

Oct 1, 2024 – 09:03 PM JST

PDB ID	:	8XI2
EMDB ID	:	EMD-38362
Title	:	Cryo-EM structure of the Chlamydomonas C [*] complex
Authors	:	Lu, Y.; Zhan, X.
Deposited on	:	2023-12-19
Resolution	:	2.60 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.dev113
Mogul	:	1.8.5 (274361), 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)	:	2.39

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.60 Å.

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



INIEUTIC	$(\# {\rm Entries})$	$(\# { m Entries})$
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 $\geq=3, 2, 1$ 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	А	2398	10%	9%	19%
2	В	111	29% 46%	·	23%
3	С	989	8%		11% 9%
4	Е	362	78%		10% 12%
5	F	101	27% 58%		6% 9%
6	q	503	8% 18% • 79%		
6	r	503	6% 22% • 74%		
6	S	503	• 13% • 86%		



Mol	Chain	Length	Quality of chain								
6	t	503	• 10% • 88%								
7	a	127	7% 63% 8%	29%							
8	Q.	77	9%	12% 16%							
	0	••	34%	12,10 10,10							
9	е	87	80%	11% 8%							
10	f	85	74%	9% 16%							
11	d	110	80%	11% 9%							
12	с	114	68%	10% 23%							
13	b	265	34% · 63%)							
14	T	925	42% 66% 5%	29%							
	-	020	33%	2370							
15	J	835	67% 5%	6 29%							
16	Р	235	3 9% 5%	56%							
17	М	563	• 13% • 86%								
18	Т	518	60% 6%	34%							
19	0	417	9% 61% ·	35%							
20	Ν	233	68% 5	% 27%							
21	R	684	33% 5% 62%	6							
22	Н	192	7% 6% 14% • 79%								
23	S	157	93%	6% ·							
24	W	576	38%	• 15%							
25	L	833	15% 49% 7%	44%							
26	Κ	303	29% 57% 12%	31%							
27	U	721	96%								
28	V	928	1 6 % 20% • 80%								
29	Q	1844	70%	- 30%							
30	5	7	71%	14% 14%							



	nam	Length		Quality of chain							
21	3	173	6%	00/	000/						



2 Entry composition (i)

There are 34 unique types of molecules in this entry. The entry contains 73326 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

• Molecule 1 is a protein called MPN domain-containing protein.

Mol	Chain	Residues		Α	AltConf	Trace			
1	А	1931	Total 15194	C 9743	N 2699	O 2682	S 70	0	0

• Molecule 2 is a RNA chain called U5 snRNA.

Mol	Chain	Residues		\mathbf{A}^{\dagger}	toms	AltConf	Trace		
2	В	86	Total 1817	C 812	N 307	0 612	Р 86	0	0

• Molecule 3 is a protein called Elongation factor Tu, chloroplastic.

Mol	Chain	Residues		Α	AltConf	Trace			
3	С	897	Total 6973	C 4431	N 1203	O 1297	$\begin{array}{c} \mathrm{S} \\ 42 \end{array}$	0	0

• Molecule 4 is a protein called U5-40K.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	Е	318	Total 2441	C 1524	N 436	0 465	S 16	0	0

• Molecule 5 is a RNA chain called U6 snRNA.

Mol	Chain	Residues		A	toms	AltConf	Trace		
5	F	92	Total 1985	C 885	N 369	O 637	Р 94	0	0

• Molecule 6 is a protein called Pre-mRNA-processing factor 19.

Mol	Chain	Residues		At	oms		AltConf	Trace	
6	q	106	Total 831	C 522	N 145	O 160	${S \over 4}$	0	0



	1					
\mathbf{Mol}	Chain	Residues	Atoms		AltConf	Trace
6	r	121	Total C N O	S	0	0
0	1	101	1021 638 183 196	4	0	0
6	G	70	Total C N O	S	0	0
0	5	70	570 353 108 107	2	0	0
6	+	69	Total C N O	S	0	0
0	t	02	504 312 95 96	1	0	0

• Molecule 7 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues		At	oms		AltConf	Trace	
7	a	90	Total 705	C 444	N 129	0 126	S 6	0	0

• Molecule 8 is a protein called Small nuclear ribonucleoprotein G.

Mol	Chain	Residues		Ato	\mathbf{ms}			AltConf	Trace
8	g	65	Total 512	C 323	N 90	0 96	S 3	0	0

• Molecule 9 is a protein called Small nuclear ribonucleoprotein E.

Mol	Chain	Residues		At	oms		AltConf	Trace	
9	е	80	Total 660	C 420	N 117	0 119	${S \atop 4}$	0	0

• Molecule 10 is a protein called Sm protein F.

Mol	Chain	Residues		At	\mathbf{oms}	AltConf	Trace		
10	f	71	Total 559	C 358	N 91	O 106	$\frac{S}{4}$	0	0

• Molecule 11 is a protein called Small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues		At	oms		AltConf	Trace	
11	d	100	Total 810	C 505	N 152	0 147	S 6	0	0

• Molecule 12 is a protein called Small nuclear ribonucleoprotein Sm D1.



Mol	Chain	Residues		At	oms			AltConf	Trace
12	с	88	Total 684	$\begin{array}{c} \mathrm{C} \\ 435 \end{array}$	N 121	O 124	$\frac{S}{4}$	0	0

• Molecule 13 is a protein called Sm domain-containing protein.

Mol	Chain	Residues		At	oms	AltConf	Trace		
13	b	99	Total 780	C 489	N 149	0 138	${f S}$ 4	0	0

• Molecule 14 is a protein called Syf1.

Mol	Chain	Residues		At	AltConf	Trace			
14	Ι	661	Total 4629	C 2900	N 855	0 861	S 13	0	0

• Molecule 15 is a protein called Crooked neck protein.

Mol	Chain	Residues		At	AltConf	Trace			
15	J	595	Total 4033	C 2511	N 759	O 753	S 10	0	0

• Molecule 16 is a protein called Cwf15/Cwc15 cell cycle control protein.

Mol	Chain	Residues		Ato	ms	AltConf	Trace	
16	Р	104	Total 867	$\begin{array}{c} \mathrm{C} \\ 536 \end{array}$	N 175	O 156	0	0

• Molecule 17 is a protein called PPIase cyclophilin-type domain-containing protein.

Mol	Chain	Residues		At	oms			AltConf	Trace
17	М	80	Total 644	C 402	N 121	O 120	S 1	0	0

• Molecule 18 is a protein called PLRG1.

Mol	Chain	Residues		At	oms			AltConf	Trace
18	Т	344	Total 2700	C 1705	N 488	0 490	S 17	0	0

• Molecule 19 is a protein called Rbm22.



Mol	Chain	Residues		At	oms			AltConf	Trace
19	0	273	Total 2136	C 1337	N 376	O 405	S 18	0	0

• Molecule 20 is a protein called G10 protein.

Mol	Chain	Residues		At	oms	AltConf	Trace		
20	Ν	171	Total 1412	C 897	N 260	0 248	${ m S} 7$	0	0

• Molecule 21 is a protein called SKI-interacting protein SKIP SNW domain-containing protein.

Mol	Chain	Residues		A	toms	5			AltConf	Trace
21	R	260	Total 1994	C 1251	N 361	0 377	Р 2	${ m S} { m 3}$	0	0

• Molecule 22 is a RNA chain called U2 snRNA.

Mol	Chain	Residues		A	AltConf	Trace			
22	Н	40	Total 838	C 375	N 134	O 289	Р 40	0	0

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

Mol	Chain	Residues		At	oms	AltConf	Trace		
23	S	155	Total 1198	C 754	N 213	0 225	S 6	0	0

• Molecule 24 is a protein called Prp17.

Mol	Chain	Residues		At	oms			AltConf	Trace
24	W	487	Total 2826	C 1721	N 553	0 549	${ m S} { m 3}$	0	0

• Molecule 25 is a protein called Cdc5L.

Mol	Chain	Residues		At	oms			AltConf	Trace
25	L	468	Total 3795	C 2349	N 722	0 712	S 12	0	0

• Molecule 26 is a protein called Pre-mRNA-splicing factor SPF27.



Mol	Chain	Residues		At	oms			AltConf	Trace
26	K	210	Total 1688	C 1045	N 318	O 321	$\frac{S}{4}$	0	0

• Molecule 27 is a protein called CWF21 domain-containing protein.

Mol	Chain	Residues		Ato	ms	AltConf	Trace		
27	U	26	Total 191	C 119	N 34	O 36	S 2	0	0

• Molecule 28 is a protein called MI domain-containing protein.

Mol	Chain	Residues		At	oms			AltConf	Trace
28	V	186	Total 1020	C 621	N 198	O 200	S 1	0	0

• Molecule 29 is a protein called Intron-binding protein aquarius.

Mol	Chain	Residues		Ato	ms		AltConf	Trace
29	Q	1299	Total 6423	C 3825	N 1299	O 1299	0	0

• Molecule 30 is a RNA chain called RNA (5'-R(P*CP*CP*GP*AP*AP*CP*G)-3').

Mol	Chain	Residues		At	oms			AltConf	Trace
30	5	7	Total 150	C 67	N 29	0 47	Р 7	0	0

• Molecule 31 is a RNA chain called RNA (173-mer).

Mol	Chain	Residues		\mathbf{A}	toms			AltConf	Trace
31	3	34	Total 694	C 311	N 111	0 238	Р 34	0	0

• Molecule 32 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).





Mol	Chain	Residues		Ate	oms			AltConf
30	С	1	Total	С	Ν	Ο	Р	0
32	U	T	32	10	5	14	3	0

• Molecule 33 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
33	С	1	Total Mg 1 1	0
33	F	6	Total Mg 6 6	0

• Molecule 34 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
34	Ο	2	Total Zn 2 2	0
34	Ν	1	Total Zn 1 1	0



