



Full wwPDB EM Validation Report ⓘ

Jun 9, 2026 – 03:37 PM EDT

PDB ID : 9DTR / pdb_00009dtr
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:

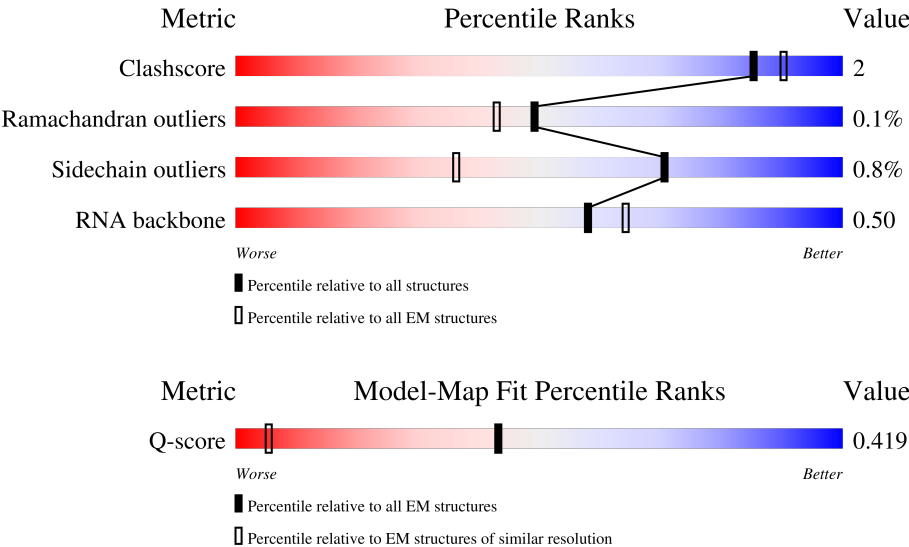
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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) : 2.49

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 2.31 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)	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	4306 (1.81 - 2.81)

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	9% 7% 89%
2	5	214	46% 69% 11% 19%
3	6	112	21% 70% 20% 9%

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Mol	Chain	Length	Quality of chain
4	A	2413	
5	C	1008	
6	D	173	
7	E	42	
8	G	235	
9	H	577	
10	I	95	
11	J	451	
12	K	379	
13	L	157	
14	M	339	
15	N	364	
16	O	590	
17	P	175	
18	R	135	
19	S	687	
20	T	859	
21	V	1145	
22	W	238	
23	Y	111	
24	Z	140	
25	a	251	
26	b	196	
26	k	196	
27	c	382	

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Mol	Chain	Length	Quality of chain
28	d	101	
28	n	101	
29	e	94	
29	p	94	
30	f	86	
30	q	86	
31	g	77	
31	r	77	
32	h	146	
32	l	146	
33	j	110	
33	m	110	
34	o	455	
35	s	175	
36	t	503	
36	u	503	
36	v	503	
36	w	503	
37	y	215	

2 Entry composition [i](#)

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
1	2	132	Total	C	N	O	P	0	0
			2779	1242	456	949	132		

- Molecule 2 is a RNA chain called U5 snRNA.

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

- Molecule 3 is a RNA chain called U6 snRNA.

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

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

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

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

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

- Molecule 6 is a protein called Protein FYV6.

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

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

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

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
8	G	28	Total	C	N	O	0	0
			139	83	28	28		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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
22	W	170	Total	C	N	O	S	0	0
			1383	866	253	257	7		

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

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

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

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

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

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

- 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		

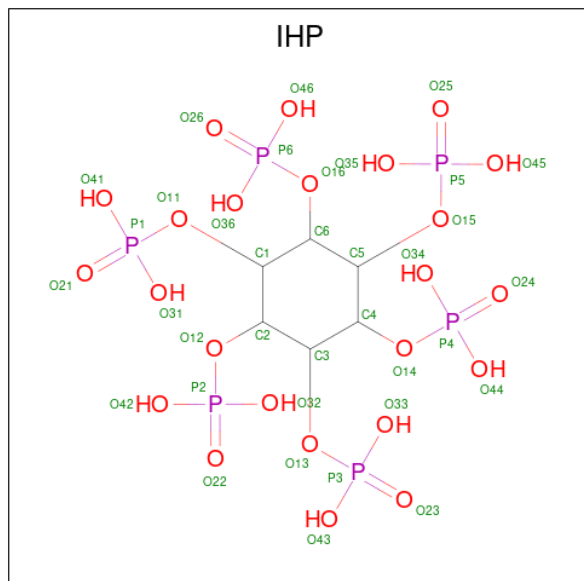
- Molecule 38 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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 (CCD ID: K) (formula: K).

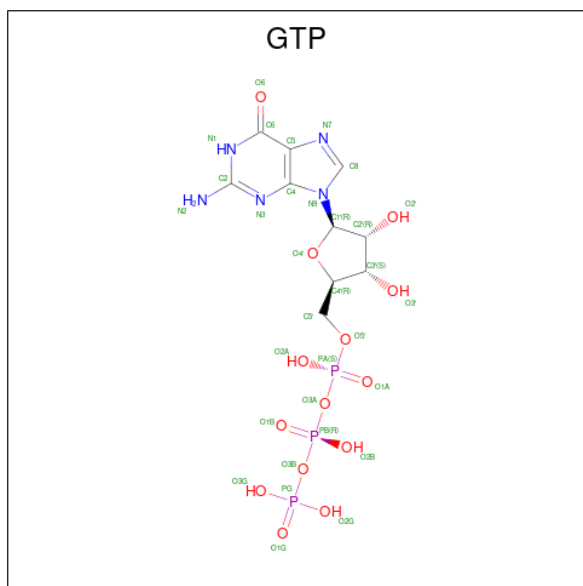
Mol	Chain	Residues	Atoms		AltConf
39	6	3	Total	K	0
			3	3	
39	E	1	Total	K	0
			1	1	

- Molecule 40 is INOSITOL HEXAKISPHOSPHATE (CCD ID: IHP) (formula: $C_6H_{18}O_{24}P_6$).



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 (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



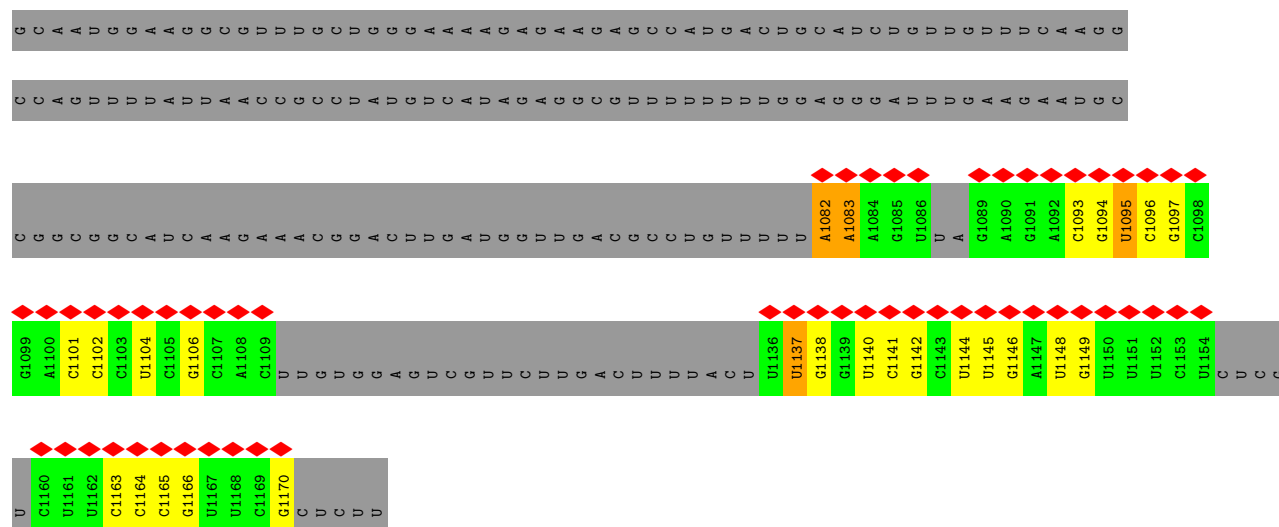
Mol	Chain	Residues	Atoms					AltConf
41	C	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 42 is ZINC ION (CCD ID: ZN) (formula: Zn).

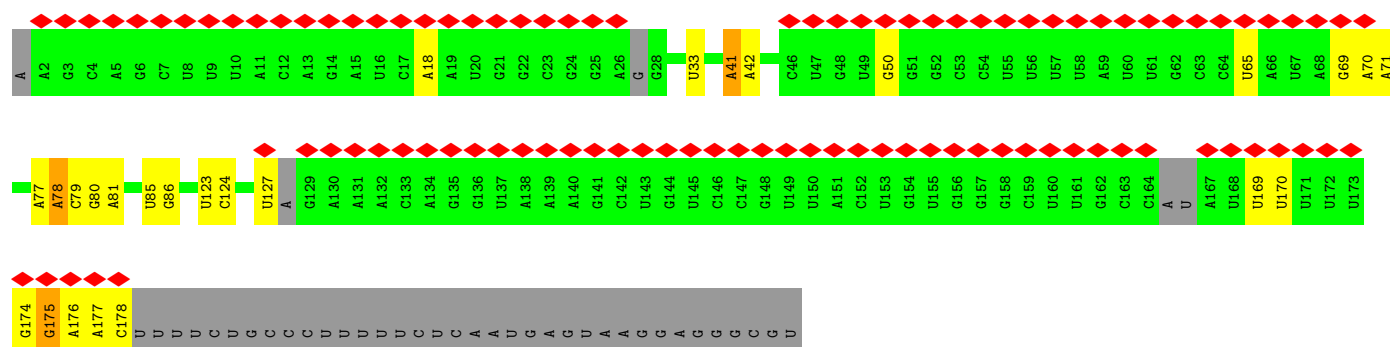
Mol	Chain	Residues	Atoms		AltConf
42	L	3	Total	Zn	0
			3	3	
42	M	1	Total	Zn	0
			1	1	
42	N	2	Total	Zn	0
			2	2	
42	c	1	Total	Zn	0
			1	1	

- Molecule 43 is water.

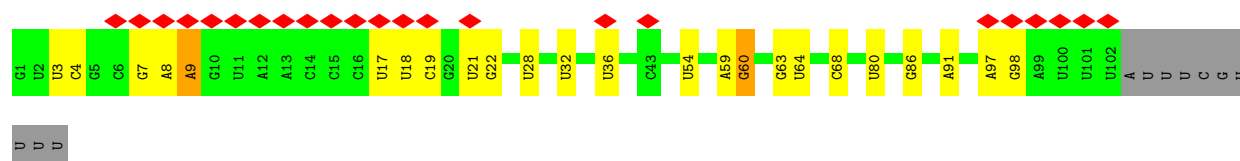
Mol	Chain	Residues	Atoms		AltConf
43	6	1	Total	O	0
			1	1	



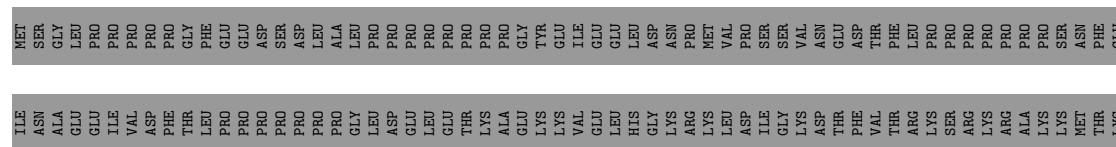
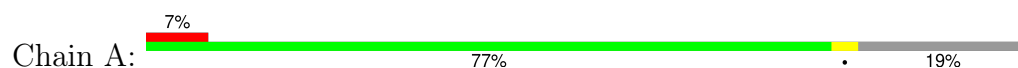
• Molecule 2: U5 snRNA



