



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 01:38 PM BST

PDB ID : 2GO5
EMDB ID: : EMD-1217
Title : Structure of signal recognition particle receptor (SR) in complex with signal recognition particle (SRP) and ribosome nascent chain complex
Authors : Halic, M.; Gartmann, M.; Schlenker, O.; Mielke, T.; Pool, M.R.; Sinning, I.; Beckmann, R.
Deposited on : 2006-04-12
Resolution : 7.40 Å(reported)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>

MolProbity : 4.02b-467
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk27241

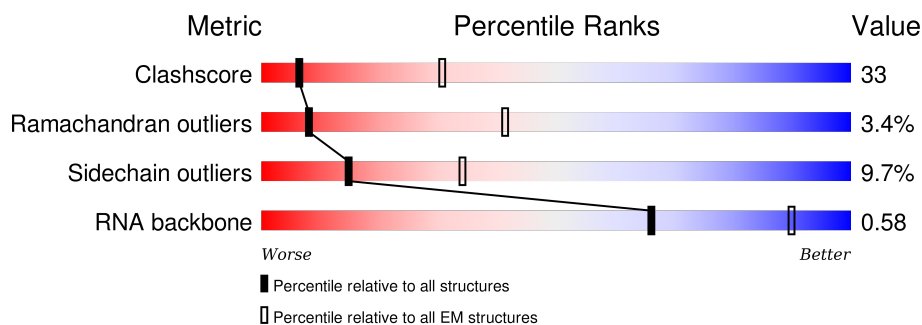
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 7.40 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	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686
RNA backbone	3027	244

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	127	33% 53% 14%
2	9	90	28% 58% 13% .
3	B	108	41% 50% 7% ..
4	W	109	69% 24% . .
5	1	185	52% 14% .. 32%
6	2	214	71% 16% . 12%
7	5	124	19% 23% 5% . 48%
8	4	152	19% 19% 10% 5% 47%

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Mol	Chain	Length	Quality of chain
9	6	123	<div><div></div><div></div><div></div><div></div><div></div><div></div></div> <div>24%24%9%9%34%</div>

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 10724 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called SRP RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	127	Total	C	N	O	P	0	0
			2728	1217	508	877	126		

- Molecule 2 is a RNA chain called ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	9	90	Total	C	N	O	P	0	0
			1935	863	364	618	90		

- Molecule 3 is a protein called Signal recognition particle 19 kDa protein (SRP19).

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	107	Total	C	N	O	S	0	0
			870	549	159	156	6		

- Molecule 4 is a protein called Signal recognition particle 54 kDa protein (SRP54).

Mol	Chain	Residues	Atoms					AltConf	Trace
4	W	109	Total	C	N	O	S	0	0
			865	540	150	164	11		

- Molecule 5 is a protein called Signal recognition particle receptor alpha subunit (SR a).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	1	125	Total	C	N	O	S	0	0
			1020	659	169	189	3		

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	-8	MET	-	CLONING ARTIFACT	UNP P08240
1	-7	SER	-	CLONING ARTIFACT	UNP P08240
1	-6	HIS	-	EXPRESSION TAG	UNP P08240

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Chain	Residue	Modelled	Actual	Comment	Reference
1	-5	HIS	-	EXPRESSION TAG	UNP P08240
1	-4	HIS	-	EXPRESSION TAG	UNP P08240
1	-3	HIS	-	EXPRESSION TAG	UNP P08240
1	-2	HIS	-	EXPRESSION TAG	UNP P08240
1	-1	HIS	-	EXPRESSION TAG	UNP P08240
1	0	SER	-	CLONING ARTIFACT	UNP P08240
1	1	MET	-	CLONING ARTIFACT	UNP P08240
1	2	VAL	-	CLONING ARTIFACT	UNP P08240

- Molecule 6 is a protein called Signal recognition particle receptor beta subunit (SR b).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	2	188	Total	C	N	O	S	0	0
			1479	940	256	278	5		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	56	MET	-	INITIATING METHIONINE	UNP P47758
2	57	ALA	-	CLONING ARTIFACT	UNP P47758

- Molecule 7 is a protein called ribosomal protein L35.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	5	64	Total	C	N	O	0	0
			504	314	99	91		

- Molecule 8 is a protein called ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	4	81	Total	C	N	O	S	0	0
			652	423	108	119	2		

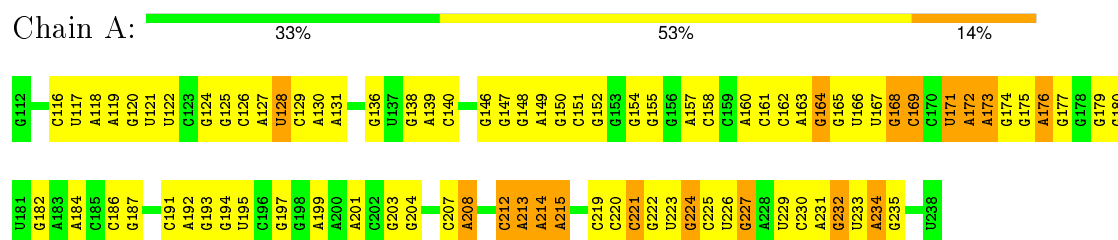
- Molecule 9 is a protein called ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	6	81	Total	C	N	O	S	0	0
			671	416	138	115	2		

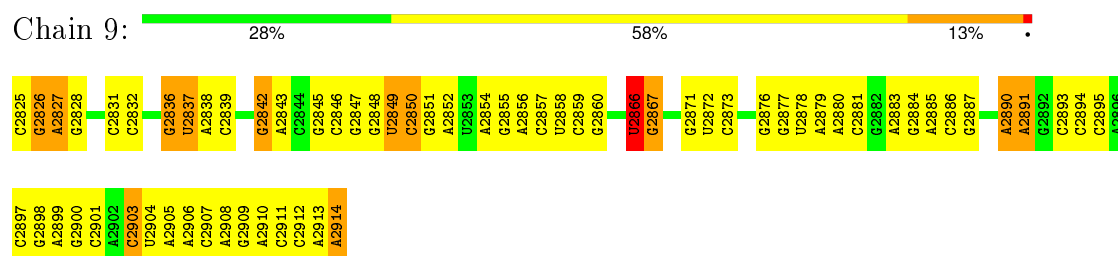
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

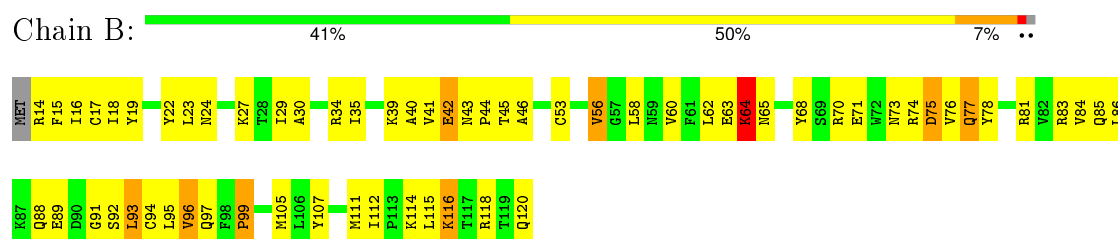
- Molecule 1: SRP RNA



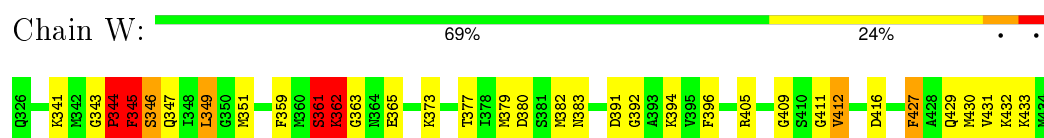
- Molecule 2: ribosomal RNA



- Molecule 3: Signal recognition particle 19 kDa protein (SRP19)

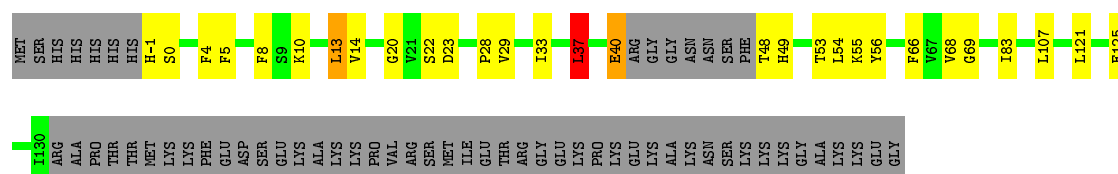


- Molecule 4: Signal recognition particle 54 kDa protein (SRP54)



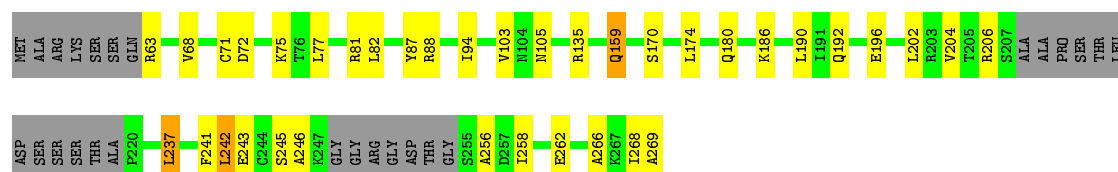
- Molecule 5: Signal recognition particle receptor alpha subunit (SR a)





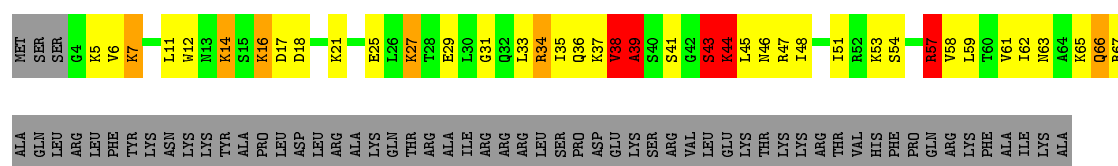
- Molecule 6: Signal recognition particle receptor beta subunit (SR b)

