



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 01:36 PM BST

PDB ID : 1YSH
EMDB ID: : EMD-1125
Title : Localization and dynamic behavior of ribosomal protein L30e
Authors : Halic, M.; Becker, T.; Frank, J.; Spahn, C.M.; Beckmann, R.
Deposited on : 2005-02-08
Resolution : 9.50 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

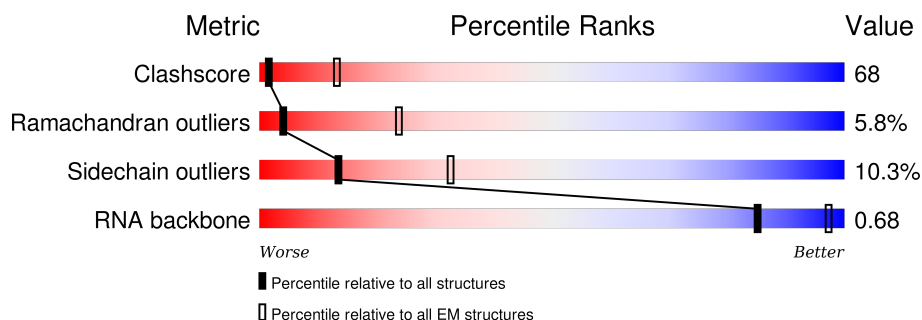
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 9.50 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	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	28	43% 50% 7%
2	F	34	47% 38% 15%
3	B	101	46% 46% 7% .
4	C	104	18% 54% 19% 9%
5	D	73	30% 55% 15%
6	E	84	29% 50% 19% .

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 5576 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 RNA (28-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	28	Total	C	N	O	P	0	0
			611	272	121	190	28		

- Molecule 2 is a RNA chain called RNA (34-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
2	F	34	Total	C	N	O	P	0	1
			717	320	139	225	33		

- Molecule 3 is a RNA chain called RNA (101-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	101	Total	C	N	O	P	0	0
			2189	973	417	698	101		

- Molecule 4 is a protein called ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	104	Total	C	N	O	S	0	0
			803	509	140	148	6		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	37	LYS	GLU	SEE REMARK 999	UNP Q5I7K9
C	57	TYR	CYS	SEE REMARK 999	UNP Q5I7K9
C	101	SER	ASN	SEE REMARK 999	UNP Q5I7K9

- Molecule 5 is a protein called ribosomal protein L37a.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	D	73	Total	C	N	O	S	0	0
			557	353	102	96	6		

- Molecule 6 is a protein called 40S RIBOSOMAL PROTEIN S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	E	84	Total	C	N	O		0	0
			699	451	131	117			

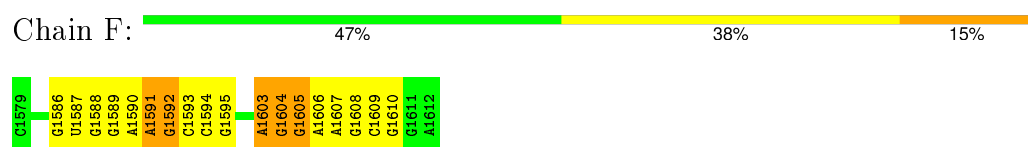
3 Residue-property plots [i](#)

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.

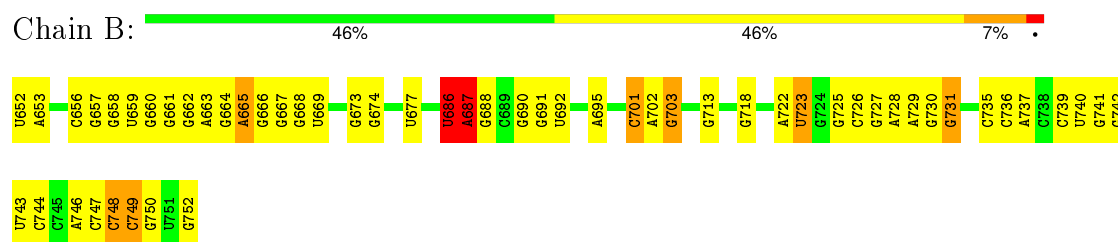
- Molecule 1: RNA (28-MER)



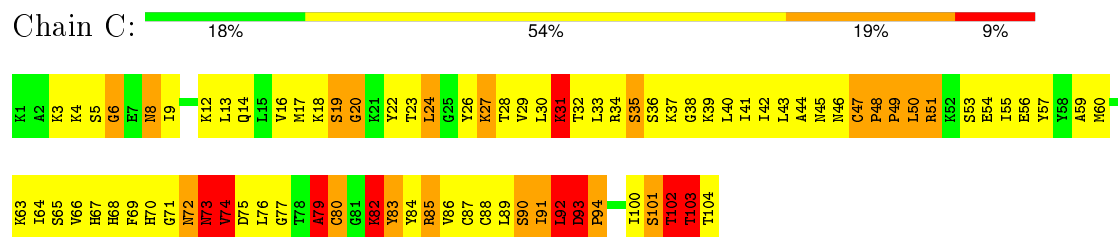
- Molecule 2: RNA (34-MER)



