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PDB ID	:	6NQB
EMDB ID	:	EMD-0482
Title	:	Role of Era in Assembly and Homeostasis of the Ribosomal Small Subunit
Authors	:	Ortega, J.
Deposited on	:	2019-01-20
Resolution	:	3.80 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 3.80 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 of chain			
			41%			
1	C	206	77%	23%		
	-	0.0	73%	_		
2	J	98	74%	24% •		
	3.7		66%			
3	N	99	76%	19% • •		
	a		84%			
4	S	74	70%	30%		
_		1 - 10	9%			
5	A	1542	38% 38%	10% 13%		
	D	207	9%			
6	D	205	79%	20% •		
_		1.10	9%			
7	E	149	82%	18%		



	11404 51011			
Mol	Chain	\mathbf{Length}	Quality of chain	
			45%	
8	F	93	71% 12%	17%
			9%	
9	Н	129	79%	21%
			5%	
10	L	123	84%	15% •
			7%	
11	0	86	83%	15% •
			<u>→</u>	
12	Р	79	81%	15% •
			5%	
13	Q	79	85%	15%
			48%	
14	R	52	67% 27%	6%
15	Т	85	78%	22%
			84%	
16	В	217	83%	17%



2 Entry composition (i)

There are 17 unique types of molecules in this entry. The entry contains 42570 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 30S ribosomal protein S3.

Mol	Chain	Residues		Ate	AltConf	Trace			
1	С	206	Total 1624	C 1028	N 305	0 288	${ m S} { m 3}$	0	0

• Molecule 2 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	Т	08	Total	С	N	0	S	0	0
	J	30	786	493	150	142	1		0

• Molecule 3 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues		At	oms	AltConf	Trace		
3	N	96	Total 774	C 483	N 160	0 128	${ m S} { m 3}$	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
N	?	-	GLU	deletion	UNP A0A090BZT4

• Molecule 4 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues		At	oms	AltConf	Trace		
4	S	74	Total 594	C 381	N 110	0 101	$\begin{array}{c} \mathrm{S} \\ \mathrm{2} \end{array}$	0	0

• Molecule 5 is a RNA chain called 16S RIBOSOMAL RNA.

Mol	Chain	Residues		A	AltConf	Trace			
5	А	1341	Total 28767	C 12830	N 5276	O 9320	Р 1341	0	0

• Molecule 6 is a protein called 30S ribosomal protein S4.



Mol	Chain	Residues	Atoms					AltConf	Trace
6	D	205	Total 1643	C 1026	N 315	O 298	$\frac{S}{4}$	0	0

• Molecule 7 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues		At	oms			AltConf	Trace
7	Е	149	Total 1089	C 675	N 209	O 199	S 6	0	0

• Molecule 8 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues		At	oms			AltConf	Trace
8	F	77	Total 630	C 401	N 109	0 114	S 6	0	0

• Molecule 9 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues		At	oms			AltConf	Trace
9	Н	129	Total 979	C 616	N 173	0 184	S 6	0	0

• Molecule 10 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues		At	oms			AltConf	Trace
10	L	123	Total 955	C 590	N 196	0 165	$\frac{S}{4}$	0	0

• Molecule 11 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues		At	oms			AltConf	Trace
11	Ο	86	Total 698	C 431	N 141	0 125	S 1	0	0

• Molecule 12 is a protein called 30S RIBOSOMAL PROTEIN bS16.

Mol	Chain	Residues		At	oms			AltConf	Trace
12	Р	79	Total 629	C 394	N 124	0 110	S 1	0	0

• Molecule 13 is a protein called 30S ribosomal protein S17.



Mol	Chain	Residues		At	oms			AltConf	Trace
13	Q	79	Total 641	C 406	N 120	0 112	${ m S} { m 3}$	0	0

• Molecule 14 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues		Aton	ıs		AltConf	Trace
14	R	49	Total 405	C 258	N 76	0 71	0	0

• Molecule 15 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues		At	oms			AltConf	Trace
15	Т	85	Total 659	C 408	N 134	0 114	${ m S} { m 3}$	0	0

• Molecule 16 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues		Ate	oms			AltConf	Trace
16	В	217	Total 1696	C 1076	N 304	O 310	S 6	0	0

• Molecule 17 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
17	А	1	Total Mg 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: 30S ribosomal protein S3























•	•	•	•	•			•	•	•	•	•	•	•	•	•		•	•	•	•	•	•	•	•	•	•	•	•
V195	D196	F197	V198	I199	P200	G201	N202	D203	D204	A205	1206	R207	T210	L211	Y212	L213	G214	A215	V216	A217	A218	T219	V220	R221	E222	G223	R224	S225



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	423567	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 $(e^-/\text{\AA}^2)$	35	Depositor
Minimum defocus (nm)	1250	Depositor
Maximum defocus (nm)	2750	Depositor
Magnification	75000	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	32.913	Depositor
Minimum map value	-13.176	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	5.18	Depositor
Map size (Å)	326.192, 326.192, 326.192	wwPDB
Map dimensions	304, 304, 304	wwPDB
Map angles $(^{\circ})$	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.073, 1.073, 1.073	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: MG

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

Mal	Chain	Bo	nd lengths	Bond angles		
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	С	0.30	0/1651	0.58	0/2225	
2	J	0.29	0/796	0.64	1/1077~(0.1%)	
3	Ν	0.28	0/785	0.62	1/1043~(0.1%)	
4	S	0.28	0/609	0.56	0/822	
5	А	0.62	0/32207	1.11	130/50237~(0.3%)	
6	D	0.37	0/1665	0.63	0/2227	
7	Е	0.36	0/1101	0.62	0/1482	
8	F	0.29	0/643	0.59	0/868	
9	Н	0.42	1/989~(0.1%)	0.70	2/1326~(0.2%)	
10	L	0.39	0/969	0.72	1/1300~(0.1%)	
11	0	0.29	0/706	0.59	0/944	
12	Р	0.41	0/639	0.71	2/859~(0.2%)	
13	Q	0.40	0/650	0.62	0/871	
14	R	0.31	0/411	0.58	0/552	
15	Т	0.31	0/665	0.53	0/881	
16	В	0.31	0/1727	0.62	0/2328	
All	All	0.55	1/46213~(0.0%)	1.00	137/69042~(0.2%)	

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	С	0	2
2	J	0	2
6	D	0	1
9	Н	0	2
10	L	0	1
16	В	0	1
All	All	0	9



All	(1)	bond	length	outliers	are	listed	below:
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Mol	Chain	Res	Type	Atoms	Ζ	Observed(Å)	Ideal(Å)
9	Н	78	SER	C-N	-5.83	1.20	1.34

All (137) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
5	А	1158	С	N1-C2-O2	14.70	127.72	118.90
5	А	1158	С	C2-N1-C1'	12.75	132.83	118.80
5	А	1158	С	N3-C2-O2	-12.14	113.40	121.90
5	А	365	U	C2-N1-C1'	11.88	131.95	117.70
5	А	866	С	C6-N1-C2	-9.31	116.58	120.30
5	А	960	U	C2-N1-C1'	9.24	128.78	117.70
5	А	365	U	N1-C2-O2	8.93	129.05	122.80
5	А	1158	С	C6-N1-C2	-8.88	116.75	120.30
5	А	365	U	C6-N1-C1'	-8.85	108.81	121.20
5	А	1158	С	C6-N1-C1'	-8.69	110.37	120.80
3	Ν	50	LEU	CA-CB-CG	8.33	134.47	115.30
5	А	960	U	N1-C2-O2	8.06	128.45	122.80
5	А	1071	С	N1-C2-O2	8.06	123.74	118.90
5	А	481	G	N1-C6-O6	-8.06	115.06	119.90
5	А	1391	U	N1-C2-O2	7.90	128.33	122.80
5	А	322	С	C2-N1-C1'	7.89	127.47	118.80
5	А	754	С	N1-C2-O2	7.66	123.50	118.90
5	А	322	С	N1-C2-O2	7.66	123.50	118.90
5	А	599	С	N1-C2-O2	7.57	123.44	118.90
5	А	339	С	N1-C2-O2	7.46	123.38	118.90
5	А	960	U	N3-C2-O2	-7.46	116.98	122.20
5	А	372	С	P-O3'-C3'	7.34	128.51	119.70
5	А	855	U	N1-C2-O2	7.28	127.89	122.80
5	А	1391	U	N3-C2-O2	-7.07	117.25	122.20
5	А	866	С	C5-C6-N1	7.07	124.53	121.00
5	А	365	U	N3-C2-O2	-7.00	117.30	122.20
5	А	599	С	N3-C2-O2	-6.99	117.01	121.90
5	А	239	U	N1-C2-O2	6.90	127.63	122.80
5	А	1065	U	P-O3'-C3'	6.87	127.94	119.70
5	А	385	С	N1-C2-O2	6.83	123.00	118.90
5	А	322	C	C6-N1-C2	-6.81	117.58	120.30
5	A	1201	A	P-O3'-C3'	6.77	127.82	119.70
5	A	1391	U	C2-N1-C1'	6.75	125.80	117.70
5	A	401	C	N1-C2-O2	6.62	122.88	118.90
5	A	754	C	C2-N1-C1'	6.62	126.08	118.80
5	А	322	C	C5-C6-N1	6.61	124.31	121.00
5	A	484	G	P-O3'-C3'	6.60	127.61	119.70

