

Mar 9, 2024 – 07:59 AM EST

PDB ID	:	6N7P
EMDB ID	:	EMD-0360
Title	:	S. cerevisiae spliceosomal E complex (UBC4)
Authors	:	Liu, S.; Li, X.; Zhou, Z.H.; Zhao, R.
Deposited on	:	2018-11-27
Resolution	:	3.60 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.dev70
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.60 Å.

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



Metric	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f EM} {f structures} \ (\#{f Entries})$
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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

Mol	Chain	Length		Quality o	of chain		
			33%				
1	А	300	1	56%	• •	38%	
	_		10%				
2	В	231		68%		14%	• 16%
			7%				
3	\mathbf{C}	350	29%	8% •		62%	
4	D	544		83%			16% •
			36%				
5	Ε	629		84%			7% 8%
			17%				
6	\mathbf{F}	523	43%	7% •		49%	
			•				
7	G	492	40%	7% •		51%	



Mol	Chain	Length	Quality of chain	
8	Н	105	21% 94%	6%
9	Ι	261	63% 9% ·	26%
10	J	583	33% • 66%	
11	Κ	196	58 % 5%	37%
12	L	146	• 70% 1:	2% 18%
13	М	110	7%	18% •
14	Ν	101	• 79%	12% • 8%
15	О	94	70% 9%	6 21%
16	Р	86	67% 16	% • 14%
17	Q	77	• 77%	14% • 8%
18	R	568	51% 52% 38%	8% ••
19	r	253	6% • 91%	
20	Х	861	96% 89%	5% • •
21	Y	208	65%	34%



2 Entry composition (i)

There are 22 unique types of molecules in this entry. The entry contains 41488 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 U1 small nuclear ribonucleoprotein 70 kDa homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	А	186	Total 1207	C 745	N 228	O 233	S 1	0	0

• Molecule 2 is a protein called U1 small nuclear ribonucleoprotein C.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	В	195	Total 1570	C 976	N 301	0 288	${ m S}{ m 5}$	0	0

• Molecule 3 is a protein called U1 small nuclear ribonucleoprotein A.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	С	132	Total 1058	C 674	N 193	0 187	$\frac{S}{4}$	0	0

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
С	299	GLY	-	expression tag	UNP P32605
С	300	ARG	-	expression tag	UNP P32605
С	301	ARG	-	expression tag	UNP P32605
С	302	ILE	-	expression tag	UNP P32605
С	303	PRO	-	expression tag	UNP P32605
С	304	GLY	-	expression tag	UNP P32605
С	305	LEU	-	expression tag	UNP P32605
С	306	ILE	-	expression tag	UNP P32605
С	307	ASN	-	expression tag	UNP P32605
С	308	PRO	-	expression tag	UNP P32605
С	309	TRP	-	expression tag	UNP P32605
С	310	LYS	-	expression tag	UNP P32605
С	311	ARG	-	expression tag	UNP P32605
С	312	ARG	-	expression tag	UNP P32605
С	313	TRP	-	expression tag	UNP P32605



Continu	iea jrom pre	vious page	· · · -	DC	
Chain	Residue	Modelled	Actual	Comment	Reference
C	314	LYS	-	expression tag	UNP P32605
C	315	LYS	-	expression tag	UNP P32605
C	316	ASN	-	expression tag	UNP P32605
С	317	PHE	-	expression tag	UNP P32605
C	318	ILE	-	expression tag	UNP P32605
C	319	ALA	-	expression tag	UNP P32605
С	320	VAL	-	expression tag	UNP P32605
С	321	SER	-	expression tag	UNP P32605
С	322	ALA	-	expression tag	UNP P32605
С	323	ALA	-	expression tag	UNP P32605
С	324	ASN	-	expression tag	UNP P32605
С	325	ARG	-	expression tag	UNP P32605
С	326	PHE	-	expression tag	UNP P32605
С	327	LYS	-	expression tag	UNP P32605
С	328	LYS	-	expression tag	UNP P32605
С	329	ILE	-	expression tag	UNP P32605
С	330	SER	-	expression tag	UNP P32605
С	331	SER	-	expression tag	UNP P32605
С	332	SER	-	expression tag	UNP P32605
С	333	GLY	-	expression tag	UNP P32605
С	334	ALA	-	expression tag	UNP P32605
С	335	LEU	-	expression tag	UNP P32605
С	336	ASP	-	expression tag	UNP P32605
С	337	TYR	-	expression tag	UNP P32605
С	338	ASP	-	expression tag	UNP P32605
С	339	ILE	-	expression tag	UNP P32605
С	340	PRO	-	expression tag	UNP P32605
С	341	THR	-	expression tag	UNP P32605
С	342	THR	-	expression tag	UNP P32605
С	343	ALA	-	expression tag	UNP P32605
С	344	SER	-	expression tag	UNP P32605
С	345	GLU	-	expression tag	UNP P32605
С	346	ASN	-	expression tag	UNP P32605
С	347	LEU	-	expression tag	UNP P32605
С	348	TYR	-	expression tag	UNP P32605
С	349	PHE	-	expression tag	UNP P32605
С	350	GLN	-	expression tag	UNP P32605

 α tio 1 0

• Molecule 4 is a protein called U1 small nuclear ribonucleoprotein component PRP42.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	544	Total 4561	C 2990	N 723	0 828	S 20	0	0



• Molecule 5 is a protein called Pre-mRNA-processing factor 39.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	Е	576	Total 3981	$\begin{array}{c} \mathrm{C} \\ 2527 \end{array}$	N 693	O 752	S 9	0	0

• Molecule 6 is a protein called Protein NAM8.

Mol	Chain	Residues		At	oms			AltConf	Trace
6	F	267	Total 1818	C 1128	N 326	O 353	S 11	0	0

• Molecule 7 is a protein called 56 kDa U1 small nuclear ribonucleoprotein component.

Mol	Chain	Residues		At		AltConf	Trace		
7	G	239	Total 1954	C 1267	N 321	0 354	S 12	0	0

• Molecule 8 is a protein called U1 small nuclear ribonucleoprotein component SNU71,U1 small nuclear ribonucleoprotein component SNU71,Snu71.

Mol	Chain	Residues		At	\mathbf{oms}			AltConf	Trace
8	Н	105	Total 685	C 425	N 127	0 132	S 1	0	0

• Molecule 9 is a protein called Protein LUC7.

Mol	Chain	Residues		\mathbf{A}	toms		AltConf	Trace	
9	Ι	192	Total 1409	C 878	N 262	O 258	S 11	0	0

• Molecule 10 is a protein called Pre-mRNA-processing protein PRP40.

Mol	Chain	Residues		Ato	ms	AltConf	Trace	
10	J	198	Total 984	C 588	N 198	O 198	0	0

• Molecule 11 is a protein called Small nuclear ribonucleoprotein-associated protein B.

Mol	Chain	Residues		At	oms			AltConf	Trace
11	K	123	Total 1008	C 636	N 191	0 178	${ m S} { m 3}$	0	0

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



Mol	Chain	Residues		At	oms			AltConf	Trace
12	L	119	Total 921	$\begin{array}{c} \mathrm{C} \\ 578 \end{array}$	N 164	O 176	${ m S} { m 3}$	0	0

• Molecule 13 is a protein called Small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues		At	oms	AltConf	Trace		
13	М	107	Total 858	C 545	N 159	0 150	$\frac{S}{4}$	0	0

• Molecule 14 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues		At	oms	AltConf	Trace		
14	N	93	Total 710	C 450	N 122	0 134	${f S}$ 4	0	0

• Molecule 15 is a protein called Small nuclear ribonucleoprotein E.

Mol	Chain	Residues		Atc	\mathbf{ms}			AltConf	Trace
15	0	74	Total	С	Ν	Ο	S	0	0
10	0	14	563	375	90	95	3	0	0

• Molecule 16 is a protein called Small nuclear ribonucleoprotein F.

Mol	Chain	Residues		At	oms	AltConf	Trace		
16	Р	74	Total 584	C 377	N 103	0 103	S 1	0	0

• Molecule 17 is a protein called Small nuclear ribonucleoprotein G.

Mol	Chain	Residues		At	\mathbf{oms}			AltConf	Trace
17	Q	71	Total 543	C 344	N 95	O 103	S 1	0	0

• Molecule 18 is a RNA chain called U1 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	558	Total 11822	$\begin{array}{c} \mathrm{C} \\ 5287 \end{array}$	N 2003	O 3974	Р 558	0	0

• Molecule 19 is a RNA chain called UBC4 pre-mRNA.



Mol	Chain	Residues	Atoms				AltConf	Trace	
19	r	22	Total 471	C 211	N 85	O 153	Р 22	0	0

• Molecule 20 is a protein called Nuclear cap-binding protein complex subunit 1.

Mol	Chain	Residues	Atoms			AltConf	Trace	
20	Х	826	Total 4101	C 2449	N 826	O 826	0	0

• Molecule 21 is a protein called Nuclear cap-binding protein subunit 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	Y	138	Total 677	C 401	N 138	0 138	0	0

• Molecule 22 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
22	В	1	Total Zn 1 1	0
22	Ι	2	Total Zn 2 2	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: U1 small nuclear ribonucleoprotein 70 kDa homolog









• Molecule 8: U1 small nuclear ribonucleoprotein component SNU71,U1 small nuclear ribonucleoprotein component SNU71,Snu71