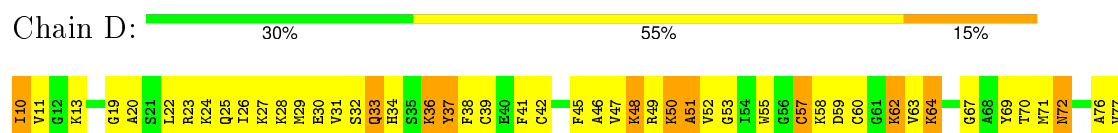
- Molecule 3: RNA (101-MER)



- Molecule 4: ribosomal protein L30

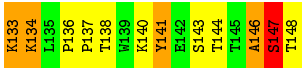
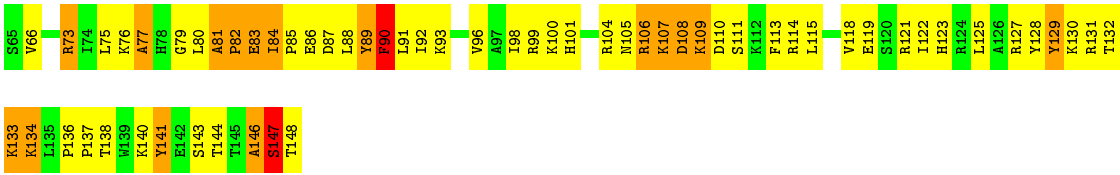
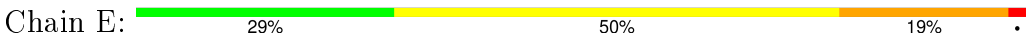


- Molecule 5: ribosomal protein L37a





● Molecule 6: 40S RIBOSOMAL PROTEIN S13



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 ($e^-/\text{\AA}^2$)	1000.00	Depositor
Minimum defocus (nm)	7000.00	Depositor
Maximum defocus (nm)	45000.00	Depositor
Magnification	38250	Depositor
Image detector	KODAK SO163 FILM	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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	0.46	0/686	0.66	0/1070
2	F	0.40	0/803	0.69	0/1252
3	B	0.51	0/2454	0.72	2/3832 (0.1%)
4	C	2.54	15/809 (1.9%)	2.58	34/1077 (3.2%)
5	D	1.05	2/566 (0.4%)	1.10	2/752 (0.3%)
6	E	2.50	7/710 (1.0%)	1.75	20/946 (2.1%)
All	All	1.36	24/6028 (0.4%)	1.25	58/8929 (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
3	B	0	1
4	C	0	8
5	D	0	2
6	E	0	5
All	All	0	16

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	E	133	LYS	CB-CG	46.84	2.79	1.52
4	C	93	ASP	CB-CG	46.73	2.49	1.51
4	C	19	SER	C-N	31.59	1.90	1.33
6	E	134	LYS	CB-CG	27.23	2.26	1.52
4	C	79	ALA	C-N	-19.82	0.88	1.34
4	C	8	ASN	CB-CG	18.22	1.93	1.51
4	C	103	THR	C-N	-16.04	0.97	1.34
6	E	132	THR	C-N	14.52	1.67	1.34
4	C	90	SER	CB-OG	-11.89	1.26	1.42
4	C	20	GLY	N-CA	9.72	1.60	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	E	82	PRO	C-N	9.52	1.55	1.34
4	C	49	PRO	N-CD	8.91	1.60	1.47
4	C	91	ILE	C-N	-8.29	1.15	1.34
4	C	94	PRO	N-CD	8.03	1.59	1.47
4	C	82	LYS	C-N	7.93	1.52	1.34
4	C	93	ASP	C-N	-7.43	1.20	1.34
6	E	84	ILE	N-CA	7.18	1.60	1.46
4	C	31	LYS	CD-CE	-6.65	1.34	1.51
5	D	64	LYS	CE-NZ	-6.15	1.33	1.49
5	D	57	CYS	CA-CB	-5.90	1.41	1.53
4	C	31	LYS	CE-NZ	5.73	1.63	1.49
6	E	133	LYS	C-O	5.39	1.33	1.23
6	E	104	ARG	CZ-NH2	5.38	1.40	1.33
4	C	35	SER	CA-CB	-5.31	1.45	1.52

