

Full wwPDB X-ray Structure Validation Report (i)

Oct 26, 2022 – 09:13 pm BST

:	2Y9H
:	Structure A of CRISPR endoribonuclease Cse3 bound to 19 nt RNA
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:	2011-02-14
:	2.50 Å(reported)
	::

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp 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:

MolProbity		4 02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.31.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 2.50 Å.

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



Metric	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R _{free}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)
RNA backbone	3102	1008 (2.84-2.16)

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

Mol	Chain	Length	Quality of chair	1	
1	А	215	4% 61%	38%	
1	С	215	3% 64%	33%	••
1	Е	215	4% 54%	44%	•
1	G	215	^{2%} 66%	26%	• 7%



Mol	Chain	Length	Quality of chain				
1	Ι	215	4%	6	26%	•	9%
1	Κ	215	4% 59%		29%	• 1	1%
1	М	215	18%		31%	1	0%
1	Ο	215	26%	9%	13%	18%	
2	В	19	5% 16%	58%		26%	
2	D	19	32%	47%		16%	5%
2	F	19	26%	53%		21%	
2	Н	19	37%	37%		21%	5%
2	J	19	5% 37%	42%		16%	5%
2	L	19	37%	37%		21%	5%
2	Ν	19	37%	53%		5%	5%
2	Р	19	58%	63%		21%	5%



2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 15663 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
1	Δ	212	Total C N O S	0	0	0
1	Л	213	1685 1074 319 290 2	0	0	0
1	C	911	Total C N O S	0	0	0
	U	211	$1676 \ 1069 \ 317 \ 288 \ 2$	0	0	0
1	F	911	Total C N O S	0	0	0
		211	1668 1064 316 286 2	0	0	0
1	C	100	Total C N O S	0	0	0
	G	199	$1587 \ 1017 \ 300 \ 268 \ 2$	0	0	0
1	T	105	Total C N O S	0	0	0
1	I	150	1545 992 289 262 2	0	0	0
1	K	101	Total C N O S	0	0	0
1	Γ	191	1519 975 282 260 2	0	0	0
1	М	103	Total C N O S	0	0	0
1	111	195	1528 982 284 260 2	0	0	0
1	0	177	Total C N O	0	0	0
			908 554 177 177	U U	0	

• Molecule 1 is a protein called CSE3.

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	-3	GLY	-	expression tag	UNP Q53WG9
А	-2	THR	-	expression tag	UNP Q53WG9
А	-1	GLY	-	expression tag	UNP Q53WG9
А	0	ALA	-	expression tag	UNP Q53WG9
С	-3	GLY	-	expression tag	UNP Q53WG9
С	-2	THR	-	expression tag	UNP Q53WG9
С	-1	GLY	-	expression tag	UNP Q53WG9
С	0	ALA	-	expression tag	UNP Q53WG9
Е	-3	GLY	-	expression tag	UNP Q53WG9
E	-2	THR	-	expression tag	UNP Q53WG9
Е	-1	GLY	-	expression tag	UNP Q53WG9
Е	0	ALA	-	expression tag	UNP Q53WG9
G	-3	GLY	-	expression tag	UNP Q53WG9



Chain	Residue	Modelled	Actual	Comment	Reference
G	-2	THR	-	expression tag	UNP Q53WG9
G	-1	GLY	-	expression tag	UNP Q53WG9
G	0	ALA	-	expression tag	UNP Q53WG9
Ι	-3	GLY	-	expression tag	UNP Q53WG9
Ι	-2	THR	-	expression tag	UNP Q53WG9
Ι	-1	GLY	-	expression tag	UNP Q53WG9
Ι	0	ALA	-	expression tag	UNP Q53WG9
K	-3	GLY	-	expression tag	UNP Q53WG9
K	-2	THR	-	expression tag	UNP Q53WG9
K	-1	GLY	-	expression tag	UNP Q53WG9
K	0	ALA	-	expression tag	UNP Q53WG9
М	-3	GLY	-	expression tag	UNP Q53WG9
М	-2	THR	-	expression tag	UNP Q53WG9
М	-1	GLY	-	expression tag	UNP Q53WG9
М	0	ALA	-	expression tag	UNP Q53WG9
0	-3	GLY	-	expression tag	UNP Q53WG9
0	-2	THR	-	expression tag	UNP Q53WG9
0	-1	GLY	-	expression tag	UNP Q53WG9
0	0	ALA	-	expression tag	UNP Q53WG9

• Molecule 2 is a RNA chain called 5'-R(*UP*CP*CP*CP*CP*AP*CP*GP*CP*GP*UP*G P*UP*GP *GP*GP*DGP*AP*UP)-3'.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
2	В	10	Total	С	Ν	0	Р	0	0	0
	D	19	385	171	69	127	18	0	0	0
0	Л	10	Total	С	Ν	0	Р	0	0	0
	D	19	385	171	69	127	18	0	0	0
0	Б	10	Total	С	Ν	0	Р	0	0	0
	Г	19	385	171	69	127	18	0	0	0
0	ц	10	Total	С	Ν	0	Р	0	0	0
	11	19	385	171	69	127	18		0	0
0	т	10	Total	С	Ν	0	Р	0	0	0
	J	19	385	171	69	127	18	0	0	U
0	т	10	Total	С	Ν	0	Р	0	0	0
		19	385	171	69	127	18	0	0	0
2	N	18	Total	С	Ν	0	Р	0	0	0
	2 IN	18	381	171	69	124	17	0	0	0
9	р	18	Total	С	Ν	0	Р	0	0	0
	1	18	381	171	69	124	17	0		0

• Molecule 3 is water.



0	V	\mathbf{O}	Ц
2	I	9.	п

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	35	$\begin{array}{cc} \text{Total} & \text{O} \\ 35 & 35 \end{array}$	0	0
3	В	13	Total O 13 13	0	0
3	С	30	Total O 30 30	0	0
3	D	19	Total O 19 19	0	0
3	Е	51	Total O 51 51	0	0
3	F	25	TotalO2525	0	0
3	G	30	Total O 30 30	0	0
3	Н	13	Total O 13 13	0	0
3	Ι	57	Total O 57 57	0	0
3	J	24	Total O 24 24	0	0
3	K	56	Total O 56 56	0	0
3	L	20	TotalO2020	0	0
3	М	44	Total O 44 44	0	0
3	Ν	23	TotalO2323	0	0
3	О	22	$\begin{array}{ccc} \text{Total} & \text{O} \\ \hline 22 & 22 \end{array}$	0	0
3	Р	13	Total O 13 13	0	0



Residue-property plots (i) 3

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 electron 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 dot above a residue indicates a poor fit to the electron density (RSRZ > 2). 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: CSE3









• Molecule 2: 5'-R(*UP*CP*CP*CP*CP*AP*CP*GP*CP*GP*UP*GP*UP*GP*GP*GP*DGP*AP*UP)-3'

	5%		
Chain B:	16%	58%	26%
	•		

• Molecule 2: 5'-R(*UP*CP*CP*CP*CP*AP*CP*GP*CP*GP*UP*GP*UP*GP*GP*GP*DGP*AP*UP)-3'



• Molecule 2: 5'-R(*UP*CP*CP*CP*CP*AP*CP*GP*CP*GP*UP*GP*UP*GP*GP*GP*DGP*AP*UP)-3'



• Molecule 2: 5'-R(*UP*CP*CP*CP*CP*AP*CP*GP*CP*GP*UP*GP*UP*GP*GP*GP*DGP*AP*UP)-3'

Chain H·	37%	37%	21%	5%
	0,10	0/10	21/0	J /0



5%

5%

5% 5%





• Molecule 2: 5'-R(*UP*CP*CP*CP*CP*AP*CP*GP*CP*GP*UP*GP*UP*GP*GP*GP*DGP*AP*UP)-3'

	58%	
Chain P: 11%	63%	21% 5%
••••	_	
U5 C6 C7 C7 C7 C3 C11 C11 C11 C11 C11 C13 C13 C13 C13	2	



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	85.86Å 149.81Å 87.26Å	Deperitor
a, b, c, α , β , γ	90.00° 94.60° 90.00°	Depositor
$\mathbf{P}_{\text{oscolution}}(\hat{\mathbf{A}})$	58.70 - 2.50	Depositor
Resolution (A)	58.70 - 2.40	EDS
% Data completeness	99.8 (58.70-2.50)	Depositor
(in resolution range)	99.9 (58.70-2.40)	EDS
R _{merge}	0.10	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.90 (at 2.40 \text{\AA})$	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
D D.	0.231 , 0.289	Depositor
Π, Π_{free}	0.219 , 0.276	DCC
R_{free} test set	1994 reflections (2.33%)	wwPDB-VP
Wilson B-factor $(Å^2)$	37.4	Xtriage
Anisotropy	0.140	Xtriage
Bulk solvent $k_{sol}(e/A^3)$, $B_{sol}(A^2)$	(Not available), (Not available)	EDS
L-test for twinning ²	$< L >=0.48, < L^2>=0.31$	Xtriage
Estimated twinning fraction	0.000 for l,-k,h	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	15663	wwPDB-VP
Average B, all atoms $(Å^2)$	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The analyses of the Patterson function reveals a significant off-origin peak that is 82.85 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.5178e-07. The detected translational NCS is most likely also responsible for the elevated intensity ratio.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



¹Intensities estimated from amplitudes.

