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PDB ID	:	8RO2
EMDB ID	:	EMD-19399
Title	:	Integrative Structure of the human intron lariat Spliceosome (ILS")
Authors	:	Rothe, P.; Vorlaender, M.K.; Plaschka, C.
Deposited on	:	2024-01-11
Resolution	:	3.50 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.dev112
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7(2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.38.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.50 Å.

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



Metric	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f EM} {f structures} \ (\#{f Entries})$
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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

Mol	Chain	Length		Quality of chain		
1	2	188	18% 7% 12% •	79%		
2	6	106	33%	80% 42%	14%	• 8%
3	С	972	5%	88%		5% 7%
4	D	285	12%	82%		
5	DX	795	56%	81%	•	18%
6	Е	357	• •	80%	•	16%
7	J	848	32%	%	34%	



Conti	nued fron	n previous	page	
Mol	Chain	Length	Quality of	chain
8	K	225	8%	• 16%
9	L1	538	51%	49%
10	Ν	144	93%	6% ••
11	Ο	420	29%	• 31%
12	Q	1485	80% 93%	7%
13	R	536	26%	• 41%
14	S	166	85%	10% • •
15	W	579	13% 24% •	73%
16	Z	166	55%	45%
17	a	126	63%	•• 34%
18	с	119	64%	• 32%
19	d	118	72%	8% • 19%
20	е	92	82%	••• 14%
21	f	86	80%	• 16%
22	g	76	84%	11% • •
23	q	504	20%	80%
23	r	504	23%	76%
23	s	504	26%	74%
23	t	504	20%	80%
24	Z	451	6% 94%	
25	3	476	13% 8	37%
26	5	116	41% 24%	13% 21%
27	А	2335	79%	5% 15%
28	Ι	855	88%	12%
29	IN	154	24% •	73%



			paye	
Mol	Chain	Length	Quality	y of chain
			27%	
30	L	802	67%	• 31%
			13%	
31	L2	894	36% • •	59%
			42%	
32	М	243	67%	• 32%
			24%	
33	Р	229	46% •	51%
			20%	
34	PX	917	32%	68%
			<u>.</u>	
35	Т	514	64%	6% 30%
			25%	
36	TF	837	67%	• 32%
			9%	
37	b	240	35% •	61%



2 Entry composition (i)

There are 40 unique types of molecules in this entry. The entry contains 81753 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

• Molecule 1 is a RNA chain called U2 snRNA.

Mol	Chain	Residues		\mathbf{A}^{\dagger}	toms	AltConf	Trace		
1	2	39	Total 823	C 368	N 137	0 279	Р 39	0	0

• Molecule 2 is a RNA chain called U6 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	6	97	Total 2075	C 928	N 381	O 669	Р 97	0	0

• Molecule 3 is a protein called 116 kDa U5 small nuclear ribonucleoprotein component.

Mol	Chain	Residues		Α	AltConf	Trace			
3	С	908	Total 7184	C 4598	N 1194	O 1357	S 35	0	0

• Molecule 4 is a protein called Pre-mRNA-splicing factor ISY1 homolog.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	D	51	Total 253	C 151	N 51	O 51	0	0

• Molecule 5 is a protein called ATP-dependent RNA helicase DHX15.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	DX	650	Total 3220	C 1920	N 650	O 650	0	0

• Molecule 6 is a protein called U5 small nuclear ribonucleoprotein 40 kDa protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	Е	299	Total 2341	C 1470	N 411	O 447	S 13	0	0



• Molecule 7 is a protein called Crooked neck-like protein 1.

Mol	Chain	Residues		Ator	AltConf	Trace		
7	J	561	Total 2793	C 1671	N 561	O 561	0	0

• Molecule 8 is a protein called Pre-mRNA-splicing factor SPF27.

Mol	Chain	Residues		Ato	ms	AltConf	Trace	
8	Κ	189	Total 941	C 563	N 189	O 189	0	0
0	К	K 189	941	563	189	189	0	

• Molecule 9 is a protein called CWF19-like protein 1.

Mol	Chain	Residues		Ato	\mathbf{ms}	AltConf	Trace	
9	L1	275	Total 1353	C 803	N 275	O 275	0	0

• Molecule 10 is a protein called Protein BUD31 homolog.

Mol	Chain	Residues		\mathbf{A}	toms			AltConf	Trace
10	Ν	143	Total 1184	С 746	N 217	O 209	S 12	0	0

• Molecule 11 is a protein called Pre-mRNA-splicing factor RBM22.

Mol	Chain	Residues		At	AltConf	Trace			
11	О	288	Total 2328	C 1463	N 412	0 433	S 20	0	0

• Molecule 12 is a protein called Intron-binding protein aquarius.

Mol	Chain	Residues		Ato	AltConf	Trace		
12	Q	1384	Total 6859	C 4091	N 1384	0 1384	0	0

• Molecule 13 is a protein called SNW domain-containing protein 1.

Mol	Chain	Residues		Ato	ms	AltConf	Trace	
13	R	317	Total 1571	C 937	N 317	O 317	0	0

• Molecule 14 is a protein called Peptidyl-prolyl cis-trans isomerase-like 1.



Mol	Chain	Residues		At	oms			AltConf	Trace
14	S	159	Total 1236	C 787	N 215	O 227	${f S}$ 7	0	0

• Molecule 15 is a protein called Pre-mRNA-processing factor 17.

Mol	Chain	Residues		At	oms			AltConf	Trace
15	W	158	Total 1276	C 803	N 217	0 252	$\frac{S}{4}$	0	0

• Molecule 16 is a protein called Coiled-coil domain-containing protein 12.

Mol	Chain	Residues		Aton	ns	AltConf	Trace	
16	Z	92	Total 459	C 275	N 92	O 92	0	0

• Molecule 17 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues		At	oms			AltConf	Trace
17	a	83	Total 651	C 408	N 114	0 122	${f S}7$	0	0

• Molecule 18 is a protein called Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues		At	AltConf	Trace			
18	с	81	Total 641	C 409	N 112	0 116	S 4	0	0

• Molecule 19 is a protein called Small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues		At	oms			AltConf	Trace
19	d	96	Total 775	C 485	N 146	0 139	${ m S}{ m 5}$	0	0

• Molecule 20 is a protein called Small nuclear ribonucleoprotein E.

Mol	Chain	Residues		At	oms		AltConf	Trace	
20	е	79	Total 653	C 412	N 116	0 120	${S \atop 5}$	0	0

• Molecule 21 is a protein called Small nuclear ribonucleoprotein F.



Mol	Chain	Residues		Ate	\mathbf{oms}			AltConf	Trace
21	f	72	Total 564	C 364	N 93	O 102	${f S}{5}$	0	0

• Molecule 22 is a protein called Small nuclear ribonucleoprotein G.

Mol	Chain	Residues		At	oms		AltConf	Trace	
22	g	73	Total 568	C 358	N 102	0 102	S 6	0	0

• Molecule 23 is a protein called Pre-mRNA-processing factor 19.

Mol	Chain	Residues		Ato	\mathbf{ms}		AltConf	Trace
23	C.	139	Total	С	Ν	Ο	0	0
20	a	152	659	395	132	132	0	0
23	a	103	Total	С	Ν	Ο	0	0
20	Ч	105	514	308	103	103	0	0
23	r	110	Total	С	Ν	Ο	0	0
20	1	119	594	356	119	119	0	0
23	+	103	Total	С	Ν	Ο	0	0
23	U	100	514	308	103	103	0	0

• Molecule 24 is a protein called Splicing regulator SDE2.

Mol	Chain	Residues		Atc	\mathbf{ms}		AltConf	Trace	
24	7	25	Total	С	Ν	Ο	\mathbf{S}	0	0
24	Z	20	198	119	35	41	3	0	0

• Molecule 25 is a protein called Splicing factor ESS-2 homolog.

Mol	Chain	Residues		Ate	\mathbf{oms}		AltConf	Trace	
25	3	60	Total 499	C 311	N 85	O 102	S 1	0	0

• Molecule 26 is a RNA chain called U5 snRNA.

Mol	Chain	Residues		\mathbf{A}^{\dagger}	toms		AltConf	Trace	
26	5	92	Total 1936	C 867	N 322	O 655	Р 92	0	0

• Molecule 27 is a protein called Pre-mRNA-processing-splicing factor 8.



Mol	Chain	Residues		At	AltConf	Trace			
27	А	1981	Total 16477	C 10621	N 2883	O 2902	S 71	0	0

• Molecule 28 is a protein called Pre-mRNA-splicing factor SYF1.

Mol	Chain	Residues		Ator	AltConf	Trace		
28	Ι	753	Total 3739	C 2233	N 753	O 753	0	0

• Molecule 29 is a RNA chain called INTRON.

Mol	Chain	Residues		Ator	ns	AltConf	Trace	
29	IN	41	Total 492	C 205	0 246	Р 41	0	0

• Molecule 30 is a protein called Cell division cycle 5-like protein.

Mol	Chain	Residues		At	AltConf	Trace			
30	L	555	Total 3623	C 2216	N 695	O 705	S 7	0	0

• Molecule 31 is a protein called CWF19-like protein 2.

Mol	Chain	Residues		At	AltConf	Trace			
31	L2	369	Total 3049	C 1930	N 527	O 569	S 23	0	0

• Molecule 32 is a protein called Pre-mRNA-splicing factor SYF2.

Mol	Chain	Residues		Ato	ms	AltConf	Trace	
32	М	166	Total 827	C 495	N 166	O 166	0	0

• Molecule 33 is a protein called Spliceosome-associated protein CWC15 homolog.

Mol	Chain	Residues		At	oms	AltConf	Trace		
33	Р	112	Total 942	C 575	N 184	0 181	${S \over 2}$	0	0

• Molecule 34 is a protein called PAX3- and PAX7-binding protein 1.



Mol	Chain	Residues		Ato	ms	AltConf	Trace	
34	РХ	295	Total 1465	C 875	N 295	O 295	0	0

• Molecule 35 is a protein called Pleiotropic regulator 1.

Mol	Chain	Residues		At	AltConf	Trace			
35	Т	360	Total 2854	C 1800	N 521	O 523	S 10	0	0

• Molecule 36 is a protein called Tuftelin-interacting protein 11.

Mol	Chain	Residues		Ator	AltConf	Trace		
36	TF	572	Total 2835	C 1690	N 572	O 573	0	0

• Molecule 37 is a protein called Small nuclear ribonucleoprotein-associated proteins B and B'.

Mol	Chain	Residues		At	oms	AltConf	Trace		
37	b	94	Total 717	C 449	N 135	0 126	S 7	0	0

• Molecule 38 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).





Mol	Chain	Residues	Residues Atoms								
38	С	1	Total	С	Ν	Ο	Р	0			
30	U	1	32	10	5	14	3	0			

• Molecule 39 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
39	Ν	3	Total Zn 3 3	0

 $\bullet \ \ \ Molecule \ 40 \ is \ INOSITOL \ HEXAKISPHOSPHATE \ (three-letter \ code: \ IHP) \ (formula: \ C_6H_{18}O_{24}P_6).$



Mol	Chain	Residues	A	Atoms								
40	А	1	Total 36	С 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: U2 snRNA







Q4995 Q4996 B1504 B504 S505 S505 S505 S505 S505 S505 S505 S505 S516 S517 S518 S518 S519 S518 S519 S518 S518 S518 S529 S521 S523 S524 S535 S554 S555 S556 S556 S556 S556 S556
1576 A577 A577 A577 S578 Y581 Y581 Y581 Y581 Y581 Y581 Y582 Y583 Y584 Y587 Y587 Y587 Y587 Y587 Y587 Y583 Y584 Y587 Y603 Y604 Y604 Y604 Y605 Y604 Y604 Y607 Y607 Y607 Y607 Y607 Y607 Y607 Y607 Y607 Y607 <t< td=""></t<>
R6 83 P6 84 F6 84 F6 84 F6 86 F6 86 F6 86 F6 86 F6 86 F6 86 F6 86 F6 86 F6 86 F6 96 F6 96 F6 96 F6 96 F6 96 F7 07 F6 96 F7 07 F6 96 F7 06 F7
V759 K760 I761 A762 A765 P765 Y765 M766 M768 A769 A769 A779 A11A A11A A11A A11A A11A A11A A11
\bullet Molecule 6: U5 small nuclear ribonucleoprotein 40 kDa protein
Chain E: 80% · 16%
MET TLE GLU GLU GLU GLU CLV GLU CLV CLV CLU CLU CLU CLU CLU CLU CLU CLU CLU CLU
L62 D120 D137 D138 D348 D348 D348 D348 D348 D349 D349 <t< td=""></t<>
• Molecule 7: Crooked neck-like protein 1
32% Chain J: 66% 34%
MET THR THR THR VAL ASN VAL ASN ASN ASN ASN ASN ASN ASN ASN ASN ASN
ASP ALA ALA ALA SER SER SER ALA ALA ALA ALA ALA ALA ALA ALA ALA AL
VAL PRO PRO PRO PRO PRO PRO PRO PRO PRO PRO
ASN LYS LYS ALA PRO GLU VAL THR THR ALA CLU GLU GLU GLU GLU GLU GLU GLU GLU GLU G
S254 M265 M261 M261 M261 M261 M261 M261 M262 M263 M264 M264 M263 M264 M263 M264 M263 M264 M264 M265 M287 M283 M284 M285 M327 M328 M329 M321 M325 M326 M325 M326 M325 M326 M325 M326 M346 M345 M345 M345 M345 M345 M345 M345 M346 M345 M346 M345 M345 M345 M345 M345 <
F365 V375 V375 V375 V375 V375 V375 V375 V37
Y438 1441 P441 P441 F443 S444 F445 P445 P446 P466 P6618 P6630 P6633 P6634 P6635 P6636 P6637 P6638 P6638 P6639 P6630 P6630 P6644 P6645 P647 P647 P647 P647







