

Dec 10, 2022 – 10:13 pm GMT

PDB ID	:	6QX9
EMDB ID	:	EMD-4665
Title	:	Structure of a human fully-assembled precatalytic spliceosome (pre-B complex).
Authors	:	Charenton, C.; Wilkinson, M.E.; Nagai, K.
Deposited on	:	2019-03-07
Resolution	:	3.28  Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org* A user guide is available at https://www.wwpdb.org/validation/2017/EMValidationReportHelp with specific help available everywhere you see the (i) 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 (1)) were used in the production of this report:

EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, 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)	:	2.31.3

# 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 3.28 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.



Motric	Whole archive	EM structures		
WIEUTC	$(\# {\it Entries})$	$(\# { m Entries})$		
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  $\geq=3, 2, 1$  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	1	104		100%					
	1	104	66%		30% ·				
9	6	106	17%		F00/				
	0	100	36% 12%	•	50%				
			/5%						
3	50	357	85%		• 14%				
			18%						
4	B4	424	18%	82%					
			64%						
5	13	126	56%	6% •	36%				
			66%						
5	23	126	66%		34%				
			53%						
5	43	126	65%	•	34%				
5	53	126	67%		33%				



Conti	nued fron	$i \ previous$	page	
Mol	Chain	Length	Quality of cha	ain
			17%	
6	4B	522	67%	• 31%
7	1	0.2	84%	
- 1	Te	92	67%	15% • 16%
7	2e	92	88%	12%
			67%	
7	4e	92	78%	• 17%
_	~		30%	
1	be	92	84%	16%
8	Т	62		60%
0	1	02	46%	80%
9	1K	437	40% 6%	54%
			6%	
10	4C	499	59% •	40%
11	11	110	68%	
	11	119	61% 67%	5% • 32%
11	21	119	67%	33%
		110	23%	
11	41	119	50% 17%	• 32%
	F 1	110	28%	
	51	119	50% 17%	• 32%
12	B	480	21%	20/
12	10	100	86%	
13	1f	86	76%	9% • 14%
	- 0		84%	
13	2f	86	84%	16%
12	٨f	86	50%	1.00/
10	41	00	55%	• 16%
13	5f	86	83%	• 15%
			90%	
14	66	80	84%	5% • 10%
15	v	155	12%	
15	А	155	32%	68%
16	12	118	71%	8% 19%
10	12	110	81%	
16	22	118	81%	19%
			26%	
16	42	118	78%	22%
16	59	110	43%	170/
10	52	110	/9% 	• 1/%
17	5	117	46%	32% 10% 11%
			75%	
18	67	103	69%	6% 25%



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Mol	Chain	Length		Quality of ch	ain	
10	69	05		100%		
19	02	90	41%	93%		5% •
20	2B	225	41%		59%	
			69%			
21	A2	209	63%		5%	31%
22	B9	805	23%		770/	
		050	22% •		//%	
23	5C	854		99%		·
0.4	ΓV	000	48%			
24	5X	820	36%		•	29%
25	1b	240	32%		64%	
			34%			
25	2b	240	34%		66%	
25	4b	240	25%		660/	
20	-TD	240	54%		00%	
25	5b	240	30%		70%	
	Dr	0.0		80%		
26	B9	80	35%	80%		20%
27	1A	282	33% •		65%	
			<b></b>			
28	S	800	15%	85%		
29	5.I	850	1470	93%		. 6%
		000	<u> </u>	5570		
30	4D	128		95%		• •
21	63	102	77	83%		70/ 1.70/
	05	102	50%	%		/% • 1/%
32	2	188	34%	13% •	50%	)
	Da	1017		97%		
33	B3	1217		97%		••
34	1g	76		86%		11% •
	-0			96%		
34	2g	76		95%		• •
24	4 m	76	720	86%		250/
- 04	4g	10	18%	0		20% •
34	5g	76	72%	6		25% •
05		0.0		99%		
35	68	96		84%		10% ••
36	5A	2311	<b></b>	95%		
			70	5%		
37	A3	501	71%		5% •	24%



Mol	Chain	Length		Quality of chain						
38	U	555	•	80	%		• 18%			
39	5D	142	•	99%						
40	64	139	53% 50% · · 47%							
41	BP	104			96% 95%					
42	1C	159	31% 27%	• •		69%				
43	Κ	1007	32% 29%			68%				
44	4A	683	34%	•		65%				
45	4	146	23%	64%		22%	14%			
46	2A	255		64% 63%		36	5%			
47	A1	647	23%	•		74%				
48	65	91		۶ 77%	34%	79	% 16%			
49	5B	2136	6%		93%		• 6%			
50	B1	1304		65% 64%		•	35%			

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# 2 Entry composition (i)

There are 54 unique types of molecules in this entry. The entry contains 137494 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 U1 snRNA.

Mol	Chain	Residues		Α	AltConf	Trace			
1	1	164	Total 3485	$\begin{array}{c} \mathrm{C} \\ 1555 \end{array}$	N 607	O 1159	Р 164	0	0

• Molecule 2 is a RNA chain called U6 snRNA.

Mol	Chain	Residues		A	toms	AltConf	Trace		
2	6	53	Total 1133	C 506	N 203	0 371	Р 53	0	0

• Molecule 3 is a protein called U5 small nuclear ribonucleoprotein 40 kDa protein.

Mol	Chain	Residues		At	AltConf	Trace			
3	50	306	Total 2394	C 1501	N 422	0 457	S 14	0	0

• Molecule 4 is a protein called Splicing factor 3B subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	Β4	78	Total 618	C 399	N 101	0 115	${ m S} { m 3}$	0	0

• Molecule 5 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues		At	oms		AltConf	Trace	
5 13	81	Total	С	Ν	0	S	0	0	
		637	400	112	119	6	0	0	
5	53	84	Total	С	Ν	0	S	0	0
0 00	04	657	412	116	123	6	0	0	
F	02	0.9	Total	С	Ν	0	S	0	0
5 23	83	652	409	115	122	6	0	U	
Б	5 43	83	Total	С	Ν	0	S	0	0
5			652	409	115	122	6		



• Molecule 6 is a protein called U4/U6 small nuclear ribonucleoprotein Prp4.

Mol	Chain	Residues		At	AltConf	Trace			
6	4B	359	Total 2842	C 1793	N 509	O 521	S 19	0	0

• Molecule 7 is a protein called Small nuclear ribonucleoprotein E.

Mol	Chain	Residues		At	oms		AltConf	Trace	
7	50	77	Total	С	Ν	0	S	0	0
1	9e	11	638	405	113	115	5	0	0
7	40	76	Total	С	Ν	0	S	0	0
1	40	70	631	400	112	114	5	0	0
7	1.0	77	Total	С	Ν	0	S	0	0
(	re	11	638	405	113	115	5	0	0
7	9.0	01	Total	С	Ν	0	S	0	0
7 2e	81	669	424	119	121	5	0	U	

• Molecule 8 is a RNA chain called AdML pre-mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	Ι	25	Total 530	C 237	N 92	0 177	Р 24	0	0

• Molecule 9 is a protein called U1 small nuclear ribonucleoprotein 70 kDa.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	1K	201	Total 1649	C 1036	N 317	0 291	${f S}{5}$	0	0

• Molecule 10 is a protein called U4/U6 small nuclear ribonucleoprotein Prp31.

Mol	Chain	Residues		At	AltConf	Trace			
10	4C	301	Total 2375	C 1486	N 418	0 456	S 15	0	0

• Molecule 11 is a protein called Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues		At	oms	AltConf	Trace		
11	41	<b>Q1</b>	Total	С	Ν	0	S	0	0
	41	01	641	408	112	118	3	0	0
11	11	<b>Q1</b>	Total	С	Ν	0	S	0	0
11	11	11 81	641	408	112	118	3	0	0



Mol	Chain	Residues	Atoms					AltConf	Trace
11	51	<b>Q1</b>	Total	С	Ν	0	S	0	0
	51	01	641	408	112	118	3	0	0
11	91	80	Total	С	Ν	0	S	0	0
11	21	21 80	634	404	111	115	4	0	U

• Molecule 12 is a protein called RNA-binding protein 42.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	R	106	Total 874	C 553	N 160	0 157	${S \atop 4}$	0	0

• Molecule 13 is a protein called Small nuclear ribonucleoprotein F.

Mol	Chain	Residues		At	oms		AltConf	Trace	
13	1f	74	Total	С	Ν	0	$\mathbf{S}$	0	0
10	11	14	576	373	95	103	5	0	0
12	Эf	72	Total	С	Ν	0	$\mathbf{S}$	0	0
10	21	12	562	364	93	100	5	0	0
12	5f	73	Total	С	Ν	0	$\mathbf{S}$	0	0
10	51	15	567	367	94	101	5	0	0
12	٨f	72	Total	С	Ν	0	S	0	0
10	-11	12	562	364	93	100	5	0	0

• Molecule 14 is a protein called U6 snRNA-associated Sm-like protein LSm6.

Mol	Chain	Residues		At	$\mathbf{oms}$	AltConf	Trace		
14	66	72	Total 567	C 360	N 97	0 108	${ m S} { m 2}$	0	0

• Molecule 15 is a protein called U4/U6.U5 small nuclear ribonucleoprotein 27 kDa protein.

Mol	Chain	Residues		Atc	$\mathbf{ms}$	AltConf	Trace		
15	Х	49	Total	C	N	0	S	0	0
			394	247	14	69	4		

• Molecule 16 is a protein called Small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues		At	oms	AltConf	Trace		
16	<u> </u>	05	Total	С	Ν	0	S	0	0
10		90	774	486	141	142	5	0	
16	49	02	Total	С	Ν	0	S	0	0
10	42	92	737	463	138	131	5	0	0



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	J	1	1 5

Mol	Chain	Residues		At	oms	AltConf	Trace		
16	50	08	Total	С	Ν	0	S	0	0
10 52	52	98	796	498	144	148	6	0	
16	10	05	Total	С	Ν	0	S	0	0
10	12	90	777	486	141	144	6	0	0

• Molecule 17 is a RNA chain called U5 snRNA.

Mol	Chain	Residues		Α	AltConf	Trace			
17	5	104	Total 2192	C 983	N 372	О 734	Р 103	0	0

• Molecule 18 is a protein called U6 snRNA-associated Sm-like protein LSm7.

Mol	Chain	Residues		At	oms	AltConf	Trace		
18	67	77	Total 604	C 383	N 102	0 116	${ m S} { m 3}$	0	0

• Molecule 19 is a protein called U6 snRNA-associated Sm-like protein LSm2.

Mol	Chain	Residues		At	oms			AltConf	Trace
19	62	95	Total 761	C 486	N 126	0 145	${S \atop 4}$	0	0

• Molecule 20 is a protein called U2 small nuclear ribonucleoprotein B".

Mol	Chain	Residues		At	oms			AltConf	Trace
20	2B	92	Total 745	C 480	N 130	O 130	${ m S}{ m 5}$	0	0

• Molecule 21 is a protein called Splicing factor 3A subunit 2.

Mol	Chain	Residues		At	oms			AltConf	Trace
21	A2	144	Total 1221	C 782	N 219	0 214	${f S}{f 6}$	0	0

• Molecule 22 is a protein called Splicing factor 3B subunit 2.

Mol	Chain	Residues		Ate	AltConf	Trace			
22	B2	208	Total 1699	C 1093	N 302	O 295	S 9	0	0



• Molecule 23 is a protein called 116 kDa U5 small nuclear ribonucleoprotein component.

Mol	Chain	Residues		Α	AltConf	Trace			
23	$5\mathrm{C}$	852	Total 6727	C 4300	N 1127	O 1266	S 34	0	0

• Molecule 24 is a protein called Probable ATP-dependent RNA helicase DDX23.

Mol	Chain	Residues		At	AltConf	Trace			
24	5X	583	Total 4780	C 3014	N 855	O 893	S 18	7	0

• Molecule 25 is a protein called Small nuclear ribonucleoprotein-associated proteins B and B'.

Mol	Chain	Residues		At	oms		AltConf	Trace	
25	1h	86	Total	С	Ν	0	S	0	0
20	10	80	692	435	126	124	7	0	0
25	9b	80	Total	С	Ν	0	S	0	0
25 20	02	664	419	121	117	7	0	0	
25	۶b	FL 79	Total	С	Ν	0	S	0	0
20	30	15	594	376	108	103	7	0	0
25	4b	80	Total	С	Ν	0	S	0	0
20	40	02	669	423	122	117	7	U	0

• Molecule 26 is a protein called Splicing factor 3B subunit 5.

Mol	Chain	Residues		At	$\mathbf{oms}$			AltConf	Trace
26	B5	69	Total 567	C 360	N 99	0 103	${S \atop 5}$	0	0

• Molecule 27 is a protein called U1 small nuclear ribonucleoprotein A.

Mol	Chain	Residues		At	oms			AltConf	Trace
27	1A	98	Total 787	C 506	N 134	0 143	$\frac{S}{4}$	0	0

• Molecule 28 is a protein called U4/U6.U5 tri-snRNP-associated protein 1.

Mol	Chain	Residues		At	oms	AltConf	Trace		
28	S	120	Total 917	C 576	N 168	0 168	${f S}{5}$	0	0

• Molecule 29 is a protein called Pre-mRNA-processing factor 6.



Mol	Chain	Residues		Α	toms			AltConf	Trace
29	$5 \mathrm{J}$	803	Total 6316	C 3963	N 1155	0 1170	S 28	0	0

• Molecule 30 is a protein called NHP2-like protein 1.

Mol	Chain	Residues		At	oms	AltConf	Trace		
30	4D	123	Total 955	C 604	N 170	0 176	${ m S}{ m 5}$	0	0

• Molecule 31 is a protein called U6 snRNA-associated Sm-like protein LSm3.

Mol	Chain	Residues		At	oms	AltConf	Trace		
31	63	85	Total 699	C 440	N 120	0 136	${ m S} { m 3}$	0	0

• Molecule 32 is a RNA chain called U2 snRNA.

Mol	Chain	Residues		A	toms	AltConf	Trace		
32	2	94	Total 1984	C 887	N 331	0 672	Р 94	0	0

• Molecule 33 is a protein called Splicing factor 3B subunit 3.

Mol	Chain	Residues		Α	toms			AltConf	Trace
33	B3	1186	Total 9296	C 5898	N 1580	0 1773	$\begin{array}{c} \mathrm{S} \\ 45 \end{array}$	0	0

• Molecule 34 is a protein called Small nuclear ribonucleoprotein G.

Mol	Chain	Residues		At	oms			AltConf	Trace
24	1 თ	72	Total	С	Ν	0	S	0	0
04	Ig	15	568	358	102	102	6	0	0
24	Ŋœ	72	Total	С	Ν	0	S	0	0
04	∠g	15	568	358	102	102	6	0	0
24	5 cr	74	Total	С	Ν	0	S	0	0
04	Jg	14	577	364	104	103	6	0	0
34	4 m	74	Total	С	Ν	0	S	0	0
- 54	4g	14	577	364	104	103	6		

• Molecule 35 is a protein called U6 snRNA-associated Sm-like protein LSm8.



Mol	Chain	Residues		At	oms			AltConf	Trace
35	68	95	Total 722	C 446	N 124	0 151	S 1	0	0

• Molecule 36 is a protein called Pre-mRNA-processing-splicing factor 8.

Mol	Chain	Residues		At	AltConf	Trace			
36	5A	2212	Total 18366	C 11840	N 3193	O 3253	S 80	0	0

• Molecule 37 is a protein called Splicing factor 3A subunit 3.

Mol	Chain	Residues		At	AltConf	Trace			
37	A3	383	Total 3227	C 2029	N 566	O 618	S 14	0	0

• Molecule 38 is a protein called U4/U6.U5 tri-snRNP-associated protein 2.

Mol	Chain	Residues		At	AltConf	Trace			
38	U	456	Total 3750	C 2427	N 635	0 674	S 14	0	0

• Molecule 39 is a protein called Thioredoxin-like protein 4A.

Mol	Chain	Residues		$\mathbf{A}$	AltConf	Trace			
39	5D	141	Total 1169	C 751	N 194	0 214	S 10	0	0

• Molecule 40 is a protein called U6 snRNA-associated Sm-like protein LSm4.

Mol	Chain	Residues		At	oms	AltConf	Trace		
40	64	73	Total 596	C 376	N 105	O 109	S 6	0	0

• Molecule 41 is a protein called PHD finger-like domain-containing protein 5A.

Mol	Chain	Residues		$\mathbf{A}$	AltConf	Trace			
41	BP	100	Total 766	C 473	N 135	0 145	S 13	0	0

• Molecule 42 is a protein called U1 small nuclear ribonucleoprotein C.



Mol	Chain	Residues		Ato	$\mathbf{ms}$	AltConf	Trace		
42	1C	50	Total 425	C 266	N 73	O 82	$\frac{S}{4}$	0	0

• Molecule 43 is a protein called Serine/threonine-protein kinase PRP4 homolog.

Mol	Chain	Residues		At	AltConf	Trace			
43	K	322	Total 2626	C 1682	N 462	O 467	S 15	0	0

• Molecule 44 is a protein called U4/U6 small nuclear ribonucleoprotein Prp3.

Mol	Chain	Residues		Ate	AltConf	Trace			
44	4A	239	Total 1946	C 1237	N 360	0 342	${f S}{7}$	0	0

• Molecule 45 is a RNA chain called U4 snRNA.