Chain C):		70%		9% 21%	-	
MET SER ASN LYS VAL LYS	THR LYS A9 P12	N15 129 W30 L31 L31 L31	V62 ASN ASN ALA ALA ASP GLU ASP CLU GLU GLU GLU	180 190 190 191 ALA ASP			
• Molec	ule 16: \$	Small nucles	ar ribonucleopro	tein F			
Chain P	2:		67%		16% • 14%		
MET SER GLU SER SER ASP	ILE SER ALA MET GLN P12	L19 L22 V27 N34	835 E37 F36 F37 F37 F36 F33 F33 F33 F33 F37 F46 M47 M47 F11 F11 E57 E57	V60 T67 R74 C75 M76	ASN ASN		
• Molec	ule 17: S	Small nucles	ar ribonucleopro	tein G			
Chain G) :		77%		14% • 8%	-	
MET V2 Y10 K13	K14 115 L16 L17 N18 19	N20 N47 GLY GLY GLU ASP ALA	N53 163 163 163 163 163 163 171 174 174 175 175	4			
• Molec	ule 18: 1	U1 snRNA	4				
Chain R	l:	52'	%	38	8%		
A1 U2 A3 A7	U10 U11 A12 A13	U16 A17 A20 G21 G23 G24 G24	A25 A26 A A A C U U A A A A A A C U U A A A C C C C C C C C C C C C C C C C C	C38 039 A40 C41 A47 A47 A48 A48 A48 A48	C55 655 C56 C56 C60 A61 A61 A64 A67 A67 A67 A67	A69 473 473 675 675	
A78 A79 G80 A86	U87 C88 A89 U90 U90	692 493 494 C95 U96 A97	U98 A99 A100 U101 U102 G103 G103 U104 U104 C106	A107 U108 U109 G110 A111 A112 G113	UI 17 UI 17 UI 18 G119 G119 A126 A126 A126 C123 C123 C123 C123 C130	U131 U132 G134 G134 G134 A139 C139 C142 C142 C142 C142 A145 A145	0146 A147
C148 G149 G150 C151 G152 C153	6154 6154 1169 1169 6170 6170	C172 C172 C172 C172 C177 C176 A179	U180 U181 C182 C183 U186 G186 A196 A196 U197	U198 G199 G200 U202 A203 A203	U205 C206 C207 C207 C208 U209 U210 G211 U213 U213 U214	2215 2216 0217 0218 0219 0220 2221 2221 2222 2223	4224 1225 1226 1227
U228 U229 G230 G231	4232 U233 U234 A235 A236	A237 C238 U239 C240 A241 U242 U242	U244 U245 0247 6247 6247 6249 6250 6250 0254 U254 U255 U255	6257 U258 U259 U260 U260 U260 U265 U265	C268 0270 6271 A271 U277 U277 U277 0280 0280 0280 A281 A281 A281 A281 A281 A281 A281 A281	A287 A288 U290 U290 C291 A292 A293 A293 A293 A293	-
	•• ••					····	
C310 G314 G314 C316 C316 C316 C317	U318 U319 U320 C321	A325 A326 A326 A326 A327 A327 A327 C326 C328 C328	A325 G334 C333 U335 U335 C335 G325 G335 C337 C337 C337 C337 C337 C337 C337 C	G338 A338 G341 G341 C342 C342 U344	0347 0347 0347 0345 0345 0355 0355 0355 0355	A356 A356 U355 U365 U365 C362 C362 C365 C365	0367 4366 6367 6367 6365 6365 6365 6371
C372 C373 A374 U375	u375 U377 U378 A379 G380	U381 U382 U383 U384 U385 G386	A38 C388 C389 C391 C391 A392 A392 A393 A394 U395 U395	C397 C398 A399 A400 A400 G402 A403	A404 C405 U406 U407 A408 A409 G410 U411 U412	A414 D415 C416 A417 A417 D418 C419 C419 A20 A22 A22	G423 U424 A425 U426 G427 G427 C429 U430 C431
U432 U433 6434 A435	4437 U438 U439 A440	U441 U442 G444 G445 G445 U446	C441 C441 6448 6449 6450 A451 V452 C453 C453 C455 C455	G457 U458 U459 U460 G461 A462 A462	G464 A465 U466 6467 6467 6467 6467 6467 6467 6463 6463 6463 6463 6463 6463 6463 6463 6463 6463 6463 6471 0471 0472 0472	U474 U475 U476 6477 A478 6479 C480 C480 C482	U483 C484 U485 A487 A488 A488 U490 U491



			- No
499 (499) (490) (490) (490) (490) (490) (490) (490) (490) (490) (490) (49)) (490) (4	650 050 050 050 050 050 050 050 050 050	0 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	
>			
• Molecule 19: UB	C4 pre-mRNA		
Chain r: 6% ·		91%	_
	•••••		
0 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2	C-8 C-7 C-7 C-7 C-7 C-7 C-7 C-7 C-7 C-7 C-7	< > 0 0 0 0 < 0 0 > > > 0 < < < > 0 0 0 0	
		A 4 0 4 D 0 0 D 4 D 0 0 4 4 0 D 4 0 4 0 4	. D U U U D A
000 4 0 0 0 0 0 4 0 0 0	00DUU4004DUU04D4D	00074040045040054004	C C C C C C C C C C C C C C C C C C C
< > 0 0 0 0 0 5 < 0 < 0 0 4 5	し < ひ ひ ひ ⊃ < C ひ < C ⊃ < O ⊃ < O	< > U > U > U < D U < > U < > U < > U < > U < > U < > U < > U < > U < > U < > U < > < >	< ひ ひ ひ < < つ つ ひ < < つ つ ひ < < つ つ ひ つ < < つ つ ひ つ つ つ つ
C P C C C			
• Molecule 20: Nuc	clear cap-binding protein	n complex subunit 1	
Chain X:	96% 89%	5%	
0		********	· · · · · · · · · · · · · · · · · · ·
MET PHE ASN ASN ARG ARG ARG ARG ASP PHE ASP ASP ASP ASP ASP ASP ASP ASP ASP ASP	ASN TYR ASP ASP PHC PRO ARG PRO PRO CYS CYS CYS ARG CIN ARG CNN ARG PRO PRO PRO PRO PRO PRO PRO PRO PRO ASP ASP ASP ASP ASP ASP ASP ASP ASP ASP	VAL VAL GLAU GLAU GLEU C36 C36 C36 C36 C36 C36 C36 C36 C36 C36	949 V50 A52 A52 E54 E54 D565 D565 C56 F59 F59 F59 F59 F59
••••	•••••	•••••	•••••
861 162 164 164 166 166 1667 1667 1667 1669 1670	D72 Y73 F74 N75 N76 A77 L78 L78 L79 S80 S80 T81 L82 N83 A84	V85 V86 V87 E88 E88 691 F90 691 F90 A95 A95 L99 L99 L99 L99 L99	M101 V102 V103 N104 N104 N106 N106 N107 N108 N1106 N1108 N1108 N1108 N1116 N1116 N1116 N1116 N1116 N1116 N1116 N1116 N1116 N1117 N116 N116
•••••			
		*****	•••••
E121 L122 Q123 V124 V125 C126 C126 C126 Q128 Y130 N131	D132 E133 F134 K135 S136 S136 T137 S138 N139 E140 T141 T141 C142 P143 P143	N146 K146 K146 K148 K148 K148 F153 F155 F155 F155 F155 F155 F155 F155	F161 L162 V163 D164 E165 L166 L166 L166 L166 L166 L166 L166 L
E121 1:22 1:22 1:22 1:22 1:25	D132 E133 F134 K135 S136 T137 S138 N139 E140 F141 C142 C142 C142 C142 C142 C142 C142 C	M145 K146 1147 K148 K149 K151 L151 R152 F153 F153 F153 F155 F155 F155 F155 F155	F161 L162 L163 P164 E165 F165 L166 T167 K171 F170 K171 F173 F173 F173 F174 F174 F174 F173 F175 F176 F176 F176 F176 F176 F176 F176 F176
N181 N182 L183 L183 L183 D184 N125 P185 N125 C126 N126 N125 C126 N125 C126 N125 C126 N125 C126 N125 C126 N125 C126 N125 C126 N125 C126 N125 C126 N125 C126 N125 C126 N125 C126 N125 C126 N125 C126 N125 C126 N125 C126 N125 C126 N125 C126 N125 C126 N125 N1	5192 0132 E193 E133 A194 F134 1195 K135 Y196 S136 T197 N133 T197 N133 T199 N133 L200 T141 N203 T141 N203 T141 N203 T141 N203 T141 P204 W144	Y205 M145 L206 K146 F207 L147 F208 K146 F208 L147 F209 L149 N210 L151 N210 L151 N211 H151 N212 H151 N213 L151 N213 L151 N213 L154 F153 N214 L154 F155 F155 T216 T156 V215 N155 N155 V216 N160	E221 F161 E222 L162 L223 L162 L224 L165 L225 L165 Y226 L166 Y226 L166 Y226 L166 Y226 L166 Y221 L166 Y231 Y170 Y231 Y170 Y231 Y170 Y231 Y170 Y233 L173 Y234 L173 Y235 L173 Y236 L176 Y237 L176 Y238 L176 Y239 L176
N181 (122 N182 (123 L183 (123 L183 (123 L183 (124 L183 (125 L185 (125 C126 N125 C126 N125 N125 N125 N126 N125 N126	\$122 \$132 E193 E133 A194 F134 1195 K135 Y196 \$133 T197 T137 T199 N139 L200 E140 L201 T141 N202 E140 L201 T141 N202 F143 P204 V144	Y205 N145 L206 K146 F207 L147 F208 K148 F209 L150 N210 L151 N211 F151 N212 F151 N213 F151 N213 F151 N213 F151 N213 F151 N213 F153 R211 L154 S155 S155 R217 L154 K218 S155 K219 S155 K219 S155 K219 M160 Y20 M160	E221 F161 E222 L162 L224 L165 L224 L166 Y226 L166 Y231 M168 Y231 M168 Y231 M168 Y231 M168 Y231 M169 Y170 Y170 Y233 Y170 Y234 L173 Y235 L173 Y236 L176 Y237 S177 Y238 L176 Y239 L176 Y238 L178 Y239 L176 Y239 L176 Y239 L176 Y239 L176 Y239 L178 Y239 L178 Y239 L178 Y239 L178 Y230 L178 Y230
L241 N181 E121 R242 N182 E172 R243 N182 E172 E243 N182 E172 E243 N182 E172 K24 D184 K124 N245 P185 K125 C246 C186 K127 F243 N187 M127 P248 N187 P128 P249 N187 Y129 P249 V189 T129 P249 V189 Y137 P249 V189 M137 P249 V189 M131 P249 V189 M131	MSE2 5192 1132 V253 E193 E133 E264 A194 F134 L265 1195 K135 V256 Y196 S133 V256 Y196 S133 V258 Y196 S133 V258 Y199 S133 V258 Y199 S133 V259 Y199 S133 V259 Y199 S134 V269 Y199 S134 V263 Y199 Y141 N202 L200 T141 N202 Y201 T141 N202 Y201 Y144 N202 Y201 Y144 N202 Y204 Y144	K265 Y205 N145 A266 L267 N146 L267 F207 N146 1268 F207 N146 1268 F208 N149 N269 F208 N146 1268 F208 N147 N269 F208 N149 N269 N210 N150 L271 N210 R115 2773 N213 F153 Q273 N213 F153 L274 D214 L154 L274 D214 1156 L274 D214 1156 L277 L217 S155 E276 L216 1156 L277 N213 S156 E276 Y219 P159 P230 V220 P159 P280 V220 P159	u281 E221 F161 N282 E222 L162 H283 L223 L165 L286 L224 L165 L286 L224 L165 L286 L224 L165 L286 V165 L166 L286 V226 L166 V226 V226 L166 V229 V226 L166 V229 V226 L166 V229 V226 L167 V229 V229 L167 V229 V233 L173 C293 V233 L173 C293 V234 L173 C293 V234 L176 V234 V234 L176 V234 V234 L176 V236 V236 L176
L241 N181 E121 R242 N182 E172 E243 N182 E172 E243 L183 Q123 Y244 D184 K124 N245 P185 W125 S246 C186 K127 P246 C186 C126 P246 N187 P185 P246 N187 P186 P246 N187 P186 P248 N187 P196 P249 V188 P128 P249 V189 P128 P249 P186 V137 P249 P189 P139 P249 P191 P139	MS52 5192 D132 V253 E193 E133 E254 A194 F134 L255 1195 K135 V256 V196 5136 V256 T197 T137 V256 T197 T137 V258 T197 T137 V259 T197 T137 V269 T199 T141 V261 T199 T141 V263 T199 T141 V264 T200 T141 V263 T200 T141 V264 P204 V144	K265 Y205 N145 A266 L206 X146 L267 F207 1147 L267 F208 X146 N269 F208 X146 N269 F208 X146 N269 F208 X146 N269 N210 1150 N210 N210 F151 N271 R211 N150 L271 N213 F153 Q273 N213 F153 Q273 N213 F153 Q273 N213 F154 N216 N213 F154 Q273 N213 F156 N275 D214 1156 N276 C315 F156 P277 N213 F157 P278 Y219 F159 P280 Y20 Y160	V281 E221 F161 N282 E222 L162 N282 E222 L165 L284 L224 D164 L286 2226 L165 P387 2225 L166 P387 2225 L166 P387 2225 L166 P387 2225 L166 P387 2223 L167 P387 2220 Y170 P381 2220 Y170 P381 2290 Y170 P291 Y231 Y170 P293 Y231 Y171 P293 Y231 Y170 P293 Y231 Y170 P293 Y231 Y170 P293 Y233 Y170 P293 Y234 Y170 P294 Y235 Y170 P295 Y236 Y170 P296 Y236 Y170 P297 Y236 Y170 P298 Y236
P301 L241 N181 E121 S302 R242 N182 1122 V303 E243 L183 0123 V303 E243 L183 0123 D304 Y244 D184 K124 D305 N245 P185 N125 L306 C246 P185 N125 K307 E247 N187 K127 S308 P249 V189 0123 F309 Y260 P186 Y126 K310 F249 N187 Y127 F309 Y260 Y189 Y129 F301 F551 L101 N131	L312 M552 S192 D122 N313 V253 E193 D122 K314 E254 A194 F134 K315 L255 1195 F134 K316 L255 1195 F134 F316 L255 1195 F134 G317 V256 Y196 S136 G317 V256 Y196 S136 S318 V258 Y197 S136 V319 V259 L1097 S136 V319 V269 L1097 S140 N322 V263 L200 F141 M323 V263 N202 G142 K324 Y264 P204 Y144	T325 K265 Y205 N145 P326 A266 L206 N146 R337 L267 F207 N146 Y328 L267 F207 N146 Y329 L267 F206 N146 A329 N266 F208 N149 F330 N269 F208 N149 F331 L374 N210 N140 Y333 L271 N210 N150 Y333 Q273 N213 E151 Y333 L274 N213 E154 P335 L274 N213 E155 Y333 L274 N213 E156 P335 L274 N213 E156 Y333 L274 N213 E156 Y335 L274 N216 E156 Y335 L274 N219 E156 Y335 L274 N219 E156 Y335 L277 N219 E156 Y336 P280 Y219 P159 Y340 N280	F341 W281 E221 F161 E342 N282 E222 L162 T343 H283 L223 L162 V345 L284 L284 L165 V345 L284 L284 L165 V345 L286 X226 L166 V345 V281 Y226 L166 V345 V281 Y226 L166 Y360 Y280 Y226 L166 Y361 Y280 Y231 L167 Y363 Y230 Y170 L167 Y361 Y231 Y170 L173 Y363 Y231 Y170 L173 Y364 Y231 Y231 L173 Y364 Y233 Y233 L173 Y364 Y233 Y234 L173 Y364 Y233 Y234 L173 Y365 Y234 Y234 L173 Y364 Y234 Y234 L173
P301 L241 N181 E121 S302 R242 N182 E172 V303 E243 N182 E172 V303 E243 N182 E172 V303 E243 N182 E172 V303 E243 N183 E183 D304 Y244 D184 K124 D305 N245 P185 V125 L306 G246 P186 V125 K307 E246 N187 K127 K307 E246 N186 C126 K307 E246 N187 N126 K307 E246 N187 N126 K308 P246 N187 N128 K309 Y260 P190 Y139 K314 K541 N149 Y134	L312 M252 5192 D122 N313 V253 E193 E133 K314 E264 A194 F134 N315 L255 1196 F134 F316 V256 Y196 5138 F317 V256 Y196 5138 F318 V256 T197 1137 V319 R257 N196 5138 V319 V258 T197 1137 V319 V259 T199 1137 V319 V259 T199 1141 V321 V259 L200 1141 M322 V263 L201 1141 M323 V263 N202 6142 M324 V263 Y203 1703 M324 V264 P204 Y144	1325 K2055 Y2055 N145 P326 A265 L207 N145 R327 L207 E207 N145 R327 L207 E207 N145 R327 L207 E208 N145 R329 N208 F200 N145 R330 N209 F200 N145 F330 N210 F211 N210 H331 L271 N210 N150 V332 E272 N213 F153 V333 L274 N213 F153 P333 L274 N213 F153 P334 L274 D214 L154 P335 L274 D214 L154 P335 L274 D214 L154 P335 L274 D214 L154 P335 L274 D214 L155 P335 L277 N215 L156 P335 E276 L216 L157 P335 E277 N210 L157 P335 E277	F341 w231 E221 F161 E342 W282 E222 L162 T343 L284 E223 L165 V344 L284 E223 L165 V345 L286 222 L165 V345 L286 222 L165 V345 L286 222 L166 V345 L286 2226 L166 V345 V286 2228 N166 T347 P286 V227 L166 Y350 T288 Y231 N170 Y351 P287 Y231 N170 Y350 Y231 Y170 Y170 Y351 P290 Y231 Y170 Y351 Y231 Y231 Y170 Y351 Y231 Y231 Y170 Y351 Y231 Y231 Y170 Y352 P293 Y233 Y170 Y352 P293 Y231 Y170