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	102	THR	O-C-N	-34.43	67.61	122.70
4	C	93	ASP	CB-CG-OD2	-27.76	93.32	118.30
4	C	93	ASP	CA-CB-CG	-24.62	59.23	113.40
4	C	93	ASP	CB-CG-OD1	23.86	139.77	118.30
4	C	103	THR	O-C-N	-18.35	93.34	122.70
4	C	82	LYS	O-C-N	-17.27	95.06	122.70
4	C	103	THR	C-N-CA	17.00	164.20	121.70
4	C	79	ALA	O-C-N	-14.88	98.90	122.70
4	C	82	LYS	C-N-CA	14.86	158.86	121.70
4	C	93	ASP	O-C-N	-14.62	93.32	121.10
6	E	133	LYS	CA-CB-CG	-13.22	84.32	113.40
4	C	103	THR	CA-C-N	12.77	145.29	117.20
4	C	92	LEU	CB-CG-CD2	-12.41	89.91	111.00
4	C	82	LYS	CA-C-N	12.21	144.06	117.20
6	E	104	ARG	NE-CZ-NH2	-10.67	114.97	120.30
5	D	51	ALA	O-C-N	-9.96	106.76	122.70
4	C	92	LEU	CB-CG-CD1	9.48	127.12	111.00
6	E	83	GLU	O-C-N	-9.31	107.81	122.70
4	C	93	ASP	CA-C-N	8.63	141.26	117.10
4	C	83	TYR	N-CA-C	8.39	133.66	111.00
4	C	49	PRO	CA-N-CD	-8.38	99.77	111.50
4	C	83	TYR	CB-CA-C	-8.33	93.73	110.40
6	E	83	GLU	CA-C-N	8.09	135.00	117.20
6	E	133	LYS	CA-C-N	8.07	134.94	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	8	ASN	CB-CG-OD1	8.06	137.72	121.60
6	E	77	ALA	CB-CA-C	-7.87	98.30	110.10
6	E	134	LYS	CA-CB-CG	-7.68	96.50	113.40
4	C	74	VAL	CB-CA-C	7.53	125.71	111.40
4	C	94	PRO	CA-N-CD	-7.48	101.03	111.50
6	E	90	PHE	CB-CG-CD1	7.44	126.01	120.80
4	C	92	LEU	CA-CB-CG	7.40	132.33	115.30
4	C	73	ASN	C-N-CA	-7.23	103.63	121.70
3	B	687	A	C2'-C3'-O3'	7.20	125.35	109.50
4	C	8	ASN	CA-CB-CG	-7.14	97.69	113.40
4	C	8	ASN	CB-CG-ND2	-7.11	99.63	116.70
6	E	104	ARG	NE-CZ-NH1	7.11	123.86	120.30
4	C	35	SER	CA-CB-OG	-6.93	92.49	111.20
4	C	17	MET	CG-SD-CE	-6.80	89.31	100.20
6	E	147	SER	N-CA-C	-6.70	92.92	111.00
6	E	147	SER	N-CA-CB	6.68	120.52	110.50
5	D	51	ALA	CB-CA-C	6.65	120.07	110.10
6	E	89	TYR	CB-CG-CD2	-6.42	117.15	121.00
4	C	73	ASN	CA-C-N	-6.41	103.10	117.20
4	C	79	ALA	CA-C-N	6.32	131.10	117.20
6	E	146	ALA	N-CA-CB	6.16	118.73	110.10
4	C	19	SER	C-N-CA	-6.12	109.44	122.30
6	E	133	LYS	CA-C-O	-5.89	107.74	120.10
4	C	6	GLY	CA-C-N	-5.78	104.49	117.20
6	E	90	PHE	CB-CG-CD2	-5.34	117.06	120.80
4	C	6	GLY	O-C-N	5.22	131.05	122.70
4	C	31	LYS	CD-CE-NZ	-5.17	99.80	111.70
6	E	66	VAL	N-CA-C	-5.17	97.04	111.00
4	C	74	VAL	N-CA-C	-5.15	97.10	111.00
6	E	77	ALA	N-CA-CB	5.13	117.29	110.10
6	E	83	GLU	CB-CA-C	-5.12	100.16	110.40
3	B	686	U	C5'-C4'-C3'	-5.10	107.83	116.00
6	E	82	PRO	C-N-CA	-5.09	108.98	121.70
6	E	108	ASP	N-CA-C	-5.01	97.48	111.00

There are no chirality outliers.

All (16) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	B	727	G	Sidechain
4	C	102	THR	Mainchain
4	C	103	THR	Peptide

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Mol	Chain	Res	Type	Group
4	C	73	ASN	Mainchain
4	C	79	ALA	Mainchain,Peptide
4	C	82	LYS	Peptide
4	C	93	ASP	Mainchain,Peptide
5	D	37	TYR	Sidechain
5	D	51	ALA	Mainchain
6	E	128	TYR	Sidechain
6	E	131	ARG	Sidechain
6	E	141	TYR	Sidechain
6	E	89	TYR	Sidechain
6	E	90	PHE	Sidechain

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	A	611	0	306	76	0
2	F	717	0	359	46	0
3	B	2189	0	1098	126	0
4	C	803	0	825	272	0
5	D	557	0	577	94	0
6	E	699	0	750	249	0
All	All	5576	0	3915	647	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 68.