5 Model quality (i)

5.1 Standard geometry (i)

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

Mol Chain		Bo	ond lengths	Bond angles		
	Ullalli	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.46	0/1721	0.62	0/2329	
1	С	0.47	0/1712	0.63	0/2317	
1	Ε	0.52	0/1703	0.65	0/2304	
1	G	0.45	0/1621	0.63	0/2194	
1	Ι	0.50	0/1577	0.67	0/2135	
1	Κ	0.49	0/1552	0.65	0/2103	
1	М	0.41	0/1561	0.59	0/2115	
1	0	0.32	0/920	0.53	0/1285	
2	В	0.99	1/429~(0.2%)	1.10	2/668~(0.3%)	
2	D	1.18	6/429~(1.4%)	1.12	0/668	
2	F	1.23	7/429~(1.6%)	1.38	9/668~(1.3%)	
2	Н	1.08	4/429~(0.9%)	1.14	3/668~(0.4%)	
2	J	0.72	0/429	1.49	6/668~(0.9%)	
2	L	0.62	0/429	1.26	5/668~(0.7%)	
2	N	0.50	0/425	0.98	0/661	
2	Р	0.37	0/425	0.90	0/661	
All	All	0.58	18/15791~(0.1%)	0.80	25/22112~(0.1%)	

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	22	А	N7-C5	-9.25	1.33	1.39
2	Н	22	А	N7-C5	-8.97	1.33	1.39
2	D	22	А	N3-C4	-8.51	1.29	1.34
2	D	22	А	N7-C5	-7.35	1.34	1.39
2	D	22	А	C6-N1	-7.20	1.30	1.35
2	F	22	А	C8-N7	-6.64	1.26	1.31
2	D	22	А	C5-C4	-6.46	1.34	1.38
2	F	22	А	P-O5'	-6.38	1.53	1.59
2	F	22	А	C6-N1	-6.09	1.31	1.35
2	В	22	А	P-O5'	-5.77	1.53	1.59
2	F	22	A	P-OP1	-5.57	1.39	1.49
2	F	22	А	C5-C4	-5.54	1.34	1.38



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Н	22	А	C6-N1	-5.40	1.31	1.35
2	Н	22	А	C8-N7	-5.38	1.27	1.31
2	Н	22	А	N9-C8	-5.32	1.33	1.37
2	D	22	А	C2-N3	-5.12	1.28	1.33
2	F	22	А	N3-C4	-5.08	1.31	1.34
2	D	22	А	N1-C2	-5.00	1.29	1.34

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	J	16	G	C5-N7-C8	-9.87	99.37	104.30
2	J	21	DG	O4'-C1'-N9	9.60	114.72	108.00
2	J	16	G	C4-C5-N7	9.46	114.58	110.80
2	F	22	А	O4'-C1'-C2'	-7.98	97.82	105.80
2	Н	15	U	C2-N1-C1'	7.93	127.22	117.70
2	J	16	G	N7-C8-N9	7.61	116.91	113.10
2	F	22	А	C8-N9-C4	-7.30	102.88	105.80
2	L	15	U	C2-N1-C1'	6.91	126.00	117.70
2	В	22	А	C3'-C2'-C1'	-6.71	96.14	101.50
2	F	22	А	P-O3'-C3'	6.32	127.28	119.70
2	J	16	G	N3-C4-C5	6.02	131.61	128.60
2	F	5	U	C2-N1-C1'	5.86	124.73	117.70
2	F	5	U	C5-C4-O4	-5.72	122.47	125.90
2	Н	15	U	C6-N1-C1'	-5.70	113.22	121.20
2	L	15	U	C6-N1-C1'	-5.67	113.26	121.20
2	В	22	A	C5'-C4'-C3'	-5.61	107.02	116.00
2	F	22	A	N7-C8-N9	5.53	116.56	113.80
2	F	14	G	C4-N9-C1'	5.43	133.56	126.50
2	F	22	A	C4'-C3'-C2'	-5.38	97.22	102.60
2	Н	15	U	C5-C6-N1	5.31	125.36	122.70
2	J	17	U	N1-C2-O2	-5.25	119.13	122.80
2	F	14	G	N3-C4-C5	-5.20	126.00	128.60
2	L	18	G	C4-N9-C1'	-5.14	119.81	126.50
2	L	15	U	C5-C6-N1	5.12	125.26	122.70
2	L	14	G	N1-C6-O6	5.03	122.92	119.90

There are no chirality outliers.

There are no planarity outliers.



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	А	1685	0	1762	98	0
1	С	1676	0	1754	71	1
1	Е	1668	0	1744	95	0
1	G	1587	0	1667	48	0
1	Ι	1545	0	1615	45	0
1	К	1519	0	1582	61	0
1	М	1528	0	1597	65	0
1	0	908	0	513	15	0
2	В	385	0	196	27	0
2	D	385	0	196	23	0
2	F	385	0	196	21	0
2	Н	385	0	196	13	0
2	J	385	0	196	18	0
2	L	385	0	196	15	0
2	Ν	381	0	197	18	0
2	Р	381	0	197	19	0
3	А	35	0	0	3	0
3	В	13	0	0	3	0
3	С	30	0	0	1	1
3	D	19	0	0	0	0
3	Е	51	0	0	7	2
3	F	25	0	0	3	0
3	G	30	0	0	3	0
3	Н	13	0	0	2	0
3	Ι	57	0	0	5	0
3	J	24	0	0	2	0
3	Κ	56	0	0	3	0
3	L	20	0	0	1	0
3	М	44	0	0	2	0
3	Ν	23	0	0	5	0
3	0	22	0	0	2	0
3	Р	13	0	0	0	0
All	All	15663	0	13804	584	2

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 20.

All (584) 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)
1:K:74:GLU:HA	1:K:76:TYR:H	1.08	1.17
1:K:74:GLU:HG3	1:K:75:GLY:HA2	1.25	1.14
2:J:21:DG:C2'	2:J:22:A:H5'	1.92	0.99
1:A:83:LYS:HE2	2:F:9:C:OP1	1.63	0.97
1:A:145:TRP:CD1	1:A:179:ARG:HB2	2.00	0.95
1:A:83:LYS:HZ1	2:F:9:C:C5'	1.80	0.94
1:K:74:GLU:HA	1:K:76:TYR:N	1.82	0.94
1:M:74:GLU:H	1:M:76:TYR:H	0.99	0.94
1:M:74:GLU:HB2	1:M:75:GLY:HA3	1.49	0.94
2:B:9:C:H2'	2:B:10:A:H8	1.32	0.93
1:M:118:THR:HG23	1:M:121:GLU:H	1.34	0.93
2:L:15:U:H4'	2:L:16:G:OP2	1.66	0.92
2:L:5:U:O2'	2:L:6:C:OP2	1.86	0.92
2:H:15:U:O2'	2:H:16:G:OP2	1.86	0.92
2:B:5:U:H2'	2:B:5:U:O2	1.66	0.90
2:N:6:C:H5'	3:N:2003:HOH:O	1.70	0.90
1:C:118:THR:HG23	1:C:121:GLU:H	1.37	0.90
1:M:73:ASP:O	1:M:76:TYR:HB3	1.71	0.90
1:M:74:GLU:H	1:M:76:TYR:N	1.71	0.88
1:C:168:LEU:HD12	1:C:169:LEU:N	1.89	0.88
1:C:144:PRO:HG3	1:E:158:ARG:HH12	1.39	0.87
1:I:95:LEU:O	1:I:179:ARG:HG2	1.74	0.87
1:C:56:PRO:HB2	1:C:57:PRO:HD2	1.55	0.87
1:E:117:LYS:HG2	1:E:121:GLU:OE1	1.75	0.86
1:M:74:GLU:N	1:M:76:TYR:H	1.74	0.86
1:E:145:TRP:CD1	1:E:179:ARG:HB2	2.11	0.85
1:0:46:TRP:0	3:O:2007:HOH:O	1.95	0.84
1:E:47:ARG:HD3	3:E:2050:HOH:O	1.77	0.84
1:A:112:LYS:NZ	2:B:5:U:H5'	1.94	0.82
2:J:21:DG:H2"	2:J:22:A:H5'	1.62	0.82
1:A:145:TRP:NE1	1:A:179:ARG:HD2	1.93	0.82
1:C:131:GLU:OE2	1:E:155:GLU:OE2	1.98	0.81
2:L:5:U:O2'	2:L:6:C:H5'	1.81	0.80
2:J:5:U:HO5'	2:J:5:U:H6	1.30	0.80
1:A:83:LYS:NZ	2:F:9:C:C5'	2.44	0.79
1:M:74:GLU:CB	1:M:75:GLY:HA3	2.11	0.79
1:A:155:GLU:HG3	1:A:168:LEU:HD11	1.63	0.79
1:G:3:LEU:HD23	1:G:83:LYS:HE3	1.66	0.78
1:I:151:ASP:OD2	3:I:2044:HOH:O	2.01	0.78
2:P:14:G:C8	2:P:15:U:C5	2.72	0.78
1:E:88:ALA:HB3	1:E:93:GLN:HE22	1.47	0.77