L263 L264	T272 1273	L274 D275	H278 L279	L280 V281	H282 C283 Y284	L285 S286	N287 L288	V289 R290	R291 E292	E293 D294	G295 H296	L297 F298	0020	L301 L302	D303	L305 K306	F307 Y308 T309	G310	E312	N314 D315	Q316 ♦ T317 ♦	G318	A320	T322	N324	A341
E358 V359	T361 R362 E363	S364 L365	V366 K367 F368	F369 G370	P371 L372	8373 8374 More	1376 T376	V380	A381	L384 C385	L386 L387 P388	T389	P391	N393	E394 D395 T355	1397 T397	D399	E401 F402	L403	E405	L407	S409	H411 E412	R413 +	I415 S416	L426 Y427
P428 T429 E430	K431 1432 1433	W434 D435	E436 N437 T438	V439 P440	T441 E442	Y443 Y444	5445 G446	6444/ 6448 7449	04150 4451	L452	K454 L455	N456 L457	L462	Y465	L466 L467	N469 N469	N471 L472	F473	L475 🔶 E476	S477	Y479 E480	1481 R482	Q483 D484	I485 E486	D487 S488	V489 S490 R491
M492 K493 P494	₩495 Q496 S497	E498 Y499	G500 G501 V502	V503 F504	G506 G506	M507 A508	M510	Abil Q512 P513	1514 V515	A516 F517	T518 V519	V520 E521	V522	K524	N526 1527	G528 E529	N530	P532	R534 V535	R536 A537	D538	T540	N542	N544	R546 D547	H548 1549 K550 D551
E552 W553 E554	G555 L556 R557	K558 H559	D560 V561 C562	F563 L564	1565 T566	NOCV R568	T570 K571	P572	G574 C	K576 F577	D578	R580 R581	P582 F583	I584 E585	Q586 V587	G588 L589	V590 Y591	V592 R593	G594 C595	E596 I597	1598 G599	M600 L601	D602 D603	K604 G605	R606 V607	E609 D610 G611
P612 E613 P614	R615 P616 N617	L618 R619	G620 E621 S622	R623 T624	F625 R626	V627 F628	D630	ц633 Ү634	цез5 Фезе	D637 M638	T639 N640	T641 I642	Q643 N644	G645 A646	E647 D648	V649 Y650	E651 T652	F653 N654	I655	M657 R658	R659 K660	P661 K662	NG 65	r060 K667 A660	V669 L670	E671 T672 1673
R674 N675 L676	M677 N678	D680 C681	VIG86 L687	H688 D689	1690 1691	1092 G693 Y694	G695 D696	P697	S699	S703	K704 M705 P706	N7 07	I709	T711	D713 F714	N715	T717 F718	L7 19 S7 20	I721 E722	H7 23 L7 24	K7 25 A7 26	S727 F728	P7 29 G7 30	H7 31	V733 K734	V735
E738 D739 P740	A741 L742 Q743	I744 P745	P746 F747 R748	1749 T750	F751	V753 R754	6756 6756 7757	G758 G758 K759	K760	K762 D763	A764 D765	V766	D7 68 🔶 E7 69	D770	E773	A774 K775	T776	1778	E780	H7 82 V7 83	I784 P785	N7 86 R7 87	G788	Y790	Y792	q794 P795 K796 R797
N7 98 T7 99 I 800	q801 F802 T803	H804 T805	1805 1807 F808	A809 I810	R811 A812	G813 M814	W821	V822 G823	P824 P825	G826 T827	G828 K829	T830 D831	V832 A833	V834 Q835	1836 • 1837 •	2838 2838 2838 2838 2838 2838 2838 2838	1849 L850		S855 NRE6	1000 1857 A 0 E 0	L859	1361 1861	F863	E804 K865 Tore	A868	L869 D870 I871
D872 E873 R874	H875 L876 L877	R878 L879	G880 H881 G882	E883 E884	E885 L886	E887 T888	F889 K890	раз 5892 5893	R894 V895	G896 R897	♦ 868N	Y900	L902 A903	R904 R905	1906 E907	◆ 606T◆ 7000	E910 E911	V912 K913	R914 L915	Q916 K917	S918 L919	G920 V921	P922	D924 A925	S926 Y927	T928 C929 E930 T931
A932 G933 Y934	F935 F936 L937	Y938	K954 G955	S956	L958 P959	U961 V961	E963 V964	S965 T966	F967	H971 E972	Y973 F974 Aq75	0164 9777	P978	P980	1981 F982 7000	6984 8985	S986 Y987	E 9 8 6	D990	E992	1993 A994 Foor	6996	F998	H1000	T1006 Q1007 T1008	E1009
F1011 R1012 A1013	S1014 E1015 L1016	L1017	51019 61020 1.1021	D1022	S1024 K1025	E1031	K1033 I1034	I1035	M1037	H1047 D1048	V1050	L1052 0 0	F1054	N1058	L1060 🔶 M1061	E1062 E1063		11067	E1069	E1071	F1073	P1075	L1076	11082	G1084 F1085	I1094
G1095 D1096 H1097	H1098 Q1099 L1100	P1101 P1102	V1103 11104 K1105	M1106	A1108 F1109	Q1110 K1111 V1110	S1112 S1113 M1114	M1115		L1119	R1122	V1124 R1125	G1127	V1128	V1131 D1132	L1133 D1134	Q1136	R1138	R1140	S1142	C1144	L1146	N1148	W1149 R1150	K1152	L1154 G1155 N1156











• Molecule 15: Pre-mRNA-processing factor 17







LIEU THR ML A THR LIEU THR ALA THR ALA T	ASP
LIEU THR THR THR THR THR THR THR THR THR THR	
THR ASP GLY GLY ASP CVAL VAL VAL VAL VAL ASP CLY CVAL ASP CLY CLY CLY CLY CLY CLY CLY CLY CLY CLY	
VAL VAL VAL VAL VAL VAL ALA ALA ALA ALA	
HIS HIS ASP ASP ASP ASP ASP ASP ASP ASP ASP AS	
TRP TRP TRP LEU LASP LASP LASP LASS LASS LASS PALEU LASS PALEU LASS ASS ASS ASS ASS ASS ASS ASS ASS AS	
THR VAL ALA GLY ALA HIS CLY THR ALA ALA ALA ARF THR ARF CLY CLY SER TYR SER TYR LEU	
• Molecule 23: Pre-mRNA-processing factor 19	
Chain q: 20% 80%	
NET ILE ILEU ILEU SRR SRR SRR SRR SRR SRR SRR SRR SRR SR	G51 LEU TLE TLE TLE LVS VAL ALA ALA ALA PRO
ALA LIVE PRO PRO PRO PRO PRO PRO PRO PRO PRO PRO	
VAL THR THR THR THR THR THR ARG ARG ARG ARG ARG ARG ARG ARG ARG AR	
AIA ASP ASP VAL VAL VAL VAL VAL VAL VAL VAL ASP ASP SER ASP CLU CLU CLU CLU CLU CLU CLU CLU CLU CLU	
VAL VAL ARG ALA ALA ALA ALA ALA ALA ALA CLY SER ALA ALA ALA ALA ALA ALA ALA ALA ALA AL	
JUL	
LANG LANG LEVEN LE	
ALA	

Chain r:

23%

76%





• Molecule 24: Splicing regulator SDE2



	5%			
Chain z:	6%		94%	
MET ALA GLU ALA ALA ALA	ULL TRP TRP TRP TRP ARG GLY PRO GLY CYS	LYS ALA ALA ALA ARG CYS SER ALA GLY GLY CYS CYS ARG ASG ASG	PHE TLE HIS ARG CAS ASP CAS ASP CAS ASP CAS ASP CAS ASP CAS ASS ASS ASS ASS ASS ASS ASS ASS ASS	LEU ILE ASN THR SER ASP
THR VAL GLN HIS GLY ALA	TYR SER LEU GLU PRO ARG LEU CYS GLY GLY	LYS LYS GLY GLY PHE GLY SER MET LEU ALA ALA ALA ALA GLN	11E GLU GLU CHYS THR ASN ASN ASN ASN ARG CYS SER ASS ASS ASS ASS ASS ASS ASS ASS ASS AS	GLU LYS MET ALA ALA GLU
			•••••	••••
TRP VAL LYS GLN GLN ALA	ALA ARG GLU GLU GLU GLU CLN CLN CLN CLN CLN CLN	GLU GLU GLU GLU GLN GLN CNS CNS CNS CNS CNS PHC	THR SER P154 P154 P154 P156 P156 P156 P156 P156 P156 P169 P169 P169 P169 P169 P169 P169	S170 V171 L172 K173 G174 M175 Q176 A177 A178 SER SER
LYS MET VAL SER ALA GLU	SER GLU ASN ARG ARG LYS ARG CLN TRP PRO PRO	LYS LYS SER GLN THR ASP GLY GLY SER ALA SER ALA SER ALA ARG ARG	CTR TRP TRP TRP TRP TRP TRP TRP GLY GLY GLY GLY GLY SER ASR SER ASR ASP ASP ASP ASP ASP ASP ASP ASP ASP ASP	SER GLU GLU ALA PRO SER
THR SER GLY MET GLY PHE	ALA PRO LYS LYS GLY SER ASN VAL VAL GLY	MET ALA ALA ALA ALA PRO PRO SER SER GLY ARG ARG ARG VAL	VAL ASN ASP ASP ASP ASP ASP ASP CLY CLU CLU CLU CLU CLU CLU CLU CLU CLU CLU	GLU ASP SIER SIER CYS ALA GLU
LEU GLY SER LYS GLU	ALL GLU SER ARG ARG MET VAL THR THR GLU GLU	GLU THR GLN GLN GLN GLU SER ALA GLU FRO FRO FRO GLU GLU	GLU PRD CLY CLY CLY CLY CLY CLY CLY CLU CLU CLU CLU CLU CLU CLU CLU CLU CLU	ALA GLU VAL ALA PRO GLU
GLU ARG GLU ASN VAL ALA	ALA LYS LFEU GLN GLN SER GLN FRO GLY ASN	ALA VAL TILE ASP ASP CYS GLU TILE ASP TILE ASP LEU LEU LEU THR THR THR	SER VAL ALA ALA ALA ALA CLEU CLEU CLEU CLEU CLEU CLEU CLEU CLEU	CYS GLY GLY LEU LEU GLN
GLU ARG ALA ALA ARG LEU	SER VAL ARG GLY GLY LEU ALA LEU GLU GLU GLU	ASP PRO ALA ALA LEU PHE PHE LEU LYS CLY LYS LYS LYS		
• Molecu	lle 25: Splicing	g factor ESS-2 home	olog	
Chain 3:	11%		87%	-
			•••••	•• •••••
MET GLU GLU PRO GLY ALA	A DEN SER SER LEU LEU PRO ALA SER	ARC PRO PRO PRO ARG CIU ARG GIU GIU GIU GIU ALA ALA	THR SER CLN CLN CLN CLN CLN CLN CLN CLN CLN CLN	R53 D54 D58 V59 E60 K61 L62 L62 L62 Q63 A64
GLN MET LYS GLU CLU THR GLU PRO LEU GLY GLU ALA	GLUM GLUU SER GLU SER GLV SER ASP LEU ASP LEU LEU LEU FLU FLU ARG ALA ARG SER	GLM TLE TLE ALA ALA PRO LYS CLV CVS CLV CLV CLV CLV CLV CLV CLV CLV CLV CLV	ARG ARG PR0 PR0 PR0 PR0 CLN PR0 CLN PR0 CLN ALA PR0 FR0 FR0 FR0 FR0 FR0 FR0 FR0 FR0 FR0 F	VAL R53 VAL D54 GLY D54 ASN D58 LYS D58 PRO E60 E60 E60 C63 C63 A64
LLM MET LYS GLU GLU THR GLU THR TTR PRO LEU ALA GLU GLU	GLU SER GLU SER GLU SER ASN SER GLV LEU LEU LEU LEU LEU GLU PRO ARG ALA ARG SER	GLM GLM GLM ALA ALA ALA ALA CLV GLV GLV GLV GLV GLV GLV GLV GLV GLV G	ARG ARG PRO PRO PRO PRO PRO PRO CLN PRO CLN PRO CLN PRO CLN PRO CLN PRO PRO PRO PRO PRO PRO PRO PRO	VAL R53 VAL B54 G17 B54 ASN P58 P70 F80 F80 C61 L62 C63 C63 C63 C63 C63 C63 C63 C63 C63 C63
ARG CLM MET PRO LYS CLU THR ARG CLU THR GLY TYR PRO ARG LEU GLY CLY CLU ALA	GUU GUU SER ASP GUU SER GUY GUU SER GUU GUU SER GUU GUU BER GUU GUU BEU GUU MET AIA AIA AGU ARG SER AIA	LTS CLU CLU GLU LLE PRO GLU LLE PRO PRO LLE PRO LEU TLE PRO LEU TLE PRO LEU TLE PRO LEU TLE PRO LEU PLE ARC L148 SER ALA D149 ALA GLU V150 CLV ALA V151 TVS GLU S153 SER ALA S153 SER ALA	R154 ARG THR R155 PR0 LV T156 PR0 CLV SER PR0 CLV M160 THR L38 A161 PR0 CH S162 THR L38 A161 PR0 E41 S163 PHE E41 S164 PHE E41 A164 PHE E41 S165 PHE E41 A164 PHE E41 M167 PHE E41 M167 PHE E41 M168 PHE E41 M167 PHE E41 M168 PHE PHE M170 PHE PHE M171 PHE PHE P171 PHE PHE	E172 VAL R53 R173 VAL R63 S174 VAL D64 S174 LYS D64 A176 LYS D68 A176 PR0 E60 H17 PR0 F00 A176 PR0 F00 A176 PR0 F00 A177 PR0 F00 A17 PR0 F00 A17 PR0 F00 A17 PR0 F00 A18 PR0 F00 A18 PR0 F00 A17 PR0 F00 A14 A14 A14
GLU ARG GLM MET GLU PR0 LVS GLU TME GLU PR0 CLU TME GLU TME GLU ARG GLU TMP PR0 GLU TME PHE GLU ARG GLU TMP PR0 GLU TME PHE GLU ARG GLU TME PR0 GLV TME PR0 LYS GLV GLY TME MLA MLA <t< th=""><th>ANN LUX LUX LUX LUX ALM ALM<th>GLU LUS CUL LUS RU ALA PRO HIS CLU LIS FRO ALA PRO GLU LED PRO ILE PRO ALA LED PRO ILE PRO ALA PRO ILE PRO ARC GLU SIA PRO ILE PRO ALA PRO ILE PRO ARC SER L148 PLE ARC CUV SER L148 SER ALA CUV ALA VIA VIA CUV ALA CLN VIA VIA CUV ALA VAL VIA CUV ALA CUV VAL L148 SER ALA CUV VAL L148 SER ALA CUV VAL L145 MA CUV CUV VAL L145 MA CUV CUV</th><th>TRP TRP ARG THR TYN T156 PR0 CLU SER TYN T156 PR0 CLN SER LYN T156 PR0 CLN SER LYN T156 PR0 CLN SER LYN T156 PR0 CLN SER LNN E158 PR0 CLN SER SER D159 PLN VAL L38 NET N160 PLN VAL L38 NET N160 PLN VAL L38 VR TNR PL0 VAL L38 VR N160 PLN VAL L38 VR A161 PR0 VAL L38 VR T18 PL0 VAL L38 VAL F163 PLN F44 PLN T166 PLN F44 VAL T165 PLN F44 VAL E165 PLN F44 VAL T166 PLN F44 PLN T166 PLN F44 VAL E165 PLN F44 VAL T166 PLN</th><th>LYS E172 (VAL R53 PRO 5174 (VAL R53 ARG 5174 (VAL B54 ARG 5174 (VAL B54 ARG 5174 (VAL B54 ARG 5174 (VAL B54 ART 5174 (CT B56 H17 (VAL B54 ATT 5174 (CT B56 H17 (CT B56) (CT B56) (CT 51 H17 (CT B56) (CT 51 H17 (CT 51) (CT 51</th></th></t<>	ANN LUX LUX LUX LUX ALM ALM <th>GLU LUS CUL LUS RU ALA PRO HIS CLU LIS FRO ALA PRO GLU LED PRO ILE PRO ALA LED PRO ILE PRO ALA PRO ILE PRO ARC GLU SIA PRO ILE PRO ALA PRO ILE PRO ARC SER L148 PLE ARC CUV SER L148 SER ALA CUV ALA VIA VIA CUV ALA CLN VIA VIA CUV ALA VAL VIA CUV ALA CUV VAL L148 SER ALA CUV VAL L148 SER ALA CUV VAL L145 MA CUV CUV VAL L145 MA CUV CUV</th> <th>TRP TRP ARG THR TYN T156 PR0 CLU SER TYN T156 PR0 CLN SER LYN T156 PR0 CLN SER LYN T156 PR0 CLN SER LYN T156 PR0 CLN SER LNN E158 PR0 CLN SER SER D159 PLN VAL L38 NET N160 PLN VAL L38 NET N160 PLN VAL L38 VR TNR PL0 VAL L38 VR N160 PLN VAL L38 VR A161 PR0 VAL L38 VR T18 PL0 VAL L38 VAL F163 PLN F44 PLN T166 PLN F44 VAL T165 PLN F44 VAL E165 PLN F44 VAL T166 PLN F44 PLN T166 PLN F44 VAL E165 PLN F44 VAL T166 PLN</th> <th>LYS E172 (VAL R53 PRO 5174 (VAL R53 ARG 5174 (VAL B54 ARG 5174 (VAL B54 ARG 5174 (VAL B54 ARG 5174 (VAL B54 ART 5174 (CT B56 H17 (VAL B54 ATT 5174 (CT B56 H17 (CT B56) (CT B56) (CT 51 H17 (CT B56) (CT 51 H17 (CT 51) (CT 51</th>	GLU LUS CUL LUS RU ALA PRO HIS CLU LIS FRO ALA PRO GLU LED PRO ILE PRO ALA LED PRO ILE PRO ALA PRO ILE PRO ARC GLU SIA PRO ILE PRO ALA PRO ILE PRO ARC SER L148 PLE ARC CUV SER L148 SER ALA CUV ALA VIA VIA CUV ALA CLN VIA VIA CUV ALA VAL VIA CUV ALA CUV VAL L148 SER ALA CUV VAL L148 SER ALA CUV VAL L145 MA CUV CUV VAL L145 MA CUV CUV	TRP TRP ARG THR TYN T156 PR0 CLU SER TYN T156 PR0 CLN SER LYN T156 PR0 CLN SER LYN T156 PR0 CLN SER LYN T156 PR0 CLN SER LNN E158 PR0 CLN SER SER D159 PLN VAL L38 NET N160 PLN VAL L38 NET N160 PLN VAL L38 VR TNR PL0 VAL L38 VR N160 PLN VAL L38 VR A161 PR0 VAL L38 VR T18 PL0 VAL L38 VAL F163 PLN F44 PLN T166 PLN F44 VAL T165 PLN F44 VAL E165 PLN F44 VAL T166 PLN F44 PLN T166 PLN F44 VAL E165 PLN F44 VAL T166 PLN	LYS E172 (VAL R53 PRO 5174 (VAL R53 ARG 5174 (VAL B54 ARG 5174 (VAL B54 ARG 5174 (VAL B54 ARG 5174 (VAL B54 ART 5174 (CT B56 H17 (VAL B54 ATT 5174 (CT B56 H17 (CT B56) (CT B56) (CT 51 H17 (CT B56) (CT 51 H17 (CT 51) (CT 51
VAL GLU ARG GLA MET HIS GLU PRO LYS GLU LYS GLU PRO LYS GLU ASN PHE GLY TYR PRO ARG LU ARG LEU GLY ARG LYS GLY GLU ALA	LEU GLM ALM ALM <td>ARC GLU LUS GLU LUS ARC CYS HIS GLU LVS GLN ARC CIN GLN LVS GLN ARC ARC CIN GLN LEU TLE PRO CIN LLE PRO LLS PRO CIN LLE PRO LLS ARC CIN GLU SER L148 ARC ALA SER L148 SER AIL ALA SER L148 SER AIL ALA SER L148 SER AIL ALA VISO CIV GUV CIV ALA VISO L148 SER AIL ALA VISO L148 SER AIL ALA VISO L148 SER AIL ALA VISO L149 SER AIL ALA VISO CIV CIV CI</td> <td>LYS TRP And THR LYS TH5 And THR GLN LYS T156 PR0 CLU VAL LYS T156 PR0 CLU VAL ALA S157 PR0 CLU VAL LYS T156 PR0 CLU CIY LYS T156 PR0 CLU ASP SER T156 PR0 CLU CIY LEU NI50 PR0 CLU ASP SER D159 VAL L38 CUU TYR D159 VAL L36 CUU TYR D159 VAL L38 CUU TYR D159 VAL L36 CUU TYR D159 VAL L36 CUU TYR D159 VAL L36 CUU TYR D164 PR0 D39 CUU TYR D169 PR0 E41 FILE PR0 Q10 E46 CUU VAL T166 Q10 E45 PR0 ALS PR0 Q10 E45 PR0 ALS PL65 PL18</td> <td>GLY LYS E172 VAL R53 PHE LYS H173 VAL R53 VAL ARG 8173 9 0AL ALA ARG 8174 9 0AL THR QLN 8175 9 0AS PRO VAL AT76 9 058 PRO VAL AT76 9 058 H17 H17 9 106 106 H17 H17 9 106 106 H17 H17 9 106 106 H18 H18 116 106 106 H18 H18 116 106 106 H18 H18 118 106 106 H18 H18 118 106 106</td>	ARC GLU LUS GLU LUS ARC CYS HIS GLU LVS GLN ARC CIN GLN LVS GLN ARC ARC CIN GLN LEU TLE PRO CIN LLE PRO LLS PRO CIN LLE PRO LLS ARC CIN GLU SER L148 ARC ALA SER L148 SER AIL ALA SER L148 SER AIL ALA SER L148 SER AIL ALA VISO CIV GUV CIV ALA VISO L148 SER AIL ALA VISO L148 SER AIL ALA VISO L148 SER AIL ALA VISO L149 SER AIL ALA VISO CIV CIV CI	LYS TRP And THR LYS TH5 And THR GLN LYS T156 PR0 CLU VAL LYS T156 PR0 CLU VAL ALA S157 PR0 CLU VAL LYS T156 PR0 CLU CIY LYS T156 PR0 CLU ASP SER T156 PR0 CLU CIY LEU NI50 PR0 CLU ASP SER D159 VAL L38 CUU TYR D159 VAL L36 CUU TYR D159 VAL L38 CUU TYR D159 VAL L36 CUU TYR D159 VAL L36 CUU TYR D159 VAL L36 CUU TYR D164 PR0 D39 CUU TYR D169 PR0 E41 FILE PR0 Q10 E46 CUU VAL T166 Q10 E45 PR0 ALS PR0 Q10 E45 PR0 ALS PL65 PL18	GLY LYS E172 VAL R53 PHE LYS H173 VAL R53 VAL ARG 8173 9 0AL ALA ARG 8174 9 0AL THR QLN 8175 9 0AS PRO VAL AT76 9 058 PRO VAL AT76 9 058 H17 H17 9 106 106 H17 H17 9 106 106 H17 H17 9 106 106 H18 H18 116 106 106 H18 H18 116 106 106 H18 H18 118 106 106 H18 H18 118 106 106
SER VAL GJU ARG GJN MET PRO HIS GJU PRO LYS GJU ALA LYS GJU ARG GJU THR PRO ASN PHE GJY TYR PRO GLY THR GJU ARG LEU GLU VAL ARG LYS GJY GJU ALA VAL ARG LYS GJY GJU ALA	CON TIL ANN LEU ANN LEU ANN LEU ANN ANN CUN SER AIN AIN <th>$\begin{array}{cccccccccccccccccccccccccccccccccccc$</th> <th>VAL LYS TRP ALS ARG THR ALS CLU SER ALG CLU SER ALS ALS CLU SER ALS CLU CLU CLU SER ALS CLU CLU CLU CLU CLU CLU CLU CLU CLU CLU</th> <th>MET CLY LYS E172 (VAL R53 ALA PHE LYS A173 (VAL R53 ALA THR CLN A173 (VAL D54 ALA THR CLN A175 (VAL D54 ALA THR CLN A175 (VAL D54 A176 (VAL D54 A177 (VAL D54 A177 (VAL D54 A176 (VAL D5</th>	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	VAL LYS TRP ALS ARG THR ALS CLU SER ALG CLU SER ALS ALS CLU SER ALS CLU CLU CLU SER ALS CLU	MET CLY LYS E172 (VAL R53 ALA PHE LYS A173 (VAL R53 ALA THR CLN A173 (VAL D54 ALA THR CLN A175 (VAL D54 ALA THR CLN A175 (VAL D54 A176 (VAL D54 A177 (VAL D54 A177 (VAL D54 A176 (VAL D5
ALA SER VAL GLU ARG GLN MET LYS PRO HIS GLU PRO LYS GLU ASN ALA LYS GLU PRO LYS GLU THR AGG PRO ASN PHE GLY TYR PRO ALA GLY THR GLU ARG LEU GLU LYS VAL ANG LYS GLY GLU ALA LYS VAL ANG LYS GLY GLU ALA	LIV CLU CLU <td>$\begin{array}{cccccccccccccccccccccccccccccccccccc$</td> <td>PRO VAL LYS TWP ALG TWP ALA ASP GLN TYS Y155 PRO GLN ARG PRO VAL LYS Y155 PRO GLN ARG PRO VAL LYS Y155 PRO GLN ARG PRO VAL LYS THE PRO GLN ARG PRO VAL LYS THE PRO GLN VLL PRO VAL SER PRO GLN VAL PRO ALA SER PRO PRO VIL PRO FIES PRO PRO PRO VAL TUE TYR PRO PRO PRO ALA ASP GLU TRR PRO PRO ALA ASP PRO PRO PRO PRO SER LUD TRR PRO PRO PRO SIR LUD PRO PRO</td> <td>THR MET GLY LYS E172 VAL R33 PR0 ALA PHE LYS E172 VAL R33 PR0 ALA PHE LYS R173 VAL R33 PR0 GUU ALA PHE R173 VAL D54 ALA ALA THR GLN R175 PLO D54 AR0 ALA THR GLN A176 PR0 E60 AR1 BLO VAL A175 PLO D54 AR1 BLO A176 PR0 D68 AR1 FR0 A176 PR0 D68 AR1 FR17 PLO PLO D68 AR1 FR18 PLO PLO PLO AR1 FR18 FR18 PLO PLO AR1 FR18 FR18 PLO PLO</td>	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	PRO VAL LYS TWP ALG TWP ALA ASP GLN TYS Y155 PRO GLN ARG PRO VAL LYS Y155 PRO GLN ARG PRO VAL LYS Y155 PRO GLN ARG PRO VAL LYS THE PRO GLN ARG PRO VAL LYS THE PRO GLN VLL PRO VAL SER PRO GLN VAL PRO ALA SER PRO PRO VIL PRO FIES PRO PRO PRO VAL TUE TYR PRO PRO PRO ALA ASP GLU TRR PRO PRO ALA ASP PRO PRO PRO PRO SER LUD TRR PRO PRO PRO SIR LUD PRO PRO	THR MET GLY LYS E172 VAL R33 PR0 ALA PHE LYS E172 VAL R33 PR0 ALA PHE LYS R173 VAL R33 PR0 GUU ALA PHE R173 VAL D54 ALA ALA THR GLN R175 PLO D54 AR0 ALA THR GLN A176 PR0 E60 AR1 BLO VAL A175 PLO D54 AR1 BLO A176 PR0 D68 AR1 FR0 A176 PR0 D68 AR1 FR17 PLO PLO D68 AR1 FR18 PLO PLO PLO AR1 FR18 FR18 PLO PLO AR1 FR18 FR18 PLO PLO
SER ALA SER VAL GLU ARG CLN NET THR LYS PR0 HIS GLU PR0 LYS GLU HIS ASN ALA LYS GLU ARG GLU TYR GLU LUU ARG PN0 LYS GLU ARG GLU TYR PN0 LYS ALA GLY THR GLU ARG GLU TYR P10 TYR LYS ALA GLY THR GLU ARG GLY ALA TYR LYS VAL ARG LYS GLY MA ALA TYR LYS VAL ARG LYS GLY ALA A	ATA GLU CLU FTD ANN CLU CLU CLU CLU GLU GLU <td>Pin Dim Dim Dim Dim Dim Dim ALA ALA ASN CUN ARG CUN LUN CUN ALA PRO ERN THR CUN ALA ALA ALA ALA ALA PRO SER THR CUN ALA PRO LEU CUN ALA ALA PRO LEU CLN ALA PRO ALA ALA PRO LEU CLN LLE PRO ALA PRO LEU CLN LLE PRO ALA PRO LEU CLN LLE PRO ALA PRO LEU ALA PRO LLE ARG CUN ALA PRO CUN LLE ARG CUN LLA PRO CUN LLA ARG CUN LLA PRO LLA ALA ARG CUN LLA PRO LLA L</td> <td>PRO PRO PRO VAL LYS TWP ALA ASP GLN TYR RER LEU ARA ASP GLN TYR Y155 GLU SER THE GLN THR LYS TYR Y155 PRO GLN SER THE GLN THR LYS TYR TH56 PRO GLN SER THE GLN THR LYS TYR TH56 PRO GLN ASP LEU RLA ASP GLN TYR PRO GLN ASP LEU RLA ASP SER D199 PLA LS9 GLN THR LEU RTR LEU TTR LS9 PTR LEU THR LUN THE PRO GLN THR LEU THR LUN THR PRO PRO PRO LEU THR LUN THR PRO PRO PRO LEU THR LUN THR PRO PLO PLO ARG THR LEU THR PLO PLO PLO ARG THR PLO THR</td> <td>THR MET CLV L/S E172 VAL R33 PRO ALA PHE L/S F173 M VAL R33 PRO CLU ALA PHE L/S F173 M VAL D54 PRO CLU ALA THR R473 M PL D54 ALA THR CLU ALA THR PL D54 ALA THR CLU AT75 PL D58 ALA PRO VAL AT75 PL D58 ALA PRO VAL AT75 PL D58 ALA PRO VAL AT6 PL D58 ALA PRO VAL AT75 PL D58 ALA PRO VAL AT76 PL D58 ALA PRO VAL AT6 PL D68 ALA PRO VAL AT6 PL D68 ALA PRO PL ALA PL D68 ALA PRO PL PL PL D68 ALA PRO PL PL PL ALA PL PL<</td>	Pin Dim Dim Dim Dim Dim Dim ALA ALA ASN CUN ARG CUN LUN CUN ALA PRO ERN THR CUN ALA ALA ALA ALA ALA PRO SER THR CUN ALA PRO LEU CUN ALA ALA PRO LEU CLN ALA PRO ALA ALA PRO LEU CLN LLE PRO ALA PRO LEU CLN LLE PRO ALA PRO LEU CLN LLE PRO ALA PRO LEU ALA PRO LLE ARG CUN ALA PRO CUN LLE ARG CUN LLA PRO CUN LLA ARG CUN LLA PRO LLA ALA ARG CUN LLA PRO LLA L	PRO PRO PRO VAL LYS TWP ALA ASP GLN TYR RER LEU ARA ASP GLN TYR Y155 GLU SER THE GLN THR LYS TYR Y155 PRO GLN SER THE GLN THR LYS TYR TH56 PRO GLN SER THE GLN THR LYS TYR TH56 PRO GLN ASP LEU RLA ASP GLN TYR PRO GLN ASP LEU RLA ASP SER D199 PLA LS9 GLN THR LEU RTR LEU TTR LS9 PTR LEU THR LUN THE PRO GLN THR LEU THR LUN THR PRO PRO PRO LEU THR LUN THR PRO PRO PRO LEU THR LUN THR PRO PLO PLO ARG THR LEU THR PLO PLO PLO ARG THR PLO THR	THR MET CLV L/S E172 VAL R33 PRO ALA PHE L/S F173 M VAL R33 PRO CLU ALA PHE L/S F173 M VAL D54 PRO CLU ALA THR R473 M PL D54 ALA THR CLU ALA THR PL D54 ALA THR CLU AT75 PL D58 ALA PRO VAL AT75 PL D58 ALA PRO VAL AT75 PL D58 ALA PRO VAL AT6 PL D58 ALA PRO VAL AT75 PL D58 ALA PRO VAL AT76 PL D58 ALA PRO VAL AT6 PL D68 ALA PRO VAL AT6 PL D68 ALA PRO PL ALA PL D68 ALA PRO PL PL PL D68 ALA PRO PL PL PL ALA PL PL<