All (647) 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)
3:B:740:U:C1'	6:E:101:HIS:CE1	1.82	1.63
3:B:740:U:H1'	6:E:101:HIS:CE1	1.33	1.61
1:A:804:C:C6	6:E:148:THR:HG23	1.13	1.61
4:C:9:ILE:HG21	4:C:69:PHE:CE1	1.30	1.60
4:C:9:ILE:CG2	4:C:69:PHE:HE1	1.09	1.56
1:A:804:C:C6	6:E:148:THR:CG2	1.88	1.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:44:ALA:HA	4:C:70:HIS:C	1.31	1.48
1:A:797:A:H5'	5:D:10:ILE:CD1	1.43	1.47
3:B:658:G:OP1	6:E:90:PHE:CE2	1.68	1.46
6:E:130:LYS:HZ2	6:E:137:PRO:N	1.04	1.46
4:C:9:ILE:CG2	4:C:69:PHE:CE1	1.91	1.45
4:C:44:ALA:N	4:C:70:HIS:HB2	1.21	1.45
4:C:44:ALA:HA	4:C:70:HIS:CA	1.49	1.43
4:C:67:HIS:HA	4:C:104:THR:CG2	1.47	1.41
4:C:8:ASN:CG	4:C:8:ASN:CB	1.93	1.37
2:F:1605:G:N7	4:C:27:LYS:HB2	1.39	1.36
4:C:93:ASP:HA	4:C:93:ASP:CG	1.34	1.36
4:C:44:ALA:CA	4:C:70:HIS:HB2	1.52	1.35
6:E:79:GLY:HA2	6:E:80:LEU:N	1.34	1.35
1:A:804:C:H6	6:E:148:THR:CG2	1.28	1.35
3:B:740:U:O4'	6:E:101:HIS:CE1	1.78	1.34
2:F:1591:A:H62	4:C:24:LEU:CD2	1.38	1.32
4:C:76:LEU:HB3	6:E:92:ILE:CG2	1.58	1.31
2:F:1591:A:N6	4:C:24:LEU:CD2	1.93	1.30
1:A:804:C:O5'	6:E:148:THR:CG2	1.79	1.29
6:E:130:LYS:NZ	6:E:137:PRO:N	1.76	1.28
3:B:668:G:C5'	6:E:107:LYS:HG2	1.61	1.28
1:A:797:A:C5'	5:D:10:ILE:CD1	2.11	1.27
4:C:44:ALA:CA	4:C:70:HIS:CB	2.10	1.27
3:B:658:G:OP1	6:E:90:PHE:HE2	0.98	1.27
3:B:728:A:N1	6:E:113:PHE:HE2	1.29	1.27
4:C:71:GLY:O	4:C:72:ASN:CG	1.74	1.25
4:C:19:SER:C	4:C:20:GLY:N	1.89	1.25
3:B:668:G:H5''	6:E:107:LYS:CG	1.65	1.25
3:B:740:U:C4'	6:E:101:HIS:ND1	1.98	1.25
3:B:741:G:OP1	6:E:98:ILE:HD11	1.09	1.24
6:E:82:PRO:O	6:E:83:GLU:CG	1.85	1.23
6:E:82:PRO:O	6:E:83:GLU:HG3	1.33	1.23
1:A:797:A:C5'	5:D:10:ILE:HD12	1.67	1.23
3:B:728:A:N1	6:E:113:PHE:CE2	2.04	1.22
6:E:75:LEU:HA	6:E:80:LEU:CD2	1.67	1.22
6:E:75:LEU:CA	6:E:80:LEU:HD21	1.55	1.22
4:C:76:LEU:CD2	6:E:92:ILE:HG22	1.69	1.22
3:B:669:U:H5'	6:E:107:LYS:NZ	1.53	1.20
4:C:44:ALA:CA	4:C:70:HIS:C	2.07	1.20
4:C:73:ASN:N	4:C:83:TYR:CE2	2.02	1.20
4:C:42:ILE:HG22	4:C:70:HIS:CD2	1.76	1.19