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:E:52:ARG:O	1:E:55:GLU:HG3	1.83	0.77
1:A:168:LEU:HD22	1:G:139:GLU:HG3	1.66	0.77
1:I:118:THR:HG23	1:I:121:GLU:H	1.49	0.77
2:J:21:DG:H2'	2:J:22:A:H5'	1.66	0.76
2:F:5:U:H2'	2:F:5:U:O2	1.86	0.76
1:I:96:ARG:HG2	1:I:210:ALA:O	1.83	0.76
1:C:1:MET:HE2	1:C:193:ARG:HH11	1.50	0.76
2:J:19:G:OP2	3:J:2014:HOH:O	2.03	0.76
2:P:14:G:H4'	2:P:15:U:OP1	1.85	0.76
1:K:74:GLU:HG3	1:K:75:GLY:CA	2.12	0.76
1:K:190:ALA:O	1:K:194:ARG:HG3	1.86	0.75
1:A:145:TRP:HD1	1:A:179:ARG:HB2	1.51	0.75
1:K:106:ARG:O	2:L:16:G:H5"	1.86	0.75
1:C:35:ARG:O	1:C:39:GLU:HG3	1.88	0.74
2:D:14:G:N3	1:E:27:ARG:HD2	2.02	0.74
1:E:96:ARG:HD3	1:E:211:PRO:HA	1.68	0.74
1:G:108:ALA:HB3	2:H:15:U:O2'	1.87	0.74
1:A:129:ARG:HD2	3:B:2009:HOH:O	1.87	0.74
2:N:22:A:O3'	3:N:2022:HOH:O	2.05	0.74
1:C:168:LEU:HD12	1:C:169:LEU:H	1.51	0.73
1:A:83:LYS:CE	2:F:9:C:OP1	2.36	0.73
2:J:12:G:C5	1:K:211:PRO:HG2	2.23	0.73
1:C:137:LEU:HD23	1:C:144:PRO:HB2	1.70	0.72
1:K:87:PRO:HG2	1:K:189:LEU:HD13	1.71	0.72
1:I:122:LYS:NZ	1:I:172:GLN:OE1	2.20	0.71
2:P:12:G:H4'	2:P:12:G:OP1	1.88	0.71
1:E:122:LYS:NZ	1:E:172:GLN:OE1	2.22	0.71
1:G:135:PHE:CZ	1:G:188:ALA:HB1	2.26	0.71
1:A:97:PHE:CD2	1:A:180:LEU:HD23	2.26	0.71
1:E:159:LYS:HE2	1:E:167:LYS:HB3	1.72	0.71
1:E:117:LYS:HG3	1:E:118:THR:HG23	1.73	0.70
1:M:73:ASP:HB3	1:M:74:GLU:HG2	1.73	0.70
1:C:144:PRO:CG	1:E:158:ARG:HH12	2.03	0.70
1:A:83:LYS:NZ	2:F:9:C:O5'	2.20	0.70
2:L:5:U:HO2'	2:L:6:C:P	2.13	0.70
1:A:83:LYS:NZ	2:F:9:C:H5"	2.07	0.70
1:E:87:PRO:HB2	1:E:89:LEU:HD13	1.74	0.70
1:A:1:MET:HB2	1:A:85:PHE:HB3	1.72	0.69
1:I:106:ARG:O	2:J:16:G:H5"	1.92	0.69
1:A:87:PRO:HG3	1:A:189:LEU:HD13	1.74	0.69
1:E:131:GLU:OE2	3:E:2026:HOH:O	2.10	0.68



	• • • • • • •	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:I:73:ASP:OD1	1:I:76:TYR:HB2	1.93	0.68
2:N:14:G:O6	3:N:2012:HOH:O	2.10	0.68
1:E:49:GLU:O	3:E:2009:HOH:O	2.11	0.68
1:E:7:VAL:HG23	1:E:80:PHE:HE2	1.57	0.67
1:M:130:LEU:HD12	1:M:137:LEU:CD1	2.24	0.67
1:A:149:LEU:HD11	1:A:177:GLU:OE1	1.95	0.67
2:B:7:C:H2'	2:B:8:C:H6	1.59	0.67
2:F:5:U:H5'	3:F:2002:HOH:O	1.93	0.67
1:M:103:PRO:HG2	1:M:122:LYS:HG2	1.77	0.66
1:K:106:ARG:HG3	1:K:106:ARG:HH11	1.60	0.66
1:A:47:ARG:HD3	3:A:2035:HOH:O	1.95	0.66
1:G:1:MET:HE2	1:G:193:ARG:HH11	1.59	0.66
1:C:3:LEU:HB2	1:C:85:PHE:HE2	1.60	0.66
1:A:55:GLU:HG2	1:A:56:PRO:HD2	1.78	0.66
2:F:19:G:OP2	3:F:2018:HOH:O	2.13	0.66
1:A:122:LYS:NZ	1:A:172:GLN:OE1	2.26	0.66
1:I:96:ARG:HD2	3:I:2057:HOH:O	1.95	0.66
2:D:5:U:H2'	2:D:6:C:C6	2.31	0.66
1:A:112:LYS:HZ1	2:B:5:U:H5'	1.58	0.65
1:E:93:GLN:HE21	1:E:95:LEU:HD21	1.61	0.65
1:G:2:TRP:CD1	3:G:2002:HOH:O	2.49	0.65
1:E:203:GLY:O	3:E:2049:HOH:O	2.13	0.65
1:A:161:ASP:OD1	1:A:162:GLY:N	2.28	0.65
1:C:127:GLU:O	1:C:131:GLU:HG3	1.97	0.65
2:D:5:U:H2'	2:D:6:C:H6	1.62	0.65
2:N:21:DG:H2'	2:N:22:A:C8	2.32	0.65
1:K:154:LEU:HB2	1:K:171:VAL:HG23	1.79	0.64
2:N:9:C:O2'	3:N:2006:HOH:O	2.14	0.64
1:A:112:LYS:HZ1	2:B:6:C:H5"	1.63	0.64
1:I:7:VAL:HB	1:I:78:GLN:HG2	1.79	0.64
1:C:202:LEU:HD11	2:D:22:A:N6	2.13	0.64
1:M:130:LEU:HD12	1:M:137:LEU:HD11	1.78	0.64
1:I:169:LEU:HB2	2:J:5:U:O2	1.97	0.64
1:K:144:PRO:N	3:K:2041:HOH:O	2.30	0.64
2:B:9:C:H2'	2:B:10:A:C8	2.24	0.63
2:H:15:U:H4'	2:H:16:G:O5'	1.98	0.63
1:E:162:GLY:N	3:E:2035:HOH:O	2.32	0.63
1:M:115:ALA:HB1	1:M:172:GLN:NE2	2.12	0.63
1:M:35:ARG:O	1:M:39:GLU:HG3	1.99	0.63
1:C:164:GLU:HG3	1:M:16:ARG:HD3	1.81	0.63
1:E:98:ARG:HH11	1:E:98:ARG:HB2	1.64	0.63



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Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:180:LEU:C	1:A:180:LEU:HD12	2.19	0.62
1:E:127:GLU:HG2	1:E:137:LEU:HD22	1.81	0.62
1:K:74:GLU:CA	1:K:76:TYR:H	1.99	0.62
1:M:50:PRO:HG2	1:M:98:ARG:HH12	1.63	0.62
1:A:64:LEU:HD13	1:A:193:ARG:NH2	2.15	0.62
1:E:149:LEU:HD11	1:E:177:GLU:OE1	1.99	0.62
1:I:184:ASP:OD2	1:I:187:ARG:HG2	1.99	0.62
1:G:8:LEU:O	1:G:10:PRO:HD3	2.00	0.62
1:0:151:ASP:HA	1:0:173:ALA:O	2.00	0.62
1:C:21:ASN:OD1	1:C:21:ASN:C	2.38	0.61
2:D:21:DG:C2'	2:D:22:A:H5'	2.30	0.61
1:C:118:THR:OG1	1:C:119:PRO:HD2	2.00	0.61
1:G:135:PHE:CE1	1:G:188:ALA:HB1	2.35	0.61
1:M:100:ARG:HH22	1:M:152:THR:CG2	2.12	0.61
1:G:207:LEU:N	3:G:2030:HOH:O	2.18	0.61
1:G:202:LEU:HD11	2:H:22:A:N6	2.15	0.61
1:O:200:LYS:HA	1:O:204:LEU:O	1.99	0.61
2:P:12:G:H2'	2:P:13:C:C6	2.36	0.61
1:C:122:LYS:NZ	1:C:172:GLN:OE1	2.23	0.61
2:B:7:C:H2'	2:B:8:C:C6	2.35	0.61
2:L:5:U:O2'	2:L:6:C:P	2.56	0.61
2:B:5:U:O2	2:B:5:U:C2'	2.44	0.61
1:C:117:LYS:HB3	1:C:121:GLU:OE1	2.01	0.61
1:C:106:ARG:HG3	1:C:106:ARG:HH11	1.66	0.60
1:A:128:ARG:O	1:A:132:GLU:HG3	2.01	0.60
2:B:20:G:O2'	2:B:21:DG:H5'	2.01	0.60
1:K:22:PRO:HB2	1:K:202:LEU:CD2	2.31	0.60
2:P:14:G:H8	2:P:15:U:C5	2.16	0.60
1:A:52:ARG:HE	1:A:55:GLU:HB2	1.66	0.60
2:D:8:C:O2'	2:D:9:C:H5'	2.01	0.60
2:L:5:U:O2	2:L:6:C:H5"	2.01	0.60
1:C:160:LYS:C	1:C:162:GLY:N	2.55	0.60
1:E:87:PRO:HG2	1:E:189:LEU:HD13	1.83	0.60
1:A:83:LYS:CE	2:F:9:C:P	2.90	0.60
1:G:2:TRP:NE1	3:G:2002:HOH:O	2.33	0.60
1:A:158:ARG:NH1	1:G:144:PRO:HD3	2.17	0.59
1:E:158:ARG:O	1:E:159:LYS:CB	2.50	0.59
1:E:94:ARG:HG2	1:E:138:LEU:HD11	1.83	0.59
1:E:35:ARG:NH2	1:K:24:GLU:OE1	2.35	0.59
1:A:15:ALA:O	1:A:19:LEU:HG	2.02	0.59
1:A:161:ASP:HB3	1:A:164:GLU:O	2.02	0.59