Mol	Chain	Residues		A	AltConf	Trace			
45	4	126	Total 2690	C 1202	N 474	0 888	Р 126	0	0

• Molecule 46 is a protein called U2 small nuclear ribonucleoprotein A'.

Mol	Chain	Residues		At	AltConf	Trace			
46	2A	162	Total 1282	C 820	N 219	0 240	${ m S} { m 3}$	0	0

• Molecule 47 is a protein called Splicing factor 3A subunit 1, Splicing factor 3A subunit 1, Splicing factor 3A subunit 1.

Mol	Chain	Residues		At	AltConf	Trace			
47	A1	168	Total 1339	C 855	N 237	0 245	${ m S} { m 2}$	0	0

• Molecule 48 is a protein called U6 snRNA-associated Sm-like protein LSm5.

Mol	Chain	Residues		Ate	$\mathbf{oms}$	AltConf	Trace		
48	65	76	Total 587	C 373	N 96	0 114	${S \atop 4}$	0	0

• Molecule 49 is a protein called U5 small nuclear ribonucleoprotein 200 kDa helicase.



Mol	Chain	Residues		At	toms			AltConf	Trace
49	5B	2001	Total 16077	C 10235	N 2767	0 2991	S 84	0	0

• Molecule 50 is a protein called Splicing factor 3B subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	B1	848	Total	С	Ν	0	$\mathbf{S}$	Ο	0
	DI	040	6749	4330	1160	1220	39	0	0

• Molecule 51 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
51	A2	1	Total Zn 1 1	0
51	U	1	Total Zn 1 1	0
51	BP	3	Total Zn 3 3	0
51	1C	1	Total Zn 1 1	0

• Molecule 52 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
52	$5\mathrm{C}$	1	Total Mg 1 1	0

• Molecule 53 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula:  $C_{10}H_{16}N_5O_{14}P_3$ ).





Mol	Chain	Residues	Atoms					AltConf
52	50	1	Total	С	Ν	Ο	Р	0
00	53 5C		32	10	5	14	3	U

• Molecule 54 is INOSITOL HEXAKISPHOSPHATE (three-letter code: IHP) (formula:  $C_6H_{18}O_{24}P_6$ ).



Mol	Chain	Residues	A	AltConf			
54	5A	1	Total 36	C 6	0 24	Р 6	0



## 3 Residue-property plots (i)

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

 $\bullet$  Molecule 1: U1 snRNA







### ILE PHE GLN LYS ARG ARG

 $\bullet$  Molecule 5: Small nuclear ribonucleoprotein Sm D3

Chain 53:	67%	33%	
M1 S2 R51 A56 A56 A56 A50 A50 A50 A50 A50 A50 A50 A50 A50 A50	GLN SER SER GLY GLY ALA ALA ALA ALA ALA ALA ALA ALA ALA A	VAL ALA ALA ALA ARG GLY ARG CLY ARG CLY ARG ARG ARG CLY ARG CLY ARG ARG ARG ARG ARG ARG ARG ARG ARG ARG	
• Molecule 5: Small nu	ıclear ribonucleoprot	ein Sm D3	-
Chain 23:	66%	34%	
MET 52 53 64 64 75 76 75 76 76 77 77 76 81 71	E14 G15 H16 H16 V18 V18 T19 C20 E21 T22 N23 T24 T24	<ul> <li>2.2</li> <li>2.2</li> <li>2.2</li> <li>2.3</li> <li>3.3</li> <li>4.3</li> <li>5.3</li> <li>4.3</li> <li>5.3</li> <li>5.3</li> <li>5.3</li> <li>6.3</li> <li>6.3</li> <li>6.3</li> <li>6.4</li> <li>7.4</li> <li>7.4</li></ul>	43 44 45 44 45 44 46 46 46 46 46 46 45 45 45 45 45 45 455 45
V61 Y62 I63 R64 G65 S66 K67 K67 F70 F70 F70 F70 F70 L71 L72 L73	P74 D75 M76 L77 L77 A80 A80 M82 L83 C84 K84 K84	MET LYS ASN ASN ASN ASN GLY GLY GLY ALA ALA ALA ALA ALA ALA ALA ALA	VALA ALA ALA ARG ARG ARG ARG ARG ALY MET ARG ALY ARG ASN
ILE PHE GLN LYS ARG ARG			
• Molecule 5: Small nu	ıclear ribonucleoprot	ein Sm D3	
Chain 43:	53% 65%	• 34%	_
MET SER 13 C C C C C C C C C C C C C C C C C C	H16 117 117 119 119 120 120 122 122 122 122 122 122 122 122	Y28 R29 G30 C31 F33 F33 F33 F33 F33 F33 F33 F33 F33 F	M45 146 747 747 749 750 753 753 855 855 456 957 957 158 856 950 960
Y62 163 566 566 F70 172 172 173 P74 P74 M76	LY7 K78 A80 P81 M82 M82 L83 K84 K84 K84 K84 K84 K84 ASN ASN	GLN GLN GLY SER GLY GLY GLY ALA ALA ALA ALA CLY CLY CLY CLY CLY CLY ALA ALA ALA ALA ALA	GLY ARG GLY GLY MET MET ARG GLY ARG GLY PHE PHE CLN
LYS ARG ARG			
• Molecule 6: U4/U6 s	small nuclear ribonuc	eleoprotein Prp4	
Chain 4B:	67%	• 31%	
MET ALA SER SER ALA ALA ALA ALA THR LYS THR LYS THR LYS ALA ALA	ASP ASP ASP VAL VAL VAL VAL VAL LYS LYS LYS TYR TYR	GLY SER CLU CLU CLU CLU CLU CLU CLU CLU CLU CLY CLY CLY CLY CLY CLY CLY CLY CLY CLY	ASP GLY LIVE CLVE ALA ALA ALA TLE TLE
GLU GLU GLY ASN TLE ASN TLE CLY CLU GLU GLU GLU GLU GLU	HIS TILE SER ARC GLU GLU CUU CUU CUU CUU CUU CUU CUU CUU CUU	ARK LYS ARG ALA ALA ARG ARG CILN CILN CILU CYS CYS CYS CYS CYS CYS CYS CYS CYS CYS	A LA LLEU GLU THLE THLE THLE
LEU PHE OLY GLU GLU PRO GLU ANG ANG ANG ANG ANG ANG ANG ANG ANG ANG	SER VAL VAL VAL CVAL ASP ASP LVS LVS LVS LVS LVS LVS LVS ASP ASP	GUN LYS SER LYS SER LYS SER LYS SER LYS SER CLU GUU GUU GUU GUU GUU GUU GUI S173 € 173 € VI76	A177



### L407 K408 • Molecule 7: Small nuclear ribonucleoprotein E 30% Chain 5e: 84% 16% MET ALA ALA ARG GLY GLN GLN GLN CLN CLN CLV CLV CLV CLV CLV CLV CLV CLV V 90 SER ASN • Molecule 7: Small nuclear ribonucleoprotein E 67% Chain 4e: 78% 17% I18 N19 L20 I21 F22 R23 MET ALA ALA ARG GLY GLN CGLN CGLN CAL CYS CGLN VAL M14 V15 330 M54 N55 L56 V57 L58 L58 D59 D60 .25 26 328 131 132 L35 Y36 E37 Q38 V39 V39 N40 N41 M41 R42 R42 I43 E44 G45 C46 F5C H65 S66 S66 K65 K65 K65 R71 R71 R71 R71 R71 R71 L73 L73 SER VAL SER ASN 15 • Molecule 7: Small nuclear ribonucleoprotein E 84% Chain 1e: 67% 15% 16% MET TYR ALA ARG GLY GLV GLN CLV CLV CLVS CLV CLV CLV CLV CLV CLVS 3 T68 K69 S70 R71 A61 E62 E63 I64 H65 H65 S66 K72 Q73 L74 G81 D82 N83 375 R76 177 K80 184 T85 L86 • Molecule 7: Small nuclear ribonucleoprotein E 88% Chain 2e: 88% 12% MET ALA TYR ARG GLY GLY GLN GLN CLY SVAL 퓓 5



A61 E62 E63 E63 H65 H65 S66 K67 K67 K69 K69	R71 K72 Q73 L74 G75 R76	177 M78 L79 K80 G81 G81 D82 N83 184 184 T85	L86 L87 Q88 S89 V90 S91 ASN			
• Molecule 8: Ad	ML pre-mI 40%	RNA				
Chain I:	31%	6% •	60%			
G-1 00 02 03 03 03 05 05 05 05 05 05 05 05 05 05 05 05 05				и и в с с с 88 8 8 8 8 8 8 9 0 0 0 0 0 0 0 0 0 0 0	U92 U92 C93 C94 095 096 096 C97 C97 C99 C99 C99	
c101						
• Molecule 9: U1	small nucl	ear ribonucleop	rotein 70 kDa			
Chain 1K:	46% 40%	6%	5	4%	-	
MET 12 F4 F4 F4 P6 P6 P6 R1 R8 R10	A11 L12 F13 A14 P15 R16	D17 P18 T19 P20 Y21 P23 P24 P24 T25	E26 K27 P29 H30 K32 K32 H33	H34 N35 Q36 P37 Y38 Y38 C39 C40 C39 C40 C40 C42	Y44 445 145 846 846 847 748 649 649 651 651	AG AG AG AG AG AG AGO
E61 162 E63 E64 E65 R66 M67 E68 R69	R71 R72 E73 K74 I75 E76	R77 R78 Q79 Q80 E81 E81 E83 E83 E85 E85	L86 K87 M88 M88 W89 P91 P91 N93	P94 P95 N96 A97 Q98 Q98 C99 D100 F101	K103 T104 F105 F105 A105 A108 N110 N111	D113 T114 T115 S117 S117 K118 K119 L119 R120
R121 E122 F123 F123 C124 V125 V126 G127 P128 F120 K130	R131 1132 H133 M134 V135 Y136	S137 K138 R139 S140 S140 G141 F143 F144 F144 C144	Y146 A147 F148 E150 Y151 E152 H153	E154 R155 M157 H157 R153 S159 A160 Y161 K162	H163 A164 A164 D165 G166 K167 K168 K168 C170 G170 R172 K172	R173 V174 L175 V176 D177 V178 E179 E179 R180
C181 R182 T183 V184 K185 C186 W187 R188 P189	R191 L192 G193 G194 G195 L196	G197 C198 T199 R200 R201 G202 G17 G17 G17 ALA ALA ASP VAF	ASN ILE ARG ARG GLY ARG ASP ASP THR	SER ARG ASP ASP GLV PRO PRO FRO LEU	PR0 HIS ARG ARG ARG ARG ARG GLU GLU GLU	
ARG ARG CLU CLU ARG ARG CLU ARG ARD ARG ARD ARG ARD ARG	ARG ARG ARG SER ARG SER ARG ARG	ARG ARG ARG ARG SER SER ARG ARG ARG ARG CLU	GLU ARG ARG ARG SER ARG GLU SER LYS	LYS LYS ASP ARG ARG ARG ARG SER SER SER SER	ABA GLU ARG ALA ARG ARG	
ARG GLU GLU GLU GLU GLU GLU CLU GLY GLY GLY	GLY GLY ASP MET ALA CLU PRO SER GLU GLU	ALA GLY GLY ALA ALA PRO PRO ASP GLY PRO CLY	GLY GLU GLU LEU GLY PRO ASP GLY ASP ASP ASP ASP	GLU GLU GLY GLY ARG ASP ARG ASP ARG ASP ARG	ARG SER HIS ARG SER SER	
GLU ARG ARG ARG ARG ARG ASP ASP ASP ASP ASP	ASF ASP ASP ASP CU CU CU CVS ARG ARG CU STV	GLU GLU GLU GLU GLU GLU ARG GLY ASP GLU ALA	ARG GLY GLY GLY GLY GLY GLN ASP ASP ASP ASV	GLU GLY GLY GLY GLY ASP ASP ASP ASP ASP ASP ASP ASP	GLU GLY GLY	
ASP GLY CLEU CLEU ALA PRO GLY CLU CLU CLU	ALA ALA PRO GLU					
• Molecule 10: U	4/U6  small	nuclear ribonu	cleoprotein Prj	p31		
Chain 4C:		59%	•	40%		
MET SER LEU LEU ALA ASP CLU LEU ALA ASP ASP CLU CLU	ALA ALA GLU GLU GLU GLU GLU GLU	SER TYR GLV GLU GLU GLU GLU FRO ALLA ALLA	GLU ASP VAL CUL CLU GLU GLU CLU CLU CLU CLU CLU CLU	SER GLY GLY GLY SER VAL THR THR THR THR THR THR THR THR THR	ASP SER LYS M59 M59	





















# PHENE CONTRACTOR OF CONTRACTON • Molecule 23: 116 kDa U5 small nuclear ribonucleoprotein component Chain 5C: 99% • Molecule 24: Probable ATP-dependent RNA helicase DDX23 48% Chain 5X: 69% 29% LYS MET LEU GLU ASP PRO PRO GLU GLU GLY GLY LYS LYS ARG ARG ARG ARG ARG ARG ARG LEU LEU ASN C4( G41 Y41 SYS E660 Q661 G662 F663 D664 P665 P666 1667 1668 1669 F670 F670 V671 N672 Q673 Q673 K675





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### PRO PRO GLY MET ARG PRO PRO PRO







 D1655

 1283

 1283

 D2877

 D2877

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 D287

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 B405

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 A449

 A476

 A476

 A476

 A476

 A476

 A449

 A553

 C533

 B548

 B544

 B544

 B544

 B544

 B544

 B544

 B544

 B544

 B544

 B544





97%

97%

• Molecule 33: Splicing factor 3B subunit 3

Chain B3:

	<b></b>	•••	•••	•••		•••	•••		•••	•••			•••			•••	•••	•••	••	••		•••	•••
	M1 F2 L3 Y4	N5 L6 T7	L8 Q9 R10	A11 T12 G13	I14 S15	F16 A17 I18	H19 G20	N21 F22 S23	G24 T25 ¥76	nz 0 q27 q28	E29 130 V31	V32 S33 R34	G35 K36	137 L38 F39	L40 L41	R42 P43	D44 P45 M46	T47 G48	K49 V50	H51 T52	L53 L54 T55	V56 E57	458 F59 G60
	****	<b>**</b>	•••	<b>**</b>	••	•••	••		•••			•••	••	•••		•••		•••	••	••	•••	•••	•••
	V61 I62 R63 S64	L65 M66 A67	F68 R69 L70	T71 G72 G73	T74 K75	D76 Y77 I78	V79 V80	G81 S82 D83	584 G85 P866	187 V88 V88	189 L90 E91	Ү92 Q93 Р94	895 K96	N97 M98 F99	E100 K101	1102 H103	E105 E105	F107 G108	K109 S110	G111 C112	R113 R114 I115	V116 P117	G118 Q119 F120
		86 64			4 5 0	9 L 8		크 더 미	4 5 6			0 0 <del>1</del>	e 9		8 5	0 0	4 D A			2 J	0 4 0	9	α σ g
	L12 A12 V12 D12	P12 K12 G12	R12 A12 V13	M13 113 S13	A13 113	E13 K13 Q13	K13 L14	V14 Y14	L14 N14	D14	A14 A15 R15	118 118 118	S15 S15	P16 E16	A16 H16	K16 A16	T16 T16	V16 Y16	H16 V17	V17 G17	717 710 717	G17 F17	N17 N17 P18
	181 182 183 184	185 186 187	88 68 68 06	191 192 193	94 95	196 197 198	199 200	201 203	204 205 206	207 208	209 210 211	212 213 214	215 216	217 218 219	220 221	222 223	224 225 276	227 228	229 230	231 232	233 234 235	236 237	238 239 240
	M F C		E X E	E E	IN IQ	2 F 3	E: A:	AC AC	885	8638		878	38	388		N N I	i X F		ы ы ы	H 9		нн 1	2 2 3
1         1	<b>***</b>	***	***	<b>**</b> *	•••	•••	•••		•••			•••	•••	•••		•••		•••	••	••	•••	•••	•••
111	6241 5242 5243 5244 5244	P245 5246 3247	V248 L249 I 250	C251 5252 E253	N254 Y255	I 256 I 257 Y 258	K259 N260	F261 3262 D263	1264 P265 D766	1267 1268 R268	0269 P270 I271	P272 R273 R274	R275 N276	0277 L278 0279	D280 P281	E282 R283	1284 M285 T286	F287 V288	5290 5290	A291 T292	H293 K294 T295	K296 S297	M298 F299 F300
																					•		
10.1         10.1 <th< td=""><td><b>***</b></td><td><b>***</b></td><td><b>***</b></td><td><b>**</b></td><td>•••</td><td>•••</td><td>•••</td><td></td><td>•••</td><td></td><td></td><td>•••</td><td>••</td><td>•••</td><td></td><td>•••</td><td>•••</td><td>•••</td><td>••</td><td>••</td><td>•••</td><td>•••</td><td>•••</td></th<>	<b>***</b>	<b>***</b>	<b>***</b>	<b>**</b>	•••	•••	•••		•••			•••	••	•••		•••	•••	•••	••	••	•••	•••	•••
111         CAL         MOI         MOI <td>F301 L302 A303 Q304</td> <td>T305 E306 Q307</td> <td>G308 D309 I310</td> <td>F311 K312 T313</td> <td>T314 L315</td> <td>E316 T317 D318</td> <td>E319 D320</td> <td>M321 V322 T323</td> <td>E324 I325 B326</td> <td>L327 L327 K328</td> <td>Y 329 F 330 D 331</td> <td>T332 V333 P334</td> <td>V335 A336</td> <td>A337 A338 M339</td> <td>C340 V341</td> <td>L342 K343</td> <td>1344 G345 F346</td> <td>L347 F348</td> <td>V349 A350</td> <td>S351 E352</td> <td>F353 G354 N355</td> <td>H356 Y357</td> <td>1.358 7.359 0.360</td>	F301 L302 A303 Q304	T305 E306 Q307	G308 D309 I310	F311 K312 T313	T314 L315	E316 T317 D318	E319 D320	M321 V322 T323	E324 I325 B326	L327 L327 K328	Y 329 F 330 D 331	T332 V333 P334	V335 A336	A337 A338 M339	C340 V341	L342 K343	1344 G345 F346	L347 F348	V349 A350	S351 E352	F353 G354 N355	H356 Y357	1.358 7.359 0.360
11.1         11.1 <th< td=""><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td></th<>																							
11         11<		⊶ ♦ ♦ ⊲ و ی			4 u	• • •	00		4 n a			0 0 <del>4</del>	<b>6 0</b>			0 0	<del>ب</del> س		••		ο 4 υ	9 1 0	
10.1         10.21         0.01         0.01         0.01         0.01         0.01         0.01           10.1         17.23         1.06         1.06         1.06         1.06         0.02           10.1         17.23         1.06         1.06         1.06         1.06         1.06           10.1         1.01         1.06         1.06         1.06         1.06         1.06           10.1         1.01         1.06         1.06         1.06         1.06         1.06           10.1         1.01         1.01         1.01         1.01         1.01         1.01           10.1         1.01         1.01         1.01         1.01         1.01         1.01           10.1         1.01         1.01         1.01         1.01         1.01         1.01           10.1         1.01         1.01         1.01         1.01         1.01         1.01           10.1         1.01         1.01         1.01         1.01         1.01         1.01           10.1         1.01         1.01         1.01         1.01         1.01         1.01           10.1         1.01         1.01         1.01         1.01 <td>I36 A36 H36 L36</td> <td>G36 D36 D36</td> <td>D36 E36 E37</td> <td>P37 E37 F37</td> <td>S37 S37</td> <td>A37 M37 P37</td> <td>L37 E38</td> <td>E38 G38 D38</td> <td>T38 F38 F38</td> <td>F38 Q38</td> <td>P38 R39 P39</td> <td>L39 K39 N39</td> <td>L39 V39</td> <td>L39 V39 D39</td> <td>E40 L40</td> <td>D40 S40</td> <td>540 540 540</td> <td>140 140 L40</td> <td>F40 C41</td> <td>Q41 I41</td> <td>A41 D41 L41</td> <td>A41 N41</td> <td>E41 D41 T42</td>	I36 A36 H36 L36	G36 D36 D36	D36 E36 E37	P37 E37 F37	S37 S37	A37 M37 P37	L37 E38	E38 G38 D38	T38 F38 F38	F38 Q38	P38 R39 P39	L39 K39 N39	L39 V39	L39 V39 D39	E40 L40	D40 S40	540 540 540	140 140 L40	F40 C41	Q41 I41	A41 D41 L41	A41 N41	E41 D41 T42
11         12.21         0.07         0.01																							
NI         1.7.1         0.01         No1         No1 </th <th>21 22 23 24</th> <th>25 26 27</th> <th>28 29</th> <th>31 32 33</th> <th>34 35</th> <th>36 37 38</th> <th>39 40</th> <th>41 42 43</th> <th>44 45 46</th> <th>47 48 48</th> <th>49 50 51</th> <th>52 53 54</th> <th>55</th> <th>57 58 59</th> <th>61</th> <th>62 63</th> <th>04 65 66</th> <th>67 68</th> <th>69 70</th> <th>71 72</th> <th>73 74 75</th> <th>76 77</th> <th>8 / 80</th>	21 22 23 24	25 26 27	28 29	31 32 33	34 35	36 37 38	39 40	41 42 43	44 45 46	47 48 48	49 50 51	52 53 54	55	57 58 59	61	62 63	04 65 66	67 68	69 70	71 72	73 74 75	76 77	8 / 80
11         1.0.1         0.	P4 Q4 L4 Y4	V4 A4 C4	G4 G4	P4 R4 S4	S4 L4	R4 V4 L4	R4 H4	64 E4 E4	V4 S4 F4	44 A4	V4 S4 E4	L4 P4 G4	N4 P4	N4 A4 V4	44 74	V4 R4	R4 14	E4 D4	E4 F4	D4 A4	Y4 14 14	V4 S4	г4 V4 N4
11         12.11         0.17         0.01	<b>****</b>	•••	•••	•••	••	•••	•••		•••			•••	•••	•••		•••	•••	••	••	••	•••	•••	•••
11         0.11         0	4481 [482 [483 /484	.485 3486 [487	1488 1489 1490	/491 2492 2493	/494 [495	3496 3497 3498	-499 -500	3501 1502 1503	504 1505 506	1507 1508	5509 1510 1511	1512 0513 0514	4515 1516	/517 4518 /519	(520 521	1522 1523	1524 1525 1526	1527 1528 1528	A529 0530	(531 (532	/533 1534 5535	4536 (537	1538 5539 3540
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11         11/2         61/N         6	<b>***</b>	<b>***</b>	<b>***</b>	•••																			
111         111 <td>K541 K542 T543 I544</td> <td>45 46 47</td> <td></td> <td></td> <td></td> <td></td> <td><b>++</b></td> <td>•••</td> <td>•••</td> <td></td> <td></td> <td>•••</td> <td><b>* * *</b></td> <td>•••</td> <td>•</td> <td></td> <td>•••</td> <td>•••</td> <td>••</td> <td>••</td> <td>•••</td> <td>•••</td> <td>•••</td>	K541 K542 T543 I544	45 46 47					<b>++</b>	•••	•••			•••	<b>* * *</b>	•••	•		•••	•••	••	••	•••	•••	•••
111         112 <td></td> <td>V5 K5 C5</td> <td>A548 V549 N550</td> <td>Q551 R552 0553</td> <td>V554 V555</td> <td>1556 A557 L558</td> <td>T559 G560</td> <td>G561 E562 L563</td> <td>V564 Y565 F566</td> <td>E567 M568</td> <td>D569 P570 S571</td> <td>G572 Q573 L574</td> <td>N575</td> <td>Y577 T578 F579</td> <td>R580 K581</td> <td>E582</td> <td>SD 54 A5 85 DF R6</td> <td>V587</td> <td>C589</td> <td>S591 ♦ L592 ♦</td> <td>A593</td> <td>P596</td> <td>E599 E599 Q600</td>		V5 K5 C5	A548 V549 N550	Q551 R552 0553	V554 V555	1556 A557 L558	T559 G560	G561 E562 L563	V564 Y565 F566	E567 M568	D569 P570 S571	G572 Q573 L574	N575	Y577 T578 F579	R580 K581	E582	SD 54 A5 85 DF R6	V587	C589	S591 ♦ L592 ♦	A593	P596	E599 E599 Q600
781         1721         4001         1071         4001           783         7223         4         1662         600           785         723         4         1662         600           785         723         4         1662         600           785         723         4         1667         600           785         723         4         1667         600           780         723         4         1667         600           781         723         4         1667         600           781         723         4         1667         600           783         7         667         660         660           784         736         736         660         660           784         736         736         660         660           784         736         7463         660         660           784         744         764         762         660           784         744         763         762         660           784         744         764         763         763           744         744         7		V5 K5 C5	A548 V549 N550	Q551 R552 Q553	V554 V555	1556 A557 L558	T559 G560	G561 E562 L563	V564 Y565	E567 M568	D509 P570 S571	G572 Q573 L574	N575 E576	Y577 T578	R580	E582	5584 A585	V587	C589 M590	S591	A593 N594 V595	P596	600 1600 1600
781         L721         L721         GLY           783         5722         5723         5662           785         7723         5665         5665           786         7723         5665         5665           785         7723         5665         5665           786         7723         1667         6665           787         782         7666         1667           789         7732         6667         1667           789         7732         6667         1667           789         7732         66672         1667           784         7732         6672         1667           784         7732         6672         1667           784         7732         6672         1667           784         7732         6672         1667           784         7734         17674         1677           784         7743         6743         1677           784         7744         6687         1676           784         7744         6687         1676           784         7743         1674         1676           7744	****		A548 • • V549 N550	(1551) (1553) (1553) (1553)	V555	1556 A557 L558	T559	G561 E562 L563	V564	E567 M568	P570	G572 G573 G573 G573 C574 G573 C574 G573 C574 G574 G574 G574 G574 G574 G574 G574 G	N575	Y577 T578	R580	E582	5584 A585	V587	C5 89	S591	A593 N594 V595	P596	6000 10000 10000
781         L1721         MCI           783         9124         9124           784         9125         91665           785         9125         91665           786         91725         91665           783         91725         91665           784         91725         91665           785         91725         91665           789         91730         91670           781         91730         91670           783         91733         91667           784         91733         91667           783         91734         91671           784         91734         91673           784         91734         91673           801         9143         91673           801         9144         91673           801         9144         91683           801         91743         91683           801         91743         91683           801         91743         91673           801         91743         91673           801         91753         91683           801         91753         91673	R601 S602 R603 F604	L605 A606 V607 C5	G608 L609 V610 V610 N550	D611 N612 T613 D553	V614 V554 V555 V555	I616 • I556 I617 • A557 S618 • L558	L619 T559 G560 G560	P621 4 G561 4 S622 4 E562 4 D623 4 L563	C624 V564 V565 V565 V565 V565 V565 V565 V56	F627 E567 E567 E667 E667 E667 E667 E667 E66	5529 P570 P570 P571 9631 5571	A632 (572 (573 (573 (573 (573 (573 (573 (573 (573	A635 0 N575 0 636 0 E576	P637 ♥ Y577 E638 ♦ T578 ♥	L640 R580 K581	I642 E582 I V643 M583 M583	E0444 S584 M645 ♠ A585 ♠ GLY D586	GLY V587 THR V588	LYS GLN M590	ASP GLU LEU LEU LEU	GLU A593 CU GLU N594 ARG GLY V595 C	SER P596	E5599 E5599 Q600
731         1.721         4.0           733         5.722         5.72           735         7.72         5.72           735         7.72         5.72           735         7.72         5.72           735         7.72         5.72           736         7.72         5.72           733         7.72         5.72           734         7.72         1.6           735         7.72         5.72           733         7.72         5.72           733         7.73         5.72           734         7.73         5.72           735         7.73         5.72           733         7.73         5.72           734         7.73         7.73           735         7.73         7.73           736         7.73         7.73           736         7.73         7.73           735         7.74         7.6           736         7.74         7.6           737         7.74         7.7           738         7.74         7.6           739         7.74         7.7           731	R601 8602 R603 F604	L605 A606 K5 V607 C5	G608 ♦ A548 L609 ♦ V549 V610 ♦ N550	D611 0612 1613 D653	V614 V554 V555 R615 V555	I616 T566 I617 A557 S618 L558	L619 T1559 G560 G560	P621 ( G561 ( S622 ( S6	C624 V564 V564 L625 Y565 L626 F5665 L626 F5665 V5665 V56655 V566555 V56655 V56655 V56555 V56555 V566555 V566555 V566555 V566555 V566555 V565555 V566555 V56555 V565555 V5655555 V5655555 V5655555 V5655555555	For the second s	5529 P570 M630 P570 G631 S571	A632 • G572 • L633 • q573 • P634 • L574 •	A635 A N575 A C636 E576	P637 ♥ Y577 E638 ♦ T578 S639 ● E579	L640 R580 C641 K581	I642   E582   I V643   M583	LO 44 C3 25 34 M645 A5	GLY V587	LYS C589 C589 C589 C589	ASP GLU S591 LEU L592	GLU A593 A ARG N594 A GLY V595 A	SER P596	66 50 B
781         1.721         1.721           783         9.722         2.721           785         9.723         2.723           786         9.723         2.724           786         9.726         2.724           786         9.725         2.724           786         9.726         2.724           789         9.726         2.724           790         9.1732         2.723           791         9.726         2.723           792         9.726         2.734           793         9.733         2.733           794         1.733         7.733           795         9.744         2.734           796         7.733         2.744           793         9.744         2.744           794         7.744         2.744           801         9.744         7.746           801         7.744         7.744           802         7.744         7.744           803         9.744         7.745           804         7.745         7.745           805         7.744         7.746           804         7.745	R601         82         8602         8602         8602         86033         8603         8603 <td< td=""><td>55 • L605 • V5 56 • A606 • K5 57 • V607 • C5</td><td>58 6 6608 6548 59 L609 50 V549 70 V610 10050</td><td>71 0 0611 0 0551 72 0 NG12 0 R552 73 1613 0 0553</td><td>74 V614 V614 V554 75 R615 V555</td><td>7 1616 1556 77 1617 1556 78 5618 1558</td><td>79 • L619 • T559 • G560 • G560</td><td>32 6521 6561 6561 6562 6562 6562 6562 656</td><td>34         C624         V564           35         L625         Y565           36         L625         T565</td><td>37     •<!--</td--><td>90 M630 P570 P570</td><td>A 6572 C 6572 C 7 J L633 C 6573 C 6574 C 65747 C 6574 C 65744 C 6574 C 6574 C 6574 C 6574 C 6574 C 6574 C</td><td>96 ♦ A635 ♦ N575 ♦ 37 ♦ q636 ♦ E576 ●</td><td>38 ♥ P637 ♥ Y577 ♥ 99 ♦ E638 ♥ T578 ♥ 00 ● S639 ● E579</td><td>01 • L640 • R580 • C641 • K581 •</td><td>33         ●         I642         ●         E582         ●           34         ●         V643         ●         M583         ●</td><td>D5 • B044 - S384 • D6 • M645 • A585 • A585 • A585 • A585 • A585 • A585 • A586 •</td><td>CLY V587 CLY V587 CILI V588</td><td>IO LYS C589 C589 C589 C589</td><td>I2 ASP SS91 CLU SS91 LEU L592</td><td>14 ↔ GLU A593 ↔ I5 ↔ GLU N594 ↔ ARG N595 ↔</td><td>IT SER PE96</td><td>19 • • • • • • • • • • • • • • • • • • •</td></td></td<>	55 • L605 • V5 56 • A606 • K5 57 • V607 • C5	58 6 6608 6548 59 L609 50 V549 70 V610 10050	71 0 0611 0 0551 72 0 NG12 0 R552 73 1613 0 0553	74 V614 V614 V554 75 R615 V555	7 1616 1556 77 1617 1556 78 5618 1558	79 • L619 • T559 • G560	32 6521 6561 6561 6562 6562 6562 6562 656	34         C624         V564           35         L625         Y565           36         L625         T565	37     • </td <td>90 M630 P570 P570</td> <td>A 6572 C 6572 C 7 J L633 C 6573 C 6574 C 65747 C 6574 C 65744 C 6574 C 6574 C 6574 C 6574 C 6574 C 6574 C</td> <td>96 ♦ A635 ♦ N575 ♦ 37 ♦ q636 ♦ E576 ●</td> <td>38 ♥ P637 ♥ Y577 ♥ 99 ♦ E638 ♥ T578 ♥ 00 ● S639 ● E579</td> <td>01 • L640 • R580 • C641 • K581 •</td> <td>33         ●         I642         ●         E582         ●           34         ●         V643         ●         M583         ●</td> <td>D5 • B044 - S384 • D6 • M645 • A585 • A585 • A585 • A585 • A585 • A585 • A586 •</td> <td>CLY V587 CLY V587 CILI V588</td> <td>IO LYS C589 C589 C589 C589</td> <td>I2 ASP SS91 CLU SS91 LEU L592</td> <td>14 ↔ GLU A593 ↔ I5 ↔ GLU N594 ↔ ARG N595 ↔</td> <td>IT SER PE96</td> <td>19 • • • • • • • • • • • • • • • • • • •</td>	90 M630 P570 P570	A 6572 C 6572 C 7 J L633 C 6573 C 6574 C 65747 C 6574 C 65744 C 6574 C 6574 C 6574 C 6574 C 6574 C 6574 C	96 ♦ A635 ♦ N575 ♦ 37 ♦ q636 ♦ E576 ●	38 ♥ P637 ♥ Y577 ♥ 99 ♦ E638 ♥ T578 ♥ 00 ● S639 ● E579	01 • L640 • R580 • C641 • K581 •	33         ●         I642         ●         E582         ●           34         ●         V643         ●         M583         ●	D5 • B044 - S384 • D6 • M645 • A585 • A585 • A585 • A585 • A585 • A585 • A586 •	CLY V587 CLY V587 CILI V588	IO LYS C589 C589 C589 C589	I2 ASP SS91 CLU SS91 LEU L592	14 ↔ GLU A593 ↔ I5 ↔ GLU N594 ↔ ARG N595 ↔	IT SER PE96	19 • • • • • • • • • • • • • • • • • • •
781         1721           782         7723           785         7723           786         7725           786         7725           786         7725           786         7725           787         787           786         7725           787         782           786         7725           789         7725           783         7725           784         7725           783         7724           784         7733           785         7733           786         7733           787         7733           786         7733           787         7733           786         7734           787         7744           803         7744           804         7744           805         7744           805         7746           816         7746           817         7756           818         7756           819         7756           814         7756           815         7756	GLY         R601 ♦           F662         \$602 ♦           L1663         \$603 ♦           Y664         F604 ♦	L665 C L605 V5 N666 A606 K6 I667 V607 C	G668         C608         A548           L669         L609         V549           Q670         V610         N550	N671 ♥ D611 ♦ Q551 G672 ♥ N612 ♥ R552 V673 ● T613 ● 0553	L674 V614 V554 V554 V555	No/o         I616         I556           T677         1617         A557           V678         5618         L558	L679 L619 T559 C560 C560 C560 C560 C560 C560 C560 C560	Foot         P621         G561           V682         5622         E562           T683         D623         L563	G684 ♥ C624 ♦ V564 ♦ D685 ♦ L625 ♦ Y565 ♦ L626 ● rese	S687 equation (1997) (1	100         55.29         1069           R690         M630         P570           T691         q631         S571	TYR A632 • 6572 • LEU L63 • 6573 • 6595 • 634 • 1574 •	S696         A635         N675            R697         Q636         E576	P698 ♦ P637 ♥ Y577 ♥ V699 ♦ E638 ♦ T578 ♦ X700 ♠ 5639 ♠ E579	1701 ♦ 1640 ♦ R580 ♦	R703         ■         I642         ■         E582         ■           V704         ●         V643         ●         M583         ●         0	R705 ← E044 5584 4585 ← A585 ← A585 ← A585 ← A586 ← A5866 ← A586 ← A586 ← A586 ← A586 ← A586 ← A586	GT 08 GLY U587 CTHR U588 CTH	E710 CLNS C589 C10 C589 C10 C589 C10	V112 • ASP S591 • S591 • L713 • LEU L592 • L80	A714 GLU A593 M715 A593 M715 A593 M715 A505 M715 A505 A505 A505 A505 A505 A505 A505 A5	S717 SER P596 R718 ILE P597	5719 ♥ Gabes 1998 1998 1998 1998 1998 1998 1998 199
731 732 732 7333 7354 7355 7355 7355 7355 7355 7355	GLY         Re01         He           F662         S022         S022<		G668 G608 ↔ A548 L669 ↔ V549 G670 ↔ V610 ↔ N550	N671         D611         Q551           0672         N612         R522           V673         T613         D553	L674 V614 V554 L675 R615 V555	No/v         1616         1556           1677         1617         A557           V678         5618         L558	L679 L619 L619 C569 C560 C560 C560 C560 C560 C560 C560 C560	root P621 9 G561 V682 5622 9 E562 9 T683 0 D623 0 L563 9	G684         C624         V564           D685         L625         Y565           L686         nene         Frace	S687         4020         1000           B688         F627         E567           D688         L628         M568           T689         C000         2000	R690 M630 P570 F570 A569 A571 A569 A571 A569 A569 A569 A569 A569 A569 A569 A569	TYR A632 C572 C572 LEU L633 C572 C572 C572 C572 C573 C573 C573 C573 C573 C573 C573 C574 C574 C574 C574 C574 C574 C574 C574	8696 A 6635 N 1575 R 1575 R 2576	P638 P637 V577 V699 E638 T578 V700 S639 E579	IT702 ← C640 ← R580 ← R581 ←	R703 1642 E582 1 V704 V643 M583	N705 ► E044 ► 5554 N706 ► M645 ► A585 0707 ► GLY D586		E710 ♦ LYS C589 ♦	V712 ASP S591 CLU L592 CLU L59	A714 011 011 011 011 011 011 011 011 011 0	R717 SER P596	8719 ♥ E599 ♥ E599 ♥
781 785 785 785 785 785 785 785 786 789 799 799 799 800 800 800 800 800 800 800 800 800 8	721         0LY         R601           722         F662         5602           723         L663         R603           724         Y664         F604	725   L665   L605   V5 726   N666   A606   K5 727   1667   V607   C5	728 ↔ G668 ↔ G608 ↔ A548 729 ↔ L669 ↔ V549 730 ↔ Q670 ↔ V610 ↔ N550	731         →         №71         →         D611         ↓         Q501           732         ↔         G672         ↔         N612         ↔         8552           733         ↔         V673         ↔         T613         ↔         0553	734 L674 V614 V564 735 L675 R615 V565	736 ↔ No <sup>1/6</sup> 1616 ↔ 1556 ↔ 737 ↔ 1677 ↔ 1617 ↔ A557 738 ↔ V678 ↔ S618 ↔ L558	739         L679         L619         T569         T569         T610         T569         T769	741         F001         P621         0561         0561           742         V682         S622         5562         0           743         T883         D623         L563         0	744 • 6684 • C624 • V564 • 1564 • 1625 • 1625 • 1625 • 1665 • 1625 • 16666 • 1666 • 1666 • 1666 • 1666 • 1666 • 1666 • 1666 • 1666 • 16	747 • 5687 • • • • • • • • • • • • • • • • • • •	750         R690         M630         P570           751         7691         9631         9570           751         7691         9631         9571	752 ♥ TYR A532 ♥ G572 ♥ 753 ♦ LEU L633 ♦ Q573 ♦ 754 ♦ G695 ♦ P634 ♥ L574 ♥	755 • S696 • A635 • N1575 • 11575 • 1576 • 1636 • 1636 • 1576	757 P698 P637 Y777 758 V699 E538 T778 759 X700 S839 E573	760 ← L701 ← L640 ← R580 ← R581 ← K581 ←	762 <b>R</b> 703 <b>1642 E582 </b>	704 ₩ KV05 ₩ K044 ₩ S504 ₩ K055 ₩ K045 ₩ K055 ₩ K045 ₩ K045 ₩ K045 ₩ K045 ₩ K055 ₩ K045 ₩ K055 ₩ K045 ₩ K055 ₩ K0	767 4 010 0LY 5000 THR 768 1HR 7588	769 € 710 € LYS C589 € 770 € 411 € GLN M590 €	771 • V712 • GLU 5591 • 772 • L713 • LEU L592 •	773 • A714 • GLY A593 • 774 • M715 • GLU N594 • 775 • s776 • GLY V595 •	776 S717 SER P596 P597	779 W7720 General Control Cont
781 785 785 785 785 785 785 785 785 785 789 789 799 799 799 811 811 811 811 811 811 811 811 811 8	L721     GLY     R601       S722     F662     \$602       Y723     L663     R603       S724     Y664     F604	Y725         L665         L605         V5           q726         №666         A606         K5           S727         1567         V607         C5	R728         G668         G608         A548           F729         L669         L609         V549           H730         Q670         V610         N550	L731   N671   D611   G51 T732   G672   N612   R522 P733   V673   T613   D553	L734 L674 v614 v554 v554 v554	Y736 ↔ <sup>No.70</sup> 1616 ↔ 1556 ↔ 1578 ↔ 1738 ↔ V678 ↔ 5618 ↔ 1558	L739         L679         L619         T559           E740         D6800         D620         G560         G560	F741 • F001 • 6621 • 6661 • 6742 • V682 • 5622 • E562 • 5622 • 5622 • E562 • 5623 • 1563 • 15	G744 ↔ G694 ↔ C624 ↔ V564 ↔ F745 ↔ D685 ↔ L625 ↔ Y565 ↔ A7AA ▲ L686 ↔ Asse ↔ steas	8687         9420         5000           8747         5687         9420         5567           8748         D688         9627         5567           8748         D688         1623         9668           9740         7628         9668         9668	4/49         500         5029         10569           C750         R690         M630         P570           P751         T691         q631         S571	E752 • TYR A632 • G572 • G572 • TYR A632 • G572 • TYR A632 • G573 • G573 • T54 • L574 • L574 • C574	V755 ♦ S696 ♦ A635 ♦ N575 ♦ A756 ♦ R697 ♦ Q636 ♦ E576	1757 P698 P637 Y677 5758 V699 E638 T578 1759 X700 S639 F573	1760 ♦ 1770 L640 ♦ 8580 ♦ 1761 ♦ 1762 ♦ 5541 ♦ 8581 ♦	L762 • R703 • 1942 • E582 • R763 • V704 • V43 • M533 • M533	L/04 ← K/05 ← E0-44 ← 35-64 ← L/765 ← M/645 ← M/645 ← A5-85 ← 47-64 ← A5-85 ←	LT67 QTOB CLY USS L767 QTOB CLY USS THR USS PTHR USS	K769 ← E710 ← LYS C589 ← L770 ← A711 ← GLN M590 ←	G771 V712 CLU EU L592 A	V773 ♥ A714 ♥ GLT A593 ♥ F774 ♥ M715 ♥ GLU N594 ♥ N775 ♥ S716 ♥ GLV V595 ♥	q776 ♦ S717 SER P596 ♦ v777 ♦ R718 • ILE P597	A//8         S/19         Good         Good         E599         E599 <t< td=""></t<>
	↓         1721         ←         GLY         R601         ←           ★         5722         ←         F662         ←         5602         ←           ★         1723         ←         L663         ←         R603         ←         R603         ←           ★         5724         ←         Y664         ←         F604         ←		●         R728         ●         G668         ●         G608         ●         A548           ●         F729         ●         L669         ●         V549           ●         H730         ●         Q670         ●         V610         N550	↓         L731         №71         ♥         D611         ¶         ¶551           ◆         1732         ♦         G672         ♥         №12         №         №52           ◆         1733         ♦         0673         ●         №13         ●         D553		Y736         R0/0         IG16         I556           E737         T677         I617         A557           T738         V678         S618         L558	↓         L739         L679         L619         T559         T559         €           ◆         E740         ●         D680         ●         D620         ●         C560         ●	F741         F001         F621         G561           A742         V682         S622         E562           A743         T683         D623         L563		ST47         S687         qozo         soco           F747         5687         9627         5567         5567           F748         D688         9627         9657         9657           F748         D688         1668         9667         9657	U 449         6-00         56.29         D969           C750         R690         M630         P570           P751         T691         q631         5571	E752         TYR         A632         G572         G572         G572         G572         G572         G573         G573 <th< td=""><td>♦ V755 ♦ S696 ♦ A635 ♦ N575 ♦ A756 ♦ R697 ♦ Q636 ♦ E576</td><td>I157         P698         P637         Y577           \$3758         V699         E638         I578           \$1759         \$1700         5539         E579</td><td>♦ N760 ♦ L701 ♦ L640 ♦ R580 ♦ 1761 ♦ F702 ♦ C641 ♦ K581</td><td>↓         L762         R703         ↓         1642         €582         ↓           ↑         N763         ↓         V643         ↑         №53         ↓</td><td>1.104 H 705 → 1044 → 2064 → 1.104 H 705 → 1.105</td><td>LT67 Q101 GLY V587 LT67 Q101 GLY V587 ET68 C1700 GLY V588</td><td>KT69 ET10 LVS C589 LVS LT70 LT70 C11M M590</td><td>A772 • LEU LE92 •</td><td></td><td>QT76 ST17 SER PE96 P597 P177 P118 P118 P597 P597 P597 P597 P597 P597 P597 P597</td><td></td></th<>	♦ V755 ♦ S696 ♦ A635 ♦ N575 ♦ A756 ♦ R697 ♦ Q636 ♦ E576	I157         P698         P637         Y577           \$3758         V699         E638         I578           \$1759         \$1700         5539         E579	♦ N760 ♦ L701 ♦ L640 ♦ R580 ♦ 1761 ♦ F702 ♦ C641 ♦ K581	↓         L762         R703         ↓         1642         €582         ↓           ↑         N763         ↓         V643         ↑         №53         ↓	1.104 H 705 → 1044 → 2064 → 1.104 H 705 → 1.105	LT67 Q101 GLY V587 LT67 Q101 GLY V587 ET68 C1700 GLY V588	KT69 ET10 LVS C589 LVS LT70 LT70 C11M M590	A772 • LEU LE92 •		QT76 ST17 SER PE96 P597 P177 P118 P118 P597 P597 P597 P597 P597 P597 P597 P597	