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R L D W I D E PDB EIN DATA BANK

α \cdot \cdot \cdot	C	•	
Continued	trom	previous	page
	J	1	1 5

Mol	Chain	\mathbf{Res}	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
5	А	1101	А	P-O3'-C3'	6.59	127.61	119.70
5	А	462	G	N3-C4-C5	-6.54	125.33	128.60
5	А	1038	С	C5-C6-N1	6.54	124.27	121.00
5	А	1071	С	N3-C2-O2	-6.51	117.35	121.90
5	А	339	С	N3-C2-O2	-6.48	117.36	121.90
5	А	284	С	N1-C2-O2	6.47	122.78	118.90
5	А	51	А	P-O3'-C3'	6.46	127.46	119.70
5	А	462	G	C4-N9-C1'	6.42	134.84	126.50
5	А	372	С	OP2-P-O3'	6.39	119.25	105.20
5	А	1158	С	C5-C6-N1	6.34	124.17	121.00
5	А	239	U	N3-C2-O2	-6.33	117.77	122.20
5	А	599	С	C6-N1-C2	-6.31	117.78	120.30
5	А	54	С	N1-C2-O2	6.27	122.66	118.90
5	А	385	С	N3-C2-O2	-6.22	117.55	121.90
12	Р	4	ILE	CG1-CB-CG2	-6.21	97.74	111.40
5	А	239	U	C2-N1-C1'	6.21	125.15	117.70
5	А	855	U	N3-C2-O2	-6.19	117.86	122.20
5	А	385	С	C2-N1-C1'	6.13	125.54	118.80
5	А	1195	С	N1-C2-O2	6.10	122.56	118.90
5	А	462	G	N3-C4-N9	6.10	129.66	126.00
5	А	365	U	C5-C6-N1	6.08	125.74	122.70
5	А	401	С	N3-C2-O2	-6.05	117.66	121.90
5	А	1038	С	C6-N1-C2	-6.04	117.88	120.30
5	А	1138	G	N3-C4-N9	6.04	129.62	126.00
5	А	823	С	C6-N1-C2	-6.02	117.89	120.30
5	А	1322	С	C2-N1-C1'	6.02	125.42	118.80
5	А	51	А	OP2-P-O3'	6.01	118.43	105.20
5	А	672	U	N1-C2-O2	6.01	127.01	122.80
5	A	284	С	N3-C2-O2	-5.98	117.71	121.90
5	A	322	С	N3-C2-O2	-5.98	117.72	121.90
5	А	355	С	C6-N1-C2	-5.97	117.91	120.30
5	А	328	С	P-O3'-C3'	5.97	126.87	119.70
5	А	929	G	P-O3'-C3'	5.97	126.87	119.70
5	А	960	U	C6-N1-C1'	-5.97	112.84	121.20
5	А	1138	G	C4-N9-C1'	5.93	134.21	126.50
5	А	1071	С	C2-N1-C1'	5.90	125.29	118.80
5	A	328	C	OP2-P-O3'	5.86	118.10	105.20
5	А	1138	G	N3-C4-C5	-5.83	125.68	128.60
9	H	120	LEU	CA-CB-CG	5.83	128.72	115.30
5	A	481	G	C5-C6-O6	5.83	132.10	128.60
10	L	23	LEU	CA-CB-CG	5.80	128.64	115.30
5	А	180	U	N3-C2-O2	-5.79	118.15	122.20



Mol	Chain	\mathbf{Res}	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
5	А	244	U	O5'-P-OP2	5.72	117.56	110.70
5	А	295	С	C6-N1-C2	-5.72	118.01	120.30
5	А	1300	G	P-O3'-C3'	5.70	126.55	119.70
5	А	401	С	C2-N1-C1'	5.70	125.07	118.80
5	А	295	С	N1-C2-O2	5.67	122.30	118.90
5	А	855	U	C2-N1-C1'	5.67	124.50	117.70
9	Н	78	SER	C-N-CA	5.63	135.78	121.70
5	А	500	G	C4-N9-C1'	5.62	133.81	126.50
5	А	614	С	C6-N1-C2	-5.62	118.05	120.30
5	А	868	С	N3-C2-O2	-5.60	117.98	121.90
5	А	882	С	C6-N1-C2	-5.59	118.06	120.30
5	А	295	С	N3-C2-O2	-5.58	117.99	121.90
5	А	328	С	N1-C2-O2	5.57	122.24	118.90
12	Р	42	ILE	CG1-CB-CG2	-5.55	99.19	111.40
5	А	413	G	N3-C4-N9	5.52	129.31	126.00
5	А	385	С	C6-N1-C2	-5.49	118.10	120.30
5	А	283	U	N3-C2-O2	-5.47	118.37	122.20
5	А	758	С	C5-C6-N1	5.47	123.73	121.00
5	А	514	С	C6-N1-C2	-5.47	118.11	120.30
5	А	243	А	P-O3'-C3'	5.41	126.19	119.70
5	А	295	С	C2-N1-C1'	5.41	124.75	118.80
5	А	854	U	N1-C2-O2	5.40	126.58	122.80
5	А	180	U	N1-C2-O2	5.39	126.58	122.80
5	А	1282	С	C6-N1-C2	-5.39	118.14	120.30
5	А	599	С	C2-N1-C1'	5.36	124.70	118.80
5	А	868	С	N1-C2-O2	5.36	122.11	118.90
5	А	156	С	N1-C2-O2	5.33	122.10	118.90
5	А	486	U	N3-C2-O2	-5.32	118.47	122.20
5	А	672	U	N3-C2-O2	-5.32	118.48	122.20
5	А	754	С	C6-N1-C1'	-5.31	114.43	120.80
5	А	672	U	C2-N1-C1'	5.30	124.07	117.70
5	А	346	G	N3-C4-N9	5.29	129.17	126.00
5	А	960	U	C5-C6-N1	5.23	125.31	122.70
5	А	500	G	C8-N9-C1'	-5.22	120.21	127.00
5	А	582	С	N1-C2-O2	5.22	122.03	118.90
5	A	209	U	N1-C2-O2	5.22	126.45	122.80
5	А	678	U	C5-C6-N1	5.21	125.30	122.70
5	A	584	G	C4-N9-C1'	5.19	133.24	126.50
5	А	108	G	C4-C5-N7	5.18	112.87	110.80
5	A	43	С	C6-N1-C2	-5.18	118.23	120.30
5	A	54	С	N3-C2-O2	-5.18	118.27	121.90
5	А	20	U	N3-C2-O2	-5.18	118.58	122.20



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
5	А	283	U	N1-C2-O2	5.18	126.42	122.80
5	А	99	С	C6-N1-C2	-5.17	118.23	120.30
5	А	180	U	C2-N1-C1'	5.16	123.89	117.70
5	А	222	С	N1-C2-O2	5.15	121.99	118.90
5	А	1369	С	N1-C2-O2	5.14	121.99	118.90
2	J	42	LEU	CA-CB-CG	5.13	127.11	115.30
5	А	530	G	C4-N9-C1'	5.10	133.13	126.50
5	А	1367	С	C6-N1-C2	-5.10	118.26	120.30
5	А	1138	G	C8-N9-C1'	-5.09	120.39	127.00
5	А	563	А	C4-N9-C1'	5.06	135.41	126.30
5	А	1056	U	N1-C2-O2	5.05	126.34	122.80
5	А	92	U	N1-C2-O2	5.05	126.34	122.80
5	А	810	С	N1-C2-O2	5.05	121.93	118.90
5	А	1125	U	C2-N1-C1'	5.05	123.76	117.70
5	А	751	U	N1-C2-O2	5.04	126.33	122.80
5	А	462	G	C8-N9-C1'	-5.04	120.45	127.00

There are no chirality outliers.