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:G:119:PRO:O	1:G:123:VAL:HG23	2.02	0.59
1:C:89:LEU:HB3	1:C:182:VAL:HG21	1.84	0.59
1:K:118:THR:HG23	1:K:121:GLU:OE1	2.01	0.59
2:J:15:U:H2'	2:J:15:U:O2	2.01	0.59
1:K:8:LEU:HD22	1:K:19:LEU:HD21	1.84	0.59
2:P:5:U:O2	2:P:5:U:H2'	2.02	0.58
1:C:56:PRO:CB	1:C:57:PRO:HD2	2.30	0.58
1:C:157:ARG:O	1:C:168:LEU:CD1	2.51	0.58
1:K:90:LYS:HB2	1:K:93:GLN:HB2	1.84	0.58
1:M:73:ASP:CB	1:M:74:GLU:HG2	2.33	0.58
1:A:87:PRO:CG	1:A:189:LEU:HD13	2.33	0.58
1:A:4:THR:HG21	1:A:69:TRP:CE2	2.39	0.58
2:D:14:G:C2	1:E:27:ARG:HD2	2.39	0.58
1:M:127:GLU:HA	1:M:137:LEU:HD13	1.86	0.58
1:A:145:TRP:HE1	1:A:179:ARG:HD2	1.65	0.58
1:E:118:THR:O	1:E:122:LYS:HG3	2.04	0.58
1:A:112:LYS:HE3	2:B:5:U:O5'	2.04	0.57
2:F:16:G:O2'	2:F:17:U:H5'	2.03	0.57
2:F:7:C:O2'	2:F:8:C:H5'	2.04	0.57
2:P:10:A:H2'	2:P:11:C:O4'	2.02	0.57
1:C:44:LEU:O	1:C:45:LEU:HD23	2.04	0.57
1:G:106:ARG:HH11	1:G:106:ARG:HG3	1.68	0.57
1:C:171:VAL:HG13	2:D:5:U:C5	2.40	0.57
1:C:202:LEU:HD11	2:D:22:A:H62	1.69	0.57
2:H:5:U:H1'	3:H:2001:HOH:O	2.04	0.57
1:A:112:LYS:NZ	2:B:6:C:H5"	2.20	0.57
1:C:118:THR:CG2	1:C:121:GLU:H	2.14	0.57
1:C:180:LEU:HD12	1:C:180:LEU:C	2.25	0.57
1:A:55:GLU:CG	1:A:56:PRO:HD2	2.35	0.57
2:P:8:C:H2'	2:P:9:C:H6	1.70	0.57
2:P:5:U:O2	2:P:5:U:C2'	2.53	0.56
1:E:35:ARG:O	1:E:39:GLU:HG3	2.05	0.56
1:C:100:ARG:HG2	1:C:204:LEU:CD2	2.36	0.56
1:E:4:THR:HG21	1:E:69:TRP:CE2	2.40	0.56
1:E:94:ARG:O	1:E:95:LEU:HD22	2.05	0.56
1:E:141:GLU:HG2	1:E:142:ARG:HA	1.86	0.56
1:G:157:ARG:HG3	1:G:169:LEU:HD12	1.86	0.56
1:I:118:THR:HG22	1:I:121:GLU:OE1	2.05	0.56
1:A:83:LYS:HZ3	2:F:9:C:H5"	1.69	0.56
1:E:90:LYS:O	1:E:93:GLN:HB2	2.05	0.56
1:E:97:PHE:CD2	1:E:180:LEU:HD23	2.40	0.56



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Atom-1	Atom-2	distance (\AA)	overlap (Å)
2:J:5:U:H6	2:J:5:U:O5'	1.85	0.56
1:K:22:PRO:HB2	1:K:202:LEU:HD22	1.87	0.56
1:A:73:ASP:O	1:A:76:TYR:HB2	2.04	0.56
1:M:169:LEU:HB3	2:N:5:U:O2	2.06	0.56
1:G:1:MET:CE	1:G:189:LEU:HD11	2.36	0.55
1:K:145:TRP:CH2	2:N:14:G:P	3.00	0.55
1:I:0:ALA:HB2	1:I:86:HIS:CE1	2.40	0.55
1:C:1:MET:N	3:C:2001:HOH:O	2.37	0.55
2:D:14:G:H2'	2:D:14:G:OP1	2.06	0.55
2:D:14:G:H4'	2:D:15:U:OP2	2.07	0.55
1:C:157:ARG:O	1:C:168:LEU:HD12	2.07	0.55
1:O:89:LEU:O	1:0:185:PRO:HB3	2.06	0.55
1:M:25:MET:HG2	1:M:46:TRP:CH2	2.42	0.55
1:A:112:LYS:HZ2	2:B:5:U:H5'	1.70	0.54
1:A:187:ARG:HH11	1:A:190:ALA:HB3	1.71	0.54
2:L:7:C:H5"	3:L:2003:HOH:O	2.06	0.54
1:I:98:ARG:NH2	3:I:2045:HOH:O	2.36	0.54
1:M:112:LYS:HE2	2:N:6:C:OP2	2.07	0.54
1:K:180:LEU:C	1:K:180:LEU:HD12	2.28	0.54
1:A:155:GLU:OE2	1:G:131:GLU:OE2	2.25	0.54
1:E:158:ARG:O	1:E:159:LYS:HB3	2.06	0.54
1:M:138:LEU:HD12	1:M:179:ARG:HG3	1.89	0.54
1:C:9:ASN:HB3	1:C:75:GLY:O	2.08	0.54
1:E:206:LEU:HB3	3:E:2051:HOH:O	2.07	0.54
1:I:118:THR:OG1	1:I:119:PRO:HD2	2.07	0.54
1:A:122:LYS:CE	1:A:172:GLN:OE1	2.56	0.54
1:E:122:LYS:HD3	1:E:174:VAL:HG21	1.90	0.54
2:B:10:A:H5'	3:B:2002:HOH:O	2.09	0.53
2:F:5:U:O2	2:F:5:U:C2'	2.56	0.53
1:M:18:ASP:HB3	1:M:25:MET:HA	1.90	0.53
2:J:5:U:H2'	2:J:6:C:H6	1.72	0.53
1:C:80:PHE:N	1:C:80:PHE:CD1	2.77	0.53
1:G:49:GLU:OE1	1:G:49:GLU:HA	2.08	0.53
1:K:184:ASP:OD2	1:K:187:ARG:HB2	2.08	0.53
2:B:19:G:N2	2:B:20:G:C4	2.76	0.53
1:C:131:GLU:HA	1:C:135:PHE:O	2.09	0.53
1:G:23:TYR:HE1	2:H:22:A:OP1	1.92	0.53
1:C:48:LEU:HD11	1:C:57:PRO:HB2	1.90	0.53
1:A:55:GLU:HG2	1:A:56:PRO:CD	2.39	0.53
1:E:201:ALA:C	1:E:202:LEU:HD12	2.29	0.53
2:F:5:U:C5'	3:F:2002:HOH:O	2.52	0.53



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:C:132:GLU:O	1:E:16:ARG:HD2	2.09	0.53
1:C:160:LYS:O	1:C:164:GLU:O	2.27	0.52
2:D:7:C:O2'	2:D:8:C:H5'	2.08	0.52
1:E:159:LYS:HD3	1:E:169:LEU:HD11	1.91	0.52
1:K:135:PHE:CZ	1:K:188:ALA:HB1	2.44	0.52
1:M:74:GLU:HB2	1:M:75:GLY:CA	2.28	0.52
1:M:115:ALA:HB1	1:M:172:GLN:HE21	1.74	0.52
1:A:187:ARG:NH1	1:A:190:ALA:HB3	2.24	0.52
1:A:200:LYS:HA	1:A:204:LEU:O	2.09	0.52
1:K:145:TRP:HZ3	2:N:14:G:H5'	1.74	0.52
1:0:133:GLY:0	1:O:188:ALA:HA	2.09	0.52
1:C:169:LEU:HB3	2:D:5:U:O2	2.09	0.52
1:M:112:LYS:HE2	2:N:6:C:P	2.50	0.52
1:M:118:THR:HG22	1:M:121:GLU:OE1	2.09	0.52
1:E:52:ARG:HB3	1:E:55:GLU:OE2	2.09	0.52
1:A:1:MET:O	1:A:85:PHE:N	2.39	0.52
1:E:155:GLU:HG3	1:E:168:LEU:HD11	1.91	0.52
1:M:155:GLU:O	1:M:156:VAL:HB	2.10	0.52
2:B:18:G:H2'	2:B:19:G:H8	1.75	0.52
1:C:118:THR:HG22	1:C:121:GLU:HG3	1.92	0.52
1:I:49:GLU:OE1	1:I:49:GLU:HA	2.10	0.52
2:B:21:DG:C2'	2:B:22:A:O5'	2.58	0.52
1:C:135:PHE:CZ	1:C:188:ALA:HB1	2.45	0.52
1:A:144:PRO:HB2	1:A:146:VAL:HG12	1.90	0.51
1:C:119:PRO:O	1:C:123:VAL:HG23	2.11	0.51
1:C:171:VAL:HG13	2:D:5:U:C4	2.45	0.51
1:E:42:GLU:OE2	1:E:63:THR:HB	2.10	0.51
1:K:3:LEU:HD23	1:K:3:LEU:C	2.31	0.51
2:D:9:C:H2'	2:D:10:A:C8	2.45	0.51
1:I:147:GLN:N	1:I:147:GLN:CD	2.63	0.51
1:M:100:ARG:HH22	1:M:152:THR:HG23	1.75	0.51
1:E:128:ARG:O	1:E:132:GLU:HG3	2.10	0.51
1:M:57:PRO:HD2	3:M:2007:HOH:O	2.11	0.51
1:C:1:MET:HE2	1:C:193:ARG:NH1	2.23	0.51
1:C:3:LEU:HB2	1:C:85:PHE:CE2	2.42	0.51
2:F:8:C:O2'	2:F:9:C:H5'	2.11	0.51
1:0:103:PRO:HB3	1:0:125:TRP:CB	2.41	0.51
1:C:74:GLU:HG2	1:C:75:GLY:N	2.25	0.51
1:E:141:GLU:CG	1:E:142:ARG:HA	2.41	0.51
1:I:95:LEU:O	1:I:179:ARG:CG	2.55	0.51
1:C:144:PRO:HD3	1:E:158:ARG:NH1	2.24	0.51