4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	124825	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 $(e^-/\text{\AA}^2)$	30	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.371	Depositor
Minimum map value	-0.206	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.065	Depositor
Map size (Å)	522.24, 522.24, 522.24	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles ($^{\circ}$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.36, 1.36, 1.36	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

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	Bond	lengths	Bond angles		
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.46	0/1224	0.59	0/1675	
2	В	0.54	0/1601	0.65	0/2154	
3	С	0.44	0/1072	0.68	0/1437	
4	D	0.76	0/4676	0.72	0/6320	
5	Е	0.55	0/4046	0.60	0/5539	
6	F	0.60	0/1844	0.68	0/2511	
7	G	0.61	0/1996	0.68	0/2682	
8	Н	0.49	0/428	0.55	0/575	
9	Ι	0.38	0/1428	0.60	0/1924	
10	J	0.37	0/983	0.49	0/1371	
11	Κ	0.66	0/1014	0.73	0/1350	
12	L	0.57	0/930	0.73	0/1261	
13	М	0.53	0/872	0.63	0/1174	
14	Ν	0.71	0/722	0.72	0/979	
15	0	0.55	0/573	0.68	0/778	
16	Р	0.65	0/597	0.74	0/809	
17	Q	0.64	0/546	0.69	0/735	
18	R	0.66	0/13201	1.19	79/20553~(0.4%)	
19	r	0.52	0/527	1.05	0/819	
20	Х	0.26	0/4100	0.59	4/5721~(0.1%)	
21	Y	0.26	0/676	0.55	0/937	
All	All	0.59	0/43056	0.87	83/61304~(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
3	С	0	2
20	Х	0	24



Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
All	All	0	26

There are no bond length outliers.

All (83) bond angle outliers are listed below:

Mol	Chain	\mathbf{Res}	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$\mathbf{Ideal}(^{o})$
18	R	227	U	N1-C2-O2	12.02	131.22	122.80
18	R	227	U	C2-N1-C1'	11.79	131.85	117.70
18	R	227	U	N3-C2-O2	-11.14	114.40	122.20
18	R	442	U	OP2-P-O3'	-10.46	82.18	105.20
18	R	442	U	OP1-P-O3'	-10.46	82.20	105.20
18	R	557	U	N3-C2-O2	-9.34	115.66	122.20
18	R	557	U	N1-C2-O2	9.16	129.21	122.80
18	R	130	С	C6-N1-C2	-8.40	116.94	120.30
18	R	130	С	C2-N1-C1'	8.35	127.99	118.80
18	R	11	U	C2-N1-C1'	8.26	127.62	117.70
18	R	227	U	C6-N1-C1'	-8.21	109.71	121.20
18	R	557	U	C2-N1-C1'	7.94	127.23	117.70
18	R	254	U	N3-C2-O2	-7.45	116.99	122.20
18	R	103	G	C4-N9-C1'	7.40	136.12	126.50
18	R	11	U	N1-C2-O2	7.32	127.92	122.80
18	R	291	С	N1-C2-O2	7.15	123.19	118.90
18	R	11	U	N3-C2-O2	-7.15	117.19	122.20
18	R	80	G	C4-N9-C1'	7.15	135.80	126.50
18	R	443	U	OP1-P-OP2	7.11	130.27	119.60
18	R	139	А	O4'-C1'-N9	6.86	113.69	108.20
18	R	148	C	C2-N1-C1'	6.80	126.28	118.80
18	R	130	C	C5-C6-N1	6.76	124.38	121.00
18	R	103	G	C8-N9-C1'	-6.74	118.24	127.00
18	R	277	U	P-O3'-C3'	6.63	127.66	119.70
18	R	498	U	N3-C2-O2	-6.58	117.59	122.20
20	Х	673	GLU	C-N-CA	6.53	138.02	121.70
18	R	291	C	C6-N1-C2	-6.45	117.72	120.30
18	R	144	С	C2-N1-C1'	6.41	125.84	118.80
18	R	258	U	P-O3'-C3'	6.38	127.35	119.70
18	R	63	U	P-O3'-C3'	6.32	127.29	119.70
18	R	180	U	C2-N1-C1'	6.22	125.16	117.70
18	R	500	C	C6-N1-C2	-6.18	117.83	120.30
18	R	265	U	N3-C2-O2	-6.13	117.91	122.20
18	R	80	G	N3-C4-C5	-6.12	125.54	128.60
18	R	63	U	C5-C6-N1	6.11	125.75	122.70
20	Х	283	HIS	C-N-CA	6.06	136.85	121.70