Mol	Chain	\mathbf{Res}	Type	Group
16	В	129	THR	Peptide
1	С	166	TRP	Peptide
1	С	24	ASN	Peptide
6	D	176	LYS	Peptide
9	Н	111	THR	Peptide
9	Н	3	GLN	Peptide
2	J	14	ASP	Peptide
2	J	41	PRO	Peptide
10	L	23	LEU	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	С	1624	0	1699	28	0
2	J	786	0	828	15	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	Ν	774	0	827	17	0
4	S	594	0	610	16	0
5	А	28767	0	14485	267	0
6	D	1643	0	1710	28	0
7	Е	1089	0	1128	19	0
8	F	630	0	626	7	0
9	Н	979	0	1033	18	0
10	L	955	0	1019	15	0
11	0	698	0	721	12	0
12	Р	629	0	643	10	0
13	Q	641	0	682	7	0
14	R	405	0	425	10	0
15	Т	659	0	703	15	0
16	В	1696	0	1723	22	0
17	А	1	0	0	0	0
All	All	42570	0	28862	431	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (431) 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)
5:A:1349:A:H62	5:A:1373:G:H21	1.36	0.71
5:A:674:G:H1	5:A:715:A:H61	1.38	0.71
5:A:993:G:H2'	5:A:995:C:H41	1.58	0.67
5:A:659:U:H3	5:A:746:A:H61	1.44	0.66
5:A:928:G:H1	5:A:1389:C:H42	1.42	0.66
5:A:988:G:H4'	5:A:1014:A:H61	1.59	0.66
5:A:1097:C:HO2'	5:A:1169:A:HO2'	1.43	0.66
5:A:551:U:O2'	10:L:82:ARG:NH1	2.29	0.66
1:C:149:LYS:HB3	1:C:200:TRP:HB2	1.78	0.65
4:S:65:MET:HA	4:S:68:HIS:HB3	1.77	0.65
12:P:14:ARG:HE	12:P:42:ILE:HD13	1.61	0.65
6:D:161:ALA:HA	6:D:164:ARG:HD3	1.79	0.65
5:A:667:G:O6	5:A:739:C:N4	2.30	0.64
5:A:655:A:H61	5:A:751:U:H3	1.46	0.63
5:A:542:G:OP1	6:D:9:LYS:NZ	2.32	0.63
5:A:978:A:OP2	5:A:1362:A:N6	2.32	0.63
5:A:617:G:H1	5:A:623:C:H42	1.47	0.62
1:C:34:SER:OG	1:C:58:ARG:NH2	2.33	0.62



	us puge	Interatomic	Clash
Atom-1	Atom-2	distance $(Å)$	overlap (Å)
5:A:1120:C:H42	5:A:1153:G:H1	1.45	0.62
6:D:61:ARG:HH21	6:D:67:LEU:HA	1.64	0.62
5:A:1089:G:N2	5:A:1097:C:N3	2.47	0.61
16:B:14:HIS:HB2	16:B:202:ASN:HD22	1.66	0.61
5:A:1121:U:H3	5:A:1152:A:H61	1.48	0.61
5:A:1064:G:O2'	5:A:1190:G:N2	2.34	0.61
14:R:35:SER:HB2	14:R:72:ARG:HH12	1.65	0.60
5:A:1103:C:H4'	16:B:96:LEU:HD22	1.83	0.60
5:A:664:G:H22	5:A:741:G:H1	1.49	0.60
5:A:1178:G:N2	5:A:1181:G:OP2	2.34	0.60
5:A:111:G:O6	5:A:330:C:N4	2.33	0.60
5:A:178:C:H2'	5:A:179:A:H8	1.66	0.60
5:A:677:U:H3	5:A:713:G:H1	1.50	0.60
5:A:916:U:H2'	5:A:917:G:H8	1.67	0.59
1:C:55:VAL:HB	1:C:66:THR:HB	1.85	0.59
5:A:363:A:N6	10:L:26:CYS:SG	2.75	0.59
5:A:987:G:H21	5:A:1014:A:H2	1.50	0.59
9:H:38:VAL:HG22	9:H:110:MET:HG3	1.84	0.59
4:S:52:ASN:O	5:A:958:A:N6	2.35	0.59
16:B:65:LYS:HB2	16:B:158:ASP:H	1.68	0.59
6:D:171:GLU:HB2	6:D:180:THR:HB	1.85	0.58
1:C:149:LYS:HB2	1:C:172:VAL:HG21	1.85	0.58
2:J:39:PRO:HB3	2:J:72:ARG:HH21	1.68	0.58
10:L:53:ARG:HA	10:L:63:THR:HA	1.85	0.58
5:A:767:A:N6	5:A:813:U:O2	2.36	0.58
16:B:31:PHE:HB2	16:B:41:ASN:HB2	1.84	0.58
16:B:87:ASP:HB3	16:B:224:ARG:HH22	1.69	0.58
5:A:178:C:OP2	15:T:59:ARG:NH1	2.36	0.58
5:A:373:A:H1'	5:A:481:G:H1'	1.85	0.58
5:A:985:C:H42	5:A:1220:G:H1	1.50	0.58
5:A:185:U:O2	15:T:75:LYS:NZ	2.36	0.58
5:A:197:A:O2'	5:A:220:G:N2	2.36	0.58
5:A:49:U:O2'	5:A:361:G:N2	2.37	0.58
5:A:486:U:H2'	5:A:487:A:H8	1.68	0.58
12:P:11:ALA:HB3	12:P:14:ARG:HB2	1.84	0.57
5:A:1097:C:H5'	16:B:138:ARG:HD3	1.86	0.57
3:N:100:TRP:OXT	5:A:1186:G:N2	2.36	0.57
5:A:977:A:O2'	5:A:1223:C:N4	2.37	0.57
5:A:344:A:OP2	5:A:345:C:N4	2.37	0.57
3:N:99:SER:O	5:A:1114:C:O2'	2.23	0.57
5:A:491:G:OP1	6:D:147:LYS:NZ	2.38	0.57



Atom-1	Atom-2	Interatomic	Clash
	1100111 2	distance $(Å)$	overlap (A)
4:S:12:LEU:HA	4:S:15:LEU:HB3	1.87	0.57
5:A:517:G:N1	5:A:533:A:OP2	2.35	0.57
5:A:764:C:OP2	5:A:765:G:N2	2.38	0.57
5:A:822:U:H3	5:A:878:A:H61	1.52	0.57
5:A:939:G:O2'	5:A:1375:A:N3	2.37	0.57
5:A:998:C:O2	5:A:1043:G:N2	2.38	0.57
1:C:33:ASP:OD1	3:N:65:GLN:NE2	2.36	0.57
5:A:662:U:O2'	5:A:836:G:OP1	2.22	0.57
5:A:1071:C:H42	5:A:1104:G:H1	1.53	0.57
5:A:108:G:H5'	5:A:109:A:H5"	1.86	0.57
5:A:411:A:OP1	6:D:25:ARG:NH2	2.37	0.57
6:D:149:LYS:NZ	6:D:177:MET:SD	2.77	0.56
7:E:77:ASN:ND2	7:E:100:GLU:OE2	2.38	0.56
5:A:16:A:OP1	7:E:19:ARG:NH2	2.38	0.56
5:A:263:A:OP1	15:T:73:ARG:NH1	2.38	0.56
6:D:10:LEU:HD21	6:D:62:ARG:HD3	1.85	0.56
9:H:6:ILE:HD12	9:H:35:ILE:HD11	1.85	0.56
9:H:83:ARG:NH1	9:H:123:GLU:OE2	2.38	0.56
2:J:8:ILE:HB	2:J:74:VAL:HB	1.88	0.56
6:D:14:GLU:OE2	6:D:55:ARG:NH1	2.38	0.56
14:R:41:SER:HB2	14:R:51:GLN:HG2	1.88	0.56
3:N:12:ARG:NH1	5:A:980:C:O3'	2.39	0.56
5:A:1305:G:N1	5:A:1331:G:N3	2.53	0.56
5:A:570:G:N2	5:A:867:G:O2'	2.38	0.55
5:A:1118:U:H3	5:A:1155:A:H61	1.54	0.55
10:L:86:VAL:HG12	10:L:88:ASP:H	1.71	0.55
4:S:49:ALA:HA	4:S:58:PRO:HA	1.89	0.55
10:L:34:THR:HG22	10:L:35:ARG:HG2	1.87	0.55
11:O:25:GLU:HG3	11:O:76:ARG:HH21	1.72	0.55
5:A:18:C:H42	5:A:917:G:H1	1.53	0.55
6:D:104:MET:HG2	6:D:170:LEU:HD13	1.89	0.55
5:A:1347:G:N2	5:A:1374:A:OP2	2.39	0.55
6:D:25:ARG:HE	6:D:30:LYS:HD2	1.71	0.55
5:A:919:A:O2'	5:A:1080:A:N1	2.39	0.55
5:A:458:U:H3	5:A:474:G:H1	1.54	0.54
5:A:952:U:O2'	5:A:969:A:N1	2.41	0.54
12:P:4:ILE:HG23	12:P:21:VAL:HG22	1.88	0.54
9:H:5:PRO:O	9:H:32:LYS:NZ	2.33	0.54
9:H:14:ARG:NH1	9:H:74:ILE:O	2.41	0.54
6:D:12:ARG:NH1	6:D:31:CYS:O	2.41	0.54
13:Q:19:SER:OG	13:Q:70:LYS:NZ	2.37	0.54