Chain 2: 71% 16% 12%



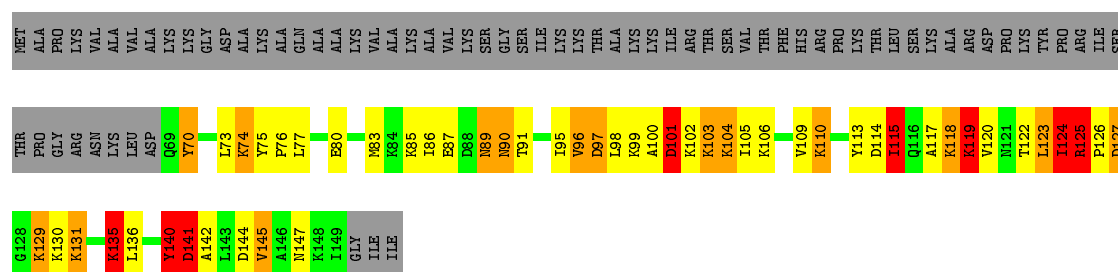
- Molecule 7: ribosomal protein L35

Chain 5: 19% 23% 5% 48%



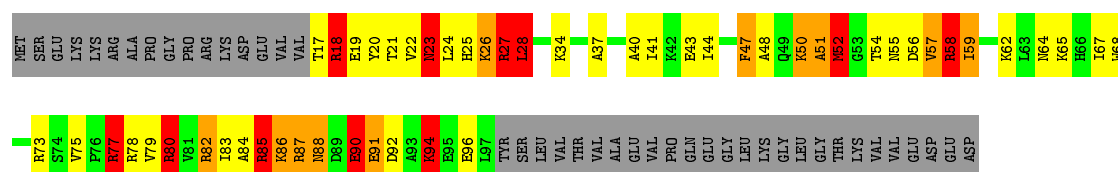
- Molecule 8: ribosomal protein L23

Chain 4: 19% 19% 10% 5% 47%



- Molecule 9: ribosomal protein L31

Chain 6: 24% 24% 9% 9% 34%



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	Depositor
Image detector	KODAK SO163 FILM	Depositor

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	Bond lengths		Bond angles	
		RMSZ	$\# Z > 2$	RMSZ	$\# Z > 2$
1	A	0.45	0/3053	0.70	0/4758
2	9	0.42	0/2167	0.72	1/3379 (0.0%)
3	B	0.46	0/884	0.69	0/1188
4	W	0.95	2/876 (0.2%)	1.26	8/1165 (0.7%)
5	1	0.60	0/1035	0.71	1/1389 (0.1%)
6	2	0.53	0/1496	0.75	2/2008 (0.1%)
7	5	1.48	4/506 (0.8%)	2.69	24/673 (3.6%)
8	4	1.43	10/660 (1.5%)	3.42	44/885 (5.0%)
9	6	1.35	3/680 (0.4%)	1.95	24/906 (2.6%)
All	All	0.76	19/11357 (0.2%)	1.29	104/16351 (0.6%)

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	A	0	3
2	9	0	2
4	W	0	5
7	5	2	2
8	4	3	7
9	6	0	11
All	All	5	30

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	W	345	PHE	C-N	-18.40	0.91	1.34
4	W	362	LYS	C-N	17.62	1.64	1.33
7	5	38	VAL	C-N	11.88	1.61	1.34
7	5	39	ALA	N-CA	-11.08	1.24	1.46
7	5	38	VAL	CA-C	10.76	1.80	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	4	97	ASP	N-CA	-9.12	1.28	1.46
8	4	125	ARG	CZ-NH2	9.02	1.44	1.33
8	4	131	LYS	CD-CE	8.06	1.71	1.51
8	4	140	TYR	CE2-CZ	-7.89	1.28	1.38
8	4	135	LYS	CD-CE	6.86	1.68	1.51
8	4	97	ASP	CB-CG	6.08	1.64	1.51
7	5	34	ARG	CZ-NH2	6.01	1.40	1.33
8	4	131	LYS	CE-NZ	5.78	1.63	1.49
9	6	85	ARG	CZ-NH1	5.62	1.40	1.33
8	4	135	LYS	CE-NZ	5.59	1.63	1.49
8	4	96	VAL	C-N	5.58	1.46	1.34
9	6	58	ARG	CZ-NH2	5.40	1.40	1.33
9	6	27	ARG	CZ-NH1	5.36	1.40	1.33
8	4	125	ARG	CD-NE	-5.31	1.37	1.46

All (104) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	4	125	ARG	NE-CZ-NH2	-72.81	83.89	120.30
7	5	39	ALA	N-CA-CB	-42.85	50.11	110.10
4	W	362	LYS	C-N-CA	-28.46	62.54	122.30
8	4	125	ARG	NE-CZ-NH1	20.51	130.55	120.30
7	5	34	ARG	NE-CZ-NH1	-20.27	110.16	120.30
8	4	97	ASP	CB-CG-OD1	17.33	133.90	118.30
7	5	39	ALA	N-CA-C	-15.52	69.10	111.00
9	6	18	ARG	NE-CZ-NH2	-14.67	112.96	120.30
7	5	38	VAL	CA-C-O	-14.15	90.39	120.10
7	5	43	SER	N-CA-CB	-13.21	90.69	110.50
7	5	38	VAL	CA-C-N	12.98	145.76	117.20
9	6	18	ARG	NE-CZ-NH1	12.94	126.77	120.30
8	4	97	ASP	CB-CG-OD2	-12.52	107.03	118.30
8	4	125	ARG	NH1-CZ-NH2	12.50	133.15	119.40
4	W	362	LYS	O-C-N	11.68	143.05	123.20
4	W	345	PHE	C-N-CA	11.67	150.86	121.70
8	4	97	ASP	CB-CA-C	11.60	133.60	110.40
4	W	361	SER	CA-C-N	-11.56	91.77	117.20
8	4	90	ASN	CB-CG-OD1	-11.35	98.89	121.60
8	4	96	VAL	C-N-CA	-11.31	93.41	121.70
8	4	141	ASP	C-N-CA	11.16	149.60	121.70
7	5	43	SER	N-CA-C	10.90	140.44	111.00
4	W	362	LYS	CA-C-N	-10.52	95.15	116.20
9	6	52	MET	CG-SD-CE	-10.06	84.10	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	5	43	SER	C-N-CA	9.85	146.31	121.70
8	4	131	LYS	CD-CE-NZ	9.66	133.93	111.70
7	5	17	ASP	CB-CG-OD2	9.59	126.94	118.30
8	4	142	ALA	CB-CA-C	-9.59	95.72	110.10
8	4	101	ASP	C-N-CA	9.47	145.37	121.70
8	4	115	ILE	CA-CB-CG1	9.31	128.69	111.00
4	W	361	SER	O-C-N	9.18	137.39	122.70
7	5	57	ARG	NE-CZ-NH1	-8.93	115.83	120.30
8	4	101	ASP	N-CA-C	8.87	134.96	111.00
9	6	57	VAL	CB-CA-C	8.61	127.77	111.40
7	5	38	VAL	C-N-CA	-8.57	100.26	121.70
8	4	145	VAL	CA-CB-CG2	-8.48	98.17	110.90
7	5	38	VAL	N-CA-C	8.34	133.52	111.00
8	4	115	ILE	CA-CB-CG2	-8.20	94.51	110.90
8	4	140	TYR	CG-CD1-CE1	-8.19	114.75	121.30
8	4	135	LYS	CA-CB-CG	8.11	131.25	113.40
7	5	44	LYS	N-CA-CB	8.05	125.09	110.60
9	6	58	ARG	NE-CZ-NH2	-8.02	116.29	120.30
8	4	131	LYS	CG-CD-CE	8.00	135.88	111.90
9	6	90	GLU	CA-CB-CG	7.87	130.72	113.40
8	4	90	ASN	CB-CG-ND2	7.87	135.58	116.70
7	5	38	VAL	CB-CA-C	7.79	126.20	111.40
8	4	96	VAL	CG1-CB-CG2	-7.74	98.52	110.90
7	5	39	ALA	CA-C-N	7.68	134.10	117.20
7	5	39	ALA	O-C-N	-7.55	110.61	122.70
9	6	28	LEU	CB-CA-C	-7.42	96.11	110.20
8	4	135	LYS	CD-CE-NZ	7.33	128.56	111.70
8	4	101	ASP	CA-C-N	-7.29	101.17	117.20
8	4	135	LYS	CB-CG-CD	7.22	130.37	111.60
7	5	43	SER	O-C-N	7.10	134.06	122.70
8	4	101	ASP	CB-CG-OD2	-7.07	111.94	118.30
8	4	119	LYS	CD-CE-NZ	7.07	127.95	111.70
9	6	52	MET	CA-CB-CG	7.03	125.24	113.30
9	6	85	ARG	CB-CA-C	-7.02	96.36	110.40
7	5	34	ARG	NH1-CZ-NH2	6.94	127.03	119.40
9	6	85	ARG	N-CA-CB	6.89	123.01	110.60
7	5	38	VAL	CA-CB-CG2	6.85	121.18	110.90
9	6	23	ASN	N-CA-C	-6.84	92.54	111.00
9	6	27	ARG	NE-CZ-NH1	-6.80	116.90	120.30
9	6	85	ARG	NE-CZ-NH1	-6.71	116.95	120.30
8	4	96	VAL	CA-C-O	-6.67	106.10	120.10
8	4	141	ASP	N-CA-C	6.58	128.75	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	W	361	SER	C-N-CA	-6.53	105.37	121.70
4	W	344	PRO	O-C-N	-6.52	112.27	122.70
8	4	70	TYR	CB-CG-CD1	6.51	124.91	121.00
8	4	141	ASP	CA-C-N	-6.46	102.98	117.20
9	6	80	ARG	N-CA-C	-6.32	93.94	111.00
8	4	115	ILE	CB-CA-C	-6.30	98.99	111.60
9	6	90	GLU	N-CA-CB	6.23	121.82	110.60
7	5	17	ASP	CB-CG-OD1	-6.21	112.71	118.30
7	5	43	SER	CA-C-N	-6.02	103.95	117.20
8	4	140	TYR	CG-CD2-CE2	-5.99	116.51	121.30
8	4	141	ASP	O-C-N	5.97	132.26	122.70
8	4	89	ASN	CB-CG-OD1	5.80	133.20	121.60
9	6	94	LYS	N-CA-CB	5.73	120.92	110.60
8	4	125	ARG	CB-CA-C	5.71	121.83	110.40
8	4	102	LYS	CB-CA-C	-5.70	99.00	110.40
5	1	37	LEU	CA-CB-CG	5.68	128.38	115.30
7	5	39	ALA	CB-CA-C	5.67	118.61	110.10
7	5	57	ARG	NE-CZ-NH2	5.66	123.13	120.30
9	6	85	ARG	NE-CZ-NH2	5.66	123.13	120.30
7	5	38	VAL	N-CA-CB	-5.64	99.08	111.50
6	2	242	LEU	CA-CB-CG	5.56	128.09	115.30
8	4	125	ARG	N-CA-CB	5.54	120.57	110.60
9	6	58	ARG	NE-CZ-NH1	5.51	123.05	120.30
9	6	96	GLU	N-CA-C	-5.50	96.15	111.00
8	4	124	ILE	N-CA-C	-5.49	96.17	111.00
8	4	140	TYR	CE1-CZ-OH	5.49	134.92	120.10
9	6	82	ARG	N-CA-C	-5.46	96.26	111.00
9	6	88	ASN	N-CA-C	-5.43	96.35	111.00
8	4	123	LEU	CB-CG-CD1	5.39	120.17	111.00
2	9	2914	A	C2'-C3'-O3'	5.38	122.31	113.70
8	4	124	ILE	O-C-N	-5.36	114.13	122.70
9	6	19	GLU	N-CA-C	-5.29	96.70	111.00
6	2	237	LEU	CA-CB-CG	5.29	127.47	115.30
8	4	101	ASP	N-CA-CB	5.26	120.07	110.60
9	6	52	MET	N-CA-C	-5.26	96.81	111.00
8	4	97	ASP	N-CA-CB	-5.23	101.19	110.60
8	4	119	LYS	CG-CD-CE	5.14	127.31	111.90
9	6	85	ARG	CD-NE-CZ	-5.09	116.48	123.60