• Molecule 3: U6 snRNA

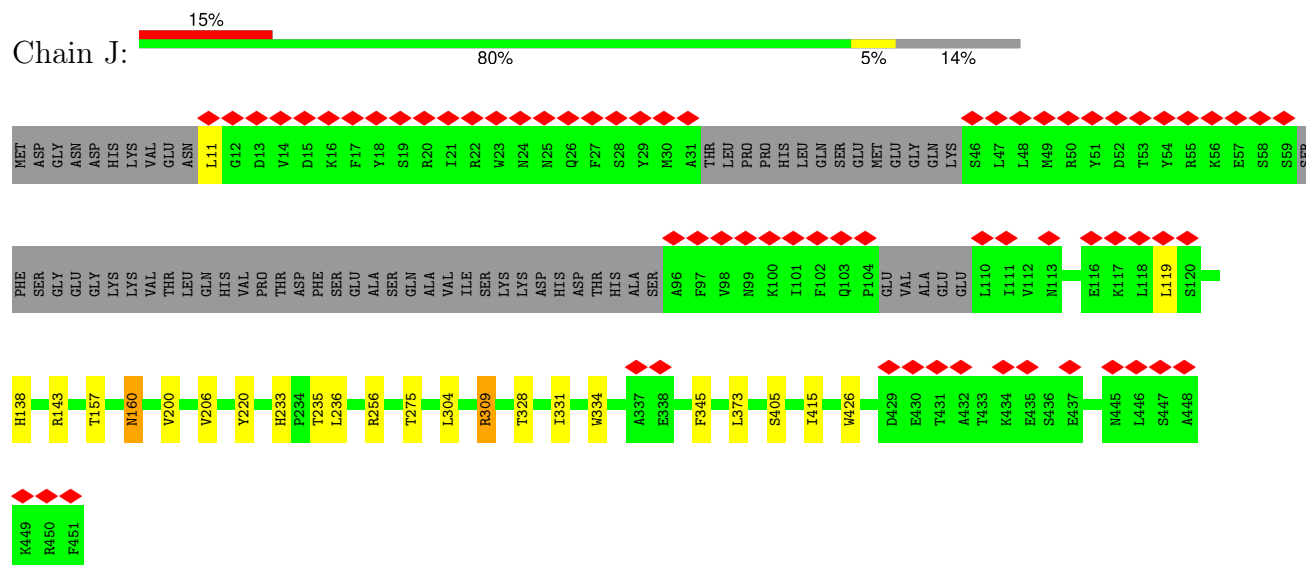


• Molecule 4: Pre-mRNA-splicing factor 8

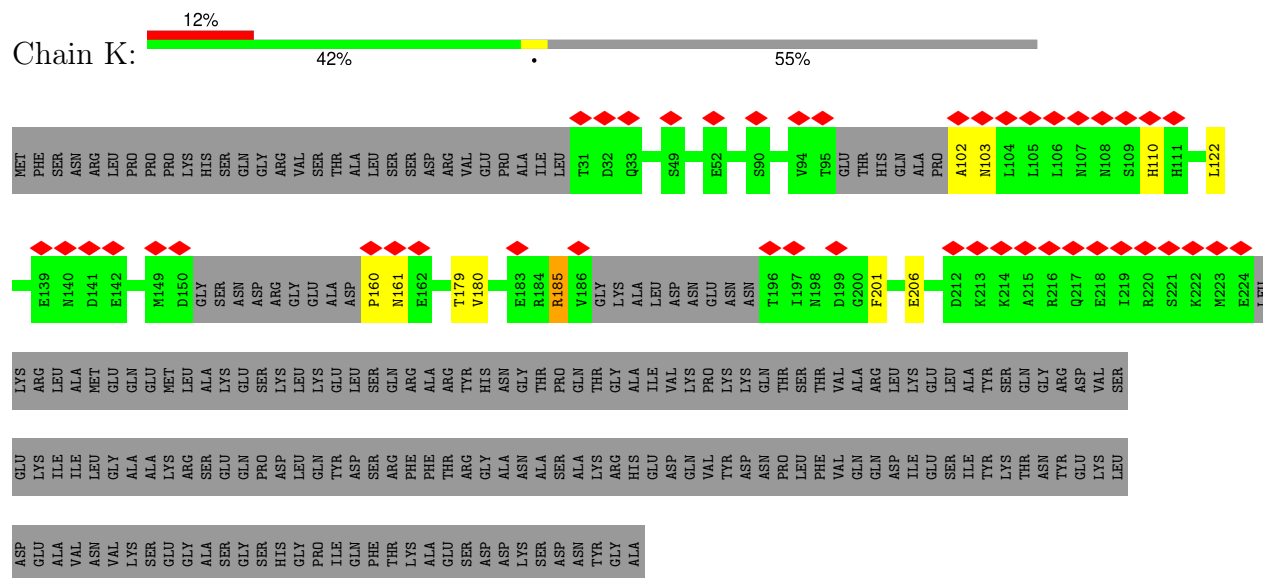




- Molecule 11: Pre-mRNA-splicing factor PRP46

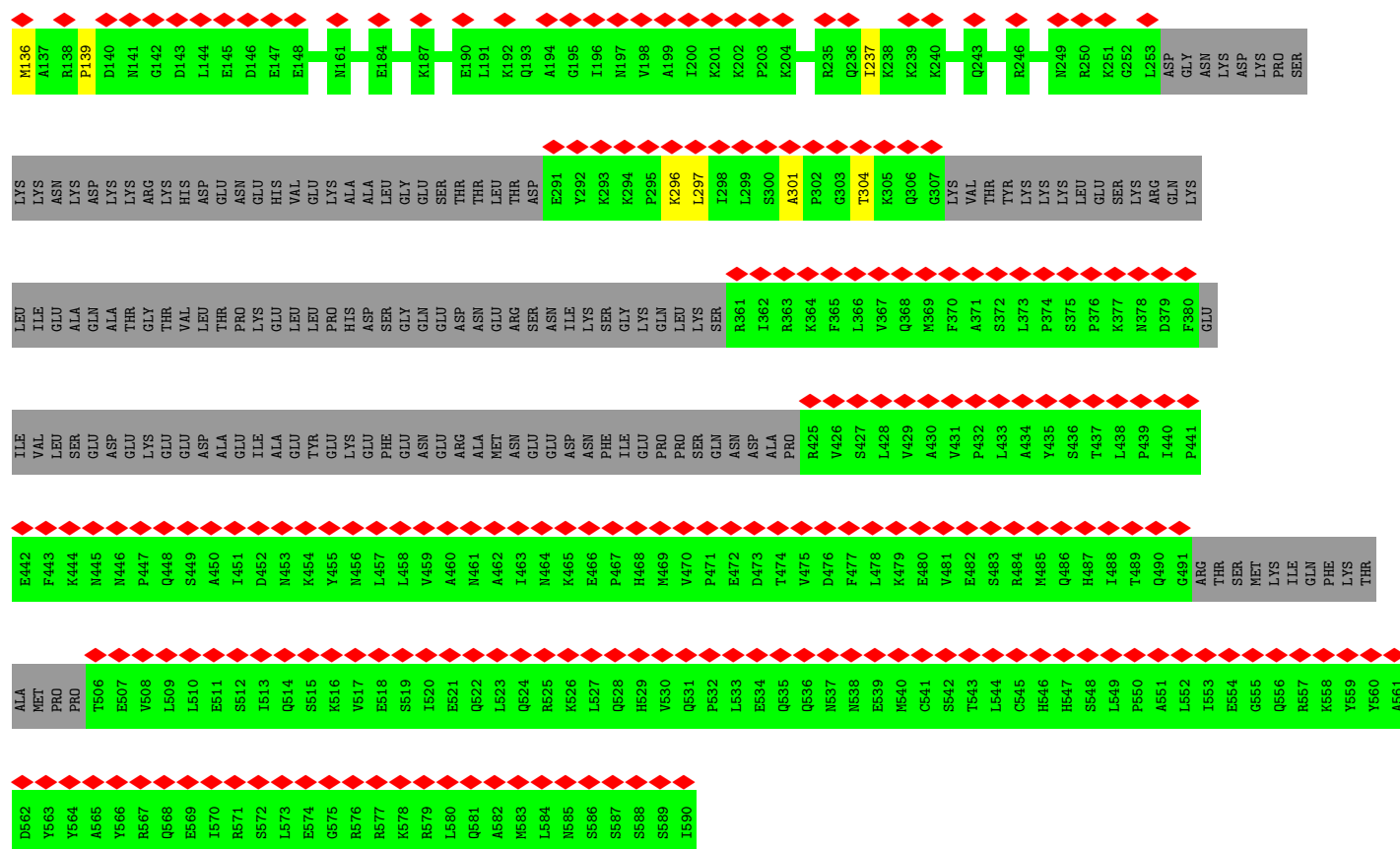


- Molecule 12: Pre-mRNA-processing protein 45

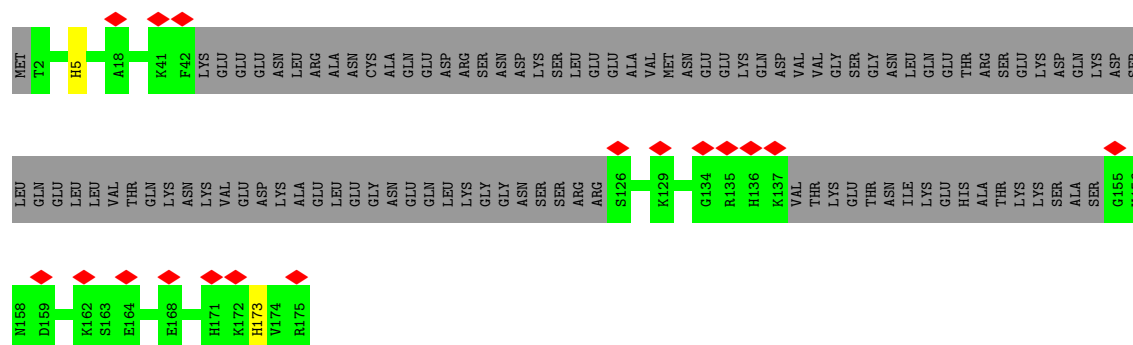


- Molecule 13: Pre-mRNA-splicing factor BUD31



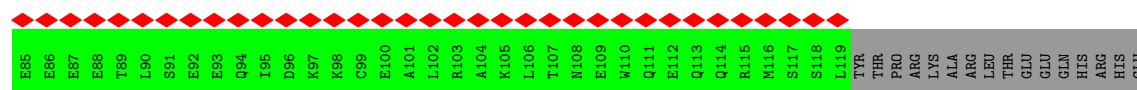


• Molecule 17: Pre-mRNA-splicing factor CWC15

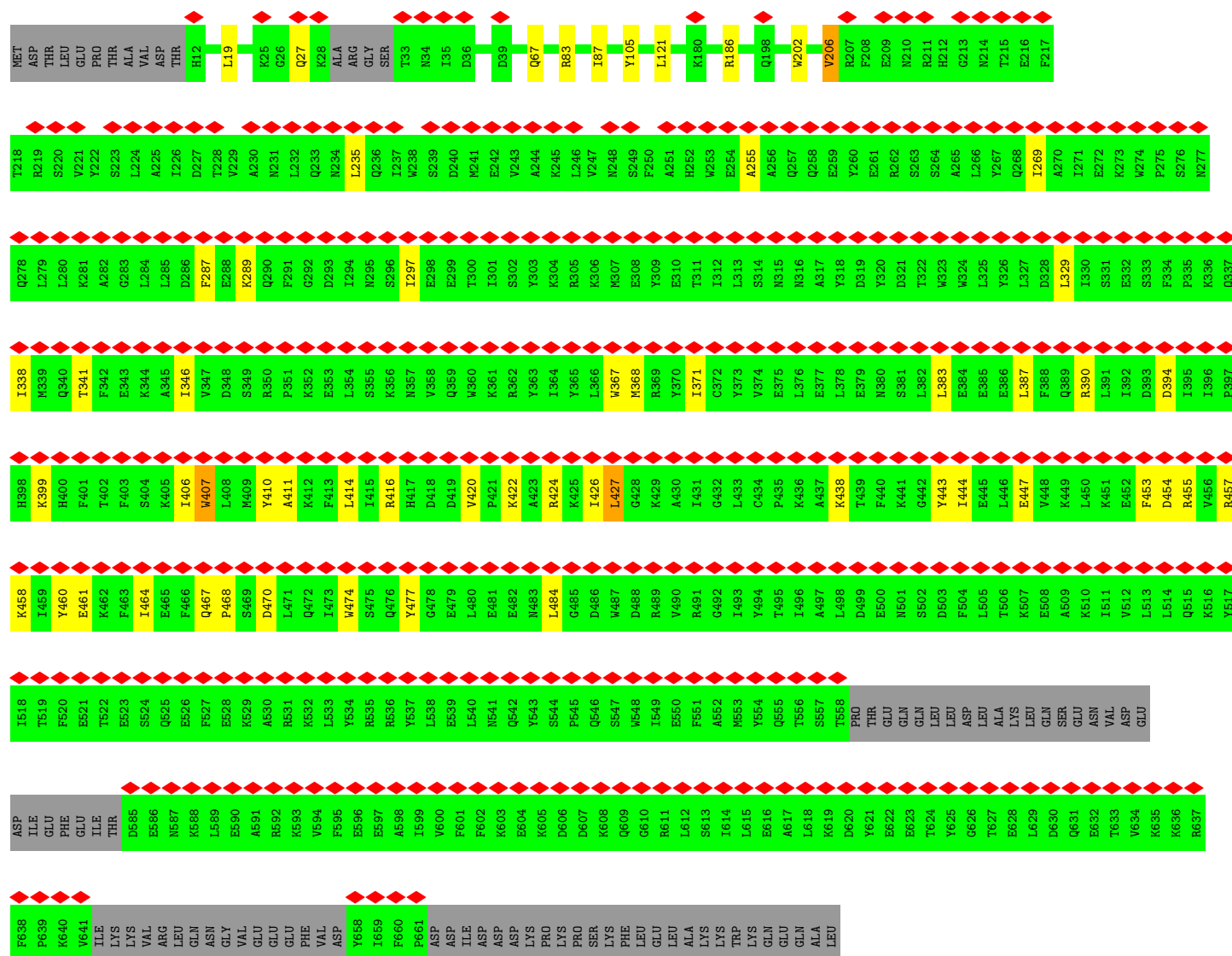
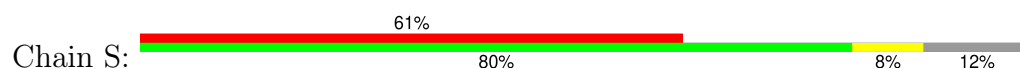


• Molecule 18: Pre-mRNA-splicing factor CWC21

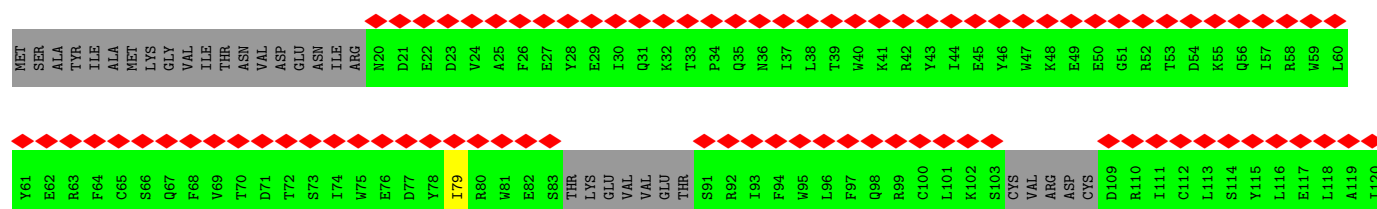
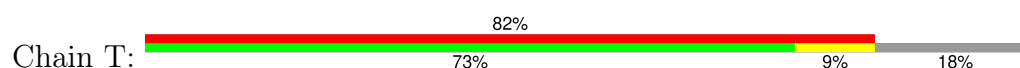




• Molecule 19: Pre-mRNA-splicing factor CLF1



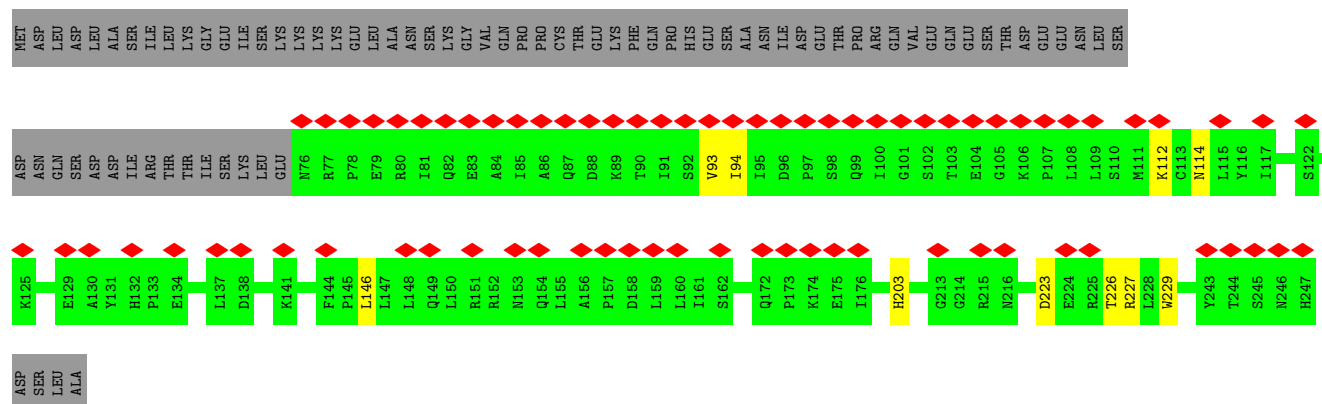
• Molecule 20: Pre-mRNA-splicing factor SYF1



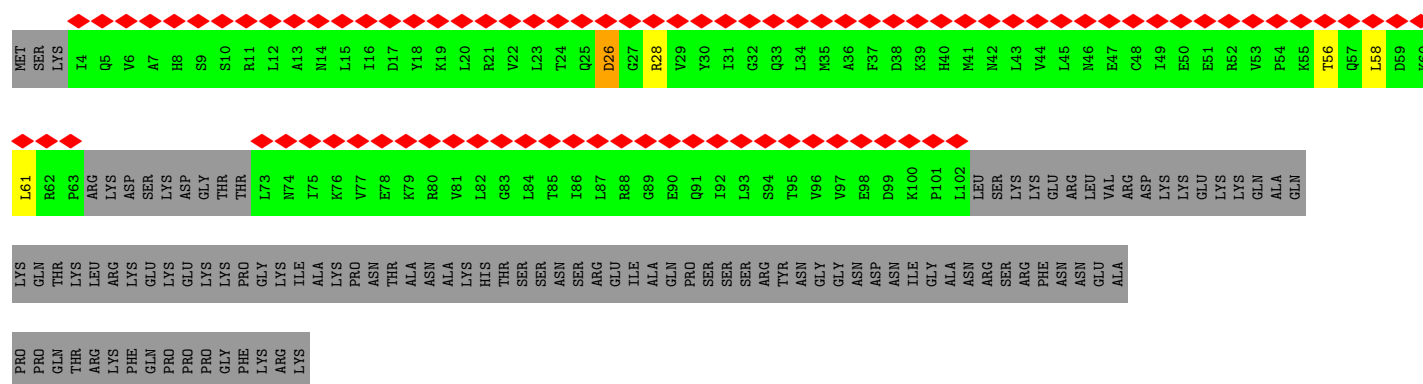
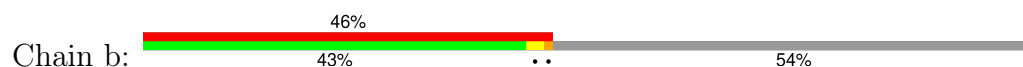


I947	A787	I727	S667	E607	R547	A487	K427	D367	A307	ASN	TYR	GLN	GLY	MET
L948	G788	L728	Q668	R608	V648	M488	Q428	G368	A308	ASN	GLU	SER	GLN	SER
M949	I789	P729	T669	T609	A549	R489	Q429	P369	S309	GLY	VAL	GLY	LEU	ASP
L850	E790	V730	P670	V610	E650	S490	S430	K370	I310	ILE	ARG	ASN	GLU	SER
K851	Q791	Y731	M671	A611	E551	E491	F431	F371	D311	LEU	ASN	GLU	LEU	LYS
A852	L792	S732	M672	D613	V652	I492	D432	K372	D312	SER	THR	THR	VAL	ILE
M853	I793	A733	D673	D613	G553	I493	D433	K373	Y313	MET	THR	THR	ARG	GLY
G854	V794	L734	Y674	V614	C554	Q494	P434	D374	P314	ASN	PHE	PHE	ASN	ALA
I855	S795	L735	I675	L615	K555	A495	T435	Q375	E315	ILE	GLY	ILE	VAL	LYS
N856	P796	S736	E676	F616	V656	V496	K436	Q376	L316	ASP	CYS	TYR	GLY	GLY
D857	I797	E737	A677	A617	G557	R497	ASN	VAL	K317	GLN	PHE	GLN	SER	SER
L858	A678	L738	A678	L618	H558	D498	LYS	LYS	ASP	HIS	VAL	VAL	SER	ASP
L859	L679	I739	L679	L619	D559	N499	ASP	ALA	ILE	SER	GLN	ALA	PRO	ASP
K860	D680	S740	V660	K620	V560	Q500	SER	LYS	GLY	GLY	PRO	LEU	LEU	PRO
F861	C681	K741	G561	K621	F501	F501	ASN	TYR	ILE	ARG	PHE	PRO	VAL	VAL
D862	V682	I742	Y562	A622	L502	V503	GLU	GLU	THR	LYS	THR	VAL	ILE	ILE
F863	I683	F743	T563	A623	I504	I504	ILE	MET	TYR	ASN	ARG	GLY	ASN	VAL
M864	D684	E744	I564	I624	R565	V505	GLN	P386	THR	THR	GLY	VAL	LEU	VAL
D865	I685	P745	R565	K625	F566	G506	LEU	K387	ALA	SER	CYS	VAL	LEU	ASN
P866	H686	T746	F567	R626	E567	E507	ASN	I388	VAL	ASP	ASP	SER	LYS	ILE
P867	I687	P747	E567	E627	E567	E507	GLN	T389	ARG	VAL	GLY	VAL	ASP	ILE
K868	N688	K748	D688	E628	V569	T508	LEU	K390	GLY	LEU	LEU	LEU	ASP	VAL
A909	E689	G749	V669	L629	V569	G509	LEU	V391	ASP	ASP	VAL	VAL	VAL	LYS
G810	G690	S750	T570	K630	T570	S510	VAL	P392	GLY	GLY	ILE	THR	THR	GLY
R811	P691	K751	G571	V631	G571	G511	THR	R393	SER	LYS	SER	LYS	ASP	ASN
T812	G692	R752	P572	I632	P572	K512	GLU	R394	ILE	SER	GLU	ILE	ASP	LEU
G813	D693	V753	D573	V633	D573	T513	TRP	G394	VAL	ASN	MET	ILE	PRO	GLU
P814	I694	V754	T574	T634	T574	T514	GLY	F395	ASN	ASP	SER	ALA	VAL	GLN
A875	L695	F755	R575	A635	R575	Q515	ASN	M396	GLY	ALA	ASP	LYS	VAL	VAL
L876	V696	A756	I576	A636	I576	I516	ARG	N397	ASN	HIS	THR	ILE	THR	ILE
T877	F697	T757	K577	T637	K577	T517	MET	R398	THR	THR	ARG	GLU	GLU	ARG
E878	L698	N758	Y578	L638	Y578	Q518	ASN	S399	GLY	ALA	THR	ALA	VAL	ASN
L879	T699	I759	T699	N639	M579	Y519	SER	A400	LYS	LEU	THR	LYS	VAL	LEU
Y880	G700	A760	S640	S640	D581	L520	ILE	I401	VAL	ASN	ASP	ILE	LEU	GLN
H881	Q701	E761	D641	A641	D581	D521	TYR	N402	SER	LYS	HIS	GLU	ILE	LEU
L882	E702	T762	G582	K642	G582	E522	GLY	G403	LEU	LYS	ASP	VAL	ASN	ASP
K883	I703	S763	M583	F643	M583	E523	ARG	S404	GLY	GLN	GLY	VAL	ALA	ALA
S884	E704	I764	S644	S644	L584	E524	THR	N405	GLN	GLN	GLY	GLN	GLY	GLY
L885	D705	T765	Q585	E645	Q585	F525	SER	I407	ARG	ARG	HIS	LEU	ASP	ASP
D886	S706	I766	R586	Y646	R586	S526	PRO	R408	GLY	THR	ILE	THR	GLU	SER
D887	C707	D767	E587	F647	E587	N527	ILE	D409	THR	THR	VAL	GLN	GLU	GLU
E888	C708	G768	L648	L648	A588	Y528	SER	H410	ASP	GLU	VAL	VAL	VAL	TYR
G889	E709	I769	L589	N649	L589	G529	ASN	R411	GLY	VAL	VAL	VAL	GLN	ASN
K890	I710	Y770	D590	C650	L590	M530	GLY	E412	ASP	GLY	VAL	VAL	LEU	ASN
L891	D591	Y771	D591	P651	I531	I531	THR	E412	D360	E298	ILE	LEU	LEU	ALA
T892	L712	T772	Y712	I652	P592	G532	GLY	E413	V361	I299	LYS	HIS	ASN	ALA
N893	D713	V773	D713	I653	E593	C533	THR	K414	E362	R300	LYS	LYS	LEU	PHE
L894	R714	D774	M594	N654	M594	T534	ARG	L415	L363	S305	GLN	GLN	LEU	GLN
G895	V715	P775	S595	I655	S595	Q535	SER	R416	T364	G306	GLY	GLY	LEU	VAL
K896	K716	G776	K596	P656	K596	P536	LEU	K417	L363	ASN	GLY	GLY	LEU	ASN
E897	T717	F777	Y597	G657	Y597	R537	PRO	K418	E362	LYS	GLY	GLY	LEU	ASN
M898	L718	K778	Y597	K658	Y597	R538	ILE	K418	T365	GLY	VAL	VAL	LEU	ASN
S899	G719	A779	V599	T659	V599	V539	SER	R419	D366	GLY	VAL	VAL	LEU	ASN
L900	D720	I780	I600	F660	I600	A540	THR	E420	D366	GLY	VAL	VAL	LEU	ASN
F901	S721	N781	M601	P661	M601	A541	GLY	I421	E362	LYS	VAL	VAL	LEU	ASN
N902	I722	I782	V662	V662	L602	V542	THR	E422	V361	GLY	VAL	VAL	LEU	ASN
M903	G723	Y783	E563	E563	D603	S543	ARG	Q423	E362	GLY	VAL	VAL	LEU	ASN
D904	E724	N784	V664	V664	E604	V544	SER	I425	L363	GLY	VAL	VAL	LEU	ASN
P905	L725	A785	A605	L665	A605	A545	THR	R426	T365	GLY	VAL	VAL	LEU	ASN
T906	L726	R786	H606	Y666	H606	K546	SER	Y486	D366	GLY	VAL	VAL	LEU	ASN