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
5:A:977:A:H8	5:A:1362:A:H61	1.55	0.54
5:A:21:G:H21	5:A:914:A:H62	1.56	0.54
5:A:764:C:N4	5:A:812:G:O6	2.41	0.54
2:J:43:PRO:HG2	2:J:71:LEU:HD12	1.89	0.54
5:A:736:C:OP1	14:R:60:ARG:NH2	2.41	0.54
5:A:1072:G:H1	5:A:1103:C:H42	1.56	0.54
14:R:25:ILE:HB	14:R:66:LEU:HD13	1.90	0.54
5:A:522:C:OP2	10:L:65:TYR:OH	2.26	0.53
5:A:1166:G:N1	5:A:1169:A:OP2	2.40	0.53
5:A:56:U:O4	5:A:357:G:N2	2.42	0.53
5:A:667:G:O2'	11:O:50:HIS:ND1	2.41	0.53
5:A:1098:C:OP1	16:B:142:LYS:NZ	2.41	0.53
1:C:27:GLU:O	1:C:31:ASN:ND2	2.41	0.53
5:A:1316:G:N2	5:A:1319:A:OP2	2.37	0.53
15:T:58:ASP:HA	15:T:61:ALA:HB3	1.90	0.53
5:A:1266:G:O2'	5:A:1269:A:N6	2.41	0.53
5:A:1310:G:H1	5:A:1328:C:H42	1.56	0.53
5:A:1289:A:N1	5:A:1371:G:O2'	2.40	0.53
11:O:81:ILE:HG22	11:O:86:LEU:HD12	1.88	0.53
5:A:62:U:OP1	5:A:385:C:O2'	2.26	0.53
7:E:156:ARG:NH2	9:H:98:LEU:O	2.42	0.53
1:C:96:VAL:HG12	1:C:98:ALA:HB2	1.91	0.53
2:J:87:LEU:HD12	2:J:90:LEU:HD12	1.90	0.53
3:N:9:GLU:OE1	3:N:60:ARG:NH2	2.41	0.52
3:N:63:CYS:HB3	3:N:68:ARG:H	1.73	0.52
5:A:528:C:N4	10:L:45:ASN:OD1	2.41	0.52
5:A:1291:U:H2'	5:A:1292:G:H8	1.74	0.52
5:A:411:A:H2	5:A:430:A:H62	1.57	0.52
4:S:15:LEU:HA	4:S:18:VAL:HG12	1.91	0.52
5:A:67:C:O2'	5:A:171:A:N3	2.43	0.52
5:A:176:C:OP1	15:T:23:ARG:NH1	2.42	0.52
5:A:773:G:H22	5:A:806:C:H42	1.58	0.52
5:A:1075:U:O2'	16:B:173:LYS:NZ	2.42	0.52
9:H:88:LYS:HE3	9:H:119:GLY:HA2	1.91	0.52
5:A:598:U:H2'	5:A:599:C:H6	1.74	0.52
5:A:734:G:N2	14:R:63:TYR:OH	2.42	0.52
5:A:1363:A:O2'	5:A:1365:G:N7	2.39	0.52
5:A:669:G:OP1	11:O:47:LYS:NZ	2.38	0.52
8:F:1:MET:HG2	8:F:67:PRO:HB3	1.91	0.52
4:S:31:ARG:HE	4:S:56:HIS:HB2	1.75	0.52
5:A:962:C:H2'	5:A:963:G:H8	1.75	0.52



	ous puge	Interstomic	Clash
Atom-1	Atom-2	distance $(Å)$	overlap (Å)
5:A:858:G:H3'	5:A:869:G:H1	1.74	0.51
5:A:1241:G:H1	5:A:1296:C:H1'	1.75	0.51
5:A:842:U:O2'	5:A:846:G:N1	2.43	0.51
16:B:11:ALA:HB3	16:B:42:LEU:HD21	1.92	0.51
1:C:153:SER:HB2	1:C:196:GLY:H	1.74	0.51
5:A:854:U:H3'	5:A:871:U:H3	1.76	0.51
5:A:1305:G:O2'	5:A:1332:A:N6	2.44	0.51
7:E:110:MET:HB3	7:E:139:THR:HG21	1.92	0.51
2:J:36:VAL:HA	2:J:76:ILE:HG22	1.93	0.51
5:A:184:G:N2	5:A:194:C:N3	2.58	0.51
5:A:501:C:OP2	10:L:113:ARG:NH2	2.44	0.51
5:A:1130:A:N6	5:A:1144:G:O2'	2.42	0.51
5:A:296:U:H2'	5:A:297:G:H8	1.76	0.51
7:E:93:VAL:HG11	7:E:139:THR:HG22	1.92	0.51
5:A:770:C:H2'	5:A:771:G:H8	1.75	0.50
5:A:1015:G:N2	5:A:1218:C:O2	2.44	0.50
16:B:75:ALA:HA	16:B:78:ALA:HB3	1.93	0.50
5:A:505:G:H2'	5:A:506:G:H8	1.76	0.50
5:A:855:U:OP2	5:A:871:U:N3	2.38	0.50
2:J:24:GLU:O	2:J:28:THR:OG1	2.29	0.50
5:A:618:C:H1'	12:P:14:ARG:HH12	1.77	0.50
11:O:45:HIS:O	11:O:47:LYS:N	2.44	0.50
11:O:53:ARG:O	11:O:57:ARG:N	2.43	0.50
5:A:1249:C:O2	5:A:1288:A:N6	2.43	0.50
1:C:149:LYS:HG3	1:C:168:ARG:HG2	1.93	0.50
5:A:571:U:O4	5:A:865:A:N6	2.42	0.50
4:S:57:VAL:HG23	4:S:74:ALA:HB1	1.94	0.50
5:A:204:G:N1	5:A:465:A:OP1	2.44	0.50
5:A:393:A:H2'	5:A:394:G:H8	1.76	0.50
5:A:826:C:O5'	9:H:12:ARG:NH1	2.45	0.50
5:A:831:A:OP1	16:B:20:ARG:NH1	2.43	0.50
1:C:117:ASP:OD1	1:C:120:THR:OG1	2.29	0.49
5:A:1055:A:N1	5:A:1205:U:O2'	2.45	0.49
5:A:384:G:H2'	5:A:385:C:H6	1.78	0.49
14:R:70:THR:HG23	14:R:73:HIS:H	1.77	0.49
2:J:62:ARG:NH2	5:A:1190:G:N7	2.44	0.49
5:A:986:U:H2'	5:A:987:G:C8	2.48	0.49
5:A:542:G:O3'	6:D:13:ARG:NH2	2.45	0.49
5:A:619:U:N3	6:D:130:ASN:OD1	2.41	0.49
5:A:501:C:H2'	5:A:502:A:C8	2.48	0.49
5:A:1268:G:N3	5:A:1326:U:O2'	2.44	0.49