• Molecule 34: Small nuclear ribonucleoprotein G



#### V61 162 R63 G64 N65 S66 167 168 168 A72 L73 A72 L73 E74 R75 E74 V76

V61

• Molecule 34: Small nuclear ribonucleoprotein G



## • Molecule 34: Small nuclear ribonucleoprotein G











• Molecule 39: Thioredoxin-like protein 4A



Chain 5D:		99%			
MET 82 81 15 822 7142					
• Molecule 40: U	J6 snRNA-associat	ed Sm-like prote	in LSm4		
Chain 64:	53% 50%		47%		
MET L2 L4 S5 K8 K8 T9	A10 A11 A12 P14 P14 M15 C116 E18 K20	N21 622 623 725 725 725 825 825 826 725 827 828	V30 531 532 532 533 633 834 835 835 835 835 835 835	N39 L40 E41 E42 V43 C45 C45 C45 C45	R45 P49 C50 C50 K52 K52 W64 R55 R55 R55 C59 C59
I61 R62 G63 S64 T65 T65 K67 Y68 Y68 L69	R70 171 P72 P72 P72 E74 A5P ASP ASP ASP ASP CUU	VAL VAL ALA LYS GLY GLY GLY GLY GLY CLEU	GLN GLN GLN GLN GLN GLY GLY GLY MET GLY	GLY ALA ALA GLY GLY PHE GLY GLY GLY GLY	ARG GLY JLE ILE
PRO GLY GLY GLY ARG GLN GLN CLN CLN CLV CLY SPRO	GLY ARG GLN ALA GLY LYS GLN				
• Molecule 41: F	PHD finger-like dor	nain-containing	protein 5A		
Chain BP:		96% 95%			
MET A2 H4 H5 P6 P6 L8 L8	C11 C11 C11 C11 C11 C11 C11 C11 C11 C11	R21 L22 C23 E24 K25 C26 C26 G28 G28 K29	C30 V31 132 C33 C33 C33 C33 C33 C33 C33 C33 C33 C	P39 C40 C40 L42 V43 R44 R44 C46 C46 C46	E448 C448 Y 51 G52 G52 Y 553 Y 553 G55 G55 C55 C55 C55 C55 C55 C55 C55 C55
C61 G62 G63 P64 P64 G65 V66 S67 S67 S67 D68 A69	Y70 Y71 C72 K73 E74 C75 C75 C75 T76 Q78 E79 E79 K80	D81 R82 D83 G84 C85 P86 F86 K87 I88 I88 V89	N90 L91 G92 S94 K95 K95 T96 D97 L96	F99 Y100 E101 LYS LYS	
• Molecule 42: U	J1 small nuclear ril	oonucleoprotein	С		
Chain 1C:	27% ••		69%		
MET P2 K3 F4 Y5 C5 C5 C5 C5 C5 C5 C5 C5 C5 C5 C5 C5 C5	711 712 113 114 714 115 817 817 819 819 819	R21 K22 T23 H24 C25 S26 G27 R28 R28 K29	H30 K31 E32 N33 V34 K35 K35 Y37 Y37 Y38	q39       K40       W41       M42       E43       E44       A46	S48 149 150 150 150 151 150 151 150 151 150 151 151
LYS TLE PRO PRO PRO PRO PRO PRO PRO PRO	ALA ALA ALA MET TLE PRO PRO PRO PRO SER SER SER SER SER SER PRO PRO	PRO ARG GLY MET MET PRO PRO HIS MET	GLY PRO PRO MET MET PRO MET MET PRO PRO	PRO PRO GLY MET MET PRO PRO GLY ALA ALA PRO	
GLY MET ARG PRO PRO PRO GLY GLY HIS MET PRO	MET PRO GLY PRO PRO PRO PRO PRO PRO PRO MET MET	MET VAL PRO THR ARG PRO GLY MET ARG PRO	ARG		
• Molecule 43: S	erine/threenine-pr	otein kinase PR	P4 homolog		
Chain K:	32% 29% •		68%		
MET ALA ALA ALA GLU GLU SER LEU ARG GLU GLU GLU	PR0 GLU GLU ALA ALA ASP ASN SER CLU CLV SER ILYS SER ASN GLU	GLU ASN GLY GLV VAL VAL SER GLU SER GLN SER	LYS HIS SER ARG HIS LYS LYS LYS LYS	HIS ARG SER LYS HIS LYS LYS LYS HIS KYS SER	
SER GLU GLU GLU ASP LYS ASP LYS HIS HIS HIS	HIS LYS LYS LYS LYS LYS LYS LYS ARG LYS GLU TILE AIA AIA	SER ASP LYS GLU GLU GLU MET SER PRO ALA ALA ALA	LEU ASP ASP ASP ASP ALA LEU CLU ASP ASP ASP LEU	GLU LYS GLN ARG ARG AIA LLYS ALA GLU LEU	
		WORLDW	IDE		










# GLY ARG GLY GLY GLY GGLY LEU LEU LYS ALA ALA ALA ASP ASP ASP ASP ASP ASP ASP TLE TLE TLE TLE TRR THR ASP GLU GLU GLU GLU MET MET GLU GLU ASP THR VAL THR VAL THR SER • Molecule 47: Splicing factor 3A subunit 1, Splicing factor 3A subunit 1, Splicing factor 3A subunit 1 23% Chain A1: 24% 74% ALALA ARGE CALLON CONTRACTOR OF A CALL ALALA ALALAN (266 (267 (271) (271) (271) (271) (271) (271) (271) (271) (271) (271) (271) (271) (271) (271) (271) (271) (272) (2 THR CLUM CONTRACTOR CONTRACTOR CLUM CO PROPERTIGATION OF THE STATE OF • Molecule 48: U6 snRNA-associated Sm-like protein LSm5 84% Chain 65: 7% 77% 16%



