



Full wwPDB EM Validation Report ⓘ

Dec 12, 2022 – 06:30 PM EST

PDB ID : 3JB9
EMDB ID : EMD-6413
Title : Cryo-EM structure of the yeast spliceosome at 3.6 angstrom resolution
Authors : Yan, C.; Hang, J.; Wan, R.; Huang, M.; Wong, C.; Shi, Y.
Deposited on : 2015-08-09
Resolution : 3.60 Å (reported)
Based on initial models : 2YTC, 1GV2, 4WZJ, 2XL2, 4I43, 3J7P, 3LRV, 2BAY, 3U1L, 4YVD

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.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

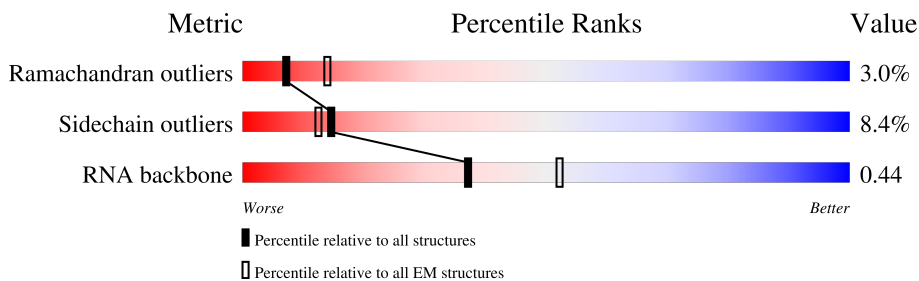
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.60 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	A	2363	<div> <div>7%</div> <div>71%</div> <div>11%</div> <div>17%</div> </div>
2	B	984	<div> <div>85%</div> <div>7%</div> <div>8%</div> </div>
3	C	120	<div> <div>42%</div> <div>45%</div> <div>12%</div> </div>
4	D	97	<div> <div>85%</div> <div>14%</div> </div>
4	Z	97	<div> <div>82%</div> <div>73%</div> <div>9%</div> <div>18%</div> </div>
5	E	147	<div> <div>62%</div> <div>5%</div> <div>33%</div> </div>
5	b	147	<div> <div>50%</div> <div>46%</div> <div>50%</div> </div>
6	F	117	<div> <div>63%</div> <div>6%</div> <div>30%</div> </div>




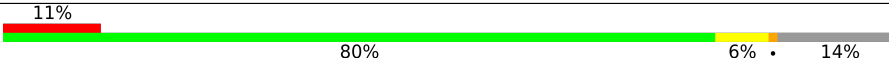
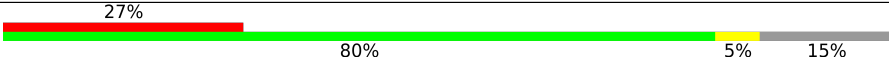

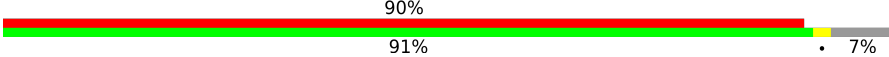



Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
6	f	117	
7	G	115	
7	l	115	
8	H	84	
8	m	84	
9	I	78	
9	n	78	
10	J	77	
10	o	77	
11	K	473	
12	L	340	
13	M	557	
14	N	99	
15	O	8	
16	Q	13	
17	P	186	
18	S	488	
18	T	488	
18	U	488	
18	V	488	
19	W	757	
20	Y	388	
21	a	354	
22	c	639	
23	d	155	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
24	e	146	
25	g	558	
26	h	265	
27	i	187	
28	R	674	
29	r	790	
30	X	1284	
31	j	239	
32	k	111	
33	x	412	

2 Entry composition

There are 37 unique types of molecules in this entry. The entry contains 86551 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Pre-mRNA-splicing factor spp42.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1964	Total	C	N	O	S	0	0
			16230	10413	2859	2893	65		

- Molecule 2 is a protein called Pre-mRNA-splicing factor cwf10.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	904	Total	C	N	O	S	0	0
			7196	4586	1235	1340	35		

- Molecule 3 is a RNA chain called U5 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	105	Total	C	N	O	P	0	0
			2209	990	364	750	105		

- Molecule 4 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	96	Total	C	N	O	S	0	0
			760	470	147	136	7		
4	Z	80	Total	C	N	O	S	0	0
			639	396	118	118	7		

- Molecule 5 is a protein called Small nuclear ribonucleoprotein-associated protein B.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	98	Total	C	N	O	S	0	0
			730	464	130	131	5		
5	b	74	Total	C	N	O	S	0	0
			576	365	99	107	5		

- Molecule 6 is a protein called Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	82	Total	C	N	O	S	0	0
			646	412	110	119	5		
6	f	82	Total	C	N	O	S	0	0
			646	412	110	119	5		

- Molecule 7 is a protein called Small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	95	Total	C	N	O	S	0	0
			751	472	141	134	4		
7	l	87	Total	C	N	O	S	0	0
			696	440	128	124	4		

- Molecule 8 is a protein called Small nuclear ribonucleoprotein E.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	76	Total	C	N	O	S	0	0
			620	401	107	110	2		
8	m	76	Total	C	N	O	S	0	0
			620	401	107	110	2		

- Molecule 9 is a protein called Small nuclear ribonucleoprotein F.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	73	Total	C	N	O	S	0	0
			570	369	95	104	2		
9	n	73	Total	C	N	O	S	0	0
			570	369	95	104	2		

- Molecule 10 is a protein called Small nuclear ribonucleoprotein G.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	73	Total	C	N	O	S	0	0
			573	366	98	108	1		
10	o	73	Total	C	N	O	S	0	0
			573	366	98	108	1		

- Molecule 11 is a protein called Pre-mRNA-splicing factor prp5.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	373	Total	C	N	O	S	0	0
			2730	1720	492	505	13		

- Molecule 12 is a protein called Pre-mRNA-splicing factor cwf17.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	293	Total	C	N	O	S	0	0
			2273	1425	407	430	11		

- Molecule 13 is a protein called Pre-mRNA-processing protein 45.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	207	Total	C	N	O	S	0	0
			1661	1044	309	304	4		

- Molecule 14 is a RNA chain called U6 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	90	Total	C	N	O	P	0	0
			1928	863	357	618	90		

- Molecule 15 is a RNA chain called RNA (5'-R(P*GP*UP*AP*UP*GP*UP*AP*U)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	8	Total	C	N	O	P	0	0
			170	76	28	58	8		

- Molecule 16 is a RNA chain called RNA (5'-R(P*UP*UP*UP*AP*UP*AP*CP*UP*AP*A P*CP*AP*C)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Q	13	Total	C	N	O	P	0	0
			270	122	44	91	13		

- Molecule 17 is a RNA chain called U2 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	P	111	Total	C	N	O	P	0	0
			2323	1039	365	808	111		

- Molecule 18 is a protein called Pre-mRNA-processing factor 19.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	S	132	Total	C	N	O	S	0	0
			1052	663	181	205	3		
18	T	134	Total	C	N	O	S	0	0
			1069	671	183	212	3		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
18	U	430	Total	C	N	O	S	0	0
			2864	1801	492	562	9		
18	V	131	Total	C	N	O	S	0	0
			1037	652	177	205	3		

- Molecule 19 is a protein called Pre-mRNA-splicing factor cdc5.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	W	426	Total	C	N	O	S	0	0
			3024	1881	562	574	7		

- Molecule 20 is a protein called Pre-mRNA-splicing factor cwf2.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	Y	261	Total	C	N	O	S	0	0
			2008	1252	365	381	10		

- Molecule 21 is a protein called Pre-mRNA-splicing factor cwf5.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	a	255	Total	C	N	O	S	0	0
			1751	1088	324	325	14		

- Molecule 22 is a protein called Pre-mRNA-splicing factor cwf19.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	c	300	Total	C	N	O	S	0	0
			2425	1541	422	447	15		

- Molecule 23 is a protein called Peptidyl-prolyl cis-trans isomerase ppi1.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	d	155	Total	C	N	O	S	0	0
			1187	755	203	224	5		

- Molecule 24 is a protein called Pre-mRNA-splicing factor cwf14.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	e	144	Total	C	N	O	S	0	0
			1176	733	216	214	13		

- Molecule 25 is a protein called Pre-mRNA-processing factor 17.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	g	148	Total	C	N	O	S	0	0
			1013	631	181	200	1		

- Molecule 26 is a protein called Pre-mRNA-splicing factor cwf15.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	h	90	Total	C	N	O	S	0	0
			752	467	146	138	1		

- Molecule 27 is a protein called Pre-mRNA-splicing factor cwf7.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	i	161	Total	C	N	O	S	0	0
			1218	758	219	238	3		

- Molecule 28 is a protein called Pre-mRNA-splicing factor cwf4.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	R	575	Total	C	N	O	S	0	0
			3800	2363	718	706	13		

- Molecule 29 is a protein called Pre-mRNA-splicing factor cwf3.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	r	573	Total	C	N	O	S	0	0
			3299	2039	619	640	1		

- Molecule 30 is a protein called Pre-mRNA-splicing factor cwf11.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	X	1195	Total	C	N	O	S	0	0
			9764	6282	1619	1820	43		

- Molecule 31 is a protein called U2 small nuclear ribonucleoprotein A'.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	j	160	Total	C	N	O	S	0	0
			1108	707	187	211	3		

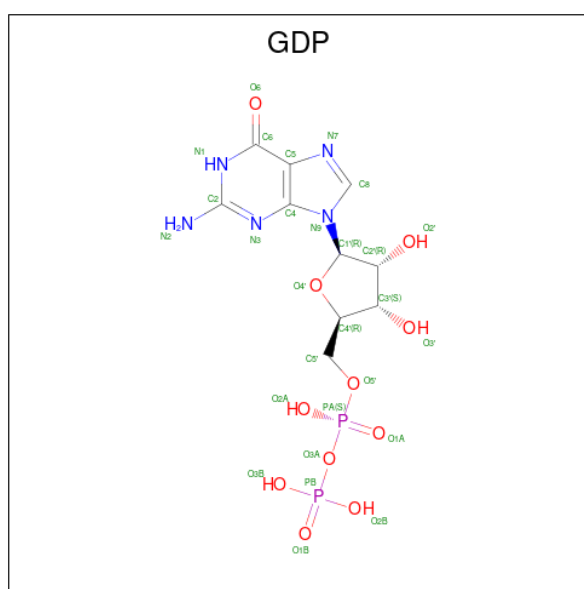
- Molecule 32 is a protein called Probable U2 small nuclear ribonucleoprotein B''.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	k	89	Total	C	N	O	S	0	0
			618	405	102	109	2		

- Molecule 33 is a protein called unknown chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	x	272	Total	C	N	O		0	0
			1360	816	272	272			

- Molecule 34 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



Mol	Chain	Residues	Atoms					AltConf
34	B	1	Total	C	N	O	P	0
			28	10	5	11	2	

- Molecule 35 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
35	N	4	Total	Mg	0
			4	4	

- Molecule 36 is ZINC ION (three-letter code: ZN) (formula: Zn).

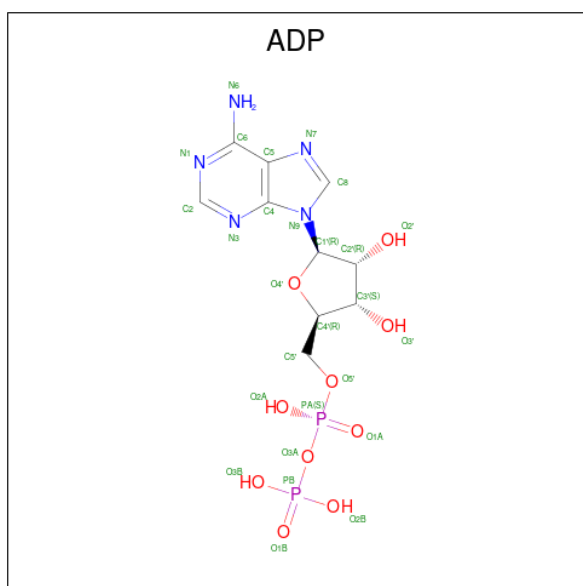
Mol	Chain	Residues	Atoms		AltConf
36	Y	1	Total	Zn	0
			1	1	

Continued on next page...

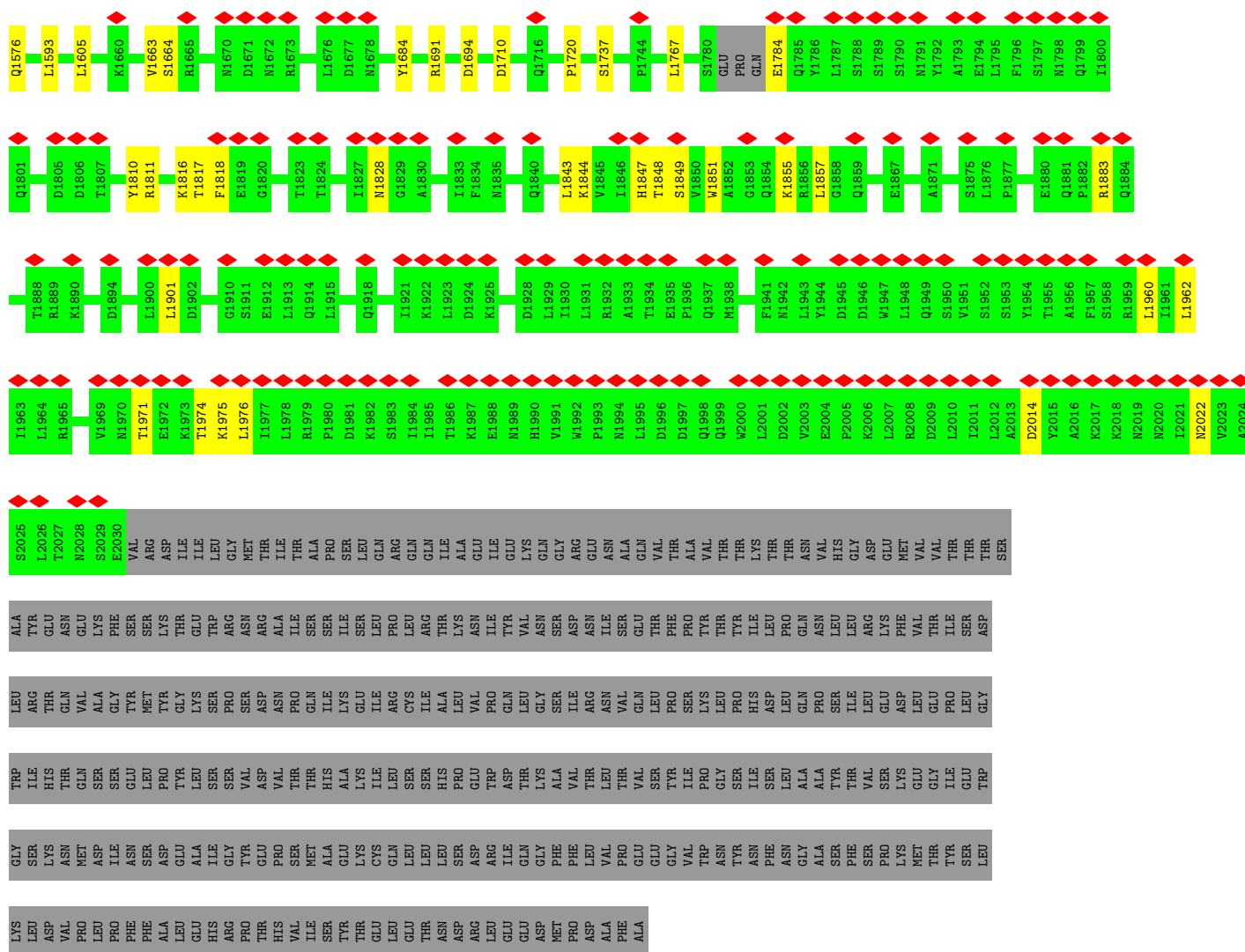
Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
36	a	2	Total Zn 2 2	0
36	c	1	Total Zn 1 1	0
36	e	3	Total Zn 3 3	0

- Molecule 37 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $\text{C}_{10}\text{H}_{15}\text{N}_5\text{O}_{10}\text{P}_2$).