- Molecule 25: Pre-mRNA-splicing factor 18

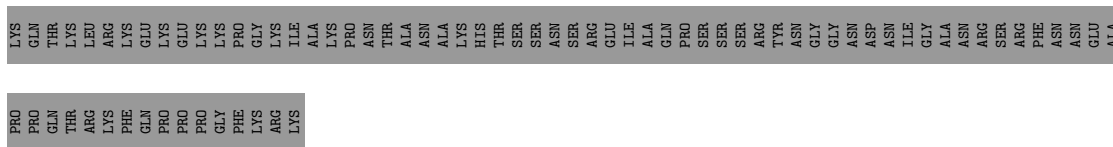


- Molecule 26: Small nuclear ribonucleoprotein-associated protein B

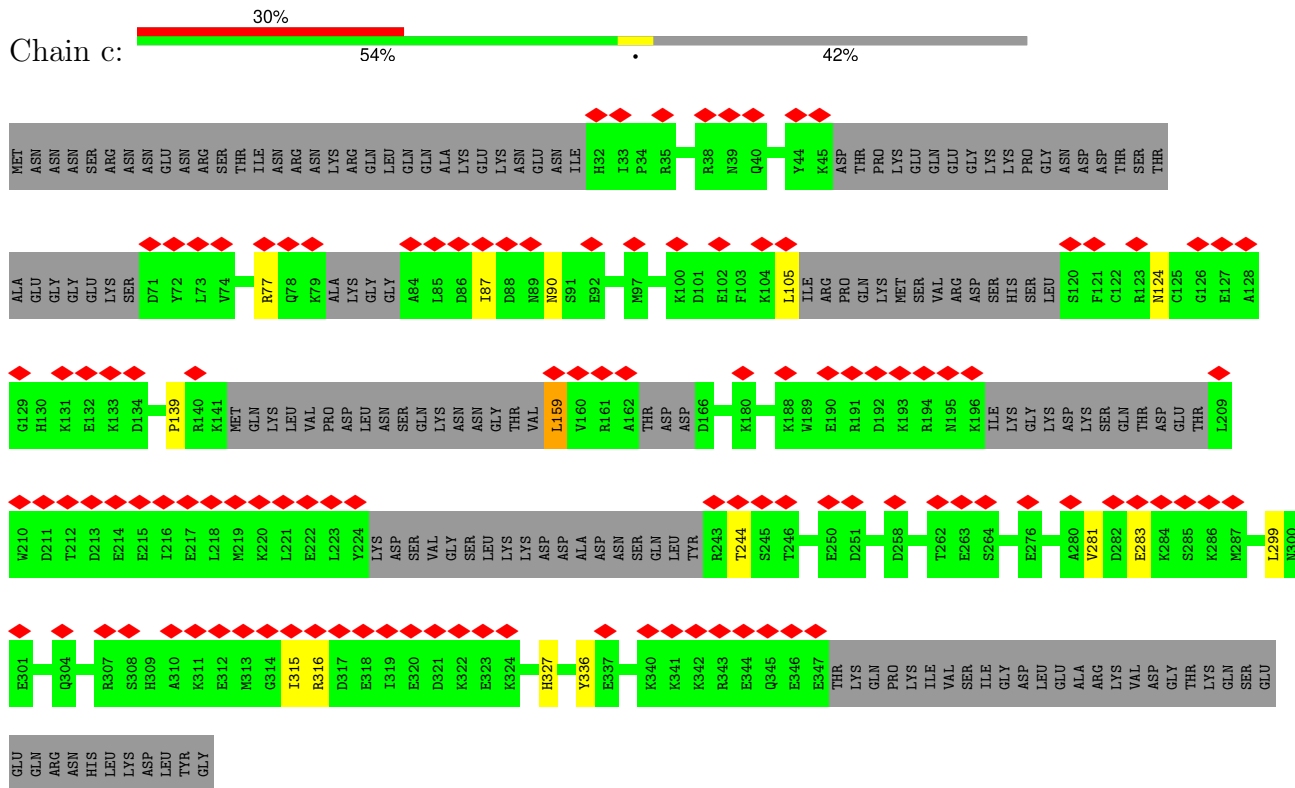


- Molecule 26: Small nuclear ribonucleoprotein-associated protein B

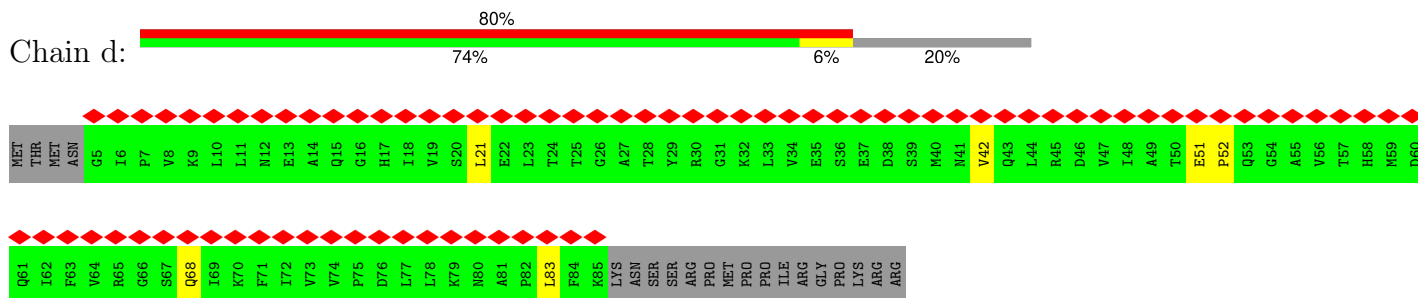




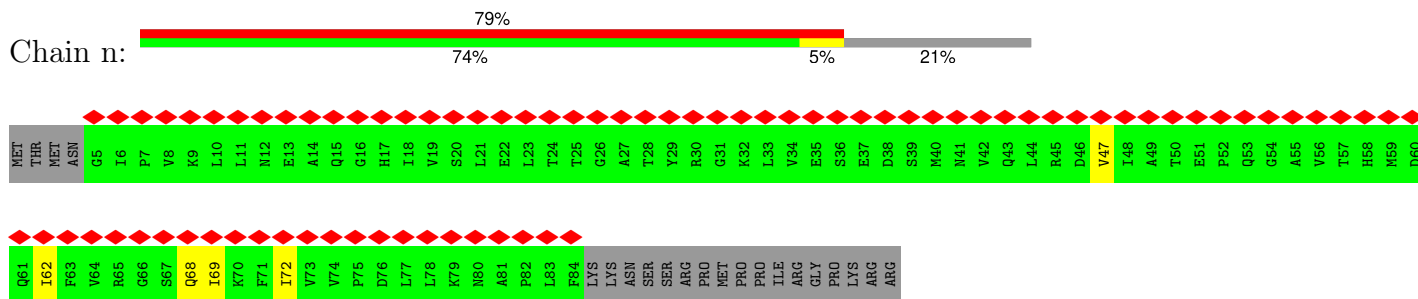
- Molecule 27: Pre-mRNA-splicing factor SLU7



- Molecule 28: Small nuclear ribonucleoprotein Sm D3

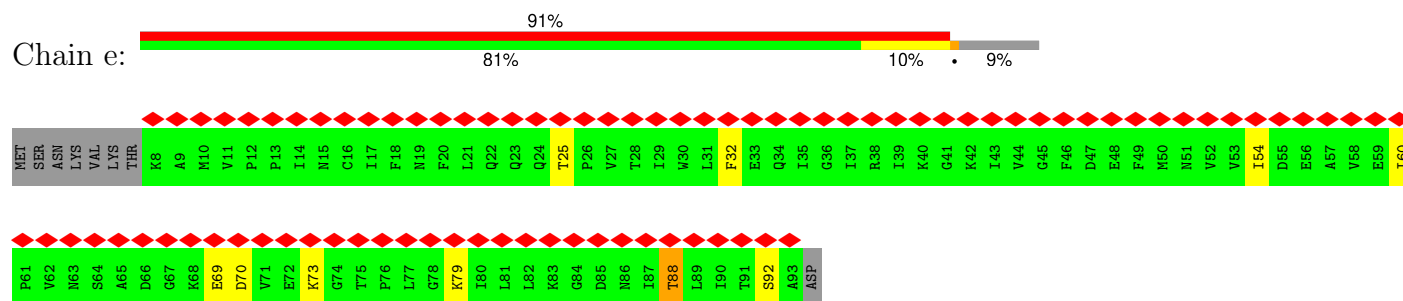


- Molecule 28: Small nuclear ribonucleoprotein Sm D3



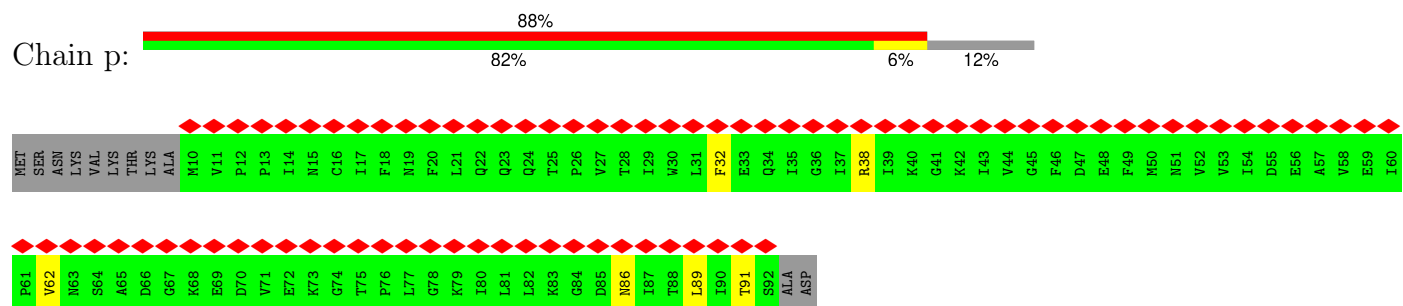
• Molecule 29: Small nuclear ribonucleoprotein E

Chain e:



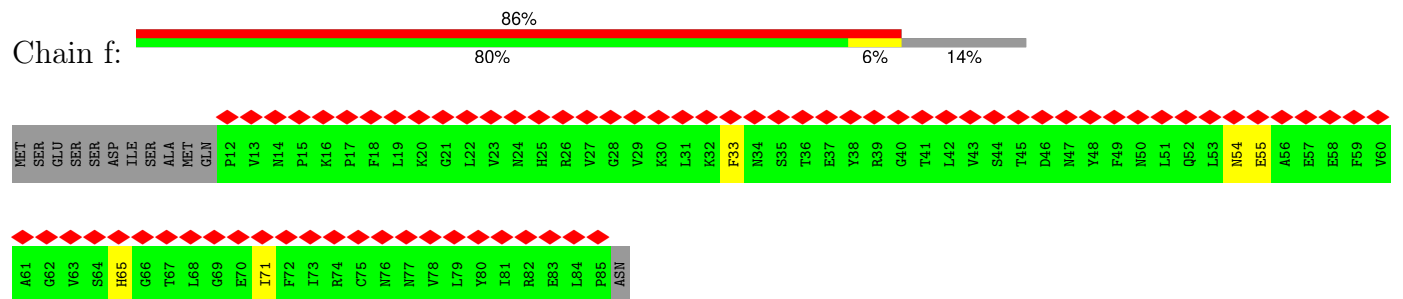
• Molecule 29: Small nuclear ribonucleoprotein E

Chain p:



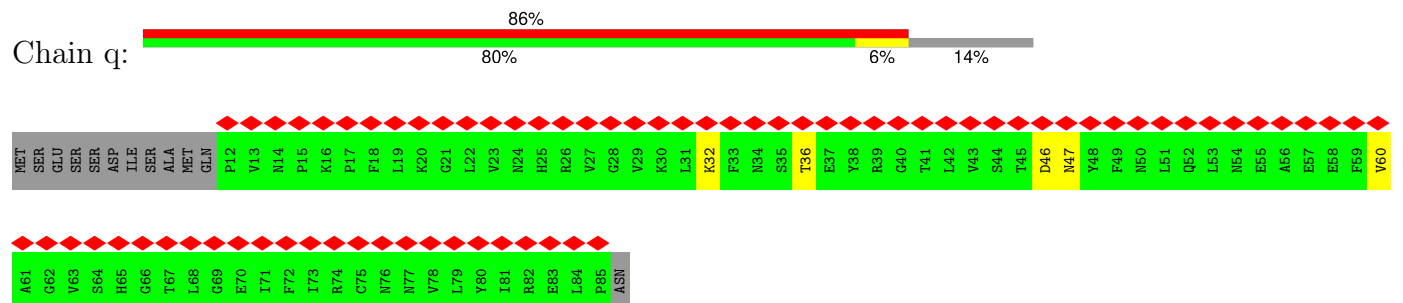
• Molecule 30: Small nuclear ribonucleoprotein F

Chain f:



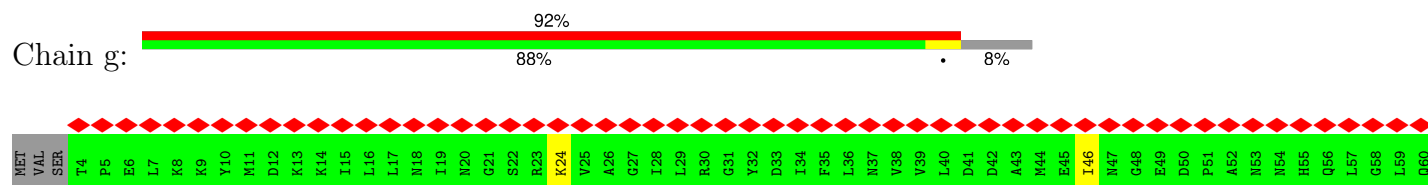
• Molecule 30: Small nuclear ribonucleoprotein F

Chain q:



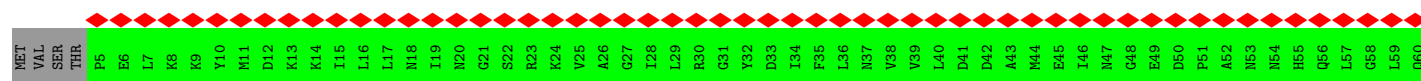
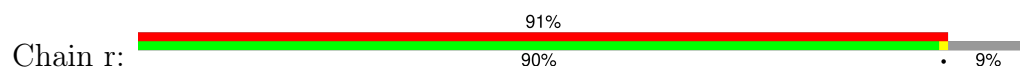
• Molecule 31: Small nuclear ribonucleoprotein G

Chain g:

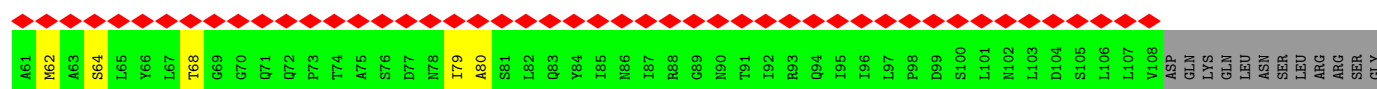
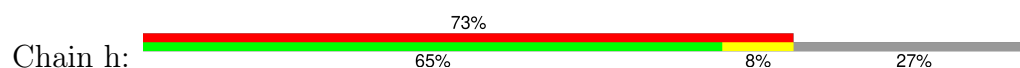




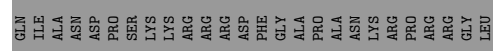
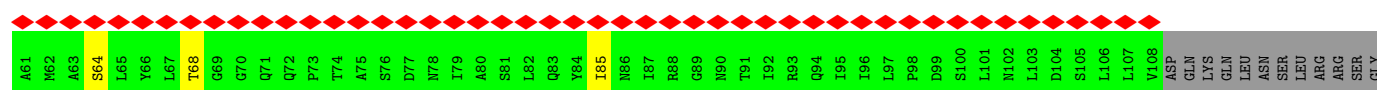
• Molecule 31: Small nuclear ribonucleoprotein G



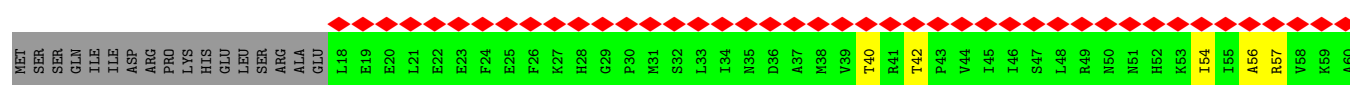
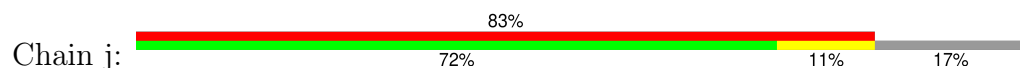
• Molecule 32: Small nuclear ribonucleoprotein Sm D1

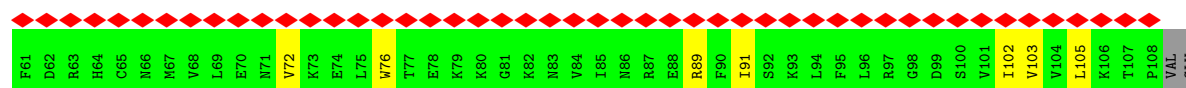


• Molecule 32: Small nuclear ribonucleoprotein Sm D1

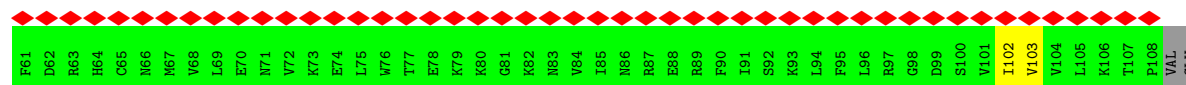
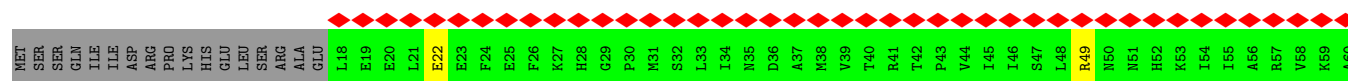
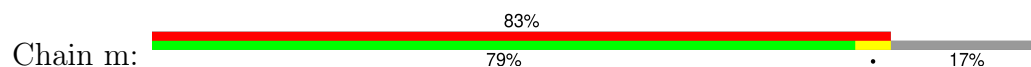