All (5) chirality outliers are listed below:

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Mol	Chain	Res	Type	Atom
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Mol	Chain	Res	Type	Atom
7	5	38	VAL	CA
7	5	39	ALA	CA
8	4	97	ASP	CA
8	4	125	ARG	CA
8	4	141	ASP	CA

All (30) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	4	101	ASP	Mainchain,Peptide
8	4	124	ILE	Peptide
8	4	125	ARG	Sidechain
8	4	140	TYR	Sidechain
8	4	141	ASP	Peptide
8	4	89	ASN	Peptide
7	5	38	VAL	Peptide
7	5	43	SER	Peptide
9	6	18	ARG	Sidechain
9	6	27	ARG	Sidechain
9	6	47	PHE	Sidechain
9	6	50	LYS	Peptide
9	6	51	ALA	Peptide
9	6	58	ARG	Sidechain
9	6	77	ARG	Sidechain
9	6	80	ARG	Sidechain
9	6	86	LYS	Peptide
9	6	87	ARG	Sidechain,Peptide
2	9	2842	G	Sidechain
2	9	2866	U	Sidechain
1	A	197	G	Sidechain
1	A	201	A	Sidechain
1	A	208	A	Sidechain
4	W	344	PRO	Mainchain,Peptide
4	W	361	SER	Mainchain,Peptide
4	W	362	LYS	Peptide

5.2 Too-close contacts ⓘ

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	A	2728	0	1366	186	0
2	9	1935	0	977	103	0
3	B	870	0	901	79	0
4	W	865	0	871	34	0
5	1	1020	0	1019	53	0
6	2	1479	0	1533	31	0
7	5	504	0	553	58	0
8	4	652	0	708	85	0
9	6	671	0	705	90	0
All	All	10724	0	8633	627	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 33.

All (627) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:9:2904:U:H4'	9:6:20:TYR:CD2	1.45	1.51
7:5:38:VAL:C	7:5:38:VAL:HA	1.20	1.49
7:5:38:VAL:C	7:5:38:VAL:CA	1.80	1.47
1:A:173:A:C1'	1:A:224:G:C4'	1.87	1.45
2:9:2856:A:H4'	9:6:78:ARG:CG	1.40	1.44
1:A:127:A:C1'	1:A:224:G:N2	1.72	1.41
1:A:127:A:C2'	1:A:224:G:C2	1.78	1.40
1:A:173:A:H1'	1:A:224:G:C4'	0.94	1.39
5:1:1:1:HIS:CB	5:1:4:PHE:CD2	1.95	1.39
5:1:0:SER:C	5:1:29:VAL:HG23	1.10	1.38
1:A:127:A:C3'	1:A:224:G:N2	1.88	1.37
1:A:173:A:C1'	1:A:224:G:H4'	1.50	1.36
1:A:173:A:H1'	1:A:224:G:C5'	1.60	1.32
1:A:125:G:C8	1:A:227:G:C6	2.12	1.31
2:9:2856:A:C4'	9:6:78:ARG:HG3	1.55	1.31
1:A:125:G:C8	1:A:227:G:O6	1.84	1.30
1:A:127:A:H2'	1:A:224:G:C2	1.38	1.30
1:A:172:A:C6	1:A:224:G:O2'	1.85	1.30
1:A:172:A:N6	1:A:225:C:O4'	1.64	1.29
1:A:172:A:C5	1:A:224:G:O2'	1.74	1.27
6:2:204:VAL:HG11	9:6:17:THR:O	1.14	1.26
2:9:2856:A:O4'	9:6:23:ASN:ND2	1.68	1.26