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:130:LYS:HG2	6:E:141:TYR:CZ	1.74	1.19
1:A:804:C:C4'	6:E:148:THR:HG21	1.73	1.18
2:F:1591:A:N6	4:C:24:LEU:HD23	1.53	1.17
3:B:668:G:H5''	6:E:107:LYS:HG3	1.25	1.17
6:E:127:ARG:HH22	6:E:141:TYR:HA	1.09	1.16
3:B:740:U:O4'	6:E:101:HIS:ND1	1.80	1.15
1:A:797:A:C4'	5:D:10:ILE:HD12	1.76	1.15
3:B:741:G:O2'	6:E:114:ARG:HG2	1.45	1.14
1:A:806:A:OP2	6:E:147:SER:N	1.79	1.14
6:E:134:LYS:CG	6:E:134:LYS:CB	2.26	1.13
4:C:76:LEU:CB	6:E:92:ILE:HG21	1.79	1.13
4:C:48:PRO:HB3	5:D:42:CYS:SG	1.88	1.13
3:B:668:G:C5'	6:E:107:LYS:CG	2.25	1.12
4:C:44:ALA:HA	4:C:70:HIS:CB	1.76	1.12
4:C:71:GLY:O	4:C:72:ASN:OD1	1.67	1.12
4:C:93:ASP:CA	4:C:93:ASP:CG	2.16	1.12
6:E:130:LYS:HZ2	6:E:137:PRO:CA	1.62	1.11
5:D:57:CYS:HB2	5:D:62:LYS:HD3	1.21	1.11
3:B:740:U:H4'	6:E:101:HIS:ND1	1.65	1.11
1:A:797:A:C4'	5:D:10:ILE:CD1	2.27	1.11
2:F:1604:G:C4'	4:C:26:TYR:HD2	1.53	1.10
3:B:668:G:O2'	6:E:105:ASN:HA	1.52	1.09
6:E:130:LYS:HZ2	6:E:137:PRO:CD	1.64	1.09
3:B:741:G:OP1	6:E:98:ILE:CD1	2.00	1.08
4:C:44:ALA:HB2	4:C:70:HIS:HB3	1.21	1.08
1:A:804:C:C5'	6:E:148:THR:HG21	1.82	1.07
6:E:84:ILE:HB	6:E:86:GLU:OE2	1.54	1.07
2:F:1591:A:H62	4:C:24:LEU:HD21	1.12	1.07
4:C:39:LYS:O	4:C:40:LEU:HD12	1.51	1.07
3:B:668:G:C4'	6:E:107:LYS:HG2	1.83	1.07
5:D:57:CYS:CB	5:D:62:LYS:HD3	1.85	1.07
4:C:9:ILE:HG22	4:C:69:PHE:HE1	1.17	1.06
4:C:26:TYR:O	4:C:29:VAL:HG12	1.53	1.06
3:B:741:G:P	6:E:98:ILE:HD11	1.94	1.06
1:A:804:C:O5'	6:E:148:THR:HG21	1.50	1.06
3:B:668:G:HO2'	6:E:105:ASN:HA	1.00	1.06
3:B:741:G:C5'	6:E:98:ILE:HD12	1.85	1.06
2:F:1604:G:C4'	4:C:26:TYR:CD2	2.38	1.05
4:C:67:HIS:CD2	4:C:103:THR:O	2.08	1.05
4:C:44:ALA:N	4:C:70:HIS:CB	2.18	1.05
3:B:669:U:C5'	6:E:107:LYS:NZ	2.19	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:130:LYS:HG2	6:E:141:TYR:CE2	1.91	1.04
1:A:797:A:H5'	5:D:10:ILE:HD11	1.09	1.04
4:C:67:HIS:CA	4:C:104:THR:HG23	1.88	1.04
1:A:797:A:H4'	5:D:10:ILE:HD12	1.31	1.03
3:B:741:G:H5''	6:E:98:ILE:HD12	1.40	1.03
3:B:658:G:P	6:E:90:PHE:HE2	1.81	1.03
6:E:133:LYS:HB3	6:E:136:PRO:HD2	1.37	1.02
4:C:76:LEU:CB	6:E:92:ILE:CG2	2.36	1.02
2:F:1604:G:H4'	4:C:26:TYR:HD2	1.21	1.02
3:B:668:G:H4'	6:E:107:LYS:HG2	1.35	1.02
3:B:669:U:C5'	6:E:107:LYS:HZ2	1.71	1.02
3:B:742:G:H5'	6:E:114:ARG:HG2	1.42	1.01
6:E:79:GLY:CA	6:E:80:LEU:N	2.23	1.01
4:C:67:HIS:CA	4:C:104:THR:CG2	2.38	1.01
4:C:76:LEU:HD22	6:E:92:ILE:HG22	1.03	1.01
6:E:83:GLU:O	6:E:86:GLU:OE2	1.78	1.00
2:F:1605:G:N7	4:C:27:LYS:CB	2.23	1.00
1:A:805:G:OP2	6:E:147:SER:C	1.99	1.00
2:F:1591:A:H61	4:C:24:LEU:HD23	1.20	0.99
4:C:20:GLY:HA2	4:C:22:TYR:HE2	1.27	0.99
3:B:668:G:O2'	6:E:107:LYS:NZ	1.78	0.98
1:A:795:G:H2'	1:A:817:G:H22	1.25	0.98
6:E:83:GLU:O	6:E:84:ILE:CG1	2.12	0.98
2:F:1604:G:N2	5:D:60:CYS:SG	2.37	0.98
6:E:83:GLU:O	6:E:84:ILE:CB	2.12	0.98
6:E:130:LYS:CG	6:E:141:TYR:CZ	2.47	0.97
4:C:44:ALA:CB	4:C:70:HIS:HB3	1.94	0.97
3:B:741:G:P	6:E:98:ILE:CD1	2.53	0.97
3:B:740:U:C4'	6:E:101:HIS:CG	2.48	0.97
3:B:668:G:H4'	6:E:107:LYS:CG	1.85	0.96
4:C:44:ALA:CB	4:C:70:HIS:CB	2.42	0.96