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# 







F1081	G1082	Y1083	11084 A1085	K1086	A1087	I1088	G1089 P1090	H1091	D1092	V1093	L1094	A1095	T1096	L1097	L1090	N1100	L1101	K1102	V1103	41104 F1105	R1106	Q1107	N1108	R1109	V1110	C1111 T1113	T1113	V1114	A1115	11116	A1117 T1118	V1119	A1120	E1121 T1122	C1123	S1124	P1125	F1125 T1127	V1128	L1129	P1130	A1131	L1132 M1133	N1134	E1135	Y1136	R1137	V1138 D1139	E1140
L1141	N1142	V1143	U1144 N1145	G1146	V1147	L1148	K1149 S1150	L1151	S1152	F1153	L1154	F1155	E1156	Y115/ T1158	G1159 G1159	E1160	M1161	G1162	K1163	V1165	I1166	Y1167	A1168	V1169	T1170	P1171 11173	L1173	E1174	D1175	A1176	L1177 M1178	D1179	R1180	D1181 11182	V1183	H1184	R1185	41180 T1187	A1188	S1189	A1190	V1191	V1192 01193	H1194	M1195	S1196	L1197	G1198 V1199	Y1200
G1201	F1202	G1203	C1204 E1205	D1206	S1207	L1208	H1210	L1211	L1212	N1213	Y1214	V1215	W1216	71214 81010	V1219	F1220	E1221	T1222	S1223	P1224 H1 225	V1226	11227	Q1228	A1229	V1230	M1231 61232	41232 A1233	L1234	E1235	G1236	L1237 B1238	V1239	A1240	11241	P1243	C1244	R1245	M1246	q1248	Y1249	C1 250	L1251	41252 61253	L1254	F1255	H1256	P1257	A1258 B1259	K1260
V1261	R1262	D1263	V1264 Y1265	W1266	K1267	I1268	Y1269 N1270	S1271	11272	Y1273	11274 21275	G1275	S1276	ц1277 D1 278	A1279	L1280	11281	A1282	H1283 ¥1564	11284 P1285	R1286	11287	Y1288	N1289	D1290	D1291 V1202	N1293	T1294	Y1295	I1296	R1297 Y1298	E1299	L1300	D1301 V1302	11303 11303	L1304													



# 4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	86146	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE	Depositor
	CORRECTION	
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{\AA}^2)$	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT $(4k \ge 4k)$	Depositor
Maximum map value	0.097	Depositor
Minimum map value	-0.048	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	429.24, 429.24, 429.24	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.022, 1.022, 1.022	Depositor



# 5 Model quality (i)

### 5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: IHP, GTP, M7M, ZN, MG  $\,$ 

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

Mal	Chain	Bo	ond lengths	Bond angles			
	Unam	RMSZ	# Z  > 5	RMSZ	# Z  > 5		
1	1	0.75	8/3891~(0.2%)	0.87	9/6061~(0.1%)		
2	6	0.72	5/1264~(0.4%)	1.19	8/1961~(0.4%)		
3	50	0.31	0/2448	0.58	0/3316		
4	B4	0.72	0/632	1.02	2/855~(0.2%)		
5	13	0.53	0/645	1.19	6/870~(0.7%)		
5	23	0.48	0/660	0.61	0/889		
5	43	0.34	0/660	0.67	1/889~(0.1%)		
5	53	0.44	0/665	0.56	0/896		
6	$4\mathrm{B}$	0.48	0/2921	0.65	0/3966		
7	1e	0.62	0/646	1.27	5/867~(0.6%)		
7	2e	0.48	0/677	0.60	0/908		
7	4e	0.37	0/639	0.78	1/857~(0.1%)		
7	5e	0.37	0/646	0.70	0/867		
8	Ι	0.86	0/590	1.30	8/916~(0.9%)		
9	1K	1.13	2/1695~(0.1%)	1.19	15/2288~(0.7%)		
10	$4\mathrm{C}$	0.34	0/2406	0.56	0/3232		
11	11	0.68	0/649	1.24	7/878~(0.8%)		
11	21	0.40	0/642	0.56	0/867		
11	41	0.40	0/649	0.73	1/878~(0.1%)		
11	51	0.40	0/649	0.73	1/878~(0.1%)		
12	R	0.39	0/891	0.77	0/1188		
13	1f	0.66	1/588~(0.2%)	1.18	4/795~(0.5%)		
13	2f	0.49	0/574	0.59	0/775		
13	4f	0.42	0/574	0.74	1/775~(0.1%)		
13	5f	0.41	0/579	0.78	0/783		
14	66	0.83	1/575~(0.2%)	1.25	3/776~(0.4%)		
15	Х	0.42	0/398	0.59	0/524		
16	12	0.69	0/786	1.15	$\overline{3/1055}~(0.3\%)$		
16	22	0.43	0/784	0.56	0/1053		
16	42	0.43	0/747	0.66	0/1000		
16	52	0.40	0/805	0.74	$\overline{1/1081}~(0.1\%)$		
17	5	0.63	0/2444	1.47	$59\overline{/3798}~(1.6\%)$		



Mal	Chain	В	ond lengths	Bond angles			
IVIOI	Chain	RMSZ	# Z  > 5	RMSZ	# Z  > 5		
18	67	0.81	1/611~(0.2%)	1.29	3/824~(0.4%)		
19	62	0.79	0/773	1.21	4/1043~(0.4%)		
20	2B	0.38	0/759	0.50	0/1016		
21	A2	0.65	0/1254	0.93	4/1682~(0.2%)		
22	B2	0.67	3/1747~(0.2%)	0.88	7/2356~(0.3%)		
23	$5\mathrm{C}$	0.54	0/6879	0.61	3/9344~(0.0%)		
24	5X	0.52	1/4859~(0.0%)	0.61	0/6522		
25	1b	0.64	0/702	1.16	3/936~(0.3%)		
25	2b	0.45	0/674	0.55	0/899		
25	4b	0.33	0/679	0.62	0/905		
25	$5\mathrm{b}$	0.38	0/602	0.57	0/801		
26	B5	0.60	0/584	0.59	0/789		
27	1A	1.04	0/801	1.02	2/1074~(0.2%)		
28	S	0.39	0/925	0.66	0/1229		
29	5 J	0.35	0/6430	0.62	6/8681~(0.1%)		
30	4D	0.51	1/967~(0.1%)	0.56	0/1305		
31	63	0.80	0/709	1.22	3/959~(0.3%)		
32	2	0.72	3/2209~(0.1%)	1.15	14/3429~(0.4%)		
33	B3	0.48	0/9485	0.61	0/12870		
34	1g	0.58	0/575	1.17	4/768~(0.5%)		
34	2g	0.48	0/575	0.62	0/768		
34	4g	0.41	0/584	0.71	1/779~(0.1%)		
34	$5\mathrm{g}$	0.41	0/584	0.72	1/779~(0.1%)		
35	68	0.80	0/728	1.30	7/987~(0.7%)		
36	5A	0.48	1/18874~(0.0%)	0.59	10/25606~(0.0%)		
37	A3	0.70	0/3294	1.07	12/4423~(0.3%)		
38	U	0.54	0/3846	0.63	2/5208~(0.0%)		
39	$5\mathrm{D}$	0.39	0/1198	0.58	1/1620~(0.1%)		
40	64	0.82	0/609	1.25	2/824~(0.2%)		
41	BP	0.65	0/779	0.56	0/1047		
42	1C	0.56	0/437	1.16	4/587~(0.7%)		
43	Κ	0.37	0/2673	0.54	0/3593		
44	4A	0.42	0/1983	0.59	2/2657~(0.1%)		
45	4	0.59	2/2967~(0.1%)	1.00	7/4610~(0.2%)		
46	2A	0.32	0/1299	0.62	0/1761		
47	A1	0.71	0/1234	1.03	4/1657~(0.2%)		
48	65	0.83	0/593	1.25	3/800~(0.4%)		
49	5B	0.44	0/16393	0.59	3/22174~(0.0%)		
50	B1	0.53	0/6878	0.65	3/9315~(0.0%)		
All	All	0.54	29/141171~(0.0%)	0.77	250/193369~(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



Mol	Chain	#Chirality outliers	#Planarity outliers
6	4B	0	3
7	$4\mathrm{e}$	0	1
9	1K	0	1
10	4C	0	2
13	4f	0	1
13	5f	0	1
14	66	0	1
16	12	0	1
16	52	0	3
18	67	0	1
19	62	0	1
21	A2	0	4
23	$5\mathrm{C}$	0	2
25	4b	0	1
29	5J	0	2
31	63	0	2
33	B3	0	1
35	68	0	3
36	5A	0	2
37	A3	0	6
38	U	0	3
40	64	0	1
44	4A	0	2
45	4	0	1
47	A1	0	4
49	5B	0	2
50	B1	0	4
All	All	0	56

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.

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	78	U	O3'-P	-19.56	1.37	1.61
1	1	2	U	O3'-P	-18.25	1.39	1.61
45	4	87	С	O3'-P	11.52	1.75	1.61
1	1	35	А	O3'-P	-7.25	1.52	1.61
22	B2	629	PRO	N-CD	-7.23	1.37	1.47
24	5X	543	CYS	CB-SG	-6.93	1.70	1.82
22	B2	629	PRO	CA-C	-6.80	1.39	1.52
2	6	87	С	C1'-N1	6.66	1.58	1.48
2	6	95	G	C1'-N9	-6.46	1.37	1.46



Mol	Chain	Res	Type	Atoms	Ζ	Observed(Å)	Ideal(Å)
32	2	11	G	C1'-N9	-6.46	1.37	1.46
30	4D	93	CYS	CB-SG	-6.33	1.71	1.82
2	6	93	G	C1'-N9	-6.29	1.38	1.46
18	67	61	GLN	C-O	-6.24	1.11	1.23
32	2	12	G	C1'-N9	-6.13	1.38	1.46
2	6	86	U	C1'-N1	5.96	1.57	1.48
1	1	25	С	O3'-P	-5.91	1.54	1.61
1	1	23	А	O3'-P	-5.83	1.54	1.61
1	1	33	С	O3'-P	-5.82	1.54	1.61
9	1K	124	GLU	CD-OE1	5.61	1.31	1.25
2	6	89	U	C1'-N1	5.60	1.57	1.48
45	4	91	А	O3'-P	-5.42	1.54	1.61
32	2	5	С	C1'-N1	5.41	1.56	1.48
9	1K	116	GLU	CD-OE1	-5.34	1.19	1.25
22	B2	629	PRO	C-N	-5.23	1.24	1.34
36	5A	492	VAL	CB-CG1	-5.11	1.42	1.52
1	1	20	G	O3'-P	-5.09	1.55	1.61
14	66	70	VAL	C-O	-5.09	1.13	1.23
13	1f	4	PRO	N-CD	5.07	1.54	1.47
1	1	22	U	03'-P	-5.05	1.55	1.61

All (250) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
29	5 J	92	GLY	C-N-CD	-13.53	90.84	120.60
17	5	57	G	O4'-C1'-N9	12.51	118.20	108.20
1	1	78	U	P-O3'-C3'	12.36	134.54	119.70
42	1C	28	ARG	NE-CZ-NH1	12.33	126.47	120.30
17	5	58	U	O5'-P-OP2	-10.23	96.50	105.70
5	13	73	LEU	CB-CG-CD2	10.20	128.34	111.00
17	5	23	С	C2-N1-C1'	10.20	130.01	118.80
17	5	22	U	N1-C2-O2	10.18	129.93	122.80
29	5 J	674	THR	N-CA-C	-10.17	83.54	111.00
13	1f	73	ARG	NE-CZ-NH1	-10.09	115.26	120.30
17	5	22	U	C2-N1-C1'	9.91	129.60	117.70
17	5	115	С	C2-N1-C1'	9.69	129.46	118.80
17	5	22	U	N3-C2-O2	-9.49	115.56	122.20
17	5	58	U	C5-C6-N1	9.46	127.43	122.70
7	1e	59	ASP	CB-CG-OD2	9.31	126.68	118.30
40	64	65	THR	CA-CB-CG2	-9.22	99.49	112.40
17	5	71	С	N1-C2-O2	9.02	124.31	118.90
47	A1	193	TYR	CB-CG-CD1	8.71	126.23	121.00



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Mol	Chain	$\mathbf{Res}$	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
17	5	23	С	N1-C2-O2	8.59	124.06	118.90
13	1f	73	ARG	NE-CZ-NH2	8.57	124.58	120.30
17	5	90	U	N1-C2-O2	8.56	128.79	122.80
21	A2	115	PRO	CA-N-CD	-8.51	99.59	111.50
18	67	69	ARG	NE-CZ-NH1	8.46	124.53	120.30
31	63	37	ARG	NE-CZ-NH1	8.30	124.45	120.30
7	1e	71	ARG	NE-CZ-NH2	-8.24	116.18	120.30
19	62	68	ARG	NE-CZ-NH1	8.21	124.41	120.30
9	1K	121	ARG	NE-CZ-NH1	8.18	124.39	120.30
47	A1	246	ARG	NE-CZ-NH1	8.17	124.38	120.30
36	5A	1551	PHE	N-CA-C	-8.10	89.14	111.00
50	B1	557	ASP	CB-CG-OD1	8.09	125.58	118.30
17	5	58	U	C2-N1-C1'	8.09	127.40	117.70
45	4	87	С	O3'-P-O5'	8.07	119.33	104.00
35	68	8	TYR	CB-CG-CD1	8.04	125.82	121.00
47	A1	193	TYR	CB-CG-CD2	-8.04	116.18	121.00
18	67	55	MET	CG-SD-CE	-8.04	87.34	100.20
17	5	71	С	C2-N1-C1'	8.01	127.61	118.80
25	1b	18	ARG	NE-CZ-NH2	-8.01	116.30	120.30
5	13	51	ARG	NE-CZ-NH2	7.96	124.28	120.30
11	11	56	GLU	OE1-CD-OE2	-7.94	113.77	123.30
5	13	69	ARG	NE-CZ-NH1	7.82	124.21	120.30
17	5	71	С	N3-C2-O2	-7.75	116.48	121.90
17	5	90	U	N3-C2-O2	-7.73	116.79	122.20
9	1K	191	ARG	NE-CZ-NH2	-7.72	116.44	120.30
17	5	58	U	N1-C2-O2	7.69	128.18	122.80
17	5	110	С	C5-C6-N1	7.67	124.83	121.00
25	1b	14	ASP	CB-CG-OD2	-7.66	111.41	118.30
17	5	23	С	N3-C2-O2	-7.66	116.54	121.90
1	1	67	U	O5'-P-OP2	-7.63	98.83	105.70
29	5J	739	CYS	C-N-CD	-7.55	104.00	120.60
17	5	90	U	C2-N1-C1'	7.52	126.72	117.70
37	A3	284	ARG	NE-CZ-NH2	7.51	124.05	120.30
17	5	110	С	C6-N1-C2	-7.50	117.30	120.30
37	A3	351	ARG	NE-CZ-NH2	7.49	124.05	120.30
37	A3	10	ARG	NE-CZ-NH2	7.45	124.02	120.30
17	5	58	U	N3-C2-O2	-7.43	117.00	122.20
8	Ι	101	С	C6-N1-C2	-7.42	117.33	120.30
48	65	49	MET	CG-SD-CE	-7.42	88.33	100.20
7	1e	86	LEU	CA-CB-CG	7.39	132.29	115.30
17	5	58	U	C6-N1-C2	-7.37	116.58	121.00
17	5	71	C	C6-N1-C2	-7.33	117.37	120.30



