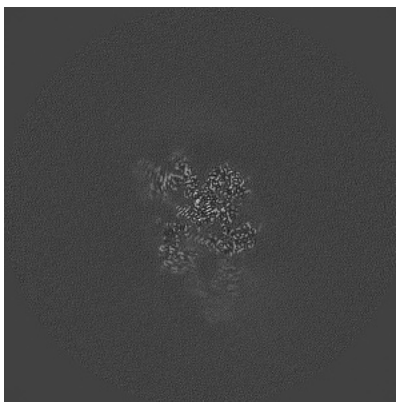
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

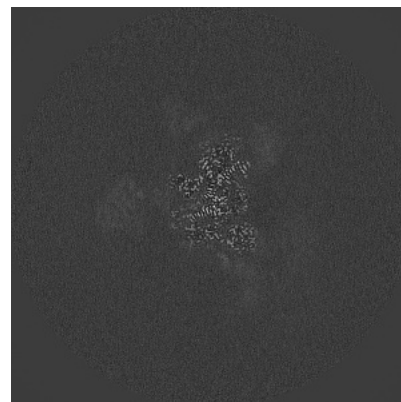
6.3.1 Primary map



X Index: 253

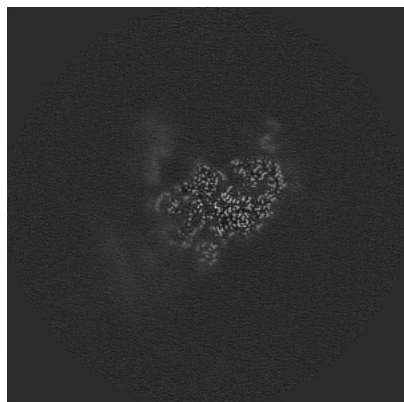


Y Index: 234

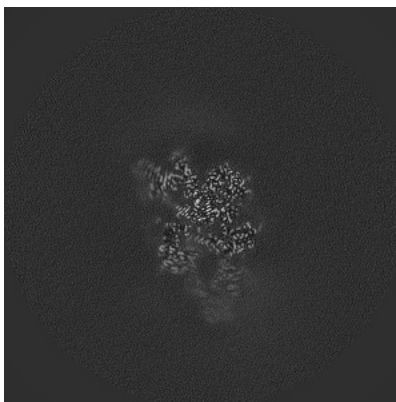


Z Index: 244

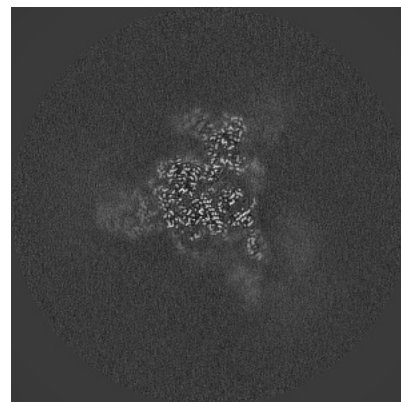
6.3.2 Raw map



X Index: 253



Y Index: 234

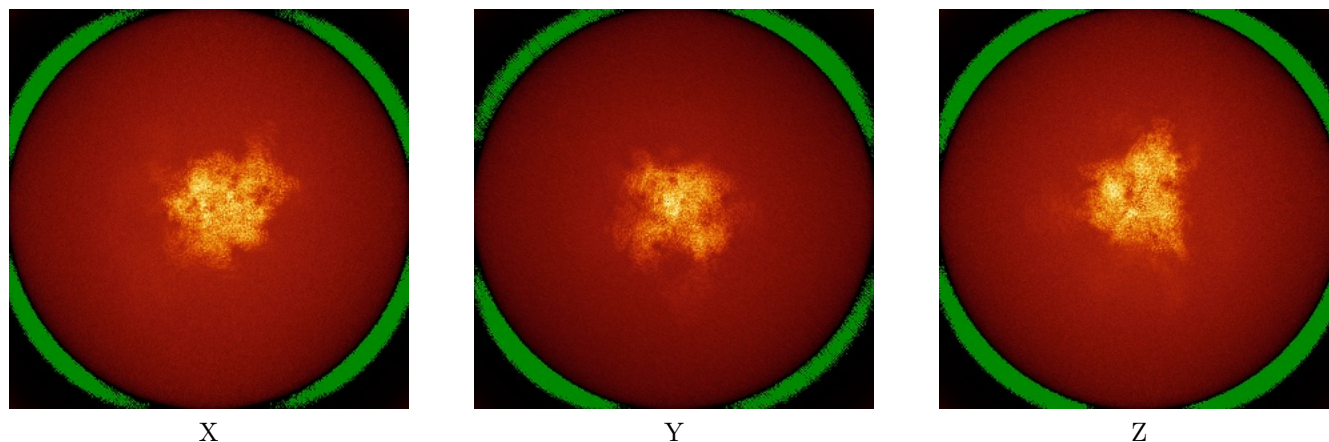


Z Index: 265

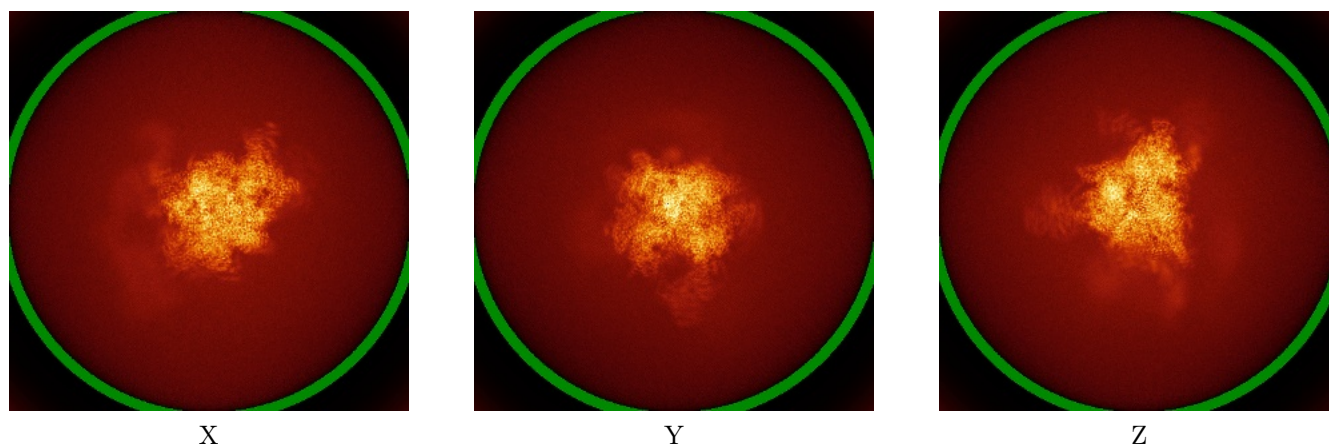