3 Residue-property plots (i)

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

• Molecule 1: MPN domain-containing protein















• Molecule 6: Pre-mRNA-processing factor 19



Cha	ain s:	– 13	3%		-	-	-	-	-	86	%	-	-	-	-	-	-				
MET PHE	SER TLE SER	GLY THR VAL PRO	ATD CLN CLU	VAL VAL SER	THR LYS SER	GLY HIS LEU	CLU GLU GLU	LEU LEU	LYS TYR	VAL ARG GLU	THR GLY LYS	CYS PRO VAL	THR GLY GLU	PRO LEU SER	THR GLU ASP	LEU LEU	LEU LEU	VAL ASN LYS	THR VAL LYS		
PRO ARG	ALA PRO ALA	T67 G71	L72 L73 S74	M84 L85	R113 V114	E121	R122 D123	A128 L129		Q134 Q135 V125	ALA ALA ALA	ASP VAL ALA	ALA ALA ALA	ALA ALA PRO	ARG GLU GLY	ATD ATD	GLY GLY	ARG ARG PRO	LYS ALA GLY	ILE PRO GLU	
ASP VAL	ALA ASP MET	THR GLU VAL ASN	ALA THR LEU	SER GLY	ARG LYS LYS	ARG PRO LEU	ASP SER	ALA SER	ASP ASP	ILE ALA ALA	MET THR LEU	ALA GLY SER	HIS PRO LEU	HIS LYS THR	THR ALA GI V	GLY	ALA ALA ILE	ASP VAL ASN	PRO GLN GLN		
GLY GLY	VAL VAL VAL THR	ALA GLY VAL ASP	THR THR LEU	GLN LEU PHE	ASP TYR LEU	GLN THR ARG	VAL LEU ALA	CER CEU	HIS THR	LYS ARG CYS	THR GLY VAL	SER TRP VAL	ALA ALA ASP	VAL ILE VAL	SER SER	ALA ASP	LIS THR ALA	ARG VAL TRP	ARG ALA GLY		
GL Y GL Y	GLY SER GLU	TRP SER CYS ALA	SER VAL LEU	ARG ASP HIS	THR ALA GLU	VAL VAL GLY	VAL THR THR	PRO SER	ARG TYR	PHE VAL THR	GLY SER THR	ASP ALA SER	TRP ALA PHE	TYR ASP VAL	ALA SER 1 FII	THR CYS	ARG GLN	VAL GLY ALA	ASP GLY GLY		
PRO GLY	PRO TYR THR	CYS LEU GLN	HIS PRO ASP	GLY LEU ILE	GLY GLY THR	GLY THR GLU	GLY LYS ALA	ARG ILE	GLU VAL	LYS ALA GLN	LYS ALA VAL	ALA ALA CYS	GLY GLY	ALA GLY ALA	ILE ARG SFR	LEU ALA	SER GLU	ASN GLY TYR	HIS MET ALA		
SER ALA	ASP ASP CYS	ILE LYS LEU TRP	ASP LEU ARG	LYS LEU ALA	ASN PHE LYS	THR ILE GLU	THT THT	GLY PRO	THR	VAL ALA PHE	ASP HIS SER	GLN GLN TYR	LEU VAL VAL	GLY GLY PRO	VAL VAL I VS	TYR	STN GLN 119	GLN GLN TRP	ALA GLU LEU		
LYS THR	SER GLU VAL	PRO LYS ARG ALA	SER ALA LEU	ARG TRP GLY	PRO ASP ALA	ARG SER VAL	VAL GLY	ALA ALA ASP	ASN	ARG VAL PHE	SER SER PRO	SERALA									
• N	folec	ule 6:	Pre	-mR	NA-	proc	essi	ng fa	actor	r 19											
Cha	ain t:	109	6•					_	_	88%	6	_	_	_		_	_				
Cha Law and co	ain t:	CLY THR VAL PRO	eLV %	VAL VAL SER	THR LYS SER	GLY HIS LEU	L YE GLU GLU	LEU LEU	LYS TYR	VAL ARG GLU SC	THR %	CYS PRO VAL	THR GLY GLU	PRO LEU SER	THR GLU ASP	LEU	rku LEU LYS	VAL ASN LYS	THR VAL LYS		
PRO ARG PHHE PHHE PHHE		CITY See CLV See VAL	G71 GLU %	T74 VAL S74 VAL LT75 SER	D78 • LYS E79 SER	W80 GLY D81 HIS A82 ♦ LEU	HR8 CTU	T92 SER LEU LEU	L105 GLU L105 TYR	ARC	V114 OLV %	A116 CVS R117 PRO T118 VAL	$\begin{array}{ccc} 1110 \\ 1119 \\ K120 \\ K120 \\ GLU \\ GLU \end{array}$	E121 R122 SER	D123 ♦ THR E124 ♦ GLU	ALA LEU ARG LEU ALA LEU	ALA PAU LEU ALA LYS	ASP VAL MET ASN LYS LYS	GLN THR GLN VAL TYR LYS	ALA ALA ASP	VAL ALA ALA
Cha ala arc PHG PHG PHG PHG			GLU GT1 GLU GLY L72 GLN GLN GLN GLN GLN GLN GLN GLU GLN GL	ARG 374 \downarrow VAL ARG 374 \downarrow VAL PRO 1.75 SER	LVS D78 + LVS ALA D78 + LVS GLY E79 SER	TLE W80 GLY PR0 D81 HIS GLU A82 ♦ LEU	ASP VAL H88 GLU TLE LYS	ALA T92 \blacklozenge SEK ASP T92 \blacklozenge LEU MET ILE	GLU L105 LYS VAL TYR	ASN H108 VAL ALA ARG ARG 6LU 688	LEU V114 CLY SER V114 CLY LYS I115 LYS	GLY A116 CYS ARG R117 PPRO LYS T118 VAL	LYS THR ARG L119 GLY PRO K120 GLU	LEU E121 PRO PRO E121 LEU ASP R122 SER	SER D123 LEU E124 ATA ASP	SER ALA LEU ALA LEU ALA ALA LEU	ASF ALA FRU ASP LEU LEU ILE ALA LYS	ALA ASP VAL ALA MET ASN MET LYS LYS	THR GLN THR LEU GLN VAL ALA TYR LYS	ALA ALA ASP	ADI ALA ALA
CUS ALA PRO MET ALA ALA PRO MET ALA ARG ANA ARG ALA ARG ARG ARG ARG ARG ARG ARG ARG ARG AR	ain t: State of the second se	LYS 6LU 100 THR 6LY 568 THR ALA 6LY 169 PY0 ALA 6LY PY0 PY0 PY0	CLY CLU 71 CLY CLU 71 CLY CLY 172 CLN 6LN 6LN 6 CLN 6LN 772 CLN 6	ALA ARC 274 VAL ALA ARC 274 VAL ILE PRO L75 SER	ASP LYS D78 + THR VAL ALA D78 + LYS ASN GLY E79 SER	PRO ILE W80 GLY GLN PRO DB1 HIS GLN GLU A82 \blacklozenge LEU	GLY VAL H88 CUU CUVL H88 CUU VAL ILE LYS	VAL ALA T92 SEK VAL ASP T92 LEU THR MET ILE THR T12 LEU	ALA INK ALOS GU GLY CLU LIOS LYS VAL VAL TYR	THR ALA HUG VAL THR ALA ARG ARG ARG ARG CUU 688	LEU LEU V114 THR S GLN SER V114 GLY LEU LYS I115 LYS	PHE GLY A116 CVS ASP ARG R117 PRO TYR LYS 118 VAL	LEU LYS LI19 GLN ARG L119 THR PRO K120 GLU	ARG LEU E121 PRO VAL PRO E121 LEU LEU ASP R122 SER	ALA SER D123 SER LEU E124 ALA ASP	GLU SER ALA LEU GLU SER ARG LEU ULY ALA ARG LEU ULY ALA ALA DEU	THR ASF AIA FWU THR ASP LAU LEU LYS ILE AIA LYS	ARG ALA ASP VAL CYS ALA MET ASN THR MET LYS LYS	GLY THR CLM THR VAL LEU CLM VAL SER ALA TYR LYS	ALA ALA ASP	VAL VAL ALA
TRP GLY ALA PRO MET VIA TRP GLY ALA PRO MET VIA TRP OF CONTRACTOR	Ain t: WIN MIN VIEW VIEW VIEW VIEW VIEW VIEW VIEW VIEW	ILE LYS GLU 100 VAL THR GLY 169 THR SER ALA GLY 169 PMA SER ALA GLY 169 PMA	SER GLY GLU G71 GLU % ALA GLY GLY 172 GLN % ASP ILE GLY 172 GLN •	LYS ALA ARG 274 VAL THR ALA ARG 274 VAL ALA ILE PRO L75 SER	ARG ASP LYS THR VAL VAL ALA D78 • LYS TRP ASN GLY E79 SER	ARG PRO ILE 480 GLY ALA GLM PRO D81 HIS GLY GLM GLU A82 \blacklozenge LEU	dur dia Ast dur dia Ast dur dia H86 diu dur val ille H86 diu urs dur val ille	GLY VAL ALA T92 + SEK SER VAL ASP T92 + LEU GLU THR MET T1E T1E	ELA ALA INA ALCA DI AL	ALA ASP ASN H108 VAL SER THR ALA ARG VAL THR THR R113 4 GLU 688	LEU LEU LEU LU LU VI14 CIY ARG GLN SRR VI15 CIY ASP LEU LYS II15 CIY	HIS PHE GLY A116 CYS THR ASP ARG R117 PRO ALA TYR LYS 1118 VAL	GLU LEU LYS THE THE VAL GLN ARG LITE CLN ARG LITE OCL	GLY ARG LEU EI21 PRO VAL VAL PRO E121 LEU THR LEU ASP R122 SER	THR ALA SER D123 HIS SER LEU BRD LEU 5124 ACP	SER GLU SER ALA LEU ARG GLU SER ARG LEU ARG UZ ALA ALA LEU	ARV THA ASY ALA FAU TYR THR ASP LEU LEU PHE LYS ILE ALA LYS	VAL ARG ALA ASP VAL THR CYS ALA ASP VAL GLY THR MET LYS LYS	SER GLY THR GLN THR THR VAL LEU GLN VAL ASP SER ALA TVR LYS	ALA ALA ASP	VAL VAL ALA
CHA TRP GLY ALA PRO MET ALA PRO MET ALA ARG PRO MET ARG PRO MET ALA ARG PRO MET ALA ARG PRO MET ARG PR	TYR VAL HIS ARG AGE AGE AGE AGE AGE AGE AGE AGE AGE AG	ASP ILE LYS GLU 100 CLY 100 CL	LEU SER GLY GLU G71 GLU ⁰ THR ALA GLY GLY L72 6 GLN • CYS ASP ILE GLY 172 6GLY •	LEU LYS ALA ARG S74 VAL ARG THR ALA ARG S74 VAL GLN ALA TLE PRO L75 SER	VAL ARG ASP LYS THR GLY VAL VAL ALA D78 + LYS ALA TRP ASN GLY E79 SER	ASP ARG PRO ILE V80 GLY GLU ALA GLN PRO D81 HIS GLY GLY GLN GLU A82 \blacklozenge LEU	PHU GLY GLA ASP GLY GLY VAL HBG GLU GLY VAL HBG GLU GLY VAL LILE DLY VAL LILE LYS	PHU GLY VAL ALA 192 FHC SER VAL ASP 192 LEU THR GLU THR MET THR OLU THR MET THR OLU THR MET THR	LUD SER GLA IIR ALS GLU LUD SER GLA GLU LIOE 1105 GLN CYS VAL VAL TYR	PHE ALA ASP ASN H108 VAL HIS SER THR ALA ALA ARG PRO VAL THR THR R113 4 GLU 688	ALP LEU LEU LEU VI14 CTIR S CLY ARG CLN SER VI14 CTIR S LEU ASP LEU LYS IIIE CLY	ILE HIS PHE CLY A116 CYS LEU THR ASP ARG R117 CPR0 GLY ALA TYR LVS R118 VAL	THR OLU LEU LVS THR CLY VAL CLM ARG L119 CLY THR VAL THR PRO K120 CU	GLU GLY ARG LEU E121 ♦ PRO GLY VAL VAL PRO E121 ♦ LEU LYS THR LEU ASP R122 ♦ EER	ALA THR ALA SER D123 🔶 THR TLE HIS SER LEU E124 🔶 GUU ARC PRO FRI ALA E124 4 GUU	TILE SER GLU SER ALA LEU TRP ARG GLU SER ARG LEU TRP ARG GLY ALA ALA LEU	VLU ARV THS ASF ALA FWU VAL TYR THR ASP LEU LEU LYS PHE LYS ILE ALA LYS	ALA VAL ARG ALA ASP VAL GLN THR OYS ALA MET LYS LYS GLY THR MET LYS LYS	ALA SER GIY THR GIN THR VAL THR VAL LEU GIN VAL ALA ASP SER ALA TVR VAL	ALA ALA ASA	VAL ALA ALA
CYS SER VIL SER ALA PRO MET ALA PRO MET CYS SER VIL SER ALA ARG PRO MET ALA PRO MET ALA ARG PRO MET ARG PRO ME	CUT ALLA PRO ALLA CON ALLA PRO ALLA CON ALLA PRO	GLY ASP ILE LYS GLU 100 CLY ALA VAL VAL THR GLY 568 TTR ILE ALA SER THR GLY 568 VAL 601 A ARG SER SER ALA GLY 770 PR0	SER LEU SER CLY $CLU C71$ $CLU 0^{\circ}$ LEU THR ALA CLY $CLY C1Y C71$ $CLU 0^{\circ}$ ALA CYS ASP ILE $CLY 172 0$ CLN	PHE LEU LYS ALA ARG CALA ARG VAL SER ARG THR ALA ARG S74 VAL GLU GLM ALA ILE PRO L75 SRR	ASN VAL ARG ASP LYS THR GLY GLY VAL VAL VAL ALA ATA D78 + LYS TYR ALA THP ASN GLY E79 SER	HIS ASP ARG PRO ILE W80 GIV MET GLU ALA GLN PRO D81 HIS ALA GLY GLY GLN GLU A82 \blacklozenge LEU	ALA GLY GLU GLA ASF ALA GLY GLU GLA VAL SER GLU GLY VAL ILE H88 GLU SER GLU GLY VAL ILE H88 LYS	ASP PRU GLY VAL ALA T92 4 SEK ASP TYR SER VAL ASP T92 4 LEU CYS THR GLU THR MET 11E	LEU CLO THE ALM THE ALMORT CONTRACT OF ALLO CLO CLO CLO CLO CLO CLO CLO CLO CLO	TRP PHE ALA ASP ASN H108 VAL ASP H1S SER THR ALA LEU PRO VAL THR ALA LEU PRO VAL THR ALA CU 688	ARG ASP LEU LEU LEU VI14 THR S LVS GIY ARG LEU LEU VI14 CIY LEU LEU ASP LEU LYS LIII VII4 LIV	ALA ILE HIS PHE GLY A116 CYS ASN LEU THR ASP ARG R117 PRO PHE GLY ALA TYR LYS 1119 VAL	LYS THR GLU LEU LYS LYS THR THR GLY VAL GLM ARG LI119 G GLY ILE THR VAL THR PRO K120 GU	GLU GLU GLY ARG LEU E121 + PRO PRO GLY VAL VAL PRO E121 + LEU TYR LYS THR LUG ASP R122 + SER	THR ALA THR ALA SER D123 🔶 THR ASP ILE HIS SER LEU E124 🔶 GU CIV ARD PRO IEU ILA E124	PRO ILE SER GLU SER ALA LEU CYS TRP ARG GLU SER ALA LEU UN ARG GLU ALA ALA LEU	THR VAL TWR THS ASP ALA FRU THR VAL TWR THR ASP LEU LEU VAL LYS PHE LYS ILE ALA LYS	ALA ALA VAL ARG ALA ASP VAL PHE GLM THR OCYS ALA MET ASN ASP LYS GLY THR MET LYS LYS	HIS ALA SER CLY THR CLN THR CLN VAL THR CLN VAL THR VAL THR VAL THR VAL THR VAL TYN VAL	ALA ALA ASP	VAL ALA ALA
CUA ALA TRP GLY ALA PRO MET AL	VAL CLY ALA PRO ALA TARA TARA TARA TARA ALA TARA ALA TARA ALA TARA ALA TYR VAL HIS ARG AGY ALA TYR VAL HIS ARG AGY	GLY GLY ASP ILE LYS GLU 100 CLY PRO ALA VAL VAL THR GLY 568 TTR VAL ILE ALA SER THR GLY 568 PRO .	LYS SER LEU SER GLY GLU G71 GLU ⁹ ILE LEU THR ALA GLY GLY L72 TYR ALA CYS ASP ILE GLY 172 GLY GLY	GLY PHE LEU LYS ALA ARG CAN VAL GLN SER ARG THR ALA ARG S74 VAL LYS GLU GLN ALA ILE PRO L75 SER	GLN ASN VAL ARG ASP LYS THR GLN GLY GLY VAL VAL ALA ANG CYS LYS TTRP TYR ALA TTRP ASN GLY E79 SER	ALA HIS ASP ARC PRO ILE W80 GLY GLU MET GLU ALA GLN PRO D81 HIS LEU ALA GLY GLY GLU A82 \blacklozenge LEU	THE ALA GLY GLA ANY THE ALA GLY GLA GLA ANY LEU SER GLU GLY VAL ILE H88 GLU LEU SER GLU GLY VAL ILE H88 LYS	SEK ASP PRU GLY VAL ALA T92 4 SEK GLU ASP TYR SER VAL ASP T92 4 LEU VAL CYS THR GLU THR MET 1LE DDD 1178 MET 11.	TYO ILE OLD THE ALL THE ALLO THE CALL THE CALL AND	ALA TRP PHE ALA ASP ASN H108 VAL SER ASP HIS SER THR ALA ALA LEU PRO VAL THR ALA EU 688	LEU ARG ASP LEU LEU LEU VII4 TIR ° ARG LYS GLY ARG GLM SER VII5 CLY TRP LEU LEU ASP LEU LYS LII5 LYS	GLY ALA ILE HIS PHE GLY A116 CYS PRO ASN LEU THR ASP ARG R17 PRO ASP PHE GLY ALA TYR LYS 1118 VAL	ALA L'AS THR OLU LEU LYS LYS THR ARG THR GLY VAL GLM ARG LI19 G GLY SER ILE THR VAL THR PRO K120 G GU	VAL GUU GUU GUY ARG LEU E121 🔶 PRO LEU PRO GLY VAL VAL PRO E121 🔶 LEU VAL TYR LYS THR LEU SEP R122 🔶 EER	GLY THR ALA THR ALA SER D123 ALA ASP ILE HIS SER LEU E124 ALA CIV ARC PIC SER LEU 124 ACD	ASP PRO ILE SER GUU SER ALA LEU HIS O'YS TRP ARG LUU SER ARG LEU ARG CUY ALA ARG LEU ARG GUY ALA ARG LEU	LEU THR VAL TAR THE ASP ALA FRU LEU THR VAL TAR THE ASP ALA LEU ARG VAL LYS PHE LYS ILE ALA LYS	VAL ALA ALA VAL ARG ALA ASP VAL PHE PHE GLN THR OT'S ALA MET ASN SER ASP LYS GLY THR MET LYS LYS	SER H1S ALA SER GLY THR GLN THR PRO SER VAL THR VAL LEU GLN VAL SER GLY ALA ASP SER ALA TYP LYS	ALA ALA ASA	VAL VAL ALA ALA