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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	1	128	U	O5'-P-OP1	-7.32	99.11	105.70
5	13	51	ARG	NE-CZ-NH1	-7.30	116.65	120.30
2	6	31	U	N1-C2-O2	7.28	127.89	122.80
45	4	87	С	P-O3'-C3'	-7.28	110.97	119.70
37	A3	184	ARG	NE-CZ-NH2	7.13	123.87	120.30
39	5D	15	ASP	CB-CG-OD1	7.11	124.70	118.30
9	1K	144	ARG	NE-CZ-NH1	7.04	123.82	120.30
17	5	115	С	N1-C2-O2	6.98	123.09	118.90
17	5	23	С	C6-N1-C1'	-6.97	112.44	120.80
32	2	103	U	OP2-P-O3'	6.93	120.45	105.20
11	11	66	ARG	NE-CZ-NH2	6.93	123.76	120.30
17	5	23	С	C6-N1-C2	-6.91	117.54	120.30
32	2	46	U	P-O3'-C3'	6.91	127.99	119.70
19	62	69	TYR	CB-CG-CD2	-6.89	116.86	121.00
11	11	45	MET	CG-SD-CE	-6.89	89.17	100.20
1	1	37	G	O5'-P-OP2	-6.88	99.51	105.70
17	5	115	С	C6-N1-C1'	-6.88	112.55	120.80
17	5	22	U	C6-N1-C1'	-6.87	111.58	121.20
37	A3	42	ARG	NE-CZ-NH2	6.87	123.73	120.30
2	6	31	U	N3-C2-O2	-6.86	117.40	122.20
13	4f	33	LEU	CA-CB-CG	6.86	131.07	115.30
22	B2	629	PRO	N-CA-CB	6.84	111.51	103.30
42	1C	28	ARG	NE-CZ-NH2	-6.77	116.91	120.30
36	5A	1557	LEU	CA-CB-CG	6.75	130.83	115.30
34	1g	32	ARG	NE-CZ-NH2	6.74	123.67	120.30
36	5A	853	LYS	N-CA-C	-6.69	92.94	111.00
45	4	87	С	OP2-P-O3'	-6.68	90.50	105.20
17	5	115	С	C5-C6-N1	6.67	124.34	121.00
17	5	55	С	C6-N1-C2	-6.64	117.64	120.30
32	2	103	U	P-O3'-C3'	6.60	127.62	119.70
38	U	378	ASP	CB-CG-OD2	6.60	124.24	118.30
17	5	105	U	N1-C2-O2	6.59	127.42	122.80
19	62	47	ASP	CB-CA-C	6.59	123.59	110.40
2	6	47	А	P-O3'-C3'	6.58	127.60	119.70
9	1K	165	ASP	CB-CG-OD1	6.54	124.19	118.30
9	1K	191	ARG	CG-CD-NE	-6.53	98.09	111.80
4	B4	74	MET	CG-SD-CE	-6.52	89.77	100.20
17	5	4	C	C2-N1-C1'	6.50	125.95	118.80
32	2	106	G	P-O3'-C3'	6.50	127.50	119.70
35	68	8	TYR	CB-CG-CD2	-6.50	117.10	121.00
36	5A	1833	LEU	CA-CB-CG	$6.4\overline{7}$	$130.1\overline{9}$	115.30
22	B2	629	PRO	CB-CA-C	-6.47	95.83	112.00



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Mol	Chain	$\mathbf{Res}$	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
17	5	57	G	P-O3'-C3'	6.46	127.45	119.70
1	1	126	A	O5'-P-OP1	-6.44	99.90	105.70
8	Ι	101	С	C2-N1-C1'	6.42	125.86	118.80
17	5	105	U	N3-C2-O2	-6.42	117.71	122.20
36	5A	779	LEU	CB-CG-CD1	-6.41	100.11	111.00
16	12	99	MET	CG-SD-CE	-6.39	89.98	100.20
19	62	69	TYR	CB-CG-CD1	6.38	124.83	121.00
17	5	110	C	N1-C2-O2	6.36	122.72	118.90
49	5B	821	LEU	CA-CB-CG	6.35	129.90	115.30
34	1g	25	ARG	NE-CZ-NH2	-6.34	117.13	120.30
42	1C	3	LYS	CB-CG-CD	6.32	128.03	111.60
36	5A	1819	LEU	CA-CB-CG	6.28	129.75	115.30
17	5	72	U	N1-C2-O2	6.28	127.19	122.80
17	5	55	С	N1-C2-O2	6.28	122.67	118.90
35	68	63	ARG	NE-CZ-NH2	-6.27	117.16	120.30
8	Ι	101	С	C5-C6-N1	6.25	124.12	121.00
17	5	96	А	N7-C8-N9	6.20	116.90	113.80
37	A3	190	LEU	CB-CG-CD1	-6.13	100.58	111.00
17	5	55	С	N3-C2-O2	-6.11	117.62	121.90
4	B4	12	ASP	CB-CG-OD2	-6.09	112.82	118.30
13	1f	3	LEU	C-N-CD	6.08	141.16	128.40
9	1K	50	ASP	CB-CG-OD1	-6.07	112.84	118.30
1	1	35	А	O5'-P-OP2	-6.07	100.24	105.70
35	68	79	SER	N-CA-CB	6.06	119.59	110.50
36	5A	851	SER	N-CA-C	-6.06	94.64	111.00
17	5	115	С	C6-N1-C2	-6.03	117.89	120.30
17	5	72	U	N3-C2-O2	-6.02	117.98	122.20
9	1K	190	ARG	NE-CZ-NH1	6.02	123.31	120.30
2	6	105	U	C5-C4-O4	5.98	129.49	125.90
47	A1	237	ARG	NE-CZ-NH1	5.96	123.28	120.30
32	2	58	U	N3-C2-O2	-5.96	118.03	122.20
14	66	52	VAL	CA-CB-CG1	5.95	119.83	110.90
8	Ι	92	U	N3-C2-O2	-5.92	118.05	122.20
14	66	56	LEU	CB-CG-CD1	-5.92	100.93	111.00
11	11	19	LEU	CB-CG-CD2	5.92	121.06	111.00
32	2	$\overline{58}$	U	N1-C2-O2	5.91	126.94	122.80
9	1K	180	ARG	NE-CZ-NH1	5.91	123.25	120.30
11	11	33	ASP	CB-CG-OD2	-5.89	113.00	118.30
8	Ι	92	U	N1-C2-O2	5.88	126.91	122.80
17	5	71	C	C5-C6-N1	5.88	123.94	121.00
9	1K	69	ARG	NE-CZ-NH1	5.87	123.23	120.30
29	5J	739	CYS	CA-CB-SG	5.87	124.57	114.00



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
31	63	46	TYR	CB-CG-CD1	-5.86	117.49	121.00
5	43	10	LEU	CA-CB-CG	5.85	128.75	115.30
8	Ι	92	U	C2-N1-C1'	5.84	124.70	117.70
45	4	8	С	C6-N1-C2	-5.83	117.97	120.30
7	4e	25	LEU	CA-CB-CG	5.79	128.61	115.30
36	5A	638	LEU	CB-CG-CD1	-5.78	101.17	111.00
34	1g	25	ARG	NE-CZ-NH1	5.78	123.19	120.30
34	$5\mathrm{g}$	19	LEU	CB-CG-CD2	-5.75	101.23	111.00
37	A3	199	ARG	NE-CZ-NH2	5.73	123.17	120.30
17	5	105	U	C2-N1-C1'	5.72	124.57	117.70
22	B2	644	SER	N-CA-CB	-5.72	101.91	110.50
34	4g	19	LEU	CB-CG-CD2	-5.72	101.27	111.00
37	A3	58	ARG	NE-CZ-NH1	5.72	123.16	120.30
23	5C	298	LEU	CA-CB-CG	5.71	128.43	115.30
11	11	66	ARG	CG-CD-NE	5.71	123.78	111.80
27	1A	47	ARG	NE-CZ-NH1	5.69	123.14	120.30
36	5A	1550	GLY	N-CA-C	5.68	127.29	113.10
37	A3	9	ARG	NE-CZ-NH1	5.67	123.14	120.30
14	66	44	ALA	N-CA-CB	5.66	118.02	110.10
9	1K	69	ARG	NE-CZ-NH2	-5.66	117.47	120.30
7	1e	74	LEU	CB-CG-CD1	5.64	120.59	111.00
50	B1	811	LEU	CA-CB-CG	5.64	128.27	115.30
17	5	96	А	C4-N9-C1'	5.62	136.42	126.30
1	1	2	U	OP1-P-O3'	5.61	117.55	105.20
17	5	32	С	C6-N1-C2	-5.60	118.06	120.30
29	5J	773	ASN	C-N-CD	-5.59	108.30	120.60
22	B2	565	ASP	CB-CG-OD1	5.58	123.33	118.30
45	4	130	U	N3-C2-O2	-5.56	118.31	122.20
45	4	3	С	C6-N1-C2	-5.54	118.08	120.30
42	1C	28	ARG	CD-NE-CZ	5.53	131.34	123.60
32	2	156	U	N1-C2-O2	5.52	126.67	122.80
31	63	50	LEU	CB-CG-CD2	-5.52	101.61	111.00
49	5B	2084	LEU	CA-CB-CG	5.52	128.00	115.30
40	64	25	TYR	CB-CG-CD2	-5.50	117.70	121.00
27	1A	47	ARG	NE-CZ-NH2	-5.50	117.55	120.30
17	5	7	U	N1-C2-O2	5.47	126.63	122.80
25	1b	7	SER	CA-CB-OG	5.46	125.94	111.20
8	Ι	95	U	C5-C6-N1	5.46	125.43	122.70
38	U	145	GLY	N-CA-C	5.45	126.73	113.10
17	5	4	C	C5-C6-N1	5.45	123.72	121.00
2	6	31	U	C2-N1-C1'	5.44	124.23	117.70
17	5	18	С	C5-C6-N1	5.44	123.72	121.00



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Mol	Chain	$\operatorname{Res}$	Type	Atoms	$\mathbf{Z}$	$Observed(^{o})$	$Ideal(^{o})$
32	2	60	U	N1-C2-O2	5.42	126.59	122.80
1	1	126	А	O5'-P-OP2	5.42	117.20	110.70
1	1	65	А	O5'-P-OP2	5.41	117.19	110.70
17	5	22	U	O4'-C1'-N1	-5.39	103.89	108.20
22	B2	619	MET	CG-SD-CE	-5.38	91.59	100.20
35	68	96	HIS	CB-CA-C	-5.35	99.70	110.40
2	6	66	С	C6-N1-C2	-5.34	118.17	120.30
8	Ι	101	C	N1-C2-O2	5.33	122.10	118.90
11	11	82	ASP	CB-CG-OD1	5.33	123.10	118.30
9	1K	179	GLU	OE1-CD-OE2	-5.32	116.91	123.30
17	5	56	С	N1-C2-O2	5.31	122.09	118.90
9	1K	16	ARG	NE-CZ-NH1	5.31	122.95	120.30
9	1K	49	GLU	OE1-CD-OE2	-5.31	116.93	123.30
22	B2	633	LEU	CB-CG-CD2	5.31	120.02	111.00
17	5	9	G	C4-N9-C1'	5.30	133.39	126.50
32	2	154	С	N3-C2-O2	-5.30	118.19	121.90
5	13	3	ILE	CA-CB-CG2	5.29	121.48	110.90
17	5	110	C	N3-C2-O2	-5.29	118.20	121.90
36	5A	422	LEU	CA-CB-CG	5.29	127.46	115.30
11	51	76	LEU	CA-CB-CG	5.29	127.46	115.30
17	5	96	A	C8-N9-C4	-5.28	103.69	105.80
23	5C	440	SER	C-N-CD	-5.27	109.00	120.60
34	1g	32	ARG	NE-CZ-NH1	-5.26	117.67	120.30
48	65	70	ASP	CA-CB-CG	5.25	124.95	113.40
37	A3	347	ARG	NE-CZ-NH2	5.25	122.92	120.30
11	41	76	LEU	CA-CB-CG	5.24	127.35	115.30
32	2	156	U	N3-C2-O2	-5.23	118.54	122.20
17	5	7	U	C2-N1-C1'	5.23	123.97	117.70
22	B2	629	PRO	N-CD-CG	5.21	111.01	103.20
21	A2	124	ASP	CB-CG-OD2	5.21	122.99	118.30
17	5	38	C	N1-C2-O2	5.21	122.02	118.90
16	52	53	LEU	CA-CB-CG	5.18	127.22	115.30
23	5C	828	MET	C-N-CA	5.18	134.65	121.70
37	A3	144	ASP	CB-CG-OD1	5.17	122.95	118.30
2	6	77	C	N1-C2-O2	5.15	121.99	118.90
32	2	156		C2-N1-C1'	5.15	123.88	117.70
48	65	65	ARG	NE-CZ-NH2	5.14	122.87	120.30
16	12	102	ARG	NE-CZ-NH1	-5.13	117.73	120.30
50	Bl	974	LEU	CA-CB-CG	5.13	127.11	115.30
5	13	73	LEU	CB-CG-CD1	-5.13	102.28	111.00
	lt	73	ARG	CG-CD-NE	5.12	122.56	111.80
32	2	40	C	N1-C2-O2	5.12	121.97	118.90



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
35	68	88	ALA	C-N-CA	5.12	134.51	121.70
2	6	105	U	C6-N1-C1'	5.12	128.37	121.20
44	4A	426	PRO	C-N-CD	5.11	139.12	128.40
44	4A	551	LEU	CA-CB-CG	5.11	127.04	115.30
16	12	61	ARG	NE-CZ-NH1	-5.09	117.75	120.30
17	5	7	U	N3-C2-O2	-5.08	118.64	122.20
9	1K	72	ARG	NE-CZ-NH1	5.08	122.84	120.30
29	5J	739	CYS	C-N-CA	5.07	143.31	122.00
45	4	3	С	C5-C6-N1	5.07	123.53	121.00
37	A3	316	ARG	NE-CZ-NH2	5.07	122.83	120.30
9	1K	53	ASP	CB-CG-OD2	5.06	122.86	118.30
32	2	45	С	C5-C6-N1	5.06	123.53	121.00
21	A2	148	ARG	NE-CZ-NH2	5.04	122.82	120.30
21	A2	58	LEU	CA-CB-CG	5.04	126.89	115.30
7	1e	73	GLN	CA-CB-CG	5.04	124.48	113.40
49	5B	299	ASP	CB-CG-OD1	5.03	122.83	118.30
18	67	69	ARG	NH1-CZ-NH2	-5.03	113.87	119.40
17	5	110	С	C2-N1-C1'	5.02	124.33	118.80
17	5	23	С	C5-C6-N1	5.02	123.51	121.00
32	2	46	U	OP2-P-O3'	5.02	116.24	105.20
35	68	63	ARG	NE-CZ-NH1	5.01	122.80	120.30
17	5	4	С	C6-N1-C2	-5.00	118.30	120.30

There are no chirality outliers.

All (	(56)	planarity	outliers	are	listed	below:
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Mol	Chain	Res	Type	Group
16	12	17	GLN	Peptide
9	1K	56	PRO	Peptide
45	4	90	G	Sidechain
44	4A	421	PRO	Peptide
44	4A	538	SER	Peptide
6	4B	420	TYR	Peptide
6	$4\mathrm{B}$	459	PRO	Peptide
6	$4\mathrm{B}$	470	TYR	Peptide
10	$4\mathrm{C}$	350	GLN	Peptide
10	$4\mathrm{C}$	386	ASP	Peptide
25	4b	53	PRO	Peptide
7	4e	51	ASP	Peptide
13	4f	40	MET	Peptide
16	52	46	CYS	Peptide
16	52	60	ASP	Peptide



Mol	Chain	Res	Type	Group
16	52	88	LYS	Peptide
36	5A	1416	ILE	Peptide
36	5A	1792	LYS	Peptide
49	5B	1265	GLN	Peptide
49	5B	526	ASN	Peptide
23	5C	167	TYR	Peptide
23	5C	439	PRO	Peptide
29	5J	624	VAL	Peptide
29	5J	724	MET	Peptide
13	5f	40	MET	Peptide
19	62	69	TYR	Sidechain
31	63	30	TYR	Sidechain
31	63	46	TYR	Sidechain
40	64	25	TYR	Sidechain
14	66	51	TYR	Sidechain
18	67	62	TYR	Sidechain
35	68	60	TYR	Sidechain
35	68	8	TYR	Sidechain
35	68	89	GLU	Peptide
47	A1	191	ARG	Sidechain
47	A1	193	TYR	Sidechain
47	A1	199	ARG	Sidechain
47	A1	255	ARG	Sidechain
21	A2	138	TYR	Sidechain
21	A2	175	PRO	Peptide
21	A2	176	TYR	Sidechain
21	A2	201	ARG	Sidechain
37	A3	163	TYR	Sidechain
37	A3	281	ARG	Sidechain
37	A3	312	ARG	Sidechain
37	A3	42	ARG	Sidechain
37	A3	58	ARG	Sidechain
37	A3	61	TYR	Sidechain
50	B1	1050	VAL	Peptide
50	B1	460	PRO	Peptide
50	B1	483	ASP	Peptide
50	B1	488	SER	Peptide
33	B3	913	LEU	Peptide
38	U	244	LEU	Peptide
38	U	423	PHE	Peptide
38	U	531	GLN	Peptide

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### 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	Perce	ntiles
3	50	304/357~(85%)	283~(93%)	19 (6%)	2(1%)	22	56
4	B4	76/424~(18%)	76 (100%)	0	0	100	100
5	13	79/126~(63%)	75 (95%)	4 (5%)	0	100	100
5	23	81/126~(64%)	76 (94%)	5 (6%)	0	100	100
5	43	81/126 (64%)	76 (94%)	5 (6%)	0	100	100
5	53	82/126~(65%)	77 (94%)	5 (6%)	0	100	100
6	4B	357/522~(68%)	330 (92%)	25 (7%)	2 (1%)	25	58
7	1e	75/92~(82%)	70 (93%)	5 (7%)	0	100	100
7	2e	79/92~(86%)	77 (98%)	2 (2%)	0	100	100
7	4e	74/92~(80%)	71 (96%)	3 (4%)	0	100	100
7	5e	75/92~(82%)	72 (96%)	3 (4%)	0	100	100
9	1K	199/437~(46%)	184 (92%)	12 (6%)	3(2%)	10	39
10	4C	293/499~(59%)	275 (94%)	18 (6%)	0	100	100
11	11	79/119~(66%)	77 (98%)	2 (2%)	0	100	100
11	21	78/119~(66%)	75 (96%)	3 (4%)	0	100	100
11	41	79/119~(66%)	75~(95%)	4 (5%)	0	100	100
11	51	79/119~(66%)	75 (95%)	4 (5%)	0	100	100
12	R	104/480~(22%)	91 (88%)	13 (12%)	0	100	100
13	1f	72/86~(84%)	69 (96%)	3 (4%)	0	100	100
13	2f	70/86~(81%)	69 (99%)	1 (1%)	0	100	100
13	4f	70/86~(81%)	69 (99%)	1 (1%)	0	100	100