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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



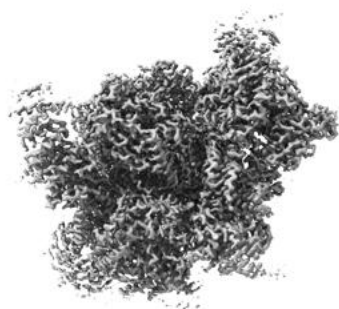
Y



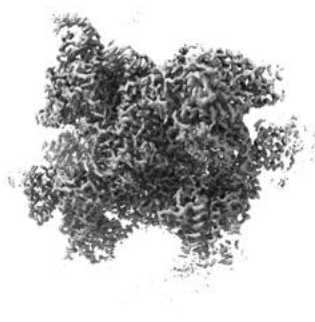
Z

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

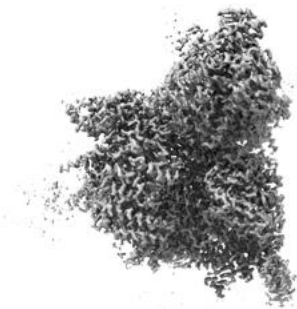
6.5.2 Raw map



X



Y



Z

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

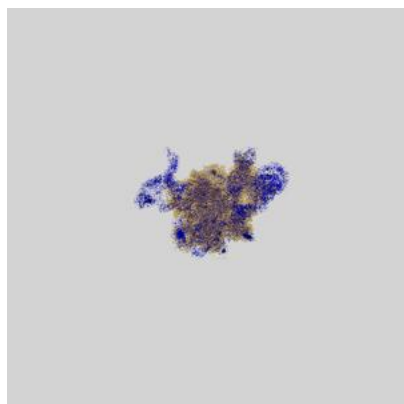
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

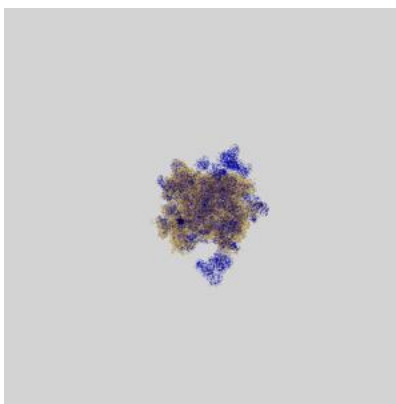
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