 \bullet Molecule 26: U5 snRNA







• Molecule 29: INTRON



Chain IN:	23% 24%		73%			
N1 N2 N3 N4 N5 N5 N7 N8	N9 N10 N11 N12 N13 N14 N15	N19 N22 N23 N N N N N N N N N	N N N N N N N N N N N N N N N N N N N		N N N N N	
<u> </u>	N N N N N N N N				a	
N N N N N N N N N N N N N N N N N N N	N N N N138 N138 M140 M141	N142 • N143 • N143 • N144 • N144 • N145 • N144 • N144 • N144 • N144 • N144 • N149 • N149 • N149 • N150 • N1	N154			
• Molecule 30:	Cell division	ı cycle 5-like protein				
Chain L:	2170	67%	• 3	1%		
MET PRIO ARIG ALLE MET K7 63 63 63 63 63 63	R12 N13 T14 E17 I18	A22 A22 V23 K26 R33 R33 R33 R33 R33 R33 R33 R33 R33 R3	R40 K44 D55 K69 E86	Q81 Q109 0111 0111 €113 €113 €114	T116 T117 D119 P120 R121 K122 L123 K124	
P125 C126 E127 D129 P130 P132 P132	T135 K135 P136 A137 R138 P139 D140	P141 1142 D143 M144 M145 E146 E146 E148 E148 E148 E148 E150 M151	E154 A155 A155 A155 A155 A157 A156 A156 A156 A156 A156 A156 A156 A156	C1164 C1165 C1166 A1167 C1168 R1168 R1168 A171 A171 A171 C173 C173	K174 K175 C175 E177 E177 A179 A184 A184 A184 A184	L185
K187 R188 R189 E190 L191 R192 A193 A194	G195 1196 E197 E198 Q199 K200 K200	K205 K205 K205 R206 G207 C207 V208 V208 V208 V208 V210 N211	1214 P215 F216 E217 K218 K219 P220 A221	S228 E229 E220 Y232 Y232 Q233 L235 L235 D236	2238 F228 F229 K241 K241 L242 R243 Q244 Q245 D245 L247 D245 D245	G249 E250
LEU ARG SER GLU CLYS GLU GLV ARG ARG ARG LYS	LYS ASP LYS CLN HIS LEU LYS ARG LYS	LYS GLU SER ASP ASP ALEU FRO FRO FRO GLN THR SER GLN VAL	SER PHE THR LYS LYS ARG SER LYS SER LYS LEU LEU	PR0 ALA PR0 GLN ILE SER ALA ALA CLU CLU GLN VAL	1HL	
VAL VAL VAL GLN GLN ALA SER GLU TLE ARG ARG	GLN THR ALA GLU GLU SER GLY THR	ASN ASN ALA ALA SER SER LEU LEU LEU CLU GLU VAL VAL VAL XSN XSN	ASN SER VAL ALA LEU LEU ARC PRO ARC PRO ASS7	S358 Q359 D360 R361 1362 L363 Q364 Q364 Q367	V375	
D376 L379 K380 G381 G381 CEU ASN THR	PRU LEU HLEU GLU SER ASP PHE SER CLY VAT.	THR PRO GLN GLN VAL VAL THR PRO ASN VAL THR VAL SER SER	THR PRO PRO APHE ARG PRO SER SER ALA ALA GLU CIV	LEU: THR PRO ARG SER GLY THR THR PRO LVS VAL	ILE	
SER THR PRO GLY ARG THR PRO LEU ASP LYS	LEU ASN ILE ASN PRO GLU ASP GLY MET	ALA ASP TYR SER ASP PRO PRO PRO CLV GLN GLN GLU	SER ARG HIS LEU LEU CLEU CLEU CLEU CLEU CLEU LEU	PRO ALA PRO LYS ASP ASP PHE CLU ILE LEU LEU		
ASN ALA GLU CLU CLU CLU GLU GLU GLU CLU CLU CLU CLU CLU CLU	ASP ASP THR TYR ILE GLU ALA ALA	D517 R536 M537 H1538 F538 F546 F553 T1554	N560 V561 F562 P563 P564 I575 F591 V592	E593 P594 S595 S595 S595 S596 K599 G600 K601	V 603 6603 7605 7605 8606 8606 8525	
K626 E627 K631 K631 A632 Q633 Q633	V637 M640 E641 V642 V642 K644	Control Contro	C673 A633 SER K883 K881 PHE			
• Molecule 31:	CWF19-like	protein 2				
Chain L2:	36%		59%			





ASN LLEU GLU ARG GLY THR ALA VAL

• Molecule 33: Spliceosome-associated protein CWC15 homolog













4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	87951	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)	750	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV $(4k \times 4k)$	Depositor
Maximum map value	5.823	Depositor
Minimum map value	0.000	Depositor
Average map value	0.016	Depositor
Map value standard deviation	0.127	Depositor
Recommended contour level	0.975	Depositor
Map size (Å)	519.75, 519.75, 519.75	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.2375, 1.2375, 1.2375	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: ZN, IHP, GTP, SEP