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:1:0:SER:C	5:1:29:VAL:CG2	2.04	1.25
1:A:234:A:OP2	5:1:49:HIS:HA	1.12	1.21
7:5:34:ARG:O	8:4:75:TYR:CD1	1.94	1.21
4:W:343:GLY:O	4:W:346:SER:HB2	1.05	1.19
2:9:2854:A:O2'	9:6:26:LYS:HE3	1.41	1.19
2:9:2854:A:O2'	9:6:26:LYS:CE	1.91	1.18
1:A:173:A:O2'	1:A:224:G:H5''	1.02	1.17
5:1:-1:HIS:HB2	5:1:4:PHE:CD2	1.79	1.16
2:9:2856:A:O2'	9:6:78:ARG:CD	1.96	1.14
4:W:361:SER:O	4:W:362:LYS:HG3	1.43	1.14
4:W:343:GLY:O	4:W:346:SER:CB	1.97	1.13
1:A:173:A:O2'	1:A:224:G:C5'	1.98	1.11
1:A:125:G:O2'	1:A:227:G:C1'	1.97	1.11
6:2:204:VAL:CG1	9:6:17:THR:O	1.99	1.10
8:4:140:TYR:CZ	8:4:145:VAL:HG21	1.88	1.09
1:A:172:A:C6	1:A:224:G:C2'	2.36	1.09
1:A:173:A:C2'	1:A:224:G:H5''	1.82	1.08
5:1:-1:HIS:HB3	5:1:4:PHE:CD2	1.73	1.07
1:A:173:A:C2	1:A:224:G:N3	2.18	1.06
2:9:2905:A:OP1	9:6:51:ALA:O	1.71	1.06
1:A:173:A:H1'	1:A:224:G:O4'	1.55	1.05
7:5:34:ARG:O	8:4:75:TYR:CE1	2.08	1.05
1:A:125:G:O2'	1:A:227:G:C8	2.08	1.05
1:A:127:A:N9	1:A:225:C:N3	2.05	1.04
2:9:2856:A:O2'	9:6:78:ARG:HD2	1.02	1.04
2:9:2904:U:C4'	9:6:20:TYR:CD2	2.40	1.03
7:5:38:VAL:O	7:5:38:VAL:HA	1.56	1.03
1:A:234:A:OP2	5:1:49:HIS:CA	2.08	1.02
1:A:172:A:H61	1:A:225:C:C1'	1.73	1.01
5:1:0:SER:O	5:1:29:VAL:HG23	1.59	1.01
1:A:125:G:O2'	1:A:227:G:N9	1.56	1.01
7:5:38:VAL:CG2	8:4:76:PRO:O	2.10	1.00
1:A:126:C:O2'	1:A:226:U:O4'	1.63	0.99
5:1:-1:HIS:HB2	5:1:4:PHE:HD2	1.09	0.98
2:9:2904:U:O2'	9:6:47:PHE:CZ	2.16	0.98
2:9:2856:A:HO2'	9:6:78:ARG:HD2	1.18	0.98
8:4:136:LEU:HD13	8:4:140:TYR:CE2	1.98	0.97
2:9:2904:U:H5''	9:6:20:TYR:HE2	1.26	0.97
2:9:2904:U:C4'	9:6:20:TYR:HD2	1.76	0.97
5:1:-1:HIS:CB	5:1:4:PHE:HD2	1.49	0.97
2:9:2904:U:H4'	9:6:20:TYR:CE2	1.99	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:220:C:H2'	1:A:221:C:H5''	1.45	0.96
7:5:34:ARG:HH12	7:5:48:ILE:HG23	1.29	0.95
5:1:-1:HIS:HB3	5:1:4:PHE:CE2	2.01	0.95
1:A:172:A:C6	1:A:225:C:O4'	1.96	0.95
8:4:119:LYS:HD3	8:4:135:LYS:HZ3	1.30	0.95
7:5:38:VAL:C	8:4:75:TYR:OH	2.04	0.95
3:B:60:VAL:HG23	3:B:83:ARG:O	1.67	0.94
1:A:172:A:C6	1:A:224:G:H2'	2.02	0.92
5:1:0:SER:CA	5:1:54:LEU:HD21	2.00	0.92
1:A:173:A:H1'	1:A:224:G:H4'	0.93	0.91
2:9:2906:A:P	9:6:50:LYS:HG2	2.11	0.91
2:9:2856:A:HO2'	9:6:21:THR:HG1	1.19	0.91
1:A:127:A:C3'	1:A:224:G:H21	1.66	0.90
1:A:126:C:O2	1:A:226:U:C6	2.24	0.90
2:9:2904:U:H5''	9:6:20:TYR:CE2	2.06	0.90
1:A:127:A:C8	1:A:225:C:N3	2.40	0.90
2:9:2905:A:O3'	9:6:50:LYS:HG2	1.71	0.89
1:A:127:A:C2'	1:A:128:U:H5''	2.02	0.89
1:A:221:C:N4	1:A:222:G:O6	2.05	0.89
3:B:64:LYS:HD3	3:B:64:LYS:N	1.88	0.89
5:1:0:SER:HA	5:1:54:LEU:HD21	1.56	0.88
1:A:172:A:N7	1:A:224:G:O2'	2.06	0.88
1:A:126:C:C2	1:A:226:U:N1	2.17	0.88
6:2:204:VAL:HG12	9:6:18:ARG:CD	2.04	0.88
7:5:38:VAL:O	7:5:38:VAL:CA	2.18	0.87
1:A:124:G:C6	1:A:126:C:C5	2.62	0.87
2:9:2890:A:H5''	2:9:2890:A:H8	1.37	0.87
1:A:127:A:H2'	1:A:128:U:H5''	1.57	0.87
5:1:-1:HIS:ND1	5:1:68:VAL:O	2.06	0.87
1:A:127:A:C2'	1:A:224:G:N2	0.72	0.87
3:B:94:CYS:O	3:B:95:LEU:HD23	1.74	0.86
8:4:122:THR:HG23	8:4:130:LYS:HD3	1.56	0.86
1:A:173:A:C1'	1:A:224:G:O4'	2.05	0.86
5:1:0:SER:HB2	5:1:29:VAL:N	1.58	0.85
1:A:126:C:O2'	1:A:226:U:C4'	2.24	0.85
2:9:2906:A:OP1	9:6:50:LYS:HG2	1.77	0.84
1:A:184:A:N3	4:W:405:ARG:NH1	2.24	0.84
1:A:127:A:C2'	1:A:224:G:H21	0.59	0.84
1:A:126:C:O2	1:A:226:U:N1	2.08	0.84
9:6:54:THR:HA	9:6:90:GLU:HB2	1.61	0.83
1:A:173:A:C1'	1:A:224:G:C5'	2.39	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:U:H5''	1:A:224:G:H21	1.44	0.82
7:5:27:LYS:HE3	7:5:27:LYS:O	1.80	0.82
1:A:127:A:O2'	1:A:224:G:N2	1.94	0.82
4:W:361:SER:O	4:W:362:LYS:CG	2.27	0.82
3:B:14:ARG:NH1	3:B:14:ARG:HB3	1.96	0.81
3:B:24:ASN:HD22	3:B:27:LYS:HG3	1.42	0.81
8:4:136:LEU:HD13	8:4:140:TYR:HE2	1.43	0.81
1:A:127:A:C3'	1:A:224:G:H22	1.66	0.81
7:5:12:TRP:HE1	7:5:61:VAL:HG22	1.45	0.81
1:A:172:A:N6	1:A:224:G:O2'	2.14	0.80
5:1:0:SER:O	5:1:29:VAL:CG2	2.23	0.80
7:5:35:ILE:HA	8:4:75:TYR:HE1	1.46	0.80
2:9:2855:G:C4	9:6:23:ASN:OD1	2.28	0.80
2:9:2854:A:C2'	9:6:26:LYS:HE3	2.10	0.80
6:2:204:VAL:HG12	9:6:18:ARG:HD2	1.63	0.79
7:5:38:VAL:HG23	8:4:76:PRO:O	1.81	0.79
1:A:128:U:H5''	1:A:224:G:N2	1.96	0.79
4:W:344:PRO:C	4:W:346:SER:N	2.34	0.79
8:4:115:ILE:HG21	8:4:140:TYR:OH	1.81	0.79
1:A:173:A:C1'	1:A:224:G:H5''	2.09	0.78
1:A:125:G:O2'	1:A:227:G:H1'	1.82	0.78
5:1:0:SER:CB	5:1:29:VAL:N	2.31	0.78
1:A:124:G:N1	1:A:126:C:C5	2.52	0.78
1:A:220:C:C2'	1:A:221:C:H5''	2.14	0.78
8:4:136:LEU:HD13	8:4:140:TYR:CD2	2.18	0.78
2:9:2905:A:OP1	9:6:51:ALA:CB	2.32	0.78
2:9:2856:A:C1'	9:6:23:ASN:HD21	1.97	0.78
6:2:204:VAL:CG1	9:6:18:ARG:HD3	2.14	0.77
4:W:344:PRO:O	4:W:346:SER:N	2.18	0.76
2:9:2904:U:C5'	9:6:20:TYR:CE2	2.69	0.76
7:5:35:ILE:HA	8:4:75:TYR:CE1	2.20	0.76
7:5:54:SER:HA	7:5:57:ARG:HE	1.51	0.76
1:A:175:G:H3'	1:A:176:A:H5'	1.68	0.75
1:A:127:A:H2'	1:A:128:U:C5'	2.17	0.75
8:4:115:ILE:HG21	8:4:140:TYR:CZ	2.21	0.75
1:A:127:A:C1'	1:A:225:C:N3	2.29	0.75
3:B:14:ARG:HB3	3:B:14:ARG:CZ	2.17	0.75
8:4:140:TYR:CE2	8:4:145:VAL:HG21	2.22	0.75
8:4:119:LYS:HD3	8:4:135:LYS:NZ	2.02	0.75
2:9:2878:U:H2'	2:9:2879:A:O4'	1.86	0.75
2:9:2904:U:C4'	9:6:20:TYR:CE2	2.66	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:5:38:VAL:HG21	8:4:76:PRO:O	1.86	0.74
1:A:173:A:C4	1:A:224:G:O2'	2.39	0.74
7:5:16:LYS:HG3	7:5:67:ARG:C	2.08	0.74
8:4:105:ILE:HD11	8:4:130:LYS:HE3	1.70	0.74
8:4:115:ILE:HG22	8:4:140:TYR:CE1	2.23	0.74
9:6:25:HIS:CE1	9:6:79:VAL:HG12	2.23	0.74
2:9:2906:A:OP1	9:6:50:LYS:CG	2.36	0.73
5:1:-1:HIS:CB	5:1:4:PHE:CE2	2.67	0.73
1:A:234:A:P	5:1:49:HIS:HA	2.28	0.73
7:5:35:ILE:CA	8:4:75:TYR:HE1	2.00	0.73
1:A:127:A:C2'	1:A:224:G:N3	2.47	0.73
1:A:117:U:H3	1:A:234:A:H61	1.37	0.73
2:9:2903:C:H5'	2:9:2903:C:H6	1.55	0.72
1:A:148:G:H4'	3:B:15:PHE:O	1.89	0.72
8:4:115:ILE:CG2	8:4:140:TYR:CZ	2.73	0.72
1:A:151:C:OP1	1:A:204:G:H4'	1.90	0.72
8:4:110:LYS:HG2	8:4:115:ILE:O	1.88	0.72
2:9:2851:G:O2'	2:9:2852:A:H5'	1.90	0.72
2:9:2866:U:H1'	2:9:2891:A:C4	2.25	0.71
1:A:125:G:C2'	1:A:227:G:C8	2.60	0.71
1:A:124:G:N1	1:A:126:C:C6	2.57	0.71
9:6:83:ILE:HG22	9:6:94:LYS:HB2	1.71	0.71
2:9:2866:U:H4'	2:9:2867:G:H5'	1.71	0.71
7:5:34:ARG:NH1	7:5:48:ILE:HG23	2.06	0.71
3:B:73:ASN:ND2	3:B:75:ASP:H	1.89	0.71
7:5:34:ARG:HH12	7:5:48:ILE:CG2	2.04	0.71
9:6:55:ASN:HD22	9:6:92:ASP:HB2	1.56	0.71
1:A:130:A:H2'	1:A:131:A:C8	2.26	0.71
6:2:204:VAL:HG12	9:6:18:ARG:HD3	1.71	0.70
8:4:140:TYR:CZ	8:4:145:VAL:CG2	2.71	0.70
8:4:122:THR:O	8:4:123:LEU:HD12	1.91	0.70
2:9:2909:G:O2'	2:9:2910:A:H5'	1.91	0.70
2:9:2827:A:H2'	2:9:2828:G:O4'	1.92	0.70
5:1:-1:HIS:CE1	5:1:68:VAL:O	2.43	0.70
2:9:2904:U:C5'	9:6:20:TYR:HE2	2.00	0.69
6:2:63:ARG:HB2	6:2:135:ARG:HB2	1.75	0.69
8:4:103:LYS:O	8:4:103:LYS:HE3	1.93	0.69
7:5:38:VAL:HG11	8:4:76:PRO:HG2	1.75	0.68
9:6:25:HIS:HE1	9:6:79:VAL:HG12	1.58	0.68
1:A:154:G:O2'	1:A:155:G:H5'	1.93	0.68
1:A:127:A:C4	1:A:225:C:C4	2.82	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:4:119:LYS:HG3	8:4:135:LYS:HB2	1.75	0.68
3:B:93:LEU:HD23	3:B:93:LEU:N	2.08	0.68
5:1:-1:HIS:HD1	5:1:68:VAL:C	1.95	0.68
5:1:-1:HIS:ND1	5:1:68:VAL:C	2.47	0.68
2:9:2895:C:OP1	9:6:77:ARG:NH1	2.27	0.67
5:1:-1:HIS:C	5:1:54:LEU:HD11	2.14	0.67
7:5:44:LYS:NZ	7:5:44:LYS:HA	2.08	0.67
1:A:175:G:H1	1:A:221:C:H42	1.42	0.67
1:A:127:A:O2'	1:A:128:U:H5''	1.93	0.67
1:A:125:G:H8	1:A:227:G:C6	2.04	0.67
9:6:22:VAL:HG12	9:6:23:ASN:O	1.95	0.67
1:A:215:A:H8	1:A:215:A:O5'	1.78	0.67
4:W:361:SER:C	4:W:362:LYS:HG3	2.13	0.67
2:9:2905:A:OP1	9:6:51:ALA:HB1	1.72	0.67
3:B:15:PHE:CE1	3:B:85:GLN:HB2	2.30	0.67
3:B:14:ARG:HG2	3:B:14:ARG:O	1.95	0.66
1:A:172:A:N6	1:A:224:G:C2'	2.59	0.66
9:6:37:ALA:HB1	9:6:68:TRP:CD1	2.31	0.66
1:A:173:A:O4'	1:A:224:G:H4'	1.95	0.66
1:A:128:U:C5'	1:A:224:G:N2	2.58	0.66
1:A:127:A:O2'	1:A:224:G:C2	2.44	0.65
1:A:233:U:O4'	5:1:40:GLU:HB3	1.68	0.65
1:A:157:A:H2'	1:A:158:C:H6	1.62	0.65
6:2:202:LEU:O	6:2:206:ARG:HB2	1.96	0.65
1:A:172:A:N6	1:A:224:G:H2'	2.11	0.65
9:6:44:ILE:CD1	9:6:67:ILE:HD11	2.26	0.65
1:A:127:A:H3'	1:A:224:G:H22	1.58	0.65
9:6:67:ILE:HG23	9:6:75:VAL:HG23	1.77	0.65
4:W:349:LEU:HD22	4:W:359:PHE:HE2	1.62	0.64
9:6:56:ASP:O	9:6:92:ASP:HB3	1.97	0.64
2:9:2894:C:O2'	2:9:2895:C:H5'	1.97	0.64
5:1:0:SER:HA	5:1:28:PRO:HB2	1.78	0.64
2:9:2890:A:H5''	2:9:2890:A:C8	2.26	0.64
2:9:2908:A:H2'	2:9:2909:G:O4'	1.98	0.64
2:9:2856:A:C4'	9:6:78:ARG:CG	2.24	0.64
8:4:125:ARG:HH22	8:4:131:LYS:HZ3	1.45	0.64
6:2:204:VAL:CG1	9:6:18:ARG:CD	2.74	0.63
2:9:2854:A:O2'	9:6:26:LYS:HE2	1.91	0.63
1:A:157:A:H2'	1:A:158:C:C6	2.32	0.63
7:5:35:ILE:O	7:5:38:VAL:HG12	1.97	0.63