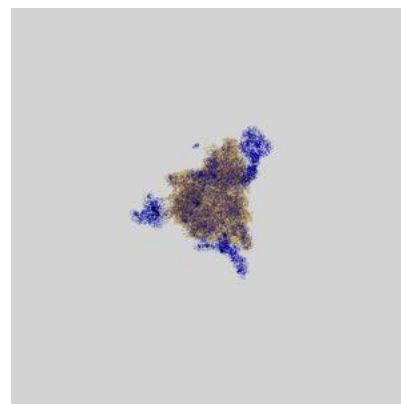
6.6.1 emd_47157_msk_1.map [i](#)



X



Y

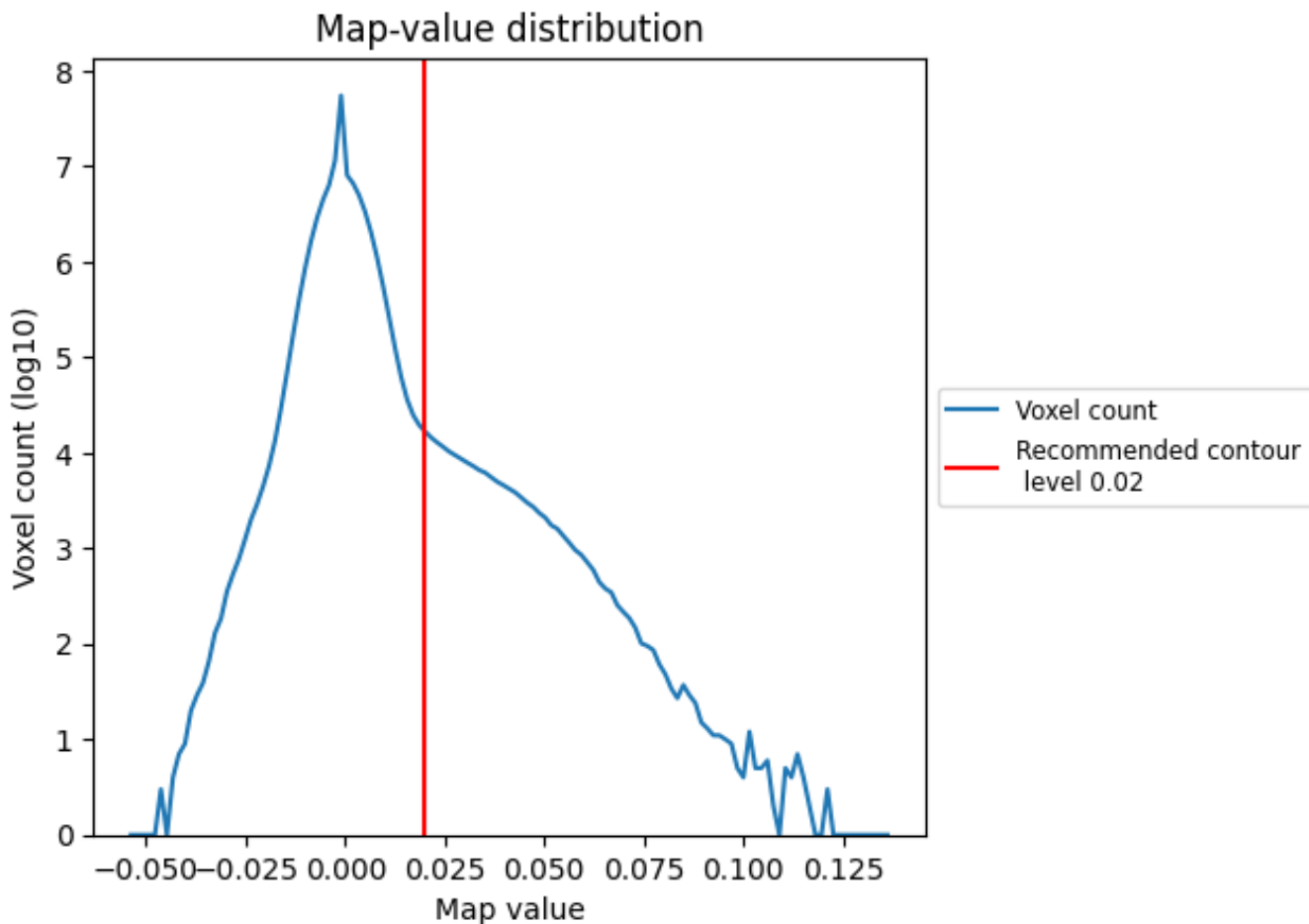


Z

7 Map analysis [i](#)