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
13	5f	71/86~(83%)	64~(90%)	7 (10%)	0	100	100
14	66	70/80~(88%)	69~(99%)	0	1 (1%)	11	40
15	Х	45/155~(29%)	39~(87%)	6(13%)	0	100	100
16	12	91/118~(77%)	85~(93%)	6 (7%)	0	100	100
16	22	91/118 (77%)	86 (94%)	5 (6%)	0	100	100
16	42	90/118~(76%)	84 (93%)	6 (7%)	0	100	100
16	52	94/118~(80%)	87~(93%)	7 (7%)	0	100	100
18	67	75/103~(73%)	72~(96%)	2 (3%)	1 (1%)	12	42
19	62	93/95~(98%)	84 (90%)	6 (6%)	3(3%)	4	23
20	2B	90/225~(40%)	88 (98%)	2 (2%)	0	100	100
21	A2	138/209~(66%)	123 (89%)	11 (8%)	4(3%)	4	25
22	B2	204/895~(23%)	181 (89%)	22 (11%)	1 (0%)	29	62
23	$5\mathrm{C}$	850/854~(100%)	817 (96%)	31 (4%)	2(0%)	47	77
24	5X	574/820~(70%)	561~(98%)	13 (2%)	0	100	100
25	1b	84/240~(35%)	82~(98%)	2 (2%)	0	100	100
25	2b	80/240~(33%)	74 (92%)	6 (8%)	0	100	100
25	4b	80/240~(33%)	71 (89%)	9 (11%)	0	100	100
25	5b	69/240~(29%)	67~(97%)	2 (3%)	0	100	100
26	B5	67/86~(78%)	61 (91%)	6 (9%)	0	100	100
27	1A	96/282~(34%)	94 (98%)	2 (2%)	0	100	100
28	S	110/800~(14%)	101 (92%)	8 (7%)	1 (1%)	17	50
29	5 J	793/850~(93%)	748 (94%)	44 (6%)	1 (0%)	51	82
30	4D	121/128~(94%)	119 (98%)	2 (2%)	0	100	100
31	63	83/102 (81%)	79~(95%)	3 (4%)	1 (1%)	13	44
33	B3	1176/1217~(97%)	1082 (92%)	92 (8%)	2(0%)	47	77
34	1g	71/76~(93%)	69~(97%)	2 (3%)	0	100	100
34	2g	71/76~(93%)	69~(97%)	2(3%)	0	100	100
34	4g	$72/\overline{76}\ (95\%)$	66 (92%)	6(8%)	0	100	100
34	$5\mathrm{g}$	72/76~(95%)	66~(92%)	6 (8%)	0	100	100
35	68	93/96~(97%)	81 (87%)	6 (6%)	6 (6%)	1	9
36	5A	$2\overline{198/2311}\ (95\%)$	2094 (95%)	102 (5%)	2(0%)	51	82



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	entiles
37	A3	377/501~(75%)	346~(92%)	26 (7%)	5 (1%)	12	42
38	U	454/555~(82%)	424 (93%)	27 (6%)	3 (1%)	22	56
39	5D	139/142~(98%)	131 (94%)	8 (6%)	0	100	100
40	64	71/139~(51%)	66 (93%)	3 (4%)	2 (3%)	5	26
41	BP	98/104 (94%)	92 (94%)	6 (6%)	0	100	100
42	1C	48/159~(30%)	47 (98%)	1 (2%)	0	100	100
43	К	316/1007~(31%)	294 (93%)	18 (6%)	4 (1%)	12	42
44	4A	229/683~(34%)	210 (92%)	18 (8%)	1 (0%)	34	67
46	2A	160/255~(63%)	147 (92%)	13 (8%)	0	100	100
47	A1	138/647~(21%)	129 (94%)	7 (5%)	2 (1%)	11	40
48	65	74/91~(81%)	70 (95%)	2 (3%)	2(3%)	5	26
49	5B	1989/2136~(93%)	1885 (95%)	103 (5%)	1 (0%)	51	82
50	B1	846/1304~(65%)	792 (94%)	53 (6%)	1 (0%)	51	82
All	All	15337/23178~(66%)	14438 (94%)	846 (6%)	53 (0%)	44	72

All (53) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	50	59	ILE
9	1K	59	ARG
9	1K	63	ARG
19	62	47	ASP
19	62	53	HIS
21	A2	165	ARG
28	S	566	ILE
29	5J	93	PRO
35	68	89	GLU
37	A3	78	PRO
38	U	408	GLN
43	Κ	697	VAL
47	A1	192	ASN
6	4B	460	ILE
9	1K	60	ALA
14	66	52	VAL
35	68	86	ILE
35	68	90	PRO
37	A3	227	PRO



Mol	Chain	Res	Type
37	A3	292	SER
43	K	851	VAL
48	65	87	GLU
33	B3	932	ASN
33	B3	933	ASN
35	68	79	SER
36	5A	189	GLU
37	A3	308	LYS
47	A1	218	ILE
3	50	58	PRO
19	62	55	LEU
23	5C	943	LEU
31	63	35	ASN
35	68	43	GLU
40	64	12	ASN
43	К	699	SER
21	A2	115	PRO
21	A2	208	LEU
23	5C	107	GLN
35	68	59	LEU
36	5A	60	ASP
37	A3	99	PRO
38	U	146	ARG
40	64	57	PRO
43	K	722	ASN
44	4A	539	GLN
18	67	19	ILE
49	5B	756	SER
6	4B	459	PRO
21	A2	188	ILE
50	B1	489	PRO
22	B2	521	PRO
38	U	362	PRO
48	65	47	VAL

#### 5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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	Perce	ntiles
3	5O	263/300~(88%)	263 (100%)	0	100	100
4	B4	66/336~(20%)	66 (100%)	0	100	100
5	13	71/101~(70%)	61 (86%)	10 (14%)	3	16
5	23	73/101~(72%)	73 (100%)	0	100	100
5	43	73/101~(72%)	73 (100%)	0	100	100
5	53	73/101~(72%)	73 (100%)	0	100	100
6	4B	306/442~(69%)	303~(99%)	3 (1%)	76	85
7	1e	72/84~(86%)	61 (85%)	11 (15%)	2	12
7	2e	76/84~(90%)	76 (100%)	0	100	100
7	4e	71/84~(84%)	69 (97%)	2(3%)	43	69
7	$5\mathrm{e}$	72/84~(86%)	72 (100%)	0	100	100
9	1K	170/373~(46%)	161 (95%)	9(5%)	22	53
10	4C	255/424~(60%)	251 (98%)	4 (2%)	62	79
11	11	76/101~(75%)	72 (95%)	4 (5%)	22	53
11	21	75/101 (74%)	75 (100%)	0	100	100
11	41	76/101~(75%)	55 (72%)	21 (28%)	0	1
11	51	76/101~(75%)	55 (72%)	21 (28%)	0	1
12	R	94/369~(26%)	91 (97%)	3 (3%)	39	67
13	1f	63/74~(85%)	56 (89%)	7 (11%)	6	24
13	2f	61/74~(82%)	61 (100%)	0	100	100
13	4f	61/74~(82%)	61 (100%)	0	100	100
13	5f	61/74~(82%)	60 (98%)	1 (2%)	62	79
14	66	62/70~(89%)	62 (100%)	0	100	100
15	Х	42/144~(29%)	42 (100%)	0	100	100
16	12	91/110 (83%)	83 (91%)	8 (9%)	10	33
16	22	91/110 (83%)	91 (100%)	0	100	100
16	42	86/110 (78%)	86 (100%)	0	100	100
16	52	93/110 (84%)	92 (99%)	1 (1%)	73	85
18	67	69/91~(76%)	68~(99%)	1 (1%)	67	82
19	62	88/88 (100%)	86 (98%)	2 (2%)	50	73
20	2B	81/195 (42%)	81 (100%)	0	100	100
21	A2	129/180~(72%)	128 (99%)	1 (1%)	81	89



Continued	fanona		
Continuea	ITOTL	DIEDIOUS	Dage
0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0		p. 0000 a0	p @ 9 0

Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles
22	B2	187/776~(24%)	185~(99%)	2(1%)	73	85
23	$5\mathrm{C}$	754/756~(100%)	751 (100%)	3~(0%)	91	95
24	5X	517/721~(72%)	501~(97%)	16 (3%)	40	67
25	1b	78/177~(44%)	70~(90%)	8 (10%)	7	26
25	2b	75/177~(42%)	75~(100%)	0	100	100
25	4b	75/177~(42%)	75~(100%)	0	100	100
25	$5\mathrm{b}$	67/177~(38%)	66~(98%)	1 (2%)	65	81
26	B5	60/77~(78%)	60 (100%)	0	100	100
27	1A	85/240~(35%)	82~(96%)	3(4%)	36	64
28	S	91/681~(13%)	91 (100%)	0	100	100
29	5J	636/715~(89%)	631 (99%)	5 (1%)	81	89
30	4D	107/111~(96%)	107 (100%)	0	100	100
31	63	79/94~(84%)	76~(96%)	3 (4%)	33	62
33	B3	1027/1051~(98%)	1021 (99%)	6 (1%)	86	91
34	1g	63/66~(96%)	57~(90%)	6 (10%)	8	29
34	2g	63/66~(96%)	62~(98%)	1 (2%)	62	79
34	4g	64/66~(97%)	46 (72%)	18 (28%)	0	1
34	$5\mathrm{g}$	64/66~(97%)	46 (72%)	18 (28%)	0	1
35	68	81/82~(99%)	77~(95%)	4(5%)	25	56
36	5A	2002/2090~(96%)	1990~(99%)	12~(1%)	86	91
37	A3	345/446~(77%)	339~(98%)	6(2%)	60	78
38	U	418/503~(83%)	414 (99%)	4 (1%)	76	85
39	$5\mathrm{D}$	129/130~(99%)	129 (100%)	0	100	100
40	64	68/111~(61%)	68~(100%)	0	100	100
41	BP	86/90~(96%)	85~(99%)	1 (1%)	71	83
42	$1\mathrm{C}$	48/135~(36%)	42 (88%)	6(12%)	4	19
43	K	$291/919$ ( $\overline{32\%}$ )	259~(89%)	32 (11%)	6	24
44	4A	210/599 (35%)	208 (99%)	2(1%)	76	85
46	2A	139/218~(64%)	138~(99%)	1 (1%)	84	90
47	A1	130/550 (24%)	127 (98%)	3~(2%)	50	73
48	65	68/80~(85%)	67~(98%)	1 (2%)	65	81



Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntile	s
49	5B	1779/1908~(93%)	1766~(99%)	13 (1%)	84	90	
50	B1	733/1104~(66%)	729 (100%)	4 (0%)	88	93	
All	All	13735/20051~(68%)	13447 (98%)	288 (2%)	56	75	

All (288) residues with a non-rotameric sidechain are listed below:

Mol	Chain	$\mathbf{Res}$	Type
5	13	3	ILE
5	13	20	CYS
5	13	24	THR
5	13	34	GLU
5	13	46	ILE
5	13	51	ARG
5	13	73	LEU
5	13	78	LYS
5	13	82	MET
5	13	83	LEU
6	4B	395	ARG
6	4B	407	LEU
6	4B	444	THR
9	1K	3	GLN
9	1K	28	LEU
9	1K	48	PHE
9	1K	50	ASP
9	1K	140	SER
9	1K	167	LYS
9	1K	168	LYS
9	1K	172	ARG
9	1K	188	ARG
10	4C	299	CYS
10	4C	315	LYS
10	4C	351	ARG
10	4C	363	LYS
11	41	2	LYS
11	41	4	VAL
11	41	8	MET
11	41	10	LEU
11	41	11	SER
11	41	16	THR
11	41	28	THR
11	41	33	ASP



Mol	Chain	Res	Type
11	41	35	SER
11	41	44	LYS
11	41	47	LEU
11	41	48	LYS
11	41	51	GLU
11	41	53	VAL
11	41	54	GLN
11	41	55	LEU
11	41	56	GLU
11	41	57	THR
11	41	74	LEU
11	41	76	LEU
11	41	81	VAL
12	R	377	ASP
12	R	379	ASP
12	R	431	ASP
13	1f	3	LEU
13	1f	8	LYS
13	1f	14	LEU
13	1f	23	LEU
13	1f	27	MET
13	1f	51	ILE
13	1f	65	ARG
7	4e	28	ARG
7	4e	30	ARG
18	67	17	LYS
19	62	44	SER
19	62	72	LEU
21	A2	189	ASP
22	B2	600	ARG
22	B2	604	LYS
23	5C	507	VAL
23	5C	735	PHE
23	5C	919	ARG
24	5X	270	ARG
24	5X	389	PRO
24	5X	395	ASP
24	5X	472	ILE
24	5X	491	PHE
24	5X	516	ARG
24	5X	532	VAL
24	5X	664	ASP



Mol	Chain	Res	Type
24	5X	674	LYS
24	5X	675	LYS
24	5X	679	VAL
24	5X	685	GLU
24	5X	703	ARG
24	5X	729	ASP
24	5X	730	ILE
24	5X	746	GLU
11	11	4	VAL
11	11	11	SER
11	11	19	LEU
11	11	82	ASP
25	1b	7	SER
25	1b	12	HIS
25	1b	54	LYS
25	1b	56	SER
25	1b	57	LYS
25	1b	58	GLN
25	1b	67	LEU
25	1b	71	LEU
27	1A	8	PRO
27	1A	61	GLU
27	1A	103	GLU
13	5f	11	LEU
29	5J	91	SER
29	5J	405	ARG
29	5J	570	PHE
29	5J	674	THR
29	5J	743	THR
11	51	2	LYS
11	51	4	VAL
11	51	8	MET
11	51	10	LEU
11	51	11	SER
11	51	16	THR
11	51	28	THR
11	51	33	ASP
11	51	35	SER
11	51	44	LYS
11	51	47	LEU
11	51	48	LYS
11	51	51	GLU



Mol	Chain	Res	Type
11	51	53	VAL
11	51	54	GLN
11	51	55	LEU
11	51	56	GLU
11	51	57	THR
11	51	74	LEU
11	51	76	LEU
11	51	81	VAL
31	63	34	ARG
31	63	39	LEU
31	63	94	LEU
33	B3	175	VAL
33	B3	248	VAL
33	B3	278	LEU
33	B3	532	ARG
33	B3	703	ARG
33	B3	1064	ASP
34	1g	27	VAL
34	1g	50	THR
34	1g	51	SER
34	1g	57	ILE
34	1g	59	MET
34	1g	69	MET
25	5b	16	ARG
35	68	13	VAL
35	68	19	ASP
35	68	90	PRO
35	68	91	LEU
7	1e	14	MET
7	1e	25	LEU
7	1e	27	ASN
7	1e	60	ASP
7	1e	62	GLU
7	1e	63	GLU
7	1e	68	THR
7	1e	70	SER
7	1e	80	LYS
7	1e	82	ASP
7	1e	86	LEU
36	5A	86	ARG
36	$5\overline{A}$	165	ARG
36	5A	284	ARG



Mol	Chain	Res	Type
36	5A	342	THR
36	5A	563	GLN
36	5A	579	GLN
36	5A	741	ARG
36	5A	1126	VAL
36	5A	1298	ARG
36	5A	1925	LYS
36	5A	1958	LYS
36	5A	2249	LYS
37	A3	78	PRO
37	A3	81	PHE
37	A3	111	GLU
37	A3	122	GLU
37	A3	195	ASP
37	A3	402	LEU
38	U	100	ARG
38	U	101	ARG
38	U	235	ASP
38	U	289	ARG
34	2g	43	ASP
16	52	33	THR
16	12	20	GLU
16	12	37	LYS
16	12	42	VAL
16	12	51	LYS
16	12	61	ARG
16	12	75	THR
16	12	94	ARG
16	12	114	LEU
41	BP	30	CYS
42	1C	3	LYS
42	1C	26	SER
42	1C	29	LYS
42	1C	39	GLN
42	1C	45	GLN
42	1C	48	SER
34	$5\mathrm{g}$	3	LYS
34	5g	10	LYS
34	5g	11	LYS
34	5g	15	LYS
34	5g	27	VAL
34	$5\mathrm{g}$	35	ASP



Mol	Chain	Res	Type
34	$5\mathrm{g}$	43	ASP
34	$5\mathrm{g}$	44	GLU
34	5g	46	VAL
34	5g	47	GLU
34	5g	50	THR
34	$5\mathrm{g}$	51	SER
34	$5\mathrm{g}$	59	MET
34	5g	62	ILE
34	5g	66	SER
34	5g	70	LEU
34	5g	71	GLU
34	5g	73	LEU
43	K	676	ARG
43	K	688	ASN
43	K	697	VAL
43	K	698	PHE
43	K	700	ASN
43	K	721	ASN
43	K	724	LEU
43	K	726	GLN
43	K	731	LYS
43	K	733	LEU
43	K	763	LEU
43	K	777	VAL
43	K	778	LEU
43	K	793	ARG
43	K	805	LEU
43	K	812	LEU
43	Κ	825	GLU
43	K	830	LEU
43	K	831	LYS
43	K	843	ASP
43	K	850	LEU
43	K	878	THR
43	K	882	LEU
43	K	886	LYS
43	K	892	LYS
43	K	920	ASP
43	K	946	MET
43	K	950	ASN
43	K	955	LEU
43	K	956	LEU