• Molecule 33: Small nuclear ribonucleoprotein Sm D2

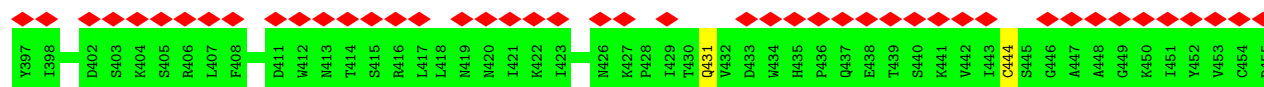
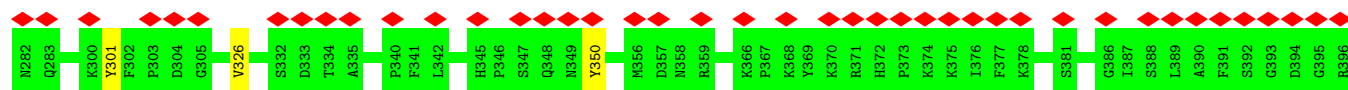
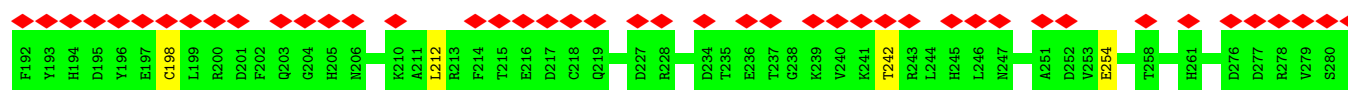
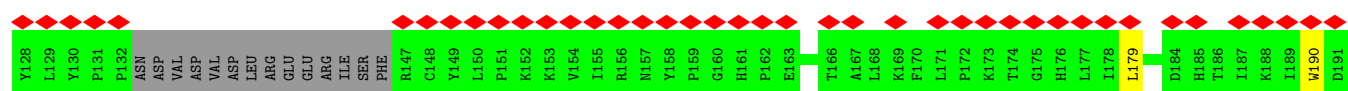
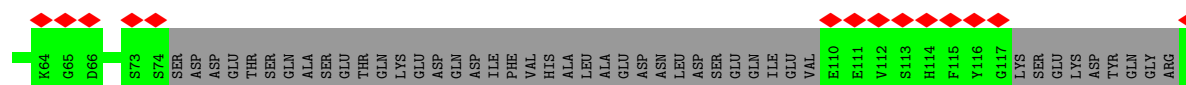
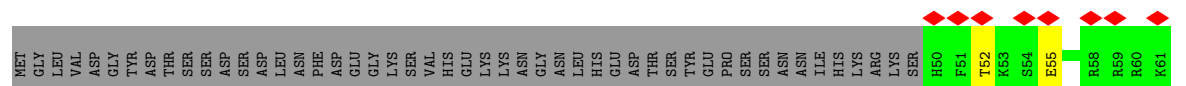
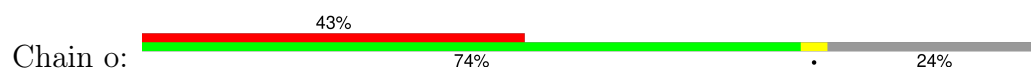




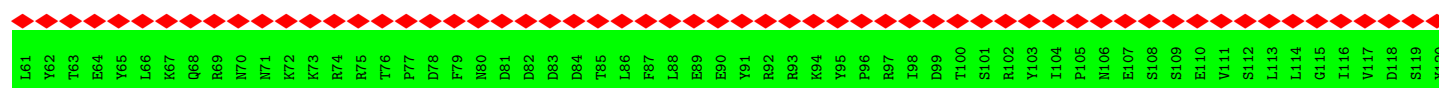
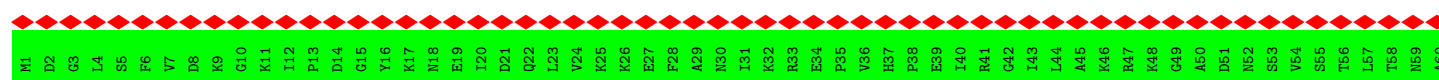
• Molecule 33: Small nuclear ribonucleoprotein Sm D2

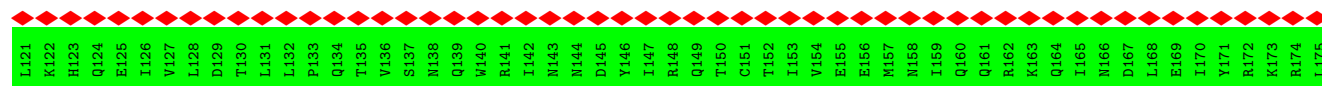


• Molecule 34: Pre-mRNA-processing factor 17

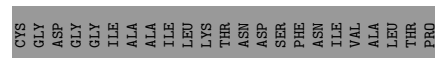
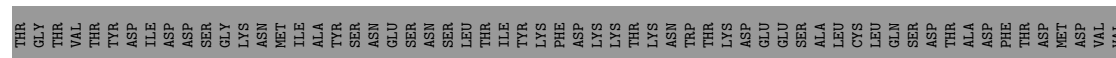
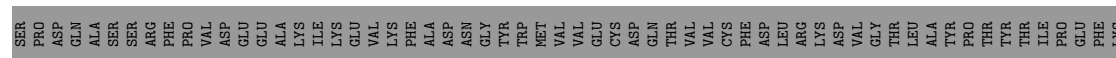
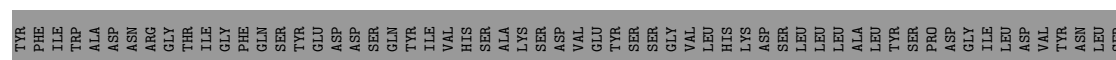
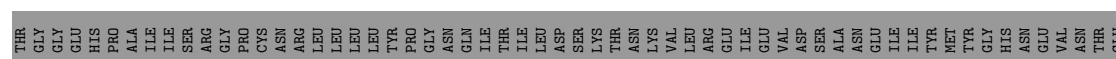
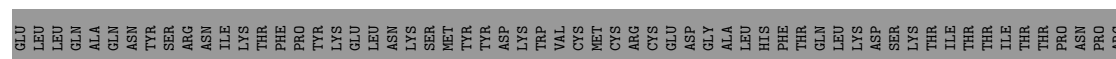
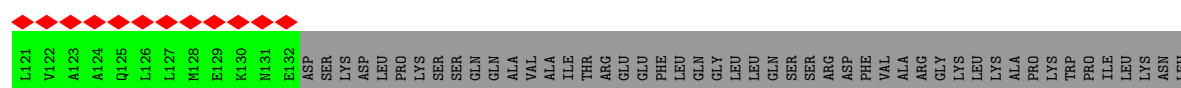
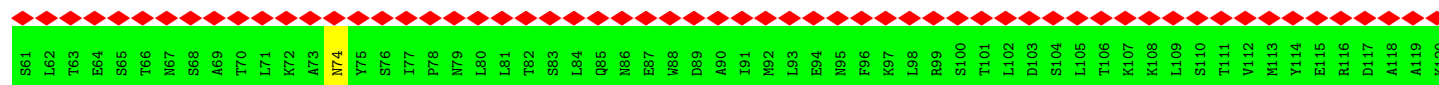
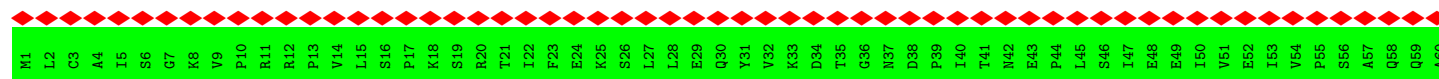


• Molecule 35: Pre-mRNA-splicing factor SNT309

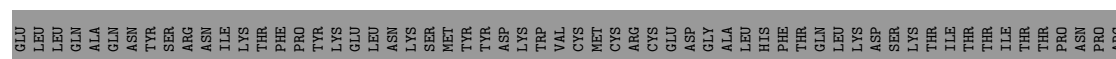
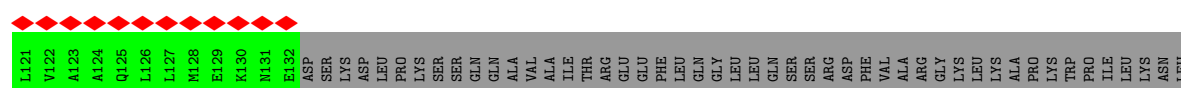
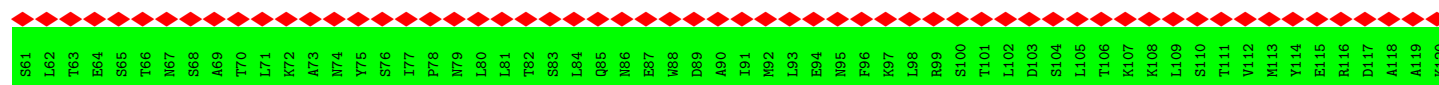
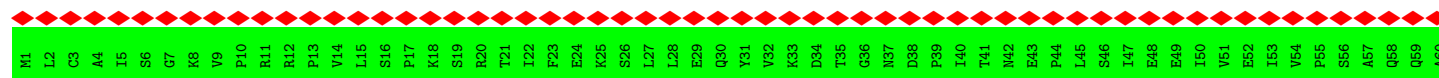




• Molecule 36: Pre-mRNA-processing factor 19



• Molecule 36: Pre-mRNA-processing factor 19



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

- Molecule 36: Pre-mRNA-processing factor 19



CYS	THR	SER	TRP	THR	GLY	PRO	SER	THR	THR	GLY	LEU	GLU	L121	S61
GLY	GLY	ASP	THR	GLY	GLY	ASP	ARG	ILE	GLY	LEU	LEU	V122	L62	L2
ASP	VAL	GLN	TRP	GLU	GLU	GLN	HIS	ALA	ALA	ALA	GLN	A123	T63	C3
GLY	THR	ALA	ASP	PRO	ASP	ASN	ASP	ALA	ASN	ASN	GLN	A124	E64	A4
ILE	TYR	SER	SER	ASP	SER	SER	ASN	ASN	ASN	ASN	GLN	Q125	S65	I5
ALA	ASP	ARG	ARG	ARG	ILE	ARG	ILE	ILE	TYR	SER	TYR	L126	T66	G7
ALA	ASP	PHE	THR	THR	THR	SER	SER	ARG	ARG	ASN	ASN	M128	S68	K8
LEU	ASP	PRO	THR	THR	THR	THR	ILE	ARG	ASN	ASN	ASN	E129	A69	V9
THR	GLY	VAL	GLY	GLY	GLY	GLY	GLY	ILE	ILE	LYS	LYS	K130	T70	P10
ASN	LYS	GLY	PHE	PRO	PRO	PRO	PRO	PRO	LYS	LYS	LYS	E132	L71	R11
ASP	ASN	GLY	GLN	CYS	CYS	THR	THR	THR	THR	THR	THR	M131	K72	P13
SER	MET	ALA	SER	ASN	ASN	ASN	ASN	ARG	ARG	PRO	PRO	ASP	A73	V14
PHE	ILE	LYS	TYR	THR	THR	THR	THR	GLY	GLY	LEU	LEU	ASP	T77	I15
ASN	ALA	ILE	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	LYS	A69	K18
ILE	TYR	LYS	ASP	ASP	ASP	ASP	ASN	ASN	ASN	ASN	ASN	LYS	T70	S19
VAL	SER	GLY	ASP	THR	THR	THR	ASN	VAL	VAL	THR	TYR	GLN	L80	R20
VAL	SER	GLY	ASP	THR	THR	THR	ASN	HIS	HIS	GLN	TYR	GLN	L81	T21
ALA	ASN	VAL	SER	LEU	LEU	LEU	LEU	ILE	ILE	THR	ASP	ALA	T82	I22
LEU	ASN	VAL	THR	ALA	ALA	ALA	ALA	THR	THR	THR	TRP	VAL	S83	F23
LEU	ASN	VAL	THR	ALA	ALA	ALA	ALA	THR	THR	THR	TRP	VAL	E24	E24
PRO	PRO	PRO	PRO	THR	THR	THR	THR	THR	THR	THR	TRP	VAL	K85	K25
				THR	THR	THR	THR	THR	THR	THR	TRP	VAL	N86	S26
				THR	THR	THR	THR	THR	THR	THR	TRP	VAL	E87	L27
				THR	THR	THR	THR	THR	THR	THR	TRP	VAL	A88	L28
				THR	THR	THR	THR	THR	THR	THR	TRP	VAL	D89	E29
				THR	THR	THR	THR	THR	THR	THR	TRP	VAL	A90	Q30
				THR	THR	THR	THR	THR	THR	THR	TRP	VAL	I91	I91
				THR	THR	THR	THR	THR	THR	THR	TRP	VAL	M92	V32
				THR	THR	THR	THR	THR	THR	THR	TRP	VAL	K93	K33
				THR	THR	THR	THR	THR	THR	THR	TRP	VAL	E94	D34
				THR	THR	THR	THR	THR	THR	THR	TRP	VAL	N95	T35
				THR	THR	THR	THR	THR	THR	THR	TRP	VAL	F96	G36
				THR	THR	THR	THR	THR	THR	THR	TRP	VAL	X97	N37
				THR	THR	THR	THR	THR	THR	THR	TRP	VAL	L98	D38
				THR	THR	THR	THR	THR	THR	THR	TRP	VAL	R99	F39
				THR	THR	THR	THR	THR	THR	THR	TRP	VAL	S100	I40
				THR	THR	THR	THR	THR	THR	THR	TRP	VAL	T101	T41
				THR	THR	THR	THR	THR	THR	THR	TRP	VAL	L102	H42
				THR	THR	THR	THR	THR	THR	THR	TRP	VAL	D103	E43
				THR	THR	THR	THR	THR	THR	THR	TRP	VAL	S104	P44
				THR	THR	THR	THR	THR	THR	THR	TRP	VAL	L105	L45
				THR	THR	THR	THR	THR	THR	THR	TRP	VAL	T106	S46
				THR	THR	THR	THR	THR	THR	THR	TRP	VAL	I107	I47
				THR	THR	THR	THR	THR	THR	THR	TRP	VAL	K108	E48
				THR	THR	THR	THR	THR	THR	THR	TRP	VAL	L109	E49
				THR	THR	THR	THR	THR	THR	THR	TRP	VAL	S110	I50
				THR	THR	THR	THR	THR	THR	THR	TRP	VAL	T111	V51
				THR	THR	THR	THR	THR	THR	THR	TRP	VAL	V112	E52
				THR	THR	THR	THR	THR	THR	THR	TRP	VAL	M113	I53
				THR	THR	THR	THR	THR	THR	THR	TRP	VAL	Y114	V54
				THR	THR	THR	THR	THR	THR	THR	TRP	VAL	E115	P55
				THR	THR	THR	THR	THR	THR	THR	TRP	VAL	R116	S56
				THR	THR	THR	THR	THR	THR	THR	TRP	VAL	D117	A57
				THR	THR	THR	THR	THR	THR	THR	TRP	VAL	A118	Q58
				THR	THR	THR	THR	THR	THR	THR	TRP	VAL	A119	Q59
				THR	THR	THR	THR	THR	THR	THR	TRP	VAL	K120	A60

- Molecule 36: Pre-mRNA-processing factor 19



M1	L2	C3	A4	I5	S6	G7	K8	V9	P10	R11	I12	P13	V14	L15	S16	G17	K18	V19	P20	R21	I22	P23	V24	L25	S26	G27	K28	V29	P30	R31	I32	P33	V34	L35	S36	G37	K38	V39	P40	R41	I42	P43	V44	L45	S46	G47	K48	V49	P50	R51	I52	P53	V54	L55	S56	G57	K58	V59	P60	R61	I62	P63	V64	L65	S66	G67	K68	V69	P70	R71	I72	P73	V74	L75	S76	G77	K78	V79	P80	R81	I82	P83	V84	L85	S86	G87	K88	V89	P90	R91	I92	P93	V94	L95	S96	G97	K98	V99	P100	R101	I102	P103	V104	L105	S106	G107	K108	V109	P110	R111	I112	P113	V114	L115	S116	G117	K118	V119	P120	R121	I122	P123	V124	L125	S126	G127	K128	V129	P130	R131	I132	P133	V134	L135	S136	G137	K138	V139	P140	R141	I142	P143	V144	L145	S146	G147	K148	V149	P150	R151	I152	P153	V154	L155	S156	G157	K158	V159	P160	R161	I162	P163	V164	L165	S166	G167	K168	V169	P170	R171	I172	P173	V174	L175	S176	G177	K178	V179	P180	R181	I182	P183	V184	L185	S186	G187	K188	V189	P190	R191	I192	P193	V194	L195	S196	G197	K198	V199	P200	R201	I202	P203	V204	L205	S206	G207	K208	V209	P210	R211	I212	P213	V214	L215	S216	G217	K218	V219	P220	R221	I222	P223	V224	L225	S226	G227	K228	V229	P230	R231	I232	P233	V234	L235	S236	G237	K238	V239	P240	R241	I242	P243	V244	L245	S246	G247	K248	V249	P250	R251	I252	P253	V254	L255	S256	G257	K258	V259	P260	R261	I262	P263	V264	L265	S266	G267	K268	V269	P270	R271	I272	P273	V274	L275	S276	G277	K278	V279	P280	R281	I282	P283	V284	L285	S286	G287	K288	V289	P290	R291	I292	P293	V294	L295	S296	G297	K298	V299	P300	R301	I302	P303	V304	L305	S306	G307	K308	V309	P310	R311	I312	P313	V314	L315	S316	G317	K318	V319	P320	R321	I322	P323	V324	L325	S326	G327	K328	V329	P330	R331	I332	P333	V334	L335	S336	G337	K338	V339	P340	R341	I342	P343	V344	L345	S346	G347	K348	V349	P350	R351	I352	P353	V354	L355	S356	G357	K358	V359	P360	R361	I362	P363	V364	L365	S366	G367	K368	V369	P370	R371	I372	P373	V374	L375	S376	G377	K378	V379	P380	R381	I382	P383	V384	L385	S386	G387	K388	V389	P390	R391	I392	P393	V394	L395	S396	G397	K398	V399	P400	R401	I402	P403	V404	L405	S406	G407	K408	V409	P410	R411	I412	P413	V414	L415	S416	G417	K418	V419	P420	R421	I422	P423	V424	L425	S426	G427	K428	V429	P430	R431	I432	P433	V434	L435	S436	G437	K438	V439	P440	R441	I442	P443	V444	L445	S446	G447	K448	V449	P450	R451	I452	P453	V454	L455	S456	G457	K458	V459	P460	R461	I462	P463	V464	L465	S466	G467	K468	V469	P470	R471	I472	P473	V474	L475	S476	G477	K478	V479	P480	R481	I482	P483	V484	L485	S486	G487	K488	V489	P490	R491	I492	P493	V494	L495	S496	G497	K498	V499	P500	R501	I502	P503	V504	L505	S506	G507	K508	V509	P510	R511	I512	P513	V514	L515	S516	G517	K518	V519	P520	R521	I522	P523	V524	L525
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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 (Å)	464.63998, 464.63998, 464.63998	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	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: IHP, ZN, MG, K, GTP, PSU