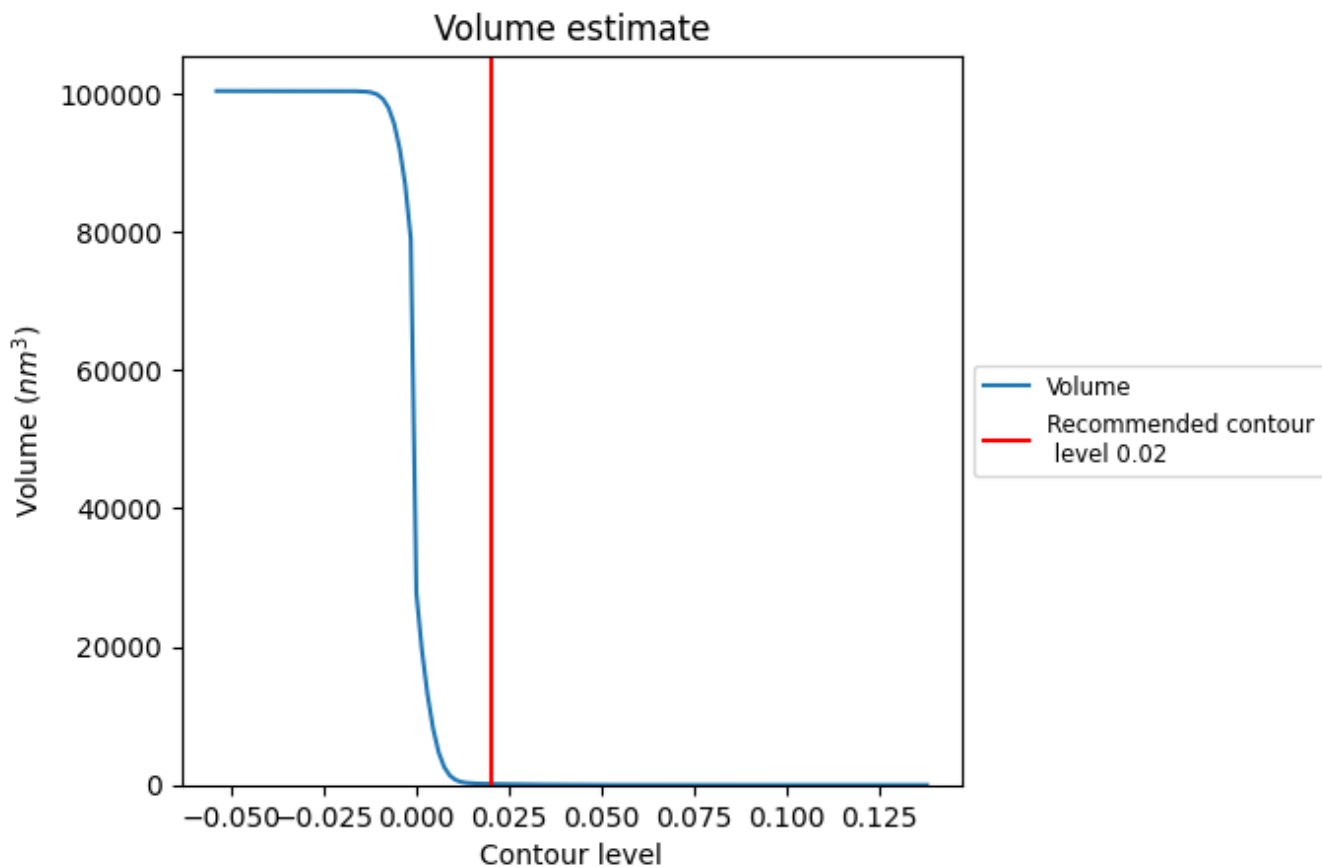
This section contains the results of statistical analysis of the map.

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.