• Molecule 12: Small nuclear ribonucleoprotein Sm D1 18% Chain c: 68% 10% 23% P87 K88 GLN GLN ARG PRO PRO PRO VAL ARG ARG ALA ALA VAL GLY ARG GLY ARG GLY ARG GLY ARG GLY ARG ARG ARG ARG ARG • Molecule 13: Sm domain-containing protein 6% Chain b: 34% 63% MET ALA LEU SER ARG 862 E63 E64 ALA ALA PRO GLY GLN ALA PRO PRODUCT CONTRACTOR CON • Molecule 14: Syf1 42% Chain I: 66% 5% 29% ALA VAL ARG ALA ALA LEU PRO GLY SER 198 96 D347







• Molecule 1	8: PLRG1				
Chain T:		60%	6%	34%	I
MET ALA ALA GLU THR THR SER GLU VAL	VAL TLE GLU GLU SER PHE PHE ASN PRO PRO SER SER ALA	ASP ALA LYS THR ILE LYS LYS ALA LEU THR LEU GLN	SER LEU LYS LYR ARG TYR GLU VAL PHE ALA SER ASN	GLY GLN PRO VAL PRO PRO LEU ASP GLU SER GLN GLN	LEU ILE ALA ALA
VAL LYS PHE ARG ASP GLU TYR GLU HIS	VAL SER HIS HIS LEU VAL ALA PRO PRO ALA PRO	LYS PRO THR ALA ALA ALA PRO PRO GLY SER	GLY ARG THR ALA ALA ALA GLY GLY GLY FRO SER SER	ALA ASP GLY GLY ASP ASP ALA SER PRO GLU SER ARG	SER ASN LEU ALA LVS
LEU ILE ASP ASN ILE PLE PRO ALA ALA VAL	ALA LYS LYS LYS LEU GLY ALA ALA ALA ALA ALA GLY GLY	GLN LEU THR LEU TYR GLN PRO GLY GLY GLY	ALA ALA ALA PRO CLY GLV ALA ALA ALA ALA ALA	VAL MET ALA ALA VAL TLE ALA ALA ASP CLY GLY GLY MI75	R1 90
V202 C212 V213 D216 C247	D270 V283 V283 V283 L306 D312 D312 D312 D314 V314	K323 H353 H353 S377 N383 F388	E396 8414 8414 8426 8466 8465 8465 8465 8465 8464	S465 L469 E485 E495 E497 E497 D498	R510 1514 F518
• Molecule 1	9: Rbm22				
Chain O:	9%	61%	·	35%	
MET ALA ALA ARG ARG LEU LEU ARG ASP PRO	GLU ALA ALA ALA ALA GLU GLU ARG SER SER E24	M35 R49 V 68 I 68 C70 C83	8110 E111 E111 E111 E124 E17 E17 E17 E17 E17 E17 E17 E17 E17 E17	GLY ALA SER SER SER \$139 ¥139 Å140 Å140	1154 1157 1157 1164 V165
C180 A192 N206 T224	P226 P226 E227 D228 L234 L234 V236	6237 C256 E257 L258 A259 Y261 R262 R262	M265 M265 V266 K267 S288 C269 C269 T272 T272 Y274	T275 S278 A279 A279 E281 K282 A283 A283	C289 C285 C295 A295 A296 R297 V298 AC0 AC0 AC0 PR0
PRO ALA PRO ALA ALA ARG ASN ALA ALA	ALA ALA ASP ASP ASP ASP GLN SER SER SER SER SER SER SER SER	ALA GLY GLY GLY GLY GLY ALA ALA ALA ALA PRO GLY SER	ALA ALA SER TYR TYR PRO PRO SER ASP PRO SER ALA MET	GLY SER ARG ALA PRO GLY PRO FRO GLY MET	ARG PRO GLY GLY GLU
GLY CLY CLY CLY GLY FRO GLY GLY GLY GLY	MET ALA PRO PRO PRO PRO GLY GLY GLY ALA	PRO PRO GLY GLY GLY PRO PRO PRO CLY TYR	MET PRO PRO PRO ARG PRO PRO MET ALA SER ALA SER ALN GLN	PRO PRO GLN GLN HIS GLN	
• Molecule 2	20: G10 proteir	L			
Chain N:		68%	5%	27%	1
MET SER LEU R4 R10 E21 V22	123 K41 L46 S72 E82 E82 S118	T134 S146 ASP GLU GLU ASP SSP	A167 K168 L169 L176 A179 CLY CLY CLY CLY CLY CLY CLY CLY CLY CLY	ASP GLY MET GLY GLY GLY GLY GLY PRO GLY GLY	PR0 SER ARG LYS ARG
PRO ALA SER THR LEU ASP GLY ASP ASP	ASP ASP GLU GLU PRO ASP GLU VAL ARG ARG	LEU GLU GLU LYS LYS CLY GLY THR THR LYS LEU	ASP		
• Molecule 2	21: SKI-interac	ting protein Sk	XIP SNW domain-	containing prot	ein
Chain R:	33%	5%	62%		1
MET SER SER LEU GLY THR LEU PRO ALA	PRO GLN GLN GLN LYS HLA ALA ALA ALA ALA PRO	VAL PRO ALA ALA ALA ALA ALA SER ALA SER SER SER	PHE LYS GLU F35 L39 K42 K42 K42 K42 K42 K42 K42 K42	V97 R105 D110 L114 K117 V118 V119	R1 28 E1 46
K152 L153 S154 S155 P158 T159 T159	101 164 164 174 174	8217 8217 1220 1223 1223 1223 8225 1231 1231	K233 C235 C267 C269 C269 C266 C266 C266 C12 C12 C12 C12 C12 C12 C12 C12 C12 C12	GLN GLN THR GLN THR GLN NZ74 NZ74 A299 SS90	1301 1901 1902 1902 1120 1120 1120
			PROTEIN DATA BANK		