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	0.34	0/3090	0.64	0/4792
2	5	0.39	0/4098	0.60	1/6373 (0.0%)
3	6	0.42	0/2405	0.57	0/3744
4	A	0.32	0/16489	0.56	0/22348
5	C	0.40	0/7189	0.59	0/9728
6	D	0.33	0/922	0.71	1/1220 (0.1%)
7	E	0.40	0/785	1.00	3/1218 (0.2%)
8	G	0.16	0/137	0.54	0/188
9	H	0.42	0/3824	0.55	2/5154 (0.0%)
10	I	0.39	0/1128	0.75	1/1747 (0.1%)
11	J	0.32	0/3052	0.60	0/4143
12	K	0.26	0/1375	0.55	0/1854
13	L	0.29	0/1307	0.55	0/1748
14	M	0.25	0/2094	0.56	0/2815
15	N	0.24	0/2124	0.51	0/2860
16	O	0.27	0/2945	0.52	0/3992
17	P	0.28	0/623	0.57	0/832
18	R	0.25	0/510	0.54	0/698
19	S	0.27	0/4780	0.46	0/6483
20	T	0.27	0/5658	0.43	0/7669
21	V	0.35	0/6210	0.58	0/8377
22	W	0.27	0/1406	0.58	0/1905
23	Y	0.26	0/706	0.54	0/941
24	Z	0.25	0/424	0.44	0/564
25	a	0.24	0/1409	0.54	0/1911
26	b	0.30	0/731	0.56	0/983
26	k	0.28	0/849	0.54	0/1138
27	c	0.31	0/1925	0.62	0/2565
28	d	0.35	0/633	0.58	0/857
28	n	0.27	0/624	0.53	0/846
29	e	0.29	0/676	0.57	0/916
29	p	0.25	0/657	0.54	0/891

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
30	f	0.29	0/605	0.52	0/819
30	q	0.28	0/605	0.53	0/819
31	g	0.30	0/556	0.55	0/749
31	r	0.26	0/549	0.54	0/738
32	h	0.29	0/835	0.56	0/1135
32	l	0.26	0/835	0.54	0/1135
33	j	0.31	0/759	0.50	0/1019
33	m	0.25	0/759	0.53	0/1019
34	o	0.22	0/2903	0.57	0/3921
35	s	0.19	0/869	0.46	0/1210
36	t	0.20	0/657	0.45	0/917
36	u	0.19	0/657	0.43	0/917
36	v	0.20	0/657	0.44	0/917
36	w	0.19	0/657	0.44	0/917
37	y	0.24	0/1085	0.42	0/1453
All	All	0.32	0/93773	0.56	8/129185 (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 (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	H	474	THR	N-CA-C	5.64	117.43	111.28
9	H	472	LEU	N-CA-C	-5.52	105.26	111.28
7	E	9	C	C4'-C3'-O3'	5.44	121.17	113.00
7	E	4	U	N1-C1'-C2'	5.27	119.90	112.00
7	E	5	C	O4'-C4'-C3'	5.19	111.29	106.10
10	I	71	C	C2'-C3'-O3'	5.15	121.42	113.70
6	D	92	LYS	N-CA-C	-5.10	105.72	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	5	41	A	C4'-C3'-O3'	5.09	117.03	109.40

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
22	W	92	ARG	Sidechain
27	c	77	ARG	Sidechain

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	2	2779	0	1411	25	0
2	5	3671	0	1856	6	0
3	6	2170	0	1095	14	0
4	A	16079	0	16079	49	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	41	0
10	I	1012	0	510	7	0
11	J	2990	0	2906	12	0
12	K	1355	0	1383	10	0
13	L	1283	0	1301	0	0
14	M	2048	0	2011	10	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	8	0
19	S	4683	0	4267	39	0
20	T	5543	0	5182	46	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	V	6096	0	6158	12	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	7	0
26	b	725	0	778	2	0
26	k	843	0	917	1	0
27	c	1893	0	1849	11	0
28	d	624	0	647	3	0
28	n	615	0	634	3	0
29	e	665	0	690	5	0
29	p	646	0	667	6	0
30	f	592	0	594	3	0
30	q	592	0	594	3	0
31	g	551	0	572	2	0
31	r	544	0	566	1	0
32	h	826	0	874	6	0
32	l	826	0	874	2	0
33	j	747	0	784	9	0
33	m	747	0	784	2	0
34	o	2821	0	2743	7	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	1	0
37	y	1075	0	1004	8	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	384	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 (384) 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
29:e:70:ASP:HB3	29:e:73:LYS:HE3	1.67	0.76
1:2:1141:C:H2'	1:2:1142:G:C8	2.20	0.76
25:a:223:ASP:HA	27:c:244:THR:HG21	1.68	0.75
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
19:S:467:GLN:HE22	19:S:470:ASP:HB2	1.54	0.73
20:T:667:ILE:HG12	20:T:711:MET:HE1	1.71	0.72
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
20:T:450:TRP:CG	20:T:473:SER:HG	2.13	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
28:d:51:GLU:HG2	28:d:52:PRO:HD2	1.80	0.64
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
33:m:49:ARG:HA	33:m:102:ILE:HD11	1.81	0.61
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
33:j:54:ILE:HG23	33:j:72:VAL:HG13	1.82	0.60
12:K:179:THR:H	37:y:200:ASN:HD21	1.49	0.60
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
26:b:58:LEU:HD12	26:b:61:LEU:HD12	1.84	0.59
37:y:149:THR:HG23	37:y:151:LYS:H	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
12:K:179:THR:H	37:y:200:ASN:ND2	2.02	0.57
20:T:291:MET:HA	20:T:291:MET:HE2	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
20:T:379:GLN:HA	20:T:382:MET:HE2	1.86	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
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
28:n:47:VAL:HG21	28:n:62:ILE:HG22	1.89	0.55
34:o:52:THR:HG23	34:o:55:GLU:H	1.71	0.55
20:T:484:LEU:HD11	20:T:535:GLN:OE1	2.06	0.55
32:h:45:LEU:HB2	32:h:80:ALA:HB3	1.89	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
27:c:327:HIS:HA	27:c:336:TYR:OH	2.07	0.53
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
33:j:57:ARG:NH1	33:j:57:ARG:HB3	2.24	0.53
10:I:65:U:H2'	10:I:66:A:C8	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
9:H:99:MET:HE3	9:H:103:VAL:HG23	1.90	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
31:g:24:LYS:HB2	31:g:46:ILE:HB	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
21:V:903:MET:HE1	21:V:911:LEU:HD22	1.92	0.51
29:p:38:ARG:HG3	29:p:62:VAL:HG21	1.93	0.51
9:H:433:LEU:HD21	9:H:472:LEU:HB2	1.92	0.51
32:h:58:ASN:O	32:h:62:MET:HG2	2.11	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
30:q:36:THR:HG22	30:q:60:VAL:HG22	1.93	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
15:N:95:ASN:C	15:N:97:GLU:H	2.21	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
20:T:542:LEU:HD22	37:y:71:THR:HG23	1.95	0.49
28:n:69:ILE:HD13	28:n:72:ILE:HD11	1.95	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
4:A:1922:ARG:CZ	25:a:227:ARG:HD3	2.43	0.48
1:2:120:G:N2	29:p:32:PHE:CD2	2.81	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
32:h:64:SER:O	32:h:68:THR:HG23	2.13	0.48
34:o:179:LEU:HG	34:o:212:LEU:HD13	1.95	0.48
4:A:1841:ALA:HA	27:c:299:LEU:HD23	1.96	0.48
34:o:431:GLN:O	34:o:444:CYS:HA	2.14	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
26:b:26:ASP:OD2	26:b:28:ARG:HD3	2.13	0.48
32:h:48:PRO:HB2	32:h:51:ARG:HG2	1.96	0.48
25:a:146:LEU:HD22	25:a:229:TRP:CE3	2.48	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
12:K:160:PRO:C	12:K:161:ASN:HD22	2.21	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
10:I:59:C:H4'	34:o:350:TYR:OH	2.13	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
9:H:99:MET:HE2	9:H:229:VAL:HG21	1.96	0.47
21:V:562:TYR:HA	21:V:578:TYR:O	2.15	0.47
4:A:1567:PHE:O	27:c:90:ASN:HB3	2.15	0.46
20:T:352:GLU:O	20:T:355:GLN:HG3	2.15	0.46
4:A:351:LYS:HA	18:R:1:MET:HE2	1.97	0.46
33:j:72:VAL:HB	33:j:91:ILE:HB	1.96	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
36:w:73:ALA:C	36:w:75:TYR:H	2.24	0.46
29:e:54:ILE:O	29:e:79:LYS:HA	2.15	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
2:5:176:A:C2	30:f:33:PHE:HB3	2.51	0.46
25:a:93:VAL:HA	25:a:112:LYS:HG3	1.97	0.46
28:d:68:GLN:HG3	31:g:69:ILE:HA	1.98	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
27:c:124:ASN:ND2	27:c:139:PRO:HA	2.30	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
32:l:43:VAL:HG21	32:l:85:ILE:HG22	1.97	0.45
4:A:2036:SER:O	4:A:2037:TYR:CG	2.70	0.45
34:o:254:GLU:HG3	34:o:301:TYR:HD2	1.81	0.45
9:H:465:PHE:O	9:H:470:LEU:N	2.44	0.45
29:p:86:ASN:OD1	30:q:32:LYS:HE2	2.17	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:a:226:THR:HA	25:a:229:TRP:CD1	2.52	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
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
10:I:93:U:OP2	25:a:203:HIS:HE1	2.01	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
19:S:368:MET:HE2	19:S:368:MET:HB3	1.86	0.44
20:T:622:GLU:O	20:T:626:GLU:HG2	2.17	0.44
33:m:102:ILE:HG22	33:m:103:VAL:HG23	1.99	0.44
29:p:38:ARG:HG2	29:p:38:ARG:HH11	1.82	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
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
28:n:68:GLN:HG3	31:r:69:ILE: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
33:j:57:ARG:HB3	33:j:57:ARG:HH11	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
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
27:c:281:VAL:HG12	27:c:283:GLU:H	1.82	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
4:A:1979:MET:HE1	34:o:326:VAL:HG21	2.00	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
9:H:474:THR:O	9:H:475:GLU:C	2.60	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
28:d:21:LEU:HD21	28:d:42:VAL:HG21	2.01	0.43
29:e:32:PHE:HA	29:e:88:THR:OG1	2.19	0.43
30:q:46:ASP:OD1	30:q:47:ASN:N	2.52	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
33:j:40:THR:OG1	33:j:42:THR:HG23	2.18	0.43
26:k:35:MET:SD	26:k:46:ASN:HB2	2.59	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
19:S:410:TYR:CE2	19:S:426:ILE:HG12	2.54	0.43
30:f:71:ILE:HG22	33:j:105:LEU:HD13	2.01	0.43
4:A:1082:ILE:HG23	4:A:1113:ILE:HD11	2.01	0.43
32:h:3:LEU:HD23	32:h:3:LEU:HA	1.87	0.43
29:p:38:ARG:HH11	29:p:38:ARG:CG	2.32	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
33:j:102:ILE:HG22	33:j:103:VAL:HG23	2.00	0.42
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
32:h:46:THR:HG22	32:h:79:ILE:HD13	2.01	0.42
4:A:1668:ILE:HD13	4:A:1801:SER:HB2	2.01	0.42
12:K:102:ALA:C	12:K:103:ASN:HD22	2.28	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
27:c:159:LEU:HD23	27:c:159:LEU:HA	1.73	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
33:j:56:ALA:HB2	33:j:72:VAL:HA	2.02	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
14:M:211:GLU:CD	14:M:211:GLU:H	2.27	0.42
22:W:43:MET:HB3	22:W:44:PRO:HD3	2.02	0.42
32:l:64:SER:O	32:l:68:THR:HG23	2.18	0.42
4:A:618:SER:HB3	4:A:725:TYR:HB3	2.02	0.42
4:A:1368:GLN:OE1	4:A:1429:MET:HE1	2.20	0.42
4:A:1570:TRP:CD1	27:c:87:ILE:HD12	2.55	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
21:V:901:PHE:HB3	21:V:903:MET:HE2	2.01	0.41
30:f:54:ASN:O	30:f:55:GLU:HG3	2.20	0.41
34:o:190:TRP:CZ3	34:o:198:CYS:HB2	2.55	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
37:y:196:ILE:H	37:y:200:ASN:HD22	1.69	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:470:LEU:HB3	4:A:471:PRO:HD2	2.02	0.41
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
25:a:94:ILE:H	25:a:94:ILE:HD12	1.86	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
37:y:110:ARG:O	37:y:114:THR:HG23	2.21	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
29:e:60:ILE:HG21	29:e:69:GLU:HB3	2.02	0.41
33:j:76:TRP:HH2	33:j:89:ARG:HG3	1.84	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
27:c:124:ASN:HD21	27:c:139:PRO:HA	1.85	0.41
29:e:73:LYS:HE2	29:e:73:LYS:HB3	1.94	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
18:R:56:ARG:O	18:R:57:PRO:C	2.64	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
20:T:582:LEU:O	37:y:71:THR:HG22	2.21	0.40
37:y:112:LEU:HD23	37:y:112:LEU: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
29:p:89:LEU:HD21	29:p:91:THR:HB	2.03	0.40
4:A:624:GLU:HG3	4:A:666:ILE:HA	2.03	0.40
6:D:82:LEU:O	16:O:125:ALA:HA	2.21	0.40
27:c:105:LEU:CD1	27:c:159:LEU:HD21	2.52	0.40
27:c:315:ILE:HG13	27:c:316:ARG:N	2.37	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 ⓘ

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	
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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	3
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	59
22	W	168/238 (71%)	152 (90%)	15 (9%)	1 (1%)	21	25
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	19

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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	19
37	y	133/215 (62%)	132 (99%)	1 (1%)	0	100	100
All	All	10223/15286 (67%)	9922 (97%)	295 (3%)	6 (0%)	49	59

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
18	R	59	ALA
21	V	943	GLN
18	R	57	PRO
36	t	74	ASN
36	w	74	ASN
22	W	76	ILE

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	
4	A	1770/2182 (81%)	1767 (100%)	3 (0%)	87	94
5	C	795/910 (87%)	795 (100%)	0	100	100
6	D	100/159 (63%)	97 (97%)	3 (3%)	36	52
9	H	429/538 (80%)	421 (98%)	8 (2%)	50	67
11	J	318/397 (80%)	315 (99%)	3 (1%)	70	83
12	K	152/328 (46%)	150 (99%)	2 (1%)	61	76
13	L	140/141 (99%)	140 (100%)	0	100	100
14	M	219/296 (74%)	217 (99%)	2 (1%)	70	83
15	N	243/332 (73%)	242 (100%)	1 (0%)	84	91
16	O	219/525 (42%)	216 (99%)	3 (1%)	59	75
17	P	61/151 (40%)	61 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	R	21/121 (17%)	21 (100%)	0	100	100
19	S	433/633 (68%)	429 (99%)	4 (1%)	70	83
20	T	551/786 (70%)	544 (99%)	7 (1%)	61	76
21	V	675/1028 (66%)	664 (98%)	11 (2%)	55	72
22	W	161/219 (74%)	158 (98%)	3 (2%)	50	67
23	Y	77/100 (77%)	77 (100%)	0	100	100
24	Z	49/128 (38%)	48 (98%)	1 (2%)	48	66
25	a	152/225 (68%)	151 (99%)	1 (1%)	76	86
26	b	83/176 (47%)	81 (98%)	2 (2%)	43	60
26	k	97/176 (55%)	97 (100%)	0	100	100
27	c	204/346 (59%)	203 (100%)	1 (0%)	81	89
28	d	70/89 (79%)	69 (99%)	1 (1%)	59	75
28	n	69/89 (78%)	69 (100%)	0	100	100
29	e	75/83 (90%)	72 (96%)	3 (4%)	28	41
29	p	74/83 (89%)	74 (100%)	0	100	100
30	f	66/77 (86%)	65 (98%)	1 (2%)	57	73
30	q	66/77 (86%)	66 (100%)	0	100	100
31	g	61/66 (92%)	61 (100%)	0	100	100
31	r	60/66 (91%)	60 (100%)	0	100	100
32	h	96/129 (74%)	95 (99%)	1 (1%)	68	81
32	l	96/129 (74%)	95 (99%)	1 (1%)	68	81
33	j	85/103 (82%)	85 (100%)	0	100	100
33	m	85/103 (82%)	84 (99%)	1 (1%)	63	78
34	o	314/413 (76%)	313 (100%)	1 (0%)	86	92
37	y	102/193 (53%)	102 (100%)	0	100	100
All	All	8268/11597 (71%)	8204 (99%)	64 (1%)	70	85

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	1652	HIS
4	A	1975	SER
4	A	2038	HIS

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Mol	Chain	Res	Type
6	D	82	LEU
6	D	87	LEU
6	D	92	LYS
9	H	65	LEU
9	H	132	GLU
9	H	136	LEU
9	H	221	THR
9	H	404	ILE
9	H	470	LEU
9	H	472	LEU
9	H	473	LEU
11	J	11	LEU
11	J	160	ASN
11	J	275	THR
12	K	110	HIS
12	K	206	GLU
14	M	211	GLU
14	M	215	ARG
15	N	51	ARG
16	O	123	LEU
16	O	135	GLN
16	O	136	MET
19	S	27	GLN
19	S	206	VAL
19	S	407	TRP
19	S	427	LEU
20	T	79	ILE
20	T	275	LEU
20	T	442	THR
20	T	471	THR
20	T	529	HIS
20	T	600	GLU
20	T	785	GLU
21	V	315	GLU
21	V	388	ILE
21	V	504	ILE
21	V	555	LYS
21	V	575	ARG
21	V	583	MET
21	V	618	LEU
21	V	676	GLU
21	V	886	ASP

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Mol	Chain	Res	Type
21	V	952	LYS
21	V	971	GLN
22	W	88	GLU
22	W	126	ASN
22	W	153	THR
24	Z	12	ASP
25	a	114	ASN
26	b	26	ASP
26	b	56	THR
27	c	159	LEU
28	d	83	LEU
29	e	25	THR
29	e	88	THR
29	e	92	SER
30	f	65	HIS
32	h	43	VAL
32	l	14	GLN
33	m	22	GLU
34	o	242	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (123) such sidechains are listed below:

Mol	Chain	Res	Type
4	A	146	HIS
4	A	178	ASN
4	A	181	HIS
4	A	271	GLN
4	A	405	ASN
4	A	487	ASN
4	A	541	ASN
4	A	542	HIS
4	A	558	GLN
4	A	559	GLN
4	A	592	HIS
4	A	658	ASN
4	A	659	HIS
4	A	676	GLN
4	A	848	ASN
4	A	1273	GLN
4	A	1404	HIS
4	A	1472	ASN
4	A	1522	ASN

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Mol	Chain	Res	Type
4	A	1548	GLN
4	A	1618	ASN
4	A	1647	GLN
4	A	1652	HIS
4	A	1718	HIS
4	A	1824	GLN
4	A	1869	ASN
4	A	1902	GLN
4	A	1929	GLN
5	C	82	ASN
5	C	103	HIS
5	C	108	GLN
5	C	158	HIS
5	C	251	GLN
5	C	255	GLN
5	C	309	ASN
5	C	334	HIS
5	C	355	HIS
5	C	398	ASN
5	C	1000	GLN
5	C	1004	ASN
9	H	48	ASN
9	H	84	ASN
9	H	105	GLN
9	H	137	GLN
9	H	260	GLN
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	214	ASN
11	J	271	GLN
11	J	280	GLN
12	K	103	ASN
12	K	148	HIS
14	M	58	HIS
14	M	191	ASN
14	M	235	GLN
15	N	30	GLN