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
6:D:201:GLU:OE2	7:E:104:ILE:N	2.44	0.49
5:A:448:A:H62	5:A:486:U:H3	1.59	0.49
5:A:1166:G:O2'	5:A:1169:A:N6	2.46	0.49
5:A:408:A:O2'	6:D:153:ARG:NH2	2.46	0.49
3:N:15:LEU:HA	3:N:18:LYS:HB2	1.93	0.48
5:A:730:G:N2	5:A:766:A:OP1	2.41	0.48
5:A:937:A:H2'	5:A:938:A:H8	1.77	0.48
5:A:52:C:H2'	5:A:53:A:H8	1.78	0.48
5:A:940:C:O2	5:A:1343:G:N2	2.30	0.48
5:A:1301:U:O2'	5:A:1303:C:OP2	2.31	0.48
16:B:119:GLN:NE2	16:B:124:THR:O	2.46	0.48
1:C:81:GLU:OE2	1:C:85:LYS:NZ	2.38	0.48
5:A:613:C:OP2	6:D:80:ARG:NH1	2.46	0.48
6:D:128:VAL:HG22	6:D:145:ARG:HD3	1.96	0.48
5:A:427:U:H3'	5:A:428:G:H2'	1.95	0.48
5:A:866:C:C4	5:A:867:G:H1'	2.49	0.48
2:J:64:GLN:HG3	3:N:98:ALA:HB3	1.95	0.48
7:E:14:LEU:HA	7:E:36:THR:HG22	1.96	0.48
5:A:662:U:H2'	5:A:663:A:C8	2.48	0.48
5:A:718:A:N1	14:R:62:ARG:NH2	2.57	0.48
5:A:994:A:H61	5:A:1046:A:H2'	1.78	0.48
5:A:897:C:H42	5:A:902:G:H1	1.62	0.48
16:B:128:LEU:HD12	16:B:132:GLU:HG2	1.96	0.48
4:S:35:ARG:NH2	5:A:1321:U:O2	2.47	0.48
5:A:209:U:H5"	5:A:210:C:H5	1.79	0.47
5:A:615:G:H2'	5:A:616:G:H8	1.79	0.47
5:A:823:C:N4	5:A:824:G:O6	2.47	0.47
8:F:11:HIS:HE1	8:F:13:ASP:HB2	1.79	0.47
5:A:390:U:O5'	12:P:28:ARG:NH1	2.47	0.47
5:A:986:U:H2'	5:A:987:G:H8	1.79	0.47
5:A:58:C:O2'	5:A:388:G:N7	2.47	0.47
5:A:59:A:H3'	5:A:331:G:H22	1.78	0.47
7:E:152:VAL:HG21	9:H:98:LEU:HD23	1.96	0.47
5:A:157:U:H3	5:A:164:G:H1	1.63	0.47
5:A:1185:G:H2'	5:A:1186:G:H8	1.79	0.47
1:C:9:ILE:HG23	1:C:10:ARG:HG3	1.94	0.47
4:S:77:ARG:NH1	5:A:1223:C:OP1	2.47	0.47
5:A:826:C:H4'	9:H:12:ARG:HG2	1.95	0.47
5:A:391:G:OP1	12:P:8:ARG:NH1	2.47	0.47
5:A:1046:A:N6	5:A:1212:U:OP2	2.48	0.47
5:A:1126:U:N3	5:A:1280:A:OP1	2.42	0.47



Interatomic Clash				
Atom-1	Atom-2	distance $(Å)$	overlap (Å)	
16:B:65:LYS:H	16:B:158:ASP:HB2	1.79	0.47	
5:A:642:A:C5	9:H:106:SER:HA	2.50	0.47	
5:A:1100:C:C4	5:A:1102:A:H5'	2.50	0.47	
5:A:1181:G:H1'	5:A:1182:G:C4	2.50	0.47	
5:A:1241:G:H2'	5:A:1242:G:C8	2.50	0.47	
5:A:1376:U:H2'	5:A:1377:A:H8	1.80	0.47	
6:D:84:ASN:HB3	6:D:87:GLU:HB3	1.96	0.47	
5:A:96:U:H2'	5:A:97:G:H8	1.80	0.47	
5:A:243:A:N6	5:A:283:U:O4	2.47	0.47	
5:A:1209:C:O2	5:A:1214:C:N4	2.38	0.47	
3:N:81:ILE:HD12	3:N:82:LYS:HG2	1.97	0.47	
5:A:121:U:N3	5:A:235:C:OP2	2.48	0.47	
5:A:1355:G:O6	5:A:1366:C:N4	2.48	0.47	
7:E:73:VAL:HG11	7:E:143:LEU:HB3	1.96	0.47	
7:E:102:THR:O	7:E:121:ASN:ND2	2.41	0.47	
5:A:462:G:H22	5:A:470:C:H42	1.64	0.47	
13:Q:4:ILE:HG13	13:Q:5:ARG:H	1.80	0.47	
5:A:130:A:H5'	13:Q:64:ARG:HD3	1.97	0.46	
2:J:92:LEU:HA	2:J:93:ALA:HA	1.56	0.46	
5:A:1238:A:H5'	5:A:1336:C:H41	1.80	0.46	
6:D:8:LEU:HD21	6:D:21:LYS:HB2	1.97	0.46	
7:E:82:HIS:HE2	7:E:147:ASN:H	1.61	0.46	
11:O:44:GLU:HA	11:O:46:LYS:HE3	1.97	0.46	
14:R:25:ILE:HD12	14:R:66:LEU:HD22	1.97	0.46	
2:J:7:ARG:HB2	2:J:101:SER:HB3	1.97	0.46	
5:A:162:A:C5	5:A:163:C:H1'	2.50	0.46	
5:A:1158:C:H5"	16:B:131:LYS:HD3	1.97	0.46	
5:A:1243:C:N4	5:A:1244:G:O6	2.48	0.46	
5:A:104:G:O6	15:T:8:LYS:NZ	2.42	0.46	
5:A:1297:G:N2	5:A:1298:U:O4	2.47	0.46	
8:F:32:ALA:HB2	8:F:70:VAL:HG21	1.98	0.46	
5:A:373:A:H2'	5:A:481:G:H21	1.81	0.46	
10:L:34:THR:O	10:L:35:ARG:NE	2.44	0.46	
1:C:152:VAL:H	1:C:165:GLU:HB2	1.80	0.46	
4:S:17:LYS:HE3	4:S:32:THR:HA	1.96	0.46	
5:A:343:U:O2'	5:A:346:G:O6	2.24	0.46	
5:A:579:A:O3'	11:O:53:ARG:NH2	2.49	0.46	
5:A:868:C:H3'	5:A:869:G:H8	1.81	0.46	
9:H:26:MET:SD	9:H:26:MET:N	2.89	0.46	
5:A:186:C:O2'	15:T:75:LYS:O	2.32	0.46	
5:A:1305:G:O2'	5:A:1306:A:O4'	2.29	0.46	



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
16:B:57:ASN:O	16:B:61:SER:N	2.48	0.46
1:C:19:SER:HB2	1:C:39:ARG:HH22	1.80	0.46
1:C:39:ARG:HH11	3:N:91:GLU:HG2	1.81	0.46
13:Q:57:VAL:H	13:Q:79:GLU:HB3	1.81	0.46
16:B:130:LYS:HA	16:B:133:ALA:HB3	1.98	0.46
4:S:52:ASN:HB2	4:S:76:THR:HA	1.98	0.45
5:A:96:U:H2'	5:A:97:G:C8	2.51	0.45
5:A:264:C:H4'	13:Q:64:ARG:HD2	1.97	0.45
15:T:43:LYS:NZ	15:T:82:ILE:O	2.40	0.45
5:A:651:C:N4	5:A:752:G:O2'	2.49	0.45
5:A:1185:G:H2'	5:A:1186:G:C8	2.51	0.45
6:D:137:SER:OG	6:D:140:ASP:OD2	2.35	0.45
16:B:86:CYS:O	16:B:88:GLN:NE2	2.50	0.45
1:C:20:THR:HA	3:N:93:PRO:HB3	1.98	0.45
5:A:410:G:H5"	6:D:25:ARG:HH22	1.81	0.45
5:A:438:U:O2'	5:A:493:A:N6	2.47	0.45
5:A:563:A:H61	5:A:884:U:H3	1.65	0.45
5:A:592:G:H1	5:A:647:C:H42	1.65	0.45
5:A:842:U:H3'	5:A:843:U:H4'	1.98	0.45
13:Q:53:GLY:N	13:Q:56:ASP:OD2	2.39	0.45
4:S:51:HIS:ND1	5:A:1220:G:O2'	2.39	0.45
6:D:169:TRP:CD2	6:D:185:PRO:HB3	2.52	0.45
9:H:29:SER:H	9:H:32:LYS:HD2	1.82	0.45
10:L:23:LEU:HB3	10:L:25:ALA:H	1.82	0.45
15:T:57:VAL:HG13	15:T:71:ALA:HB1	1.99	0.45
5:A:673:A:N3	5:A:674:G:N2	2.65	0.45
5:A:925:G:N2	5:A:927:G:O4'	2.50	0.45
5:A:1094:G:O2'	5:A:1108:G:N2	2.46	0.45
4:S:36:ARG:HG2	5:A:1320:C:H41	1.81	0.45
5:A:236:A:H2'	5:A:237:G:H8	1.82	0.45
5:A:671:G:O2'	8:F:79:ARG:NH1	2.50	0.45
1:C:160:GLU:OE2	5:A:1206:G:N2	2.51	0.44
5:A:1162:C:H2'	5:A:1163:A:C8	2.52	0.44
5:A:539:A:H2'	5:A:540:G:H8	1.83	0.44
5:A:623:C:H2'	5:A:624:C:H6	1.83	0.44
5:A:1004:A:OP1	5:A:1024:G:N1	2.50	0.44
16:B:118:THR:HA	16:B:121:GLN:HE21	1.81	0.44
1:C:186:SER:OG	1:C:187:GLU:N	2.49	0.44
3:N:50:LEU:HA	4:S:12:LEU:HD22	1.99	0.44
6:D:189:ASP:OD1	6:D:189:ASP:N	2.48	0.44
5:A:995:C:H2'	5:A:996:A:H8	1.82	0.44