	A L O	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:C:55:GLU:HB2	1:C:56:PRO:HD2	1.93	0.51
1:E:145:TRP:HD1	1:E:179:ARG:N	2.08	0.51
1:K:145:TRP:HH2	2:N:14:G:P	2.33	0.51
1:M:135:PHE:CE1	1:M:182:VAL:HG22	2.46	0.51
1:O:95:LEU:N	1:O:180:LEU:O	2.40	0.51
1:K:0:ALA:HB2	1:K:86:HIS:CE1	2.46	0.50
1:K:123:VAL:HG13	1:K:146:VAL:HG11	1.92	0.50
1:K:100:ARG:NH1	3:K:2031:HOH:O	2.44	0.50
1:A:52:ARG:HG2	1:A:55:GLU:OE1	2.11	0.50
1:C:56:PRO:HB2	1:C:57:PRO:CD	2.35	0.50
1:E:93:GLN:NE2	1:E:95:LEU:HD21	2.26	0.50
1:K:36:ALA:HB2	1:K:41:ARG:NH2	2.26	0.50
1:A:52:ARG:HG2	1:A:55:GLU:HB3	1.93	0.50
1:E:7:VAL:HG23	1:E:80:PHE:CE2	2.43	0.50
1:G:2:TRP:O	1:G:62:GLN:HA	2.11	0.50
1:M:135:PHE:HE1	1:M:182:VAL:HG22	1.76	0.50
1:E:34:SER:O	1:E:38:GLU:HG3	2.12	0.50
1:G:180:LEU:C	1:G:180:LEU:HD12	2.32	0.50
1:M:106:ARG:NE	2:N:17:U:O4	2.42	0.50
2:L:6:C:H5'	2:L:6:C:H6	1.76	0.50
1:M:43:ARG:HG3	1:M:43:ARG:O	2.12	0.50
1:A:74:GLU:OE1	1:A:75:GLY:HA2	2.12	0.50
1:K:103:PRO:HG2	1:K:122:LYS:HG2	1.94	0.49
1:C:97:PHE:HA	1:C:208:SER:O	2.12	0.49
1:I:31:LYS:HB3	1:I:71:VAL:HG21	1.93	0.49
1:A:96:ARG:NE	1:A:211:PRO:O	2.45	0.49
2:B:7:C:O2'	2:B:8:C:H5'	2.13	0.49
1:M:73:ASP:O	1:M:76:TYR:CB	2.51	0.49
1:C:4:THR:HG22	1:C:5:LYS:N	2.28	0.49
1:A:52:ARG:HG2	1:A:55:GLU:CB	2.42	0.49
1:A:129:ARG:NH2	1:A:197:GLY:H	2.10	0.49
2:D:13:C:H4'	2:D:14:G:OP1	2.05	0.49
1:E:136:ARG:O	1:E:180:LEU:HB2	2.13	0.49
1:A:35:ARG:O	1:A:39:GLU:HG3	2.13	0.49
1:A:122:LYS:HE2	1:A:172:GLN:OE1	2.11	0.49
1:E:149:LEU:HD11	1:E:177:GLU:CD	2.33	0.49
2:H:15:U:O2'	2:H:16:G:P	2.70	0.49
1:I:24:GLU:OE1	1:I:24:GLU:HA	2.13	0.49
1:C:118:THR:HG22	1:C:121:GLU:CG	2.42	0.49
1:C:135:PHE:CE1	1:C:188:ALA:HB1	2.48	0.49
1:G:3:LEU:HD23	1:G:83:LYS:CE	2.40	0.49



	A L O	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:K:106:ARG:HG3	1:K:106:ARG:NH1	2.27	0.49
1:A:35:ARG:NH2	1:I:24:GLU:OE1	2.46	0.49
1:A:83:LYS:NZ	2:F:9:C:P	2.86	0.49
1:E:53:GLY:C	1:E:54:LEU:HD12	2.33	0.48
1:K:31:LYS:HB3	1:K:71:VAL:HG21	1.95	0.48
1:M:135:PHE:CD1	1:M:180:LEU:HD13	2.48	0.48
1:M:138:LEU:C	1:M:145:TRP:HD1	2.16	0.48
2:P:10:A:H2	2:P:17:U:O2	1.96	0.48
1:A:24:GLU:O	1:A:27:ARG:N	2.47	0.48
1:K:23:TYR:CE1	2:L:22:A:H5'	2.48	0.48
2:L:20:G:O2'	2:L:21:DG:H5'	2.13	0.48
1:M:97:PHE:HA	1:M:208:SER:O	2.14	0.48
1:E:149:LEU:HD12	1:E:177:GLU:HB2	1.96	0.48
2:J:21:DG:H2"	2:J:22:A:C5'	2.37	0.48
1:K:74:GLU:CG	1:K:75:GLY:HA2	2.19	0.48
1:E:5:LYS:O	1:E:80:PHE:HD2	1.96	0.48
1:E:7:VAL:CG1	1:E:56:PRO:HB2	2.44	0.48
1:E:135:PHE:CE1	1:E:188:ALA:HB1	2.48	0.48
2:J:12:G:C6	1:K:211:PRO:HG2	2.48	0.48
1:C:155:GLU:HA	1:C:170:GLN:HB3	1.95	0.48
2:J:5:U:H2'	2:J:6:C:C6	2.48	0.48
1:O:93:GLN:O	1:O:181:GLU:HA	2.14	0.48
1:G:168:LEU:HD13	1:G:170:GLN:HG3	1.96	0.48
2:J:14:G:N7	1:K:94:ARG:NH1	2.61	0.48
1:K:112:LYS:HD3	2:L:5:U:H3'	1.96	0.48
1:M:97:PHE:CD2	1:M:180:LEU:HD23	2.49	0.48
1:C:9:ASN:HD21	1:C:11:ALA:HB3	1.78	0.47
1:E:94:ARG:C	1:E:95:LEU:HD22	2.34	0.47
1:K:64:LEU:HD13	1:K:193:ARG:NH2	2.29	0.47
2:L:15:U:HO2'	2:L:16:G:P	2.37	0.47
1:M:8:LEU:O	1:M:10:PRO:HD3	2.14	0.47
1:K:13:ARG:HD3	3:K:2005:HOH:O	2.14	0.47
1:K:68:ASP:O	1:K:71:VAL:HG13	2.15	0.47
1:M:49:GLU:OE2	1:M:60:LEU:HD22	2.15	0.47
1:A:83:LYS:HZ1	2:F:9:C:P	2.36	0.47
2:B:13:C:O2	2:B:13:C:O4'	2.30	0.47
1:M:127:GLU:HA	1:M:137:LEU:CD1	2.44	0.47
1:G:184:ASP:HA	1:G:185:PRO:HD3	1.74	0.47
1:K:145:TRP:HH2	2:N:14:G:O5'	1.97	0.47
1:G:21:ASN:OD1	1:G:21:ASN:C	2.52	0.47
1:G:126:LEU:HD22	1:G:176:PHE:CG	2.50	0.47