Mol	Chain	Res	Type	Atoms	Ζ	$Observed(^{o})$	$Ideal(^{o})$
18	R	180	U	N1-C2-O2	6.04	127.03	122.80
18	R	148	С	N1-C2-O2	6.03	122.52	118.90
18	R	80	G	C8-N9-C1'	-6.00	119.20	127.00
18	R	112	А	P-O3'-C3'	5.96	126.85	119.70
18	R	151	С	P-O3'-C3'	5.90	126.78	119.70
18	R	144	С	N1-C2-O2	5.88	122.43	118.90
18	R	148	С	N3-C2-O2	-5.88	117.78	121.90
18	R	80	G	N3-C4-N9	5.81	129.49	126.00
18	R	291	С	N3-C2-O2	-5.80	117.84	121.90
18	R	268	С	P-O3'-C3'	5.70	126.54	119.70
18	R	310	С	C5-C6-N1	5.66	123.83	121.00
18	R	279	U	P-O3'-C3'	5.66	126.49	119.70
18	R	399	А	P-O3'-C3'	5.64	126.47	119.70
18	R	123	С	C6-N1-C2	-5.63	118.05	120.30
20	Х	403	TYR	C-N-CA	5.63	135.77	121.70
20	Х	391	GLU	C-N-CA	5.62	145.63	122.00
18	R	254	U	N1-C2-N3	5.62	118.27	114.90
18	R	103	G	N3-C4-N9	5.62	129.37	126.00
18	R	127	С	C6-N1-C2	-5.59	118.06	120.30
18	R	99	А	C4-N9-C1'	5.56	136.31	126.30
18	R	342	С	C6-N1-C2	-5.54	118.08	120.30
18	R	206	С	N1-C2-O2	5.50	122.20	118.90
18	R	291	С	C5-C6-N1	5.45	123.72	121.00
18	R	180	U	N3-C2-O2	-5.34	118.46	122.20
18	R	63	U	C2-N1-C1'	5.31	124.07	117.70
18	R	140	С	N1-C2-O2	5.28	122.07	118.90
18	R	154	G	C4-N9-C1'	5.28	133.36	126.50
18	R	11	U	C6-N1-C1'	-5.28	113.81	121.20
18	R	480	С	C6-N1-C2	-5.24	118.20	120.30
18	R	144	С	N3-C2-O2	-5.23	118.24	121.90
18	R	347	U	N3-C2-O2	-5.22	118.55	122.20
18	R	342	С	C5-C6-N1	5.22	123.61	121.00
18	R	310	С	C6-N1-C2	-5.20	118.22	120.30
18	R	557	U	C6-N1-C1'	-5.20	113.92	121.20
18	R	342	С	C2-N1-C1'	5.15	124.46	118.80
18	R	56	C	C6-N1-C2	-5.13	118.25	120.30
18	R	496	С	C6-N1-C2	-5.13	118.25	120.30
18	R	151	С	N1-C2-O2	5.13	121.97	118.90
18	R	118	U	N3-C2-O2	-5.12	118.62	122.20
18	R	11	U	C5-C6-N1	5.12	125.26	122.70
18	R	516	U	C5-C6-N1	5.10	125.25	122.70
18	R	187	G	O5'-P-OP2	5.10	116.82	110.70



Mol	Chain	Res	Type	Atoms	Ζ	$Observed(^{o})$	$Ideal(^{o})$
18	R	114	U	O5'-P-OP2	-5.08	101.12	105.70
18	R	277	U	C2'-C3'-O3'	5.06	121.79	113.70
18	R	316	С	C6-N1-C2	-5.05	118.28	120.30
18	R	501	С	C5-C6-N1	5.05	123.53	121.00
18	R	90	U	C5-C6-N1	5.03	125.22	122.70

There are no chirality outliers.

Mol	Chain	Res	Type	Group
3	С	12	ARG	Peptide,Sidechain
20	Х	281	TRP	Peptide
20	Х	284	LEU	Peptide
20	Х	342	GLU	Peptide
20	Х	379	THR	Peptide
20	Х	380	LEU	Peptide
20	Х	381	ASP	Peptide
20	Х	383	PHE	Peptide
20	Х	388	ILE	Peptide
20	Х	389	PHE	Peptide
20	Х	405	GLU	Peptide
20	Х	408	LEU	Peptide
20	Х	410	PRO	Peptide
20	Х	550	THR	Peptide
20	Х	570	THR	Peptide
20	Х	669	PHE	Peptide
20	Х	671	LYS	Peptide
20	Х	672	ILE	Peptide
20	Х	674	LEU	Peptide
20	Х	69	GLY	Peptide
20	Х	70	HIS	Peptide
20	Х	728	ASN	Peptide
20	Х	730	GLY	Peptide
20	Х	785	GLU	Peptide
20	Х	786	ILE	Peptide

All (26) planarity outliers are listed below:

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



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	А	1207	0	927	14	0
2	В	1570	0	1553	33	0
3	С	1058	0	1118	26	0
4	D	4561	0	4549	72	0
5	Е	3981	0	3282	35	0
6	F	1818	0	1567	29	0
7	G	1954	0	1961	44	0
8	Н	685	0	477	4	0
9	Ι	1409	0	1285	24	0
10	J	984	0	416	1	0
11	K	1008	0	1109	9	0
12	L	921	0	972	10	0
13	М	858	0	882	13	0
14	Ν	710	0	730	16	0
15	0	563	0	594	5	0
16	Р	584	0	586	11	0
17	Q	543	0	560	7	0
18	R	11822	0	5939	99	0
19	r	471	0	236	0	0
20	Х	4101	0	1779	14	0
21	Y	677	0	298	1	0
22	В	1	0	0	0	0
22	Ι	2	0	0	0	0
All	All	41488	0	30820	413	0

the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

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 6.

All (413) 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 (Å)	overlap (Å)
4:D:303:LEU:CD1	4:D:312:VAL:HG11	1.70	1.21
2:B:8:TYR:CE1	14:N:82:PRO:HG3	1.80	1.15
3:C:13:PRO:HD2	3:C:19:TYR:CD1	1.82	1.14
2:B:136:LEU:HD23	2:B:137:PRO:HD2	1.11	1.09
2:B:8:TYR:HE1	14:N:82:PRO:CG	1.64	1.09
3:C:13:PRO:HD2	3:C:19:TYR:HD1	0.94	1.06
4:D:303:LEU:CD1	4:D:312:VAL:CG1	2.36	1.03
4:D:303:LEU:HD11	4:D:312:VAL:CG1	1.90	1.01
1:A:7:LYS:HD3	1:A:7:LYS:H	1.25	1.01



	bus puge	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
4:D:303:LEU:HD12	4:D:312:VAL:HG11	1.43	1.00
18:R:380:G:H1	18:R:438:U:H3	1.07	0.99
2:B:8:TYR:CE1	14:N:82:PRO:CG	2.44	0.98
18:R:384:U:H3	18:R:434:G:H1	1.01	0.98
2:B:8:TYR:CD1	14:N:82:PRO:HG3	1.99	0.97
4:D:303:LEU:HD11	4:D:312:VAL:HG12	1.45	0.95
2:B:136:LEU:HD23	2:B:137:PRO:CD	1.95	0.95
16:P:22:LEU:HD22	16:P:27:VAL:HG12	1.48	0.95
3:C:13:PRO:CD	3:C:19:TYR:HD1	1.82	0.93
2:B:8:TYR:HE1	14:N:82:PRO:CD	1.84	0.90
9:I:45:CYS:HB2	9:I:70:GLN:HB2	1.52	0.89
7:G:68:SER:HB2	7:G:224:PHE:CD2	2.07	0.89
7:G:68:SER:HB2	7:G:224:PHE:HD2	1.38	0.89
3:C:62:LEU:HD21	3:C:79:LEU:HD11	1.58	0.85
18:R:55:G:N2	18:R:151:C:C2	2.45	0.85
18:R:389:G:H1	18:R:430:U:H3	0.86	0.84
16:P:22:LEU:HD22	16:P:27:VAL:CG1	2.09	0.83
5:E:321:LEU:HD22	5:E:322:PRO:HD2	1.60	0.83
7:G:68:SER:HA	7:G:224:PHE:CD2	2.14	0.82
2:B:6:CYS:SG	2:B:30:HIS:CE1	2.72	0.81
2:B:8:TYR:CE1	14:N:82:PRO:CD	2.63	0.79
5:E:321:LEU:HD22	5:E:322:PRO:CD	2.13	0.79
4:D:448:TYR:CD2	5:E:480:SER:HA	2.18	0.78
4:D:7:LEU:O	4:D:7:LEU:HD22	1.84	0.77
9:I:201:CYS:SG	9:I:226:HIS:HE1	2.09	0.76
3:C:15:ASN:OD1	3:C:16:LYS:N	2.19	0.76
12:L:51:ARG:HD3	13:M:87:ARG:HH12	1.52	0.75
7:G:68:SER:CB	7:G:224:PHE:CD2	2.70	0.74
18:R:171:A:H61	18:R:540:G:H1	1.35	0.74
9:I:44:ILE:N	9:I:44:ILE:HD12	2.02	0.74
9:I:41:ASP:HB3	9:I:42:PRO:CD	2.18	0.73
6:F:411:GLN:HA	6:F:411:GLN:NE2	2.04	0.73
7:G:68:SER:CB	7:G:224:PHE:HD2	2.01	0.73
2:B:136:LEU:CD2	2:B:137:PRO:HD2	2.05	0.72
4:D:24:PRO:HD2	7:G:260:LEU:CB	2.20	0.72
4:D:33:LEU:O	4:D:33:LEU:HD22	1.90	0.71
1:A:5:LEU:O	1:A:5:LEU:HD23	1.90	0.70
6:F:410:LEU:HD23	6:F:410:LEU:O	1.91	0.70
5:E:582:GLN:HE21	5:E:606:ARG:HD2	1.56	0.69
5:E:317:ALA:O	5:E:321:LEU:HB2	1.92	0.69
1:A:5:LEU:HD23	1:A:5:LEU:C	2.13	0.69