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
3:N:63:CYS:SG	3:N:64:ARG:N	2.90	0.44
5:A:712:A:C6	5:A:713:G:H1'	2.53	0.44
5:A:825:A:H2	9:H:11:THR:HG21	1.82	0.44
5:A:881:G:OP1	10:L:8:ARG:NH1	2.46	0.44
5:A:1328:C:H2'	5:A:1329:A:C8	2.53	0.44
7:E:156:ARG:O	9:H:63:LYS:NZ	2.50	0.44
5:A:455:G:H1	5:A:477:C:H42	1.65	0.44
5:A:1020:G:H2'	5:A:1021:A:C8	2.53	0.44
5:A:1278:G:H1'	5:A:1279:G:H21	1.80	0.44
5:A:1073:U:H3	5:A:1102:A:H61	1.65	0.44
5:A:833:G:H1	5:A:853:C:H42	1.66	0.43
8:F:26:THR:HG23	8:F:29:ILE:HD12	1.99	0.43
5:A:1099:G:N1	5:A:1100:C:O2	2.52	0.43
5:A:1250:A:H61	5:A:1354:U:H4'	1.82	0.43
5:A:31:G:H8	5:A:31:G:H5"	1.83	0.43
5:A:360:G:H2'	5:A:361:G:C8	2.53	0.43
5:A:539:A:H2'	5:A:540:G:C8	2.52	0.43
5:A:974:A:H4'	5:A:975:A:H3'	1.99	0.43
5:A:141:G:H2'	5:A:142:G:H8	1.83	0.43
5:A:741:G:H2'	5:A:742:G:H8	1.83	0.43
5:A:1305:G:H1	5:A:1331:G:H1'	1.84	0.43
6:D:24:VAL:HG12	6:D:25:ARG:H	1.82	0.43
16:B:199:ILE:HG22	16:B:201:GLY:H	1.84	0.43
5:A:1125:U:H2'	5:A:1126:U:H2'	1.99	0.43
10:L:54:VAL:N	10:L:62:VAL:O	2.46	0.43
15:T:6:ALA:O	15:T:10:ALA:N	2.42	0.43
5:A:202:G:H21	5:A:465:A:H61	1.67	0.43
6:D:32:LYS:HB3	6:D:35:GLN:HB2	2.01	0.43
10:L:82:ARG:HB3	10:L:95:HIS:HB3	1.99	0.43
4:S:22:VAL:HG22	4:S:46:LEU:HG	2.01	0.43
7:E:79:THR:HB	7:E:121:ASN:HB2	2.01	0.43
5:A:105:G:O6	15:T:8:LYS:NZ	2.37	0.43
5:A:392:C:H4'	12:P:13:LYS:HE3	2.01	0.43
5:A:404:G:O2'	5:A:439:U:N3	2.43	0.43
5:A:865:A:N3	5:A:918:A:O2'	2.49	0.43
5:A:1037:C:H2'	5:A:1038:C:H6	1.84	0.43
12:P:20:VAL:HG13	12:P:32:PHE:HB3	2.00	0.43
5:A:1070:U:H2'	5:A:1071:C:H6	1.83	0.43
10:L:55:ARG:HA	10:L:61:GLU:HG2	2.01	0.43
5:A:824:G:H2'	5:A:825:A:C8	2.54	0.42
2:J:7:ARG:NH2	2:J:102:LEU:O	2.51	0.42



	A 4	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
3:N:2:LYS:HD3	5:A:1049:U:H2'	2.02	0.42
5:A:536:C:H2'	5:A:537:G:H8	1.84	0.42
5:A:868:C:H3'	5:A:869:G:C8	2.54	0.42
1:C:70:ALA:HA	1:C:104:GLU:HG3	2.01	0.42
3:N:81:ILE:H	3:N:81:ILE:HG13	1.56	0.42
5:A:541:G:H2'	5:A:542:G:H8	1.84	0.42
5:A:74:A:H2'	5:A:75:G:C8	2.54	0.42
5:A:200:G:O2'	5:A:381:C:N4	2.53	0.42
5:A:764:C:H4'	11:O:49:HIS:HB3	2.00	0.42
5:A:891:U:H2'	5:A:892:A:H8	1.83	0.42
5:A:1110:A:N7	5:A:1111:A:N6	2.68	0.42
3:N:5:MET:O	3:N:9:GLU:N	2.53	0.42
2:J:15:HIS:CD2	5:A:1152:A:H4'	2.55	0.42
5:A:588:G:H1	5:A:651:C:H42	1.68	0.42
6:D:9:LYS:HE3	6:D:9:LYS:HB2	1.80	0.42
8:F:25:TYR:HB3	8:F:74:LEU:HD11	2.01	0.42
16:B:33:ALA:HA	16:B:38:HIS:HA	2.01	0.42
5:A:1096:C:H2'	5:A:1097:C:C6	2.53	0.42
14:R:58:ILE:HA	14:R:61:ALA:HB2	2.01	0.42
1:C:15:LYS:HD2	1:C:16:PRO:HD2	2.02	0.42
11:O:39:GLN:O	11:O:43:ALA:N	2.53	0.42
15:T:23:ARG:HB3	15:T:60:GLN:HE22	1.84	0.42
2:J:40:ILE:HD12	2:J:42:LEU:HD11	2.02	0.41
5:A:229:U:H2'	5:A:230:G:H8	1.84	0.41
5:A:1144:G:H21	5:A:1146:A:H62	1.68	0.41
1:C:39:ARG:HG3	1:C:54:ILE:HD12	2.02	0.41
5:A:296:U:H2'	5:A:297:G:C8	2.54	0.41
5:A:352:C:H42	5:A:357:G:H22	1.68	0.41
5:A:639:G:H2'	5:A:640:A:H8	1.85	0.41
5:A:1040:U:H2'	5:A:1041:G:C8	2.55	0.41
7:E:20:VAL:O	7:E:31:SER:N	2.54	0.41
5:A:9:G:H5'	7:E:107:GLY:HA3	2.02	0.41
5:A:362:G:H5"	10:L:30:ARG:HH12	1.85	0.41
5:A:579:A:N3	5:A:763:G:N2	2.69	0.41
5:A:1261:A:N6	5:A:1274:A:O2'	2.45	0.41
12:P:23:ASP:OD1	12:P:24:SER:N	2.53	0.41
1:C:10:ARG:NH2	1:C:174:LEU:O	2.41	0.41
3:N:52:ARG:NH1	5:A:1220:G:OP2	2.52	0.41
5:A:10:A:H2'	5:A:11:G:H8	1.85	0.41
5:A:1250:A:H2	5:A:1353:G:H21	1.67	0.41
4:S:77:ARG:NH2	5:A:1322:C:OP1	2.53	0.41