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Mol	Chain	Res	Type
15	N	54	ASN
15	N	72	GLN
16	O	26	GLN
16	O	31	HIS
16	O	47	GLN
17	P	34	HIS
19	S	67	GLN
19	S	116	ASN
19	S	467	GLN
20	T	183	ASN
20	T	293	GLN
20	T	403	GLN
20	T	406	ASN
20	T	540	ASN
20	T	634	HIS
21	V	402	ASN
21	V	518	GLN
21	V	649	ASN
21	V	781	ASN
21	V	784	ASN
21	V	833	ASN
21	V	841	GLN
21	V	845	HIS
21	V	986	HIS
21	V	1070	HIS
21	V	1082	GLN
22	W	13	GLN
22	W	20	ASN
22	W	105	ASN
22	W	106	ASN
22	W	115	GLN
22	W	126	ASN
22	W	143	HIS
23	Y	47	ASN
23	Y	64	ASN
25	a	154	GLN
25	a	177	ASN
25	a	203	HIS
25	a	208	HIS
25	a	212	GLN
26	b	5	GLN
27	c	89	ASN

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Mol	Chain	Res	Type
27	c	124	ASN
27	c	257	ASN
27	c	291	HIS
28	d	43	GLN
31	g	18	ASN
33	j	35	ASN
32	l	71	GLN
32	l	78	ASN
32	l	86	ASN
28	n	17	HIS
34	o	157	ASN
34	o	185	HIS
34	o	330	GLN
34	o	431	GLN
29	p	24	GLN
30	q	47	ASN
31	r	60	GLN
37	y	73	GLN
37	y	185	ASN
37	y	200	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	126/1175 (10%)	27 (21%)	5 (3%)
10	I	45/95 (47%)	15 (33%)	6 (13%)
2	5	169/214 (78%)	17 (10%)	4 (2%)
3	6	101/112 (90%)	9 (8%)	0
7	E	32/42 (76%)	17 (53%)	6 (18%)
All	All	473/1638 (28%)	85 (17%)	21 (4%)

All (85) 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

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Mol	Chain	Res	Type
1	2	120	G
1	2	121	C
1	2	122	A
1	2	123	C
1	2	145	G
1	2	146	A
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	71	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

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Mol	Chain	Res	Type
3	6	60	G
3	6	68	C
3	6	80	U
3	6	91	A
7	E	-13	G
7	E	-11	G
7	E	-10	A
7	E	-7	U
7	E	-6	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	16	A
7	E	17	U
7	E	18	G
7	E	21	G
10	I	10	A
10	I	58	U
10	I	59	C
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

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Mol	Chain	Res	Type
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
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 ⓘ

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
40	IHP	S	701	-	36,36,36	0.69	0	60,60,60	0.85	2 (3%)
41	GTP	C	2501	38	33,34,34	0.96	1 (3%)	50,54,54	1.65	9 (18%)
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
40	IHP	S	701	-	-	2/30/54/54	0/1/1/1
41	GTP	C	2501	38	-	2/22/38/38	0/3/3/3
40	IHP	A	2500	-	-	1/30/54/54	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	C	2501	GTP	C5-N7	-2.33	1.34	1.39

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	C	2501	GTP	C5-C4-N3	-5.06	120.33	128.39
41	C	2501	GTP	C2-N3-C4	4.84	120.64	112.30
41	C	2501	GTP	N9-C4-N3	3.17	132.29	125.95
41	C	2501	GTP	N9-C8-N7	-3.01	107.83	113.40
41	C	2501	GTP	C2-N1-C6	-2.97	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	C8-N7-C5	2.71	109.09	104.26
41	C	2501	GTP	C5-C6-N1	2.65	119.99	113.25
41	C	2501	GTP	O6-C6-C5	-2.21	120.69	126.53
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

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Mol	Chain	Res	Type	Atoms
40	S	701	IHP	C4-O14-P4-O34
41	C	2501	GTP	PA-O3A-PB-O1B
41	C	2501	GTP	PB-O3B-PG-O3G

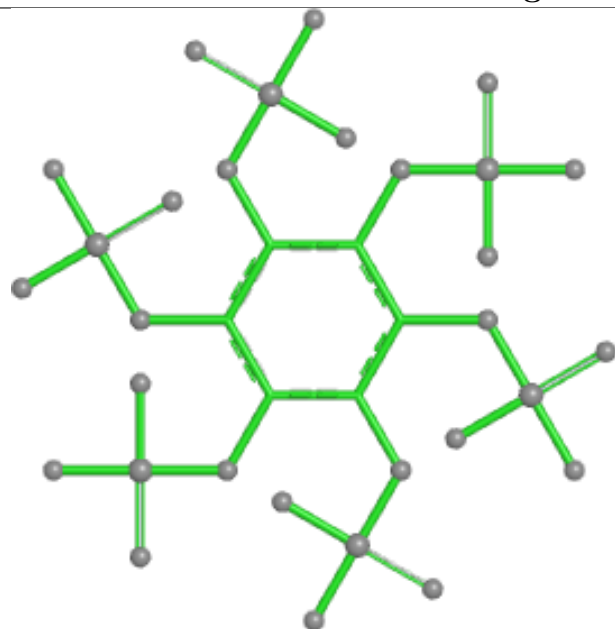
There are no ring outliers.

2 monomers are involved in 2 short contacts:

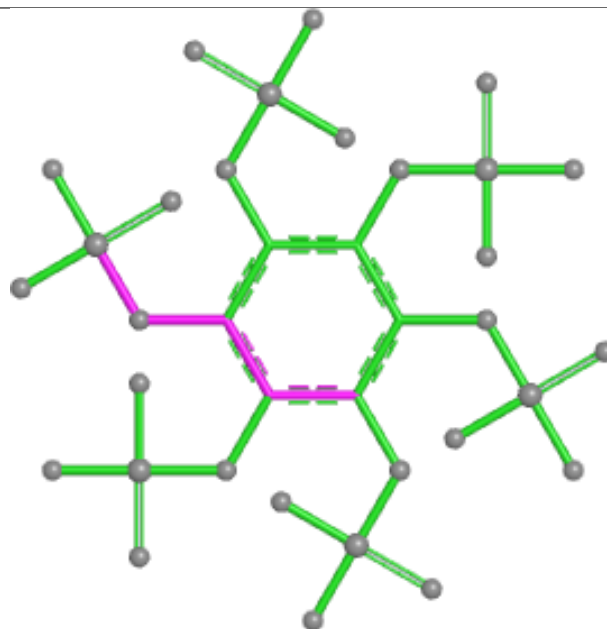
Mol	Chain	Res	Type	Clashes	Symm-Clashes
40	S	701	IHP	1	0
40	A	2500	IHP	1	0

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.

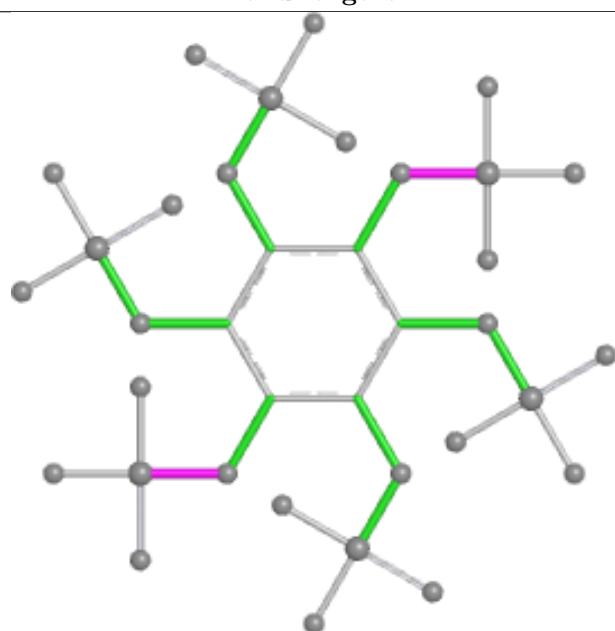
Ligand IHP S 701



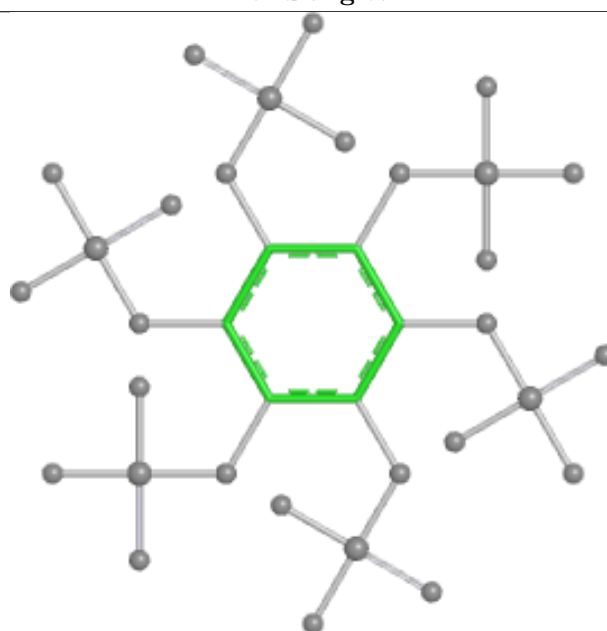
Bond lengths



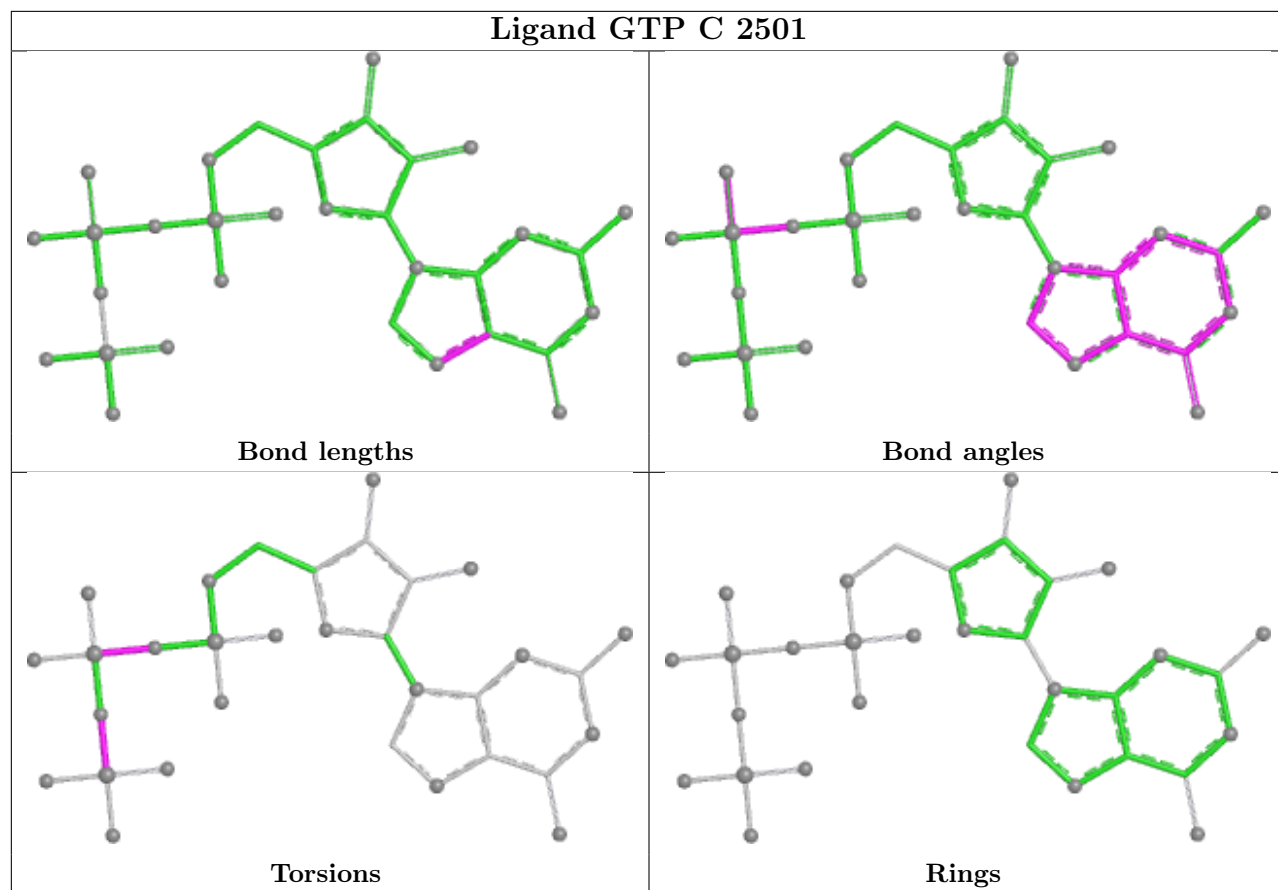
Bond angles

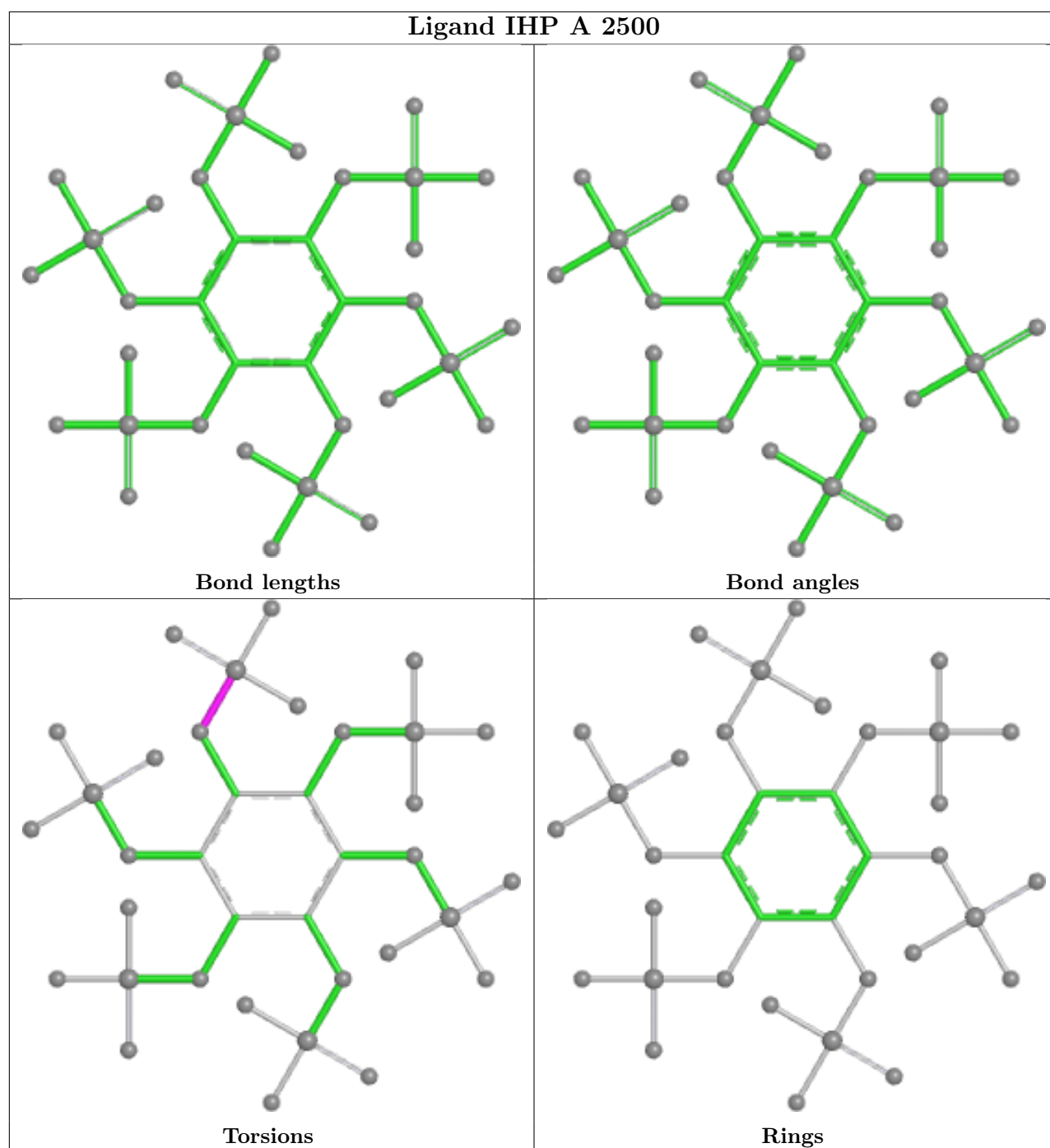


Torsions



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.