3:B:728:A:C6	6:E:113:PHE:CD2	2.54	0.95
4:C:73:ASN:H	4:C:83:TYR:HE2	1.04	0.95
4:C:67:HIS:HA	4:C:104:THR:HG23	0.97	0.95
1:A:804:C:N1	6:E:148:THR:HG23	1.82	0.94
3:B:658:G:OP1	6:E:90:PHE:CZ	2.20	0.94
4:C:42:ILE:O	4:C:70:HIS:CD2	2.20	0.94
5:D:76:ALA:O	5:D:79:VAL:HG22	1.68	0.94
4:C:73:ASN:OD1	4:C:84:TYR:O	1.86	0.94
3:B:669:U:H5'	6:E:107:LYS:HZ2	1.14	0.94
4:C:76:LEU:HD22	6:E:92:ILE:CG2	1.96	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:67:HIS:HA	4:C:104:THR:HG21	1.48	0.93
4:C:44:ALA:HB2	4:C:70:HIS:CB	1.96	0.93
3:B:740:U:C1'	6:E:101:HIS:ND1	2.28	0.93
3:B:668:G:HO2'	6:E:105:ASN:CA	1.82	0.92
3:B:668:G:C4'	6:E:107:LYS:CG	2.39	0.92
3:B:664:G:H22	3:B:741:G:H1	1.15	0.92
1:A:797:A:H4'	5:D:10:ILE:HG23	1.50	0.92
6:E:83:GLU:O	6:E:84:ILE:HG13	1.67	0.92
4:C:69:PHE:CD2	4:C:70:HIS:HA	2.03	0.91
6:E:134:LYS:HD3	6:E:134:LYS:O	1.69	0.91
2:F:1604:G:H4'	4:C:26:TYR:CD2	2.03	0.90
5:D:11:VAL:HG11	5:D:23:ARG:O	1.71	0.90
4:C:83:TYR:C	4:C:84:TYR:HA	1.92	0.90
4:C:75:ASP:O	4:C:79:ALA:HB2	1.72	0.90
6:E:123:HIS:CD2	6:E:144:THR:HB	2.06	0.89
5:D:62:LYS:HD2	5:D:62:LYS:H	1.35	0.89
4:C:13:LEU:O	4:C:13:LEU:HD23	1.70	0.89
3:B:741:G:O2'	6:E:114:ARG:CG	2.21	0.89
4:C:76:LEU:HB3	6:E:92:ILE:HG21	0.89	0.89
6:E:127:ARG:NE	6:E:141:TYR:CE1	2.36	0.88
4:C:31:LYS:O	4:C:31:LYS:HE2	1.74	0.87
3:B:741:G:H5''	6:E:98:ILE:CD1	2.05	0.87
6:E:82:PRO:O	6:E:83:GLU:HG2	1.72	0.87
6:E:82:PRO:C	6:E:83:GLU:HG3	1.92	0.87
3:B:742:G:H5'	6:E:114:ARG:CG	2.05	0.87
6:E:83:GLU:C	6:E:84:ILE:HG13	1.94	0.87
3:B:740:U:O3'	6:E:98:ILE:HD13	1.75	0.87
3:B:741:G:C5'	6:E:98:ILE:CD1	2.53	0.86
1:A:804:C:O5'	6:E:148:THR:CB	2.22	0.86
3:B:728:A:C6	6:E:113:PHE:HD2	1.91	0.86
1:A:804:C:H6	6:E:148:THR:HG22	1.41	0.86
4:C:44:ALA:CA	4:C:70:HIS:CA	2.38	0.86
4:C:89:LEU:HD23	4:C:90:SER:N	1.90	0.85
2:F:1604:G:N1	5:D:42:CYS:SG	2.44	0.85
3:B:656:C:O2'	6:E:121:ARG:NH2	2.09	0.85
4:C:42:ILE:HG22	4:C:70:HIS:NE2	1.92	0.85
4:C:73:ASN:OD1	4:C:84:TYR:C	2.15	0.85
1:A:804:C:O5'	6:E:148:THR:HG22	1.77	0.84
6:E:123:HIS:CD2	6:E:146:ALA:HB2	2.11	0.84
1:A:806:A:OP2	6:E:147:SER:CA	2.26	0.84
6:E:130:LYS:CB	6:E:141:TYR:CZ	2.61	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:728:A:N6	6:E:113:PHE:CD2	2.46	0.84
6:E:85:PRO:HG3	6:E:129:TYR:CE1	2.12	0.84
6:E:83:GLU:O	6:E:84:ILE:HB	1.76	0.84
4:C:24:LEU:O	4:C:24:LEU:HD22	1.78	0.83
4:C:49:PRO:C	5:D:41:PHE:CZ	2.50	0.83
4:C:70:HIS:HB3	4:C:71:GLY:N	1.92	0.83
1:A:797:A:C4'	5:D:10:ILE:HD13	2.07	0.83
3:B:740:U:H4'	6:E:101:HIS:CG	2.08	0.83
4:C:93:ASP:OD1	4:C:93:ASP:HA	1.77	0.83
6:E:130:LYS:H	6:E:140:LYS:NZ	1.77	0.82
1:A:804:C:C5	6:E:148:THR:HG23	2.08	0.82
1:A:795:G:H2'	1:A:817:G:N2	1.94	0.82
4:C:49:PRO:C	5:D:41:PHE:HZ	1.83	0.82
6:E:130:LYS:O	6:E:133:LYS:O	1.98	0.82
4:C:24:LEU:H	4:C:24:LEU:HD13	1.43	0.82
3:B:728:A:N6	6:E:110:ASP:HA	1.94	0.82
4:C:42:ILE:C	4:C:70:HIS:HD2	1.83	0.81
4:C:69:PHE:CD2	4:C:70:HIS:CA	2.62	0.81
4:C:66:VAL:O	4:C:104:THR:HG21	1.79	0.81
4:C:23:THR:HG22	4:C:90:SER:OG	1.78	0.81
4:C:43:LEU:C	4:C:70:HIS:HB2	2.00	0.81
1:A:795:G:N2	1:A:817:G:H2'	1.94	0.81