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
5:A:222:C:H2'	5:A:223:A:C8	2.55	0.41
5:A:370:C:H42	5:A:391:G:H1	1.69	0.41
5:A:398:U:H2'	5:A:399:G:H8	1.85	0.41
5:A:579:A:O2'	11:O:53:ARG:NH2	2.53	0.41
7:E:35:LEU:HD11	7:E:133:ILE:HG12	2.03	0.41
1:C:107:LYS:HB3	1:C:110:LEU:HD12	2.01	0.41
1:C:137:VAL:HG13	1:C:148:ILE:HG21	2.03	0.41
1:C:149:LYS:HE3	1:C:168:ARG:HD3	2.02	0.41
5:A:114:U:H1'	5:A:353:A:H1'	2.02	0.41
11:O:53:ARG:HA	11:O:56:LEU:HB3	2.03	0.41
5:A:1237:C:O2	5:A:1334:G:O2'	2.37	0.41
7:E:110:MET:HA	7:E:113:VAL:HG22	2.03	0.41
9:H:51:GLU:O	9:H:57:GLU:N	2.48	0.41
1:C:63:ILE:HG23	1:C:96:VAL:HG11	2.03	0.41
5:A:62:U:O2'	5:A:379:C:O2	2.29	0.41
5:A:451:A:H2	5:A:480:U:C2	2.38	0.41
5:A:829:G:H2'	5:A:830:G:H8	1.86	0.41
5:A:1254:A:O2'	5:A:1356:G:OP1	2.39	0.41
9:H:83:ARG:HB2	13:Q:36:PHE:HE2	1.86	0.41
16:B:182:VAL:HB	16:B:195:VAL:HG13	2.03	0.41
5:A:81:A:N7	5:A:83:C:N4	2.69	0.41
5:A:908:A:H2'	5:A:909:A:C8	2.56	0.41
5:A:1000:A:N3	5:A:1041:G:N1	2.68	0.41
5:A:1072:G:H22	5:A:1104:G:H1'	1.85	0.41
6:D:92:LEU:O	6:D:135:GLN:NE2	2.54	0.41
5:A:60:A:N7	5:A:108:G:O2'	2.54	0.41
15:T:28:ARG:HA	15:T:31:ILE:HD12	2.02	0.41
1:C:145:ALA:O	1:C:147:GLY:N	2.54	0.40
5:A:219:U:H2'	5:A:220:G:C8	2.55	0.40
14:R:62:ARG:HD2	14:R:69:TYR:HA	2.03	0.40
5:A:398:U:H2'	5:A:399:G:C8	2.56	0.40
5:A:878:A:P	9:H:79:ARG:HH11	2.44	0.40
7:E:81:GLN:HG2	7:E:82:HIS:HD2	1.86	0.40
8:F:11:HIS:CE1	8:F:13:ASP:HB2	2.56	0.40
1:C:13:ILE:HG22	1:C:14:VAL:H	1.85	0.40
2:J:11:LYS:HE3	2:J:71:LEU:HD21	2.03	0.40
12:P:28:ARG:HG2	12:P:29:ASN:H	1.85	0.40
2:J:11:LYS:HG2	2:J:71:LEU:HD23	2.02	0.40
5:A:331:G:O3'	15:T:2:ASN:HB3	2.21	0.40
5:A:572:A:H5"	5:A:917:G:H4'	2.04	0.40
5:A:894:G:H1	5:A:905:U:H3	1.68	0.40



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1270:G:H2'	5:A:1271:A:C8	2.56	0.40
7:E:37:VAL:HA	7:E:47:PHE:HA	2.03	0.40
15:T:53:MET:HA	15:T:56:ILE:HD12	2.03	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	С	204/206~(99%)	178 (87%)	26 (13%)	0	100	100
2	J	96/98~(98%)	76~(79%)	20 (21%)	0	100	100
3	Ν	92/99~(93%)	79~(86%)	13 (14%)	0	100	100
4	S	72/74~(97%)	67~(93%)	5 (7%)	0	100	100
6	D	203/205~(99%)	179 (88%)	24 (12%)	0	100	100
7	Е	147/149~(99%)	126 (86%)	21 (14%)	0	100	100
8	F	73/93~(78%)	68~(93%)	5 (7%)	0	100	100
9	Н	127/129~(98%)	114 (90%)	13 (10%)	0	100	100
10	L	121/123~(98%)	88 (73%)	33 (27%)	0	100	100
11	Ο	84/86~(98%)	75~(89%)	8 (10%)	1 (1%)	13	50
12	Р	77/79~(98%)	61 (79%)	16 (21%)	0	100	100
13	Q	77/79~(98%)	68 (88%)	9 (12%)	0	100	100
14	R	45/52~(86%)	45 (100%)	0	0	100	100
15	Т	83/85~(98%)	76 (92%)	7 (8%)	0	100	100
16	В	215/217~(99%)	181 (84%)	34 (16%)	0	100	100
All	All	1716/1774 (97%)	1481 (86%)	234 (14%)	1 (0%)	54	83

All (1) Ramachandran outliers are listed below:



Mol	Chain	Res	Type
11	0	46	LYS

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	Percer	ntiles
1	\mathbf{C}	170/170~(100%)	169~(99%)	1 (1%)	86	92
2	J	86/86~(100%)	86 (100%)	0	100	100
3	Ν	79/82~(96%)	77~(98%)	2(2%)	47	70
4	S	65/65~(100%)	64 (98%)	1 (2%)	65	81
6	D	172/172~(100%)	169~(98%)	3(2%)	60	78
7	Ε	111/112~(99%)	111 (100%)	0	100	100
8	F	69/82~(84%)	69 (100%)	0	100	100
9	Н	104/104~(100%)	103~(99%)	1 (1%)	76	86
10	L	103/103~(100%)	103 (100%)	0	100	100
11	Ο	74/74~(100%)	73~(99%)	1 (1%)	67	81
12	Р	64/64~(100%)	61~(95%)	3~(5%)	26	56
13	Q	73/73~(100%)	71~(97%)	2(3%)	44	69
14	R	43/45~(96%)	43 (100%)	0	100	100
15	Т	64/65~(98%)	64 (100%)	0	100	100
16	В	179/179~(100%)	178 (99%)	1 (1%)	86	92
All	All	1456/1476~(99%)	1441 (99%)	15 (1%)	77	86

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	С	184	ASN
3	Ν	27	LYS
3	Ν	60	ARG
4	S	28	LYS
6	D	151	GLN
6	D	176	LYS



COULL	Continueu from previous page				
Mol	Chain	\mathbf{Res}	Type		
6	D	177	MET		
9	Н	93	LYS		
11	0	53	ARG		
12	Р	5	ARG		
12	Р	28	ARG		
12	Р	51	ARG		
13	Q	$\overline{76}$	ARG		
13	Q	80	LYS		
16	B	224	ARG		

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	С	24	ASN
15	Т	74	HIS
16	В	119	GLN
16	В	121	GLN
16	В	202	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
5	А	1338/1542~(86%)	471 (35%)	15~(1%)

All (471) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
5	А	7	А
5	А	9	G
5	А	14	U
5	А	16	А
5	А	21	G
5	А	22	G
5	А	30	U
5	А	31	G
5	А	32	А
5	А	39	G
5	А	47	С
5	А	48	С
5	А	50	А



Mol	Chain	Res	Type
5	А	51	А
5	А	52	С
5	А	58	С
5	А	60	А
5	А	61	G
5	А	66	А
5	А	69	G
5	А	70	U
5	А	71	А
5	А	72	А
5	А	75	G
5	А	76	G
5	А	83	С
5	A	84	U
5	A	85	U
5	A	86	G
5	А	87	С
5	А	88	U
5	А	89	U
5	А	95	С
5	А	108	G
5	А	110	С
5	А	112	G
5	А	119	А
5	А	120	А
5	А	121	U
5	А	125	U
5	А	130	А
5	A	131	A
5	A	134	G
5	A	135	С
5	A	136	С
5	А	144	G
5	A	145	G
5	A	151	А
5	A	163	С
5	A	173	U
5	A	174	A
5	A	175	С
5	A	177	G
5	A	182	A
5	A	196	A



Mol	Chain	Res	Type
5	А	197	А
5	А	200	G
5	А	202	G
5	А	204	G
5	А	205	А
5	А	208	U
5	А	209	U
5	А	210	C
5	А	211	G
5	А	212	G
5	А	213	G
5	А	214	С
5	А	220	G
5	A	226	G
5	А	228	А
5	A	239	U
5	А	240	G
5	А	243	А
5	А	244	U
5	А	245	U
5	А	247	G
5	А	250	А
5	А	251	G
5	А	257	G
5	А	258	G
5	А	265	G
5	А	266	G
5	А	267	С
5	А	279	A
5	A	283	U
5	А	289	G
5	A	290	C
5	А	299	G
5	A	300	A
5	А	303	A
5	A	305	G
5	А	306	A
5	A	312	С
5	А	315	A
5	A	316	С
5	A	319	G
5	А	321	A



Mol	Chain	Res	Type
5	А	328	С
5	А	329	А
5	А	332	G
5	А	336	А
5	А	337	G
5	А	339	С
5	А	345	С
5	А	347	G
5	А	348	G
5	А	350	G
5	А	351	G
5	А	352	С
5	А	353	A
5	A	354	G
5	А	362	G
5	А	367	U
5	А	368	U
5	А	369	G
5	А	372	С
5	А	373	А
5	А	375	U
5	А	380	G
5	А	381	С
5	А	382	А
5	А	397	А
5	А	398	U
5	А	406	G
5	А	407	U
5	А	408	A
5	А	411	A
5	А	412	A
5	А	413	G
5	А	414	A
5	А	415	A
5	А	417	G
5	А	421	U
5	А	422	С
5	А	423	G
5	А	424	G
5	А	429	U
5	А	435	A
5	А	439	U