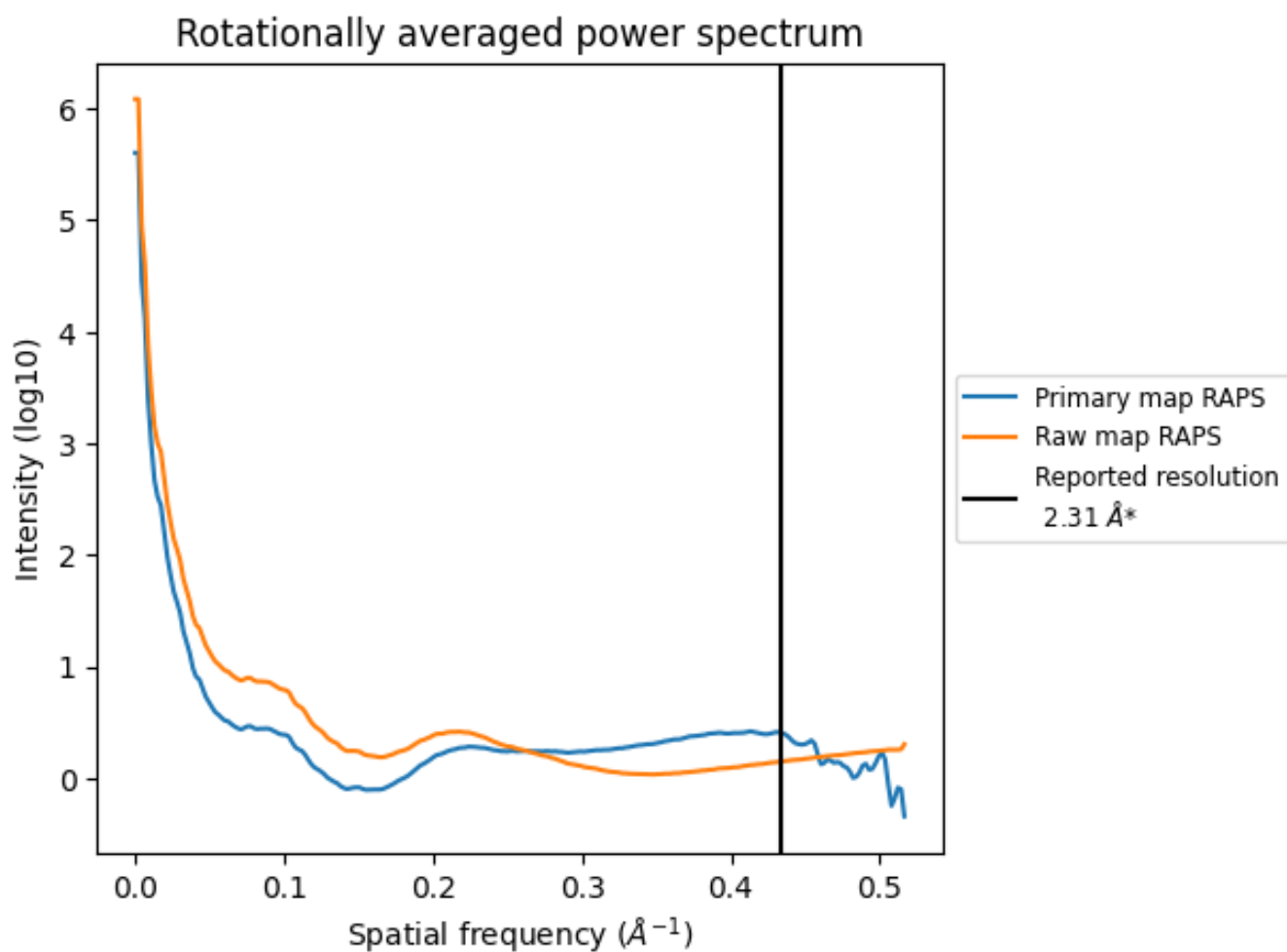
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 146 nm^3 ; this corresponds to an approximate mass of 132 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum [i](#)