Mol	Chain	Res	Type
43	K	1004	GLN
43	K	1005	GLU
44	4A	597	LEU
44	4A	646	MET
34	4g	3	LYS
34	4g	10	LYS
34	4g	11	LYS
34	4g	15	LYS
34	4g	27	VAL
34	4g	35	ASP
34	4g	43	ASP
34	4g	44	GLU
34	4g	46	VAL
34	4g	47	GLU
34	4g	50	THR
34	4g	51	SER
34	4g	59	MET
34	4g	62	ILE
34	4g	66	SER
34	4g	70	LEU
34	4g	71	GLU
34	4g	73	LEU
46	2A	120	ILE
47	A1	163	ASP
47	A1	223	LYS
47	A1	237	ARG
48	65	16	GLU
49	5B	287	ASP
49	5B	300	ARG
49	5B	406	ARG
49	5B	681	ARG
49	5B	753	ARG
49	5B	992	TYR
49	5B	998	VAL
49	5B	1030	ARG
49	5B	1152	ARG
49	5B	1228	VAL
49	5B	1518	VAL
49	5B	1521	VAL
49	5B	1843	ARG
50	B1	614	ARG
50	B1	632	PHE



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Mol	Chain	$\mathbf{Res}$	Type
50	B1	695	VAL
50	B1	970	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (168) such sidechains are listed below:

Mol	Chain	Res	Type
3	50	101	ASN
3	50	165	GLN
3	50	225	ASN
6	4B	282	HIS
6	4B	414	ASN
7	5e	32	GLN
7	5e	38	GLN
7	5e	88	GLN
9	1K	36	GLN
9	1K	133	HIS
9	1K	158	HIS
10	4C	389	GLN
11	41	24	GLN
12	R	393	ASN
12	R	471	GLN
14	66	69	ASN
19	62	53	HIS
19	62	71	GLN
20	2B	15	ASN
5	53	42	GLN
21	A2	79	GLN
21	A2	149	HIS
22	B2	496	ASN
13	2f	68	ASN
23	5C	137	HIS
23	5C	154	HIS
23	5C	571	ASN
23	5C	583	ASN
23	5C	702	ASN
23	$5\mathrm{C}$	719	GLN
23	$5\mathrm{C}$	743	ASN
23	$5\mathrm{C}$	771	GLN
23	5C	903	HIS
23	5C	905	GLN
24	5X	297	GLN
24	5X	359	GLN



Mol	Chain	Res	Type
24	5X	420	GLN
24	5X	428	ASN
24	5X	535	ASN
24	5X	597	HIS
24	5X	731	GLN
16	42	49	ASN
16	42	69	ASN
16	42	112	ASN
26	B5	34	ASN
26	B5	51	ASN
26	B5	58	ASN
28	S	728	GLN
13	5f	6	ASN
13	5f	68	ASN
29	5J	140	GLN
29	5J	308	HIS
29	5J	353	GLN
29	5J	587	HIS
29	5J	733	ASN
29	5J	741	HIS
29	5J	839	HIS
29	5J	865	HIS
11	51	63	ASN
11	51	64	ASN
30	4D	111	GLN
25	2b	76	ASN
33	B3	138	GLN
33	B3	260	ASN
33	B3	264	GLN
33	B3	760	ASN
33	B3	796	ASN
33	B3	885	ASN
33	B3	988	ASN
33	B3	1172	ASN
5	23	40	ASN
5	23	45	ASN
25	5b	22	GLN
36	5A	221	ASN
36	5A	325	HIS
36	5A	434	HIS
36	$5\overline{\mathrm{A}}$	448	GLN
36	5A	579	GLN



Mol	Chain	Res	Type
36	5A	654	ASN
36	5A	711	GLN
36	5A	775	ASN
36	5A	875	HIS
36	5A	1003	HIS
36	5A	1014	ASN
36	5A	1159	ASN
36	5A	1172	ASN
36	5A	1332	HIS
36	5A	1345	GLN
36	5A	1487	HIS
36	5A	1543	ASN
36	5A	1737	ASN
36	5A	1752	GLN
36	5A	1830	GLN
36	5A	1875	HIS
36	5A	2166	HIS
36	5A	2203	ASN
36	5A	2260	GLN
36	5A	2276	GLN
36	5A	2306	HIS
37	A3	143	HIS
38	U	144	GLN
38	U	158	GLN
38	U	205	ASN
38	U	234	ASN
38	U	242	GLN
38	U	298	HIS
38	U	413	GLN
38	U	531	GLN
38	U	541	GLN
34	2g	26	HIS
39	5D	7	HIS
39	5D	32	HIS
16	52	41	GLN
7	2e	19	ASN
7	2e	88	GLN
34	5g	26	HIS
34	5g	55	ASN
43	K	695	GLN
43	K	707	ASN
43	K	722	ASN



Mol	Chain	Res	Type
43	K	740	ASN
43	K	840	HIS
43	K	895	ASN
43	K	896	HIS
43	K	921	GLN
43	K	926	ASN
43	K	928	ASN
43	K	950	ASN
43	K	995	ASN
44	4A	425	ASN
44	4A	524	GLN
11	21	64	ASN
34	4g	26	HIS
34	4g	55	ASN
46	2Ă	72	ASN
49	5B	259	HIS
49	5B	304	ASN
49	5B	313	ASN
49	5B	485	GLN
49	5B	498	ASN
49	5B	524	HIS
49	5B	638	ASN
49	5B	702	GLN
49	5B	785	HIS
49	5B	884	ASN
49	5B	885	GLN
49	5B	968	ASN
49	5B	999	GLN
49	5B	1003	GLN
49	5B	1086	GLN
49	5B	1209	GLN
49	5B	1247	GLN
49	5B	1265	GLN
49	5B	1423	ASN
49	5B	1441	GLN
49	5B	1659	HIS
49	5B	1674	HIS
49	5B	1769	ASN
49	5B	1885	ASN
49	5B	1994	ASN
50	B1	457	ASN
50	B1	533	ASN



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Mol	Chain	Res	Type
50	B1	698	GLN
50	B1	832	GLN
50	B1	1002	ASN
50	B1	1107	GLN
50	B1	1252	GLN
50	B1	1256	HIS

### 5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	163/164~(99%)	49 (30%)	6(3%)
17	5	101/117~(86%)	42 (41%)	4(3%)
2	6	50/106~(47%)	5 (10%)	2(4%)
32	2	90/188~(47%)	23~(25%)	4 (4%)
45	4	120/146~(82%)	25 (20%)	3~(2%)
8	Ι	23/62~(37%)	5 (21%)	0
All	All	547/783~(69%)	149(27%)	19(3%)

All (149) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	10	U
1	1	12	G
1	1	15	G
1	1	16	G
1	1	17	G
1	1	20	G
1	1	21	А
1	1	22	U
1	1	23	А
1	1	28	G
1	1	29	А
1	1	35	А
1	1	41	G
1	1	47	С
1	1	48	С
1	1	50	G
1	1	51	G
1	1	55	А
1	1	62	U
1	1	72	U


Mol	Chain	Res	Type
1	1	73	С
1	1	75	G
1	1	88	С
1	1	90	U
1	1	91	G
1	1	92	С
1	1	93	G
1	1	94	А
1	1	103	А
1	1	105	U
1	1	108	G
1	1	112	А
1	1	114	С
1	1	115	U
1	1	117	G
1	1	118	А
1	1	119	С
1	1	123	А
1	1	124	U
1	1	126	А
1	1	128	U
1	1	130	G
1	1	132	G
1	1	133	G
1	1	135	А
1	1	136	G
1	1	137	U
1	1	138	G
1	1	158	U
2	6	48	А
2	6	49	G
2	6	74	U
2	6	77	С
2	6	106	U
8	Ι	0	G
8	Ι	5	G
8	Ι	92	U
8	Ι	100	A
8	Ι	101	С
17	5	4	С
17	5	5	U
17	5	6	С



Mol	Chain	Res	Type
17	5	7	U
17	5	9	G
17	5	20	G
17	5	21	А
17	5	22	U
17	5	23	С
17	5	24	G
17	5	25	С
17	5	26	А
17	5	28	А
17	5	36	С
17	5	37	G
17	5	38	С
17	5	47	A
17	5	48	А
17	5	57	G
17	5	58	U
17	5	59	G
17	5	63	А
17	5	66	А
17	5	67	А
17	5	71	С
17	5	75	G
17	5	78	U
17	5	86	С
17	5	88	А
17	5	89	U
17	5	90	U
17	5	94	U
17	5	95	G
17	5	97	G
17	5	98	G
17	5	102	U
17	5	104	С
17	5	105	U
17	5	106	U
17	5	107	U
17	5	108	G
17	5	109	G
32	2	37	U
32	2	38	A
32	2	40	С



Mol	Chain	Res	Type
32	2	43	U
32	2	45	С
32	2	46	U
32	2	47	U
32	2	48	А
32	2	49	U
32	2	63	G
32	2	65	U
32	2	98	G
32	2	100	U
32	2	101	U
32	2	102	U
32	2	103	U
32	2	104	U
32	2	105	G
32	2	106	G
32	2	107	А
32	2	157	G
32	2	171	U
32	2	178	А
45	4	2	G
45	4	19	U
45	4	20	A
45	4	25	A
45	4	26	G
45	4	30	A
45	4	36	U
45	4	37	U
45	4	38	U
45	4	40	U
45	4	44	A
45	4	45	G
45	4	51	A
45	4	52	U
45	4	67	A
45	4	68	A
45	4	69	С
45	4	114	U
45	4	115	G
45	4	121	U
45	4	122	U
45	4	123	U



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Mol	Chain	Res	Type
45	4	125	G
45	4	126	А
45	4	140	G

All (19) KINA pucker outliers are listed belo	All (	(19)	RNA	pucker	outliers	are	listed	below
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Mol	Chain	Res	Type
1	1	15	G
1	1	90	U
1	1	92	С
1	1	123	А
1	1	126	А
1	1	128	U
2	6	47	А
2	6	104	U
17	5	57	G
17	5	58	U
17	5	96	А
17	5	105	U
32	2	37	U
32	2	46	U
32	2	103	U
32	2	106	G
45	4	1	А
45	4	68	А
45	4	114	U

### 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 9 ligands modelled in this entry, 7 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).

Mal	Turne	Chain	Dec	Timle	Bo	ond leng	ths	В	ond ang	les
WIOI	туре	Unain	nes	LIIIK	Link Counts		# Z >2	Counts	RMSZ	# Z >2
54	IHP	5A	2401	-	36,36,36	0.71	0	$54,\!60,\!60$	0.58	0
53	GTP	5C	1002	52	26,34,34	1.36	3 (11%)	32,54,54	1.61	7 (21%)

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
54	IHP	5A	2401	-	-	8/30/54/54	0/1/1/1
53	GTP	$5\mathrm{C}$	1002	52	-	4/18/38/38	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\operatorname{Ideal}(\operatorname{\AA})$
53	$5\mathrm{C}$	1002	GTP	C5-C6	-4.45	1.38	1.47
53	5C	1002	GTP	C5-C4	-2.15	1.37	1.43
53	5C	1002	GTP	O4'-C4'	-2.11	1.40	1.45

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
53	$5\mathrm{C}$	1002	GTP	PB-O3B-PG	-3.54	120.68	132.83
53	$5\mathrm{C}$	1002	GTP	C5-C6-N1	3.51	120.14	113.95
53	$5\mathrm{C}$	1002	GTP	C8-N7-C5	3.05	108.80	102.99
53	$5\mathrm{C}$	1002	GTP	C2-N1-C6	-3.00	119.58	125.10
53	$5\mathrm{C}$	1002	GTP	PA-O3A-PB	-2.50	124.26	132.83
53	$5\mathrm{C}$	1002	GTP	O6-C6-C5	-2.35	119.79	124.37
53	$5\mathrm{C}$	1002	GTP	C3'-C2'-C1'	2.22	104.32	100.98

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
54	5A	2401	IHP	C1-O11-P1-O41



Mol	Chain	Res	Type	Atoms
54	5A	2401	IHP	C3-O13-P3-O23
53	$5\mathrm{C}$	1002	GTP	O4'-C4'-C5'-O5'
53	5C	1002	GTP	PB-O3A-PA-O2A
53	$5\mathrm{C}$	1002	GTP	C3'-C4'-C5'-O5'
54	5A	2401	IHP	C5-O15-P5-O25
54	5A	2401	IHP	C6-O16-P6-O26
54	5A	2401	IHP	C4-O14-P4-O34
54	5A	2401	IHP	C5-O15-P5-O35
54	5A	2401	IHP	C5-O15-P5-O45
54	5A	2401	IHP	C6-O16-P6-O46
53	$5\mathrm{C}$	1002	GTP	C5'-O5'-PA-O1A

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There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and sufficient must be 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)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
47	A1	2
1	1	2
29	5J	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A1	282:VAL	С	422:UNK	Ν	108.26
1	5J	165:ASP	С	236:GLY	Ν	34.19
1	A1	447:UNK	С	455:VAL	Ν	4.52
1	1	2:U	O3'	3:A	Р	1.39



Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	1	78:U	O3'	79:G	Р	1.37



# 6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-4665. 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



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

### 6.2 Central slices (i)

#### 6.2.1 Primary map



X Index: 210

Y Index: 210



Z Index: 210

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: 177

Y Index: 193

Z Index: 218

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



The images above show the 3D surface view of the map at the recommended contour level 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.



# 6.5 Mask visualisation (i)

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



# 7 Map analysis (i)

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

## 7.1 Map-value distribution (i)



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



## 7.2 Volume estimate (i)



The volume at the recommended contour level is 726  $\text{nm}^3$ ; this corresponds to an approximate mass of 656 kDa.

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



## 7.3 Rotationally averaged power spectrum (i)



\*Reported resolution corresponds to spatial frequency of 0.305  ${\rm \AA^{-1}}$ 



# 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 0.305  $\mathrm{\AA^{-1}}$ 



# 8.2 Resolution estimates (i)

$\begin{bmatrix} Bosolution ostimato (Å) \end{bmatrix}$	Estimation criterion (FSC cut-off)		
Resolution estimate (A)	0.143	0.5	Half-bit
Reported by author	3.28	-	-
Author-provided FSC curve	3.24	3.88	3.29
Unmasked-calculated*	-	-	-

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.



# 9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-4665 and PDB model 6QX9. Per-residue inclusion information can be found in section 3 on page 16.

## 9.1 Map-model overlay (i)



The images above show the 3D surface view of the map at the recommended contour level 0.01 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 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 (0.01).



### 9.4 Atom inclusion (i)



At the recommended contour level, 47% of all backbone atoms, 42% of all non-hydrogen atoms, are inside the map.



1.0

0.0 <0.0

## 9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	$\mathbf{Q} extsf{-score}$
All	0.4194	0.2070
1	0.0023	0.0020
11	0.0000	0.0070
12	0.0000	0.0170
13	0.0000	-0.0180
1A	0.0000	0.0280
1C	0.0000	0.0100
1K	0.0006	-0.0000
1b	0.0030	0.0140
1e	0.0000	0.0140
1f	0.0018	0.0020
1g	0.0000	0.0360
2	0.0010	0.0100
21	0.0000	0.0000
22	0.0000	0.0000
23	0.0000	0.0000
2A	0.0000	0.0000
2B	0.0000	0.0000
2b	0.0000	0.0000
2e	0.0000	0.0000
2f	0.0000	0.0000
$2\mathrm{g}$	0.0000	0.0000
4	0.6367	0.2560
41	0.4715	0.1690
42	0.4716	0.2320
43	0.2394	0.0950
4A	0.4885	0.1430
4B	0.5560	0.1550
4C	0.6882	0.3260
4D	0.6862	0.3020
4b	0.2844	0.0870
4e	0.2407	0.0760
4f	0.3333	0.1270
4g	0.2039	0.0230
5	0.7532	0.2890



Chain	Atom inclusion	Q-score
51	0.4684	0.1360
52	0.4128	0.1040
53	0.7283	0.3880
5A	0.8233	0.4690
5B	0.7650	0.3870
5C	0.8727	0.5100
5D	0.8171	0.4650
5J	0.6497	0.2450
50	0.1712	0.0160
5X	0.3058	0.1470
5b	0.5769	0.2660
5e	0.4727	0.1160
5f	0.3573	0.0930
5g	0.5677	0.2690
6	0.5613	0.1810
62	0.0053	0.0140
63	0.0103	-0.0020
64	0.0000	-0.0400
65	0.0017	0.0290
66	0.0000	-0.0130
67	0.0017	-0.0100
68	0.0014	0.0270
A1	0.1031	0.0580
A2	0.0000	-0.0020
A3	0.0003	0.0040
B1	0.0008	0.0020
B2	0.0024	0.0090
B3	0.0014	-0.0030
B4	0.0000	-0.0010
B5	0.0036	-0.0090
BP	0.0013	-0.0110
Ι	0.0038	-0.0000
K	0.0124	0.0130
R	0.5998	0.2310
S	0.6347	0.3130
U	0.8799	0.5060
Х	0.5431	0.2760