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

Mol Chain		Bo	nd lengths	Bond angles		
	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	2	0.62	1/917~(0.1%)	1.56	19/1425~(1.3%)	
2	6	0.56	1/2323~(0.0%)	1.52	50/3619~(1.4%)	
3	С	0.34	0/7346	0.70	6/9980~(0.1%)	
4	D	0.35	0/252	0.57	0/350	
5	DX	0.30	0/3219	0.59	0/4487	
6	Ε	0.36	0/2394	0.79	7/3243~(0.2%)	
7	J	0.29	0/2792	0.48	0/3900	
8	Κ	0.33	0/940	0.49	0/1312	
9	L1	0.29	0/1352	0.59	0/1878	
10	Ν	0.38	0/1210	0.76	1/1622~(0.1%)	
11	0	0.40	1/2378~(0.0%)	0.81	2/3211~(0.1%)	
12	Q	0.30	0/6858	0.52	0/9563	
13	R	0.34	0/1558	0.67	0/2168	
14	S	0.33	0/1268	0.73	2/1714~(0.1%)	
15	W	0.36	0/1306	0.75	3/1760~(0.2%)	
16	Ζ	0.31	0/458	0.54	0/639	
17	а	0.38	0/659	0.92	2/888~(0.2%)	
18	с	0.37	0/649	1.00	3/877~(0.3%)	
19	d	0.43	0/785	1.02	3/1049~(0.3%)	
20	е	0.38	0/661	0.96	0/886	
21	f	0.43	0/575	1.01	3/776~(0.4%)	
22	g	0.45	0/575	1.01	4/768~(0.5%)	
23	q	0.33	0/512	0.47	0/713	
23	r	0.35	0/592	0.56	0/825	
23	s	0.31	0/658	0.55	0/919	
23	t	0.32	0/512	0.49	0/713	
24	Z	0.28	0/200	0.56	0/266	
25	3	0.31	0/504	0.59	0/675	
26	5	0.52	0/2157	1.59	58/3351~(1.7%)	
27	A	0.35	1/16926~(0.0%)	0.73	$2\overline{1/22947}~(0.1\%)$	
28	Ι	0.30	0/3737	0.50	0/5213	
30	L	0.31	0/3657	0.64	4/4979~(0.1%)	



Mal	Chain	Bond lengths		Bond angles		
IVIOI		RMSZ	# Z > 5	RMSZ	# Z > 5	
31	L2	0.36	1/3117~(0.0%)	0.77	6/4183~(0.1%)	
32	М	0.30	0/825	0.47	0/1150	
33	Р	0.34	0/957	0.75	2/1276~(0.2%)	
34	PX	0.31	0/1463	0.49	0/2039	
35	Т	0.36	1/2927~(0.0%)	0.81	5/3980~(0.1%)	
36	TF	0.31	0/2830	0.55	0/3937	
37	b	0.36	0/726	0.90	2/966~(0.2%)	
All	All	0.36	6/82775~(0.0%)	0.78	203/114247~(0.2%)	

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	С	0	1
17	a	0	2
19	d	0	3
20	е	0	1
22	g	0	1
27	А	0	3
All	All	0	11

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms		Observed(Å)	Ideal(Å)
11	0	225	PRO	C-N	6.48	1.46	1.34
2	6	35	А	N9-C4	5.92	1.41	1.37
31	L2	678	CYS	CB-SG	-5.63	1.72	1.81
1	2	35	А	N9-C8	-5.43	1.33	1.37
35	Т	306	CYS	CB-SG	-5.37	1.73	1.81
27	А	1307	MET	C-N	5.19	1.44	1.34

All (203) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	6	36	А	C8-N9-C4	-14.35	100.06	105.80
26	5	86	С	N1-C2-O2	13.81	127.18	118.90
2	6	36	A	N7-C8-N9	13.30	120.45	113.80
26	5	86	С	C2-N1-C1'	12.61	132.67	118.80
26	5	24	G	O4'-C1'-N9	-11.78	98.78	108.20
26	5	99	С	C6-N1-C2	-11.62	115.65	120.30



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	6	37	С	N1-C2-O2	11.29	125.67	118.90
26	5	86	С	N3-C2-O2	-11.04	114.17	121.90
26	5	103	С	C6-N1-C2	-10.06	116.28	120.30
2	6	81	С	C6-N1-C2	-9.79	116.39	120.30
1	2	35	А	O4'-C1'-N9	-9.42	100.66	108.20
2	6	37	С	N3-C2-O2	-9.30	115.39	121.90
1	2	7	U	C6-N1-C2	-9.29	115.42	121.00
1	2	7	U	C5-C6-N1	9.14	127.27	122.70
26	5	99	C	C2-N1-C1'	9.06	128.77	118.80
2	6	36	A	C5-N7-C8	-8.98	99.41	103.90
1	2	7	U	N3-C2-O2	-8.97	115.92	122.20
2	6	35	A	C8-N9-C4	-8.78	102.29	105.80
26	5	23	C	C2-N1-C1'	8.76	128.43	118.80
2	6	37	С	C6-N1-C2	-8.71	116.82	120.30
26	5	86	С	C6-N1-C2	-8.70	116.82	120.30
30	L	77	LEU	CA-CB-CG	8.69	135.29	115.30
26	5	86	C	C6-N1-C1'	-8.59	110.49	120.80
2	6	37	C	C2-N1-C1'	8.50	128.15	118.80
27	А	259	ASP	CB-CG-OD1	8.37	125.83	118.30
2	6	97	U	C5-C6-N1	8.33	126.86	122.70
26	5	11	U	C2-N1-C1'	8.32	127.69	117.70
21	f	70	LEU	CA-CB-CG	8.30	134.38	115.30
2	6	34	G	P-O3'-C3'	8.10	129.42	119.70
18	с	32	VAL	CG1-CB-CG2	-8.06	98.01	110.90
1	2	8	С	O4'-C1'-N1	8.04	114.63	108.20
2	6	81	С	O4'-C1'-N1	7.98	114.58	108.20
26	5	103	С	C5-C6-N1	7.91	124.95	121.00
27	A	519	ASP	CB-CG-OD1	7.86	125.38	118.30
37	b	23	ASP	CB-CG-OD1	7.72	125.25	118.30
3	С	860	ASP	CB-CG-OD1	7.67	125.20	118.30
26	5	10	U	C2-N1-C1'	7.64	126.87	117.70
35	Т	300	ILE	CG1-CB-CG2	-7.62	94.64	111.40
26	5	37	G	N9-C1'-C2'	7.61	123.90	114.00
2	6	42	С	P-O3'-C3'	7.58	128.80	119.70
22	g	35	ASP	CB-CG-OD1	7.55	125.10	118.30
1	2	7	U	N1-C2-O2	7.50	128.05	122.80
2	6	35	A	N7-C8-N9	7.50	117.55	113.80
1	2	8	C	C6-N1-C2	-7.41	117.34	120.30
19	d	60	ASP	CB-CG-OD1	7.39	124.95	118.30
2	6	81	C	C6-N1-C1'	7.36	129.63	120.80
26	5	11	U	C5-C6-N1	7.34	126.37	122.70
26	5	36	C	C2-N1-C1'	7.30	126.83	118.80



Mol	Chain	\mathbf{Res}	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
35	Т	225	ASP	CB-CG-OD1	7.19	124.77	118.30
2	6	41	А	O5'-P-OP1	7.15	119.28	110.70
26	5	36	С	N1-C2-O2	7.08	123.15	118.90
2	6	35	А	C2-N3-C4	7.02	114.11	110.60
26	5	86	С	C5-C6-N1	7.01	124.50	121.00
30	L	222	LEU	CA-CB-CG	6.99	131.38	115.30
27	А	1467	LEU	CA-CB-CG	6.99	131.38	115.30
27	А	371	LEU	CA-CB-CG	6.93	131.23	115.30
2	6	37	С	C5-C6-N1	6.91	124.45	121.00
18	с	79	LEU	CA-CB-CG	6.88	131.13	115.30
27	А	1670	ASP	CB-CG-OD1	6.88	124.49	118.30
15	W	193	LEU	CA-CB-CG	6.82	130.99	115.30
1	2	7	U	O4'-C1'-N1	6.80	113.64	108.20
6	Е	180	ASP	CB-CG-OD1	6.78	124.40	118.30
27	А	488	ASP	CB-CG-OD1	6.76	124.38	118.30
6	Е	130	ASP	CB-CG-OD1	6.73	124.36	118.30
26	5	99	С	C5-C6-N1	6.69	124.34	121.00
26	5	92	U	P-O3'-C3'	6.64	127.67	119.70
26	5	10	U	C5-C6-N1	6.64	126.02	122.70
26	5	36	С	C6-N1-C2	-6.61	117.66	120.30
1	2	22	U	N3-C2-O2	-6.58	117.59	122.20
3	С	300	LEU	CA-CB-CG	6.58	130.43	115.30
2	6	36	А	C6-C5-N7	-6.58	127.70	132.30
26	5	95	G	P-O3'-C3'	6.57	127.59	119.70
27	А	1473	ASP	CB-CG-OD1	6.51	124.16	118.30
1	2	13	С	N1-C2-O2	6.49	122.79	118.90
22	g	68	ILE	CG1-CB-CG2	-6.47	97.17	111.40
22	g	70	LEU	CA-CB-CG	6.44	130.11	115.30
2	6	33	G	P-O3'-C3'	6.41	127.39	119.70
26	5	105	U	N3-C2-O2	-6.40	117.72	122.20
2	6	36	А	C4-C5-N7	6.37	113.89	110.70
26	5	37	G	O4'-C1'-N9	-6.36	103.11	108.20
1	2	8	С	C6-N1-C1'	6.36	128.43	120.80
26	5	103	С	C2-N1-C1'	6.30	125.73	118.80
6	Е	120	ASP	CB-CG-OD1	6.28	123.95	118.30
21	f	37	ASP	CB-CG-OD1	6.28	123.95	118.30
26	5	23	С	N1-C2-O2	6.27	122.67	118.90
2	6	52	U	N3-C2-O2	-6.27	117.81	122.20
2	6	35	А	O4'-C1'-N9	6.25	113.20	108.20
3	С	230	ASP	CB-CG-OD1	6.20	123.88	118.30
2	6	45	А	C2-N3-C4	6.20	113.70	110.60
26	5	35	U	N3-C2-O2	-6.15	117.89	122.20



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Mol	Chain	\mathbf{Res}	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	6	81	С	C5-C6-N1	6.15	124.08	121.00
33	Р	63	LEU	CA-CB-CG	6.14	129.42	115.30
26	5	23	С	C6-N1-C1'	-6.13	113.44	120.80
27	А	260	LEU	CA-CB-CG	6.10	129.34	115.30
3	С	298	LEU	CA-CB-CG	6.10	129.32	115.30
26	5	45	С	C6-N1-C2	-6.09	117.86	120.30
2	6	52	U	N1-C2-O2	6.04	127.03	122.80
2	6	35	A	P-O3'-C3'	6.03	126.94	119.70
27	А	1233	ASP	CB-CG-OD1	6.02	123.72	118.30
3	С	469	ASP	CB-CG-OD1	6.00	123.70	118.30
35	Т	351	ASP	CB-CG-OD1	6.00	123.70	118.30
2	6	62	С	C6-N1-C2	-6.00	117.90	120.30
11	0	64	ARG	CG-CD-NE	5.97	124.34	111.80
27	А	1109	LEU	CA-CB-CG	5.97	129.03	115.30
6	Е	348	ASP	CB-CG-OD1	5.93	123.64	118.30
35	Т	257	ARG	C-N-CA	5.91	136.47	121.70
19	d	77	VAL	CG1-CB-CG2	-5.87	101.51	110.90
26	5	105	U	N1-C2-O2	5.85	126.90	122.80
31	L2	599	LEU	CA-CB-CG	5.84	128.74	115.30
27	А	413	LEU	CA-CB-CG	5.84	128.73	115.30
1	2	27	U	N3-C2-O2	-5.82	118.12	122.20
27	А	1593	LEU	CA-CB-CG	5.81	128.66	115.30
2	6	41	А	C2-N3-C4	5.80	113.50	110.60
2	6	58	G	P-O3'-C3'	5.80	126.66	119.70
27	А	1185	LEU	CA-CB-CG	5.75	128.53	115.30
27	А	1639	VAL	CA-CB-CG1	5.75	119.53	110.90
2	6	45	А	O5'-P-OP1	5.75	117.60	110.70
2	6	61	С	C6-N1-C2	-5.71	118.02	120.30
2	6	97	U	C6-N1-C2	-5.71	117.57	121.00
26	5	36	С	N3-C2-O2	-5.70	117.91	121.90
6	Ε	137	ASP	CB-CG-OD1	5.69	123.42	118.30
14	\mathbf{S}	106	ASP	CB-CG-OD1	5.67	123.40	118.30
11	Ο	191	ASP	CB-CG-OD1	5.66	123.39	118.30
21	f	33	LEU	CA-CB-CG	5.66	128.32	115.30
15	W	140	ASP	CB-CG-OD1	5.63	123.37	118.30
27	A	941	LYS	N-CA-C	5.62	$1\overline{26.17}$	111.00
15	W	193	LEU	CB-CG-CD1	5.60	120.53	111.00
1	2	13	C	C6-N1-C2	-5.58	118.07	120.30
17	a	61	VAL	CG1-CB-CG2	-5.57	101.99	110.90
26	5	39	C	N1-C2-O2	5.55	$122.2\overline{3}$	118.90
26	5	43	U	N1-C2-O2	$5.5\overline{5}$	126.68	122.80
26	5	23	C	N3-C2-O2	-5.54	118.02	121.90