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
2:H:5:U:H2'	2:H:6:C:C6	2.49	0.47
1:M:127:GLU:HG3	1:M:137:LEU:HD13	1.97	0.47
1:C:68:ASP:OD2	1:C:71:VAL:HG13	2.15	0.47
1:M:15:ALA:O	1:M:19:LEU:HG	2.15	0.47
1:A:68:ASP:O	1:A:71:VAL:HG22	2.15	0.47
1:I:118:THR:HG22	1:I:121:GLU:CG	2.45	0.47
1:K:22:PRO:HB2	1:K:202:LEU:HD23	1.97	0.47
2:J:5:U:O2'	2:J:6:C:H5'	2.15	0.47
1:A:145:TRP:CD1	1:A:179:ARG:CB	2.87	0.46
1:G:35:ARG:O	1:G:38:GLU:HB2	2.15	0.46
1:M:4:THR:HG21	1:M:69:TRP:NE1	2.30	0.46
1:O:81:PRO:HA	1:0:82:PRO:HD2	1.80	0.46
1:E:94:ARG:CG	1:E:138:LEU:HD11	2.45	0.46
1:I:106:ARG:HG3	1:I:106:ARG:HH11	1.80	0.46
1:K:36:ALA:HA	1:K:41:ARG:NH1	2.30	0.46
1:I:42:GLU:OE1	1:I:43:ARG:N	2.45	0.46
1:0:113:ARG:0	2:P:5:U:H5"	2.15	0.46
1:A:83:LYS:HZ2	2:F:10:A:P	2.37	0.46
1:C:146:VAL:HG22	1:C:147:GLN:N	2.31	0.46
1:C:160:LYS:C	1:C:162:GLY:H	2.19	0.46
1:C:160:LYS:O	1:C:162:GLY:N	2.48	0.46
1:E:91:PRO:C	1:E:93:GLN:H	2.19	0.46
2:D:13:C:C4'	2:D:14:G:OP1	2.63	0.46
1:E:145:TRP:CD1	1:E:145:TRP:O	2.68	0.46
1:E:6:LEU:CD2	1:E:79:VAL:HG23	2.46	0.46
1:E:158:ARG:HD2	1:E:166:GLY:O	2.16	0.46
1:I:12:SER:O	1:I:15:ALA:HB3	2.16	0.46
1:I:135:PHE:CZ	1:I:188:ALA:HB1	2.51	0.46
1:0:56:PRO:HA	1:0:57:PRO:HD2	1.86	0.46
2:B:20:G:H2'	2:B:21:DG:O4'	2.16	0.45
1:E:96:ARG:NH1	1:E:96:ARG:HB2	2.30	0.45
1:G:146:VAL:HG22	1:G:147:GLN:N	2.30	0.45
1:I:68:ASP:O	1:I:71:VAL:HG13	2.16	0.45
1:K:23:TYR:OH	1:K:27:ARG:HD2	2.16	0.45
1:M:94:ARG:HD3	1:M:138:LEU:HD11	1.98	0.45
1:C:132:GLU:OE1	1:E:13:ARG:HD2	2.16	0.45
1:I:73:ASP:OD1	1:I:76:TYR:CB	2.62	0.45
1:0:200:LYS:CB	3:O:2020:HOH:O	2.64	0.45
1:A:171:VAL:HG22	1:A:172:GLN:N	2.30	0.45
1:E:196:VAL:O	1:E:205:GLY:HA2	2.17	0.45
2:P:7:C:C2	2:P:21:DG:N2	2.84	0.45



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:A:98:ARG:HG3	1:A:175:LEU:HD11	1.98	0.45
2:B:11:C:H2'	2:B:11:C:O2	2.16	0.45
2:F:5:U:H5'	2:F:6:C:OP2	2.16	0.45
1:A:81:PRO:HA	1:A:82:PRO:HD2	1.78	0.45
1:G:80:PHE:CD1	1:G:80:PHE:N	2.84	0.45
2:P:10:A:C2	2:P:17:U:O2	2.70	0.45
2:D:9:C:H2'	2:D:10:A:H8	1.80	0.45
1:G:1:MET:HE1	1:G:193:ARG:HG2	1.99	0.45
1:I:98:ARG:NH1	1:I:175:LEU:HD21	2.31	0.45
2:D:14:G:H3'	2:D:15:U:H5'	1.99	0.45
1:E:96:ARG:HB2	1:E:210:ALA:O	2.16	0.45
1:G:33:VAL:HG21	1:G:42:GLU:OE1	2.17	0.45
1:M:135:PHE:CZ	1:M:188:ALA:HB1	2.51	0.45
1:A:103:PRO:HA	1:A:125:TRP:CE2	2.52	0.45
1:A:157:ARG:HD3	2:B:22:A:O2'	2.17	0.45
1:G:9:ASN:HB3	1:G:75:GLY:O	2.16	0.45
1:G:83:LYS:HA	1:G:84:PRO:HD3	1.79	0.45
1:I:2:TRP:O	1:I:62:GLN:HA	2.17	0.45
1:I:35:ARG:HD2	1:I:35:ARG:HA	1.60	0.45
1:M:171:VAL:HG22	2:N:5:U:C4	2.51	0.45
1:A:64:LEU:N	1:A:64:LEU:HD23	2.32	0.45
1:I:44:LEU:HD23	1:I:45:LEU:N	2.32	0.45
1:A:135:PHE:CD1	1:A:180:LEU:HD13	2.52	0.44
1:E:23:TYR:HE2	1:E:27:ARG:NH2	2.15	0.44
1:E:106:ARG:O	2:F:16:G:H5"	2.16	0.44
2:P:12:G:H8	2:P:12:G:H5"	1.81	0.44
1:K:199:GLY:HA3	1:K:204:LEU:HD12	1.98	0.44
1:M:118:THR:HG22	1:M:121:GLU:CG	2.47	0.44
1:M:138:LEU:HD23	1:M:138:LEU:HA	1.76	0.44
2:D:20:G:H2'	2:D:21:DG:O4'	2.17	0.44
1:E:7:VAL:HG13	1:E:56:PRO:HB2	2.00	0.44
1:E:127:GLU:CG	1:E:137:LEU:HD22	2.48	0.44
1:K:91:PRO:HD3	1:K:185:PRO:CG	2.48	0.44
2:D:5:U:C2'	2:D:6:C:O5'	2.65	0.44
1:E:98:ARG:HB2	1:E:98:ARG:NH1	2.32	0.44
1:A:97:PHE:HA	1:A:208:SER:O	2.18	0.44
1:K:73:ASP:O	1:K:74:GLU:C	2.56	0.44
1:K:97:PHE:CD2	1:K:180:LEU:HD23	2.53	0.44
1:C:56:PRO:CB	1:C:57:PRO:CD	2.96	0.44
1:I:146:VAL:HG13	1:I:146:VAL:O	2.17	0.44
1:K:42:GLU:OE1	1:K:43:ARG:N	2.46	0.44



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:A:115:ALA:HB1	1:A:172:GLN:NE2	2.33	0.43
1:E:1:MET:HB2	1:E:85:PHE:CE2	2.53	0.43
1:E:23:TYR:CE2	1:E:27:ARG:NH2	2.85	0.43
1:E:37:LEU:HD23	1:E:37:LEU:HA	1.84	0.43
1:I:97:PHE:HA	1:I:208:SER:O	2.17	0.43
1:K:147:GLN:HB3	2:N:15:U:O4'	2.18	0.43
1:G:167:LYS:C	1:G:167:LYS:HD2	2.39	0.43
1:G:192:LEU:HD23	1:G:207:LEU:HD23	2.00	0.43
1:I:44:LEU:HD22	1:I:46:TRP:HD1	1.83	0.43
1:A:31:LYS:O	1:A:31:LYS:HG2	2.18	0.43
1:A:74:GLU:HA	1:A:76:TYR:H	1.83	0.43
1:C:44:LEU:HD11	1:C:61:VAL:HG13	2.01	0.43
1:A:52:ARG:O	1:A:52:ARG:HG3	2.17	0.43
1:A:103:PRO:HA	1:A:125:TRP:CD2	2.54	0.43
1:C:89:LEU:O	1:C:185:PRO:HB3	2.19	0.43
1:E:145:TRP:CD1	1:E:179:ARG:CB	2.92	0.43
2:J:5:U:H1'	3:J:2001:HOH:O	2.18	0.43
1:M:129:ARG:NH1	3:M:2030:HOH:O	2.29	0.43
1:A:150:GLN:HG2	1:A:175:LEU:HB3	2.00	0.43
2:D:14:G:N2	1:E:24:GLU:OE1	2.33	0.43
1:A:73:ASP:O	1:A:76:TYR:CB	2.67	0.43
2:P:20:G:H2'	2:P:21:DG:O4'	2.17	0.43
2:B:9:C:O4'	3:B:2003:HOH:O	2.21	0.43
1:C:6:LEU:HD22	1:C:79:VAL:HG22	2.01	0.43
1:C:18:ASP:HB3	1:C:25:MET:HA	2.00	0.43
1:C:81:PRO:O	1:C:82:PRO:C	2.57	0.43
1:G:33:VAL:HG22	1:G:36:ALA:HB3	1.99	0.43
1:M:96:ARG:HG2	1:M:179:ARG:HE	1.83	0.43
1:A:3:LEU:HD13	1:A:3:LEU:HA	1.88	0.43
1:A:126:LEU:HD22	1:A:176:PHE:CD1	2.54	0.43
2:H:10:A:H2'	2:H:11:C:O4'	2.19	0.43
1:K:145:TRP:CH2	2:N:14:G:O5'	2.72	0.43
1:K:200:LYS:HA	1:K:204:LEU:O	2.18	0.43
1:M:130:LEU:HD12	1:M:137:LEU:HD12	1.99	0.43
1:A:13:ARG:HG2	2:H:18:G:H5'	2.00	0.43
1:A:21:ASN:HA	1:A:22:PRO:HD3	1.90	0.43
1:I:95:LEU:HD13	1:I:95:LEU:HA	1.69	0.43
2:P:7:C:H2'	2:P:8:C:C6	2.54	0.43
2:B:17:U:H2'	2:B:18:G:C8	2.54	0.42
1:E:138:LEU:O	1:E:145:TRP:HB3	2.19	0.42
1:E:141:GLU:HA	1:E:142:ARG:C	2.38	0.42