Mol	Chain	Res	Type
5	А	448	А
5	А	451	А
5	А	455	G
5	А	457	G
5	А	460	А
5	А	461	А
5	А	462	G
5	А	463	U
5	А	466	А
5	А	467	U
5	А	468	А
5	А	469	С
5	А	470	С
5	А	479	U
5	А	483	С
5	А	484	G
5	А	485	U
5	А	494	G
5	А	497	G
5	А	500	G
5	А	505	G
5	А	508	U
5	А	509	А
5	А	510	А
5	А	511	С
5	А	517	G
5	А	518	С
5	А	519	С
5	А	520	A
5	А	521	G
5	A	527	G
5	А	531	U
5	А	532	A
5	А	533	A
5	А	536	С
5	A	540	G
5	А	547	A
5	А	548	G
5	A	550	G
5	A	556	С
5	A	559	A
5	А	562	U



Mol	Chain	Res	Type
5	А	564	С
5	А	567	G
5	А	572	A
5	А	573	А
5	А	576	С
5	А	577	G
5	А	580	С
5	А	581	G
5	А	582	С
5	А	587	G
5	А	588	G
5	А	602	А
5	А	604	G
5	А	606	G
5	А	607	A
5	А	610	U
5	А	620	С
5	А	623	С
5	А	633	G
5	А	641	U
5	А	642	A
5	А	646	G
5	А	652	U
5	А	653	U
5	А	654	G
5	А	661	G
5	А	663	А
5	А	665	А
5	А	666	G
5	А	667	G
5	А	671	G
5	A	673	A
5	А	674	G
5	A	675	A
5	А	677	U
5	A	678	U
5	A	713	G
5	А	714	G
5	A	717	U
5	A	718	A
5	A	721	G
5	А	722	G



Mol	Chain	Res	Type
5	А	731	G
5	А	733	G
5	А	736	С
5	А	737	С
5	А	745	G
5	А	748	G
5	А	753	А
5	А	755	G
5	А	760	G
5	А	761	G
5	А	763	G
5	А	765	G
5	А	768	А
5	А	777	А
5	А	778	G
5	А	779	С
5	А	780	А
5	А	802	А
5	А	803	G
5	А	804	U
5	А	805	С
5	А	812	G
5	А	815	А
5	А	816	А
5	А	817	С
5	А	818	G
5	А	819	А
5	А	820	U
5	А	821	G
5	A	825	А
5	A	828	U
5	A	829	G
5	A	832	G
5	A	835	U
5	A	837	U
5	A	838	G
5	A	841	С
5	А	843	U
5	A	844	G
5	А	846	G
5	А	849	G
5	A	851	G



Mol	Chain	Res	Type
5	А	853	С
5	А	857	С
5	А	858	G
5	А	865	А
5	А	867	G
5	А	873	А
5	А	876	С
5	А	885	G
5	А	890	G
5	А	895	G
5	А	900	А
5	А	901	А
5	А	914	А
5	А	918	А
5	А	921	U
5	А	922	G
5	А	926	G
5	А	927	G
5	А	930	С
5	А	931	С
5	А	934	С
5	А	942	G
5	А	945	G
5	А	948	С
5	А	953	G
5	А	954	G
5	А	955	U
5	А	958	А
5	А	960	U
5	A	961	U
5	A	962	C
5	А	963	G
5	А	966	G
5	A	968	A
5	А	969	А
5	А	971	G
5	А	972	С
5	A	973	G
5	A	974	А
5	А	975	А
5	A	976	G
5	А	977	А



Mol	Chain	Res	Type
5	А	982	U
5	А	984	С
5	А	986	U
5	А	987	G
5	А	991	U
5	А	992	U
5	А	993	G
5	А	999	С
5	А	1004	А
5	А	1005	А
5	А	1010	U
5	А	1016	А
5	А	1020	G
5	А	1025	U
5	А	1026	G
5	А	1030	U
5	А	1032	G
5	А	1033	G
5	А	1034	G
5	А	1036	А
5	А	1037	С
5	А	1044	А
5	А	1045	С
5	А	1049	U
5	А	1052	U
5	А	1054	С
5	А	1055	А
5	А	1063	С
5	A	1064	G
5	A	1065	U
5	A	1066	С
5	A	1067	A
5	A	1070	U
5	A	1072	G
5	A	1077	G
5	A	1079	G
5	A	1080	A
5	A	1081	A
5	A	1085	U
5	A	1089	G
5	A	1091	U
5	A	1094	G



Mol	Chain	Res	Type
5	А	1095	U
5	А	1098	С
5	А	1100	С
5	А	1101	А
5	А	1102	А
5	А	1105	А
5	А	1111	А
5	А	1112	С
5	А	1118	U
5	А	1119	С
5	А	1124	G
5	А	1125	U
5	А	1129	С
5	A	1133	G
5	А	1136	С
5	А	1137	С
5	А	1138	G
5	А	1139	G
5	А	1143	G
5	А	1145	А
5	А	1146	А
5	А	1152	А
5	А	1155	А
5	А	1157	А
5	А	1159	U
5	А	1160	G
5	А	1161	С
5	А	1168	U
5	А	1179	А
5	А	1181	G
5	A	1183	U
5	A	1184	G
5	A	1191	A
5	A	1193	G
5	A	1195	С
5	A	1197	А
5	А	1199	U
5	A	1200	С
5	A	1201	A
5	А	1202	U
5	A	1207	G
5	А	1209	С



Mol	Chain	Res	Type
5	А	1210	С
5	А	1212	U
5	А	1213	А
5	А	1214	С
5	А	1215	G
5	А	1222	G
5	А	1224	U
5	А	1225	А
5	А	1226	С
5	А	1229	А
5	А	1230	С
5	А	1231	G
5	А	1236	А
5	А	1239	А
5	А	1240	U
5	А	1242	G
5	А	1243	С
5	А	1244	G
5	А	1246	А
5	А	1247	U
5	А	1248	А
5	А	1249	С
5	А	1253	G
5	А	1256	А
5	А	1257	А
5	А	1258	G
5	А	1260	G
5	А	1263	С
5	А	1265	С
5	А	1269	А
5	А	1270	G
5	A	1272	G
5	А	1274	А
5	A	1278	G
5	А	1280	А
5	A	1281	С
5	А	1285	A
5	A	1286	U
5	A	1290	G
5	A	1294	G
5	А	1296	С
5	A	1298	U



Mol	Chain	Res	Type
5	А	1300	G
5	А	1301	U
5	А	1302	С
5	А	1304	G
5	А	1305	G
5	А	1309	G
5	А	1312	G
5	А	1313	U
5	А	1315	U
5	А	1316	G
5	А	1318	A
5	А	1319	А
5	А	1320	С
5	А	1322	С
5	А	1323	G
5	А	1324	A
5	А	1331	G
5	А	1332	A
5	А	1336	С
5	А	1337	G
5	А	1340	A
5	А	1347	G
5	А	1348	U
5	А	1350	А
5	А	1355	G
5	А	1362	А
5	А	1363	А
5	А	1364	U
5	А	1365	G
5	А	1368	A
5	А	1369	С
5	А	1378	С
5	А	1380	U
5	А	1381	U
5	А	1392	G
5	А	1394	A
5	А	1395	С
5	А	1396	A

Continued from previous page...

All (15) RNA pucker outliers are listed below: Continued on next page...



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Continued fro	<i>m</i> previous	page

Type

Mol | Chain | Res

Mol	Chain	\mathbf{Res}	Type
5	А	51	А
5	А	238	А
5	А	243	А
5	А	328	С
5	А	372	С
5	А	428	G
5	А	484	G
5	А	913	А
5	А	929	G
5	А	930	С
5	А	1065	U
5	А	1101	А
5	А	1201	А
5	А	1213	А
5	А	1300	G

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 1 ligands modelled in this entry, 1 is 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)

There are no chain breaks in this entry.



6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-0482. 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: 152

Y Index: 152



Z Index: 152

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: 122

Y Index: 167

Z Index: 149

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 5.18. 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 332 nm^3 ; this corresponds to an approximate mass of 300 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 0.263 ${\rm \AA^{-1}}$



8 Fourier-Shell correlation (i)

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



9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-0482 and PDB model 6NQB. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay (i)



The images above show the 3D surface view of the map at the recommended contour level 5.18 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 (5.18).



9.4 Atom inclusion (i)



At the recommended contour level, 73% of all backbone atoms, 71% 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 (5.18) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score	
All	0.7080	0.3320	
А	0.7950	0.3320	
В	0.1660	0.2570	— 10
С	0.4450	0.3340	
D	0.6980	0.3840	
Е	0.6940	0.3880	
F	0.3860	0.2530	
Н	0.7020	0.3730	
J	0.2560	0.2670	
L	0.7690	0.4250	
N	0.2760	0.2540	
0	0.6820	0.3300	0.0
Р	0.8170	0.4350	<0.0
Q	0.7650	0.4330	
R	0.4200	0.2920]
S	0.1790	0.1500	
Т	0.7000	0.3540	