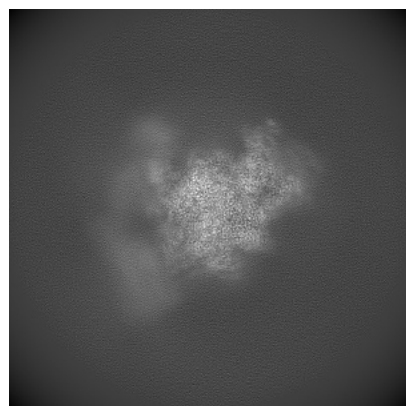
6 Map visualisation [i](#)

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

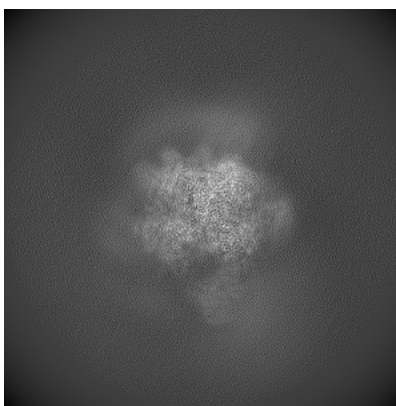
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

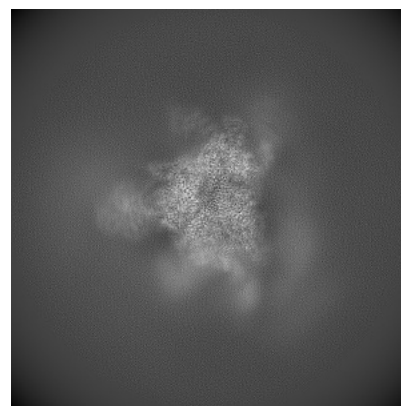
6.1.1 Primary map



X

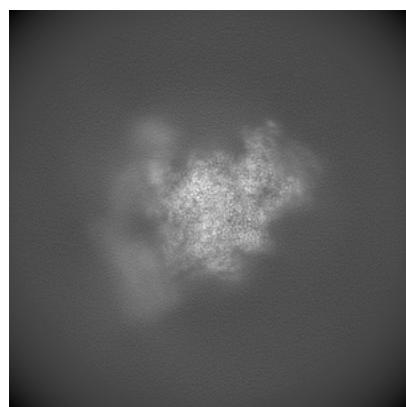


Y

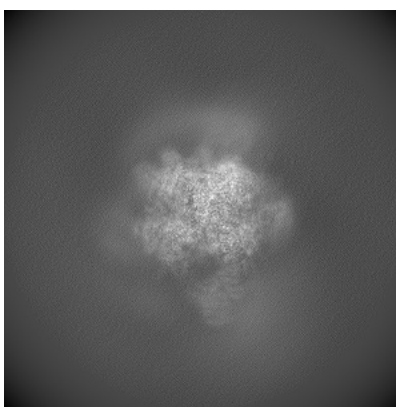


Z

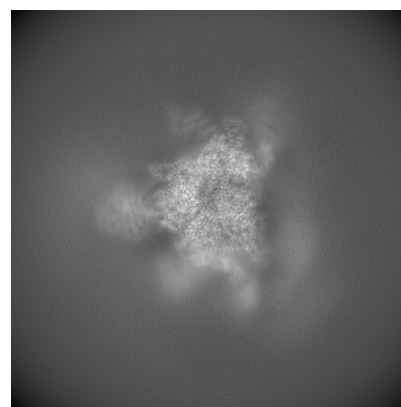
6.1.2 Raw map



X



Y

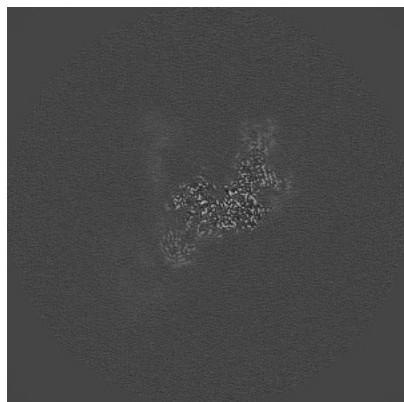


Z

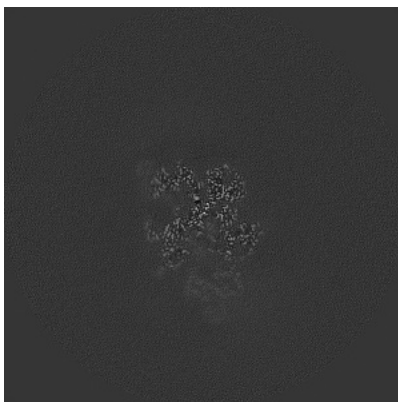
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

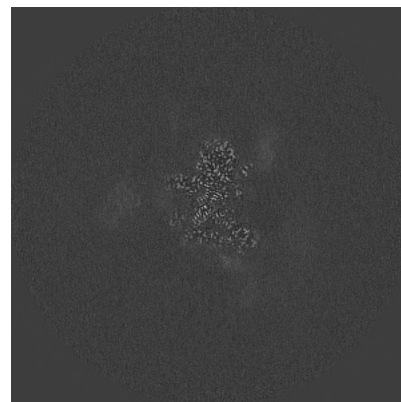
6.2.1 Primary map



X Index: 240

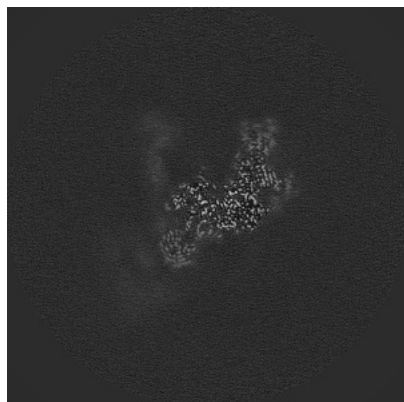


Y Index: 240

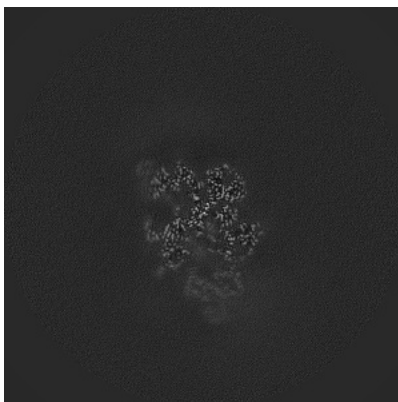


Z Index: 240

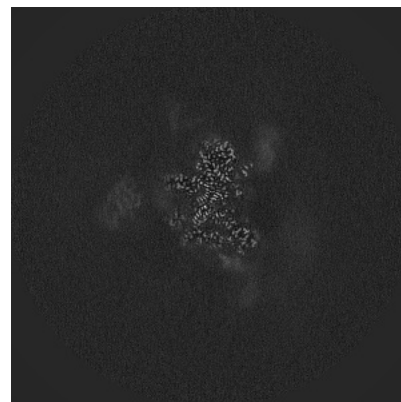
6.2.2 Raw map



X Index: 240



Y Index: 240

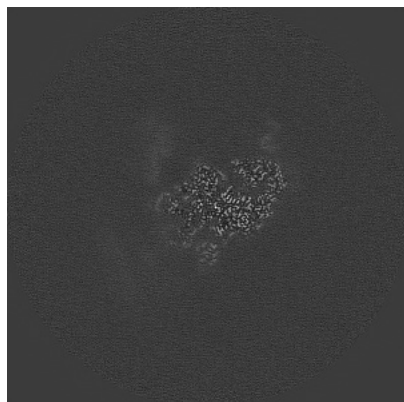


Z Index: 240

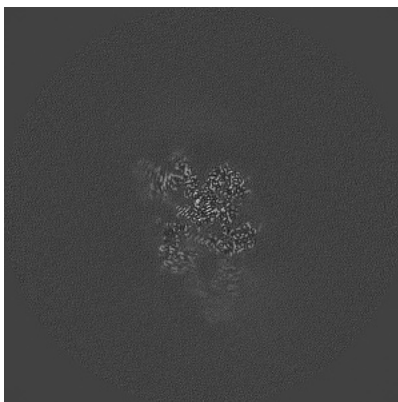
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

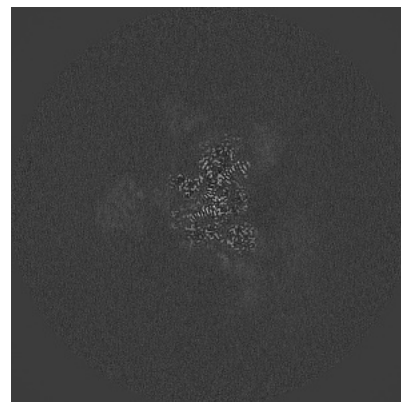
6.3.1 Primary map



X Index: 253

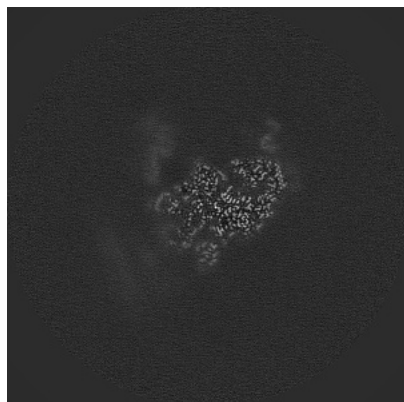


Y Index: 234

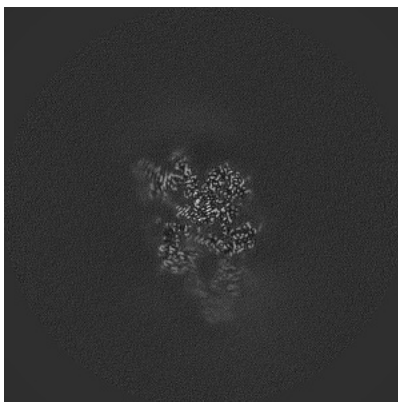


Z Index: 244

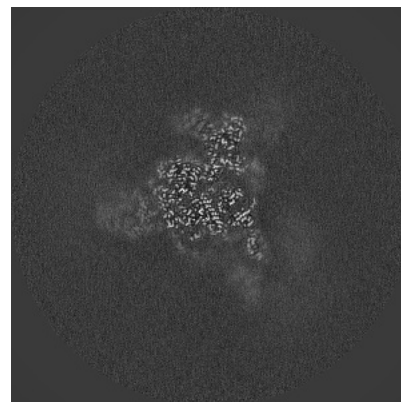
6.3.2 Raw map



X Index: 253



Y Index: 234

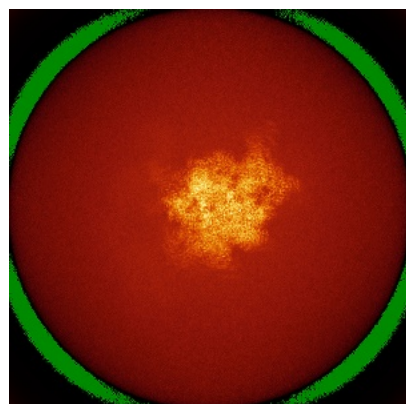


Z Index: 265

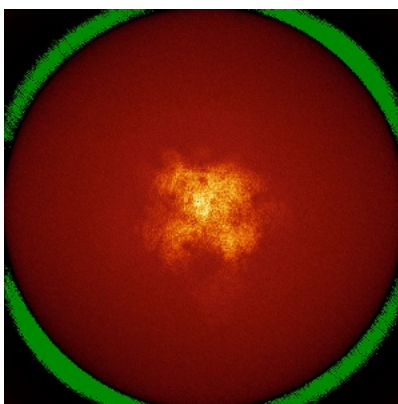
The images above show the largest variance slices of the map in three orthogonal directions.

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

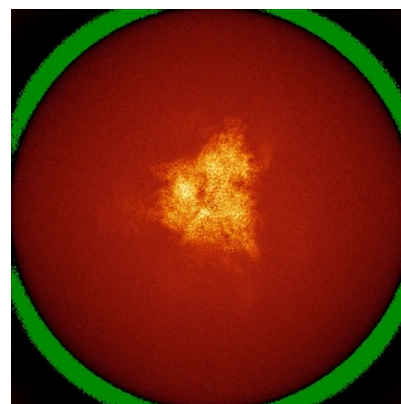
6.4.1 Primary map



X

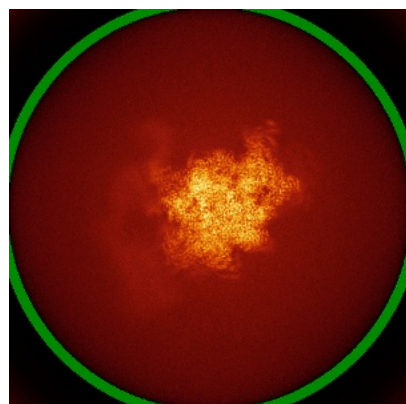


Y

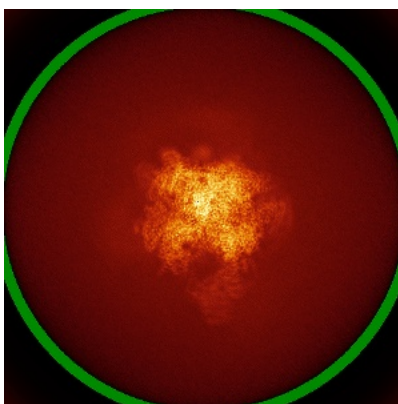


Z

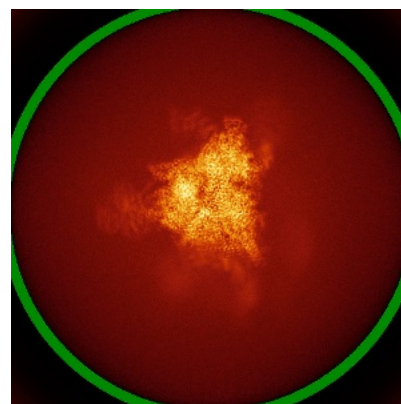
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



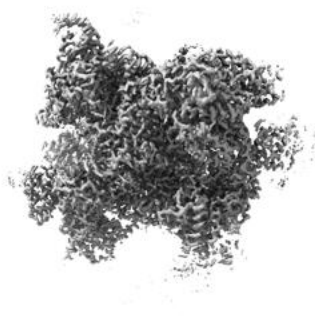
Z

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

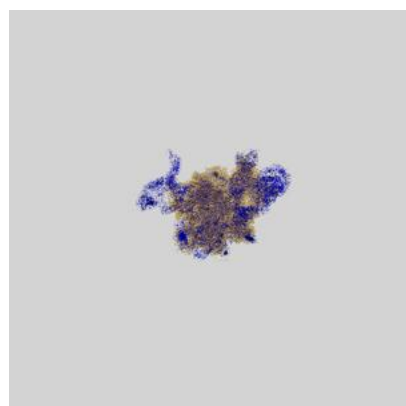
6.6 Mask visualisation [i](#)

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

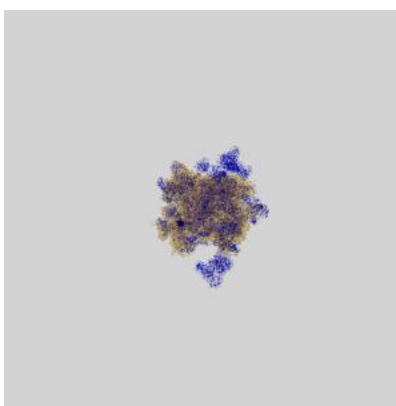
A mask typically either:

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

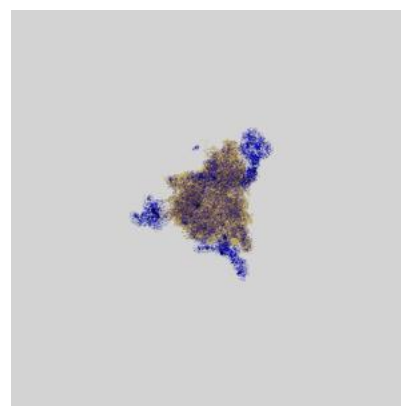
6.6.1 emd_47157_msk_1.map [i](#)



X



Y

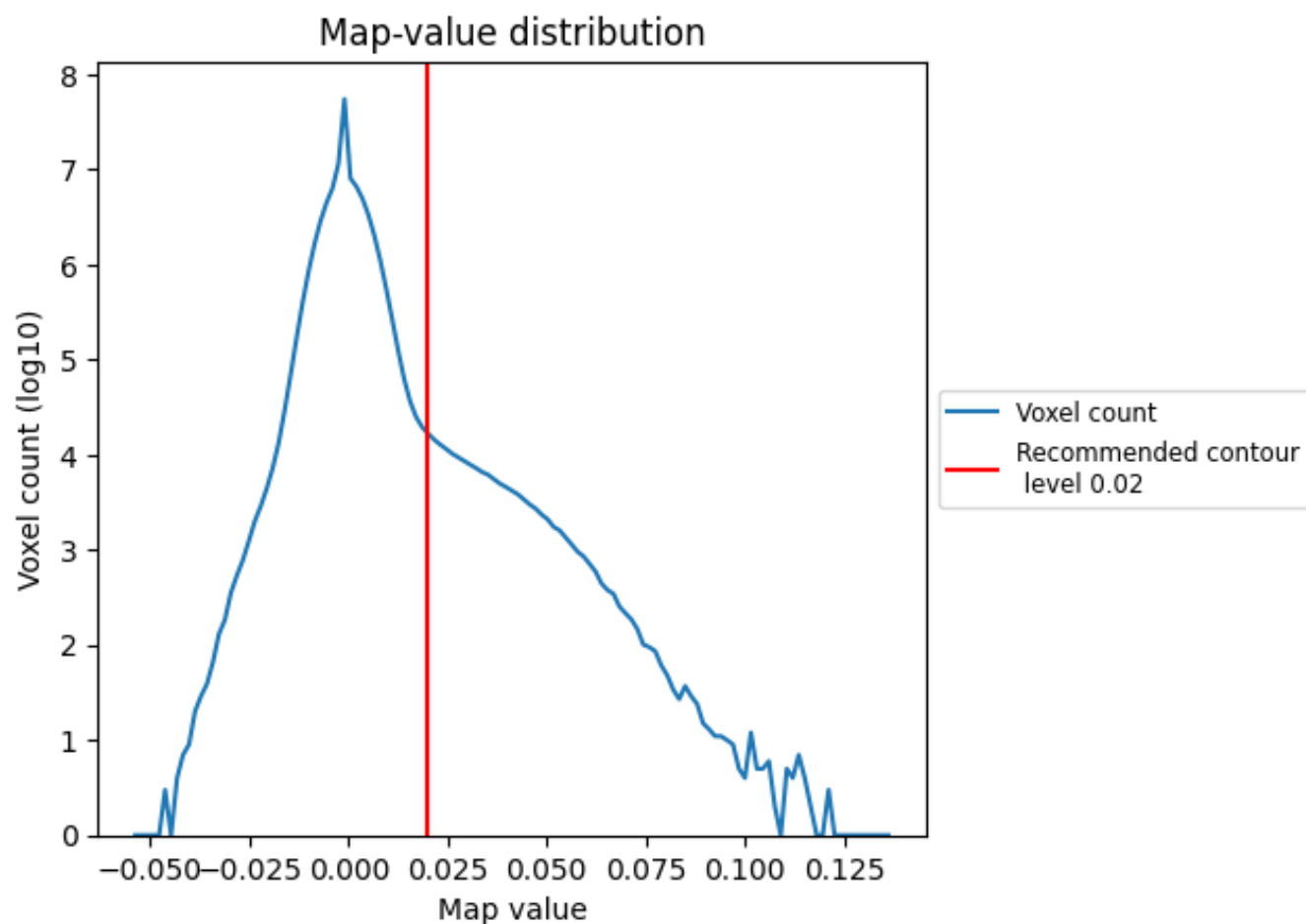


Z

7 Map analysis [i](#)

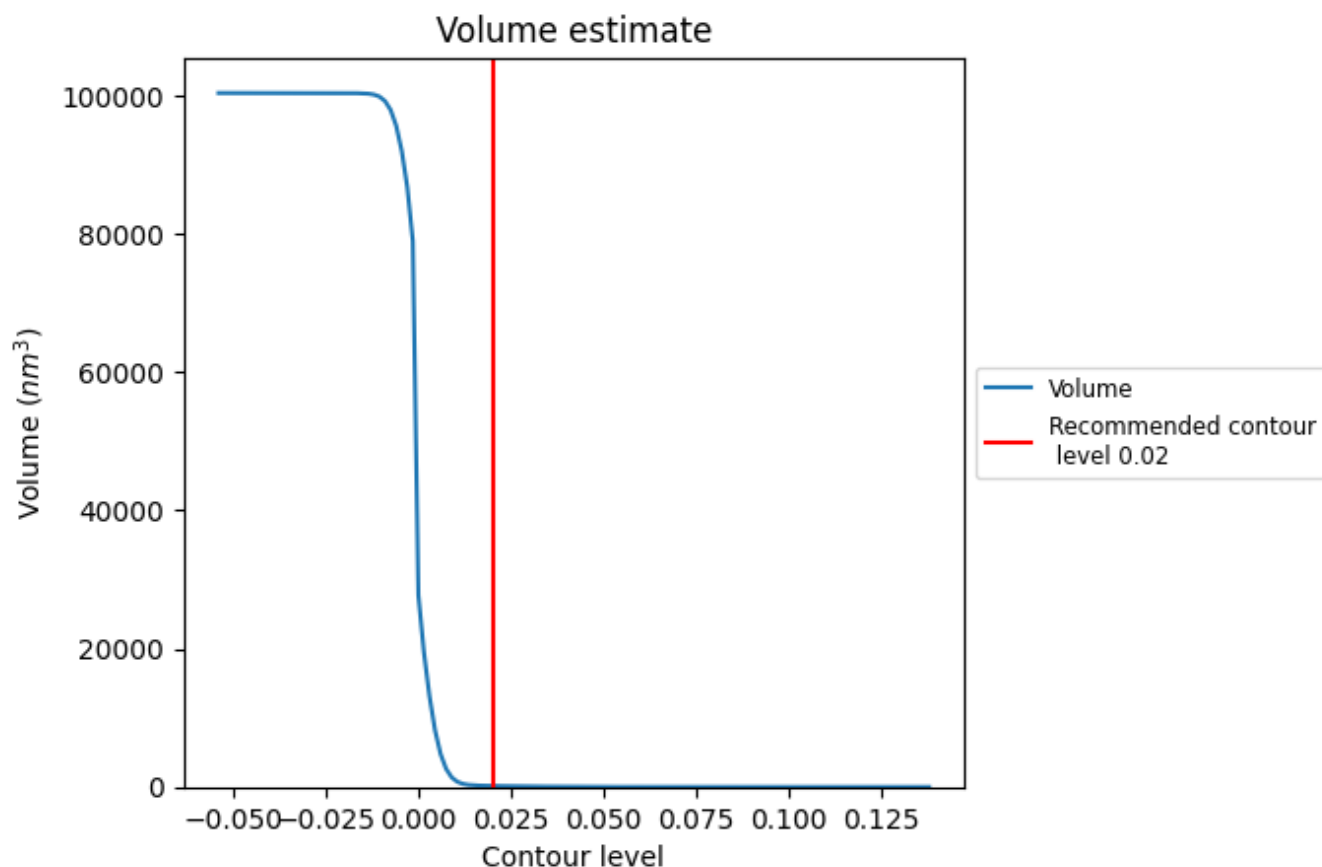
This section contains the results of statistical analysis of the map.