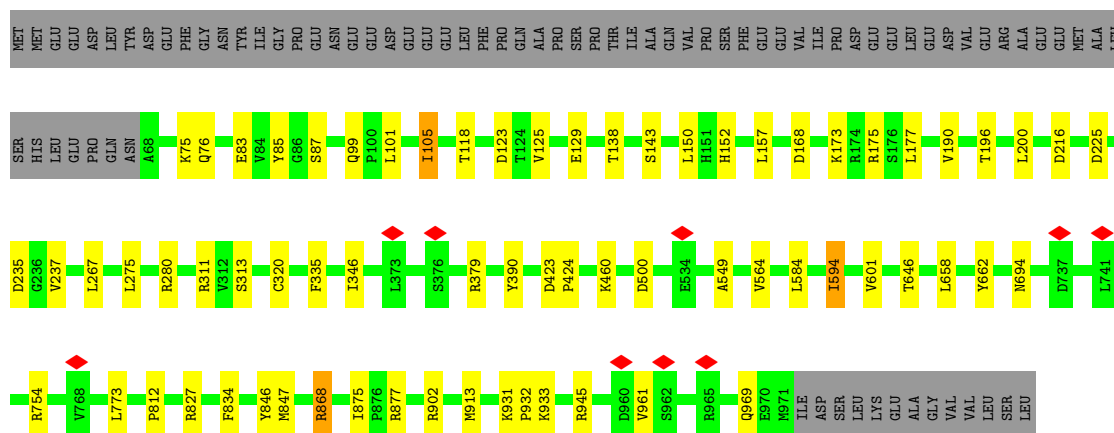


Mol	Chain	Residues	Atoms					AltConf
37	X	1	Total 27	C 10	N 5	O 10	P 2	0

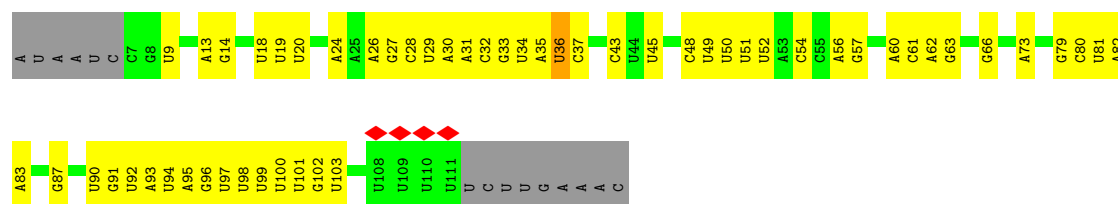


• Molecule 2: Pre-mRNA-splicing factor cwf10

Chain B: 85% 7% 8%

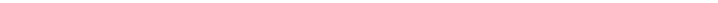


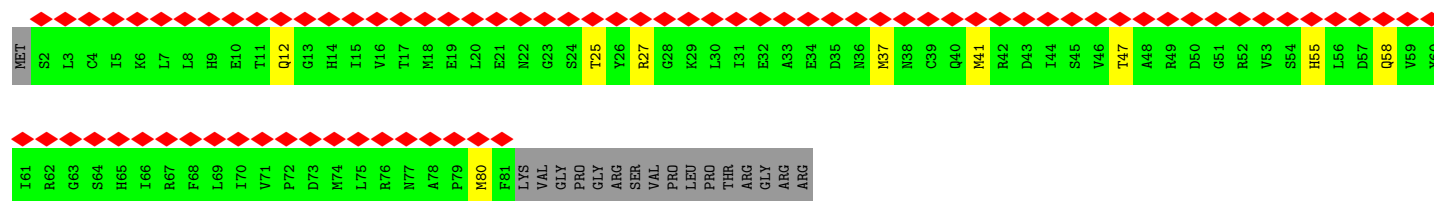
• Molecule 3: U5 snRNA



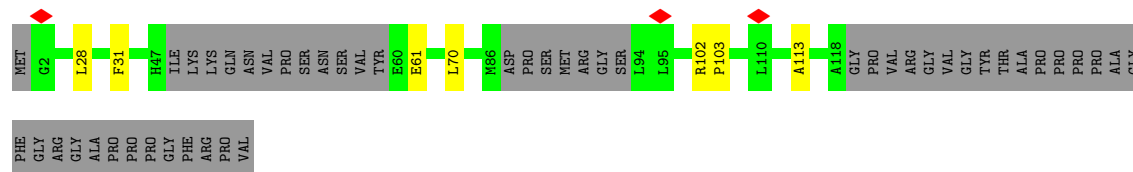
- Chain D: 85% 14%



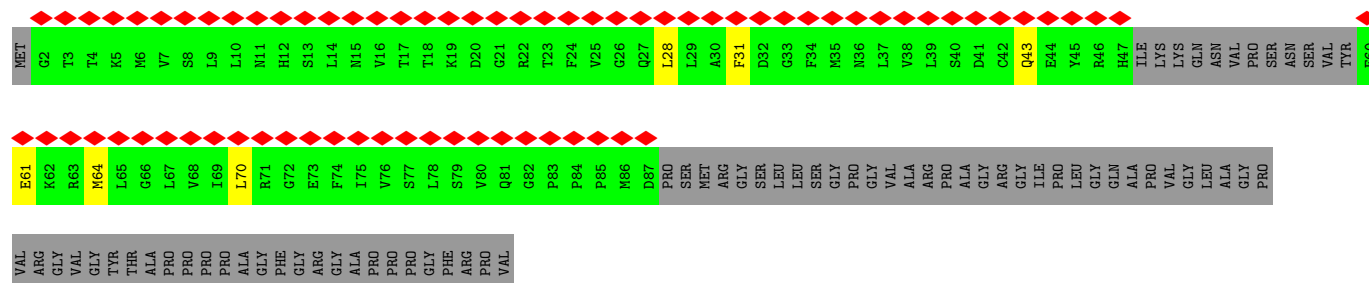
- Chain Z:  82% 73% 9% 18%



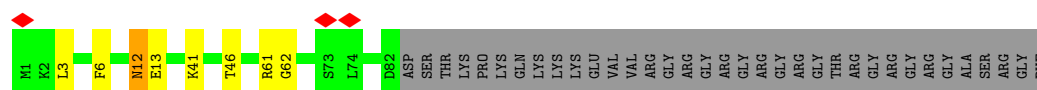
- Chain E:  62% 5% 33%



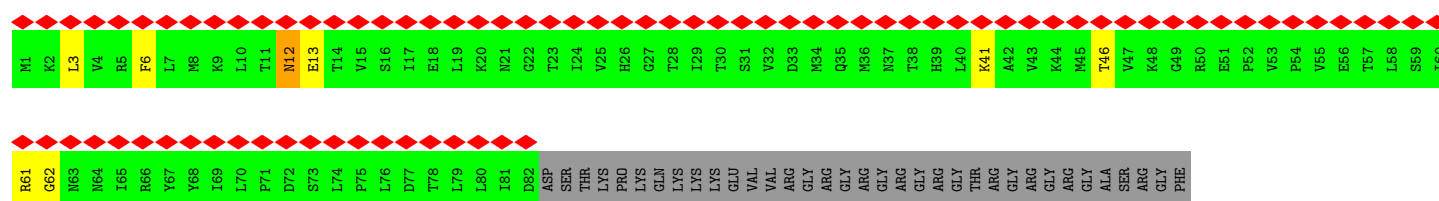
- Chain b:  50% 46% 50%



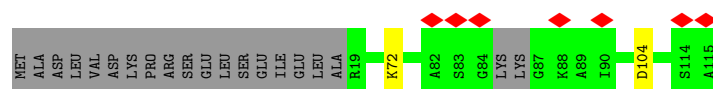
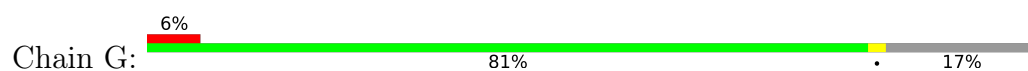
- Molecule 6: Small nuclear ribonucleoprotein Sm D1



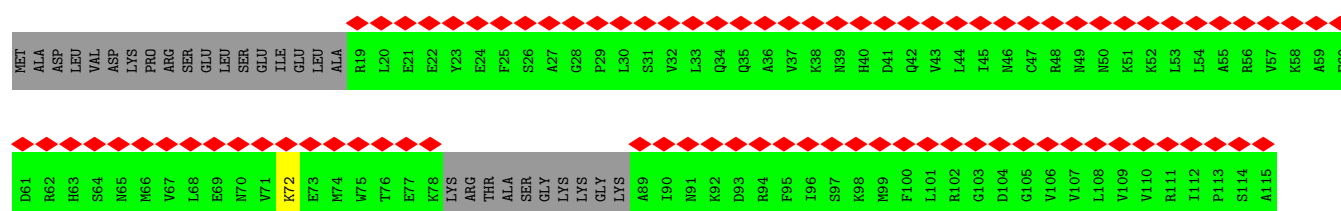
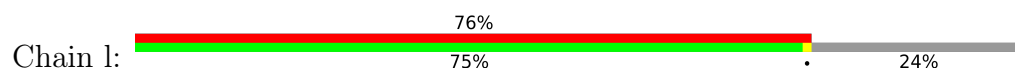
- Molecule 6: Small nuclear ribonucleoprotein Sm D1



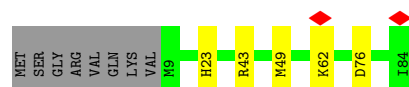
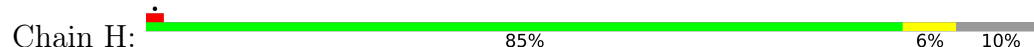
- Molecule 7: Small nuclear ribonucleoprotein Sm D2



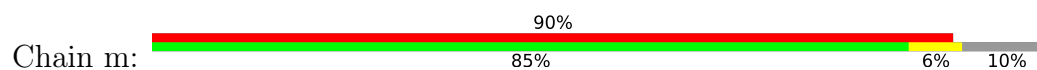
- Molecule 7: Small nuclear ribonucleoprotein Sm D2

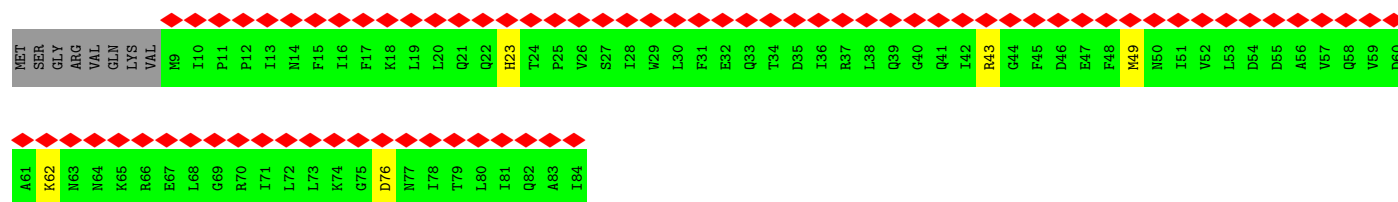


- Molecule 8: Small nuclear ribonucleoprotein E

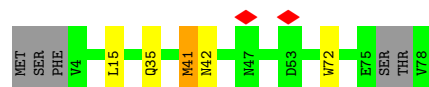
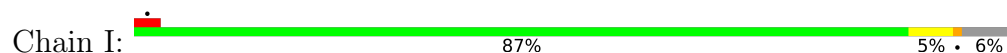


- Molecule 8: Small nuclear ribonucleoprotein E

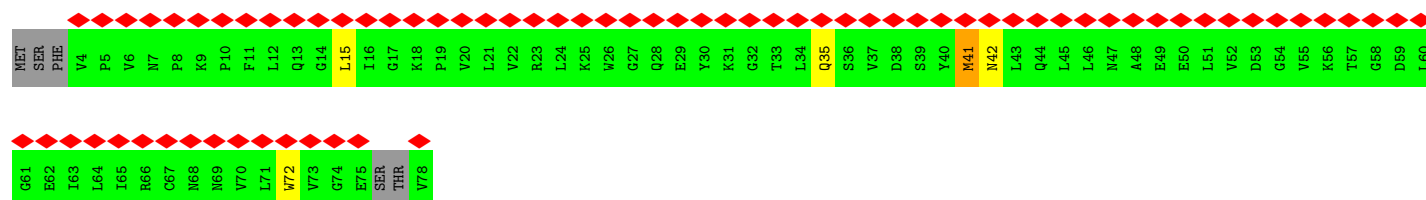
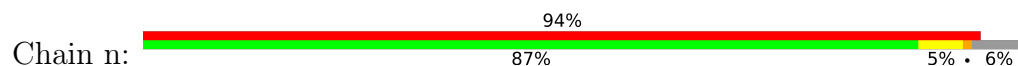




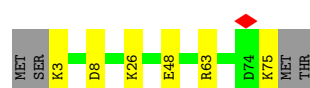
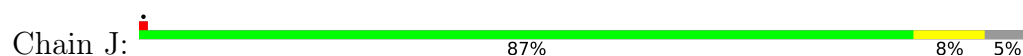
• Molecule 9: Small nuclear ribonucleoprotein F



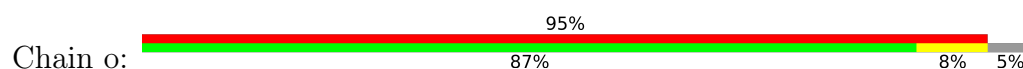
• Molecule 9: Small nuclear ribonucleoprotein F



• Molecule 10: Small nuclear ribonucleoprotein G



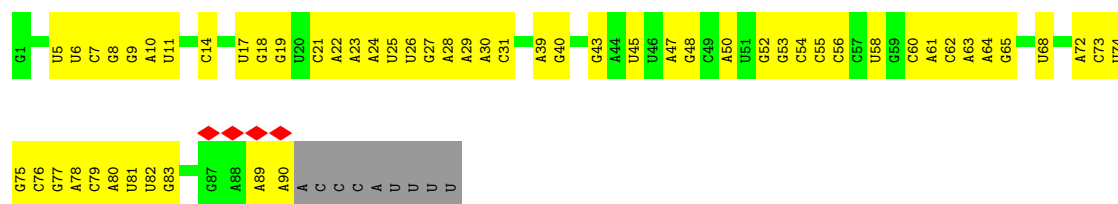
• Molecule 10: Small nuclear ribonucleoprotein G



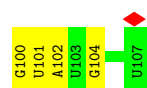
• Molecule 11: Pre-mRNA-splicing factor prp5



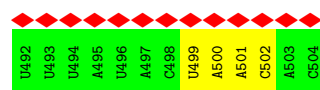
WORLDWIDE
PDB
PROTEIN DATA BANK



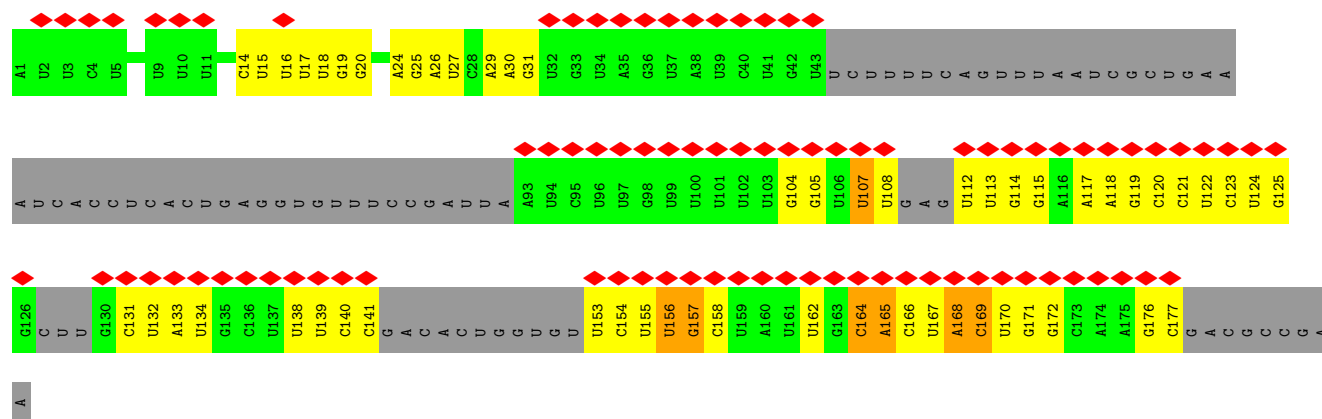
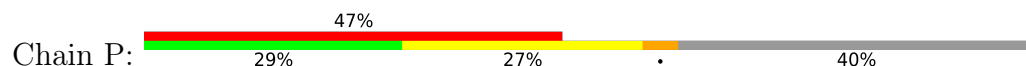
- Molecule 15: RNA (5'-R(P*GP*UP*AP*UP*GP*UP*AP*U)-3')



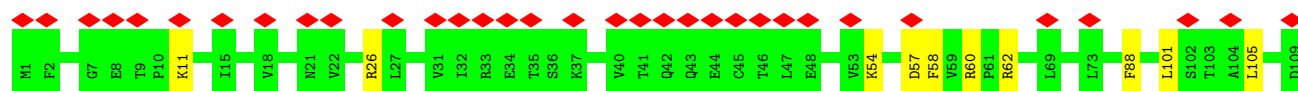
- Molecule 16: RNA (5'-R(P*UP*UP*UP*AP*UP*AP*CP*UP*AP*AP*CP*AP*C)-3')