5:1:0:SER:N	5:1:54:LEU:HD11	2.12	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:60:VAL:HG23	3:B:83:ARG:C	2.18	0.63
1:A:148:G:O2'	3:B:83:ARG:NH2	2.31	0.63
2:9:2904:U:H4'	9:6:20:TYR:HD2	0.88	0.63
1:A:124:G:O6	1:A:126:C:C5	2.51	0.63
4:W:344:PRO:O	4:W:346:SER:HB3	1.99	0.63
5:1:20:GLY:C	5:1:22:SER:H	2.01	0.63
6:2:103:VAL:HG12	6:2:105:ASN:H	1.62	0.63
3:B:88:GLN:HE21	3:B:92:SER:HB2	1.63	0.63
1:A:195:U:O4'	4:W:411:GLY:HA3	1.99	0.63
9:6:28:LEU:HD23	9:6:75:VAL:HG11	1.80	0.63
1:A:139:A:H2'	1:A:140:C:H6	1.63	0.63
8:4:119:LYS:C	8:4:119:LYS:HD2	2.18	0.63
1:A:149:A:H4'	3:B:17:CYS:SG	2.39	0.62
3:B:76:VAL:HG13	3:B:77:GLN:N	2.14	0.62
2:9:2849:U:O2'	2:9:2850:C:OP2	2.16	0.62
1:A:124:G:C6	1:A:126:C:H5	2.13	0.62
4:W:341:LYS:O	4:W:345:PHE:CD1	2.52	0.62
3:B:107:TYR:CZ	3:B:111:MET:HG3	2.35	0.62
1:A:193:G:N1	4:W:409:GLY:O	2.32	0.62
8:4:122:THR:HG23	8:4:130:LYS:CD	2.30	0.62
1:A:127:A:C2'	1:A:224:G:H22	1.27	0.62
8:4:119:LYS:NZ	8:4:135:LYS:HD3	2.14	0.62
1:A:139:A:H2'	1:A:140:C:C6	2.35	0.61
4:W:361:SER:C	4:W:362:LYS:CG	2.66	0.61
1:A:117:U:H3	1:A:234:A:N6	1.98	0.61
2:9:2855:G:N3	9:6:23:ASN:ND2	2.49	0.60
1:A:234:A:OP2	5:1:48:THR:O	2.19	0.60
1:A:173:A:H2	1:A:224:G:N3	1.55	0.60
8:4:110:LYS:O	8:4:110:LYS:HE3	2.01	0.60
3:B:73:ASN:HD21	3:B:75:ASP:H	1.50	0.60
1:A:120:G:N2	1:A:230:C:O2	2.32	0.60
4:W:394:LYS:HB3	4:W:394:LYS:HZ2	1.67	0.60
4:W:344:PRO:O	4:W:346:SER:CB	2.50	0.60
8:4:91:THR:HG22	8:4:135:LYS:HG3	1.83	0.59
8:4:83:MET:HA	8:4:86:ILE:HG22	1.84	0.59
8:4:114:ASP:C	8:4:115:ILE:HG23	2.15	0.59
6:2:159:GLN:CD	6:2:206:ARG:HH22	2.06	0.59
5:1:-1:HIS:CG	5:1:69:GLY:CA	2.85	0.59
7:5:31:GLY:O	7:5:35:ILE:HG12	2.03	0.59
1:A:126:C:N3	1:A:226:U:N3	2.51	0.59
8:4:113:TYR:HB2	8:4:115:ILE:HD12	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:9:2900:G:H2'	2:9:2901:C:O4'	2.02	0.59
1:A:172:A:C5	1:A:224:G:C2'	2.77	0.59
2:9:2866:U:H4'	2:9:2867:G:C5'	2.32	0.58
3:B:73:ASN:ND2	3:B:75:ASP:N	2.51	0.58
8:4:125:ARG:HD3	8:4:127:ASP:HB3	1.84	0.58
1:A:212:C:H4'	1:A:213:A:OP1	2.03	0.58
3:B:73:ASN:HD21	3:B:75:ASP:CB	2.16	0.58
5:1:-1:HIS:N	5:1:4:PHE:CZ	2.52	0.58
1:A:214:A:H5'	1:A:215:A:P	2.43	0.58
1:A:233:U:H2'	1:A:234:A:H5''	1.84	0.58
1:A:233:U:H3'	1:A:234:A:H5'	1.86	0.58
5:1:0:SER:HB2	5:1:28:PRO:C	2.19	0.58
2:9:2907:C:H2'	2:9:2908:A:O4'	2.04	0.57
1:A:128:U:H6	1:A:128:U:H5'	1.68	0.57
1:A:233:U:H1'	5:1:40:GLU:HA	1.84	0.57
8:4:115:ILE:CG2	8:4:140:TYR:CE1	2.85	0.57
3:B:112:ILE:HG23	3:B:115:LEU:HD12	1.87	0.57
3:B:60:VAL:CG2	3:B:84:VAL:HG12	2.35	0.57
1:A:163:A:O5'	1:A:163:A:H8	1.87	0.57
6:2:180:GLN:HG3	6:2:243:GLU:HB3	1.87	0.57
1:A:235:G:OP1	5:1:48:THR:N	2.37	0.57
2:9:2825:C:H4'	2:9:2826:G:O5'	2.05	0.57
3:B:86:LEU:HD13	3:B:99:PRO:O	2.05	0.56
5:1:121:LEU:O	5:1:125:GLU:HG3	2.06	0.56
5:1:0:SER:CA	5:1:29:VAL:N	2.69	0.56
8:4:96:VAL:HG23	8:4:130:LYS:HE2	1.87	0.56
7:5:44:LYS:HZ2	7:5:44:LYS:HA	1.70	0.56
1:A:127:A:C2'	1:A:128:U:C5'	2.79	0.56
1:A:173:A:C4	1:A:224:G:C2'	2.56	0.56
8:4:125:ARG:NH2	8:4:131:LYS:HZ3	2.04	0.56
1:A:125:G:C4	1:A:226:U:O2	2.47	0.56
1:A:171:U:C3'	1:A:172:A:H5''	2.35	0.56
9:6:17:THR:HG22	9:6:82:ARG:HE	1.71	0.56
9:6:41:ILE:HD12	9:6:64:ASN:HD22	1.71	0.56
8:4:106:LYS:HG3	8:4:117:ALA:HB3	1.88	0.55
1:A:220:C:C3'	1:A:221:C:H5''	2.36	0.55
5:1:-1:HIS:CG	5:1:69:GLY:HA3	2.42	0.55
1:A:220:C:H2'	1:A:221:C:C5'	2.29	0.55
3:B:62:LEU:HD12	3:B:81:ARG:O	2.07	0.55
1:A:127:A:N9	1:A:225:C:C4	2.74	0.55
2:9:2856:A:H5'	9:6:23:ASN:HA	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:1:0:SER:CB	5:1:54:LEU:HD21	2.36	0.55
1:A:173:A:N1	1:A:224:G:N3	2.53	0.55
8:4:109:VAL:HG22	8:4:115:ILE:HD11	1.89	0.55
5:1:0:SER:C	5:1:29:VAL:H	2.09	0.55
2:9:2854:A:HO2'	9:6:26:LYS:HE3	1.65	0.55
3:B:76:VAL:HG13	3:B:77:GLN:H	1.71	0.55
4:W:429:GLN:O	4:W:432:LYS:HG2	2.06	0.55
4:W:379:MET:HA	4:W:382:MET:HG3	1.87	0.55
1:A:125:G:N9	1:A:227:G:O6	2.10	0.55
7:5:27:LYS:HE3	7:5:27:LYS:C	2.28	0.55
2:9:2904:U:O2'	9:6:47:PHE:CE2	2.58	0.55
8:4:83:MET:O	8:4:86:ILE:HG22	2.07	0.54
2:9:2856:A:H5''	9:6:78:ARG:HB2	1.89	0.54
3:B:77:GLN:HG2	3:B:77:GLN:O	2.05	0.54
8:4:73:LEU:HD23	8:4:96:VAL:HG12	1.88	0.54
5:1:0:SER:N	5:1:54:LEU:HD21	2.23	0.54
3:B:60:VAL:HB	3:B:84:VAL:HG12	1.90	0.54
8:4:125:ARG:HG3	8:4:129:LYS:O	2.08	0.54
3:B:116:LYS:N	3:B:116:LYS:HD2	2.23	0.54
2:9:2909:G:O2'	2:9:2910:A:C5'	2.56	0.54
3:B:64:LYS:NZ	3:B:65:ASN:H	2.06	0.54
6:2:192:GLN:O	6:2:196:GLU:HG3	2.08	0.54
7:5:33:LEU:HD13	7:5:48:ILE:HG13	1.89	0.54
1:A:125:G:C4	1:A:227:G:N7	2.74	0.54
2:9:2904:U:C5'	9:6:20:TYR:CD2	2.91	0.53
7:5:34:ARG:C	8:4:75:TYR:CD1	2.79	0.53
1:A:233:U:H3'	1:A:234:A:C5'	2.39	0.53
3:B:73:ASN:HD21	3:B:75:ASP:N	2.05	0.53
7:5:14:LYS:NZ	7:5:14:LYS:HA	2.23	0.53
2:9:2856:A:H4'	9:6:78:ARG:CB	2.32	0.53
5:1:29:VAL:O	5:1:33:ILE:HD13	2.09	0.53
3:B:88:GLN:O	3:B:91:GLY:N	2.42	0.53
3:B:116:LYS:O	3:B:120:GLN:HG2	2.09	0.53
1:A:208:A:H1'	4:W:380:ASP:O	2.08	0.53
1:A:127:A:C4	1:A:225:C:N3	2.77	0.53
4:W:341:LYS:O	4:W:345:PHE:CE1	2.62	0.53
7:5:34:ARG:NH1	7:5:48:ILE:CG2	2.70	0.53
5:1:8:PHE:HB3	5:1:14:VAL:HA	1.91	0.53
6:2:245:SER:O	6:2:256:ALA:HB1	2.09	0.53
2:9:2866:U:O2'	2:9:2867:G:P	2.67	0.53
1:A:195:U:H4'	4:W:411:GLY:O	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:A:O2'	1:A:224:G:N3	2.34	0.52
1:A:172:A:N1	1:A:224:G:H2'	2.24	0.52
3:B:112:ILE:C	3:B:114:LYS:H	2.13	0.52
2:9:2912:C:H2'	2:9:2913:A:O4'	2.09	0.52
3:B:64:LYS:HZ3	3:B:65:ASN:H	1.55	0.52
3:B:71:GLU:OE2	3:B:78:TYR:HD2	1.92	0.52
3:B:41:VAL:CG1	3:B:42:GLU:N	2.72	0.52
2:9:2858:U:H2'	2:9:2859:C:C6	2.44	0.52
8:4:85:LYS:HB3	8:4:91:THR:OG1	2.10	0.52
6:2:103:VAL:CG1	6:2:266:ALA:HA	2.40	0.52
1:A:164:G:OP2	1:A:164:G:H8	1.92	0.52
2:9:2906:A:H5'	2:9:2907:C:O4'	2.10	0.52
5:1:53:THR:O	5:1:69:GLY:HA2	2.10	0.52
8:4:114:ASP:C	8:4:115:ILE:CG2	2.75	0.52
1:A:126:C:C2	1:A:226:U:C6	2.86	0.51
3:B:64:LYS:H	3:B:64:LYS:HD3	1.71	0.51
8:4:119:LYS:CD	8:4:135:LYS:HZ3	2.13	0.51
1:A:175:G:H1	1:A:221:C:N4	2.08	0.51
7:5:35:ILE:CA	8:4:75:TYR:CE1	2.87	0.51
3:B:15:PHE:CZ	3:B:85:GLN:HB2	2.45	0.51
1:A:199:A:H8	1:A:199:A:OP1	1.93	0.51
6:2:81:ARG:HD3	6:2:246:ALA:O	2.09	0.51
3:B:60:VAL:CG2	3:B:83:ARG:O	2.52	0.51
3:B:93:LEU:HD23	3:B:93:LEU:H	1.75	0.51
3:B:64:LYS:HZ3	3:B:65:ASN:HB2	1.75	0.51
7:5:11:LEU:HD22	7:5:58:VAL:HG22	1.92	0.51
3:B:56:VAL:HG21	3:B:107:TYR:CE2	2.45	0.50
2:9:2905:A:O3'	9:6:50:LYS:HE2	2.06	0.50
1:A:127:A:C5	1:A:225:C:N4	2.79	0.50
8:4:96:VAL:HG21	8:4:130:LYS:HE3	1.94	0.50
8:4:125:ARG:CZ	8:4:131:LYS:CD	2.90	0.50
1:A:126:C:O2'	1:A:226:U:H4'	2.10	0.50
1:A:126:C:C2	1:A:226:U:N3	2.46	0.50
1:A:233:U:C4'	5:1:40:GLU:HB3	2.38	0.50
5:1:10:LYS:HG2	6:2:94:ILE:HD11	1.92	0.50
2:9:2857:C:H5'	9:6:78:ARG:NE	2.26	0.50
1:A:233:U:H1'	5:1:40:GLU:CA	1.99	0.50
1:A:121:U:H2'	1:A:122:U:C6	2.46	0.50
3:B:68:TYR:CE2	3:B:70:ARG:HB2	2.46	0.50
7:5:29:GLU:O	7:5:33:LEU:HG	2.11	0.50
8:4:119:LYS:CE	8:4:135:LYS:HD3	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:6:52:MET:CE	9:6:83:ILE:HD11	2.42	0.50
7:5:16:LYS:HE2	7:5:16:LYS:N	2.27	0.50
7:5:12:TRP:NE1	7:5:61:VAL:HG22	2.23	0.49
1:A:136:G:N3	1:A:214:A:H2	2.09	0.49
9:6:28:LEU:CD1	9:6:43:GLU:HG3	2.42	0.49
1:A:125:G:C8	1:A:227:G:N1	2.76	0.49
2:9:2856:A:OP1	9:6:77:ARG:HB3	2.12	0.49
3:B:24:ASN:ND2	3:B:27:LYS:HG3	2.22	0.49
8:4:125:ARG:CZ	8:4:131:LYS:HG3	2.42	0.49
2:9:2855:G:C4	9:6:23:ASN:CG	2.82	0.49
7:5:7:LYS:NZ	7:5:7:LYS:HA	2.27	0.49
4:W:394:LYS:HB3	4:W:394:LYS:NZ	2.27	0.49
1:A:231:A:H5''	1:A:232:G:OP2	2.12	0.49
1:A:127:A:H2'	1:A:224:G:N2	0.45	0.49
2:9:2885:A:H2'	2:9:2886:C:H6	1.78	0.49
2:9:2856:A:H4'	9:6:78:ARG:HG3	0.59	0.49
1:A:130:A:H2'	1:A:131:A:H8	1.72	0.49
2:9:2842:G:H2'	2:9:2843:A:H5'	1.95	0.49
4:W:349:LEU:HD22	4:W:359:PHE:CE2	2.45	0.49
2:9:2912:C:O2'	2:9:2913:A:H5'	2.12	0.49
4:W:392:GLY:O	4:W:396:PHE:HD1	1.95	0.49
1:A:124:G:N7	1:A:125:G:N7	2.42	0.48
8:4:103:LYS:HE3	8:4:103:LYS:C	2.33	0.48
4:W:373:LYS:O	4:W:377:THR:HG23	2.13	0.48
7:5:36:GLN:O	7:5:39:ALA:O	2.31	0.48
2:9:2903:C:O2'	2:9:2904:U:H5'	2.12	0.48
1:A:192:A:H2'	1:A:193:G:O4'	2.13	0.48
1:A:160:A:H2'	1:A:161:C:C6	2.49	0.48
3:B:29:ILE:HG22	3:B:30:ALA:N	2.28	0.48
2:9:2886:C:O2'	2:9:2887:G:H5'	2.14	0.48
6:2:186:LYS:HD3	6:2:190:LEU:HD23	1.95	0.48
1:A:165:G:N7	1:A:176:A:C6	2.82	0.48
8:4:119:LYS:HD2	8:4:120:VAL:N	2.29	0.48
8:4:119:LYS:HZ3	8:4:135:LYS:HD3	1.78	0.48
6:2:170:SER:HB3	6:2:237:LEU:HD23	1.95	0.48
7:5:35:ILE:C	8:4:75:TYR:HE1	2.16	0.48
8:4:140:TYR:OH	8:4:145:VAL:HG11	2.14	0.48
9:6:54:THR:CA	9:6:90:GLU:HB2	2.39	0.48
7:5:16:LYS:HZ2	7:5:65:LYS:HE2	1.78	0.48
5:1:13:LEU:HD11	5:1:107:LEU:HD21	1.96	0.48