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.

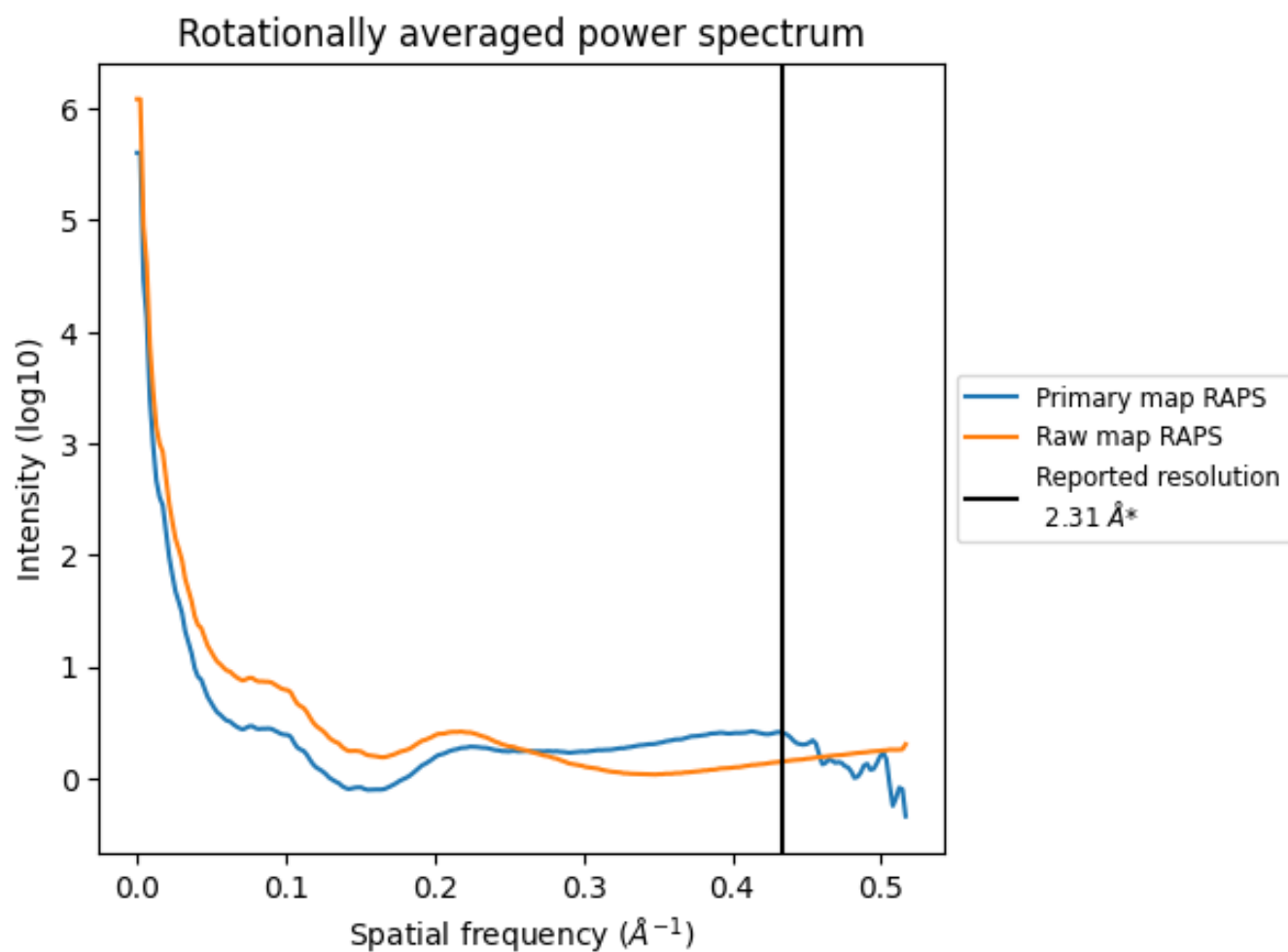
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 146 nm³; 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 ⓘ

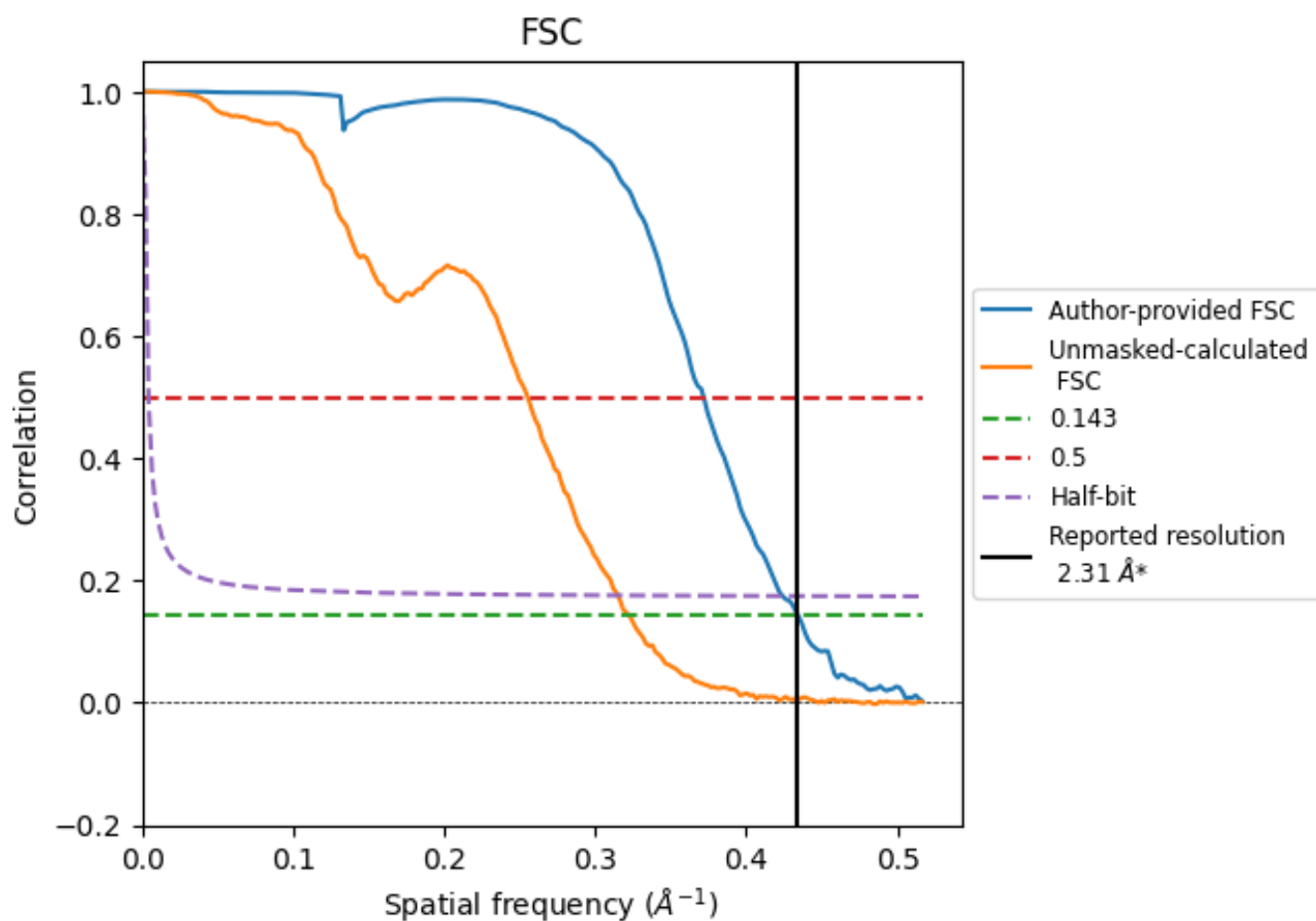


*Reported resolution corresponds to spatial frequency of 0.433 Å⁻¹

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 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

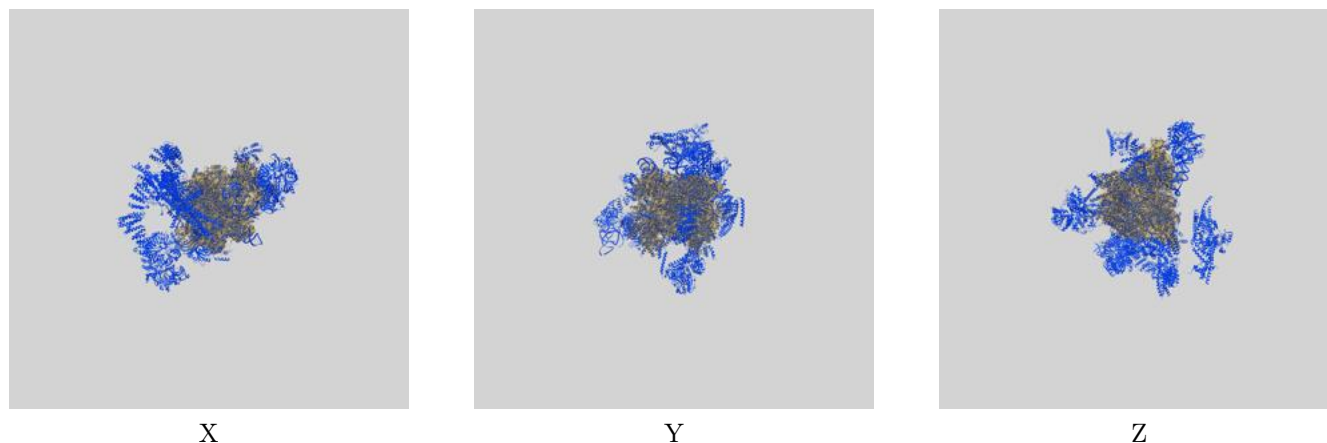
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.31	-	-
Author-provided FSC curve	2.30	2.69	2.36
Unmasked-calculated*	3.10	3.92	3.18

*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](#)

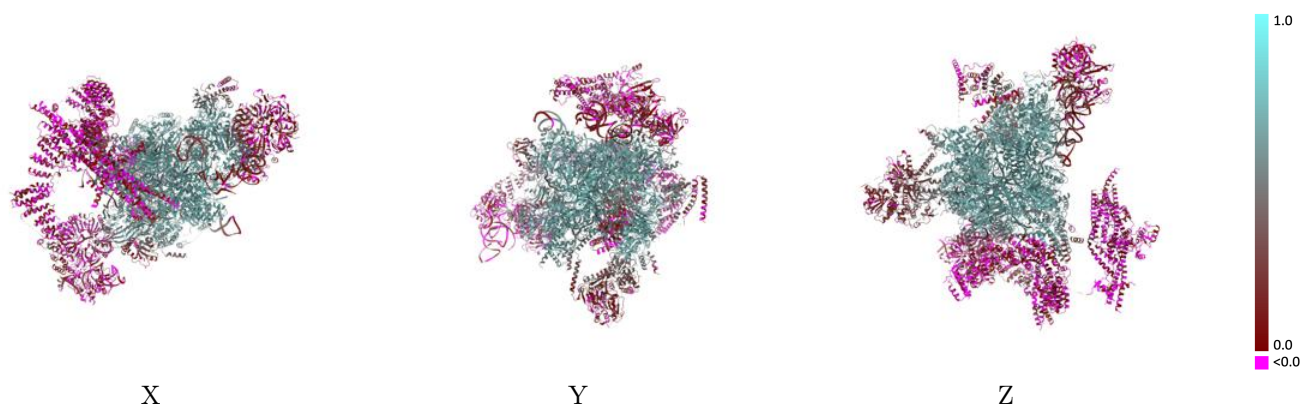
This section contains information regarding the fit between EMDB map EMD-47157 and PDB model 9DTR. Per-residue inclusion information can be found in [section 3](#) on [page 13](#).

9.1 Map-model overlay [i](#)



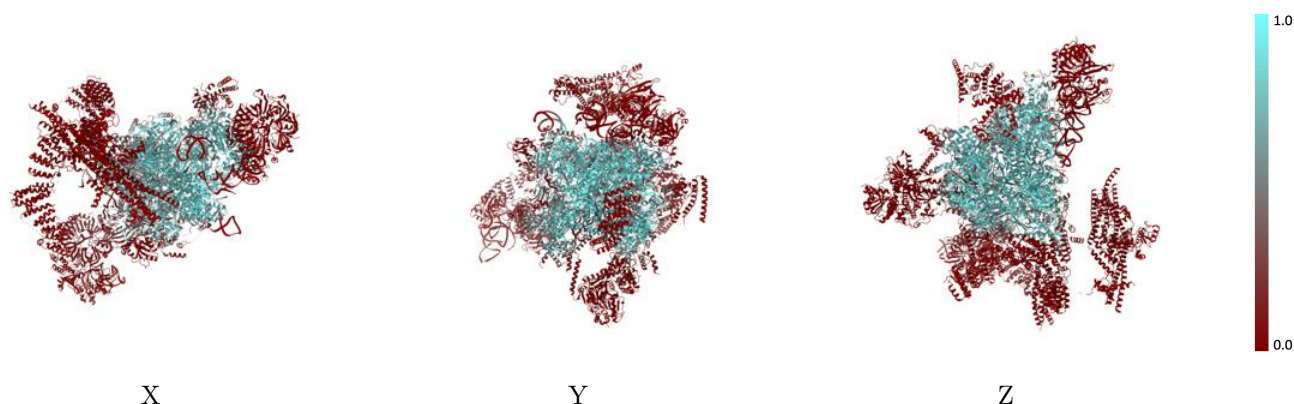
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



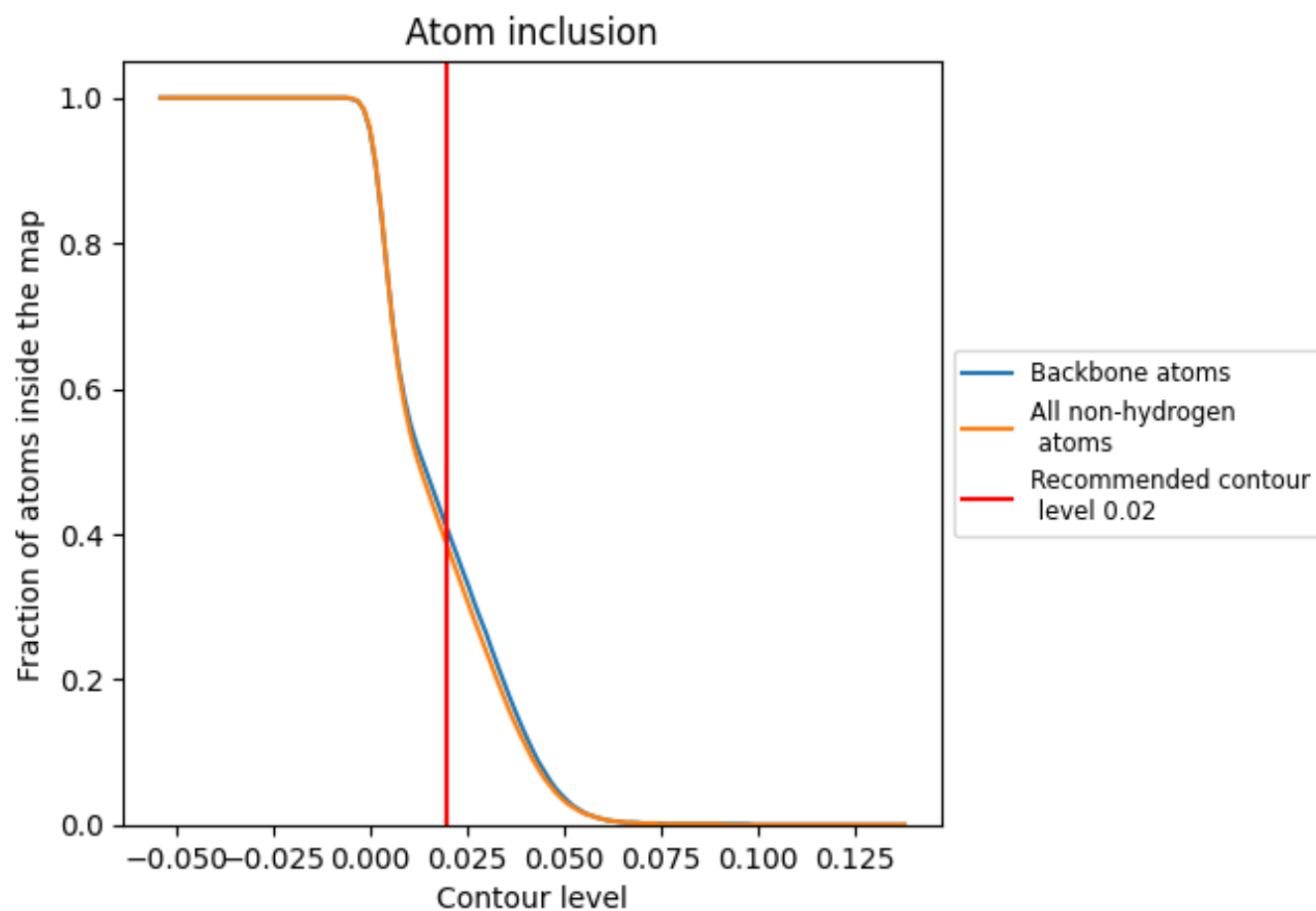
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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