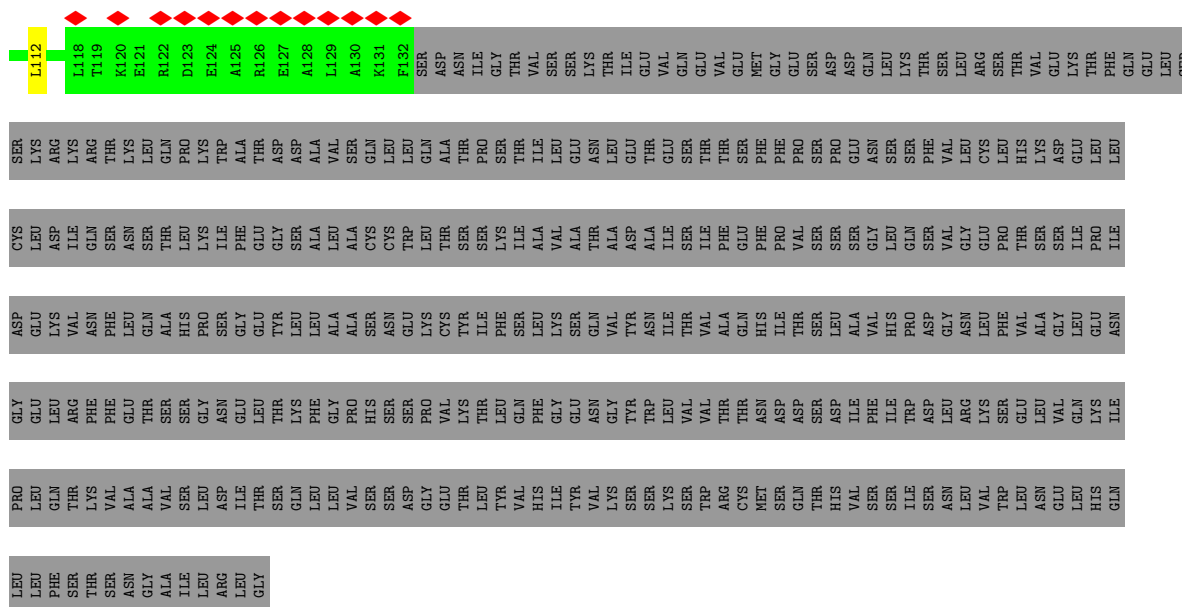


- Molecule 17: U2 snRNA

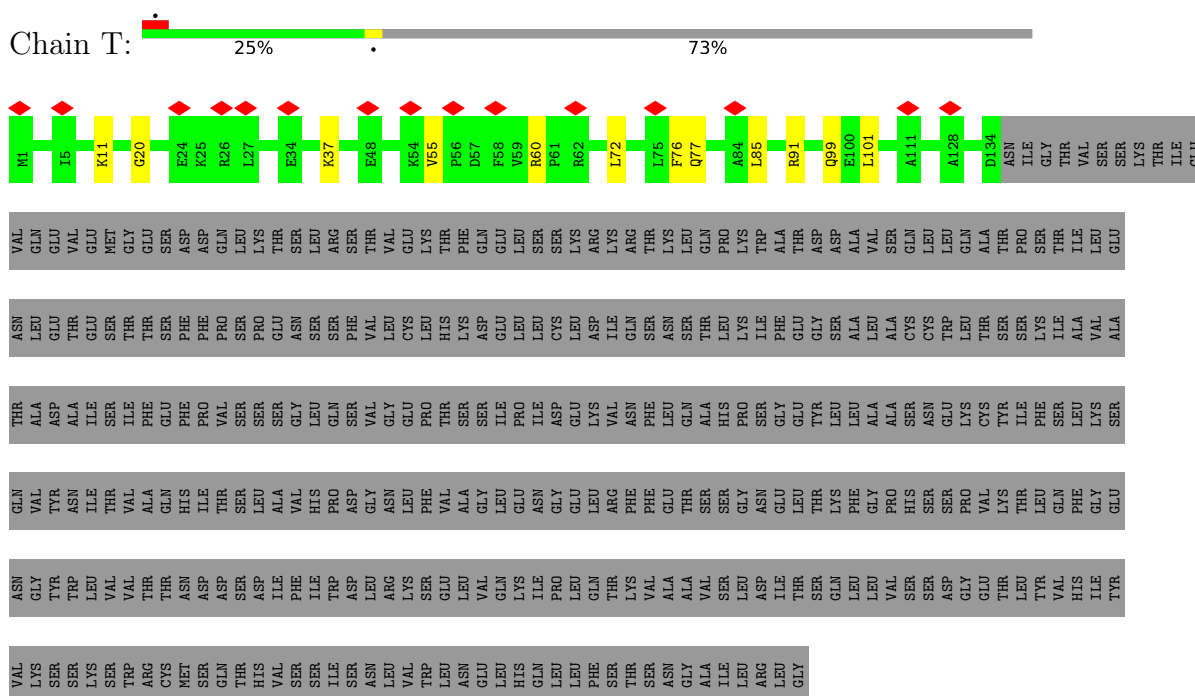


- Molecule 18: Pre-mRNA-processing factor 19

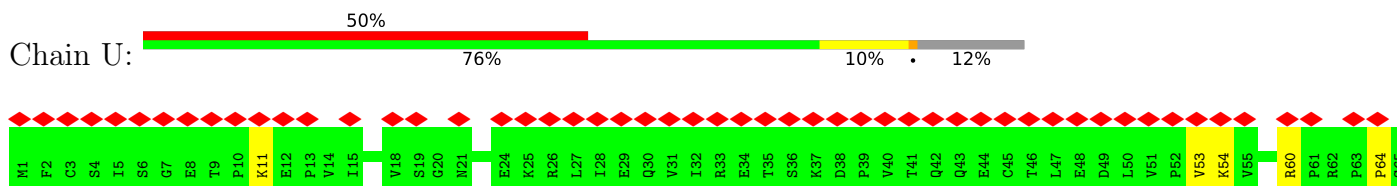


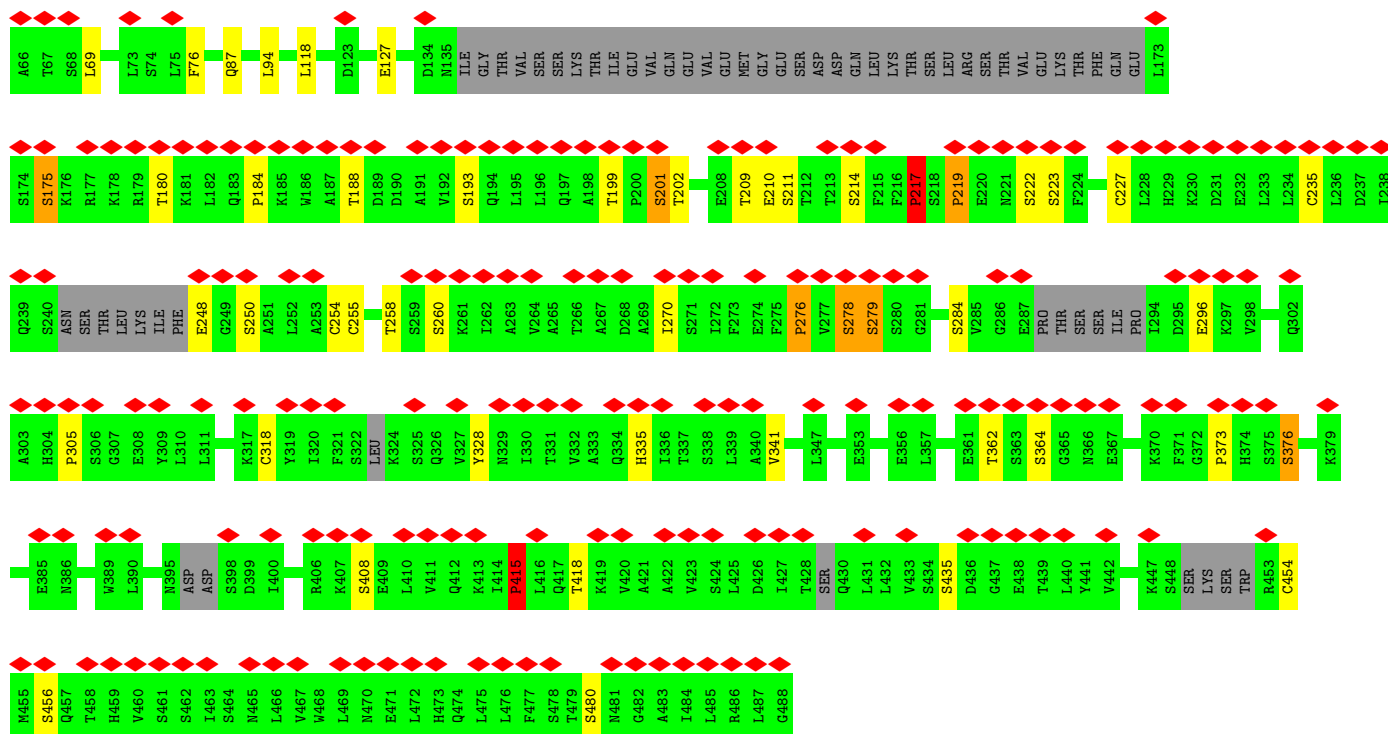


- Molecule 18: Pre-mRNA-processing factor 19

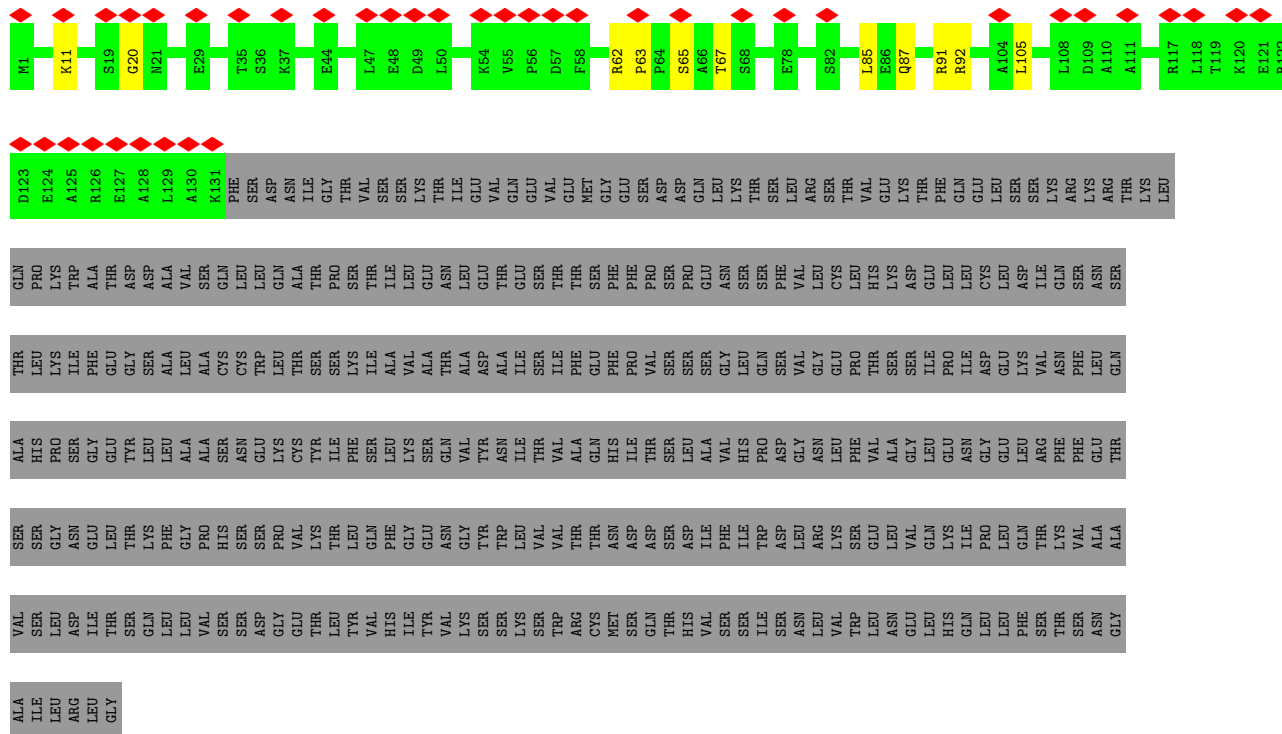


- Molecule 18: Pre-mRNA-processing factor 19

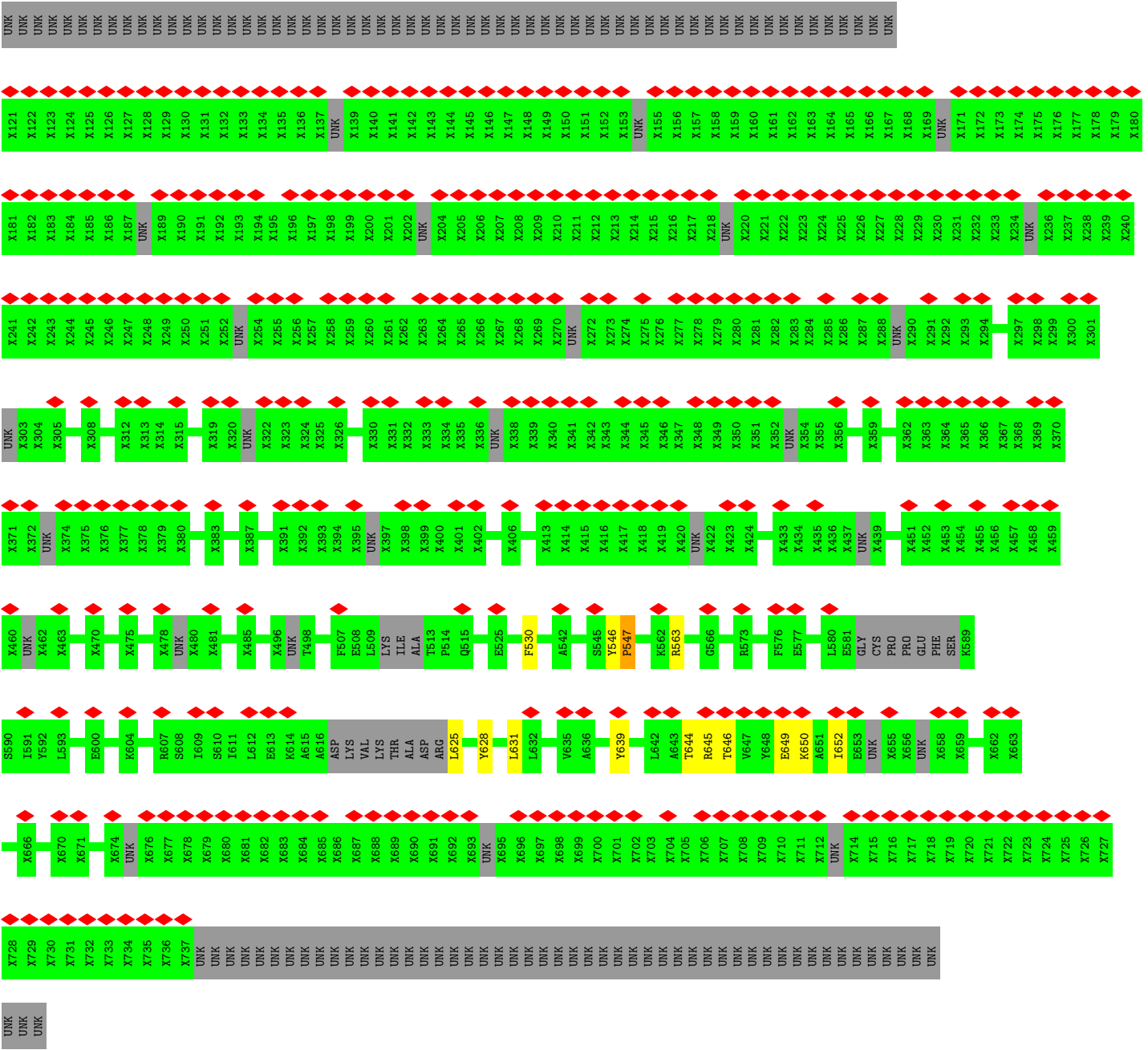




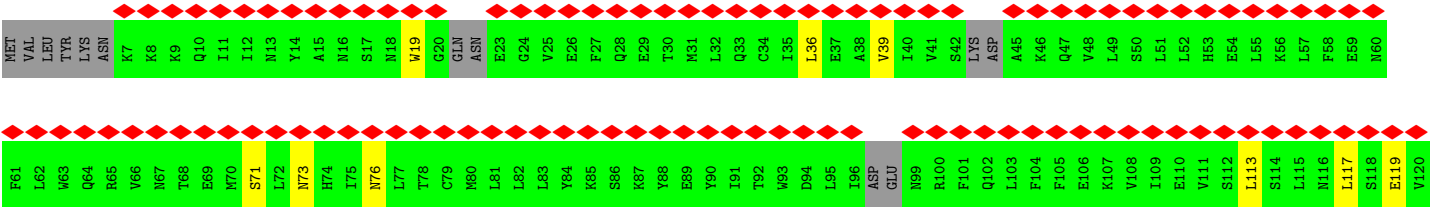
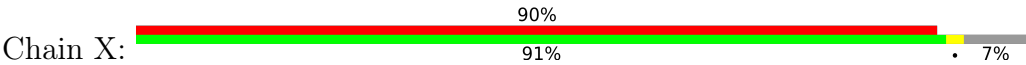
• Molecule 18: Pre-mRNA-processing factor 19



• Molecule 19: Pre-mRNA-splicing factor cdc5



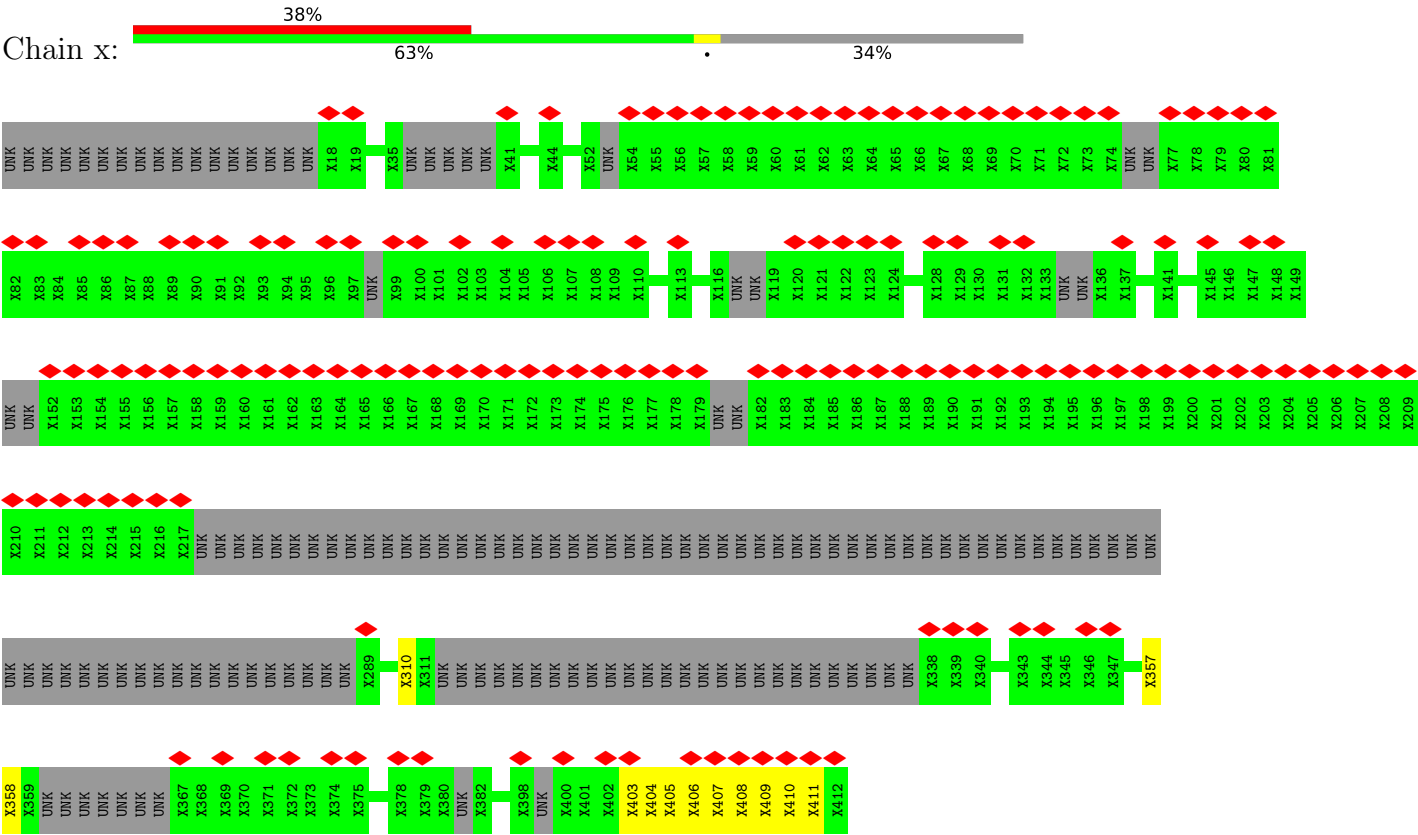
● Molecule 30: Pre-mRNA-splicing factor cwf11