1:A:224:G:H5'	1:A:224:G:H8	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:9:2883:A:H2'	2:9:2884:G:O4'	2.13	0.48
8:4:96:VAL:CG2	8:4:130:LYS:CE	2.92	0.47
8:4:125:ARG:HH22	8:4:131:LYS:NZ	2.11	0.47
2:9:2855:G:N3	9:6:23:ASN:CG	2.68	0.47
1:A:125:G:H2'	1:A:126:C:C6	2.48	0.47
9:6:55:ASN:HD21	9:6:85:ARG:HB3	1.79	0.47
9:6:55:ASN:ND2	9:6:92:ASP:HB2	2.26	0.47
2:9:2842:G:C2'	2:9:2843:A:H5'	2.45	0.47
1:A:160:A:H2'	1:A:161:C:O4'	2.14	0.47
8:4:125:ARG:CZ	8:4:125:ARG:HA	2.45	0.47
1:A:173:A:C2'	1:A:224:G:C5'	2.64	0.47
2:9:2831:C:H2'	2:9:2832:C:H5'	1.96	0.47
2:9:2897:C:O2'	2:9:2898:G:H5'	2.15	0.47
3:B:62:LEU:HD12	3:B:63:GLU:N	2.30	0.47
2:9:2836:G:H4'	2:9:2837:U:OP1	2.15	0.47
1:A:167:U:H2'	1:A:168:G:O4'	2.15	0.47
2:9:2854:A:O2'	9:6:26:LYS:NZ	2.43	0.47
8:4:91:THR:HG22	8:4:135:LYS:CG	2.44	0.47
3:B:14:ARG:CB	3:B:14:ARG:CZ	2.88	0.47
3:B:73:ASN:HD21	3:B:75:ASP:HB3	1.80	0.47
4:W:391:ASP:HB3	4:W:394:LYS:HZ2	1.79	0.47
9:6:94:LYS:HZ2	9:6:94:LYS:HB3	1.80	0.47
1:A:171:U:H3'	1:A:172:A:H5''	1.96	0.47
7:5:35:ILE:HA	7:5:38:VAL:HG12	1.95	0.46
1:A:116:C:H2'	1:A:117:U:C6	2.50	0.46
2:9:2871:G:H2'	2:9:2872:U:C6	2.51	0.46
9:6:40:ALA:HB2	9:6:75:VAL:HG21	1.98	0.46
5:1:56:TYR:HA	5:1:66:PHE:O	2.15	0.46
8:4:144:ASP:OD1	8:4:145:VAL:HG23	2.14	0.46
7:5:53:LYS:O	7:5:57:ARG:HD3	2.15	0.46
6:2:103:VAL:HG13	6:2:266:ALA:HA	1.97	0.46
2:9:2871:G:H2'	2:9:2872:U:H6	1.80	0.46
9:6:52:MET:HE1	9:6:83:ILE:HD11	1.96	0.46
8:4:110:LYS:HZ2	8:4:115:ILE:N	2.14	0.46
7:5:5:LYS:NZ	7:5:47:ARG:HD2	2.31	0.46
8:4:125:ARG:HD3	8:4:127:ASP:CB	2.45	0.46
2:9:2911:C:O2'	2:9:2912:C:H5'	2.15	0.46
9:6:28:LEU:HD11	9:6:40:ALA:HA	1.97	0.46
7:5:38:VAL:HG21	8:4:76:PRO:N	2.31	0.45
1:A:223:U:H2'	1:A:224:G:H5''	1.98	0.45
7:5:14:LYS:HB3	7:5:18:ASP:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:G:C6	1:A:147:G:C5	3.03	0.45
3:B:75:ASP:OD1	3:B:76:VAL:N	2.47	0.45
1:A:125:G:N3	1:A:227:G:N7	2.64	0.45
2:9:2856:A:C1'	9:6:23:ASN:ND2	2.58	0.45
1:A:207:C:C4	1:A:208:A:N7	2.84	0.45
3:B:43:ASN:C	3:B:118:ARG:HH22	2.20	0.45
5:1:0:SER:O	5:1:29:VAL:HG21	2.13	0.45
5:1:68:VAL:HG11	5:1:83:ILE:HD11	1.98	0.45
8:4:125:ARG:HB3	8:4:126:PRO:C	2.36	0.45
4:W:427:PHE:O	4:W:431:VAL:HG23	2.17	0.45
7:5:59:LEU:O	7:5:59:LEU:HD13	2.17	0.45
1:A:229:U:H2'	1:A:230:C:C6	2.51	0.45
7:5:65:LYS:O	7:5:66:GLN:HB3	2.16	0.45
5:1:20:GLY:C	5:1:22:SER:N	2.69	0.45
7:5:37:LYS:C	7:5:39:ALA:O	2.55	0.45
7:5:37:LYS:N	7:5:41:SER:HB3	2.32	0.45
1:A:166:U:H2'	1:A:167:U:O4'	2.17	0.45
1:A:127:A:H2'	1:A:224:G:H22	1.14	0.44
8:4:83:MET:CA	8:4:86:ILE:HG22	2.47	0.44
3:B:116:LYS:CD	3:B:116:LYS:N	2.80	0.44
2:9:2831:C:C2'	2:9:2832:C:H5'	2.46	0.44
1:A:168:G:H3'	1:A:169:C:H5'	1.99	0.44
1:A:172:A:C6	1:A:224:G:HO2'	1.69	0.44
3:B:76:VAL:C	3:B:78:TYR:N	2.70	0.44
3:B:76:VAL:O	3:B:78:TYR:N	2.50	0.44
1:A:162:C:H2'	1:A:163:A:C8	2.52	0.44
9:6:25:HIS:CE1	9:6:79:VAL:CG1	2.99	0.44
3:B:76:VAL:CG1	3:B:77:GLN:N	2.80	0.44
3:B:35:ILE:HD11	3:B:40:ALA:HA	1.99	0.44
8:4:85:LYS:HB3	8:4:91:THR:HG1	1.83	0.44
9:6:56:ASP:H	9:6:91:GLU:HA	1.83	0.44
2:9:2885:A:H2'	2:9:2886:C:C6	2.52	0.44
7:5:36:GLN:HB3	7:5:41:SER:HA	2.00	0.44
1:A:163:A:H2'	1:A:164:G:N9	2.32	0.44
4:W:344:PRO:C	4:W:346:SER:CB	2.85	0.44
7:5:16:LYS:HG3	7:5:67:ARG:O	2.17	0.44
3:B:45:THR:O	3:B:46:ALA:C	2.56	0.44
1:A:186:C:H6	1:A:186:C:O5'	2.01	0.44
2:9:2846:C:H2'	2:9:2847:G:H8	1.82	0.44
1:A:124:G:H1	1:A:125:G:H2'	1.31	0.44
7:5:66:GLN:HG2	7:5:66:GLN:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:2:82:LEU:HD23	6:2:258:ILE:HD12	2.00	0.44
1:A:138:G:H2'	1:A:139:A:H8	1.83	0.44
8:4:119:LYS:HE2	8:4:135:LYS:HD3	1.99	0.44
3:B:88:GLN:HG3	3:B:92:SER:O	2.18	0.44
2:9:2859:C:O2'	2:9:2860:G:H5'	2.18	0.44
7:5:47:ARG:O	7:5:51:ILE:HG12	2.17	0.44
1:A:179:G:N2	1:A:180:G:H1'	2.33	0.44
9:6:51:ALA:HB3	9:6:52:MET:HG3	1.99	0.43
8:4:110:LYS:HE3	8:4:110:LYS:C	2.37	0.43
4:W:430:MET:HA	4:W:433:LYS:HB3	2.00	0.43
3:B:96:VAL:HG23	3:B:97:GLN:N	2.33	0.43
2:9:2890:A:C2'	2:9:2891:A:OP2	2.65	0.43
8:4:74:LYS:NZ	8:4:74:LYS:HA	2.33	0.43
6:2:268:ILE:C	6:2:268:ILE:HD12	2.39	0.43
1:A:125:G:H2'	1:A:126:C:H6	1.81	0.43
1:A:221:C:N4	1:A:222:G:C6	2.82	0.43
3:B:15:PHE:O	3:B:83:ARG:NH2	2.52	0.43
7:5:65:LYS:O	7:5:66:GLN:CB	2.66	0.43
3:B:116:LYS:H	3:B:116:LYS:HE3	1.83	0.43
8:4:77:LEU:HD13	8:4:95:ILE:HD11	1.99	0.43
1:A:171:U:H3'	1:A:172:A:C5'	2.49	0.43
1:A:117:U:H2'	1:A:118:A:C8	2.53	0.43
3:B:24:ASN:HD22	3:B:27:LYS:CG	2.22	0.43
2:9:2899:A:O2'	2:9:2900:G:H5'	2.19	0.43
2:9:2872:U:H2'	2:9:2873:C:H6	1.84	0.43
3:B:53:CYS:O	3:B:58:LEU:HB2	2.19	0.43
3:B:73:ASN:ND2	3:B:74:ARG:N	2.67	0.43
6:2:192:GLN:HG3	6:2:241:PHE:CE1	2.54	0.43
3:B:23:LEU:HB2	3:B:44:PRO:HG3	2.01	0.43
1:A:150:G:O2'	1:A:203:G:N3	2.49	0.43
5:1:37:LEU:C	5:1:37:LEU:HD12	2.38	0.43
8:4:110:LYS:HZ1	8:4:114:ASP:HA	1.83	0.43
8:4:118:LYS:NZ	8:4:118:LYS:HA	2.33	0.43
3:B:60:VAL:CB	3:B:84:VAL:HG12	2.49	0.43
3:B:94:CYS:C	3:B:95:LEU:HD23	2.38	0.43
7:5:62:ILE:HG23	7:5:67:ARG:HA	2.01	0.43
3:B:41:VAL:HG12	3:B:42:GLU:N	2.34	0.43
2:9:2838:A:H2'	2:9:2839:C:C6	2.54	0.43
7:5:66:GLN:O	7:5:67:ARG:CB	2.67	0.42
2:9:2885:A:O2'	2:9:2886:C:H5'	2.19	0.42
6:2:258:ILE:O	6:2:262:GLU:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:4:119:LYS:CD	8:4:119:LYS:C	2.85	0.42
7:5:54:SER:CA	7:5:57:ARG:HE	2.26	0.42
8:4:125:ARG:NE	8:4:131:LYS:HG3	2.34	0.42
4:W:347:GLN:O	4:W:351:MET:HG3	2.18	0.42
2:9:2909:G:H2'	2:9:2910:A:H8	1.83	0.42
2:9:2847:G:O2'	2:9:2848:G:H5'	2.19	0.42
1:A:195:U:C4'	4:W:411:GLY:HA3	2.50	0.42
3:B:19:TYR:CE2	3:B:81:ARG:HD3	2.55	0.42
3:B:42:GLU:HG3	3:B:43:ASN:N	2.34	0.42
4:W:344:PRO:HB2	4:W:345:PHE:H	1.69	0.42
1:A:160:A:H2'	1:A:161:C:H6	1.84	0.42
8:4:98:LEU:HA	8:4:130:LYS:HB2	2.01	0.42
9:6:48:ALA:O	9:6:52:MET:HB2	2.19	0.42
9:6:83:ILE:HG22	9:6:94:LYS:CB	2.44	0.42
1:A:173:A:O3'	1:A:223:U:O2'	2.38	0.42
2:9:2856:A:O2'	9:6:21:THR:OG1	2.08	0.42
5:1:0:SER:C	5:1:29:VAL:N	2.73	0.42
1:A:117:U:H2'	1:A:118:A:H8	1.83	0.42
3:B:16:ILE:HG12	3:B:84:VAL:HG22	2.02	0.42
3:B:93:LEU:CD2	3:B:93:LEU:N	2.77	0.42
3:B:56:VAL:O	3:B:56:VAL:HG12	2.20	0.42
6:2:87:TYR:O	6:2:88:ARG:HG2	2.19	0.42
1:A:149:A:C4'	3:B:17:CYS:SG	3.08	0.42
3:B:107:TYR:O	3:B:111:MET:HG2	2.19	0.42
1:A:233:U:C3'	1:A:234:A:C5'	2.98	0.41
4:W:344:PRO:O	4:W:345:PHE:C	2.53	0.41
3:B:18:ILE:HD12	3:B:105:MET:HG2	2.02	0.41
6:2:71:CYS:O	6:2:72:ASP:HB2	2.19	0.41
1:A:171:U:H5'	1:A:172:A:OP2	2.20	0.41
1:A:126:C:C4	1:A:226:U:C2	2.99	0.41
1:A:223:U:H2'	1:A:224:G:C5'	2.49	0.41
9:6:84:ALA:O	9:6:92:ASP:HA	2.19	0.41
2:9:2836:G:O2'	2:9:2837:U:P	2.78	0.41
3:B:22:TYR:CD1	3:B:34:ARG:HG3	2.56	0.41
9:6:59:ILE:HG22	9:6:94:LYS:HD2	2.01	0.41
1:A:126:C:H2'	1:A:127:A:O4'	2.21	0.41
8:4:125:ARG:HH22	8:4:131:LYS:CE	2.34	0.41
2:9:2858:U:H2'	2:9:2859:C:H6	1.85	0.41
7:5:36:GLN:O	7:5:41:SER:HA	2.20	0.41
6:2:103:VAL:HG21	6:2:269:ALA:HB2	2.02	0.41
7:5:5:LYS:HG3	7:5:6:VAL:HG23	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:2:174:LEU:HD11	6:2:242:LEU:HG	2.03	0.41
2:9:2893:C:O2'	2:9:2894:C:H5'	2.20	0.41
1:A:151:C:H2'	1:A:152:G:H8	1.86	0.41
3:B:76:VAL:CG1	3:B:77:GLN:H	2.34	0.41
3:B:88:GLN:O	3:B:89:GLU:C	2.58	0.41
3:B:116:LYS:H	3:B:116:LYS:CE	2.34	0.41
1:A:124:G:N1	1:A:125:G:C4	2.50	0.41
2:9:2854:A:C2'	9:6:26:LYS:CE	2.83	0.41
2:9:2877:G:N2	2:9:2879:A:H3'	2.36	0.41
1:A:193:G:H2'	1:A:194:G:O4'	2.21	0.41
2:9:2825:C:C2	2:9:2826:G:C5	3.09	0.41
8:4:100:ALA:O	8:4:104:LYS:HG3	2.21	0.41
2:9:2906:A:P	9:6:50:LYS:HE2	2.61	0.41
9:6:51:ALA:HB3	9:6:52:MET:CG	2.51	0.41
1:A:207:C:O2'	1:A:208:A:H5'	2.21	0.41
8:4:119:LYS:HE2	8:4:135:LYS:CB	2.52	0.40
2:9:2845:G:O2'	2:9:2846:C:H5'	2.20	0.40
6:2:88:ARG:HG2	6:2:88:ARG:HH11	1.85	0.40
8:4:124:ILE:HD12	8:4:124:ILE:O	2.20	0.40
6:2:68:VAL:C	6:2:75:LYS:HD3	2.41	0.40
1:A:127:A:H2'	1:A:128:U:H5'	1.99	0.40
1:A:118:A:H2'	1:A:119:A:H5'	2.03	0.40
1:A:164:G:OP2	1:A:164:G:C8	2.73	0.40
6:2:77:LEU:HG	6:2:246:ALA:HB1	2.02	0.40
5:1:55:LYS:HB2	5:1:55:LYS:HE3	1.87	0.40
2:9:2880:A:H2'	2:9:2881:C:O4'	2.21	0.40
8:4:106:LYS:O	8:4:109:VAL:HG12	2.20	0.40
9:6:54:THR:HA	9:6:90:GLU:CB	2.41	0.40
4:W:412:VAL:HG22	4:W:416:ASP:OD2	2.20	0.40
9:6:20:TYR:CE1	9:6:52:MET:HE3	2.56	0.40
1:A:182:G:H21	1:A:215:A:H62	1.68	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	B	105/108 (97%)	87 (83%)	11 (10%)	7 (7%)	1	24
4	W	107/109 (98%)	100 (94%)	2 (2%)	5 (5%)	3	32
5	1	115/185 (62%)	107 (93%)	7 (6%)	1 (1%)	21	67
6	2	182/214 (85%)	177 (97%)	5 (3%)	0	100	100
7	5	62/124 (50%)	55 (89%)	2 (3%)	5 (8%)	1	19
8	4	79/152 (52%)	71 (90%)	4 (5%)	4 (5%)	2	30
9	6	79/123 (64%)	66 (84%)	10 (13%)	3 (4%)	4	37
All	All	729/1015 (72%)	663 (91%)	41 (6%)	25 (3%)	8	40