	ous page	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
3:C:12:ARG:NH2	18:R:60:C:C5	2.60	0.68
4:D:306:LEU:O	4:D:306:LEU:HD12	1.93	0.68
7:G:70:LEU:HD23	7:G:70:LEU:C	2.14	0.68
18:R:425:A:H2'	18:R:426:U:H4'	1.76	0.67
7:G:43:GLN:HE22	7:G:53:ARG:HG3	1.59	0.67
20:X:670:ALA:HB3	20:X:676:ILE:HA	1.77	0.67
1:A:7:LYS:HD3	1:A:7:LYS:N	2.04	0.66
4:D:307:ALA:O	4:D:313:TRP:NE1	2.25	0.66
2:B:138:GLN:O	2:B:140:ALA:N	2.29	0.66
4:D:304:LEU:HB2	4:D:305:PRO:HD3	1.78	0.65
7:G:98:LEU:HD23	7:G:98:LEU:C	2.18	0.64
7:G:68:SER:CA	7:G:224:PHE:CD2	2.81	0.64
4:D:24:PRO:HD2	7:G:260:LEU:HB2	1.80	0.63
4:D:140:HIS:HB3	4:D:143:SER:HB3	1.80	0.63
2:B:75:VAL:HG22	4:D:224:PRO:HB3	1.80	0.63
18:R:55:G:N2	18:R:151:C:O2	2.31	0.63
18:R:386:G:H1	18:R:433:U:H3	1.45	0.63
18:R:171:A:N6	18:R:540:G:H1	1.97	0.62
9:I:42:PRO:O	9:I:70:GLN:NE2	2.32	0.62
4:D:310:ASP:HA	4:D:313:TRP:HD1	1.64	0.62
7:G:226:LYS:NZ	18:R:119:G:N7	2.47	0.62
3:C:12:ARG:NH2	18:R:60:C:C4	2.68	0.62
7:G:72:LEU:O	7:G:72:LEU:HG	1.99	0.62
5:E:405:THR:O	5:E:409:ASN:HB2	2.00	0.61
2:B:6:CYS:SG	2:B:30:HIS:HE1	2.17	0.61
5:E:355:VAL:HG11	5:E:372:TYR:HB2	1.80	0.61
21:Y:48:ILE:HA	21:Y:121:LEU:HA	1.82	0.61
3:C:68:SER:OG	3:C:73:MET:SD	2.59	0.61
6:F:407:GLN:HG3	6:F:408:PRO:HD2	1.83	0.61
18:R:78:A:H4'	18:R:79:A:H5'	1.81	0.61
11:K:85:THR:HG22	14:N:73:VAL:HG22	1.82	0.61
18:R:342:C:H2'	18:R:343:A:H4'	1.82	0.60
7:G:186:SER:HB3	7:G:214:GLU:HG2	1.83	0.60
11:K:88:ARG:NH1	14:N:66:GLY:O	2.35	0.60
3:C:100:LYS:HE3	3:C:100:LYS:O	2.02	0.59
18:R:320:U:H3	18:R:521:G:H1	1.50	0.59
9:I:44:ILE:HD12	9:I:44:ILE:H	1.66	0.59
3:C:14:ALA:O	3:C:69:ARG:NH1	2.36	0.59
6:F:330:ARG:HE	6:F:342:VAL:HG21	1.67	0.59
13:M:30:PRO:HG2	16:P:46:ASP:HB2	1.83	0.59
18:R:217:U:O2	18:R:220:G:O6	2.20	0.59



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
4:D:445:VAL:HG23	4:D:445:VAL:O	2.01	0.59
9:I:193:SER:O	9:I:197:LYS:N	2.36	0.58
11:K:121:LYS:NZ	18:R:280:G:O6	2.35	0.58
7:G:92:TYR:HD1	7:G:92:TYR:N	2.01	0.58
1:A:97:ASP:O	1:A:99:HIS:N	2.36	0.58
4:D:266:SER:O	4:D:269:THR:HG22	2.04	0.58
6:F:377:ARG:O	6:F:379:ARG:NH2	2.34	0.58
18:R:88:C:N3	18:R:111:A:N6	2.52	0.58
4:D:440:LEU:O	4:D:444:LEU:HD12	2.04	0.58
3:C:62:LEU:CD2	3:C:79:LEU:HD21	2.34	0.57
4:D:374:SER:O	8:H:50:ARG:NH2	2.37	0.57
7:G:68:SER:HA	7:G:224:PHE:HD2	1.68	0.57
9:I:45:CYS:HB2	9:I:70:GLN:CB	2.31	0.57
16:P:34:ASN:HB3	16:P:36:THR:HG23	1.86	0.57
20:X:674:LEU:HA	20:X:677:GLU:H	1.67	0.57
18:R:131:U:O2'	18:R:132:U:H5'	2.04	0.57
4:D:411:GLN:HE22	4:D:449:SER:HB2	1.68	0.57
5:E:326:LYS:O	5:E:326:LYS:HG2	2.04	0.57
11:K:127:LYS:NZ	18:R:173:G:OP1	2.37	0.57
14:N:34:VAL:HG12	14:N:35:GLU:HG2	1.85	0.57
15:O:12:PRO:HD2	15:O:15:ASN:HD22	1.68	0.57
18:R:524:G:H2'	18:R:525:G:H8	1.69	0.57
4:D:7:LEU:HD22	4:D:7:LEU:C	2.25	0.57
7:G:92:TYR:N	7:G:92:TYR:CD1	2.73	0.57
12:L:33:SER:HB3	12:L:37:ASN:HB2	1.87	0.57
13:M:47:SER:OG	13:M:53:LYS:NZ	2.38	0.57
7:G:68:SER:CA	7:G:224:PHE:HD2	2.16	0.56
6:F:345:PRO:HD2	6:F:350:CYS:O	2.06	0.56
2:B:138:GLN:C	2:B:140:ALA:H	2.07	0.56
2:B:142:GLU:HA	2:B:145:ALA:HB3	1.88	0.56
6:F:320:LEU:HD22	6:F:324:VAL:HG11	1.87	0.56
9:I:45:CYS:SG	9:I:47:SER:OG	2.63	0.56
18:R:209:U:H3	18:R:229:U:H3	1.54	0.56
6:F:385:SER:OG	6:F:386:ALA:N	2.39	0.56
7:G:58:LYS:HB3	7:G:61:ALA:HB2	1.87	0.56
13:M:41:ARG:O	13:M:57:ARG:NH1	2.39	0.56
17:Q:17:LEU:HB3	17:Q:71:LEU:HD12	1.87	0.55
9:I:198:LEU:HD12	9:I:207:TYR:HB3	1.88	0.55
4:D:372:GLU:OE1	4:D:391:TYR:OH	2.23	0.55
9:I:41:ASP:HB3	9:I:42:PRO:HD2	1.89	0.55
18:R:502:C:H2'	18:R:503:G:H8	1.71	0.55



	o uo puge	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
6:F:339:ILE:HD11	6:F:342:VAL:HG13	1.89	0.55
4:D:448:TYR:CE2	5:E:480:SER:HA	2.41	0.55
2:B:40:ASN:HD21	18:R:298:G:H21	1.53	0.55
4:D:334:LEU:HD22	4:D:347:ILE:HG23	1.88	0.55
18:R:239:U:H2'	18:R:240:G:H8	1.72	0.55
6:F:326:GLU:HG2	6:F:344:ILE:HG23	1.89	0.55
7:G:68:SER:CB	7:G:224:PHE:CE2	2.90	0.55
15:O:89:LEU:HD13	17:Q:63:ILE:HG13	1.89	0.54
18:R:448:G:H2'	18:R:449:G:H8	1.72	0.54
16:P:37:GLU:OE2	16:P:39:ARG:NH2	2.40	0.54
4:D:193:ILE:HG22	4:D:230:LYS:HE2	1.90	0.54
18:R:198:U:H3	18:R:240:G:H1	1.54	0.54
6:F:411:GLN:HA	6:F:411:GLN:HE21	1.73	0.54
18:R:384:U:O4	18:R:434:G:O6	2.25	0.54
20:X:834:PHE:O	20:X:839:ASP:N	2.40	0.54
3:C:13:PRO:HG2	3:C:19:TYR:HB2	1.88	0.54
4:D:24:PRO:HD2	7:G:260:LEU:HB3	1.90	0.54
7:G:187:ILE:HD11	7:G:215:LEU:HD22	1.90	0.53
13:M:98:GLY:O	16:P:74:ARG:NH1	2.41	0.53
9:I:41:ASP:CB	9:I:42:PRO:CD	2.86	0.53
5:E:274:LEU:O	5:E:278:LEU:N	2.38	0.53
11:K:50:GLU:OE2	11:K:52:ARG:NH2	2.37	0.53
3:C:67:ILE:HG22	3:C:77:ALA:HB1	1.90	0.53
4:D:369:GLU:HA	4:D:372:GLU:HG2	1.91	0.53
9:I:73:LEU:HB3	9:I:76:HIS:HD2	1.74	0.53
2:B:186:THR:OG1	4:D:242:MET:SD	2.66	0.53
7:G:228:GLU:OE1	7:G:230:ASN:N	2.42	0.53
9:I:39:LEU:HD13	9:I:79:GLN:OE1	2.09	0.53
15:O:80:ILE:HG22	16:P:82:ARG:HB3	1.91	0.53
6:F:197:HIS:HA	6:F:204:SER:HA	1.90	0.53
7:G:95:LYS:HZ2	7:G:95:LYS:HB2	1.73	0.53
5:E:573:HIS:HD2	5:E:576:ILE:HB	1.73	0.52
18:R:62:A:H8	18:R:65:G:HO2'	1.57	0.52
4:D:437:GLN:NE2	4:D:472:TYR:OH	2.39	0.52
9:I:39:LEU:HG	9:I:39:LEU:O	2.08	0.52
18:R:391:C:N4	18:R:423:G:O2'	2.37	0.52
4:D:489:ASP:OD2	4:D:492:ARG:NH2	2.42	0.52
18:R:131:U:H2'	18:R:132:U:C6	2.45	0.52
7:G:68:SER:HB2	7:G:224:PHE:CE2	2.45	0.52
13:M:45:ILE:HG12	13:M:55:ILE:HG12	1.91	0.52
5:E:383:ASN:OD1	5:E:383:ASN:N	2.43	0.51