V121	K181	F241	L301	Y364	Q426	T486	N546	L606	V666	T786	S846	N906
Y122	R182	A242	V302	A365	Y427	S487	A547	K607	A667	L787	H847	F907
M123	P183	H243	Q307	I366	L428	V488	L548	F608	R668	F788	D848	F908
I124	SER	P244	L308	K367	S429	A489	D549	N609	N669	T789	A849	D909
Q125	V186	P245	L309	V368	I430	P490	P650	F610	L670	L790	S850	Y910
I126	E187	I246	T309	D369	S431	GLN	GLN	A611	N671	L791	P851	A911
T128	K188	E247	L310	F370	F432	I1E	GLY	L612	N672	E792	D852	T912
L129	E189	D248	F311	E371	M434	GLN	GLY	V613	T673	K793	T853	K913
C130	P190	S249	S312	F372	R435	VAL	V554	L614	V674	A794	A854	L914
F131	L191	C250	D313	L373	Q436	L497	D556	S615	E676	R795	L855	Y915
Q132	H192	F251	F314	K374	Q437	P498	F557	GLU	Q676	C796	Y856	G916
F133	N193	Y252	Q315	F377	S438	Q499	T558	ALA	L677	F797	P857	E917
S134	L194	A254	GLU	I378	K439	Q900	I559	N619	Q678	H798	R858	L918
N135	L195	L255	LEU	N379	A440	V501	A560	K620	S679	GLN	D859	E919
I136	S196	R256	ASP	D382	Y441	K502	T561	Y621	V680	GLY	A860	Y920
E137	R197	M257	VAL	R383	K442	C503	I562	N622	L681	H801	Y861	M921
K138	W198	S258	PHE	THR	K443	Q504	C563	L623	P682	L802	T862	F922
L139	I199	L259	CYS	R385	K444	M505	N564	D624	N683	L803	K863	Q923
R140	H200	Y260	THR	L445	L445	G506	N564	L625	C684	Y804	R864	Q924
K141	S201	Y261	THR	L446	L446	L507	D566	N626	H685	L805	L865	L925
L142	L202	Y262	SER	V387	R447	S508	V567	L627	V686	S806	W866	E926
V143	L203	S263	L329	N388	S448	R509	G568	L628	P687	D807	D867	E927
Y144	I204	N264	Q330	D389	L449	P510	M569	V629	S688	E808	E868	I928
Q145	K205	E265	Q331	Y390	Y450	GLY	F570	S630	N689	L809	Y869	R929
L146	S206	L266	R332	D391	A451	P490	GLN	L631	L690	ASP	L870	P930
T147	I207	F267	Q333	E392	E452	SER	ASP	L632	S691	GLU	N871	F931
N148	S208	K268	K334	I393	L453	HIS	N574	N633	T692	T813	T872	G932
I149	Y209	K269	L335	I394	L454	A516	Q575	R634	E693	L814	V873	L933
S150	A210	M270	E336	N395	N455	L517	S576	A635	S694	E815	D874	L934
I151	Q211	T271	E337	F396	F456	R518	S577	K636	L696	Y817	ASP	R935
L152	THR	T272	I338	T397	S457	D519	D577	E637	L697	G818	K876	Y936
N153	GLU	D272	T339	L398	E458	L520	S578	F638	T697	L757	D877	Y937
S154	Q215	L274	S340	K399	Q459	K521	D579	P639	K698	T758	S878	E938
L155	E216	N275	F341	D400	Y460	N522	N580	K640	F699	C759	V879	D939
ASP	A217	Y276	L342	V401	R461	S523	K581	N641	Y700	K760	D880	Q940
L158	K218	L277	S343	G403	R462	I1E	S582	F642	T701	L761	S822	E941
D159	V219	T278	F344	E404	L463	LYS	I583	E643	M702	L762	W823	L942
K160	T220	K279	N345	R405	S464	S526	N584	D644	Q703	E763	T824	Y943
V161	P221	F280	S346	R406	I465	P527	V585	L645	M704	V764	S825	A944
K162	L222	P281	S347	S406	K466	F528	V586	F646	K705	L765	K826	L945
Y163	L223	F282	L347	V407	N467	L529	L587	L647	I1E	Q766	L827	C946
L164	A224	D283	K348	M408	A468	C530	S588	G648	S707	D767	P828	Q947
L165	N284	N284	S349	D409	T469	L531	P589	F649	A708	T768	G829	Q948
H166	I225	T285	L350	E411	K470	Y533	F590	G650	D709	S769	L830	S949
D167	I226	R286	C351	M412	N471	L534	Y591	T651	Y710	P770	L831	Q950
N227	G287	K353	S352	S413	L472	S535	H593	P652	T711	M771	R832	I951
M228	M228	C354	THR	S415	L414	K536	S594	D653	A712	D772	E833	I952
S229	S229	Y355	LYS	T415	ASP	D537	L595	T654	S713	R773	G835	Q953
S170	L230	L356	L356	M416	N476	M538	A596	A656	D714	T774	R836	C954
L171	V231	E291	R357	PHE	F477	E539	G597	F657	R715	V775	L837	T955
T172	L232	K292	T358	LEU	F478	Y540	L598	P658	H716	V776	A838	W956
K173	L233	E293	S359	LEU	S479	K541	G599	N659	F717	L777	R839	R957
A174	S234	Q294	F360	GLN	L480	L542	E600	A660	LEU	S778	S840	P958
F175	A235	K295	P361	ASN	N481	L543	N481	G602	PRO	D779	T841	I959
D176	F236	I296	E362	T423	N482	H544	G545	GLY	S721	S780	N781	E960
S177	P237	R297	K363	A424	F483	H544	G545	LEU	N722	N781	Q842	T961
Y178	T238	N298		I425	N483				L723	F782	A843	R962
K179	R239	D299			K484				L724	S783	P844	L963
E180	R240	E300			V485				L725	N785	G845	Q964
												T965



● Molecule 33: unknown chain



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	112795	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	
Minimum defocus (nm)	3.0	Depositor
Maximum defocus (nm)	1.5	Depositor
Magnification	Not provided	
Image detector	GATAN K2 (4k x 4k)	Depositor
Maximum map value	0.189	Depositor
Minimum map value	-0.087	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.0203	Depositor
Map size (\AA)	475.2, 475.2, 475.2	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.32, 1.32, 1.32	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ADP, GDP, ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.35	0/16654	0.57	0/22571
2	B	0.33	0/7357	0.57	0/9980
3	C	0.32	0/2463	0.72	1/3829 (0.0%)
4	D	0.29	0/772	0.56	0/1038
4	Z	0.29	0/648	0.54	0/871
5	E	0.30	0/741	0.54	0/998
5	b	0.32	0/584	0.55	0/785
6	F	0.27	0/654	0.50	0/885
6	f	0.27	0/654	0.50	0/885
7	G	0.27	0/760	0.46	0/1016
7	l	0.27	0/705	0.47	0/945
8	H	0.28	0/630	0.47	0/851
8	m	0.28	0/630	0.47	0/851
9	I	0.28	0/579	0.50	0/785
9	n	0.28	0/579	0.50	0/785
10	J	0.27	0/578	0.51	0/774
10	o	0.27	0/578	0.51	0/774
11	K	0.39	0/2539	0.67	2/3453 (0.1%)
12	L	0.30	0/2317	0.56	0/3130
13	M	0.33	0/1698	0.54	0/2295
14	N	0.22	0/2160	0.68	0/3365
15	O	0.19	0/189	0.65	0/292
16	Q	0.18	0/300	0.63	0/463
17	P	0.92	22/2580 (0.9%)	1.48	66/4000 (1.6%)
18	S	0.30	0/1069	0.48	0/1449
18	T	0.29	0/1086	0.51	0/1472
18	U	1.33	36/2888 (1.2%)	0.78	4/3898 (0.1%)
18	V	0.30	0/1053	0.48	0/1429
19	W	0.30	0/2300	0.50	1/3087 (0.0%)
20	Y	0.44	5/1934 (0.3%)	0.69	7/2609 (0.3%)
21	a	0.57	5/1479 (0.3%)	0.60	2/1980 (0.1%)
22	c	0.31	0/2486	0.52	1/3360 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
23	d	0.30	0/1214	0.47	0/1646
24	e	0.33	0/1199	0.60	0/1609
25	g	0.47	2/1033 (0.2%)	0.65	6/1412 (0.4%)
26	h	0.33	0/767	0.55	0/1028
27	i	0.30	0/1231	0.44	0/1657
28	R	0.31	0/2243	0.52	0/3016
29	r	0.42	0/1161	0.57	1/1565 (0.1%)
30	X	0.32	0/9957	0.53	0/13430
31	j	1.67	12/1118 (1.1%)	1.71	18/1513 (1.2%)
32	k	0.81	2/624 (0.3%)	1.36	5/838 (0.6%)
All	All	0.48	84/82191 (0.1%)	0.67	114/112619 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	5
11	K	0	2
20	Y	0	3
33	x	0	12
All	All	0	22

All (84) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	j	118	SER	CB-OG	31.06	1.82	1.42
18	U	318	CYS	CB-SG	-19.87	1.48	1.82
18	U	227	CYS	CB-SG	-19.43	1.49	1.82
31	j	70	CYS	CB-SG	-17.93	1.51	1.82
31	j	111	CYS	CB-SG	-17.52	1.52	1.82
31	j	76	THR	CB-OG1	17.41	1.78	1.43
18	U	254	CYS	CB-SG	-17.29	1.52	1.82
18	U	235	CYS	CB-SG	-17.10	1.53	1.82
31	j	119	CYS	CB-SG	-16.82	1.53	1.82
18	U	454	CYS	CB-SG	-16.22	1.54	1.82
18	U	255	CYS	CB-SG	-15.77	1.55	1.82
17	P	153	U	O3'-P	-10.06	1.49	1.61
18	U	211	SER	CB-OG	9.98	1.55	1.42
32	k	93	ALA	CA-CB	-9.92	1.31	1.52
18	U	222	SER	CB-OG	9.74	1.54	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	j	93	SER	CB-OG	9.69	1.54	1.42
18	U	193	SER	CA-CB	-9.28	1.39	1.52
18	U	364	SER	CB-OG	9.03	1.53	1.42
18	U	408	SER	CB-OG	8.99	1.53	1.42
18	U	250	SER	CB-OG	8.87	1.53	1.42
18	U	279	SER	CB-OG	8.06	1.52	1.42
21	a	267	SER	CB-OG	8.05	1.52	1.42
21	a	240	SER	CB-OG	7.83	1.52	1.42
21	a	259	SER	CB-OG	7.81	1.52	1.42
18	U	214	SER	CB-OG	7.80	1.52	1.42
18	U	284	SER	CB-OG	7.73	1.52	1.42
18	U	260	SER	CB-OG	7.73	1.52	1.42
31	j	9	SER	CB-OG	7.67	1.52	1.42
17	P	141	C	C1'-N1	7.51	1.60	1.48
18	U	456	SER	CB-OG	7.50	1.52	1.42
18	U	175	SER	CB-OG	7.44	1.51	1.42
31	j	16	SER	CB-OG	7.16	1.51	1.42
31	j	140	SER	CB-OG	7.16	1.51	1.42
18	U	480	SER	CA-CB	-7.02	1.42	1.52
17	P	138	U	C1'-N1	6.94	1.59	1.48
17	P	112	U	C1'-N1	6.88	1.59	1.48
17	P	153	U	C1'-N1	6.88	1.59	1.48
17	P	122	U	C1'-N1	6.88	1.59	1.48
17	P	113	U	C1'-N1	6.87	1.59	1.48
17	P	132	U	C1'-N1	6.86	1.59	1.48
17	P	134	U	C1'-N1	6.85	1.59	1.48
17	P	139	U	C1'-N1	6.85	1.59	1.48
18	U	435	SER	CB-OG	6.84	1.51	1.42
17	P	124	U	C1'-N1	6.82	1.58	1.48
17	P	158	C	C1'-N1	6.76	1.58	1.48
18	U	278	SER	CB-OG	6.71	1.50	1.42
17	P	172	G	C1'-N9	-6.50	1.37	1.46
21	a	226	TYR	CB-CG	-6.41	1.42	1.51
17	P	154	C	C1'-N1	6.37	1.58	1.48
17	P	123	C	C1'-N1	6.37	1.58	1.48
17	P	121	C	C1'-N1	6.34	1.58	1.48
17	P	120	C	C1'-N1	6.34	1.58	1.48
17	P	140	C	C1'-N1	6.30	1.58	1.48
17	P	131	C	C1'-N1	6.26	1.58	1.48
18	U	202	THR	CB-OG1	6.25	1.55	1.43
18	U	210	GLU	CB-CG	-6.14	1.40	1.52
18	U	328	TYR	CB-CG	-6.13	1.42	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	U	219	PRO	CA-CB	-6.12	1.41	1.53
18	U	376	SER	CA-CB	-6.12	1.43	1.52
17	P	166	C	C1'-N1	5.98	1.57	1.48
17	P	154	C	O3'-P	5.88	1.68	1.61
18	U	180	THR	CB-OG1	5.87	1.54	1.43
18	U	296	GLU	CB-CG	-5.86	1.41	1.52
18	U	201	SER	CA-CB	-5.75	1.44	1.52
31	j	13	SER	CB-OG	5.75	1.49	1.42
31	j	81	ASP	CA-CB	-5.67	1.41	1.53
18	U	188	THR	CB-OG1	5.67	1.54	1.43
31	j	58	ASN	CA-CB	-5.62	1.38	1.53
18	U	199	THR	CB-OG1	5.59	1.54	1.43
18	U	248	GLU	CB-CG	-5.51	1.41	1.52
18	U	418	THR	CB-OG1	5.50	1.54	1.43
18	U	362	THR	CB-OG1	5.45	1.54	1.43
32	k	89	GLU	CB-CG	-5.44	1.41	1.52
20	Y	67	PRO	N-CD	5.38	1.55	1.47
18	U	335	HIS	CB-CG	-5.35	1.40	1.50
20	Y	64	PRO	N-CD	5.29	1.55	1.47
25	g	144	PRO	N-CD	5.23	1.55	1.47
21	a	233	GLU	CB-CG	-5.21	1.42	1.52
18	U	223	SER	CB-OG	5.17	1.49	1.42
25	g	156	PRO	N-CD	5.14	1.55	1.47
20	Y	275	PRO	N-CD	5.12	1.55	1.47
17	P	107	U	C1'-N1	5.10	1.56	1.48
20	Y	252	PRO	N-CD	5.09	1.54	1.47
20	Y	250	PRO	N-CD	5.05	1.54	1.47

All (114) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	Y	57	ARG	C-N-CD	-16.30	84.75	120.60
31	j	54	ARG	NE-CZ-NH1	14.95	127.77	120.30
31	j	54	ARG	CD-NE-CZ	13.77	142.87	123.60
17	P	167	U	C5-C4-O4	11.99	133.10	125.90
31	j	54	ARG	NE-CZ-NH2	-11.81	114.40	120.30
31	j	74	ARG	NE-CZ-NH1	-11.35	114.62	120.30
17	P	164	C	N1-C2-O2	-10.00	112.90	118.90
20	Y	49	PRO	CA-N-CD	-9.42	98.31	111.50
17	P	166	C	O4'-C1'-N1	8.88	115.30	108.20
17	P	162	U	N3-C2-O2	-8.68	116.12	122.20
17	P	169	C	P-O3'-C3'	8.30	129.66	119.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	P	164	C	C5'-C4'-O4'	-8.27	99.17	109.10
17	P	167	U	N3-C4-O4	-8.04	113.77	119.40
18	U	217	PRO	N-CA-CB	7.83	112.70	103.30
31	j	106	ASP	CB-CG-OD1	7.55	125.10	118.30
17	P	164	C	P-O3'-C3'	7.54	128.74	119.70
17	P	164	C	N3-C2-O2	7.46	127.12	121.90
17	P	167	U	N1-C2-O2	7.43	128.00	122.80
31	j	26	ARG	NE-CZ-NH2	-7.42	116.59	120.30
32	k	56	PRO	CA-CB-CG	7.33	118.72	104.80
17	P	138	U	OP2-P-O3'	7.23	121.11	105.20
17	P	119	G	OP2-P-O3'	7.23	121.10	105.20
17	P	124	U	OP2-P-O3'	7.23	121.10	105.20
17	P	114	G	OP2-P-O3'	7.22	121.09	105.20
17	P	132	U	OP2-P-O3'	7.22	121.09	105.20
17	P	112	U	OP2-P-O3'	7.22	121.09	105.20
17	P	120	C	OP2-P-O3'	7.22	121.08	105.20
17	P	121	C	OP2-P-O3'	7.22	121.08	105.20
17	P	115	G	OP2-P-O3'	7.21	121.07	105.20
17	P	122	U	OP2-P-O3'	7.21	121.07	105.20
17	P	125	G	OP2-P-O3'	7.21	121.07	105.20
17	P	113	U	OP2-P-O3'	7.21	121.06	105.20
17	P	140	C	OP2-P-O3'	7.21	121.06	105.20
17	P	123	C	OP2-P-O3'	7.21	121.06	105.20
17	P	131	C	OP2-P-O3'	7.21	121.05	105.20
17	P	134	U	OP2-P-O3'	7.21	121.05	105.20
17	P	133	A	OP2-P-O3'	7.19	121.03	105.20
17	P	139	U	OP2-P-O3'	7.18	121.00	105.20
18	U	415	PRO	N-CA-CB	7.08	111.79	103.30
17	P	168	A	P-O5'-C5'	-7.07	109.58	120.90
17	P	167	U	N3-C2-O2	-7.02	117.28	122.20
19	W	77	PRO	N-CA-CB	6.89	111.56	103.30
29	r	547	PRO	N-CA-CB	6.87	111.54	103.30
31	j	4	ASN	N-CA-CB	-6.84	98.29	110.60
17	P	121	C	O3'-P-O5'	-6.81	91.05	104.00
17	P	112	U	O3'-P-O5'	-6.81	91.06	104.00
17	P	124	U	O3'-P-O5'	-6.80	91.08	104.00
17	P	125	G	O3'-P-O5'	-6.79	91.10	104.00
17	P	139	U	O3'-P-O5'	-6.78	91.11	104.00
17	P	119	G	O3'-P-O5'	-6.78	91.12	104.00
17	P	140	C	O3'-P-O5'	-6.78	91.12	104.00
17	P	113	U	O3'-P-O5'	-6.78	91.12	104.00
17	P	120	C	O3'-P-O5'	-6.78	91.13	104.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	P	132	U	O3'-P-O5'	-6.78	91.13	104.00
17	P	138	U	O3'-P-O5'	-6.78	91.13	104.00
17	P	131	C	O3'-P-O5'	-6.77	91.13	104.00
17	P	114	G	O3'-P-O5'	-6.77	91.13	104.00
17	P	123	C	O3'-P-O5'	-6.77	91.13	104.00
17	P	133	A	O3'-P-O5'	-6.77	91.13	104.00
17	P	134	U	O3'-P-O5'	-6.76	91.15	104.00
17	P	122	U	O3'-P-O5'	-6.76	91.16	104.00
17	P	115	G	O3'-P-O5'	-6.74	91.19	104.00
31	j	22	GLU	OE1-CD-OE2	-6.73	115.22	123.30
17	P	155	U	P-O3'-C3'	6.72	127.76	119.70
31	j	12	PRO	N-CA-CB	6.68	111.32	103.30
21	a	268	PRO	N-CA-CB	6.41	110.99	103.30
17	P	157	G	C5-C6-O6	-6.41	124.76	128.60
3	C	36	U	C4'-C3'-O3'	6.40	125.81	113.00
17	P	157	G	N1-C6-O6	6.29	123.67	119.90
17	P	165	A	O4'-C1'-N9	-6.26	103.19	108.20
21	a	237	PRO	N-CA-CB	6.23	110.77	103.30
11	K	460	PRO	N-CA-CB	6.19	110.73	103.30
17	P	162	U	N1-C2-O2	5.99	126.99	122.80
31	j	131	ARG	CD-NE-CZ	5.96	131.95	123.60
25	g	23	PRO	N-CA-CB	5.96	110.45	103.30
17	P	164	C	C5-C4-N4	-5.94	116.05	120.20
31	j	26	ARG	CB-CA-C	-5.87	98.65	110.40
25	g	155	GLY	C-N-CD	5.82	140.63	128.40
25	g	94	VAL	C-N-CD	5.82	140.62	128.40
17	P	168	A	C5'-C4'-C3'	-5.82	106.69	116.00
31	j	80	PRO	N-CA-CB	5.82	110.28	103.30
17	P	172	G	P-O3'-C3'	5.80	126.66	119.70
17	P	167	U	O3'-P-O5'	-5.78	93.01	104.00
18	U	276	PRO	N-CA-CB	5.78	110.23	103.30
18	U	305	PRO	N-CA-CB	5.78	110.23	103.30
25	g	32	PRO	N-CA-CB	5.78	110.23	103.30
11	K	466	PRO	N-CA-CB	5.75	110.20	103.30
31	j	74	ARG	NH1-CZ-NH2	5.74	125.71	119.40
17	P	156	U	P-O3'-C3'	-5.71	112.85	119.70
25	g	19	PRO	N-CA-CB	5.68	110.12	103.30
20	Y	86	PRO	N-CA-CB	5.68	110.11	103.30
22	c	334	PRO	N-CA-CB	5.64	110.06	103.30
20	Y	66	GLN	C-N-CD	5.63	140.23	128.40
20	Y	274	LEU	C-N-CD	5.60	140.16	128.40
25	g	143	ASP	C-N-CD	5.60	140.16	128.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	Y	63	GLU	C-N-CD	5.53	140.00	128.40
17	P	154	C	O3'-P-O5'	-5.50	93.55	104.00
31	j	17	PRO	N-CA-CB	5.50	109.91	103.30
32	k	36	ASP	CB-CG-OD2	-5.43	113.42	118.30
17	P	156	U	OP2-P-O3'	5.36	117.00	105.20
32	k	36	ASP	CB-CG-OD1	5.36	123.12	118.30
31	j	46	ILE	N-CA-CB	5.30	122.99	110.80
31	j	112	PRO	N-CA-CB	5.26	109.61	103.30
32	k	56	PRO	N-CA-CB	5.25	109.60	103.30
20	Y	281	ASP	CB-CG-OD2	5.23	123.01	118.30
17	P	157	G	P-O5'-C5'	-5.15	112.66	120.90
17	P	170	U	O4'-C1'-C2'	-5.14	100.66	105.80
17	P	156	U	C4'-C3'-C2'	5.12	107.72	102.60
17	P	176	G	OP1-P-OP2	-5.11	111.93	119.60
32	k	43	PRO	CA-CB-CG	5.09	114.48	104.80
17	P	153	U	OP2-P-O3'	5.03	116.26	105.20
31	j	98	HIS	CA-CB-CG	-5.02	105.06	113.60
17	P	162	U	C2-N3-C4	-5.02	123.99	127.00
31	j	45	ALA	CB-CA-C	-5.00	102.59	110.10

There are no chirality outliers.