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
33	Р	215	ASP	CB-CG-OD1	5.54	123.29	118.30
2	6	62	С	C2-N1-C1'	5.54	124.89	118.80
26	5	105	U	C5-C6-N1	5.53	125.47	122.70
30	L	375	VAL	CG1-CB-CG2	-5.51	102.09	110.90
26	5	23	С	C6-N1-C2	-5.50	118.10	120.30
26	5	22	U	N1-C2-O2	5.48	126.64	122.80
2	6	17	С	C5-C6-N1	5.47	123.74	121.00
1	2	38	А	N7-C8-N9	5.46	116.53	113.80
1	2	27	U	O4'-C1'-N1	5.44	112.55	108.20
2	6	34	G	C8-N9-C4	-5.43	104.23	106.40
1	2	13	С	N3-C2-O2	-5.43	118.10	121.90
26	5	12	U	N1-C2-O2	5.42	126.59	122.80
27	А	1547	VAL	CA-CB-CG1	5.41	119.01	110.90
26	5	105	U	C6-N1-C2	-5.40	117.76	121.00
2	6	35	А	OP1-P-O3'	5.39	117.06	105.20
2	6	35	А	N3-C4-C5	-5.37	123.04	126.80
1	2	35	А	N7-C8-N9	5.36	116.48	113.80
2	6	50	А	P-O3'-C3'	5.35	126.12	119.70
31	L2	676	LEU	CA-CB-CG	5.35	127.61	115.30
6	Е	221	ASP	CB-CG-OD1	5.35	123.12	118.30
14	S	27	LEU	CA-CB-CG	5.35	127.61	115.30
1	2	3	С	C6-N1-C2	-5.34	118.16	120.30
2	6	57	U	C2-N1-C1'	5.33	124.10	117.70
26	5	36	С	C5-C6-N1	5.32	123.66	121.00
26	5	99	С	N3-C2-O2	-5.32	118.17	121.90
2	6	45	А	C4-N9-C1'	5.31	135.86	126.30
26	5	98	С	C6-N1-C2	-5.30	118.18	120.30
31	L2	666	ARG	NE-CZ-NH1	5.30	122.95	120.30
27	А	1690	ASP	CB-CG-OD1	5.30	123.07	118.30
31	L2	811	ARG	NE-CZ-NH1	5.30	122.95	120.30
2	6	4	С	C6-N1-C2	-5.29	118.18	120.30
26	5	11	U	C6-N1-C1'	-5.29	113.80	121.20
2	6	8	С	C6-N1-C2	-5.28	118.19	120.30
26	5	12	U	N3-C2-O2	-5.28	118.50	122.20
2	6	36	А	N1-C6-N6	5.28	121.77	118.60
1	2	7	U	C2-N1-C1'	5.27	124.02	117.70
$\overline{26}$	5	114	С	N1-C2-O2	5.27	122.06	118.90
$\overline{26}$	5	47	A	O4'-C1'-N9	5.25	112.40	108.20
18	С	65	ILE	CG1-CB-CG2	-5.23	99.89	111.40
26	5	14	U	N3-C2-O2	-5.23	118.54	122.20
19	d	110	LEU	CA-CB-CG	5.23	$1\overline{27.32}$	115.30
26	5	22	U	C2-N1-C1'	5.23	123.97	117.70



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
26	5	38	С	C6-N1-C2	-5.23	118.21	120.30
31	L2	811	ARG	CD-NE-CZ	5.22	130.91	123.60
27	А	830	LEU	CA-CB-CG	5.22	127.31	115.30
6	Е	173	ASP	CB-CG-OD1	5.18	122.96	118.30
26	5	11	U	C6-N1-C2	-5.18	117.89	121.00
35	Т	309	ASP	CB-CG-OD1	5.18	122.96	118.30
30	L	55	ASP	CB-CG-OD1	5.17	122.96	118.30
10	N	97	TYR	CA-CB-CG	5.15	123.19	113.40
2	6	6	С	O5'-P-OP2	-5.15	101.06	105.70
22	g	60	VAL	CG1-CB-CG2	-5.14	102.67	110.90
3	С	190	LEU	CA-CB-CG	5.12	127.07	115.30
31	L2	811	ARG	CG-CD-NE	5.11	122.53	111.80
17	a	76	MET	CA-CB-CG	5.10	121.97	113.30
26	5	43	U	N3-C2-O2	-5.09	118.64	122.20
26	5	103	С	O4'-C1'-N1	5.09	112.27	108.20
27	А	1284	LEU	CA-CB-CG	5.08	126.98	115.30
27	А	1753	LEU	CA-CB-CG	5.08	126.98	115.30
26	5	10	U	C6-N1-C1'	-5.08	114.09	121.20
37	b	31	PHE	CB-CG-CD1	5.08	124.35	120.80
2	6	4	С	C5-C6-N1	5.07	123.53	121.00
2	6	5	U	C2-N1-C1'	5.06	123.78	117.70
26	5	99	С	C6-N1-C1'	-5.05	114.73	120.80
2	6	61	С	C5-C6-N1	5.05	123.52	121.00
2	6	64	U	N3-C2-O2	-5.05	118.67	122.20
26	5	9	G	C4-N9-C1'	5.04	133.06	126.50
26	5	104	С	C6-N1-C2	-5.04	118.28	120.30
26	5	10	U	C6-N1-C2	-5.03	117.98	121.00
27	А	1702	LEU	CA-CB-CG	5.03	126.86	115.30
2	6	31	U	N1-C2-O2	5.01	126.31	122.80

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
27	А	165	ARG	Peptide
27	А	707	ARG	Sidechain
27	А	995	ARG	Sidechain
3	С	940	ARG	Sidechain
17	a	51	ARG	Sidechain
17	a	69	ARG	Sidechain
19	d	110	LEU	Peptide
19	d	55	ARG	Sidechain



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Mol	Chain	Res	Type	Group
19	d	61	ARG	Sidechain
20	е	50	PHE	Peptide
22	g	33	GLY	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2	823	0	416	2	0
2	6	2075	0	1048	12	0
3	С	7184	0	7206	20	0
4	D	253	0	120	0	0
5	DX	3220	0	1416	2	0
6	Ε	2341	0	2275	4	0
7	J	2793	0	1241	0	0
8	K	941	0	424	0	0
9	L1	1353	0	620	0	0
10	Ν	1184	0	1189	5	0
11	0	2328	0	2317	8	0
12	Q	6859	0	2971	0	0
13	R	1571	0	725	3	0
14	S	1236	0	1210	7	0
15	W	1276	0	1221	11	0
16	Ζ	459	0	204	0	0
17	a	651	0	669	0	0
18	с	641	0	689	0	0
19	d	775	0	818	0	0
20	е	653	0	668	0	0
21	f	564	0	572	0	0
22	g	568	0	590	0	0
23	q	514	0	236	0	0
23	r	594	0	270	0	0
23	S	659	0	299	0	0
23	t	514	0	236	0	0
24	Z	198	0	184	0	0
25	3	499	0	479	0	0
26	5	1936	0	982	10	0
27	А	16477	0	16462	46	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	Ι	3739	0	1699	2	0
29	IN	492	0	330	4	0
30	L	3623	0	2842	6	0
31	L2	3049	0	2973	21	0
32	М	827	0	380	1	0
33	Р	942	0	929	2	0
34	PX	1465	0	620	0	0
35	Т	2854	0	2812	15	0
36	TF	2835	0	1200	4	0
37	b	717	0	736	0	0
38	С	32	0	12	0	0
39	N	3	0	0	0	0
40	А	36	0	6	1	0
All	All	81753	0	62296	154	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 1.

All (154) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
2:6:59:G:H1	2:6:76:A:H61	1.01	0.96
2:6:59:G:H1	2:6:76:A:N6	1.75	0.84
14:S:56:ILE:HG12	14:S:62:ILE:HG23	1.78	0.65
14:S:57:ILE:HD13	15:W:97:ASN:HB3	1.80	0.63
2:6:1:G:O2'	10:N:99:ASN:ND2	2.33	0.62
26:5:12:U:H3	26:5:65:G:H1	1.48	0.61
27:A:435:CYS:SG	27:A:439:GLN:NE2	2.73	0.61
6:E:62:LEU:HB2	6:E:351:LEU:HB2	1.85	0.58
27:A:1304:ASN:ND2	27:A:1565:LYS:O	2.36	0.58
27:A:929:GLU:OE1	27:A:933:ARG:NH1	2.38	0.57
35:T:390:GLY:HA3	35:T:416:ILE:HD11	1.87	0.56
33:P:57:ARG:NH1	35:T:472:GLN:O	2.38	0.56
35:T:314:ILE:HD12	35:T:324:HIS:HB2	1.87	0.56
26:5:36:C:N4	26:5:37:G:O6	2.39	0.55
27:A:1335:ILE:HG23	27:A:1365:ILE:HD11	1.88	0.55
1:2:10:C:H2'	1:2:11:G:H8	1.72	0.55
27:A:1255:THR:HA	27:A:1531:ASN:HD21	1.72	0.55
26:5:59:G:OP1	27:A:417:ARG:NH2	2.40	0.54
27:A:549:GLU:OE1	27:A:552:ARG:NH1	2.40	0.54
3:C:451:HIS:O	3:C:578:ARG:NH1	2.41	0.54



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
27:A:71:ARG:NH1	27:A:177:ASP:OD2	2.41	0.54
31:L2:844:TYR:OH	31:L2:862:ARG:NH2	2.41	0.54
11:O:169:VAL:HG13	15:W:216:LEU:HD22	1.90	0.54
27:A:1333:VAL:HG13	27:A:1365:ILE:HD13	1.90	0.54
11:O:20:PHE:O	11:O:72:GLN:NE2	2.41	0.54
27:A:1310:ARG:NH1	27:A:1546:ASN:O	2.42	0.53
26:5:46:U:OP2	27:A:597:LYS:NZ	2.42	0.52
27:A:881:ILE:HG23	27:A:918:THR:HG23	1.90	0.52
31:L2:685:PRO:O	31:L2:687:HIS:ND1	2.43	0.52
3:C:93:ILE:HD12	35:T:275:LEU:HD22	1.91	0.51
3:C:213:ASP:N	3:C:213:ASP:OD1	2.44	0.51
2:6:49:G:OP1	30:L:33:ARG:NH2	2.44	0.51
36:TF:790:PRO:HA	36:TF:802:TYR:HA	1.92	0.51
27:A:1155:TRP:O	27:A:1159:ASN:ND2	2.43	0.51
27:A:1617:ARG:NH1	31:L2:586:GLU:OE2	2.44	0.51
3:C:313:GLN:O	3:C:417:ARG:NH1	2.44	0.50
10:N:139:CYS:SG	10:N:140:ARG:N	2.85	0.50
36:TF:617:GLY:O	36:TF:621:GLY:N	2.44	0.50
6:E:161:ARG:HD2	6:E:203:ASP:HA	1.93	0.49
11:O:66:LYS:NZ	29:IN:19:N:OP1	2.45	0.49
3:C:92:PRO:HA	35:T:278:ASN:HD21	1.77	0.49
3:C:236:MET:SD	3:C:837:GLN:NE2	2.83	0.49
30:L:376:ASP:OD1	30:L:376:ASP:N	2.46	0.49
35:T:346:ILE:HD13	35:T:380:LEU:HD11	1.94	0.49
3:C:772:TRP:NE1	3:C:776:GLU:OE2	2.44	0.49
27:A:211:GLN:OE1	27:A:214:ARG:NH1	2.44	0.49
36:TF:789:MET:O	36:TF:803:THR:N	2.40	0.49
27:A:1580:HIS:NE2	31:L2:595:ASP:OD1	2.45	0.49
11:0:229:LYS:O	11:O:277:ARG:NH1	2.45	0.49
32:M:156:HIS:O	32:M:160:PHE:N	2.43	0.49
27:A:425:PRO:HB2	27:A:428:LYS:HB2	1.95	0.48
3:C:381:LEU:HG	3:C:416:LEU:HD21	1.95	0.48
15:W:126:GLU:HG3	15:W:130:ARG:HE	1.78	0.48
27:A:109:PRO:HG3	27:A:630:TRP:HE1	1.77	0.48
27:A:991:THR:HG22	30:L:81:GLN:HE22	1.76	0.48
30:L:37:LEU:HD11	30:L:155:ALA:HA	1.96	0.48
2:6:14:C:H2'	2:6:15:A:H8	1.77	0.48
30:L:119:ASP:OD2	30:L:122:LYS:NZ	2.46	0.48
35:T:244:GLY:H	35:T:273:TRP:HH2	1.62	0.48
26:5:97:G:N2	26:5:115:U:O2	2.47	0.48
27:A:1870:ASP:OD2	31:L2:556:ARG:NH1	2.43	0.47