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V1321	P1322	A1324	E1325	51326 V1327	A1328	Y1329 T1330	C1331	E1332 T1333	A1334	G1335	Y1336	F1337 W1338	L1339	I1340	H1341	V1342 L1343	A1344	R1345	W1346 E1347	K1348	F1349 T1360	A1351	A1352 V1353	E1354	R1355 A1356	R1357	A1358	G1360	A1361	41362 A1363	A1364	V1365 I1366	A1367	E1368 11369	E1370	P1371	F1372 V1272	E1374	Y1375	F1376	D1378	ALA PRO
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GLN	V1383	F1384	A1385 G1386	A1387	S1388 F1389	D1390	A1391 D1392	M1393	E1394	R1395 A1396	R1397	G1398	C1399	F1400	H1402	L1403	K1404	L1406	F1407	Q 1408 F1409	L1410	E1411 E1412	C1413	R1414 A1415	F1416	E1417 M1418	L1419	K1420 G1421	Q1422	A1423	R1425	V1426	V1427 Y1428	L1429	S1430 T1431	K1432	Q1433	A1434 V1435	11436 II436	V1437	A1438 M1430	T1440
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C1441	T1442	A1444	A1445	L1440 K1447	R1448	R1449 E1450	F1451	L1452 01453	L1454	A1455	F1456	K1457 Y1458	D1459	N1460	L1461	L1462 M1463	E1464	E1465	A1466 A1467	Q 1468	11469 1470	E1471	I1472 E1473	T1474	F1475 T1476	P1477	M1478	L1480	Q1481	K1482 P1483	E1484	D1485 G1486	V1487	S1488 D1/80	L1490	K1491	R1492 W1402	V1494	L1495	I1496	D1498	H1499 H1500
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Q1501	L1502 D1502	P1504	V1505 V1505	V1505 K1507	N1508	Q1509 A1510	F1511	Q1512 K1513	Y1514	S1515	H1516	L1517 D1518	q1519	S1520	L1521 74500	r1522 T1523	R1524	F1525	I1526 R1527	L1528	G1529 T1520	P1531	Y1532 V1533	Q1534	L1535 N1536	M1537	Q1538 01530	R1540	A1541	K1542 A1543	S1544	L1545 A1546	Q1547	L1548 v1540	N1550	W1551	R1552 v1 c c 2	K1554	A1555	L1556	D1558	L1559 P1560
A 1561	V1562 01562	41564	L1565	41567	F1568	R1569 A1570	A1571	N1572 D1573	31574	F1575	V1576	H1577 E1578	Y1579	q1580	F1581 11500	V1582 D1583	V1584	P1585	01586 Y1587	L1588	31589 1 E 00	31591	E1592 81593	E1594	P1595 L1596	P 1597	Y 1598 51500	Y1600	q1601	N1602 L1603	31604	E1605 A1606	E1607	Y1608 V1609	V1610	A1611	r1612 51212	C1017	F1615	M1616	L1618	L1619 31620
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1621	01622	11624	(1625	.1625	1628	.1629	1631	1632	1634	1635	(1636	1637 1638	1639	1640	01641	1642	c1644	1645	11646	1648	01649	1651	11652	:1654	11655	1657	t1658	1660	1661	1663	(1664	1665	:1667	11668	11670	1671	1672	1674	.1675 🔶	31676	1678	11679
Y1621	P1622	H1624	K1625	11626 S1627	I1628	L1629	T1631	Y1632	G1634	Q1635	K1636	A1637 L1638	I1639	R1640	D1641	V1642 11643	E1644	Q1645	R1646 C1647	A1648 🔶	P1649	P1651	M1652 F1653	G1654	R1655	¥1657	R1658	A1660	T1661	V1662 D1663	K1664	Y1665 Q1666	G1667	A1668	N1670	D1671	Y1672	L1674	L1675	S1676		R1679 S1680
1681 🔶 Y1621	1682 P1622	1684 H1624	1685 + K1625 +	1687 • 11626 • 11626 • 11687 •	1688 • 11628 •	1689 Tile29 Tile30 Tile30	1691 • T1631	1692 • Y1632 •	1694 • G1634 •	1695 🔶 Q1635 🔶	1696 • K1636	1697 • A1637 • A1638 • 1698 • 1.1638 •	1699 • I1639	1700 🔶 R1640 🔶	1701 D1641	1/02 V1642	1704 E1644	1705 Q 1645	1706 • R1646 • 1707 • C1647 •	1708 🄶 🛛 A1648 🄶	1709 P1649	1711 P1651	1712 💎 M1652 🕈 1713 🔶 F1653 🔶	1714 🔶 G1654 🔶	1715 V R1655 V 1716 V 1656 V	1717 Y1657	1718 R1658	1720 • A1660	1721 • T1661	1723 V1663	1724 🔶 K1664 🔶	1725 V Y1665 V 1726 V 01666	1727 og G1667	1728 🔷 A1668 🔶	1730 • N1670	1731 D1671	1732 Y1672	1734 • L1674	1735 🔶 L1675 🔶	1736 S1676		ER R1679 YR S1680
R1681 🔶 Y1621	A1682	G1684 H1624	H1685 K1625	L1680 T1626 L1626 L1626 L1626 L1626 L1626 L1626 L1627	D1688	V1689 V1629 V1629 V1630 V16300 V1630	R1691 T1631	L1692 Y1632	V1694 G1634	A1695	M1696 K1636	S1697 A A1637 R A1637 B B1698 C A1638 A	A1699	R1700 🔶 R1640 🔶	L1701 D1641	G1/02 V1642	Y1704 E1644	V1705 4 Q1645	F1706 R1646 C1707 C1647	R1708 🔶 A1648 🔶	K1709 P1649	L1711 P1651	F1712 • M1652 • A1713 • F1653 •	N1714 • G1654 •	C1715 C1715 C1716 C17176 C1716	E1717 Y1657	L1718 R1658	N1720 A A1660	T1721 T1661	R1723 D1663	L1724 🔶 K1664 🔶	L1725 V Y1665 V M1726 01666	A1727 0 G1667	R1728 A A1668	T1730 • N1670	K1731 D1671	L1732 Y Y1672	L1734 L1674	V1735 🔶 L1675 🔶	K1736 S1676	E1738 V1678	SER R1679
Y R1681 🔶 Y1621	742 • A1682 • P1622 • 743 •	$744 \textcircled{0} \qquad 01684 \textcircled{0} \qquad H1624 \textcircled{0}$	7 45 + H1685 + K1625 + 746 + 746 + 746 + 746 + 746 + 746 + 746 + 746 + 74600 + 746000 + 74600 + 74600 + 746000 + 7460	747 \bullet $B1687$ \bullet $S1627$ \bullet	748 • D1688 • I1628 •	750 • V1689 • L1629 • T1630 •	751 A R1691 A T1631	752 V L1692 V Y1632 V 753 V V1693 V N1633 V	754 • V1694 • G1634 •	755 A A1695 A Q1635	756 M1696 W1636	758 • 81697 • 81637 • 758 • 81638 • 11	759 • A1699 • I1639 •	760 🔮 R1700 🄶 R1640 🄶	762 L1701 D1641	763 • L1703 • 11643 •	764 • Y1704 • E1644 •	765 V1705 Q1645 V 766	767 • F1706 • R1646 • 7167 • C1647 • C1647	768 🔶 R1708 🄶 A1648 🔶	770 K1709 P1649	771 L1711 P1651	773 • F1712 • M1652 • 773	774 🔷 N1714 🍨 G1654 🔶	776 • C1715 • R1655 • 776 • 7176 • 7176 • 71716 • 71656	777	R L1718 R1658	A N1/19 A 11009 A	R T1721 T1661	R F1/22 V1662	L L1724 🔶 K1664 🔶	A L1725 V Y1665 V A D1666 V	A A1727 G1667	R1728 A A1668		M K1731 D1671	N L1732 V1672	M L1733 L1673	A V1735 🔶 L1675 🔶	K1736 S1676		SER TYR S1679 S1680
GLY R1681 Y1621	V1742 A A1682 P P1622 C C1743 A C1743 A C1743 A C1743 A C1744	S1744 G1684 HI624	R1745 H1685 K1625 C17746 T1700 L1776	V1747 C R1687 C S1627 C	D1748 D1688 T1628	D1/49 V1689 L1629 V1689 T1630 V1689 V1750 V1630	V1751 A1691 T1631	A1752 L1692 V1632 Q1753 V1632 V1633	P1754 V1694 G1634	D1755 • A1695 • Q1635 •	L1756 M1696 K1636 M1757	D1758 R1698 L1638	G1759 A A1699 I1639	V1760 R1700 R1640	$E1761 \qquad L1701 \qquad 01641 \qquad \qquad$	M1763 C L1703 L17643	S1764 • Y1704 • E1644 •	G1765 V1705 Q1645	VIT67 CI647 CI647	A1768 A R1708 A A1648	$\begin{array}{cccccccccccccccccccccccccccccccccccc$		E1773 A1712 M1652 E1773 E1773 A1713 F1653 A	Q1774 A N1714 G1654	$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	A1777 • E1717 • Y1657 •	TYR L1718 R1658	ALA NIT20 A1660	TYR T1721 T1661	THR F1/22 V1052 C	VAL L1724 K1664 PRO	ALA L1725 V Y1665 V GLN M1726 D1666	ALA A1727 O G1667	GLU R1728 A1668 CU		GLN K1731 GLY 5111	GLN L1732 Y1672	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	ALA V1735 🔶 L1675 🔶	K1736 S1676		SER R1679 TYR S1680
GLU GLY R1681 Y1621	GLN C1743 A1682 P1622 C	ASP S1744 01684 0 H1624 0	LYS R1745 H1685 K1625 PR0 01746 11000 01746 11000	MET 4-1-22 LI686 11626 ALA V1747 R1687 S1627	GLU D1748 D1688 11628	ALA D1/43 V1689 1629	GLU V1751 R1691 T1631	VAL 01753 VIEG2 VIEG2 VIEG3	LYS P1754 V1694 G1634 G	LYS D1755 GLU 17765 A1695 Q1635	GLY M1757 M1696 K1636	GLU D1758 B1698 11638	ALA G1759 A1699 I1639	LYS V1760 R1700 R1640	PR0 E1761 L1701 D1641 CLU A1762 A1766 A176	GLY M1763 61/02 7 11643 6	AHG S1764 Y1704 E1644	THR G1765 V1705 Q1645 V VAL 11766 C	GLU L100 F1706 F1646	LYS A1768 A R1708 A A1648	$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	ALA TI771 ALA TI771 ALA TI71 ALA TI771 ALA TI7711 ALA TI771 ALA TI771 ALA TI771 ALA TI	VAL E1/72 ♥ N1652 ♥ M652 ♥ M654 ♥ M6540 V M654 ♥ M	GLU Q1774 • N1714 • G1654 •	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	A1777 E1717 Y1657	TYR L1718 R1658	ALA N.1.19 11059 ALA A1660	TYR T1721 T17661	THR $F1/22$ V1062 GLN $R1/23$ \bigcirc D1663 \bigcirc	VAL L1724 K1664 PRO	ALA L1725 Y1665 Y GLN M1726 D1666	ALA A1727 6 G1667	GLU R1728 A1668		GLV K1731 D1671	GLN L1732 Y1672	GLN L1734 L1674	ALA V1735 🔶 L1675 🄶	K1736 S1676		SER R1 679
CLU GLY R1681 Y1621	M dui V1742 A1682 P1622	$d = \frac{1}{3}$	LYS R1745 H1685 K1625	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	GLU D1748 D1688 T1628	ALA DITA VI689 LI629		W MI/52 L1692 Y1632 Y1632 <thy1632< th=""> Y1632 Y163</thy1632<>	CT L78 P1754 V1694 G1634 G1634	LYS D1755 A1695 A1695 A1695 A1695 A1695 A1695	(L) (LI756 M1696 (K1636 (LI7636 (LI763	+ GLU m1758 → B1697 → A1637 → A1637 → A1638 → GLU D1758 → B1698 → 1.1638 →	d ALA G1759 ♦ A1699 ♦ 11639 ♦	× ALA V1760 • R1700 • R1640 •	Ho PRO E1761 L1701 D1641 GLU A1762 C1702 D1641	* GIY M1763 0 11/02 11/042 1643	d GLU S1764 • V1704 • E1644 •	VAL 11765 V1705 Q1645		A1768 A1768 A1708 A1648	* GLY I1770 K1709 P1649	CLAR IIII IIII IIII IIII	× VAL 51/12 € M1652 € M1653 €	C dLU 01774 N1714 G1654	$\begin{pmatrix} \\ \\ \\ \\ A1776 \\ \\ Y1716 \\ \\ Y1676 \\ \\ Y1716 \\ \\ Y1676 \\ \\ Y1716 \\ \\ Y1$	A1777 E1717 Y1657	TYR L1718 R1658	ALA N1/19 11009 4	TYR T1721 T1661	THR $F1/22$ V1962 GLN $R1/23$ \bigcirc D1663 \bigcirc	VAL L1724 A K1664	ALA L1725 Y1665 Y GLN M1726 D1666	ALA A1727 O G1667			GLN K1731 D1671	GLN L1732 Y1672	GLN L1734 L1674	ALA V1735 O L1675 O	K1736 S1676		SER R1679
C GLU GLY R1681 V1621	P1742 P1622	$d_{\rm LU}$	25: LYS R1745 H1685 K1625	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	GLU D1748 D1688 D1688 D1688 D1688	ALA DIVES V1689 11629		Value A1752 L1692 Y1632 Y1633 Y1632 Y16323 Y1632 Y1632 <t< td=""><td>CT LYS P1754 • 11694 • G1634 •</td><td>TXR D1755 A A1695 A G1635 A CT C C C C C C C C C C C C C C C C C</td><td>L1756 M1696 M1636</td><td>* GLU m1/0 S1697 A1637 A 61037 A 61037</td><td></td><td>× ALA V1760 R1700 R1700 K1640</td><td>L BRO E1761 L1701 D1641</td><td>* CLY M1763 0 L1703 1 1643</td><td>d_{LU} s_{1764} \bullet r_{1704} \bullet r_{1644} \bullet</td><td>VAL 11766 V1705 Q1645</td><td></td><td>A A1768 A1768 A1768 A1648 A1648</td><td>$\begin{array}{c ccccccccccccccccccccccccccccccccccc$</td><td></td><td>* VAL E1/12 M1652 M165</td><td></td><td>$\begin{pmatrix} & & & \\ & & & & \\ & & & & \\ & & & \\ & & &$</td><td></td><td>TYR L1718 R1658</td><td></td><td>GLN T1721 T1661</td><td>THR F1/22 V1962 C</td><td>VAL L1724 K1664</td><td>ALA L1725 V Y1665 V GLN M1726 D1666 V</td><td>ALA A1727 O G1667</td><td>GLU R1728 A1668</td><td></td><td>GLY K1731 OI671 O</td><td>GLN L1732 11672</td><td>GLN L1734 L1674</td><td>ALA V1735 🔶 L1675 🄶</td><td></td><td></td><td>SER RIG79</td></t<>	CT LYS P1754 • 11694 • G1634 •	TXR D1755 A A1695 A G1635 A CT C C C C C C C C C C C C C C C C C	L1756 M1696 M1636	* GLU m1/0 S1697 A1637 A 61037		× ALA V1760 R1700 R1700 K1640	L BRO E1761 L1701 D1641	* CLY M1763 0 L1703 1 1643	d_{LU} s_{1764} \bullet r_{1704} \bullet r_{1644} \bullet	VAL 11766 V1705 Q1645		A A1768 A1768 A1768 A1648 A1648	$\begin{array}{c ccccccccccccccccccccccccccccccccccc$		* VAL E1/12 M1652 M165		$\begin{pmatrix} & & & \\ & & & & \\ & & & & \\ & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & $		TYR L1718 R1658		GLN T1721 T1661	THR F1/22 V1962 C	VAL L1724 K1664	ALA L1725 V Y1665 V GLN M1726 D1666 V	ALA A1727 O G1667	GLU R1728 A1668		GLY K1731 OI671 O	GLN L1732 11672	GLN L1734 L1674	ALA V1735 🔶 L1675 🄶			SER RIG79

• Molecule 21, DNA (172

 \bullet Molecule 31: RNA (173-mer)