4:C:42:ILE:O	4:C:70:HIS:HD2	1.63	0.81
4:C:42:ILE:C	4:C:70:HIS:CD2	2.55	0.80
4:C:40:LEU:HG	4:C:65:SER:OG	1.81	0.80
4:C:83:TYR:C	4:C:84:TYR:N	2.33	0.80
1:A:817:G:H4'	1:A:818:A:OP1	1.80	0.80
4:C:101:SER:O	4:C:103:THR:N	2.13	0.80
1:A:797:A:H4'	5:D:10:ILE:CD1	2.01	0.80
4:C:75:ASP:HA	4:C:83:TYR:CZ	2.17	0.80
3:B:728:A:C6	6:E:113:PHE:CE2	2.70	0.80
1:A:804:C:O4'	6:E:148:THR:HG21	1.82	0.80
2:F:1605:G:C8	4:C:27:LYS:HG3	2.16	0.80
4:C:83:TYR:C	4:C:84:TYR:CA	2.51	0.79
4:C:9:ILE:HG22	4:C:69:PHE:CE1	1.96	0.79
4:C:4:LYS:C	4:C:5:SER:C	2.40	0.79
2:F:1591:A:N6	4:C:24:LEU:CG	2.46	0.79
3:B:728:A:N1	6:E:113:PHE:CD2	2.50	0.79
3:B:673:G:H2'	3:B:674:G:C8	2.17	0.79
3:B:740:U:C5'	6:E:101:HIS:HB2	2.13	0.79
5:D:57:CYS:SG	5:D:62:LYS:HD3	2.23	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:39:CYS:HB3	5:D:62:LYS:HZ2	1.48	0.79
3:B:741:G:H5'	6:E:98:ILE:HD12	1.64	0.79
1:A:804:C:C4'	6:E:148:THR:CG2	2.58	0.79
3:B:661:G:OP2	4:C:3:LYS:NZ	2.15	0.79
6:E:88:LEU:HD11	6:E:122:ILE:HG23	1.65	0.78
4:C:83:TYR:O	4:C:84:TYR:HD1	1.66	0.78
2:F:1591:A:H62	4:C:24:LEU:CG	1.96	0.78
4:C:45:ASN:H	4:C:70:HIS:C	1.86	0.78
2:F:1590:A:N6	2:F:1605:G:H1'	1.99	0.78
6:E:130:LYS:H	6:E:140:LYS:HZ1	1.28	0.78
4:C:75:ASP:O	4:C:79:ALA:CB	2.32	0.78
4:C:23:THR:CG2	4:C:90:SER:OG	2.32	0.77
2:F:1604:G:C4	4:C:51:ARG:HG3	2.19	0.77
6:E:75:LEU:HA	6:E:80:LEU:HD21	0.81	0.77
6:E:73:ARG:NH2	6:E:77:ALA:HB2	2.00	0.77
6:E:81:ALA:N	6:E:82:PRO:HD3	2.00	0.77
4:C:76:LEU:CG	6:E:92:ILE:HG22	2.15	0.77
4:C:30:LEU:HD23	4:C:30:LEU:O	1.85	0.76
6:E:127:ARG:NH2	6:E:141:TYR:HA	1.84	0.76
4:C:31:LYS:HZ1	4:C:35:SER:CB	1.99	0.76
1:A:797:A:O4'	5:D:10:ILE:HD13	1.85	0.76
3:B:740:U:H1'	6:E:101:HIS:HE1	0.65	0.75
5:D:53:GLY:HA2	5:D:67:GLY:O	1.87	0.75
4:C:71:GLY:HA3	4:C:86:VAL:O	1.86	0.75
4:C:49:PRO:O	5:D:41:PHE:CZ	2.39	0.75
4:C:9:ILE:HG21	4:C:69:PHE:CD1	2.15	0.75
1:A:804:C:C6	6:E:148:THR:HG22	2.13	0.74
4:C:39:LYS:C	4:C:40:LEU:HD12	2.06	0.74
1:A:796:A:N6	1:A:817:G:H1'	2.01	0.74
3:B:750:G:H1'	6:E:83:GLU:OE1	1.87	0.74
3:B:740:U:O4'	6:E:101:HIS:CG	2.38	0.74
4:C:42:ILE:CG2	4:C:70:HIS:NE2	2.51	0.73
3:B:750:G:C1'	6:E:83:GLU:OE1	2.36	0.73
3:B:667:G:H22	6:E:101:HIS:HE2	1.37	0.73
2:F:1589:G:N2	2:F:1605:G:H2'	2.05	0.72
6:E:130:LYS:HZ2	6:E:137:PRO:CG	2.01	0.72
3:B:669:U:C5'	6:E:107:LYS:HZ1	1.99	0.72
6:E:130:LYS:HZ3	6:E:137:PRO:N	1.88	0.72
4:C:70:HIS:CB	4:C:71:GLY:N	2.52	0.72
3:B:748:C:H1'	3:B:749:C:H5	1.53	0.72
4:C:8:ASN:ND2	4:C:8:ASN:CB	2.52	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:24:LEU:HD22	4:C:24:LEU:C	2.10	0.71
6:E:84:ILE:N	6:E:86:GLU:CB	2.54	0.71
4:C:8:ASN:O	4:C:12:LYS:HB2	1.90	0.71
2:F:1604:G:O5'	4:C:51:ARG:NH2	2.21	0.71
3:B:740:U:H5'	6:E:101:HIS:HB2	1.70	0.71
3:B:740:U:H4'	6:E:101:HIS:CB	2.20	0.70
3:B:668:G:H5'	6:E:107:LYS:HG2	1.70	0.70
4:C:48:PRO:CB	5:D:42:CYS:SG	2.75	0.70
4:C:20:GLY:HA2	4:C:22:TYR:CE2	2.19	0.70
4:C:45:ASN:N	4:C:70:HIS:C	2.45	0.70
4:C:73:ASN:C	4:C:75:ASP:N	2.44	0.70
6:E:125:LEU:O	6:E:140:LYS:HE3	1.91	0.70
4:C:44:ALA:CB	4:C:70:HIS:C	2.60	0.70