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
6:E:321:TYR:OH	6:E:357:GLN:O	2.31	0.47
31:L2:550:ARG:HB3	31:L2:660:LYS:HB3	1.95	0.47
27:A:523:ASN:OD1	27:A:552:ARG:NH2	2.47	0.47
27:A:1865:ARG:NH2	31:L2:726:ASP:OD2	2.43	0.47
35:T:391:SER:OG	35:T:393:ASP:OD1	2.32	0.47
27:A:1243:ARG:NH1	27:A:1246:GLN:OE1	2.46	0.47
27:A:1242:ASN:OD1	27:A:1245:ARG:NH1	2.47	0.47
14:S:51:THR:HB	14:S:66:ASP:H	1.80	0.47
26:5:12:U:H5'	27:A:224:THR:HG23	1.97	0.47
35:T:416:ILE:HA	35:T:431:ALA:HA	1.95	0.46
13:R:134:ARG:HA	35:T:385:TYR:HB2	1.97	0.46
36:TF:452:ILE:O	36:TF:456:LYS:N	2.47	0.46
10:N:101:CYS:SG	10:N:139:CYS:HB2	2.56	0.46
11:O:64:ARG:NH1	29:IN:19:N:OP2	2.49	0.46
27:A:1504:GLU:O	27:A:1533:ARG:NH1	2.48	0.46
31:L2:60:LEU:HD11	31:L2:876:ALA:HB1	1.97	0.46
31:L2:677:TYR:HB3	31:L2:714:VAL:HG11	1.97	0.46
27:A:251:ASP:OD2	27:A:253:ASN:ND2	2.49	0.45
35:T:201:SER:OG	35:T:455:GLN:NE2	2.49	0.45
3:C:800:PRO:HA	3:C:803:ARG:HE	1.82	0.45
26:5:45:C:H4'	27:A:596:TYR:HB3	1.98	0.45
31:L2:548:LEU:HD22	31:L2:661:ALA:HB1	1.98	0.45
2:6:2:U:H2'	2:6:3:G:H8	1.82	0.45
31:L2:675:CYS:SG	31:L2:678:CYS:N	2.86	0.45
33:P:38:HIS:HB2	35:T:282:ARG:HD3	1.99	0.44
15:W:180:LYS:HD3	15:W:197:ALA:HB3	1.99	0.44
27:A:609:LYS:NZ	40:A:3000:IHP:O12	2.50	0.44
27:A:1144:LYS:HE2	27:A:1148:ASN:HD21	1.82	0.44
31:L2:805:LEU:HD11	31:L2:832:ALA:HB2	1.99	0.44
2:6:34:G:H2'	2:6:35:A:H8	1.82	0.44
28:I:565:ILE:HA	28:I:569:GLY:HA3	1.99	0.44
3:C:354:ARG:NH1	27:A:381:PRO:O	2.50	0.44
35:T:393:ASP:OD1	35:T:393:ASP:N	2.51	0.44
27:A:1278:VAL:HG13	27:A:1284:LEU:HD12	2.00	0.44
10:N:103:LEU:HD13	27:A:59:GLU:HB2	2.00	0.44
14:S:52:LYS:HA	14:S:158:LYS:HA	2.00	0.44
13:R:9:ALA:O	13:R:11:THR:N	2.45	0.43
14:S:60:PHE:HB2	15:W:99:PHE:HE2	1.83	0.43
26:5:23:C:H5'	26:5:24:G:H5"	1.99	0.43
27:A:1491:LYS:O	27:A:1710:ASN:ND2	2.49	0.43
3:C:737:PRO:HB2	3:C:775:ARG:HE	1.82	0.43



Atom-1	Atom-2	Interatomic	Clash
	1100111-2	distance (Å)	overlap (Å)
27:A:578:LEU:HA	27:A:581:ILE:HD12	2.00	0.43
6:E:307:ARG:NH1	15:W:116:GLU:OE1	2.51	0.43
27:A:1544:ARG:HB2	27:A:1547:VAL:HG12	2.00	0.43
31:L2:810:ILE:H	31:L2:810:ILE:HG13	1.56	0.43
2:6:30:A:O2'	15:W:223:ARG:NH1	2.51	0.43
10:N:70:ILE:HG23	10:N:74:LEU:HB3	2.01	0.43
26:5:12:U:O2	26:5:65:G:N2	2.41	0.43
35:T:220:VAL:HG11	35:T:261:LEU:HD21	1.99	0.43
14:S:83:GLU:HA	14:S:106:ASP:HB2	1.99	0.43
31:L2:580:SER:O	31:L2:589:ARG:NH1	2.52	0.43
27:A:1321:GLU:OE1	27:A:1471:ARG:NH1	2.51	0.43
3:C:189:VAL:HG12	3:C:199:LEU:HA	2.00	0.43
31:L2:868:SER:HB2	31:L2:872:GLN:H	1.84	0.43
31:L2:56:ASP:OD1	31:L2:56:ASP:N	2.52	0.42
1:2:33:G:OP1	31:L2:666:ARG:NH2	2.49	0.42
27:A:1941:ARG:HH22	27:A:2013:GLY:HA2	1.84	0.42
3:C:181:ILE:HG13	3:C:182:LYS:HG2	2.02	0.42
3:C:282:VAL:O	3:C:286:ASN:ND2	2.44	0.42
27:A:1072:LEU:HD22	27:A:1087:LEU:HD22	2.02	0.42
3:C:151:GLU:OE1	3:C:421:LYS:NZ	2.52	0.42
3:C:225:VAL:HG23	3:C:251:LEU:HD12	2.02	0.42
27:A:546:LEU:HD13	27:A:648:LEU:HD21	2.02	0.42
29:IN:149:N:H3'	31:L2:839:HIS:HE1	1.85	0.42
2:6:22:A:H62	15:W:167:VAL:HG11	1.84	0.42
3:C:210:ASN:HB3	3:C:636:TYR:HB2	2.01	0.42
5:DX:279:VAL:O	5:DX:283:ARG:N	2.44	0.42
27:A:802:THR:HB	27:A:805:GLU:HG3	2.02	0.42
13:R:61:GLY:HA3	14:S:136:ILE:HG21	2.02	0.41
35:T:294:LEU:HD12	35:T:303:LEU:HD11	2.02	0.41
27:A:200:ASP:OD1	27:A:240:ARG:NH2	2.53	0.41
31:L2:805:LEU:HD13	31:L2:810:ILE:HG12	2.03	0.41
27:A:1002:ASP:OD1	27:A:1004:ASN:ND2	2.49	0.41
2:6:14:C:H2'	2:6:15:A:C8	2.55	0.41
27:A:1597:PHE:HB3	27:A:1609:VAL:HG11	2.03	0.41
2:6:2:U:H2'	2:6:3:G:C8	2.56	0.41
3:C:474:LEU:HA	3:C:499:GLY:HA3	2.03	0.41
28:I:564:PHE:O	28:I:569:GLY:N	2.53	0.41
3:C:177:ARG:NH2	3:C:638:ASP:OD2	2.49	0.41
5:DX:214:GLY:N	5:DX:217:VAL:O	2.53	0.41
26:5:100:U:H2'	26:5:101:U:H6	1.85	0.41
27:A:964:ASP:OD1	27:A:964:ASP:N	2.52	0.41



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:A:1835:GLN:HB3	31:L2:557:VAL:HG11	2.02	0.41
31:L2:752:ILE:HD12	31:L2:773:LEU:HD21	2.03	0.41
29:IN:145:N:H1'2	29:IN:146:N:H5'	2.02	0.41
11:O:72:GLN:HA	11:O:75:SER:HB3	2.02	0.41
15:W:116:GLU:HA	15:W:117:PRO:HD3	1.93	0.41
2:6:55:C:OP2	2:6:74:U:O2'	2.33	0.40
30:L:236:ASP:OD1	30:L:236:ASP:N	2.49	0.40
11:O:22:ILE:HG21	15:W:111:LEU:HD23	2.03	0.40
15:W:209:SER:HB2	15:W:212:GLU:HB2	2.03	0.40
3:C:328:ALA:HA	3:C:334:ILE:HD12	2.04	0.40
11:O:64:ARG:HH21	11:O:163:HIS:CE1	2.40	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	С	906/972~(93%)	868~(96%)	35 (4%)	3~(0%)	37 68
4	D	49/285~(17%)	48 (98%)	0	1 (2%)	6 33
5	DX	648/795~(82%)	631~(97%)	15 (2%)	2 (0%)	37 68
6	Е	297/357~(83%)	285~(96%)	12 (4%)	0	100 100
7	J	559/848~(66%)	548 (98%)	9 (2%)	2 (0%)	30 64
8	K	187/225~(83%)	182 (97%)	3 (2%)	2(1%)	12 45
9	L1	273/538~(51%)	264 (97%)	9 (3%)	0	100 100
10	Ν	141/144~(98%)	125~(89%)	16 (11%)	0	100 100
11	Ο	286/420~(68%)	265~(93%)	21 (7%)	0	100 100
12	Q	1382/1485~(93%)	1346 (97%)	35(2%)	1 (0%)	48 79
13	R	313/536~(58%)	281 (90%)	27 (9%)	5 (2%)	8 38



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	entiles
14	S	157/166~(95%)	143 (91%)	11 (7%)	3~(2%)	6	34
15	W	156/579~(27%)	137~(88%)	19 (12%)	0	100	100
16	Ζ	90/166~(54%)	83 (92%)	7 (8%)	0	100	100
17	a	81/126 (64%)	71 (88%)	10 (12%)	0	100	100
18	с	79/119~(66%)	69~(87%)	10 (13%)	0	100	100
19	d	94/118~(80%)	82 (87%)	12 (13%)	0	100	100
20	е	77/92~(84%)	63 (82%)	13 (17%)	1 (1%)	10	41
21	f	70/86~(81%)	64 (91%)	6 (9%)	0	100	100
22	g	71/76~(93%)	65~(92%)	6 (8%)	0	100	100
23	q	99/504~(20%)	97~(98%)	2 (2%)	0	100	100
23	r	115/504~(23%)	112 (97%)	2 (2%)	1 (1%)	14	49
23	s	130/504~(26%)	126 (97%)	4 (3%)	0	100	100
23	t	99/504~(20%)	97~(98%)	2 (2%)	0	100	100
24	Z	23/451~(5%)	23~(100%)	0	0	100	100
25	3	56/476~(12%)	56 (100%)	0	0	100	100
27	А	1977/2335~(85%)	1863 (94%)	112 (6%)	2 (0%)	48	79
28	Ι	749/855~(88%)	728 (97%)	20 (3%)	1 (0%)	48	79
30	L	547/802~(68%)	514 (94%)	32 (6%)	1 (0%)	44	75
31	L2	363/894~(41%)	321~(88%)	37 (10%)	5 (1%)	9	40
32	М	162/243~(67%)	159 (98%)	3 (2%)	0	100	100
33	Р	108/229~(47%)	103~(95%)	5 (5%)	0	100	100
34	PX	291/917~(32%)	286~(98%)	5 (2%)	0	100	100
35	Т	$\overline{356/514}~(69\%)$	337~(95%)	19 (5%)	0	100	100
36	TF	562/837~(67%)	549 (98%)	12 (2%)	1 (0%)	44	75
37	b	88/240~(37%)	78~(89%)	8 (9%)	2 (2%)	5	31
All	All	$11\overline{641}/18942~(62\%)$	11069 (95%)	539 (5%)	33 (0%)	38	68

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All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
31	L2	579	VAL
3	С	166	CYS
13	R	47	ARG

Mol	Chain	Res	Type
13	R	277	THR
3	С	126	SER
3	С	948	SER
7	J	448	ALA
7	J	505	ALA
14	S	12	PRO
14	S	80	LYS
27	А	1656	THR
28	Ι	812	GLN
31	L2	644	ALA
31	L2	776	GLU
14	S	86	LEU
20	е	69	LYS
5	DX	427	SER
8	К	45	PRO
13	R	82	MET
13	R	97	LYS
31	L2	584	GLU
36	TF	560	GLN
23	r	52	LEU
5	DX	714	LYS
8	K	60	ALA
12	Q	956	SER
31	L2	684	PHE
37	b	87	PRO
13	R	10	PRO
27	А	1785	VAL
30	L	208	VAL
4	D	155	ILE
37	b	113	GLY

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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	Percentiles
3	\mathbf{C}	807/866~(93%)	797~(99%)	10 (1%)	67 82