Chain 3:	6% 8%	9% •		80%	
G1 U2 A3 G7 C8	G12 C13 A14 U15 U16	A17 G18 U19 A20 C21 U22 U22	0000<000<0000<	. < 0 0 0 0 0 0 0 < 0 0 0 0 0 < 0 0 0 0	Ð
A Q D C C A C	כככטט	U D D D D T	а и с с с с с с с с с с с с с с с с с с		o u u u





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	518369	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{\AA}^2)$	50.00	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV $(4k \ge 4k)$	Depositor
Maximum map value	2.593	Depositor
Minimum map value	-1.565	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.038	Depositor
Recommended contour level	0.08	Depositor
Map size (Å)	404.80002, 404.80002, 404.80002	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.92, 0.92, 0.92	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: GTP, MG, SEP, G5J, ZN

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

Mal	Chain	Bo	ond lengths	B	ond angles
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.86	19/15581~(0.1%)	0.67	7/21167~(0.0%)
2	В	1.22	6/2024~(0.3%)	1.16	5/3144~(0.2%)
3	С	0.41	0/7126	0.57	1/9683~(0.0%)
4	Е	0.40	0/2496	0.58	1/3382~(0.0%)
5	F	1.60	43/2188~(2.0%)	1.31	17/3409~(0.5%)
6	q	0.30	0/847	0.57	0/1148
6	r	0.31	0/1040	0.58	0/1411
6	s	0.30	0/580	0.59	0/784
6	t	0.33	0/514	0.62	0/698
7	a	0.30	0/716	0.53	0/960
8	g	0.31	0/516	0.56	0/691
9	е	0.28	0/667	0.52	0/891
10	f	0.29	0/567	0.56	0/764
11	d	0.28	0/821	0.50	0/1097
12	с	0.29	0/691	0.61	0/933
13	b	0.30	0/792	0.60	0/1059
14	Ι	0.28	0/4712	0.48	0/6427
15	J	0.65	0/4092	0.52	1/5574~(0.0%)
16	Р	0.74	1/882~(0.1%)	0.60	0/1173
17	М	0.39	0/654	0.56	0/874
18	Т	1.14	5/2773~(0.2%)	0.81	0/3765
19	0	0.54	0/2179	0.59	0/2944
20	N	0.82	0/1446	0.64	2/1944~(0.1%)
21	R	0.64	0/2020	0.59	0/2736
22	Н	1.25	4/932~(0.4%)	1.29	4/1447~(0.3%)
23	S	0.43	0/1224	0.56	0/1652
24	W	0.44	2/2852~(0.1%)	0.57	2/3908~(0.1%)
25	L	0.46	0/3847	0.57	1/5158~(0.0%)
26	K	0.29	0/1717	0.55	3/2320~(0.1%)
27	U	0.32	0/194	0.60	0/259
28	V	0.28	0/1023	0.42	0/1413
29	Q	0.28	0/6411	0.48	1/8913~(0.0%)



Mal	Chain	Bo	ond lengths	E	Bond angles
INIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5
30	5	1.29	0/167	1.52	4/258~(1.6%)
31	3	0.55	0/771	1.19	4/1193~(0.3%)
All	All	0.69	80/75062~(0.1%)	0.68	53/103179~(0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	А	0	11
3	С	0	1
6	s	0	1
6	t	0	1
25	L	0	1
28	V	0	1
All	All	0	16

All (80) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
24	W	89	PRO	N-CA	13.08	1.69	1.47
5	F	58	G	C8-N7	-7.87	1.26	1.30
5	F	58	G	C5-C4	-7.64	1.33	1.38
5	F	60	G	C8-N7	-7.22	1.26	1.30
5	F	57	U	C2-N3	-7.16	1.32	1.37
5	F	65	G	C5-C4	-7.13	1.33	1.38
5	F	47	G	C2-N3	-7.11	1.27	1.32
5	F	60	G	C6-N1	-6.90	1.34	1.39
5	F	58	G	N9-C8	-6.88	1.33	1.37
22	Н	21	G	C6-N1	-6.84	1.34	1.39
5	F	62	А	N7-C5	-6.76	1.35	1.39
1	А	1092	TYR	CD2-CE2	-6.74	1.29	1.39
5	F	68	G	C8-N7	-6.66	1.26	1.30
2	В	56	U	C2-N3	-6.52	1.33	1.37
5	F	62	А	C8-N7	-6.50	1.26	1.31
5	F	63	А	C6-N1	-6.47	1.31	1.35
5	F	58	G	C6-O6	-6.38	1.18	1.24
1	А	1083	TYR	CD1-CE1	-6.29	1.29	1.39
1	A	190	GLU	CB-CG	-6.17	1.40	1.52
5	F	49	А	C5-C4	-6.11	1.34	1.38
2	В	34	С	N3-C4	-6.05	1.29	1.33



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	63	А	N9-C8	-6.03	1.32	1.37
1	А	190	GLU	CG-CD	-5.96	1.43	1.51
5	F	65	G	N1-C2	-5.89	1.33	1.37
5	F	60	G	N1-C2	-5.88	1.33	1.37
18	Т	426	ASN	CB-CG	-5.86	1.37	1.51
24	W	88	GLY	C-N	5.86	1.45	1.34
5	F	60	G	N7-C5	-5.84	1.35	1.39
5	F	65	G	N9-C4	-5.80	1.33	1.38
5	F	64	G	C5-C4	-5.79	1.34	1.38
5	F	58	G	N1-C2	-5.75	1.33	1.37
1	А	1083	TYR	CD2-CE2	-5.71	1.30	1.39
1	А	154	VAL	CB-CG1	-5.70	1.40	1.52
2	В	54	G	C2-N3	-5.67	1.28	1.32
5	F	62	A	C5-C6	-5.67	1.35	1.41
2	В	51	A	C6-N1	-5.63	1.31	1.35
1	А	957	GLU	CB-CG	-5.60	1.41	1.52
5	F	64	G	C2-N3	-5.55	1.28	1.32
5	F	59	С	N3-C4	-5.51	1.30	1.33
18	Т	485	GLU	CG-CD	-5.49	1.43	1.51
1	А	179	TYR	CD1-CE1	-5.49	1.31	1.39
16	Р	233	TYR	CD2-CE2	-5.43	1.31	1.39
1	А	858	TYR	CD1-CE1	-5.39	1.31	1.39
5	F	47	G	C5-C4	-5.39	1.34	1.38
5	F	64	G	C8-N7	-5.38	1.27	1.30
5	F	56	С	N3-C4	-5.36	1.30	1.33
5	F	62	A	C5-C4	-5.36	1.34	1.38
18	Т	202	VAL	CB-CG2	-5.36	1.41	1.52
1	А	742	GLU	CB-CG	-5.36	1.42	1.52
22	Н	22	C	N3-C4	-5.34	1.30	1.33
5	F	48	C	N3-C4	-5.32	1.30	1.33
22	Н	21	G	C2-N3	-5.31	1.28	1.32
1	А	283	TYR	CD1-CE1	-5.25	1.31	1.39
1	А	644	TYR	CD2-CE2	-5.23	1.31	1.39
22	Н	25	A	N7-C5	-5.23	1.36	1.39
5	F	68	G	C5-C4	-5.22	1.34	1.38
5	F	59	C	N1-C6	-5.20	1.34	1.37
1	A	237	TYR	CD1-CE1	-5.20	1.31	1.39
1	A	179	TYR	CD2-CE2	-5.20	1.31	1.39
5	F	60	G	N9-C4	-5.19	1.33	1.38
1	А	1044	GLU	CB-CG	-5.18	1.42	1.52
5	F	60	G	C5-C4	-5.17	1.34	1.38
18	Т	283	VAL	CB-CG2	-5.17	1.42	1.52



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	Т	495	GLU	CB-CG	-5.16	1.42	1.52
1	А	169	TRP	CE3-CZ3	-5.15	1.29	1.38
2	В	55	А	N9-C4	-5.14	1.34	1.37
5	F	60	G	N9-C8	-5.14	1.34	1.37
1	А	973	TYR	CD2-CE2	-5.13	1.31	1.39
5	F	57	U	N3-C4	-5.13	1.33	1.38
5	F	64	G	C6-N1	-5.13	1.35	1.39
1	А	1340	GLU	CG-CD	-5.11	1.44	1.51
5	F	63	А	C8-N7	-5.08	1.27	1.31
2	В	52	G	C6-N1	-5.07	1.36	1.39
5	F	17	G	C8-N7	-5.04	1.27	1.30
5	F	47	G	N9-C4	-5.04	1.33	1.38
5	F	56	С	N1-C6	-5.03	1.34	1.37
5	F	55	С	N3-C4	-5.03	1.30	1.33
1	А	634	ASP	CB-CG	-5.01	1.41	1.51
5	F	59	С	C2-N3	-5.00	1.31	1.35
5	F	69	А	C5-C4	-5.00	1.35	1.38

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
22	Н	22	С	O5'-P-OP1	-18.02	89.07	110.70
20	Ν	46	LEU	CA-CB-CG	7.61	132.81	115.30
1	А	843	LEU	CA-CB-CG	7.12	131.67	115.30
5	F	39	G	C5-C6-O6	-6.80	124.52	128.60
5	F	68	G	N9-C4-C5	-6.78	102.69	105.40
24	W	89	PRO	CA-N-CD	-6.59	102.28	111.50
4	Е	357	LEU	CA-CB-CG	6.53	130.32	115.30
1	А	711	LEU	CA-CB-CG	6.43	130.09	115.30
5	F	39	G	N1-C6-O6	6.41	123.74	119.90
5	F	52	G	C4-C5-N7	6.39	113.36	110.80
20	Ν	169	LEU	CA-CB-CG	6.37	129.96	115.30
31	3	20	А	P-O3'-C3'	6.31	127.27	119.70
5	F	65	G	C8-N9-C4	6.21	108.89	106.40
5	F	68	G	C4-C5-N7	6.11	113.24	110.80
5	F	58	G	C8-N9-C4	6.08	108.83	106.40
5	F	58	G	C5-C6-N1	6.05	114.52	111.50
22	Н	4	С	N3-C2-O2	-6.03	117.68	121.90
25	L	740	LEU	CA-CB-CG	5.99	129.08	115.30
1	А	303	LEU	CA-CB-CG	5.98	129.05	115.30
2	В	70	U	C2-N1-C1'	5.96	124.85	117.70
5	F	46	А	N1-C6-N6	-5.83	115.10	118.60



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
26	K	62	PRO	N-CA-CB	5.80	110.26	103.30
1	А	1156	LEU	CA-CB-CG	5.65	128.29	115.30
29	Q	788	ALA	N-CA-C	-5.64	95.76	111.00
30	5	-6	С	C2-N1-C1'	5.59	124.95	118.80
2	В	29	U	N3-C2-O2	-5.52	118.34	122.20
5	F	7	С	C2-N1-C1'	5.52	124.87	118.80
30	5	-2	С	C2-N3-C4	-5.51	117.14	119.90
1	А	749	LEU	CA-CB-CG	5.51	127.96	115.30
30	5	-6	С	N1-C2-O2	5.47	122.18	118.90
3	С	415	GLY	N-CA-C	-5.43	99.53	113.10
22	Н	21	G	N7-C8-N9	5.43	115.81	113.10
5	F	54	С	N1-C2-O2	-5.35	115.69	118.90
5	F	47	G	N3-C4-C5	5.33	131.26	128.60
24	W	91	HIS	CB-CA-C	5.31	121.01	110.40
2	В	29	U	O4'-C1'-N1	5.25	112.40	108.20
15	J	21	ASP	CB-CG-OD2	5.25	123.03	118.30
5	F	58	G	C4-C5-C6	-5.24	115.66	118.80
5	F	26	G	N3-C4-N9	-5.20	122.88	126.00
5	F	19	U	C2-N1-C1'	5.19	123.93	117.70
1	А	1004	VAL	C-N-CA	-5.18	108.75	121.70
31	3	8	С	C5-C6-N1	5.18	123.59	121.00
5	F	63	А	N1-C6-N6	-5.17	115.50	118.60
5	F	47	G	C8-N9-C4	5.16	108.46	106.40
31	3	13	С	C6-N1-C2	-5.15	118.24	120.30
22	Н	21	G	C8-N9-C4	-5.13	104.35	106.40
2	В	56	U	C2-N3-C4	-5.13	123.92	127.00
30	5	-2	С	N3-C2-O2	-5.12	118.31	121.90
1	А	1154	ARG	NE-CZ-NH2	-5.10	117.75	120.30
26	К	106	LEU	CA-CB-CG	5.09	127.02	115.30
31	3	16	U	C2-N1-C1'	5.09	123.81	117.70
2	В	49	А	O4'-C1'-N9	5.07	112.25	108.20
26	К	219	LEU	CA-CB-CG	5.00	126.81	115.30

There are no chirality outliers.