	• • • • • •	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:E:158:ARG:O	1:E:159:LYS:HG2	2.19	0.42
2:H:19:G:O2'	2:H:20:G:H5'	2.19	0.42
2:L:15:U:O2'	2:L:16:G:P	2.77	0.42
1:A:4:THR:HG21	1:A:69:TRP:NE1	2.33	0.42
1:A:155:GLU:OE2	1:G:127:GLU:OE2	2.36	0.42
2:D:19:G:C2'	2:D:20:G:H5'	2.49	0.42
2:N:8:C:H1'	3:N:2005:HOH:O	2.19	0.42
1:G:193:ARG:HH11	1:G:193:ARG:HG2	1.83	0.42
1:I:28:THR:CG2	1:I:72:LEU:HD21	2.49	0.42
1:K:149:LEU:CD2	1:M:108:ALA:HB3	2.49	0.42
1:M:148:ILE:HG23	1:M:174:VAL:HG13	2.01	0.42
1:I:11:ALA:O	1:I:16:ARG:NH1	2.52	0.42
1:E:105:LYS:O	1:E:113:ARG:HA	2.20	0.42
1:G:1:MET:HE1	1:G:193:ARG:CG	2.49	0.42
1:I:100:ARG:NH2	1:I:154:LEU:HD21	2.35	0.42
1:K:2:TRP:O	1:K:62:GLN:HA	2.19	0.42
2:P:12:G:C5'	2:P:12:G:C8	3.03	0.42
1:E:145:TRP:HE1	1:E:179:ARG:HG3	1.83	0.42
2:H:5:U:C1'	3:H:2001:HOH:O	2.67	0.42
1:M:100:ARG:HH21	1:M:154:LEU:HD21	1.83	0.42
1:0:152:THR:O	1:O:153:PHE:C	2.57	0.42
1:E:150:GLN:HG2	1:E:175:LEU:HB3	2.02	0.42
1:G:24:GLU:OE1	1:G:24:GLU:HA	2.19	0.42
1:E:52:ARG:HD2	1:E:52:ARG:HA	1.57	0.42
1:O:83:LYS:HA	1:0:84:PRO:HD2	1.91	0.42
2:P:14:G:C4'	2:P:15:U:OP1	2.62	0.42
1:A:169:LEU:HD22	2:B:5:U:O2'	2.19	0.42
1:E:135:PHE:CZ	1:E:188:ALA:HB1	2.54	0.42
1:E:154:LEU:HB2	1:E:171:VAL:HG12	2.00	0.42
1:G:131:GLU:HA	1:G:135:PHE:O	2.20	0.42
1:M:37:LEU:HD23	1:M:42:GLU:HB3	2.01	0.42
1:G:33:VAL:HG22	1:G:33:VAL:O	2.20	0.42
1:G:127:GLU:OE2	1:G:131:GLU:OE2	2.38	0.42
1:I:190:ALA:O	1:I:194:ARG:HG3	2.19	0.42
1:G:145:TRP:O	1:G:178:GLY:HA3	2.20	0.41
1:C:8:LEU:HA	1:C:77:ALA:HB2	2.00	0.41
1:C:105:LYS:HE2	1:C:116:LEU:CD2	2.50	0.41
1:E:97:PHE:HB3	1:E:209:VAL:HG12	2.02	0.41
1:E:157:ARG:HD2	3:E:2034:HOH:O	2.19	0.41
1:G:138:LEU:HD21	1:G:181:GLU:HB2	2.01	0.41
1:K:23:TYR:CD1	2:L:22:A:H5'	2.55	0.41



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:M:146:VAL:HG22	1:M:147:GLN:N	2.34	0.41
1:A:179:ARG:NH1	3:A:2027:HOH:O	2.53	0.41
1:A:31:LYS:O	1:A:71:VAL:HG21	2.20	0.41
1:C:210:ALA:HA	1:C:211:PRO:HD3	1.87	0.41
1:E:97:PHE:CE2	1:E:180:LEU:HD23	2.56	0.41
1:G:106:ARG:HG3	1:G:106:ARG:NH1	2.34	0.41
1:I:169:LEU:HD12	1:I:169:LEU:C	2.40	0.41
1:M:107:LEU:HB2	1:M:110:THR:OG1	2.21	0.41
1:A:135:PHE:CZ	1:A:188:ALA:HB1	2.55	0.41
1:I:4:THR:HG22	1:I:6:LEU:HD12	2.03	0.41
1:K:194:ARG:O	1:K:200:LYS:HE2	2.21	0.41
2:B:9:C:O2'	2:B:10:A:H5'	2.21	0.41
1:K:119:PRO:O	1:K:123:VAL:HG23	2.21	0.41
1:A:137:LEU:HD12	1:A:137:LEU:HA	1.76	0.41
1:A:142:ARG:NH2	3:A:2023:HOH:O	2.54	0.41
1:A:168:LEU:HG	1:A:169:LEU:N	2.35	0.41
1:E:81:PRO:HA	1:E:82:PRO:HD2	1.92	0.41
1:A:43:ARG:O	1:A:43:ARG:HG3	2.19	0.41
1:A:162:GLY:C	1:A:164:GLU:H	2.24	0.41
1:G:43:ARG:NH1	1:G:200:LYS:HD3	2.36	0.41
1:I:56:PRO:HA	1:I:57:PRO:HD3	1.84	0.41
1:I:177:GLU:CD	3:I:2045:HOH:O	2.59	0.41
1:K:91:PRO:HD3	1:K:185:PRO:HG3	2.02	0.41
1:M:9:ASN:OD1	1:M:11:ALA:HB3	2.21	0.41
1:O:30:SER:C	1:O:32:ALA:H	2.24	0.41
2:P:9:C:O2	2:P:9:C:H2'	2.21	0.41
1:A:23:TYR:CE2	1:A:27:ARG:NH1	2.89	0.41
1:C:89:LEU:HA	1:C:93:GLN:OE1	2.21	0.41
1:E:35:ARG:NH2	1:K:27:ARG:HB3	2.36	0.41
1:I:98:ARG:NE	3:I:2045:HOH:O	2.53	0.41
1:K:155:GLU:HG2	1:K:170:GLN:OE1	2.21	0.41
1:M:27:ARG:HH11	1:M:27:ARG:HG3	1.86	0.41
1:A:9:ASN:OD1	1:A:11:ALA:HB3	2.20	0.40
1:E:100:ARG:HG2	1:E:204:LEU:CD2	2.51	0.40
2:N:21:DG:H2'	2:N:22:A:H8	1.84	0.40
2:B:19:G:C2	2:B:20:G:C4	3.09	0.40
1:E:145:TRP:HD1	1:E:179:ARG:H	1.67	0.40
1:K:49:GLU:OE1	1:K:49:GLU:HA	2.21	0.40
1:M:145:TRP:O	1:M:178:GLY:HA3	2.22	0.40
1:E:139:GLU:OE1	1:E:144:PRO:HA	2.21	0.40
1:G:200:LYS:HA	1:G:204:LEU:O	2.22	0.40



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:12:SER:HB3	1:M:15:ALA:HB3	2.02	0.40
1:M:118:THR:OG1	1:M:119:PRO:HD2	2.20	0.40
1:A:24:GLU:O	1:A:25:MET:C	2.59	0.40
1:A:49:GLU:OE1	1:A:49:GLU:HA	2.21	0.40
1:C:80:PHE:HD1	1:C:80:PHE:H	1.69	0.40
2:H:15:U:HO2'	2:H:16:G:P	2.39	0.40
1:M:97:PHE:CD1	1:M:97:PHE:C	2.94	0.40
1:A:96:ARG:O	1:A:209:VAL:HA	2.20	0.40
1:C:100:ARG:NH2	1:C:154:LEU:HD13	2.36	0.40
2:J:10:A:H2'	2:J:11:C:O4'	2.22	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:2021:HOH:O	3:E:2020:HOH:O[2_445]	2.01	0.19
1:C:155:GLU:OE2	3:E:2026:HOH:O[2_445]	2.16	0.04

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 X-ray entries followed by that with respect to entries of similar resolution.

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	Percentile	s
1	А	211/215~(98%)	198 (94%)	12 (6%)	1 (0%)	29 48	
1	С	209/215~(97%)	194 (93%)	14 (7%)	1 (0%)	29 48	
1	Е	207/215~(96%)	196 (95%)	10 (5%)	1 (0%)	29 48	
1	G	193/215~(90%)	185 (96%)	5 (3%)	3 (2%)	9 17	
1	Ι	185/215~(86%)	175 (95%)	10 (5%)	0	100 100)
1	Κ	183/215~(85%)	174 (95%)	7 (4%)	2 (1%)	14 26	
1	М	185/215~(86%)	174 (94%)	11 (6%)	0	100 100)



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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Ο	167/215~(78%)	139~(83%)	24 (14%)	4 (2%)	6 9	
All	All	1540/1720~(90%)	1435~(93%)	93~(6%)	12 (1%)	19 35	

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	33	VAL
1	Κ	145	TRP
1	0	8	LEU
1	0	31	LYS
1	0	34	SER
1	G	73	ASP
1	G	145	TRP
1	Κ	74	GLU
1	А	82	PRO
1	С	162	GLY
1	0	82	PRO
1	Е	92	GLY

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 X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles
1	А	172/173~(99%)	172 (100%)	0	100	100
1	С	172/173~(99%)	167 (97%)	5(3%)	42	69
1	Ε	170/173~(98%)	168~(99%)	2(1%)	71	88
1	G	164/173~(95%)	162 (99%)	2(1%)	71	88
1	Ι	159/173~(92%)	155~(98%)	4 (2%)	47	73
1	Κ	157/173~(91%)	157 (100%)	0	100	100
1	М	158/173~(91%)	158 (100%)	0	100	100
1	Ο	17/173~(10%)	17 (100%)	0	100	100
All	All	1169/1384 (84%)	1156 (99%)	13 (1%)	73	89



Mol	Chain	Res	Type
1	С	54	LEU
1	С	80	PHE
1	С	168	LEU
1	С	171	VAL
1	С	187	ARG
1	Ε	46	TRP
1	Е	202	LEU
1	G	46	TRP
1	G	187	ARG
1	Ι	6	LEU
1	Ι	71	VAL
1	Ι	94	ARG
1	Ι	168	LEU

All (13) residues with a non-rotameric sidechain are listed below:

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such side chains are listed below:

Mol	Chain	Res	Type
1	А	93	GLN
1	G	147	GLN
1	Ι	86	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	В	17/19~(89%)	5(29%)	1 (5%)
2	D	16/19~(84%)	4 (25%)	1 (6%)
2	F	16/19~(84%)	6 (37%)	1 (6%)
2	Н	16/19~(84%)	6 (37%)	1 (6%)
2	J	16/19~(84%)	3 (18%)	1 (6%)
2	L	17/19~(89%)	6 (35%)	2(11%)
2	Ν	16/19~(84%)	3(18%)	0
2	Р	16/19~(84%)	6 (37%)	2(12%)
All	All	130/152~(85%)	39~(30%)	9(6%)

All (39) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	В	6	С
2	В	11	С



Mol	Chain	Res	Type
2	В	13	C
2	B	15	U
2	В	16	G
2	D	6	С
2	D	13	С
2	D	14	G
2	D	22	А
2	F	6	С
2	F	11	С
2	F	12	G
2	F	14	G
2	F	15	U
2	F	16	G
2	Н	6	С
2	Н	11	С
2	Н	12	G
2	Н	14	G
2	Н	15	U
2	Н	16	G
2	J	15	U
2	J	16	G
2	J	22	А
2	L	6	С
2	L	7	С
2	L	8	С
2	L	13	С
2	L	15	U
2	L	16	G
2	N	11	C
2	N	15	U
2	N	16	G
2	Р	6	С
2	Р	11	C
2	Р	12	G
2	Р	15	U
2	Р	16	G
2	Р	22	А

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All (9) RNA pucker outliers are listed below:

Mol	Chain	Res	Type		
2	В	5	U		
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Mol	Chain	Res	Type
2	D	13	С
2	F	14	G
2	Н	15	U
2	J	15	U
2	L	5	U
2	L	15	U
2	Р	12	G
2	Р	14	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)

There are no ligands in this entry.

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 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	$<$ RSRZ $>$	#RSRZ>2	$\mathbf{OWAB}(\mathbf{\AA}^2)$	Q<0.9
1	А	213/215~(99%)	0.41	8 (3%) 40 43	23, 41, 78, 118	0
1	С	211/215~(98%)	0.36	7 (3%) 46 50	21, 41, 82, 115	0
1	Е	211/215~(98%)	0.36	8 (3%) 40 43	18, 41, 75, 112	0
1	G	199/215~(92%)	0.29	4 (2%) 65 68	21, 41, 64, 95	0
1	Ι	195/215~(90%)	0.26	9 (4%) 32 34	12, 32, 64, 98	0
1	K	191/215~(88%)	0.28	8 (4%) 36 39	15, 35, 63, 99	0
1	М	193/215~(89%)	1.11	39 (20%) 1 0	27, 47, 78, 109	0
1	Ο	177/215~(82%)	1.49	56 (31%) 0 0	63, 85, 116, 132	0
2	В	19/19~(100%)	0.18	1 (5%) 26 28	43, 57, 104, 110	0
2	D	19/19~(100%)	0.44	0 100 100	36, 52, 68, 69	0
2	F	19/19~(100%)	0.25	0 100 100	34, 42, 58, 74	0
2	Н	19/19~(100%)	0.25	0 100 100	41, 55, 72, 84	0
2	J	19/19~(100%)	0.54	1 (5%) 26 28	25, 37, 104, 118	0
2	L	19/19~(100%)	0.35	1 (5%) 26 28	28, 46, 88, 148	0
2	N	18/19~(94%)	1.43	7 (38%) 0 0	41, 57, 87, 99	0
2	Р	18/19~(94%)	2.45	11 (61%) 0 0	116, 128, 162, 176	0
All	All	1740/1872 (92%)	0.57	160 (9%) 9 9	12, 43, 95, 176	0

All (160) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	А	142	ARG	9.0
1	0	101	ALA	7.9
2	J	5	U	7.0
2	Р	22	А	6.5
1	0	178	GLY	6.3



Mol	Chain	Res	Type	RSRZ
1	Е	108	ALA	6.0
1	М	23	TYR	6.0
2	Р	21	DG	5.9
1	Ι	168	LEU	5.6
1	С	162	GLY	5.4
1	М	13	ARG	5.2
1	Ο	15	ALA	5.1
2	Ν	22	A	5.0
1	М	145	TRP	5.0
1	М	33	VAL	4.9
1	Ο	84	PRO	4.9
1	Κ	51	ALA	4.9
1	0	36	ALA	4.9
1	М	74	GLU	4.7
1	М	75	GLY	4.7
1	Ο	198	PRO	4.7
1	М	147	GLN	4.7
1	А	54	LEU	4.6
1	0	112	LYS	4.5
1	М	153	PHE	4.4
1	0	32	ALA	4.4
1	0	13	ARG	4.3
1	0	208	SER	4.3
1	0	205	GLY	4.2
1	Ι	169	LEU	4.1
1	М	37	LEU	3.9
1	0	41	ARG	3.9
1	С	15	ALA	3.8
1	0	199	GLY	3.8
2	Р	9	C	3.7
1	0	103	PRO	3.6
1	0	33	VAL	3.6
1	0	114	VAL	3.6
1	Ο	39	GLU	3.6
1	0	99	LEU	3.6
1	0	195	GLY	3.6
1	0	34	SER	3.5
2	Р	19	G	3.5
1	А	145	TRP	3.5
1	E	211	PRO	3.5
2	Р	8	C	3.5
1	0	16	ARG	3.4



Mol	Chain	Res	Type	RSRZ
1	М	69	TRP	3.4
1	0	29	LEU	3.4
1	0	40	GLY	3.4
1	А	80	PHE	3.4
1	А	140	GLY	3.4
1	М	36	ALA	3.3
2	N	9	С	3.3
1	Е	141	GLU	3.3
2	Р	20	G	3.3
1	А	161	ASP	3.3
1	Е	80	PHE	3.3
2	Ν	21	DG	3.3
1	0	174	VAL	3.3
1	K	108	ALA	3.2
1	М	32	ALA	3.2
2	Р	7	С	3.2
2	Ν	5	U	3.1
1	Κ	171	VAL	3.1
1	Ε	79	VAL	3.1
1	М	112	LYS	3.1
1	Ο	67	PRO	3.0
1	М	138	LEU	3.0
1	А	13	ARG	3.0
2	Ν	20	G	3.0
1	С	165	ALA	3.0
1	М	156	VAL	2.9
1	0	30	SER	2.9
1	Ι	110	THR	2.9
1	М	194	ARG	2.9
1	М	38	GLU	2.9
1	E	109	ALA	2.9
1	М	155	GLU	2.9
1	0	26	HIS	2.9
1	0	35	ARG	2.8
1	0	147	GLN	2.8
1	Ō	85	PHE	2.8
1	М	102	ASN	2.8
1	0	207	LEU	2.8
1	Ō	97	PHE	2.7
1	0	124	ALA	2.7
1	М	34	SER	2.7
1	М	170	GLN	2.7



Mol	Chain	Res	Type	RSRZ
1	0	9	ASN	2.7
1	Ι	170	GLN	2.7
2	Ν	8	С	2.7
1	М	73	ASP	2.7
1	М	14	ALA	2.7
1	Ι	51	ALA	2.6
1	0	135	PHE	2.6
1	С	52	ARG	2.6
1	K	35	ARG	2.6
1	0	100	ARG	2.6
1	М	149	LEU	2.6
1	М	41	ARG	2.6
1	Ι	145	TRP	2.6
1	Ι	95	LEU	2.6
1	0	48	LEU	2.5
2	L	5	U	2.5
1	0	113	ARG	2.5
1	М	30	SER	2.5
1	0	173	ALA	2.5
1	0	175	LEU	2.4
1	М	39	GLU	2.4
1	0	50	PRO	2.4
1	0	59	VAL	2.4
1	С	160	LYS	2.4
1	0	110	THR	2.4
1	Е	145	TRP	2.4
1	G	201	ALA	2.4
1	С	159	LYS	2.4
1	0	63	THR	2.4
1	0	28	THR	2.4
1	М	71	VAL	2.4
2	P	6	C	2.4
1	М	72	LEU	2.4
1	M	101	ALA	2.3
1	A	-1	GLY	2.3
1	М	9	ASN	2.3
2	Р	14	G	2.3
1	0	197	GLY	2.3
1	G	141	GLU	2.3
1	0	125	TRP	2.3
1	0	18	ASP	2.3
1	0	23	TYR	2.3



Mol	Chain	Res	Type	RSRZ
2	N	7	С	2.3
1	М	139	GLU	2.3
1	Е	210	ALA	2.3
1	0	105	LYS	2.2
1	0	38	GLU	2.2
1	М	171	VAL	2.2
1	М	209	VAL	2.2
1	М	35	ARG	2.2
1	K	74	GLU	2.2
1	М	124	ALA	2.2
1	K	111	GLY	2.2
1	0	22	PRO	2.2
1	0	69	TRP	2.2
2	В	13	С	2.2
1	K	13	ARG	2.1
1	М	174	VAL	2.1
1	0	194	ARG	2.1
2	Р	18	G	2.1
1	G	35	ARG	2.1
1	0	91	PRO	2.1
1	М	179	ARG	2.1
1	С	140	GLY	2.1
1	Ι	109	ALA	2.1
1	0	14	ALA	2.1
1	K	139	GLU	2.1
2	Р	15	U	2.1
1	G	108	ALA	2.0
1	Ι	11	ALA	2.0
1	М	114	VAL	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.



6.5 Other polymers (i)

There are no such residues in this entry.