	bus puge	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
7:G:72:LEU:HD23	7:G:115:ILE:HB	1.93	0.51
4:D:496:ASP:OD1	4:D:496:ASP:N	2.36	0.51
5:E:619:LEU:HD13	6:F:379:ARG:HB3	1.93	0.51
3:C:44:ASN:ND2	3:C:55:LEU:O	2.44	0.51
20:X:815:PHE:O	20:X:819:ILE:N	2.43	0.51
13:M:8:ARG:NH1	13:M:17:GLU:OE1	2.43	0.51
5:E:321:LEU:CD2	5:E:322:PRO:CD	2.88	0.51
12:L:19:LEU:HD12	12:L:23:THR:HG23	1.92	0.51
16:P:76:ASN:ND2	18:R:559:G:OP2	2.43	0.51
1:A:4:ASN:HD22	1:A:6:SER:HB3	1.76	0.50
1:A:8:TYR:HB3	1:A:12:VAL:HB	1.93	0.50
3:C:89:ARG:O	3:C:93:LYS:HB2	2.12	0.50
4:D:428:LEU:HA	4:D:437:GLN:HE22	1.75	0.50
7:G:98:LEU:HD23	7:G:99:ARG:N	2.25	0.50
18:R:439:U:H2'	18:R:440:A:C8	2.46	0.50
13:M:54:ILE:HG22	13:M:74:GLU:HG2	1.93	0.50
1:A:25:LYS:HD3	11:K:78:GLU:HB3	1.93	0.50
6:F:358:ARG:NH2	6:F:362:GLU:OE2	2.44	0.50
5:E:326:LYS:HG3	5:E:330:TYR:HE2	1.76	0.50
7:G:117:LEU:HD11	7:G:128:VAL:HG11	1.94	0.50
4:D:506:TRP:HE1	4:D:521:LEU:HD11	1.76	0.50
6:F:341:TYR:C	6:F:341:TYR:CD2	2.85	0.50
4:D:88:SER:HB2	18:R:114:U:H4'	1.94	0.50
5:E:321:LEU:CD2	5:E:322:PRO:HD3	2.42	0.50
20:X:830:LEU:O	20:X:834:PHE:N	2.40	0.50
18:R:21:G:H2'	18:R:22:A:H8	1.75	0.50
2:B:8:TYR:CD1	2:B:8:TYR:N	2.79	0.49
3:C:135:LEU:HD12	18:R:426:U:H2'	1.94	0.49
18:R:249:G:H2'	18:R:250:G:H8	1.77	0.49
14:N:63:PHE:HB3	17:Q:71:LEU:HB3	1.94	0.49
11:K:88:ARG:HH12	14:N:67:SER:HA	1.77	0.49
6:F:407:GLN:HG3	6:F:408:PRO:CD	2.41	0.49
6:F:417:TYR:HB2	7:G:281:MET:HE2	1.94	0.49
10:J:522:ALA:O	10:J:526:LEU:N	2.45	0.49
20:X:811:THR:O	20:X:815:PHE:N	2.40	0.49
20:X:379:THR:O	20:X:381:ASP:N	2.44	0.49
18:R:392:A:N6	18:R:424:U:O3'	2.46	0.49
5:E:322:PRO:HD2	5:E:325:PHE:CE2	2.48	0.49
18:R:401:U:H2'	18:R:402:G:H8	1.78	0.49
4:D:33:LEU:HD22	4:D:33:LEU:C	2.32	0.49
4:D:195:ASP:OD1	4:D:195:ASP:N	2.46	0.49



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
4:D:503:ARG:NH2	5:E:386:ASP:OD1	2.46	0.49
9:I:213:THR:HG23	9:I:215:ARG:H	1.78	0.49
20:X:64:ILE:O	20:X:68:TYR:N	2.45	0.49
5:E:581:PRO:HG3	5:E:611:ILE:HG22	1.95	0.48
18:R:389:G:O6	18:R:430:U:O4	2.30	0.48
5:E:383:ASN:HD22	5:E:392:ILE:HA	1.78	0.48
5:E:409:ASN:ND2	5:E:414:GLN:O	2.46	0.48
11:K:93:LEU:HD12	12:L:91:THR:HG21	1.96	0.48
2:B:138:GLN:C	2:B:140:ALA:N	2.67	0.48
6:F:381:SER:OG	6:F:382:TRP:N	2.46	0.48
7:G:61:ALA:HB1	7:G:123:LEU:CD1	2.44	0.48
4:D:442:ASN:OD1	4:D:484:ARG:NH1	2.47	0.48
18:R:20:A:H2'	18:R:21:G:H8	1.78	0.48
2:B:195:SER:H	6:F:301:GLN:HE22	1.62	0.47
7:G:71:ILE:HG23	7:G:116:VAL:HG22	1.95	0.47
4:D:424:VAL:HG11	4:D:444:LEU:HD11	1.97	0.47
16:P:36:THR:HG22	16:P:60:VAL:HG22	1.97	0.47
18:R:16:U:O2'	18:R:168:C:OP2	2.23	0.47
18:R:521:G:H2'	18:R:522:A:H8	1.80	0.47
2:B:124:ARG:O	2:B:128:GLY:HA3	2.14	0.47
20:X:776:LEU:O	20:X:780:ALA:N	2.47	0.47
7:G:71:ILE:HD12	7:G:198:PHE:CE2	2.50	0.47
13:M:48:LEU:HD11	13:M:96:LEU:HD11	1.96	0.47
7:G:68:SER:OG	7:G:224:PHE:HE2	1.97	0.47
8:H:22:ASP:OD1	8:H:22:ASP:N	2.47	0.47
9:I:203:VAL:HG12	9:I:229:TYR:HD2	1.80	0.47
18:R:497:G:N2	18:R:498:U:O4	2.46	0.47
18:R:342:C:N4	18:R:480:C:OP2	2.48	0.47
1:A:9:PRO:O	1:A:12:VAL:N	2.45	0.47
4:D:276:ILE:HG23	4:D:311:LEU:HD12	1.97	0.47
18:R:21:G:H2'	18:R:22:A:C8	2.50	0.47
3:C:9:LEU:CD2	3:C:101:VAL:HG21	2.45	0.47
7:G:45:PHE:HB3	7:G:153:LYS:HD3	1.97	0.47
18:R:239:U:H2'	18:R:240:G:C8	2.49	0.47
6:F:195:ILE:HA	6:F:208:GLY:HA3	1.97	0.46
14:N:41:ASN:ND2	14:N:64:VAL:O	2.48	0.46
6:F:323:LEU:HD23	6:F:323:LEU:O	2.14	0.46
9:I:41:ASP:CB	9:I:42:PRO:HD3	2.46	0.46
18:R:24:G:H2'	18:R:25:A:C8	2.50	0.46
3:C:74:THR:OG1	3:C:75:ASN:N	2.48	0.46
13:M:77:THR:HG22	13:M:86:ASN:HD22	1.80	0.46



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:B:8:TYR:HD1	14:N:82:PRO:HG3	1.71	0.46
4:D:345:THR:HG22	4:D:387:ILE:HD11	1.97	0.46
2:B:104:THR:O	2:B:108:LEU:HB2	2.16	0.46
18:R:429:C:H2'	18:R:430:U:H6	1.81	0.46
9:I:48:TYR:HB2	9:I:53:CYS:HB2	1.98	0.46
15:O:31:LEU:HD12	15:O:37:ILE:HG13	1.97	0.46
18:R:125:A:H2'	18:R:126:A:H8	1.80	0.46
5:E:624:PHE:HE2	6:F:389:THR:HG21	1.79	0.46
7:G:129:LEU:O	7:G:133:LEU:HB2	2.16	0.46
18:R:424:U:H2'	18:R:425:A:C8	2.49	0.46
2:B:59:ARG:HH12	2:B:67:SER:HB3	1.81	0.46
4:D:306:LEU:HB2	4:D:309:TYR:HB2	1.97	0.46
18:R:47:A:H2'	18:R:48:A:C8	2.51	0.46
4:D:208:LEU:HB3	4:D:214:ILE:HG23	1.97	0.45
11:K:60:LYS:NZ	11:K:74:ASN:O	2.37	0.45
7:G:69:LEU:HD23	7:G:164:PRO:CG	2.46	0.45
18:R:180:U:O5'	18:R:533:A:N6	2.48	0.45
4:D:451:ASP:N	4:D:451:ASP:OD1	2.48	0.45
18:R:170:G:H2'	18:R:171:A:H8	1.81	0.45
5:E:321:LEU:HD22	5:E:322:PRO:HD3	1.95	0.45
18:R:486:C:H2'	18:R:487:A:C8	2.52	0.45
4:D:400:ASN:ND2	4:D:413:ASN:O	2.50	0.45
4:D:438:GLU:OE2	4:D:475:ASN:ND2	2.49	0.45
4:D:303:LEU:HD12	4:D:312:VAL:CG1	2.23	0.45
6:F:313:THR:O	6:F:313:THR:OG1	2.35	0.45
18:R:20:A:H2'	18:R:21:G:C8	2.52	0.45
18:R:47:A:H2'	18:R:48:A:H8	1.81	0.45
4:D:57:ARG:NE	4:D:81:GLU:OE2	2.50	0.45
7:G:98:LEU:C	7:G:98:LEU:CD2	2.85	0.45
18:R:334:U:H2'	18:R:335:G:C8	2.52	0.45
18:R:478:A:H2'	18:R:479:G:H8	1.81	0.45
12:L:3:LEU:HD21	13:M:68:VAL:HG23	1.98	0.44
3:C:9:LEU:HD23	3:C:101:VAL:HG21	1.99	0.44
7:G:261:PHE:O	7:G:262:ASP:C	2.53	0.44
18:R:314:G:H2'	18:R:315:G:H8	1.82	0.44
18:R:455:U:H2'	18:R:456:A:H8	1.82	0.44
20:X:369:ASN:O	20:X:373:VAL:N	2.50	0.44
4:D:178:SER:O	4:D:178:SER:OG	2.29	0.44
6:F:306:HIS:HB3	6:F:384:ARG:HG2	1.99	0.44
18:R:55:G:C2	18:R:151:C:O2	2.70	0.44
18:R:403:A:H2'	18:R:404:A:H8	1.81	0.44