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	B	42	GLU
3	B	75	ASP
4	W	344	PRO
4	W	345	PHE
4	W	362	LYS
7	5	39	ALA
7	5	45	LEU
8	4	101	ASP
8	4	125	ARG
9	6	24	LEU
9	6	52	MET
9	6	90	GLU
3	B	99	PRO
4	W	346	SER
7	5	66	GLN
8	4	127	ASP
8	4	141	ASP
7	5	38	VAL
7	5	43	SER
3	B	64	LYS
3	B	77	GLN
5	1	23	ASP
4	W	363	GLY
3	B	56	VAL
3	B	96	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	B	96/97 (99%)	92 (96%)	4 (4%)	36	70
4	W	96/96 (100%)	91 (95%)	5 (5%)	29	65
5	1	115/166 (69%)	111 (96%)	4 (4%)	43	74
6	2	164/182 (90%)	163 (99%)	1 (1%)	90	95
7	5	55/109 (50%)	44 (80%)	11 (20%)	1	11
8	4	72/128 (56%)	53 (74%)	19 (26%)	0	5
9	6	72/108 (67%)	51 (71%)	21 (29%)	0	3
All	All	670/886 (76%)	605 (90%)	65 (10%)	15	40

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	B	39	LYS
3	B	64	LYS
3	B	93	LEU
3	B	116	LYS
4	W	349	LEU
4	W	365	GLU
4	W	383	ASN
4	W	412	VAL
4	W	427	PHE
5	1	5	PHE
5	1	13	LEU
5	1	37	LEU
5	1	40	GLU
6	2	159	GLN
7	5	7	LYS
7	5	14	LYS
7	5	16	LYS
7	5	21	LYS
7	5	25	GLU
7	5	27	LYS