Mol	Chain	Analysed	Rotameric	Outliers	Perce	entile	s
6	Е	256/300~(85%)	254 (99%)	2 (1%)	79	88	
10	Ν	130/130~(100%)	128 (98%)	2(2%)	60	77	
11	Ο	258/361 (72%)	254 (98%)	4 (2%)	58	76	
14	S	129/134~(96%)	125~(97%)	4 (3%)	35	63	
15	W	135/502~(27%)	130 (96%)	5 (4%)	29	58	
17	a	73/101~(72%)	72 (99%)	1 (1%)	62	79	
18	с	76/101~(75%)	74 (97%)	2(3%)	41	66	
19	d	90/110 (82%)	84 (93%)	6 (7%)	13	40	
20	е	74/84~(88%)	71~(96%)	3~(4%)	26	55	
21	f	61/74~(82%)	61 (100%)	0	100	100	
22	g	63/66~(96%)	58~(92%)	5(8%)	10	34	
24	z	21/371~(6%)	21 (100%)	0	100	100	
25	3	55/395~(14%)	55~(100%)	0	100	100	
27	А	1792/2108~(85%)	1761 (98%)	31 (2%)	56	75	
30	L	231/709~(33%)	224 (97%)	7 (3%)	36	63	
31	L2	334/806~(41%)	323~(97%)	11 (3%)	33	61	
33	Р	103/203~(51%)	101 (98%)	2(2%)	52	73	
35	Т	313/441~(71%)	309~(99%)	4 (1%)	65	81	
37	b	74/177~(42%)	68~(92%)	6 (8%)	9	33	
All	All	5075/8039~(63%)	4970 (98%)	105 (2%)	49	71	

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All (105) residues with a non-rotameric side chain are listed below:

Mol	Chain	Res	Type
3	С	103	THR
3	С	199	LEU
3	С	213	ASP
3	С	219	LEU
3	С	298	LEU
3	С	300	LEU
3	С	327	TYR
3	С	339	PHE
3	С	707	ILE
3	С	903	HIS
6	Е	203	ASP



Mol	Chain	Res	Type
6	Е	231	MET
10	Ν	97	TYR
10	Ν	115	THR
11	0	131	THR
11	0	245	GLU
11	0	254	GLN
11	0	259	ARG
14	S	27	LEU
14	S	61	MET
14	S	102	ASN
14	S	152	ARG
15	W	73	ASP
15	W	87	THR
15	W	93	PHE
15	W	129	ARG
15	W	212	GLU
17	a	76	MET
18	с	12	HIS
18	с	72	ASP
19	d	43	LEU
19	d	53	LEU
19	d	74	TRP
19	d	93	ASP
19	d	111	ARG
19	d	112	ASN
20	е	50	PHE
20	е	72	LYS
20	е	87	LEU
22	g	9	LEU
22	g	13	MET
22	g	14	ASP
22	g	32	ARG
22	g	35	ASP
$\overline{27}$	А	97	HIS
27	A	166	PHE
$\overline{27}$	A	319	LEU
$\overline{27}$	А	327	VAL
$\overline{27}$	А	351	TYR
27	A	409	ARG
27	A	413	LEU
27	А	479	THR
27	А	579	GLN



Mol	Chain	Res	Type
27	А	642	ARG
27	А	676	ARG
27	А	705	LYS
27	А	884	HIS
27	А	964	ASP
27	А	1021	ASP
27	А	1089	CYS
27	А	1195	ARG
27	А	1293	ASN
27	А	1402	ARG
27	А	1467	LEU
27	А	1536	LEU
27	А	1582	TRP
27	А	1622	MET
27	А	1636	LYS
27	А	1702	LEU
27	А	1763	LEU
27	А	1813	ARG
27	А	1833	LEU
27	А	1918	ASN
27	А	1946	ASN
27	А	1966	HIS
30	L	13	ASN
30	L	202	ARG
30	L	206	ARG
30	L	213	GLU
30	L	222	LEU
30	L	244	GLN
30	L	250	GLU
31	L2	539	GLU
31	L2	550	ARG
31	L2	589	ARG
31	L2	624	LYS
31	L2	628	LYS
31	L2	657	GLN
31	L2	658	ARG
31	L2	676	LEU
31	L2	702	ASN
31	L2	737	ARG
31	L2	810	ILE
33	Р	83	HIS
33	Р	102	ASN



Mol	Chain	Res	Type
35	Т	29	ASN
35	Т	216	ASN
35	Т	416	ILE
35	Т	432	ASP
37	b	10	LEU
37	b	16	ARG
37	b	23	ASP
37	b	$\overline{25}$	ARG
37	b	48	PHE
37	b	81	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
10	N	99	ASN
10	N	116	ASN
11	0	163	HIS
14	S	102	ASN
15	W	213	GLN
18	с	64	ASN
19	d	45	ASN
20	е	32	GLN
27	А	368	GLN
27	А	439	GLN
27	А	579	GLN
27	А	1096	HIS
27	А	1282	GLN
27	А	1293	ASN
27	А	1468	ASN
27	А	1487	HIS
27	А	1531	ASN
27	А	1830	GLN
27	А	1918	ASN
30	L	13	ASN
30	L	81	GLN
31	L2	702	ASN
31	L2	839	HIS
35	Т	50	ASN
35	Т	278	ASN
35	Т	283	HIS
35	Т	324	HIS
35	Т	455	GLN



Continued from previous page...

Mol	Chain	Res	Type
37	b	11	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	38/188~(20%)	19~(50%)	1 (2%)
2	6	96/106~(90%)	42 (43%)	7~(7%)
26	5	90/116~(77%)	26 (28%)	2(2%)
29	IN	0/154	-	-
All	All	224/564~(39%)	87~(38%)	10 (4%)

All (87) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	8	С
1	2	14	С
1	2	15	U
1	2	16	U
1	2	19	G
1	2	20	G
1	2	24	А
1	2	28	С
1	2	29	А
1	2	30	А
1	2	31	G
1	2	32	U
1	2	33	G
1	2	34	U
1	2	35	А
1	2	36	G
1	2	37	U
1	2	38	А
1	2	39	U
2	6	5	U
2	6	6	С
2	6	7	G
2	6	9	U
2	6	10	U
2	6	12	G
2	6	22	А
2	6	25	С



Mol	Chain	Res	Type
2	6	26	U
2	6	27	А
2	6	28	А
2	6	29	А
2	6	33	G
2	6	34	G
2	6	35	А
2	6	36	А
2	6	37	С
2	6	41	А
2	6	42	С
2	6	43	А
2	6	44	G
2	6	45	А
2	6	46	G
2	6	48	А
2	6	51	U
2	6	53	А
2	6	54	G
2	6	56	А
2	6	59	G
2	6	60	С
2	6	61	С
2	6	68	С
2	6	69	А
2	6	74	U
2	6	78	А
2	6	79	С
2	6	81	С
2	6	82	А
2	6	84	A
2	6	87	С
2	6	88	G
2	6	91	А
26	5	10	U
26	5	11	U
26	5	20	G
26	5	21	A
26	5	34	U
26	5	35	U
26	5	36	С
26	5	38	С



Mol	Chain	Res	Type
26	5	39	С
26	5	42	U
26	5	45	С
26	5	47	А
26	5	52	U
26	5	53	U
$\overline{26}$	5	57	G
26	5	69	А
26	5	86	С
26	5	89	U
26	5	91	U
26	5	92	U
26	5	93	U
$\overline{26}$	5	94	U
$\overline{26}$	5	95	G
26	5	96	A
$\overline{26}$	5	104	C
$2\overline{6}$	5	115	U

Continued from previous page...

All (10) RNA pucker outliers are listed below:

Mol	Chain	\mathbf{Res}	Type
1	2	28	С
2	6	5	U
2	6	33	G
2	6	35	А
2	6	50	А
2	6	58	G
2	6	81	С
2	6	82	А
26	5	92	Ū
26	5	95	G

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the



Mol Type	Chain	Dec	Timle	Bond lengths			Bond angles			
	туре	Ullaili	nes	LINK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
13	SEP	R	232	13	3,4,10	0.75	0	2,4,14	1.37	0
13	SEP	R	224	13	3,4,10	0.71	0	2,4,14	1.30	0

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).

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
13	SEP	R	232	13	-	0/0/2/10	-
13	SEP	R	224	13	-	0/0/2/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 5 ligands modelled in this entry, 3 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	Tinle	Bo	ond leng	\mathbf{ths}	B	ond ang	les
	туре	Chain	nes	LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2
38	GTP	С	1500	-	26,34,34	1.22	2 (7%)	32,54,54	1.56	7 (21%)
40	IHP	А	3000	-	36,36,36	1.50	6 (16%)	54,60,60	0.78	3 (5%)

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
38	GTP	С	1500	-	-	3/18/38/38	0/3/3/3
40	IHP	А	3000	-	-	4/30/54/54	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\operatorname{Ideal}(\operatorname{\AA})$
38	С	1500	GTP	C5-C6	-4.25	1.38	1.47
40	А	3000	IHP	P1-011	3.22	1.65	1.59
40	А	3000	IHP	P3-O13	3.21	1.65	1.59
40	А	3000	IHP	P6-O16	3.18	1.65	1.59
40	А	3000	IHP	P2-O12	3.15	1.65	1.59
40	А	3000	IHP	P5-O15	3.11	1.65	1.59
40	А	3000	IHP	P4-014	3.05	1.65	1.59
38	С	1500	GTP	C2-N3	2.17	1.38	1.33

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
38	С	1500	GTP	PA-O3A-PB	-3.90	119.43	132.83
38	С	1500	GTP	C5-C6-N1	2.96	119.18	113.95
40	А	3000	IHP	C5-C6-C1	2.86	116.68	110.41
38	С	1500	GTP	PB-O3B-PG	-2.85	123.05	132.83
38	С	1500	GTP	C2-N1-C6	-2.77	120.00	125.10
38	С	1500	GTP	C8-N7-C5	2.62	107.98	102.99
40	А	3000	IHP	C6-C1-C2	2.11	115.02	110.41
40	А	3000	IHP	O11-C1-C6	-2.10	103.72	108.69
38	C	1500	GTP	O6-C6-C5	-2.08	120.30	124.37
38	С	1500	GTP	O5'-C5'-C4'	2.03	115.96	108.99

There are no chirality outliers.

All (7) torsion outliers are listed below:



Mol	Chain	Res	Type	Atoms
38	С	1500	GTP	C5'-O5'-PA-O3A
38	С	1500	GTP	C5'-O5'-PA-O2A
38	С	1500	GTP	C5'-O5'-PA-O1A
40	А	3000	IHP	C1-O11-P1-O21
40	А	3000	IHP	C3-O13-P3-O23
40	А	3000	IHP	C4-O14-P4-O24
40	А	3000	IHP	C3-O13-P3-O43

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
40	А	3000	IHP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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 the outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-19399. 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: 208

Y Index: 181

Z Index: 164

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

6.4 Orthogonal standard-deviation projections (False-color) (i)

6.4.1 Primary map



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



6.5 Orthogonal surface views (i)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.975. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.6 Mask visualisation (i)

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



7 Map analysis (i)

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

7.1 Map-value distribution (i)



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



7.2 Volume estimate (i)



The volume at the recommended contour level is $632~\mathrm{nm^3};$ this corresponds to an approximate mass of 571 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 0.286 ${\rm \AA^{-1}}$



8 Fourier-Shell correlation (i)

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



9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-19399 and PDB model 8RO2. Per-residue inclusion information can be found in section 3 on page 12.

9.1 Map-model overlay (i)



The images above show the 3D surface view of the map at the recommended contour level 0.975 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 (0.975).



9.4 Atom inclusion (i)



At the recommended contour level, 61% of all backbone atoms, 55% 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 (0.975) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	$\mathbf{Q} extsf{-score}$
All	0.5500	0.2970
2	0.1030	0.1420
3	0.1130	0.2610
5	0.7420	0.3420
6	0.1140	0.1380
А	0.6610	0.4410
С	0.7990	0.4230
D	0.3200	0.1480
DX	0.3170	0.0420
Е	0.7530	0.4590
Ι	0.7640	0.2170
IN	0.1340	0.1400
J	0.4970	0.2040
Κ	0.8930	0.2380
L	0.5120	0.2490
L1	0.0050	-0.0160
L2	0.5040	0.3570
М	0.3880	0.2140
Ν	0.7100	0.4570
О	0.4830	0.3360
Р	0.3950	0.3060
PX	0.3900	0.0850
Q	0.1440	0.0730
R	0.5260	0.3470
\mathbf{S}	0.6770	0.3700
Т	0.8480	0.4350
TF	0.6370	0.1070
W	0.4190	0.3350
Z	0.5930	0.1980
a	0.7150	0.4790
b	0.5820	0.4170
c	0.5730	0.4140
d	0.4780	0.3430
e	0.5900	0.4110
f	0.6080	0.4210



Chain	Atom inclusion	Q-score
g	0.5840	0.4440
q	0.6130	0.2030
r	0.5660	0.1850
s	0.9060	0.2290
t	0.5800	0.1830
Z	0.0260	-0.0320