	A	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:B:121:ASP:O	2:B:131:VAL:HG21	2.17	0.44
14:N:43:GLN:HG2	14:N:63:PHE:HD1	1.82	0.44
18:R:2:U:H2'	18:R:3:A:H8	1.98	0.44
4:D:303:LEU:O	4:D:307:ALA:HB2	2.18	0.44
5:E:323:LEU:H	5:E:323:LEU:HG	1.39	0.44
2:B:8:TYR:CE1	14:N:82:PRO:HD3	2.49	0.44
4:D:501:ILE:HA	4:D:505:ILE:HD13	2.00	0.44
4:D:473:LEU:HD13	4:D:479:TRP:HZ2	1.82	0.44
18:R:321:C:H2'	18:R:322:A:C8	2.52	0.44
18:R:380:G:O6	18:R:438:U:O4	2.36	0.44
4:D:243:VAL:HG11	5:E:583:ILE:HG13	2.00	0.44
4:D:310:ASP:HB3	4:D:341:SER:HB2	2.00	0.44
7:G:105:GLU:HG2	7:G:108:ASP:HA	1.99	0.44
1:A:5:LEU:C	1:A:5:LEU:CD2	2.85	0.44
18:R:6:U:H2'	18:R:7:A:H8	1.83	0.44
4:D:17:THR:HG21	8:H:31:ILE:HA	2.00	0.43
2:B:177:PRO:HB3	4:D:177:HIS:O	2.18	0.43
4:D:303:LEU:CD2	4:D:313:TRP:CH2	3.01	0.43
12:L:92:ILE:HD12	12:L:95:ILE:HD11	2.00	0.43
9:I:58:PHE:HE1	9:I:225:ILE:HA	1.83	0.43
18:R:321:C:H2'	18:R:322:A:H8	1.83	0.43
3:C:13:PRO:HG3	3:C:19:TYR:HA	1.99	0.43
12:L:50:PRO:HB2	12:L:55:LEU:HD23	1.99	0.43
18:R:396:U:H5	18:R:416:G:H1	1.65	0.43
2:B:55:HIS:CE1	18:R:133:G:H2'	2.53	0.43
2:B:124:ARG:O	2:B:128:GLY:CA	2.67	0.43
5:E:621:THR:HA	5:E:625:LEU:HB2	1.99	0.43
18:R:389:G:N2	18:R:430:U:O2	2.33	0.43
1:A:114:LEU:N	1:A:149:GLY:O	2.45	0.43
4:D:460:ILE:O	4:D:464:ILE:HG12	2.18	0.43
9:I:41:ASP:HB3	9:I:42:PRO:HD3	2.00	0.43
18:R:328:G:H2'	18:R:329:A:H8	1.82	0.43
3:C:16:LYS:HG2	3:C:67:ILE:HD11	2.00	0.43
2:B:120:VAL:HG13	2:B:123:ASN:H	1.83	0.43
7:G:97:ILE:HD12	7:G:97:ILE:HA	1.77	0.43
18:R:125:A:H2'	18:R:126:A:C8	2.53	0.43
18:R:219:U:H3'	18:R:220:G:H8	1.83	0.43
18:R:350:U:H1'	18:R:351:U:H5	1.84	0.43
18:R:448:G:H2'	18:R:449:G:C8	2.54	0.43
20:X:414:ILE:O	20:X:418:ALA:N	2.46	0.43
7:G:61:ALA:O	7:G:122:ILE:HG22	2.17	0.43



	bus puge	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
7:G:70:LEU:C	7:G:70:LEU:CD2	2.85	0.42
4:D:60:TYR:OH	4:D:76:ASP:OD2	2.27	0.42
6:F:168:GLY:HA2	6:F:207:TYR:HA	2.02	0.42
6:F:438:LEU:HD23	6:F:438:LEU:HA	1.85	0.42
9:I:43:LYS:HD3	9:I:43:LYS:HA	1.79	0.42
5:E:126:LEU:O	5:E:130:LYS:N	2.47	0.42
18:R:328:G:H2'	18:R:329:A:C8	2.55	0.42
4:D:18:LEU:HD21	8:H:35:ASP:HB3	2.01	0.42
4:D:447:PHE:HD2	4:D:456:VAL:HG21	1.85	0.42
5:E:605:PHE:HB3	5:E:608:LEU:HD23	2.02	0.42
9:I:213:THR:OG1	9:I:214:ASP:N	2.52	0.42
13:M:99:ASP:HB3	18:R:558:U:H1'	2.01	0.42
16:P:57:GLU:HG2	16:P:67:THR:HG22	2.02	0.42
18:R:418:U:H2'	18:R:419:G:C8	2.55	0.42
3:C:13:PRO:CD	3:C:19:TYR:CD1	2.72	0.42
3:C:65:VAL:HA	3:C:79:LEU:HA	2.02	0.42
6:F:341:TYR:CD2	6:F:341:TYR:O	2.72	0.42
18:R:443:U:H2'	18:R:444:G:H8	1.84	0.42
3:C:103:GLY:HA3	18:R:67:A:N3	2.35	0.42
4:D:169:ARG:NH2	4:D:173:GLU:OE2	2.53	0.42
18:R:68:G:H2'	18:R:69:A:H8	1.85	0.42
12:L:25:VAL:HG22	12:L:45:LEU:HD23	2.01	0.42
12:L:37:ASN:OD1	12:L:89:GLY:N	2.53	0.42
18:R:79:A:H5"	18:R:79:A:H8	1.85	0.42
18:R:91:U:H2'	18:R:92:G:C8	2.55	0.42
18:R:444:G:H2'	18:R:445:G:C8	2.55	0.42
4:D:108:LEU:HD23	4:D:108:LEU:HA	1.88	0.42
5:E:366:ILE:HG21	6:F:522:PHE:HB2	2.02	0.42
14:N:9:LYS:HE3	14:N:9:LYS:HB2	1.89	0.42
18:R:337:A:H2'	18:R:338:G:H8	1.84	0.42
17:Q:13:LYS:HE2	17:Q:77:ILE:HA	2.00	0.42
3:C:3:ALA:HB2	3:C:115:SER:HB2	2.02	0.41
18:R:246:U:H2'	18:R:247:G:C8	2.56	0.41
4:D:289:LEU:HA	5:E:568:TRP:HZ3	1.85	0.41
4:D:447:PHE:CD2	4:D:456:VAL:HG21	2.56	0.41
4:D:310:ASP:HA	4:D:313:TRP:CD1	2.50	0.41
5:E:427:ASP:HB2	5:E:463:LEU:HD22	2.02	0.41
18:R:37:C:H2'	18:R:38:C:C6	2.55	0.41
18:R:403:A:H2'	18:R:404:A:C8	2.55	0.41
2:B:127:ILE:O	2:B:131:VAL:CG2	2.68	0.41
4:D:273:SER:N	6:F:414:ASN:O	2.50	0.41



	lous page	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
17:Q:73:ALA:HB3	17:Q:77:ILE:HD11	2.02	0.41
18:R:282:C:H2'	18:R:283:A:H8	1.85	0.41
18:R:443:U:H2'	18:R:444:G:C8	2.55	0.41
18:R:510:G:H2'	18:R:511:A:C8	2.55	0.41
4:D:441:LEU:O	4:D:445:VAL:HG13	2.20	0.41
7:G:70:LEU:HD23	7:G:71:ILE:N	2.35	0.41
18:R:438:U:H2'	18:R:439:U:C6	2.56	0.41
1:A:8:TYR:OH	2:B:34:THR:HG21	2.19	0.41
4:D:424:VAL:HG13	4:D:440:LEU:HD12	2.02	0.41
5:E:321:LEU:HD23	5:E:321:LEU:HA	1.68	0.41
17:Q:19:ILE:HD13	17:Q:19:ILE:HA	1.89	0.41
18:R:248:G:H2'	18:R:249:G:H8	1.85	0.41
18:R:413:U:H2'	18:R:414:A:C8	2.56	0.41
5:E:536:ASP:HA	5:E:537:PRO:HD3	1.97	0.41
4:D:417:ASN:HD22	4:D:418:LYS:H	1.69	0.41
9:I:203:VAL:HB	9:I:226:HIS:CE1	2.56	0.41
12:L:15:VAL:HG21	12:L:29:LEU:HD12	2.03	0.41
18:R:444:G:H2'	18:R:445:G:H8	1.85	0.41
18:R:453:U:H2'	18:R:454:G:C8	2.56	0.41
20:X:283:HIS:CB	20:X:292:GLU:H	2.34	0.41
20:X:275:ASN:HA	20:X:409:ALA:HB3	2.03	0.41
2:B:16:ASP:OD2	2:B:21:ARG:NH2	2.54	0.40
5:E:137:ALA:C	5:E:139:SER:H	2.24	0.40
5:E:455:PHE:HD1	5:E:455:PHE:HA	1.76	0.40
1:A:7:LYS:H	1:A:7:LYS:CD	1.97	0.40
3:C:13:PRO:CG	3:C:19:TYR:HA	2.51	0.40
15:O:29:ILE:HG12	15:O:90:ILE:HG12	2.04	0.40
17:Q:10:TYR:HB3	17:Q:15:ILE:HD11	2.02	0.40
1:A:134:GLU:N	1:A:154:VAL:O	2.44	0.40
4:D:365:ARG:HH22	4:D:402:LEU:HD21	1.86	0.40
13:M:99:ASP:HA	16:P:74:ARG:HH12	1.87	0.40
18:R:416:G:H4'	18:R:417:A:H5'	2.03	0.40
18:R:454:G:H2'	18:R:455:U:H6	1.86	0.40
20:X:679:LYS:O	20:X:683:ILE:N	2.48	0.40
7:G:111:MET:SD	7:G:111:MET:N	2.94	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	Perce	entiles
1	А	182/300~(61%)	162 (89%)	17 (9%)	3~(2%)	9	46
2	В	193/231~(84%)	180 (93%)	10 (5%)	3~(2%)	9	46
3	С	126/350~(36%)	120 (95%)	6 (5%)	0	100	100
4	D	542/544~(100%)	515 (95%)	27 (5%)	0	100	100
5	Е	570/629~(91%)	532 (93%)	38 (7%)	0	100	100
6	F	259/523~(50%)	240 (93%)	19 (7%)	0	100	100
7	G	235/492~(48%)	218 (93%)	17 (7%)	0	100	100
8	Н	50/105~(48%)	47 (94%)	3 (6%)	0	100	100
9	Ι	186/261~(71%)	174 (94%)	11 (6%)	1 (0%)	29	68
10	J	196/583~(34%)	185 (94%)	10 (5%)	1 (0%)	29	68
11	К	119/196~(61%)	111 (93%)	8 (7%)	0	100	100
12	L	117/146 (80%)	111 (95%)	6 (5%)	0	100	100
13	М	105/110~(96%)	103 (98%)	2 (2%)	0	100	100
14	Ν	91/101 (90%)	84 (92%)	7 (8%)	0	100	100
15	Ο	70/94~(74%)	68~(97%)	2 (3%)	0	100	100
16	Р	72/86~(84%)	68 (94%)	4 (6%)	0	100	100
17	Q	67/77~(87%)	62 (92%)	5 (8%)	0	100	100
20	Х	824/861 (96%)	727 (88%)	80 (10%)	17 (2%)	7	40
21	Y	136/208~(65%)	120 (88%)	15 (11%)	1 (1%)	22	61
All	All	4140/5897~(70%)	3827 (92%)	287 (7%)	26 (1%)	29	64