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Mol	Chain	Res	Type
7	5	38	VAL
7	5	44	LYS
7	5	46	ASN
7	5	57	ARG
7	5	63	ASN
8	4	70	TYR
8	4	74	LYS
8	4	80	GLU
8	4	87	GLU
8	4	90	ASN
8	4	97	ASP
8	4	99	LYS
8	4	101	ASP
8	4	103	LYS
8	4	104	LYS
8	4	110	LYS
8	4	115	ILE
8	4	118	LYS
8	4	119	LYS
8	4	125	ARG
8	4	129	LYS
8	4	135	LYS
8	4	141	ASP
8	4	147	ASN
9	6	18	ARG
9	6	23	ASN
9	6	26	LYS
9	6	27	ARG
9	6	28	LEU
9	6	34	LYS
9	6	57	VAL
9	6	58	ARG
9	6	59	ILE
9	6	62	LYS
9	6	65	LYS
9	6	73	ARG
9	6	77	ARG
9	6	80	ARG
9	6	85	ARG
9	6	86	LYS
9	6	87	ARG
9	6	88	ASN

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Mol	Chain	Res	Type
9	6	90	GLU
9	6	91	GLU
9	6	94	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
3	B	24	ASN
3	B	59	ASN
3	B	65	ASN
3	B	73	ASN
3	B	88	GLN
4	W	383	ASN
4	W	385	GLN
4	W	429	GLN
5	1	49	HIS
5	1	99	GLN
6	2	91	GLN
6	2	194	GLN
7	5	22	GLN
7	5	63	ASN
7	5	66	GLN
8	4	71	GLN
8	4	116	GLN
9	6	23	ASN
9	6	29	HIS
9	6	39	ASN
9	6	64	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	124/127 (97%)	22 (17%)	1 (0%)
2	9	89/90 (98%)	10 (11%)	4 (4%)
All	All	213/217 (98%)	32 (15%)	5 (2%)

All (32) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	128	U

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Mol	Chain	Res	Type
1	A	129	C
1	A	164	G
1	A	168	G
1	A	169	C
1	A	171	U
1	A	172	A
1	A	173	A
1	A	174	G
1	A	176	A
1	A	177	G
1	A	187	G
1	A	191	C
1	A	213	A
1	A	214	A
1	A	215	A
1	A	219	C
1	A	221	C
1	A	224	G
1	A	227	G
1	A	232	G
1	A	234	A
2	9	2826	G
2	9	2827	A
2	9	2837	U
2	9	2850	C
2	9	2867	G
2	9	2876	G
2	9	2890	A
2	9	2891	A
2	9	2903	C
2	9	2914	A

All (5) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	212	C
2	9	2836	G
2	9	2849	U
2	9	2866	U
2	9	2890	A

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 carbohydrates 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.