All (22) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1191	THR	Peptide
1	A	1440	ILE	Peptide
1	A	187	PHE	Peptide
1	A	457	HIS	Peptide
1	A	964	LYS	Peptide
11	K	301	ASP	Peptide
11	K	359	PHE	Peptide
20	Y	301	UNK	Mainchain
20	Y	302	UNK	Mainchain
20	Y	303	UNK	Mainchain
33	x	310	UNK	Mainchain
33	x	357	UNK	Mainchain
33	x	358	UNK	Mainchain
33	x	403	UNK	Mainchain
33	x	404	UNK	Mainchain
33	x	405	UNK	Mainchain
33	x	406	UNK	Mainchain
33	x	407	UNK	Mainchain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
33	x	408	UNK	Mainchain
33	x	409	UNK	Mainchain
33	x	410	UNK	Mainchain
33	x	411	UNK	Mainchain

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1956/2363 (83%)	1657 (85%)	220 (11%)	79 (4%)	3	26
2	B	902/984 (92%)	783 (87%)	97 (11%)	22 (2%)	6	37
4	D	94/97 (97%)	80 (85%)	8 (8%)	6 (6%)	1	17
4	Z	78/97 (80%)	71 (91%)	6 (8%)	1 (1%)	12	50
5	E	92/147 (63%)	81 (88%)	9 (10%)	2 (2%)	6	39
5	b	70/147 (48%)	67 (96%)	3 (4%)	0	100	100
6	F	80/117 (68%)	72 (90%)	6 (8%)	2 (2%)	5	36
6	f	80/117 (68%)	72 (90%)	6 (8%)	2 (2%)	5	36
7	G	91/115 (79%)	88 (97%)	3 (3%)	0	100	100
7	l	83/115 (72%)	81 (98%)	2 (2%)	0	100	100
8	H	74/84 (88%)	69 (93%)	5 (7%)	0	100	100
8	m	74/84 (88%)	69 (93%)	5 (7%)	0	100	100
9	I	70/78 (90%)	64 (91%)	4 (6%)	2 (3%)	4	33
9	n	70/78 (90%)	65 (93%)	3 (4%)	2 (3%)	4	33
10	J	71/77 (92%)	66 (93%)	5 (7%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	o	71/77 (92%)	66 (93%)	5 (7%)	0	100	100
11	K	320/473 (68%)	246 (77%)	50 (16%)	24 (8%)	1	12
12	L	285/340 (84%)	239 (84%)	41 (14%)	5 (2%)	8	43
13	M	203/557 (36%)	172 (85%)	22 (11%)	9 (4%)	2	23
18	S	130/488 (27%)	122 (94%)	7 (5%)	1 (1%)	19	59
18	T	132/488 (27%)	123 (93%)	8 (6%)	1 (1%)	19	59
18	U	414/488 (85%)	383 (92%)	20 (5%)	11 (3%)	5	35
18	V	129/488 (26%)	121 (94%)	4 (3%)	4 (3%)	4	32
19	W	266/757 (35%)	244 (92%)	13 (5%)	9 (3%)	3	31
20	Y	234/388 (60%)	200 (86%)	24 (10%)	10 (4%)	2	24
21	a	189/354 (53%)	167 (88%)	18 (10%)	4 (2%)	7	40
22	c	298/639 (47%)	254 (85%)	31 (10%)	13 (4%)	2	23
23	d	153/155 (99%)	137 (90%)	13 (8%)	3 (2%)	7	41
24	e	142/146 (97%)	120 (84%)	17 (12%)	5 (4%)	3	30
25	g	146/558 (26%)	123 (84%)	15 (10%)	8 (6%)	2	19
26	h	86/265 (32%)	75 (87%)	7 (8%)	4 (5%)	2	22
27	i	157/187 (84%)	144 (92%)	10 (6%)	3 (2%)	8	42
28	R	248/674 (37%)	219 (88%)	20 (8%)	9 (4%)	3	29
29	r	130/790 (16%)	120 (92%)	6 (5%)	4 (3%)	4	32
30	X	1143/1284 (89%)	1032 (90%)	87 (8%)	24 (2%)	7	40
31	j	156/239 (65%)	140 (90%)	14 (9%)	2 (1%)	12	50
32	k	87/111 (78%)	85 (98%)	2 (2%)	0	100	100
All	All	9004/14646 (62%)	7917 (88%)	816 (9%)	271 (3%)	7	33

All (271) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	67	GLY
1	A	68	VAL
1	A	155	ARG
1	A	188	PRO
1	A	232	ALA
1	A	275	TYR
1	A	378	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	438	SER
1	A	441	THR
1	A	562	ARG
1	A	615	TYR
1	A	621	LEU
1	A	648	PRO
1	A	650	CYS
1	A	695	ILE
1	A	965	PRO
1	A	1005	SER
1	A	1038	VAL
1	A	1299	ARG
1	A	1492	ASN
1	A	1523	GLU
1	A	1971	THR
2	B	75	LYS
2	B	105	ILE
2	B	190	VAL
2	B	379	ARG
2	B	932	PRO
4	D	83	VAL
11	K	207	THR
11	K	276	MET
11	K	288	HIS
11	K	302	PRO
11	K	360	PRO
11	K	460	PRO
12	L	221	ILE
13	M	113	HIS
13	M	141	PRO
13	M	190	ASN
13	M	200	ARG
13	M	209	GLN
18	U	53	VAL
18	U	64	PRO
18	U	69	LEU
18	U	201	SER
18	U	217	PRO
18	U	373	PRO
18	V	67	THR
19	W	77	PRO
20	Y	66	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
20	Y	73	LEU
21	a	22	ILE
21	a	107	PRO
22	c	391	VAL
22	c	415	CYS
22	c	563	GLY
22	c	564	TYR
24	e	145	CYS
25	g	74	VAL
25	g	158	ALA
27	i	86	PRO
28	R	69	ALA
28	R	169	PRO
28	R	272	PRO
29	r	546	TYR
29	r	547	PRO
30	X	396	PHE
30	X	935	ARG
30	X	1070	SER
30	X	1098	GLN
1	A	73	GLY
1	A	301	LEU
1	A	317	ASP
1	A	415	ASP
1	A	444	ALA
1	A	457	HIS
1	A	691	VAL
1	A	692	ALA
1	A	749	TRP
1	A	753	GLY
1	A	790	VAL
1	A	1115	ILE
1	A	1217	PHE
1	A	1663	VAL
2	B	125	VAL
2	B	150	LEU
2	B	311	ARG
2	B	390	TYR
2	B	549	ALA
2	B	594	ILE
4	D	37	MET
5	E	103	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	F	12	ASN
9	I	41	MET
11	K	232	TRP
11	K	350	SER
11	K	413	VAL
11	K	459	HIS
11	K	469	LEU
12	L	263	GLY
12	L	331	ASP
13	M	199	GLN
18	S	57	ASP
18	U	270	ILE
19	W	232	ALA
20	Y	58	PRO
20	Y	211	GLY
22	c	379	ALA
22	c	426	VAL
24	e	118	ILE
24	e	132	VAL
25	g	49	ASN
25	g	152	ALA
26	h	233	ASN
27	i	83	LEU
28	R	42	ILE
30	X	36	LEU
30	X	121	VAL
30	X	621	TYR
30	X	1275	GLU
31	j	159	GLU
4	Z	37	MET
6	f	12	ASN
1	A	71	LYS
1	A	205	LEU
1	A	211	ILE
1	A	240	ASN
1	A	246	ARG
1	A	271	ASP
1	A	316	ASN
1	A	494	SER
1	A	618	LYS
1	A	641	THR
1	A	721	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	725	ARG
1	A	791	ASP
1	A	2022	ASN
2	B	87	SER
2	B	123	ASP
11	K	249	GLY
11	K	338	SER
11	K	344	PHE
12	L	133	GLY
18	V	65	SER
19	W	226	PRO
20	Y	57	ARG
20	Y	143	PHE
20	Y	183	PRO
21	a	21	SER
22	c	335	THR
22	c	457	ILE
22	c	614	THR
26	h	43	GLY
28	R	86	PHE
28	R	185	HIS
28	R	202	PRO
29	r	530	PHE
29	r	563	ARG
30	X	363	LYS
30	X	428	LEU
30	X	1186	VAL
1	A	135	ARG
1	A	352	HIS
1	A	355	SER
1	A	391	SER
1	A	486	HIS
1	A	552	THR
1	A	613	GLY
1	A	1324	LYS
1	A	1331	MET
1	A	1543	THR
1	A	1664	SER
2	B	754	ARG
2	B	868	ARG
4	D	96	ARG
11	K	173	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
11	K	359	PHE
11	K	466	PRO
12	L	177	LYS
13	M	174	VAL
18	V	63	PRO
19	W	63	ARG
19	W	92	THR
20	Y	251	ASN
20	Y	281	ASP
22	c	385	ARG
22	c	442	GLU
22	c	537	ARG
22	c	539	ILE
23	d	95	PRO
24	e	116	THR
24	e	117	CYS
25	g	70	ALA
26	h	240	ASP
30	X	19	TRP
30	X	311	PHE
30	X	355	TYR
30	X	567	VAL
30	X	1004	ARG
31	j	31	PRO
1	A	269	ARG
1	A	325	HIS
1	A	327	ILE
1	A	622	MET
1	A	643	PRO
1	A	761	MET
2	B	83	GLU
2	B	177	LEU
2	B	662	TYR
2	B	750	GLY
4	D	90	PRO
6	F	62	GLY
9	I	42	ASN
11	K	150	HIS
11	K	161	GLY
11	K	257	PRO
11	K	455	THR
13	M	140	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
13	M	196	LEU
18	U	60	ARG
19	W	9	TRP
19	W	37	VAL
20	Y	163	MET
25	g	31	ALA
28	R	87	ALA
30	X	76	ASN
30	X	415	THR
30	X	846	SER
6	f	62	GLY
9	n	41	MET
9	n	42	ASN
1	A	187	PHE
1	A	432	HIS
1	A	793	THR
1	A	825	THR
2	B	812	PRO
4	D	91	LEU
11	K	287	GLY
11	K	324	LEU
18	U	415	PRO
21	a	267	SER
25	g	143	ASP
30	X	465	ILE
30	X	528	PHE
30	X	970	GLY
30	X	1192	SER
1	A	723	GLY
5	E	113	ALA
11	K	203	GLY
25	g	64	GLN
30	X	39	VAL
1	A	326	PRO
1	A	1720	PRO
2	B	424	PRO
4	D	95	GLY
18	U	219	PRO
27	i	11	PRO
1	A	642	GLY
1	A	1143	PRO
18	T	20	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
19	W	231	PRO
26	h	241	THR
28	R	201	HIS
1	A	129	MET
18	V	20	GLY
19	W	225	ILE
23	d	86	GLY
1	A	206	GLU
1	A	668	VAL
2	B	601	VAL
18	U	376	SER
23	d	69	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1775/2138 (83%)	1565 (88%)	210 (12%)	5	28
2	B	809/881 (92%)	758 (94%)	51 (6%)	18	53
4	D	85/86 (99%)	77 (91%)	8 (9%)	8	38
4	Z	72/86 (84%)	64 (89%)	8 (11%)	6	31
5	E	80/118 (68%)	75 (94%)	5 (6%)	18	53
5	b	66/118 (56%)	60 (91%)	6 (9%)	9	39
6	F	77/102 (76%)	70 (91%)	7 (9%)	9	39
6	f	77/102 (76%)	70 (91%)	7 (9%)	9	39
7	G	81/101 (80%)	79 (98%)	2 (2%)	47	75
7	l	76/101 (75%)	75 (99%)	1 (1%)	69	86
8	H	69/76 (91%)	64 (93%)	5 (7%)	14	47
8	m	69/76 (91%)	64 (93%)	5 (7%)	14	47
9	I	64/69 (93%)	60 (94%)	4 (6%)	18	53
9	n	64/69 (93%)	60 (94%)	4 (6%)	18	53

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	J	63/67 (94%)	57 (90%)	6 (10%)	8	37
10	o	63/67 (94%)	57 (90%)	6 (10%)	8	37
11	K	261/278 (94%)	239 (92%)	22 (8%)	11	42
12	L	251/292 (86%)	234 (93%)	17 (7%)	16	50
13	M	182/477 (38%)	160 (88%)	22 (12%)	5	26
18	S	120/443 (27%)	110 (92%)	10 (8%)	11	42
18	T	123/443 (28%)	112 (91%)	11 (9%)	9	40
18	U	223/443 (50%)	206 (92%)	17 (8%)	13	45
18	V	118/443 (27%)	111 (94%)	7 (6%)	19	55
19	W	234/294 (80%)	213 (91%)	21 (9%)	9	39
20	Y	194/253 (77%)	158 (81%)	36 (19%)	1	10
21	a	142/222 (64%)	123 (87%)	19 (13%)	4	23
22	c	259/579 (45%)	224 (86%)	35 (14%)	4	23
23	d	129/129 (100%)	125 (97%)	4 (3%)	40	71
24	e	130/132 (98%)	123 (95%)	7 (5%)	22	57
25	g	78/496 (16%)	62 (80%)	16 (20%)	1	7
26	h	79/240 (33%)	70 (89%)	9 (11%)	5	29
27	i	118/163 (72%)	108 (92%)	10 (8%)	10	41
28	R	224/224 (100%)	192 (86%)	32 (14%)	3	21
29	r	117/136 (86%)	107 (92%)	10 (8%)	10	41
30	X	1106/1188 (93%)	1100 (100%)	6 (0%)	88	95
31	j	87/214 (41%)	83 (95%)	4 (5%)	27	61
32	k	49/96 (51%)	46 (94%)	3 (6%)	18	53
All	All	7814/11442 (68%)	7161 (92%)	653 (8%)	14	42