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	98	PRO
2	В	139	ARG



Mol	Chain	Res	Type
10	J	370	PRO
20	Х	71	GLU
20	Х	284	LEU
20	Х	380	LEU
20	Х	672	ILE
20	Х	673	GLU
20	Х	674	LEU
21	Y	24	TYR
1	А	99	HIS
20	Х	70	HIS
20	Х	289	THR
20	Х	343	THR
20	Х	571	VAL
20	Х	390	THR
20	Х	670	ALA
2	В	70	ASN
20	Х	290	GLY
20	Х	449	ASN
9	Ι	41	ASP
2	В	136	LEU
20	Х	278	PHE
20	Х	389	PHE
20	Х	410	PRO
1	А	97	ASP

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	А	82/265~(31%)	78~(95%)	4(5%)	25 59
2	В	171/214~(80%)	161 (94%)	10 (6%)	20 55
3	С	117/317~(37%)	112 (96%)	5 (4%)	29 63
4	D	508/519~(98%)	491 (97%)	17 (3%)	38 69
5	Е	316/603~(52%)	307~(97%)	9~(3%)	43 72



Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles
6	F	157/451~(35%)	149 (95%)	8 (5%)	24	58
7	G	218/448~(49%)	207~(95%)	11 (5%)	24	59
8	Н	48/48 (100%)	46 (96%)	2 (4%)	30	63
9	Ι	130/234~(56%)	124 (95%)	6 (5%)	27	61
11	Κ	114/176~(65%)	114 (100%)	0	100	100
12	L	107/129~(83%)	106 (99%)	1 (1%)	78	90
13	М	95/103~(92%)	94 (99%)	1 (1%)	73	88
14	Ν	81/89~(91%)	78~(96%)	3 (4%)	34	66
15	Ο	62/83~(75%)	62 (100%)	0	100	100
16	Р	64/77~(83%)	59~(92%)	5 (8%)	12	44
17	Q	59/66~(89%)	55 (93%)	4 (7%)	16	50
All	All	2329/3822~(61%)	2243 (96%)	86 (4%)	37	66

All (86) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	5	LEU
1	А	7	LYS
1	А	46	ASN
1	А	70	ARG
2	В	3	ARG
2	В	29	ASN
2	В	47	ASN
2	В	80	ASN
2	В	124	ARG
2	В	131	VAL
2	В	135	LYS
2	В	136	LEU
2	В	138	GLN
2	В	172	LYS
3	С	62	LEU
3	С	101	VAL
3	С	107	ARG
3	С	108	MET
3	С	117	LEU
4	D	5	THR
4	D	7	LEU
4	D	8	ILE



Mol	Chain	Res	Type
4	D	33	LEU
4	D	102	ASN
4	D	263	TYR
4	D	265	THR
4	D	306	LEU
4	D	310	ASP
4	D	366	ASN
4	D	381	ASN
4	D	416	LEU
4	D	417	ASN
4	D	444	LEU
4	D	445	VAL
4	D	446	GLN
4	D	515	GLN
5	Е	314	TYR
5	Е	321	LEU
5	Е	323	LEU
5	Е	324	ASP
5	Е	349	ASN
5	Ε	352	ASN
5	Е	409	ASN
5	Е	472	LEU
5	Ε	617	ASN
6	F	312	ASN
6	F	314	THR
6	F	322	SER
6	F	341	TYR
6	F	342	VAL
6	F	343	LYS
6	F	344	ILE
6	F	410	LEU
7	G	69	LEU
7	G	72	LEU
7	G	90	HIS
7	G	92	TYR
7	G	95	LYS
7	G	97	ILE
7	G	122	ILE
7	G	123	LEU
7	G	200	GLN
7	G	260	LEU
7	G	261	PHE



Mol	Chain	Res	Type
8	Н	2	ARG
8	Н	51	ASN
9	Ι	39	LEU
9	Ι	43	LYS
9	Ι	44	ILE
9	Ι	73	LEU
9	Ι	88	LYS
9	Ι	118	ASN
12	L	114	ASN
13	М	51	ASN
14	Ν	3	MET
14	Ν	30	ARG
14	Ν	41	ASN
16	Р	19	LEU
16	Р	39	ARG
16	Р	47	ASN
16	Р	51	LEU
16	Р	82	ARG
17	Q	20	ASN
17	Q	66	ASN
17	Q	75	ASP
17	Q	77	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	46	ASN
2	В	29	ASN
2	В	40	ASN
2	В	47	ASN
2	В	80	ASN
3	С	18	ASN
4	D	102	ASN
4	D	153	GLN
4	D	298	ASN
4	D	366	ASN
4	D	381	ASN
4	D	400	ASN
4	D	411	GLN
4	D	417	ASN
4	D	437	GLN
4	D	443	ASN



Mol	Chain	Res	Type
4	D	474	GLN
5	Е	349	ASN
5	Е	352	ASN
5	Е	409	ASN
5	Е	488	ASN
5	Е	582	GLN
5	Е	617	ASN
6	F	301	GLN
6	F	306	HIS
6	F	311	ASN
6	F	312	ASN
6	F	334	GLN
6	F	407	GLN
6	F	411	GLN
6	F	497	GLN
7	G	43	GLN
7	G	90	HIS
7	G	200	GLN
8	Н	51	ASN
9	Ι	40	HIS
9	Ι	76	HIS
9	Ι	118	ASN
9	Ι	226	HIS
12	L	114	ASN
13	М	51	ASN
13	М	86	ASN
14	Ν	41	ASN
15	0	15	ASN
16	Р	24	ASN
16	Р	47	ASN
16	Р	50	ASN
17	Q	66	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
18	R	556/568~(97%)	134 (24%)	18(3%)
19	r	21/253~(8%)	6 (28%)	0
All	All	577/821 (70%)	140 (24%)	18 (3%)

All (140) RNA backbone outliers are listed below:



Mol	Chain	Res	Type
18	R	10	U
18	R	11	U
18	R	12	А
18	R	13	А
18	R	17	А
18	R	26	G
18	R	40	А
18	R	41	С
18	R	53	G
18	R	54	С
18	R	55	G
18	R	56	С
18	R	62	А
18	R	63	U
18	R	64	А
18	R	65	G
18	R	66	U
18	R	67	А
18	R	72	G
18	R	74	С
18	R	75	G
18	R	79	А
18	R	80	G
18	R	87	U
18	R	90	U
18	R	92	G
18	R	93	А
18	R	97	А
18	R	98	U
18	R	99	А
18	R	100	А
18	R	101	U
18	R	103	G
18	R	104	U
18	R	107	A
18	R	113	G
18	R	114	U
18	R	117	U
18	R	134	G
18	R	139	А
18	R	141	А
18	R	$14\overline{2}$	C
18	R	145	A



Mol	Chain	Res	Type
18	R	147	А
18	R	149	G
18	R	150	G
18	R	151	С
18	R	152	G
18	R	153	С
18	R	154	G
18	R	176	U
18	R	178	С
18	R	179	А
18	R	180	U
18	R	181	U
18	R	182	С
18	R	183	С
18	R	186	U
18	R	187	G
18	R	205	U
18	R	206	С
18	R	217	U
18	R	218	U
18	R	219	U
18	R	220	G
18	R	227	U
18	R	228	U
18	R	230	G
18	R	254	U
18	R	255	U
18	R	257	G
18	R	258	U
18	R	259	U
18	R	260	U
18	R	262	U
18	R	269	U
18	R	270	G
18	R	271	G
18	R	272	A
18	R	278	U
18	R	279	U
18	R	280	G
18	R	287	A
18	R	290	U
18	R	325	A



Mol	Chain	Res	Type
18	R	327	А
18	R	328	G
18	R	343	А
18	R	352	G
18	R	365	U
18	R	369	G
18	R	377	U
18	R	378	U
18	R	385	U
18	R	386	G
18	R	389	G
18	R	393	G
18	R	394	А
18	R	395	U
18	R	399	А
18	R	400	А
18	R	407	U
18	R	409	А
18	R	416	G
18	R	418	U
18	R	422	G
18	R	424	U
18	R	426	U
18	R	427	G
18	R	443	U
18	R	460	U
18	R	466	U
18	R	468	U
18	R	477	G
18	R	482	G
18	R	493	G
18	R	504	U
18	R	505	U
18	R	506	A
18	R	508	G
18	R	513	A
18	R	540	G
18	R	542	U
18	R	545	A
18	R	551	U
18	R	553	A
18	R	555	U



Mol	Chain	Res	Type
18	R	559	G
18	R	560	А
18	R	561	U
18	R	562	U
18	R	563	U
18	R	564	А
18	R	565	U
19	r	-8	С
19	r	-6	А
19	r	-5	G
19	r	-4	А
19	r	-2	А
19	r	-1	G

All (1	8) RNA	pucker	outliers	are	listed	below:
--------	--------	-------------------------	----------	-----	--------	--------

Mol	Chain	\mathbf{Res}	Type
18	R	63	U
18	R	64	А
18	R	66	U
18	R	79	А
18	R	86	А
18	R	100	А
18	R	112	А
18	R	113	G
18	R	133	G
18	R	151	С
18	R	152	G
18	R	186	U
18	R	258	U
18	R	268	С
18	R	277	U
18	R	279	U
18	R	399	А
18	R	505	U

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

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



5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

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.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
8	Н	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	Н	52:SER	С	1262:UNK	Ν	64.87



6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-0360. 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: 192

Y Index: 192





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: 182

Z Index: 189

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 0.065. 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 $190~{\rm nm^3};$ this corresponds to an approximate mass of 171 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 0.278 $\mathrm{\AA^{-1}}$



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 0.278 \AA^{-1}

8.2 Resolution estimates (i)

B osolution ostimato $(\hat{\lambda})$	Estimation criterion (FSC cut-off)		
Resolution estimate (A)	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.59	4.12	3.65
Unmasked-calculated*	-	-	-

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

9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-0360 and PDB model 6N7P. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlay (i)

The images above show the 3D surface view of the map at the recommended contour level 0.065 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 (0.065).

9.4 Atom inclusion (i)

At the recommended contour level, 52% of all backbone atoms, 52% 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 (0.065) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5230	0.3520
А	0.4790	0.3590
В	0.7210	0.4940
С	0.6150	0.4190
D	0.8350	0.5290
Ε	0.5890	0.3960
F	0.6130	0.4260
G	0.7570	0.5030
Н	0.6720	0.4630
Ι	0.5690	0.4080
J	0.0000	0.0480
К	0.7590	0.5120
L	0.7970	0.5130
М	0.7630	0.5140
Ν	0.7880	0.5370
0	0.8070	0.5180
Р	0.8310	0.5250
Q	0.8020	0.5270
R	0.4330	0.2710
Х	0.0000	0.0480
Y	0.0000	0.0440
r	0.4310	0.2910