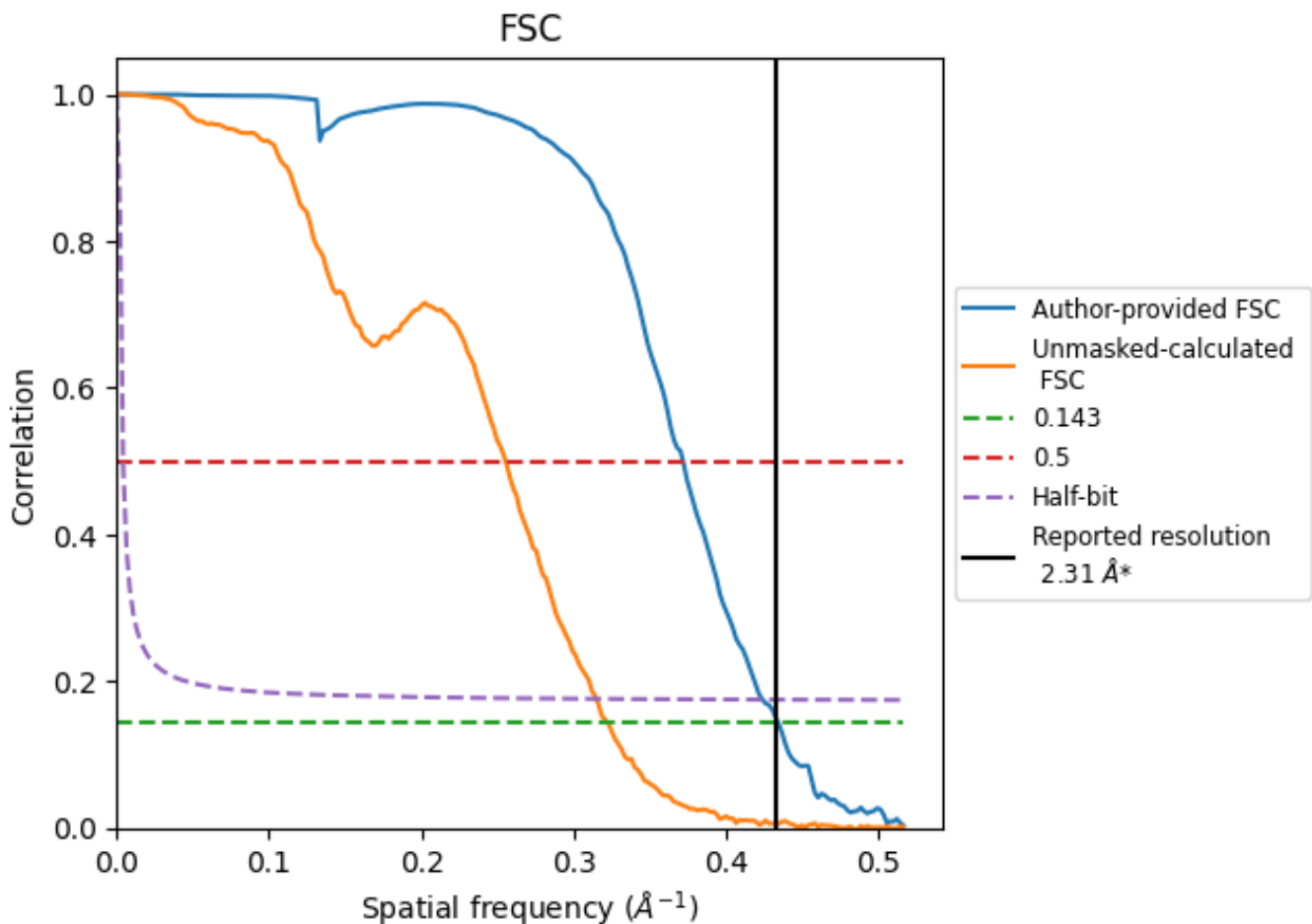


*Reported resolution corresponds to spatial frequency of 0.433 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.433 Å⁻¹

8.2 Resolution estimates [i](#)

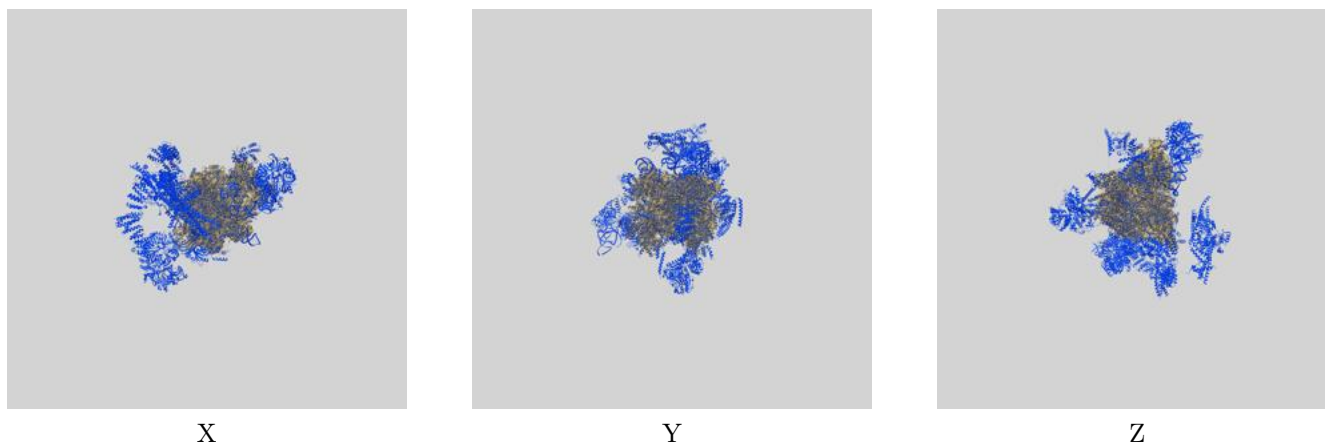
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.31	-	-
Author-provided FSC curve	2.30	2.69	2.36
Unmasked-calculated*	3.10	3.92	3.18

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.10 differs from the reported value 2.31 by more than 10 %