All (16) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	А	1004	VAL	Peptide
1	А	1005	LYS	Peptide
1	А	1045	PHE	Peptide
1	А	1338	TYR	Peptide
1	А	1470	ASP	Peptide



Mol	Chain	Res	Type	Group
1	А	1480	ILE	Peptide
1	А	1701	TRP	Peptide
1	А	1751	TYR	Peptide
1	А	1783	PHE	Peptide
1	А	532	LYS	Peptide
1	А	686	GLY	Peptide
3	С	69	GLU	Peptide
25	L	670	TRP	Peptide
28	V	703	PHE	Peptide
6	s	67	THR	Peptide
6	t	67	THR	Peptide

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
1	А	1923/2398~(80%)	1730 (90%)	182 (10%)	11 (1%)	22	43
3	С	895/989~(90%)	816 (91%)	78~(9%)	1 (0%)	48	71
4	Ε	316/362~(87%)	289~(92%)	26 (8%)	1 (0%)	37	59
6	q	102/503~(20%)	102 (100%)	0	0	100	100
6	r	129/503~(26%)	120~(93%)	8~(6%)	1 (1%)	16	34
6	s	68/503~(14%)	65~(96%)	3~(4%)	0	100	100
6	t	60/503~(12%)	56~(93%)	4 (7%)	0	100	100
7	a	88/127~(69%)	86~(98%)	2 (2%)	0	100	100
8	g	$\overline{63/77}~(82\%)$	60~(95%)	$\overline{3}(5\%)$	0	100	100
9	е	78/87~(90%)	74 (95%)	4 (5%)	0	100	100



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
10	f	69/85~(81%)	68~(99%)	1 (1%)	0	100	100
11	d	98/110~(89%)	97~(99%)	1 (1%)	0	100	100
12	с	86/114~(75%)	82 (95%)	4 (5%)	0	100	100
13	b	95/265~(36%)	89 (94%)	6~(6%)	0	100	100
14	Ι	657/925~(71%)	641 (98%)	16 (2%)	0	100	100
15	J	587/835~(70%)	551 (94%)	30~(5%)	6 (1%)	13	29
16	Р	98/235~(42%)	90~(92%)	8 (8%)	0	100	100
17	М	74/563~(13%)	68~(92%)	6 (8%)	0	100	100
18	Т	342/518~(66%)	326~(95%)	15 (4%)	1 (0%)	37	59
19	Ο	269/417~(64%)	245~(91%)	24 (9%)	0	100	100
20	Ν	167/233~(72%)	154 (92%)	13 (8%)	0	100	100
21	R	254/684~(37%)	240 (94%)	14 (6%)	0	100	100
23	S	153/157~(98%)	137 (90%)	16 (10%)	0	100	100
24	W	475/576~(82%)	431 (91%)	38~(8%)	6 (1%)	10	21
25	L	454/833~(54%)	429 (94%)	25~(6%)	0	100	100
26	K	208/303~(69%)	191 (92%)	16 (8%)	1 (0%)	25	47
27	U	24/721~(3%)	23~(96%)	1 (4%)	0	100	100
28	V	184/928~(20%)	177 (96%)	7 (4%)	0	100	100
29	Q	1275/1844~(69%)	1217 (96%)	49 (4%)	9 (1%)	19	38
All	All	9291/16398~(57%)	8654 (93%)	600 (6%)	37 (0%)	32	52

Continued from previous page...

All (37) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	389	VAL
1	А	449	GLU
15	J	26	ALA
15	J	27	GLU
29	Q	893	ARG
1	А	246	PRO
3	С	422	THR
6	r	58	THR
15	J	37	GLN
15	J	40	ASP
15	J	53	GLU


Mol	Chain	Res	Type
26	K	62	PRO
29	Q	155	GLU
29	Q	158	GLY
29	Q	719	ALA
29	Q	789	SER
1	А	247	LEU
1	А	528	PRO
4	Е	47	GLY
24	W	86	VAL
29	Q	154	GLN
1	А	1266	MET
1	А	1717	ASP
1	А	2011	PRO
29	Q	153	LYS
1	А	1426	ASP
1	А	1718	GLN
24	W	87	LEU
24	W	92	PRO
24	W	91	HIS
29	Q	898	ASP
29	Q	$13\overline{65}$	VAL
1	A	1822	PRO
15	J	52	PRO
24	W	84	ALA
24	W	198	GLN
18	Т	247	GLY

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 side chain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	А	1505/2124~(71%)	1306 (87%)	199 (13%)	3 6
3	С	753/825~(91%)	647~(86%)	106 (14%)	3 5
4	Е	264/300~(88%)	231 (88%)	33 (12%)	3 7
6	q	94/398~(24%)	79~(84%)	15 (16%)	2 3



Mol	Chain	Analysed	Rotameric	Outliers	Perce	entiles
6	r	113/398~(28%)	93~(82%)	20 (18%)	1	2
6	\mathbf{S}	59/398~(15%)	54 (92%)	5 (8%)	8	18
6	\mathbf{t}	54/398~(14%)	45 (83%)	9~(17%)	2	3
7	a	76/97~(78%)	66~(87%)	10 (13%)	3	6
8	g	58/67~(87%)	49~(84%)	9~(16%)	2	3
9	е	73/79~(92%)	63~(86%)	10 (14%)	3	5
10	f	62/75~(83%)	54 (87%)	8 (13%)	3	6
11	d	92/100~(92%)	80~(87%)	12~(13%)	3	6
12	с	78/95~(82%)	67~(86%)	11 (14%)	3	5
13	b	84/211~(40%)	76~(90%)	8 (10%)	7	14
14	Ι	357/743~(48%)	308~(86%)	49 (14%)	3	5
15	J	260/676~(38%)	228 (88%)	32 (12%)	4	8
16	Р	88/188~(47%)	77~(88%)	11 (12%)	3	7
17	М	63/424~(15%)	56~(89%)	7 (11%)	5	10
18	Т	291/416~(70%)	263~(90%)	28 (10%)	7	14
19	Ο	228/318~(72%)	210~(92%)	18 (8%)	10	21
20	Ν	148/193~(77%)	137~(93%)	11 (7%)	11	24
21	R	209/507~(41%)	179~(86%)	30 (14%)	2	5
23	S	128/130~(98%)	119~(93%)	9~(7%)	12	27
24	W	118/474~(25%)	95~(80%)	23 (20%)	1	2
25	L	388/648~(60%)	333~(86%)	55 (14%)	2	5
26	Κ	177/221~(80%)	144 (81%)	33 (19%)	1	2
27	U	20/572~(4%)	16 (80%)	4 (20%)	1	2
28	V	28/746~(4%)	24 (86%)	4 (14%)	2	5
All	All	5868/11821 (50%)	5099~(87%)	769 (13%)	6	6

All (769) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	85	GLN
1	А	95	LYS
1	А	96	TRP
1	А	108	ARG
1	А	114	GLU



Mol	Chain	Res	Type
1	А	127	LYS
1	А	130	ARG
1	А	137	SER
1	А	145	ARG
1	А	146	VAL
1	А	148	LEU
1	А	167	MET
1	А	175	VAL
1	А	177	VAL
1	А	181	ILE
1	А	185	ILE
1	А	229	ASP
1	А	276	LYS
1	А	279	ASN
1	А	288	LEU
1	А	296	LEU
1	А	299	LEU
1	А	303	LEU
1	А	305	THR
1	А	310	ARG
1	А	311	ASN
1	А	321	PHE
1	А	331	ILE
1	А	342	ARG
1	А	368	THR
1	А	380	ASN
1	А	385	VAL
1	А	386	ARG
1	А	387	LEU
1	A	391	HIS
1	A	396	LEU
1	A	478	ARG
1	A	489	PRO
1	A	492	ASN
1	A	493	CYS
1	A	498	HIS
1	A	502	THR
1	A	503	TYR
1	A	$52\overline{2}$	LEU
1	A	529	LYS
1	A	530	SER
1	А	540	LEU



Mol	Chain	Res	Type
1	А	547	GLN
1	А	548	SER
1	А	549	THR
1	А	587	ASN
1	А	593	THR
1	А	595	THR
1	А	596	THR
1	А	599	ARG
1	А	610	LEU
1	А	618	THR
1	А	619	LYS
1	А	633	VAL
1	А	634	ASP
1	A	640	ASP
1	А	643	GLN
1	А	675	LEU
1	А	691	VAL
1	А	706	ARG
1	А	708	ILE
1	А	712	LEU
1	А	714	ARG
1	А	729	SER
1	А	732	ILE
1	А	738	LYS
1	А	756	ASP
1	А	800	GLU
1	А	809	GLN
1	А	834	THR
1	А	866	THR
1	A	884	ARG
1	А	899	ASP
1	A	909	ARG
1	A	923	SER
1	A	935	TYR
1	A	946	LYS
1	A	952	GLN
1	A	954	SER
1	A	978	LEU
1	A	980	LYS
1	A	984	CYS
1	A	986	LEU
1	А	987	ASP



Mol	Chain	Res	Type
1	А	993	GLU
1	А	999	LEU
1	А	1004	VAL
1	А	1005	LYS
1	А	1015	LEU
1	А	1024	ASN
1	А	1027	THR
1	А	1042	GLN
1	А	1043	SER
1	А	1059	ARG
1	А	1085	ASP
1	А	1087	SER
1	А	1091	SER
1	А	1094	LEU
1	А	1120	THR
1	А	1133	ASN
1	А	1142	LYS
1	А	1153	SER
1	А	1157	ASN
1	А	1163	PHE
1	А	1164	ARG
1	А	1188	ASN
1	А	1196	LYS
1	А	1201	ASP
1	А	1213	LEU
1	А	1224	ARG
1	А	1230	THR
1	А	1231	THR
1	А	1240	SER
1	А	1245	ASP
1	А	1246	ASN
1	A	1248	ASN
1	A	1265	ARG
1	A	1283	VAL
1	А	1285	THR
1	A	1289	THR
1	A	1319	THR
1	A	1321	THR
1	A	1322	LYS
1	А	1331	LEU
1	A	1336	THR
1	А	1340	GLU



Mol	Chain	Res	Type
1	А	1348	LEU
1	А	1362	ARG
1	А	1365	ILE
1	А	1402	SER
1	А	1417	PHE
1	А	1421	MET
1	А	1428	LEU
1	А	1434	ARG
1	А	1441	SER
1	А	1447	GLU
1	А	1452	GLU
1	А	1456	LYS
1	А	1457	LYS
1	А	1459	GLU
1	А	1461	LYS
1	А	1465	ARG
1	А	1468	THR
1	A	1470	ASP
1	A	1472	LEU
1	A	1490	ASP
1	A	1491	ARG
1	А	1493	THR
1	A	1502	VAL
1	A	1512	THR
1	A	1513	LYS
1	A	1514	MET
1	A	1538	VAL
1	A	1545	VAL
1	A	1557	THR
1	A	1558	TYR
1	A	1590	LEU
1	A	1592	GLN
1	A	1593	ILE
1	A	1600	LEU
1	A	1601	TRP
1	A	1605	THR
1	A	1608	ARG
1	A	1630	ILE
1	A	1632	THR
1	A	1633	LEU
1	A	1635	ILE
1	A	1658	CYS



Mol	Chain	Res	Type
1	А	1665	LEU
1	А	1679	HIS
1	А	1683	SER
1	А	1700	LYS
1	А	1701	TRP
1	А	1702	ASN
1	А	1705	LYS
1	А	1707	SER
1	А	1712	THR
1	А	1725	TRP
1	А	1726	VAL
1	А	1728	VAL
1	А	1729	GLN
1	А	1732	TRP
1	А	1747	LYS
1	А	1754	ASP
1	А	1756	MET
1	А	1757	SER
1	А	1783	PHE
1	А	1786	ILE
1	А	1807	LEU
1	А	1810	ARG
1	А	1813	LYS
1	А	1816	GLN
1	А	1817	LEU
1	А	1819	SER
3	С	67	LEU
3	С	69	GLU
3	С	76	SER
3	С	92	GLU
3	С	109	LYS
3	С	111	GLU
3	С	112	THR
3	C	113	LEU
3	С	118	LEU
3	С	119	ARG
3	С	127	LEU
3	C	135	GLU
3	C	140	VAL
3	C	150	LYS
3	C	162	HIS
3	С	166	LYS



Mol	Chain	Res	Type
3	С	171	GLN
3	С	176	LYS
3	С	197	MET
3	С	200	SER
3	С	204	GLU
3	С	210	SER
3	С	212	LEU
3	С	218	CYS
3	С	269	MET
3	С	306	CYS
3	С	313	GLU
3	С	319	VAL
3	С	330	SER
3	С	337	GLN
3	С	339	PHE
3	С	355	GLU
3	С	356	PHE
3	С	358	LYS
3	С	365	TYR
3	С	384	ARG
3	С	397	MET
3	С	416	LEU
3	С	419	TYR
3	С	421	ARG
3	С	429	THR
3	С	465	LYS
3	С	482	MET
3	С	485	CYS
3	С	508	ASP
3	С	525	LYS
3	С	527	LEU
3	С	537	GLU
3	С	550	TYR
3	С	560	ARG
3	С	566	LEU
3	С	572	VAL
3	С	585	ASP
3	С	591	VAL
3	С	606	LYS
3	С	610	GLU
3	С	616	GLU
3	С	620	MET