All (653) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	63	LYS
1	A	65	LYS
1	A	69	LYS
1	A	77	THR
1	A	85	GLU
1	A	91	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	108	SER
1	A	109	TYR
1	A	110	LEU
1	A	127	MET
1	A	129	MET
1	A	137	VAL
1	A	139	VAL
1	A	148	THR
1	A	153	SER
1	A	156	VAL
1	A	167	THR
1	A	169	TRP
1	A	183	LYS
1	A	197	PHE
1	A	206	GLU
1	A	211	ILE
1	A	214	ASP
1	A	229	GLU
1	A	239	VAL
1	A	246	ARG
1	A	250	ASN
1	A	254	MET
1	A	263	GLN
1	A	269	ARG
1	A	277	PHE
1	A	284	THR
1	A	289	ASN
1	A	292	ILE
1	A	316	ASN
1	A	319	TYR
1	A	328	LYS
1	A	331	TYR
1	A	344	ARG
1	A	365	ASP
1	A	366	LEU
1	A	388	LEU
1	A	403	PHE
1	A	404	GLU
1	A	408	ASP
1	A	414	GLU
1	A	428	LEU
1	A	435	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	436	LYS
1	A	443	ARG
1	A	445	GLN
1	A	451	LYS
1	A	458	CYS
1	A	467	ARG
1	A	469	SER
1	A	473	LEU
1	A	474	LEU
1	A	484	MET
1	A	494	SER
1	A	495	LEU
1	A	497	ARG
1	A	500	LYS
1	A	503	LYS
1	A	518	GLN
1	A	521	ARG
1	A	522	GLN
1	A	536	LEU
1	A	537	THR
1	A	538	TYR
1	A	547	LEU
1	A	553	LEU
1	A	569	LEU
1	A	570	MET
1	A	572	GLU
1	A	574	LEU
1	A	575	ARG
1	A	587	TYR
1	A	588	ARG
1	A	589	LEU
1	A	593	ASP
1	A	597	LEU
1	A	608	VAL
1	A	616	ARG
1	A	619	TYR
1	A	622	MET
1	A	628	CYS
1	A	646	LYS
1	A	656	SER
1	A	667	ILE
1	A	670	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	671	LEU
1	A	675	LEU
1	A	678	LEU
1	A	693	LYS
1	A	699	ARG
1	A	705	ASP
1	A	708	LEU
1	A	714	ASN
1	A	728	LYS
1	A	741	ARG
1	A	754	LEU
1	A	759	GLU
1	A	761	MET
1	A	768	SER
1	A	781	ARG
1	A	785	ARG
1	A	792	LYS
1	A	796	LYS
1	A	808	LYS
1	A	810	GLU
1	A	812	GLU
1	A	814	GLN
1	A	817	TYR
1	A	839	TRP
1	A	856	LYS
1	A	860	LYS
1	A	862	LEU
1	A	868	ARG
1	A	878	ARG
1	A	879	LEU
1	A	884	ARG
1	A	900	MET
1	A	912	ARG
1	A	920	GLU
1	A	935	ASP
1	A	937	MET
1	A	949	LEU
1	A	952	GLU
1	A	969	GLU
1	A	974	LEU
1	A	978	TRP
1	A	980	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	996	CYS
1	A	1001	GLU
1	A	1010	LYS
1	A	1012	ASP
1	A	1015	LEU
1	A	1017	ASN
1	A	1050	SER
1	A	1053	LEU
1	A	1055	ARG
1	A	1066	PHE
1	A	1069	LEU
1	A	1076	LEU
1	A	1078	LEU
1	A	1121	MET
1	A	1130	ARG
1	A	1153	LYS
1	A	1174	LEU
1	A	1188	ARG
1	A	1196	GLU
1	A	1210	LEU
1	A	1222	LEU
1	A	1228	ASN
1	A	1230	GLU
1	A	1233	LEU
1	A	1251	GLN
1	A	1270	GLN
1	A	1282	LYS
1	A	1289	THR
1	A	1305	THR
1	A	1308	LEU
1	A	1318	LYS
1	A	1329	SER
1	A	1334	ARG
1	A	1352	LEU
1	A	1358	LEU
1	A	1392	LEU
1	A	1412	GLU
1	A	1431	ASP
1	A	1440	ILE
1	A	1458	LYS
1	A	1465	GLU
1	A	1472	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1480	THR
1	A	1482	GLN
1	A	1546	GLN
1	A	1560	LEU
1	A	1576	GLN
1	A	1593	LEU
1	A	1605	LEU
1	A	1684	TYR
1	A	1691	ARG
1	A	1694	ASP
1	A	1710	ASP
1	A	1737	SER
1	A	1767	LEU
1	A	1784	GLU
1	A	1810	TYR
1	A	1811	ARG
1	A	1816	LYS
1	A	1817	THR
1	A	1818	PHE
1	A	1828	ASN
1	A	1843	LEU
1	A	1844	LYS
1	A	1847	HIS
1	A	1848	THR
1	A	1849	SER
1	A	1851	TRP
1	A	1855	LYS
1	A	1857	LEU
1	A	1883	ARG
1	A	1901	LEU
1	A	1960	LEU
1	A	1962	LEU
1	A	1974	THR
1	A	1975	LYS
1	A	1976	LEU
1	A	2014	ASP
2	B	76	GLN
2	B	85	TYR
2	B	99	GLN
2	B	101	LEU
2	B	105	ILE
2	B	118	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	129	GLU
2	B	138	THR
2	B	143	SER
2	B	152	HIS
2	B	157	LEU
2	B	168	ASP
2	B	173	LYS
2	B	175	ARG
2	B	196	THR
2	B	200	LEU
2	B	216	ASP
2	B	225	ASP
2	B	235	ASP
2	B	237	VAL
2	B	267	LEU
2	B	275	LEU
2	B	280	ARG
2	B	313	SER
2	B	320	CYS
2	B	335	PHE
2	B	346	ILE
2	B	423	ASP
2	B	460	LYS
2	B	500	ASP
2	B	564	VAL
2	B	584	LEU
2	B	594	ILE
2	B	646	THR
2	B	658	LEU
2	B	694	ASN
2	B	773	LEU
2	B	827	ARG
2	B	834	PHE
2	B	846	TYR
2	B	847	MET
2	B	868	ARG
2	B	875	ILE
2	B	877	ARG
2	B	902	ARG
2	B	913	MET
2	B	931	LYS
2	B	933	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	945	ARG
2	B	961	VAL
2	B	969	GLN
4	D	12	GLN
4	D	25	THR
4	D	41	MET
4	D	47	THR
4	D	55	HIS
4	D	58	GLN
4	D	80	MET
4	D	94	ARG
5	E	28	LEU
5	E	31	PHE
5	E	61	GLU
5	E	70	LEU
5	E	102	ARG
6	F	3	LEU
6	F	6	PHE
6	F	12	ASN
6	F	13	GLU
6	F	41	LYS
6	F	46	THR
6	F	61	ARG
7	G	72	LYS
7	G	104	ASP
8	H	23	HIS
8	H	43	ARG
8	H	49	MET
8	H	62	LYS
8	H	76	ASP
9	I	15	LEU
9	I	35	GLN
9	I	41	MET
9	I	72	TRP
10	J	3	LYS
10	J	8	ASP
10	J	26	LYS
10	J	48	GLU
10	J	63	ARG
10	J	75	LYS
11	K	154	THR
11	K	169	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
11	K	170	ASP
11	K	191	ASP
11	K	200	THR
11	K	216	ARG
11	K	226	ASP
11	K	231	CYS
11	K	248	SER
11	K	253	LEU
11	K	272	ARG
11	K	282	VAL
11	K	291	THR
11	K	352	ASP
11	K	356	HIS
11	K	359	PHE
11	K	371	HIS
11	K	379	SER
11	K	383	ASP
11	K	388	SER
11	K	392	ASN
11	K	447	ILE
12	L	44	LEU
12	L	46	MET
12	L	71	ASP
12	L	85	ASN
12	L	98	ASP
12	L	104	ASP
12	L	110	CYS
12	L	154	VAL
12	L	157	ASP
12	L	215	LEU
12	L	218	HIS
12	L	219	LYS
12	L	222	ILE
12	L	240	ASP
12	L	269	GLU
12	L	306	LEU
12	L	315	HIS
13	M	118	GLN
13	M	130	ARG
13	M	131	LEU
13	M	139	GLU
13	M	161	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
13	M	180	ASP
13	M	192	MET
13	M	202	ILE
13	M	217	PHE
13	M	221	LYS
13	M	224	ARG
13	M	234	LEU
13	M	247	GLN
13	M	254	SER
13	M	258	TRP
13	M	260	ASN
13	M	261	PRO
13	M	283	GLU
13	M	305	GLU
13	M	309	ARG
13	M	312	MET
13	M	315	LYS
18	S	11	LYS
18	S	26	ARG
18	S	54	LYS
18	S	58	PHE
18	S	60	ARG
18	S	62	ARG
18	S	88	PHE
18	S	101	LEU
18	S	105	LEU
18	S	112	LEU
18	T	11	LYS
18	T	37	LYS
18	T	55	VAL
18	T	60	ARG
18	T	72	LEU
18	T	76	PHE
18	T	77	GLN
18	T	85	LEU
18	T	91	ARG
18	T	99	GLN
18	T	101	LEU
18	U	11	LYS
18	U	54	LYS
18	U	76	PHE
18	U	87	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
18	U	94	LEU
18	U	118	LEU
18	U	127	GLU
18	U	175	SER
18	U	184	PRO
18	U	209	THR
18	U	217	PRO
18	U	258	THR
18	U	276	PRO
18	U	278	SER
18	U	279	SER
18	U	341	VAL
18	U	415	PRO
18	V	11	LYS
18	V	62	ARG
18	V	85	LEU
18	V	87	GLN
18	V	91	ARG
18	V	92	ARG
18	V	105	LEU
19	W	10	LYS
19	W	23	LYS
19	W	35	LEU
19	W	39	LYS
19	W	40	THR
19	W	68	LYS
19	W	79	GLN
19	W	82	THR
19	W	170	LEU
19	W	172	ASN
19	W	177	LYS
19	W	186	GLN
19	W	228	GLU
19	W	687	TYR
19	W	693	LEU
19	W	704	LEU
19	W	707	GLU
19	W	708	ARG
19	W	723	LEU
19	W	728	ARG
19	W	743	GLU
20	Y	52	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
20	Y	53	GLN
20	Y	55	GLU
20	Y	56	THR
20	Y	59	GLU
20	Y	60	TYR
20	Y	65	GLU
20	Y	66	GLN
20	Y	69	GLN
20	Y	71	TYR
20	Y	75	TYR
20	Y	117	CYS
20	Y	127	GLU
20	Y	140	ASP
20	Y	147	ASN
20	Y	153	ARG
20	Y	171	ARG
20	Y	188	GLU
20	Y	203	ARG
20	Y	205	ARG
20	Y	225	PHE
20	Y	227	LYS
20	Y	230	MET
20	Y	241	LEU
20	Y	242	ASN
20	Y	247	THR
20	Y	248	THR
20	Y	251	ASN
20	Y	259	GLN
20	Y	260	ARG
20	Y	261	ARG
20	Y	262	LEU
20	Y	265	ARG
20	Y	271	LYS
20	Y	274	LEU
20	Y	286	LYS
21	a	21	SER
21	a	27	LEU
21	a	38	GLU
21	a	42	GLN
21	a	45	LYS
21	a	47	CYS
21	a	49	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
21	a	60	ARG
21	a	62	GLN
21	a	78	ASN
21	a	87	LEU
21	a	91	LEU
21	a	101	LYS
21	a	109	ASN
21	a	118	GLN
21	a	237	PRO
21	a	244	SER
21	a	246	ARG
21	a	268	PRO
22	c	345	LEU
22	c	350	ARG
22	c	351	LYS
22	c	352	TYR
22	c	356	TYR
22	c	366	LYS
22	c	378	ASN
22	c	385	ARG
22	c	401	ASP
22	c	414	LEU
22	c	418	TYR
22	c	429	LEU
22	c	430	SER
22	c	432	ARG
22	c	440	GLN
22	c	443	LEU
22	c	449	LEU
22	c	467	TRP
22	c	471	ARG
22	c	490	PHE
22	c	492	GLU
22	c	499	ARG
22	c	515	LEU
22	c	523	ARG
22	c	549	TYR
22	c	552	TRP
22	c	560	LYS
22	c	562	LEU
22	c	564	TYR
22	c	568	TRP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
22	c	600	LEU
22	c	601	ASN
22	c	610	LYS
22	c	616	LYS
22	c	630	LYS
23	d	71	LYS
23	d	115	LYS
23	d	136	ARG
23	d	151	LYS
24	e	8	ARG
24	e	17	ASP
24	e	30	MET
24	e	85	ASP
24	e	100	LEU
24	e	113	PHE
24	e	126	LEU
25	g	56	ASN
25	g	67	LEU
25	g	71	ASN
25	g	77	GLU
25	g	81	ILE
25	g	86	THR
25	g	91	ARG
25	g	92	GLU
25	g	101	GLN
25	g	102	GLU
25	g	137	ARG
25	g	138	ARG
25	g	143	ASP
25	g	145	SER
25	g	148	GLU
25	g	154	LYS
26	h	40	GLU
26	h	42	GLN
26	h	44	THR
26	h	59	ARG
26	h	227	GLU
26	h	236	LYS
26	h	241	THR
26	h	243	ARG
26	h	250	MET
27	i	31	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
27	i	83	LEU
27	i	88	THR
27	i	102	GLN
27	i	111	LEU
27	i	114	LYS
27	i	118	LYS
27	i	150	ARG
27	i	155	TYR
27	i	156	GLN
28	R	41	ASN
28	R	48	LEU
28	R	65	ARG
28	R	68	LEU
28	R	70	MET
28	R	83	GLN
28	R	86	PHE
28	R	88	ARG
28	R	101	SER
28	R	122	HIS
28	R	127	PHE
28	R	134	LEU
28	R	136	ARG
28	R	148	GLU
28	R	149	GLU
28	R	161	PHE
28	R	162	GLU
28	R	171	GLU
28	R	174	TRP
28	R	180	MET
28	R	194	TYR
28	R	201	HIS
28	R	203	GLU
28	R	206	ASN
28	R	238	PHE
28	R	258	GLU
28	R	271	MET
28	R	272	PRO
28	R	273	ARG
28	R	275	LYS
28	R	279	LEU
28	R	285	HIS
29	r	625	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
29	r	628	TYR
29	r	631	LEU
29	r	639	TYR
29	r	644	THR
29	r	645	ARG
29	r	646	THR
29	r	649	GLU
29	r	650	LYS
29	r	652	ILE
30	X	71	SER
30	X	73	ASN
30	X	113	LEU
30	X	117	LEU
30	X	119	GLU
30	X	377	PHE
31	j	54	ARG
31	j	64	ARG
31	j	80	PRO
31	j	91	THR
32	k	14	LYS
32	k	43	PRO
32	k	56	PRO
4	Z	12	GLN
4	Z	25	THR
4	Z	27	ARG
4	Z	41	MET
4	Z	47	THR
4	Z	55	HIS
4	Z	58	GLN
4	Z	80	MET
5	b	28	LEU
5	b	31	PHE
5	b	43	GLN
5	b	61	GLU
5	b	64	MET
5	b	70	LEU
6	f	3	LEU
6	f	6	PHE
6	f	12	ASN
6	f	13	GLU
6	f	41	LYS
6	f	46	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	f	61	ARG
7	l	72	LYS
8	m	23	HIS
8	m	43	ARG
8	m	49	MET
8	m	62	LYS
8	m	76	ASP
9	n	15	LEU
9	n	35	GLN
9	n	41	MET
9	n	72	TRP
10	o	3	LYS
10	o	8	ASP
10	o	26	LYS
10	o	48	GLU
10	o	63	ARG
10	o	75	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (137) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	201	GLN
1	A	240	ASN
1	A	258	HIS
1	A	263	GLN
1	A	272	ASN
1	A	289	ASN
1	A	316	ASN
1	A	340	ASN
1	A	356	ASN
1	A	376	ASN
1	A	435	ASN
1	A	462	GLN
1	A	522	GLN
1	A	532	HIS
1	A	591	ASN
1	A	596	GLN
1	A	698	GLN
1	A	714	ASN
1	A	980	GLN
1	A	983	ASN
1	A	1017	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1027	ASN
1	A	1037	ASN
1	A	1065	GLN
1	A	1140	ASN
1	A	1320	GLN
1	A	1384	ASN
1	A	1407	GLN
1	A	1470	GLN
1	A	1490	GLN
1	A	1552	GLN
1	A	1629	GLN
1	A	1734	ASN
1	A	1815	HIS
1	A	1847	HIS
1	A	1854	GLN
2	B	76	GLN
2	B	99	GLN
2	B	120	ASN
2	B	166	HIS
2	B	300	ASN
2	B	318	ASN
2	B	449	HIS
2	B	694	ASN
2	B	716	ASN
4	D	38	ASN
4	D	58	GLN
4	D	65	HIS
5	E	36	ASN
6	F	12	ASN
7	G	34	GLN
8	H	33	GLN
8	H	77	ASN
9	I	13	GLN
9	I	35	GLN
9	I	44	GLN
10	J	22	ASN
11	K	217	HIS
11	K	298	GLN
11	K	329	HIS
12	L	73	GLN
12	L	90	ASN
12	L	218	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
13	M	118	GLN
13	M	167	GLN
13	M	191	GLN
13	M	219	HIS
18	V	87	GLN
19	W	172	ASN
19	W	186	GLN
19	W	719	ASN
20	Y	66	GLN
20	Y	69	GLN
20	Y	194	HIS
20	Y	222	ASN
20	Y	232	HIS
20	Y	233	GLN
20	Y	242	ASN
20	Y	251	ASN
20	Y	259	GLN
21	a	62	GLN
21	a	78	ASN
21	a	81	GLN
21	a	88	GLN
21	a	118	GLN
21	a	121	GLN
21	a	134	GLN
22	c	371	ASN
22	c	378	ASN
22	c	395	GLN
24	e	53	HIS
25	g	56	ASN
25	g	78	GLN
26	h	32	HIS
26	h	39	GLN
26	h	235	HIS
27	i	102	GLN
27	i	156	GLN
28	R	41	ASN
28	R	83	GLN
28	R	117	ASN
28	R	159	GLN
28	R	219	ASN
28	R	225	GLN
28	R	240	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
29	r	629	ASN
30	X	53	HIS
30	X	73	ASN
30	X	76	ASN
30	X	166	HIS
30	X	192	HIS
30	X	243	HIS
30	X	275	ASN
30	X	305	HIS
30	X	416	ASN
30	X	605	GLN
30	X	740	GLN
30	X	755	HIS
30	X	906	ASN
30	X	983	ASN
30	X	1084	HIS
30	X	1087	GLN
30	X	1108	GLN
30	X	1142	GLN
30	X	1156	HIS
30	X	1252	HIS
4	Z	58	GLN
4	Z	65	HIS
5	b	36	ASN
6	f	12	ASN
7	l	34	GLN
8	m	33	GLN
8	m	77	ASN
9	n	13	GLN
9	n	35	GLN
9	n	44	GLN
10	o	22	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
14	N	89/99 (89%)	53 (59%)	12 (13%)
15	O	8/8 (100%)	3 (37%)	1 (12%)
16	Q	12/13 (92%)	4 (33%)	2 (16%)
17	P	106/186 (56%)	28 (26%)	8 (7%)
3	C	104/120 (86%)	54 (51%)	13 (12%)

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
All	All	319/426 (74%)	142 (44%)	36 (11%)

All (142) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	C	9	U
3	C	14	G
3	C	18	U
3	C	19	U
3	C	20	U
3	C	24	A
3	C	26	A
3	C	27	G
3	C	28	C
3	C	29	U
3	C	30	A
3	C	31	A
3	C	32	C
3	C	33	G
3	C	34	U
3	C	35	A
3	C	36	U
3	C	37	C
3	C	43	C
3	C	45	U
3	C	48	C
3	C	49	U
3	C	50	U
3	C	51	U
3	C	52	U
3	C	54	C
3	C	56	A
3	C	57	G
3	C	60	A
3	C	61	C
3	C	62	A
3	C	63	G
3	C	66	G
3	C	73	A
3	C	79	G
3	C	80	C
3	C	81	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	82	A
3	C	83	A
3	C	87	G
3	C	90	U
3	C	91	G
3	C	92	U
3	C	93	A
3	C	94	U
3	C	95	A
3	C	96	G
3	C	97	U
3	C	98	U
3	C	99	U
3	C	100	U
3	C	101	U
3	C	102	G
3	C	103	U
14	N	5	U
14	N	6	U
14	N	7	C
14	N	8	G
14	N	9	G
14	N	11	U
14	N	14	C
14	N	18	G
14	N	19	G
14	N	21	C
14	N	22	A
14	N	23	A
14	N	24	A
14	N	25	U
14	N	26	U
14	N	27	G
14	N	28	A
14	N	29	A
14	N	30	A
14	N	31	C
14	N	40	G
14	N	43	G
14	N	45	U
14	N	47	A
14	N	48	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
14	N	50	A
14	N	52	G
14	N	53	G
14	N	54	C
14	N	55	C
14	N	56	C
14	N	58	U
14	N	60	C
14	N	61	A
14	N	62	C
14	N	63	A
14	N	64	A
14	N	65	G
14	N	68	U
14	N	72	A
14	N	73	C
14	N	74	U
14	N	75	G
14	N	76	C
14	N	77	G
14	N	78	A
14	N	79	C
14	N	80	A
14	N	81	U
14	N	82	U
14	N	83	G
14	N	89	A
14	N	90	A
15	O	101	U
15	O	102	A
15	O	104	G
16	Q	499	U
16	Q	500	A
16	Q	501	A
16	Q	502	C
17	P	14	C
17	P	15	U
17	P	16	U
17	P	17	U
17	P	18	U
17	P	19	G
17	P	20	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
17	P	24	A
17	P	25	G
17	P	26	A
17	P	27	U
17	P	29	A
17	P	30	A
17	P	31	G
17	P	104	G
17	P	105	G
17	P	107	U
17	P	108	U
17	P	117	A
17	P	118	A
17	P	156	U
17	P	157	G
17	P	164	C
17	P	165	A
17	P	168	A
17	P	169	C
17	P	171	G
17	P	177	C