9 Map-model fit [i](#)

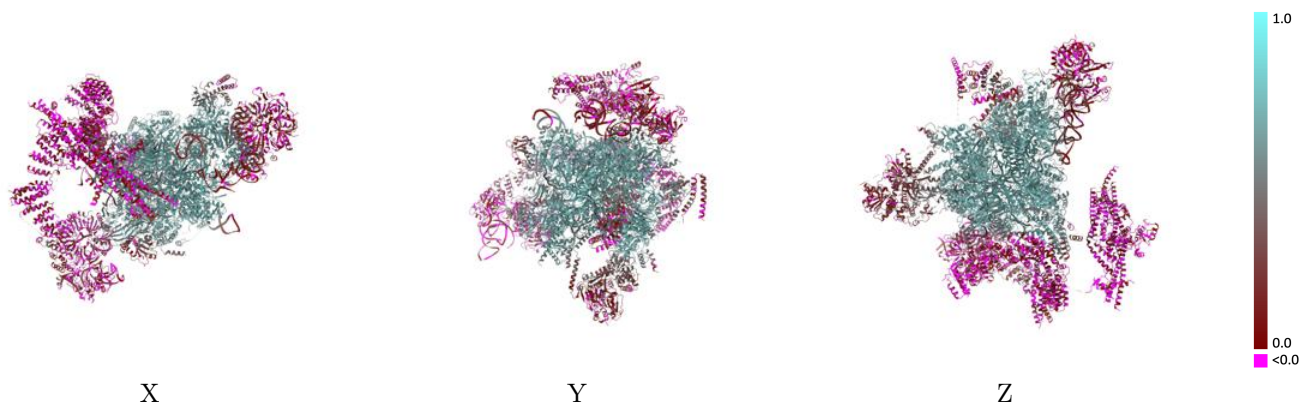
This section contains information regarding the fit between EMDB map EMD-47157 and PDB model 9DTR. Per-residue inclusion information can be found in section [3](#) on page [13](#).

9.1 Map-model overlay [i](#)



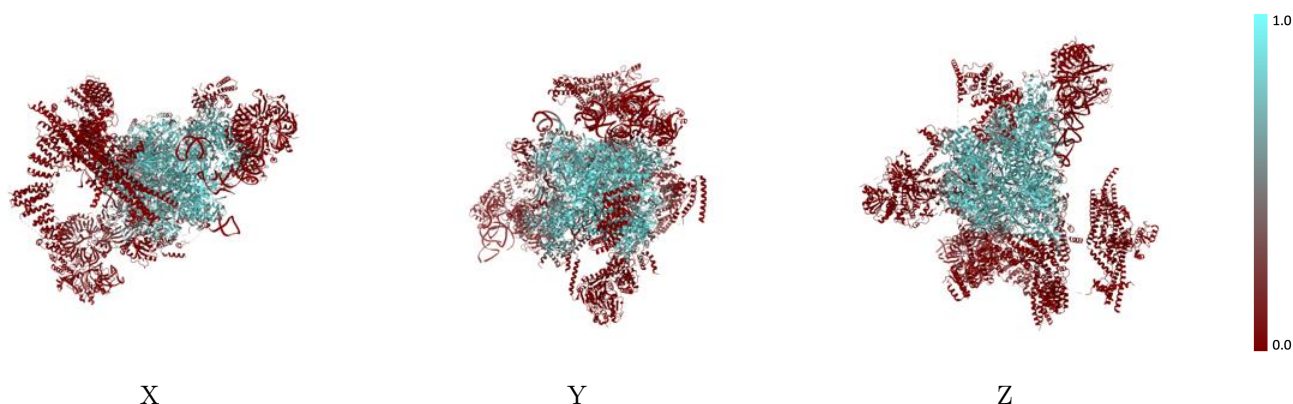
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