Mol	Chain	Res	Type
3	С	622	GLU
3	С	634	CYS
3	С	636	THR
3	С	640	GLU
3	С	643	GLU
3	С	649	THR
3	С	654	LEU
3	С	658	MET
3	С	662	ARG
3	С	676	VAL
3	С	690	LYS
3	С	700	ASN
3	С	709	LEU
3	С	710	ASP
3	С	721	ASN
3	С	725	ASP
3	С	729	LYS
3	С	747	ARG
3	С	749	LEU
3	С	763	LEU
3	С	770	GLU
3	С	772	ASN
3	С	773	LYS
3	С	781	ASP
3	С	784	ILE
3	С	785	GLN
3	С	787	PHE
3	С	789	TRP
3	С	809	LEU
3	C	810	ASP
3	С	826	ILE
3	С	839	MET
3	С	843	ARG
3	C	849	TYR
3	С	855	THR
3	C	858	ASP
3	С	865	ASN
3	С	874	VAL
3	С	878	VAL
3	С	895	VAL
3	С	901	GLU
3	С	902	THR



Mol	Chain	Res	Type
3	С	905	ARG
3	С	932	SER
3	С	936	ARG
3	С	938	LEU
3	С	948	ARG
3	С	961	SER
4	Е	53	ASN
4	Е	54	LEU
4	Е	72	ARG
4	Е	76	ASP
4	Е	96	ASP
4	Е	103	VAL
4	Е	104	ILE
4	Е	118	THR
4	Е	127	SER
4	Е	130	LYS
4	Е	157	CYS
4	Е	181	ARG
4	Е	184	LYS
4	Е	200	PHE
4	Е	202	ASP
4	Е	212	VAL
4	Е	214	ASN
4	Е	223	ARG
4	Е	228	ASP
4	Е	232	SER
4	Е	243	THR
4	Е	256	SER
4	Е	265	GLU
4	E	266	TRP
4	E	277	CYS
4	E	284	HIS
4	E	288	PHE
4	E	300	ASP
4	E	302	SER
4	E	306	CYS
4	E	311	ARG
4	E	333	SER
4	E	337	VAL
6	q	1	MET
6	q	3	CYS
6	q	12	GLN



Mol	Chain	Res	Type
6	q	18	LYS
6	q	33	ARG
6	q	46	SER
6	q	48	GLU
6	q	50	LEU
6	q	72	LEU
6	q	78	ASP
6	q	92	THR
6	q	97	THR
6	q	113	ARG
6	q	114	VAL
6	q	117	ARG
6	r	2	PHE
6	r	6	SER
6	r	12	GLN
6	r	14	VAL
6	r	31	TYR
6	r	41	THR
6	r	45	LEU
6	r	55	VAL
6	r	57	LYS
6	r	59	VAL
6	r	63	THR
6	r	67	THR
6	r	88	HIS
6	r	95	HIS
6	r	106	TYR
6	r	113	ARG
6	r	115	ILE
6	r	119	LEU
6	r	120	LYS
6	r	129	LEU
6	S	74	SER
6	S	84	MET
6	S	85	LEU
6	S	113	ARG
6	S	131	ASP
6	t	74	SER
6	t	75	LEU
6	t	80	TRP
6	t	88	HIS
6	t	105	LEU



Mol	Chain	Res	Type
6	t	108	HIS
6	t	117	ARG
6	t	119	LEU
6	t	123	ASP
7	a	19	GLU
7	a	34	ARG
7	a	47	GLN
7	a	57	ASP
7	a	59	ARG
7	a	61	THR
7	a	66	LEU
7	a	68	ILE
7	a	89	LYS
7	a	90	ARG
8	g	21	LEU
8	g	24	ASN
8	g	27	VAL
8	g	38	MET
8	g	53	ASP
8	g	56	MET
8	g	60	ARG
8	g	65	GLN
8	g	70	LEU
9	е	9	MET
9	е	24	GLN
9	е	35	ASP
9	е	50	ASN
9	е	55	GLU
9	е	61	MET
9	е	63	ARG
9	е	77	ASP
9	е	82	ILE
9	е	85	THR
10	f	12	PHE
10	f	23	VAL
10	f	42	MET
10	f	48	SER
10	f	63	GLU
10	f	68	CYS
10	f	69	ASN
10	f	74	LEU
11	d	17	GLU



Mol	Chain	Res	Type
11	d	22	THR
11	d	42	CYS
11	d	44	ASN
11	d	51	ARG
11	d	63	LEU
11	d	68	GLU
11	d	69	MET
11	d	71	THR
11	d	81	LYS
11	d	84	ARG
11	d	98	ARG
12	с	2	VAL
12	с	6	ARG
12	с	21	LYS
12	с	24	THR
12	с	38	ASN
12	с	45	LYS
12	с	49	ARG
12	с	62	ARG
12	с	64	ASN
12	с	75	LEU
12	с	85	ASP
13	b	9	LEU
13	b	20	THR
13	b	25	ARG
13	b	30	ARG
13	b	44	ASP
13	b	55	LYS
13	b	61	GLU
13	b	62	ARG
14	Ι	347	ASP
14	I	354	GLU
14	Ι	356	LEU
14	I	365	SER
14	Ι	367	VAL
14	Ι	370	ARG
14	I	382	ARG
14	Ι	384	LYS
14	Ι	392	LYS
14	Ι	395	LEU
14	I	402	ARG
14	I	412	LYS



Mol	Chain	Res	Type
14	Ι	416	LEU
14	Ι	420	PHE
14	Ι	434	ARG
14	Ι	438	GLN
14	Ι	444	ARG
14	Ι	456	CYS
14	Ι	466	SER
14	Ι	473	ASP
14	Ι	480	THR
14	Ι	487	ARG
14	Ι	492	GLU
14	Ι	500	ASP
14	Ι	537	ILE
14	Ι	546	TYR
14	Ι	548	LEU
14	Ι	601	LEU
14	Ι	613	GLU
14	Ι	614	CYS
14	Ι	615	LYS
14	Ι	628	TYR
14	Ι	640	ARG
14	Ι	651	LYS
14	Ι	655	ASP
14	Ι	659	SER
14	Ι	670	VAL
14	Ι	687	SER
14	Ι	688	ASP
14	Ι	692	ARG
14	Ι	702	GLU
14	Ι	712	ARG
14	Ι	735	ARG
14	Ι	737	PHE
14	Ι	745	ASP
14	Ι	746	THR
14	Ι	747	PHE
14	Ι	752	ARG
14	Ι	758	LYS
15	J	24	ILE
15	J	38	LEU
15	J	54	GLU
15	J	57	GLU
15	J	61	SER



Mol	Chain	Res	Type
15	J	65	GLN
15	J	71	ARG
15	J	77	ASN
15	J	96	ARG
15	J	126	ARG
15	J	139	VAL
15	J	140	SER
15	J	144	ARG
15	J	167	GLN
15	J	175	PHE
15	J	196	ASP
15	J	202	PHE
15	J	213	LYS
15	J	223	MET
15	J	237	ARG
15	J	242	LEU
15	J	244	GLU
15	J	247	GLN
15	J	248	THR
15	J	249	GLU
15	J	255	PHE
15	J	257	GLU
15	J	273	ARG
15	J	279	ILE
15	J	288	TYR
15	J	311	LYS
15	J	313	ARG
16	Р	13	ILE
16	Р	40	LYS
16	Р	48	GLN
16	Р	62	GLU
16	Р	68	ARG
16	Р	194	ARG
16	Р	199	ASP
16	P	204	ASN
16	Р	211	LYS
16	Р	231	GLN
16	P	234	ILE
17	М	447	GLN
17	М	464	GLU
17	М	484	LYS
17	М	499	MET



Mol	Chain	Res	Type
17	М	531	ARG
17	М	535	PHE
17	М	538	LYS
18	Т	190	ARG
18	Т	199	MET
18	Т	212	CYS
18	Т	213	VAL
18	Т	216	ASP
18	Т	270	ASP
18	Т	286	SER
18	Т	306	LEU
18	Т	312	ASP
18	Т	314	VAL
18	Т	323	LYS
18	Т	353	HIS
18	Т	377	SER
18	Т	383	MET
18	Т	388	PHE
18	Т	396	GLU
18	Т	414	SER
18	Т	446	ARG
18	Т	450	CYS
18	Т	462	SER
18	Т	464	GLU
18	Т	465	SER
18	Т	469	LEU
18	Т	485	GLU
18	Т	497	GLU
18	Т	498	ASP
18	Т	510	ARG
18	Т	514	ASP
19	0	24	GLU
19	0	35	MET
19	0	49	ARG
19	0	68	VAL
19	0	70	CYS
19	Ο	83	CYS
19	0	110	SER
19	0	111	GLU
19	0	151	LEU
19	0	154	SER
19	0	157	TYR



Mol	Chain	Res	Type
19	0	164	ARG
19	0	165	VAL
19	0	180	CYS
19	0	206	ASN
19	0	224	THR
19	0	233	THR
19	0	282	LYS
20	Ν	10	LYS
20	N	21	GLU
20	N	23	ILE
20	Ν	41	LYS
20	N	72	SER
20	N	82	GLU
20	N	118	SER
20	Ν	134	THR
20	Ν	146	SER
20	N	169	LEU
20	N	176	TRP
21	R	39	LEU
21	R	42	LYS
21	R	83	ILE
21	R	88	LYS
21	R	97	VAL
21	R	105	ARG
21	R	110	ASP
21	R	114	LEU
21	R	117	LYS
21	R	118	VAL
21	R	119	ASP
21	R	128	ARG
21	R	146	GLU
21	R	152	LYS
21	R	154	SER
21	R	155	SER
21	R	161	LEU
21	R	168	SER
21	R	174	THR
21	R	195	ASP
21	R	211	VAL
21	R	220	VAL
21	R	223	LEU
21	R	231	THR



Mol	Chain	Res	Type
21	R	233	LYS
21	R	236	GLN
21	R	257	LEU
21	R	259	LYS
21	R	264	ASP
21	R	286	THR
23	S	9	ASP
23	S	28	CYS
23	S	73	LYS
23	S	80	ARG
23	S	85	THR
23	S	91	SER
23	S	133	ARG
23	S	134	LEU
23	S	146	VAL
24	W	47	THR
24	W	50	VAL
24	W	51	LEU
24	W	65	LEU
24	W	66	GLN
24	W	72	LYS
24	W	77	LEU
24	W	81	ASP
24	W	87	LEU
24	W	89	PRO
24	W	91	HIS
24	W	102	LEU
24	W	107	VAL
24	W	112	ASP
24	W	118	ILE
24	W	122	GLN
24	W	134	GLU
24	W	139	ILE
24	W	167	THR
24	W	171	ARG
24	W	202	SER
24	W	212	GLU
24	W	225	LYS
$\overline{25}$	L	24	LYS
25	L	35	SER
25	L	38	VAL
25	L	61	GLU



Mol	Chain	Res	Type
25	L	70	LEU
25	L	103	LEU
25	L	120	ARG
25	L	122	LEU
25	L	130	ASN
25	L	148	LYS
25	L	152	SER
25	L	161	THR
25	L	171	ARG
25	L	175	LEU
25	L	180	ARG
25	L	183	GLN
25	L	184	LEU
25	L	217	LEU
25	L	220	GLN
25	L	237	GLN
25	L	541	ASP
25	L	543	ARG
25	L	545	ARG
25	L	548	ARG
25	L	552	GLU
25	L	553	ARG
25	L	563	LYS
25	L	571	ARG
25	L	596	LEU
25	L	599	ARG
25	L	614	HIS
25	L	619	TYR
25	L	622	LYS
25	L	654	SER
25	L	660	ASP
25	L	665	TYR
25	L	675	LEU
25	L	696	SER
25	L	699	ARG
25	L	702	ARG
25	L	718	GLU
25	L	720	ASP
25	L	731	LYS
25	L	748	GLN
25	L	749	ARG
25	L	757	ARG



Mol	Chain	Res	Type
25	L	779	HIS
25	L	780	GLU
25	L	781	ARG
25	L	800	THR
25	L	816	ARG
25	L	817	ARG
25	L	818	ARG
25	L	828	LYS
25	L	833	SER
26	K	28	HIS
26	K	29	LEU
26	K	55	LYS
26	K	58	SER
26	K	59	THR
26	K	65	TYR
26	K	68	GLU
26	K	69	MET
26	K	77	PHE
26	K	86	GLU
26	К	87	TYR
26	K	94	GLU
26	К	104	TYR
26	К	105	ARG
26	K	114	ARG
26	K	116	ASP
26	K	122	SER
26	K	123	SER
26	К	130	GLN
26	K	131	LEU
26	К	136	LEU
26	K	145	LEU
26	K	149	ASP
26	K	159	ASP
26	K	177	THR
26	K	188	GLN
26	К	197	LYS
26	K	202	TYR
26	K	205	GLN
26	K	208	LYS
26	K	214	ARG
26	K	216	CYS
26	K	226	MET