All (36) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	C	13	A
3	C	27	G
3	C	28	C
3	C	30	A
3	C	31	A
3	C	36	U
3	C	50	U
3	C	60	A
3	C	90	U
3	C	91	G
3	C	94	U
3	C	96	G
3	C	100	U
14	N	10	A
14	N	14	C
14	N	17	U
14	N	21	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
14	N	22	A
14	N	24	A
14	N	30	A
14	N	39	A
14	N	52	G
14	N	60	C
14	N	72	A
14	N	77	G
15	O	100	G
16	Q	500	A
16	Q	501	A
17	P	14	C
17	P	17	U
17	P	18	U
17	P	24	A
17	P	104	G
17	P	156	U
17	P	164	C
17	P	168	A

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 11 are monoatomic - leaving 2 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
34	GDP	B	1000	-	24,30,30	1.02	1 (4%)	30,47,47	1.12	3 (10%)
37	ADP	X	1500	-	24,29,29	0.96	1 (4%)	29,45,45	1.50	4 (13%)

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
34	GDP	B	1000	-	-	5/12/32/32	0/3/3/3
37	ADP	X	1500	-	-	6/12/32/32	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	X	1500	ADP	C5-C4	2.51	1.47	1.40
34	B	1000	GDP	C6-N1	-2.49	1.34	1.37

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	X	1500	ADP	PA-O3A-PB	-3.59	120.52	132.83
37	X	1500	ADP	C3'-C2'-C1'	3.50	106.25	100.98
37	X	1500	ADP	N3-C2-N1	-3.14	123.77	128.68
37	X	1500	ADP	C4-C5-N7	-2.70	106.59	109.40
34	B	1000	GDP	O6-C6-C5	-2.36	119.77	124.37
34	B	1000	GDP	C5-C6-N1	2.18	117.79	113.95
34	B	1000	GDP	C8-N7-C5	2.05	106.90	102.99

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
34	B	1000	GDP	C5'-O5'-PA-O3A
34	B	1000	GDP	C3'-C4'-C5'-O5'
37	X	1500	ADP	C5'-O5'-PA-O3A
37	X	1500	ADP	C4'-C5'-O5'-PA
34	B	1000	GDP	O4'-C4'-C5'-O5'
37	X	1500	ADP	PB-O3A-PA-O1A
34	B	1000	GDP	C5'-O5'-PA-O1A

Continued on next page...

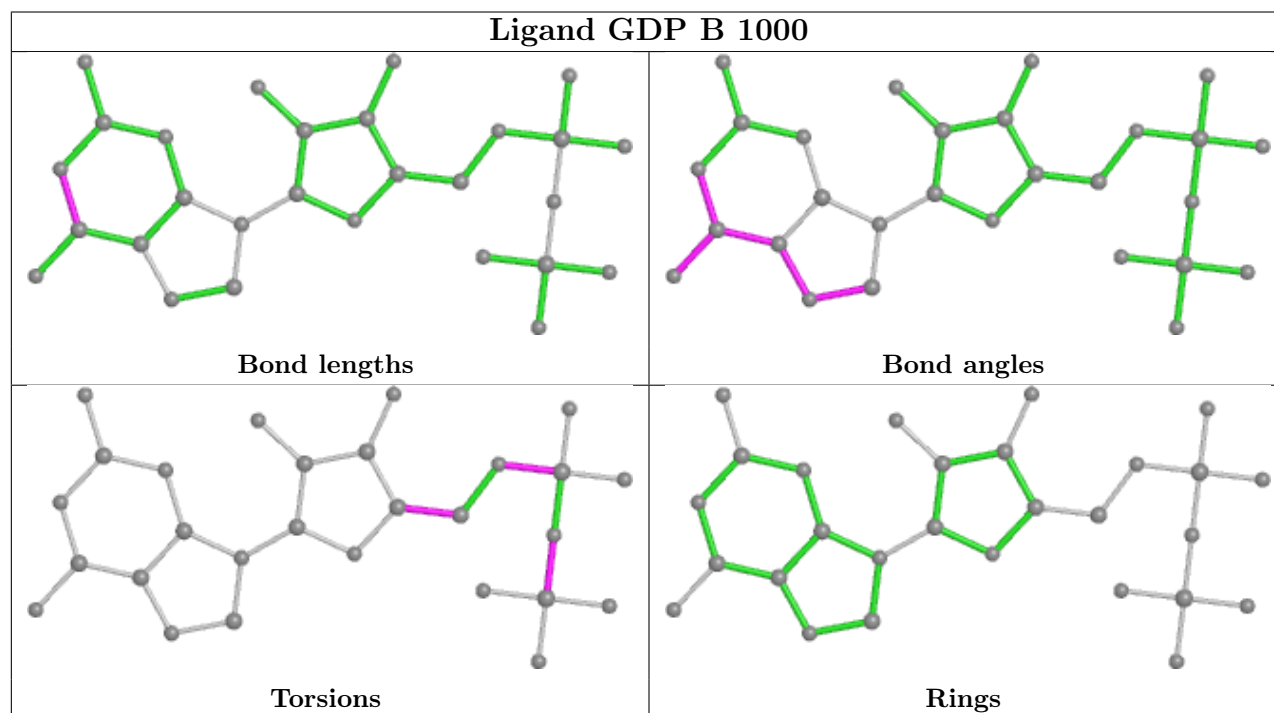
Continued from previous page...

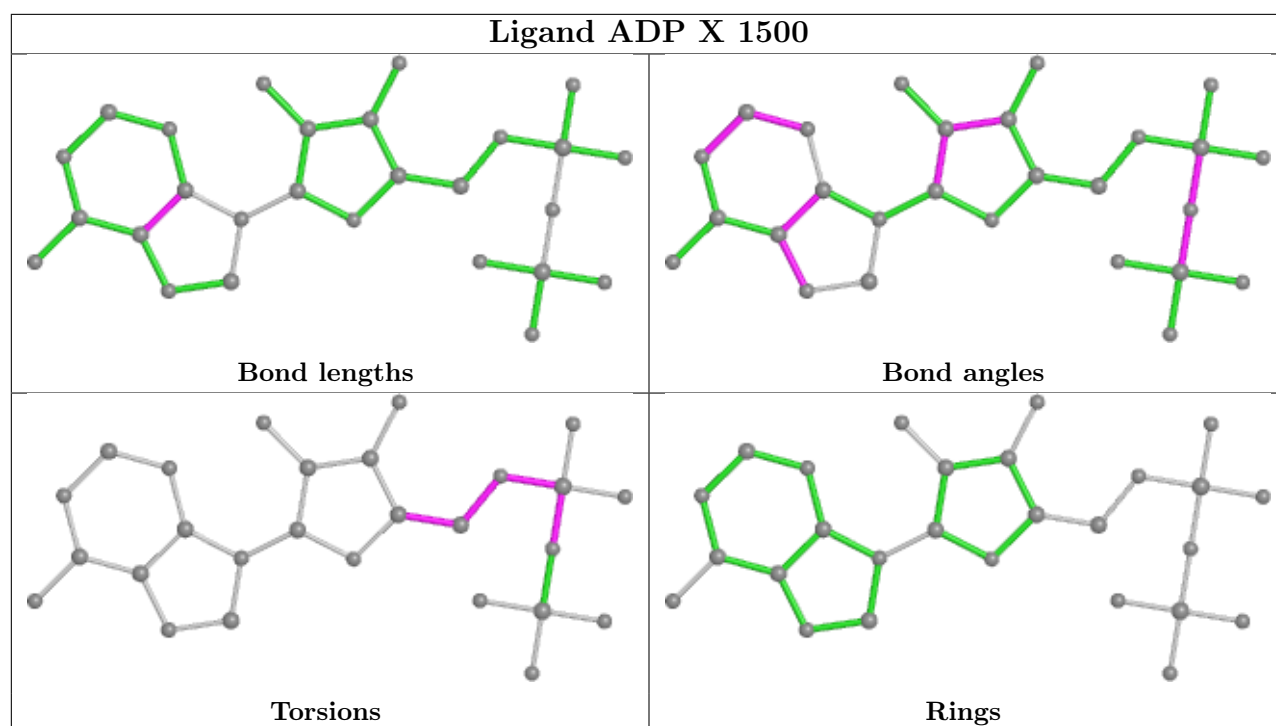
Mol	Chain	Res	Type	Atoms
37	X	1500	ADP	C5'-O5'-PA-O1A
37	X	1500	ADP	PB-O3A-PA-O2A
34	B	1000	GDP	PA-O3A-PB-O2B
37	X	1500	ADP	O4'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

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

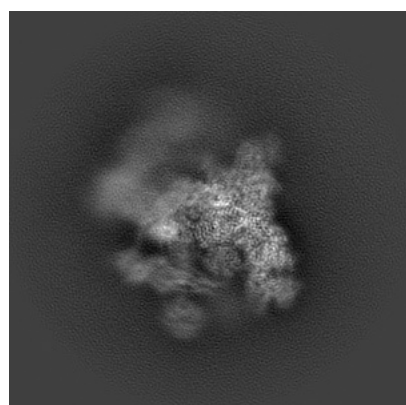
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6413. These allow visual inspection of the internal detail of the map and identification of artifacts.

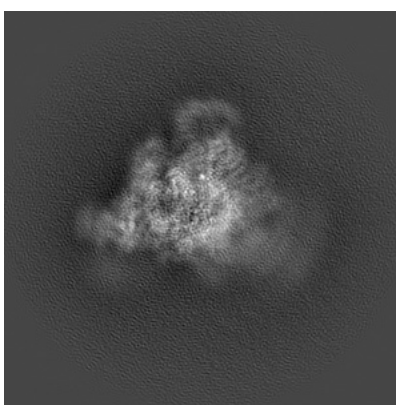
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

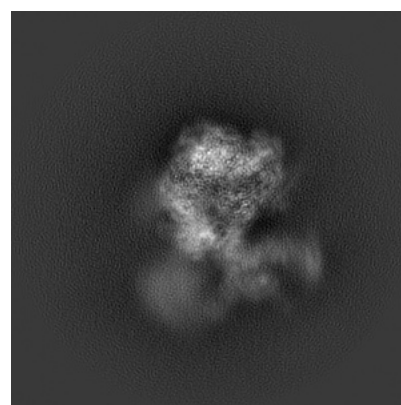
6.1.1 Primary map



X



Y

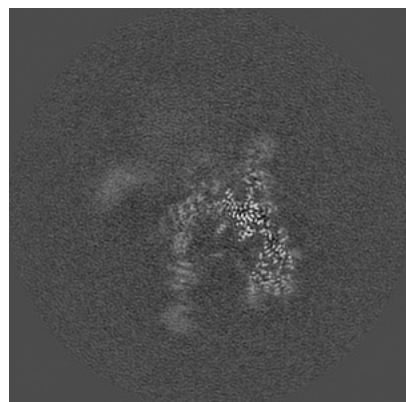


Z

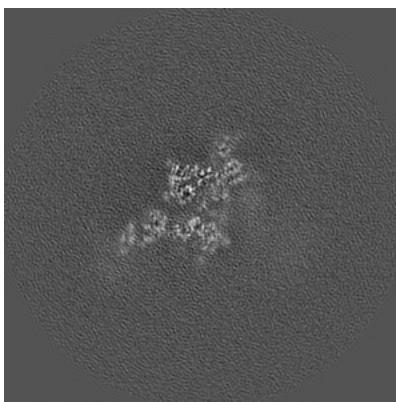
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

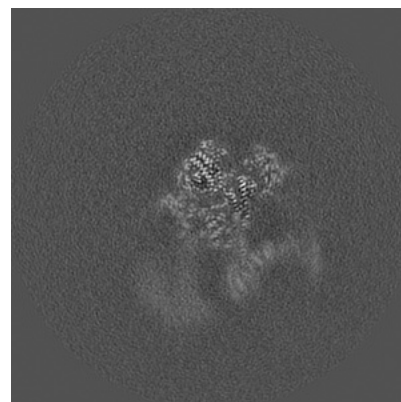
6.2.1 Primary map



X Index: 180



Y Index: 180

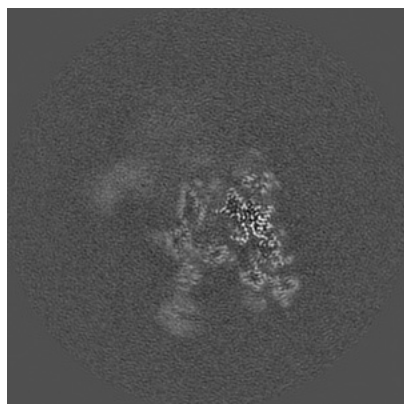


Z Index: 180

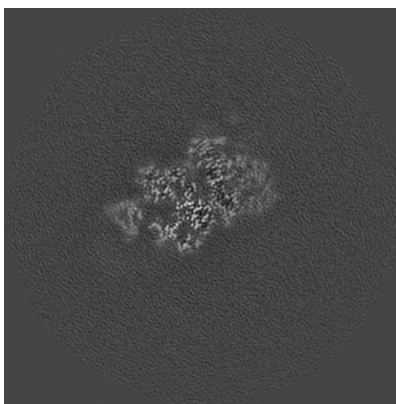
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

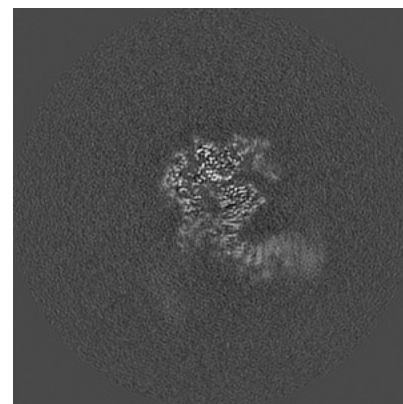
6.3.1 Primary map



X Index: 174



Y Index: 217

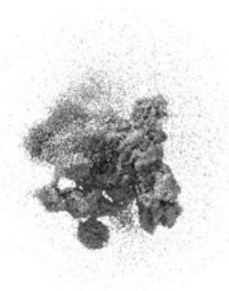


Z Index: 165

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

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0203. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