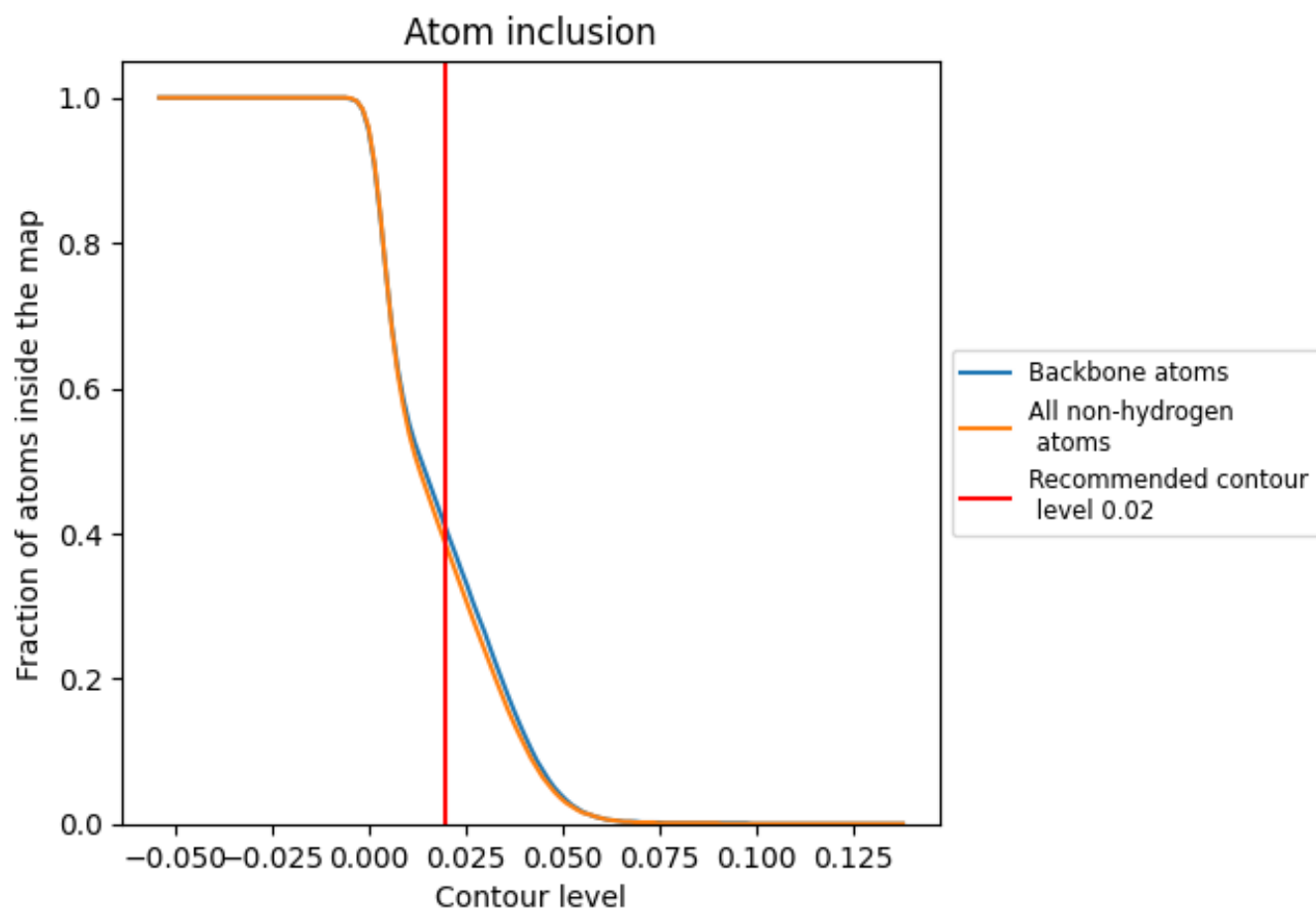
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.02).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 41% of all backbone atoms, 38% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary



























The table lists the average atom inclusion at the recommended contour level (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.3830	 0.4190
2	 0.1890	 0.1990
5	 0.4020	 0.3860
6	 0.6940	 0.6010
A	 0.8090	 0.6900
C	 0.6380	 0.6380
D	 0.1020	 0.3640
E	 0.3640	 0.4890
G	 0.0000	 0.2440
H	 0.2550	 0.3880
I	 0.4820	 0.5290
J	 0.7740	 0.6530
K	 0.6140	 0.6310
L	 0.7560	 0.6820
M	 0.5670	 0.6180
N	 0.3400	 0.4580
O	 0.4200	 0.4350
P	 0.6700	 0.6760
R	 0.3160	 0.3600
S	 0.3100	 0.3250
T	 0.0000	 0.0850
V	 0.0330	 0.2770
W	 0.0000	 0.0680
Y	 0.0000	 0.0490
Z	 0.0000	 0.0240
a	 0.4950	 0.5960
b	 0.0000	 0.1840
c	 0.3990	 0.5810
d	 0.0000	 0.2890
e	 0.0000	 0.0740
f	 0.0000	 0.0680
g	 0.0000	 0.1370
h	 0.0000	 0.1120
j	 0.0000	 0.0920
k	 0.0000	 0.0590



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Chain	Atom inclusion	Q-score
l	 0.0000	 0.0350
m	 0.0000	 0.0140
n	 0.0000	 0.0770
o	 0.3940	 0.5910
p	 0.0000	 0.0230
q	 0.0000	 0.0210
r	 0.0000	 0.0590
s	 0.0000	 0.0340
t	 0.0000	 0.0360
u	 0.0000	 0.0180
v	 0.0000	 0.0450
w	 0.0000	 0.0390
y	 0.4080	 0.4650