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Mol	Chain	Res	Type
27	U	2	TYR
27	U	15	THR
27	U	19	VAL
27	U	23	LYS
28	V	656	ARG
28	V	658	THR
28	V	668	ASP
28	V	669	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (156) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	100	ASN
1	А	124	HIS
1	А	132	HIS
1	А	269	HIS
1	А	279	ASN
1	А	311	ASN
1	А	379	ASN
1	А	391	HIS
1	А	461	ASN
1	А	481	HIS
1	А	492	ASN
1	А	496	GLN
1	А	512	GLN
1	А	521	ASN
1	А	A 581	
1	А	625	ASN
1	А	627	GLN
1	А	648	HIS
1	А	674	HIS
1	А	728	GLN
1	А	739	GLN
1	А	744	HIS
1	А	755	HIS
1	А	809	GLN
1	А	852	GLN
1	А	855	GLN
1	А	895	ASN
1	А	939	HIS
1	А	948	HIS
1	А	952	GLN



Mol	Chain	Res	Type
1	А	968	HIS
1	А	1024	ASN
1	А	1025	ASN
1	А	1033	ASN
1	А	1078	ASN
1	А	1133	ASN
1	А	1147	HIS
1	А	1157	ASN
1	А	1160	HIS
1	А	1175	GLN
1	А	1194	ASN
1	А	1223	ASN
1	А	1246	ASN
1	A	1282	ASN
1	А	1284	HIS
1	А	1291	GLN
1	А	1310	GLN
1	А	1325	ASN
1	А	1346	GLN
1	А	1357	ASN
1	А	1360	GLN
1	А	1401	GLN
1	А	1437	GLN
1	А	1464	ASN
1	А	1504	GLN
1	А	1521	HIS
1	А	1524	HIS
1	А	1616	GLN
1	A	1639	GLN
1	A	1702	ASN
1	А	1801	ASN
3	С	68	HIS
3	С	133	ASN
3	С	147	HIS
3	С	214	ASN
3	C	337	GLN
3	C	388	GLN
3	C	502	GLN
3	C	757	GLN
3	C	760	ASN
3	C	865	ASN
3	C	915	GLN



Mol	Chain	Res	Type
3	С	944	GLN
4	Е	100	ASN
4	Е	275	ASN
4	Е	284	HIS
4	Е	330	HIS
6	q	83	ASN
6	q	95	HIS
6	q	99	GLN
6	r	21	HIS
6	r	56	ASN
6	r	108	HIS
6	t	88	HIS
6	t	107	GLN
7	a	16	HIS
7	a	47	GLN
7	a	84	ASN
8	g	65	GLN
9	е	21	GLN
9	е	27	GLN
9	е	50	ASN
9	е	78	ASN
11	d	44	ASN
11	d	58	HIS
11	d	80	GLN
12	с	65	ASN
12	с	76	ASN
14	Ι	374	HIS
14	Ι	393	GLN
14	Ι	427	HIS
14	Ι	432	ASN
14	Ι	445	HIS
14	Ι	453	HIS
14	Ι	465	HIS
14	I	512	HIS
14	Ι	545	ASN
14	Ι	553	GLN
14	Ι	743	ASN
15	J	154	HIS
15	J	207	GLN
15	J	224	GLN
15	J	247	GLN
16	Р	38	HIS



Mol	Chain	Res	Type
16	Р	48	GLN
17	М	495	ASN
17	М	540	GLN
18	Т	261	HIS
18	Т	347	GLN
18	Т	353	HIS
19	0	45	HIS
19	0	60	ASN
19	0	71	GLN
19	0	119	GLN
19	0	149	GLN
19	0	152	GLN
20	N	29	GLN
20	N	51	HIS
20	N	111	ASN
20	N	119	HIS
20	N	138	GLN
20	N	172	ASN
21	R	79	GLN
21	R	150	GLN
21	R	235	GLN
21	R	236	GLN
21	R	274	ASN
23	S	30	ASN
23	S	98	ASN
23	S	138	GLN
24	W	66	GLN
24	W	91	HIS
24	W	114	HIS
24	W	125	HIS
24	W	195	GLN
24	W	198	GLN
25	L	29	GLN
25	L	130	ASN
25	L	568	GLN
25	L	688	HIS
26	K	26	ASN
26	K	28	HIS
26	K	134	GLN
26	K	187	GLN
26	K	233	HIS
28	V	674	HIS



5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	В	83/111~(74%)	48 (57%)	2(2%)
22	Н	39/192~(20%)	28~(71%)	3~(7%)
30	5	6/7~(85%)	1 (16%)	0
31	3	33/173~(19%)	16 (48%)	6 (18%)
5	F	90/101~(89%)	48 (53%)	5(5%)
All	All	251/584~(42%)	141~(56%)	16~(6%)

All (141) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	В	8	А
2	В	9	С
2	В	10	G
2	В	11	А
2	В	15	G
2	В	16	А
2	В	17	А
2	В	20	С
2	В	27	А
2	В	28	А
2	В	35	U
2	В	39	G
2	В	40	С
2	В	41	С
2	В	42	U
2	В	48	U
2	В	49	А
2	В	52	G
2	В	53	А
2	В	58	С
2	В	59	G
2	В	62	А
2	В	63	G
2	В	64	U
2	В	65	U
2	В	66	U
2	В	68	G
2	В	69	С
2	В	70	U
2	В	71	С
2	В	72	А



Mol	Chain	Res	Type
2	В	73	С
2	В	74	G
2	B 75 C		
2	В	76	А
2	В	77	G
2	В	79	С
2	В	80	G
2	В	88	А
2	В	89	U
2	В	90	С
2	В	91	U
2	В	92	U
2	В	94	U
2	В	95	U
2	В	96	G
2	В	97	U
2	В	98	G
5	F	4	С
5	F	5	U
5	F	6	U
5	F	7	С
5	F	8	G
5	F	9	G
5	F	13	А
5	F	14	А
5	F	19	U
5	F	20	А
5	F	21	А
5	F	22	А
5	F	24	U
5	F	26	G
5	F	27	G
5	F	29	A
5	F	37	G
5	F	40	A
5	F	41	A
5	F	42	G
5	F	47	G
5	F	51	G
5	F	61	С
5	F	62	A
5	F	67	U



Mol	Chain	Res	Type
5	F	68	G
5	F	71	А
5	F	72	С
5	F	73	G
5	F	74	С
5	F	75	А
5	F	76	U
5	F	77	А
5	F	78	А
5	F	79	А
5	F	80	U
5	F	81	С
5	F	82	G
5	F	83	А
5	F	84	G
5	F	85	А
5	F	86	А
5	F	87	А
5	F	88	U
5	F	89	G
5	F	90	G
5	F	91	U
5	F	92	U
22	Н	2	U
22	Н	3	А
22	Н	4	С
22	Н	5	С
22	Н	6	U
22	Н	7	U
22	Н	8	U
22	Н	9	С
22	Н	10	U
22	Н	11	C
22	Н	12	G
22	Н	13	G
22	Н	14	С
22	Н	16	U
22	Н	17	U
22	Н	18	U
22	Н	19	U
22	Н	20	G
22	Н	21	G



Mol	Chain	Type	
22	Н	24	С
22	Н	25	А
22	Н	26	G
22	Н	30	А
22	Н	31	U
22	Н	32	G
22	Н	34	G
22	Н	38	U
22	Н	40	U
30	5	-6	С
31	3	2	U
31	3	3	А
31	3	7	G
31	3	8	C
31	3	12	G
31	3	13	C
31	3	14	А
31	3	17	А
31	3	19	U
31	3	20	А
31	3	21	С
31	3	22	U
31	3	91	А
31	3	96	U
31	3	98	U
31	3	100	C

All (16) RNA pucker outliers are listed below:

Mol	Chain	Res	Type	
2	В	16	А	
2	В	97	U	
5	F	19	U	
5	F	26	G	
5 F 76		U		
5	F	78	А	
5	F	80	U	
22	22 H		U	
22	H 30		A	
22	Н	31	U	
31	1 3 16		U	
31	3	20	А	



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Mol	Chain	Res	Type
31	3	21	С
31	3	90	С
31	3	95	U
31	3	97	А

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 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	Mol Tuno Chain Bog Lin		Tink	Bond lengths		Bond angles				
IVI01	туре	Unam	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
21	SEP	R	225	21	8,9,10	1.19	1 (12%)	8,12,14	1.31	2 (25%)
21	SEP	R	217	21	8,9,10	1.16	1 (12%)	8,12,14	1.38	1 (12%)

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
21	SEP	R	225	21	-	0/5/8/10	-
21	SEP	R	217	21	-	1/5/8/10	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
21	R	217	SEP	P-O1P	2.38	1.58	1.50
21	R	225	SEP	P-O1P	2.18	1.57	1.50

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
21	R	217	SEP	O2P-P-OG	3.08	114.92	106.73



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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
21	R	225	SEP	OG-CB-CA	2.72	110.79	108.14
21	R	225	SEP	O3P-P-OG	2.09	112.30	106.73

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
21	R	217	SEP	CA-CB-OG-P

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 11 ligands modelled in this entry, 10 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	anin Ros		Bo	ond leng	ths	B	ond ang	gles
	туре	Ullalli	nes	LINK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2
32	GTP	С	1001	33	26,34,34	1.11	3 (11%)	32,54,54	0.89	1 (3%)

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	\mathbf{Res}	Link	Chirals	Torsions	Rings
32	GTP	С	1001	33	-	5/18/38/38	0/3/3/3



Mol	Chain	Res	Type	Atoms	Ζ	$\operatorname{Observed}(\operatorname{\AA})$	$\mathrm{Ideal}(\mathrm{\AA})$
32	С	1001	GTP	C5-C6	-2.67	1.42	1.47
32	С	1001	GTP	C8-N7	-2.23	1.31	1.35
32	С	1001	GTP	C5-C4	-2.16	1.37	1.43

All (3) bond length outliers are listed below:

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
32	С	1001	GTP	C3'-C2'-C1'	2.08	104.11	100.98

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	С	1001	GTP	C5'-O5'-PA-O1A
32	С	1001	GTP	C5'-O5'-PA-O2A
32	С	1001	GTP	PA-O3A-PB-O3B
32	С	1001	GTP	PG-O3B-PB-O2B
32	С	1001	GTP	C5'-O5'-PA-O3A

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 any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-38362. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections (i)

6.1.1 Primary map



6.1.2 Raw map



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



6.2 Central slices (i)

6.2.1 Primary map



X Index: 220



Y Index: 220



Z Index: 220

6.2.2 Raw map



X Index: 220

Y Index: 220

Z Index: 220 $\,$

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: 203



Y Index: 234



Z Index: 222

6.3.2 Raw map



X Index: 213

Y Index: 224



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



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

6.4.1 Primary map



6.4.2 Raw map



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


6.5 Orthogonal surface views (i)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.08. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

6.6 Mask visualisation (i)

This section 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 1131 nm^3 ; this corresponds to an approximate mass of 1022 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 0.385 $\mathrm{\AA^{-1}}$



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 0.385 $\mathrm{\AA^{-1}}$



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	2.60	-	-
Author-provided FSC curve	2.59	2.89	2.61
Unmasked-calculated*	3.12	3.63	3.13

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.12 differs from the reported value 2.6 by more than 10 %



9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-38362 and PDB model 8XI2. Per-residue inclusion information can be found in section 3 on page 11.

9.1 Map-model overlay (i)



The images above show the 3D surface view of the map at the recommended contour level 0.08 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 (0.08).



9.4 Atom inclusion (i)



At the recommended contour level, 62% of all backbone atoms, 68% of all non-hydrogen atoms, are inside the map.



9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.08) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	$\mathbf{Q} extsf{-score}$
All	0.6850	0.3810
3	0.7060	0.2340
5	0.9530	0.6210
А	0.8830	0.5470
В	0.8690	0.3780
С	0.7990	0.3620
E	0.9280	0.4580
F	0.9130	0.4530
Н	0.6630	0.2840
Ι	0.4210	0.1850
J	0.6150	0.3610
K	0.4830	0.2310
L	0.6460	0.3640
М	0.7050	0.3600
N	0.9860	0.6290
0	0.7890	0.4460
Р	0.9320	0.5920
Q	0.0410	0.1050
R	0.9330	0.5620
S	0.9540	0.5290
Т	0.9960	0.6770
U	0.4390	0.3290
V	0.2680	0.2470
W	0.5890	0.3040
a	0.7190	0.2760
b	0.6710	0.2880
С	0.5790	0.2130
d	0.5490	0.2310
e	0.5280	0.2160
f	0.4730	0.2010
g	0.6610	0.2630
q	0.4630	0.2050
r	0.5790	0.2140
S	0.6220	0.2370
t	0.5040	0.2050