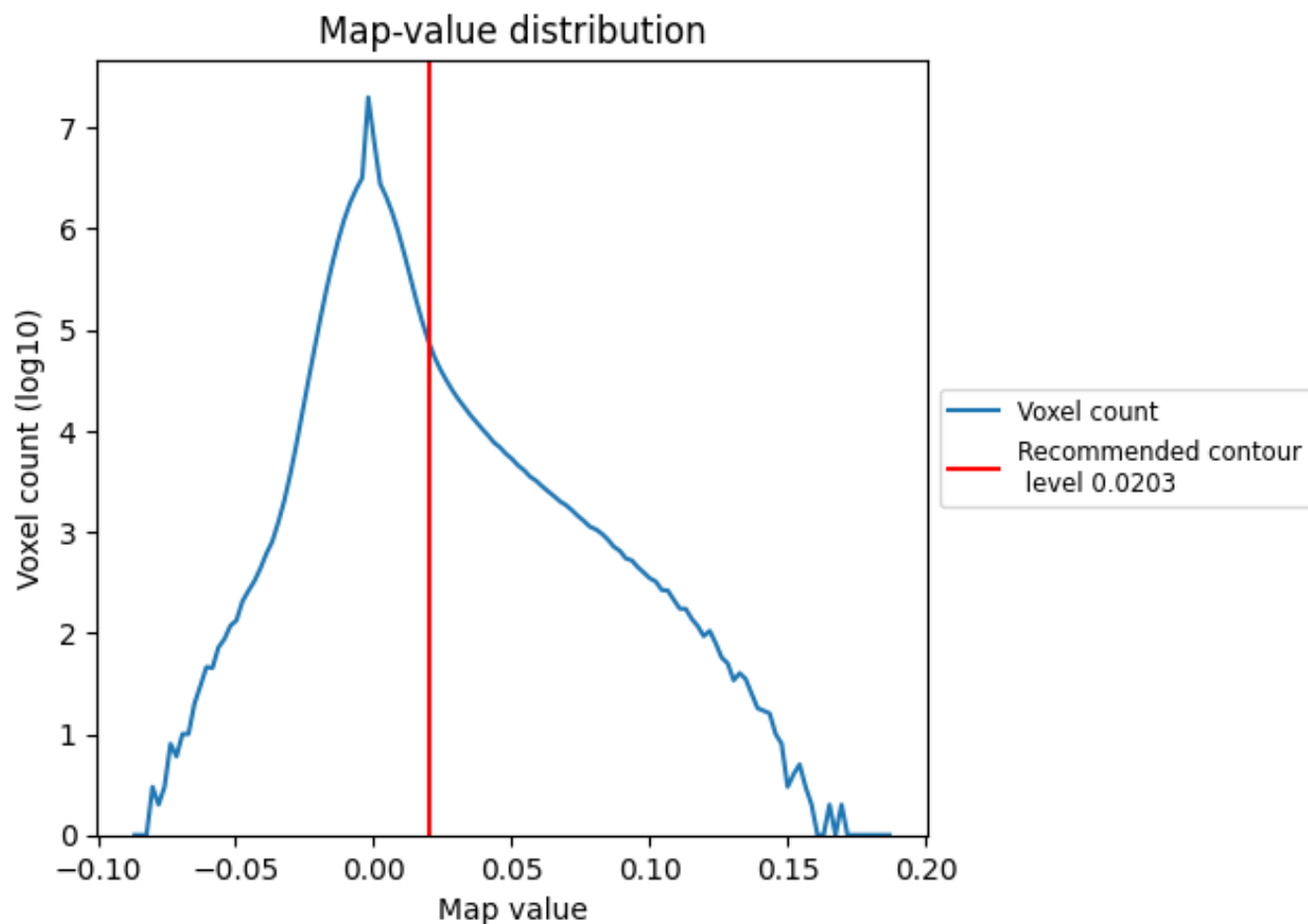
6.5 Mask visualisation

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

7 Map analysis [i](#)

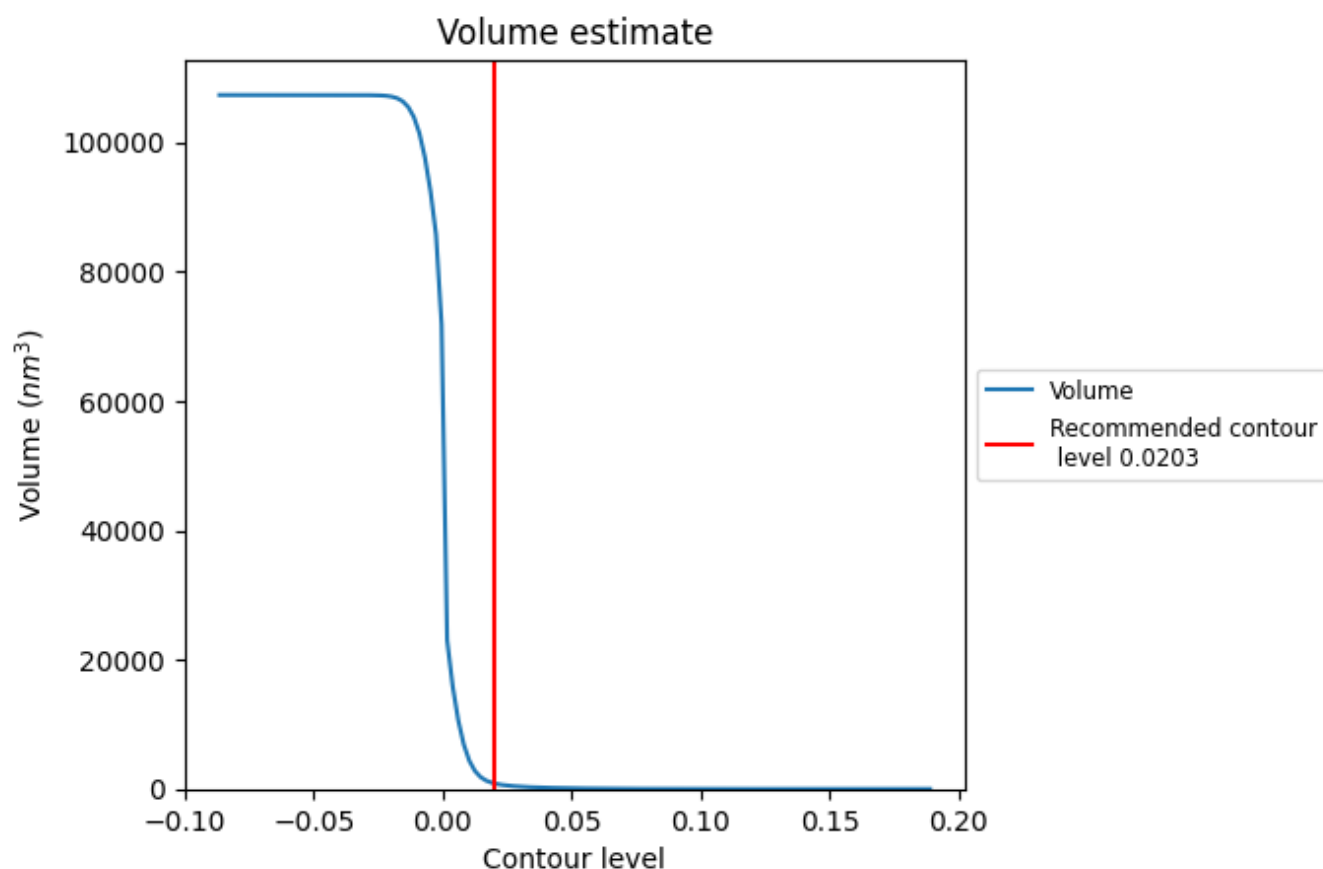
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

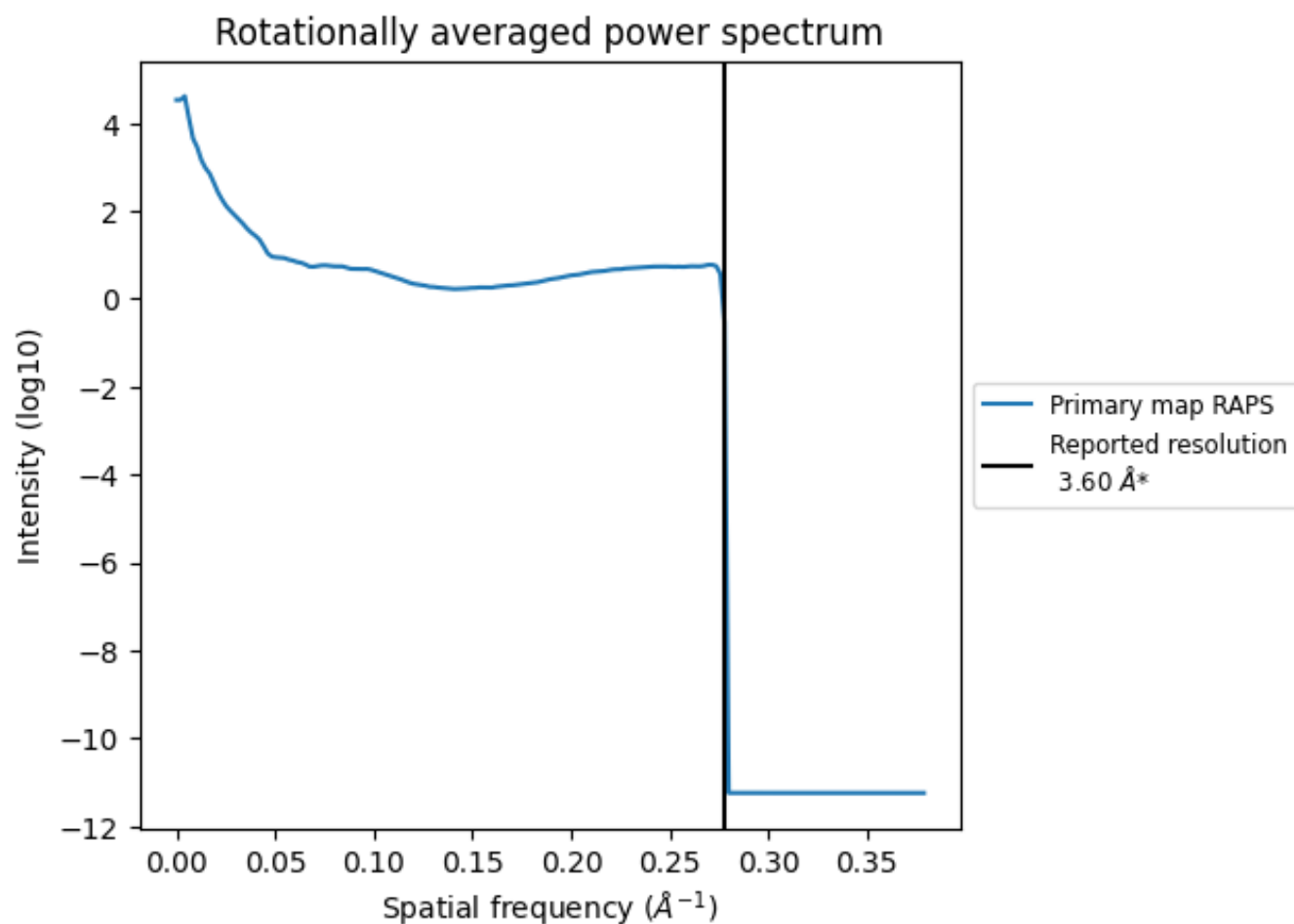
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 836 nm^3 ; this corresponds to an approximate mass of 755 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 0.278 Å⁻¹

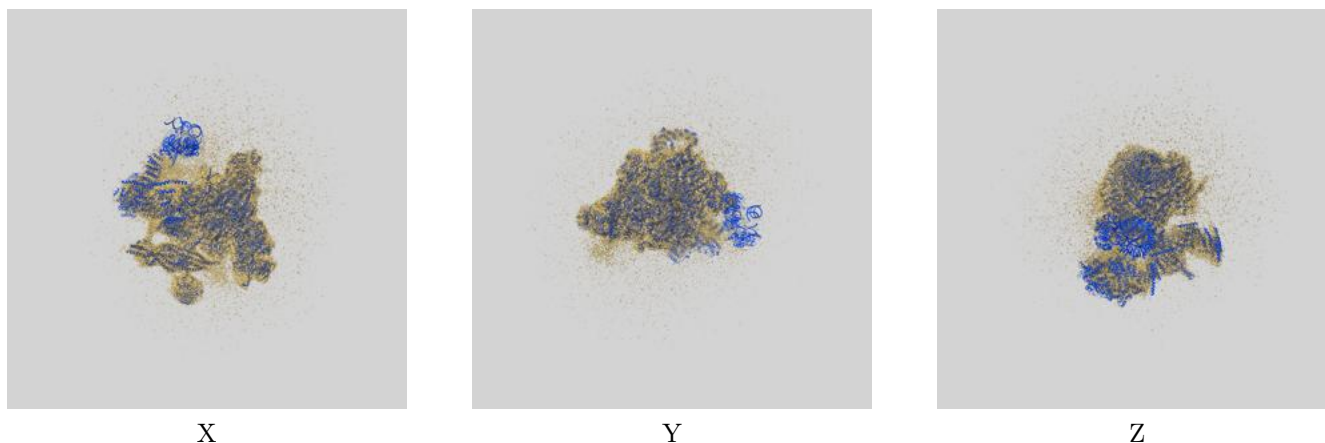
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

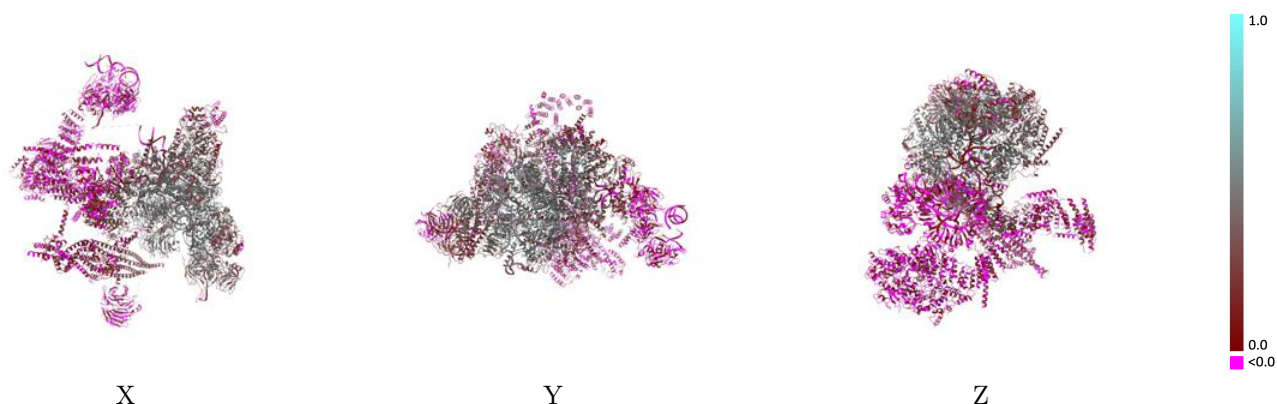
This section contains information regarding the fit between EMDB map EMD-6413 and PDB model 3JB9. Per-residue inclusion information can be found in [section 3](#) on [page 12](#).

9.1 Map-model overlay [i](#)



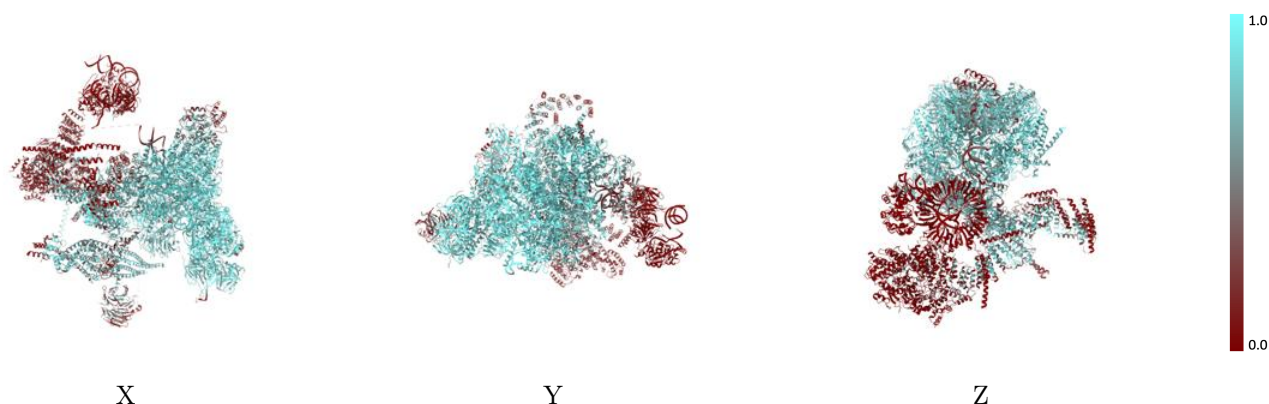
The images above show the 3D surface view of the map at the recommended contour level 0.0203 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



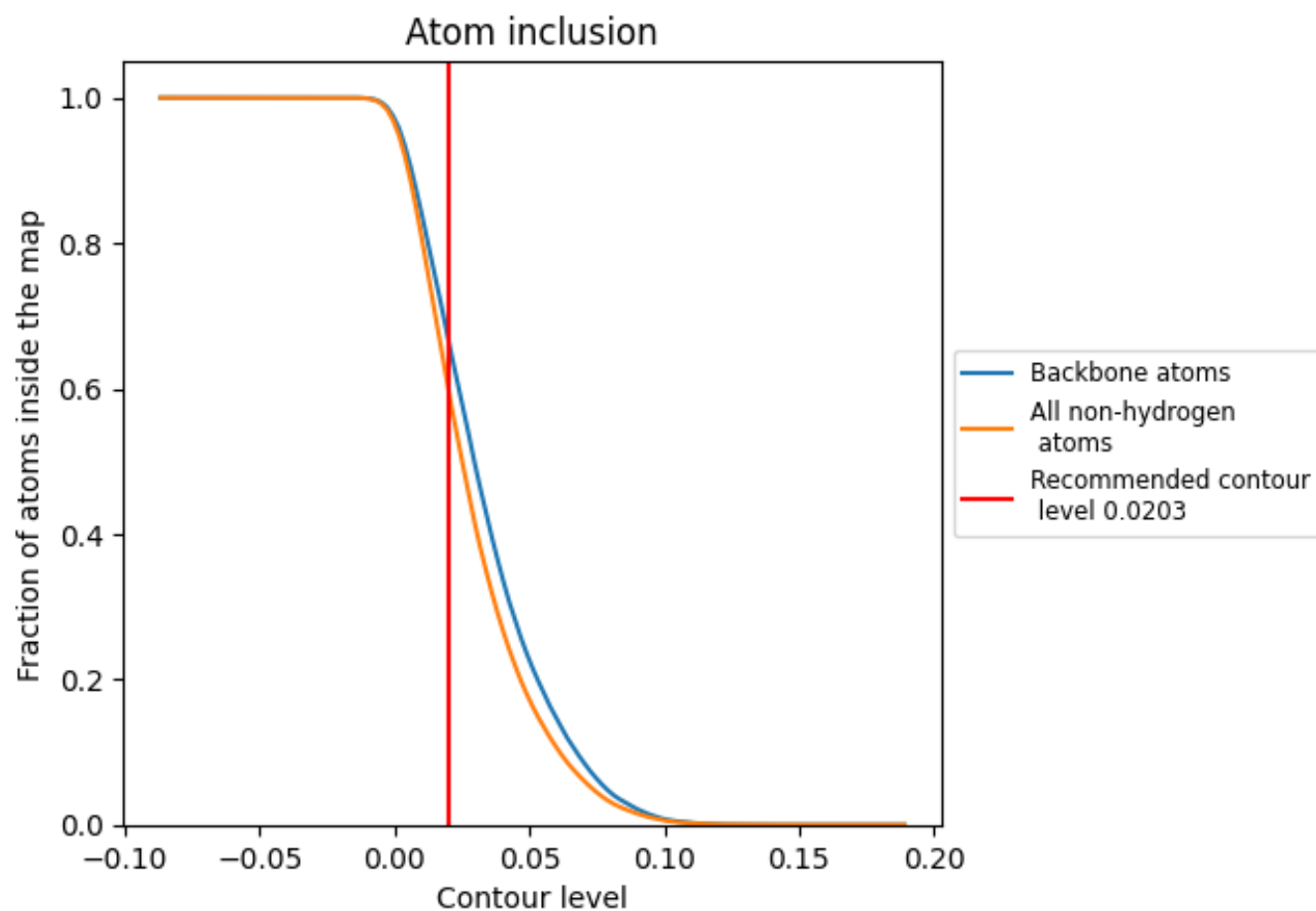
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0203).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 66% of all backbone atoms, 59% 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 (0.0203) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5928	 0.2520
A	 0.8041	 0.4010
B	 0.8677	 0.4180
C	 0.9294	 0.4420
D	 0.8886	 0.4500
E	 0.8480	 0.3960
F	 0.7736	 0.3100
G	 0.7333	 0.2220
H	 0.8069	 0.3130
I	 0.7740	 0.2540
J	 0.8221	 0.3800
K	 0.8765	 0.4390
L	 0.8577	 0.4210
M	 0.7384	 0.3490
N	 0.8106	 0.3390
O	 0.7118	 0.2310
P	 0.1830	 0.0590
Q	 0.2222	 0.0640
R	 0.6467	 0.2420
S	 0.5141	 0.1110
T	 0.6351	 0.1600
U	 0.3927	 0.0610
V	 0.5483	 0.1070
W	 0.6940	 0.2420
X	 0.0763	 0.0030
Y	 0.7698	 0.2860
Z	 0.0080	 0.0210
a	 0.6502	 0.2880
b	 0.0053	 0.0380
c	 0.6499	 0.3140
d	 0.7451	 0.3010
e	 0.8977	 0.4560
f	 0.0031	 0.0210
g	 0.7292	 0.3180
h	 0.7500	 0.4070



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
i	 0.6583	 0.1600
j	 0.0037	 -0.0160
k	 0.0049	 0.0040
l	 0.0029	 -0.0040
m	 0.0000	 -0.0030
n	 0.0018	 -0.0110
o	 0.0036	 -0.0400
r	 0.4199	 0.0610
x	 0.4110	 0.0850