4:C:49:PRO:O	5:D:41:PHE:HZ	1.74	0.70
4:C:70:HIS:CA	4:C:71:GLY:N	2.54	0.70
6:E:81:ALA:N	6:E:82:PRO:CD	2.55	0.70
6:E:73:ARG:HH22	6:E:77:ALA:HB2	1.55	0.70
6:E:123:HIS:NE2	6:E:144:THR:HB	2.06	0.70
4:C:49:PRO:HG2	5:D:41:PHE:CG	1.55	0.70
3:B:740:U:O3'	6:E:98:ILE:CD1	2.39	0.70
3:B:667:G:N2	6:E:101:HIS:HE2	1.89	0.69
1:A:805:G:OP2	6:E:148:THR:N	2.24	0.69
3:B:686:U:HO2'	3:B:687:A:H8	1.39	0.69
1:A:804:C:O5'	6:E:148:THR:HB	1.91	0.69
5:D:57:CYS:HB2	5:D:62:LYS:CD	2.12	0.69
3:B:701:C:H5'	3:B:703:G:O4'	1.92	0.69
3:B:740:U:C1'	6:E:101:HIS:HE1	1.54	0.69
4:C:26:TYR:OH	4:C:54:GLU:CB	2.41	0.69
4:C:9:ILE:HG23	4:C:69:PHE:HE1	1.45	0.69
4:C:40:LEU:HD23	4:C:67:HIS:CE1	2.28	0.69
4:C:8:ASN:CG	4:C:8:ASN:CA	2.61	0.69
4:C:20:GLY:CA	4:C:22:TYR:HE2	2.02	0.68
2:F:1605:G:C8	4:C:27:LYS:CG	2.76	0.68
2:F:1605:G:O6	4:C:28:THR:N	2.23	0.68
5:D:20:ALA:O	5:D:24:LYS:HG2	1.94	0.68
4:C:91:ILE:CG2	4:C:94:PRO:HD3	2.23	0.68
4:C:31:LYS:NZ	4:C:35:SER:CB	2.57	0.67
4:C:76:LEU:HD22	6:E:92:ILE:C	2.14	0.67
4:C:31:LYS:CE	4:C:35:SER:OG	2.42	0.67
5:D:57:CYS:HB3	5:D:59:ASP:OD1	1.95	0.67
4:C:27:LYS:NZ	4:C:27:LYS:HA	2.10	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1590:A:H61	2:F:1605:G:H1'	1.58	0.67
4:C:70:HIS:HA	4:C:71:GLY:N	2.09	0.67
4:C:85:ARG:O	4:C:85:ARG:NE	2.28	0.67
1:A:806:A:O3'	6:E:144:THR:O	2.11	0.67
1:A:804:C:H6	6:E:148:THR:HG21	1.48	0.67
2:F:1591:A:N3	4:C:84:TYR:HD2	1.92	0.67
6:E:85:PRO:HG3	6:E:129:TYR:HE1	1.57	0.66
3:B:662:G:H2'	3:B:663:A:C8	2.30	0.66
3:B:667:G:O2'	6:E:108:ASP:HA	1.95	0.66
4:C:29:VAL:CG2	4:C:41:ILE:HD12	2.26	0.66
6:E:134:LYS:CD	6:E:134:LYS:O	2.43	0.66
2:F:1591:A:N6	4:C:24:LEU:HG	2.11	0.66
4:C:50:LEU:O	4:C:54:GLU:HG2	1.95	0.66
4:C:24:LEU:C	4:C:24:LEU:CD2	2.64	0.66
3:B:750:G:O2'	6:E:84:ILE:HG12	1.96	0.66
4:C:73:ASN:O	4:C:75:ASP:N	2.29	0.66
3:B:668:G:O2'	6:E:105:ASN:CA	2.36	0.66
6:E:127:ARG:HA	6:E:141:TYR:HE1	1.60	0.66
4:C:76:LEU:CB	6:E:92:ILE:HG22	2.15	0.66
4:C:32:THR:HG22	4:C:38:GLY:N	2.11	0.66
4:C:32:THR:HG22	4:C:38:GLY:H	1.61	0.65
6:E:130:LYS:HB3	6:E:141:TYR:CZ	2.31	0.65
4:C:76:LEU:HD13	6:E:92:ILE:HB	1.77	0.65
6:E:123:HIS:CD2	6:E:144:THR:CB	2.80	0.65
5:D:62:LYS:HG3	5:D:64:LYS:HZ2	1.61	0.65
4:C:73:ASN:N	4:C:83:TYR:HE2	1.67	0.64
6:E:130:LYS:HZ2	6:E:137:PRO:CB	2.10	0.64
6:E:82:PRO:C	6:E:83:GLU:CG	2.60	0.64
6:E:91:LEU:HD11	6:E:121:ARG:NH1	2.13	0.64
3:B:748:C:H1'	3:B:749:C:C5	2.30	0.64
6:E:133:LYS:HB2	6:E:136:PRO:HG2	1.79	0.64
5:D:39:CYS:HB3	5:D:62:LYS:NZ	2.12	0.64
4:C:26:TYR:O	4:C:29:VAL:CG1	2.39	0.64
4:C:76:LEU:HD21	6:E:93:LYS:HA	1.78	0.63
6:E:130:LYS:HB2	6:E:141:TYR:CE1	2.33	0.63
3:B:723:U:O2	3:B:723:U:H2'	1.98	0.63
4:C:42:ILE:HB	4:C:70:HIS:HE2	1.63	0.63
1:A:795:G:H1'	1:A:818:A:N6	2.14	0.63
3:B:677:U:H3	3:B:713:G:H22	1.45	0.63
6:E:130:LYS:NZ	6:E:137:PRO:CD	2.39	0.63
2:F:1604:G:O4'	4:C:26:TYR:HD2	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:56:GLU:O	4:C:60:MET:HG2	1.98	0.63
4:C:100:ILE:HG13	4:C:101:SER:N	2.12	0.63
4:C:43:LEU:HD21	4:C:55:ILE:HD13	1.80	0.63
4:C:69:PHE:HD2	4:C:70:HIS:CA	2.10	0.62
1:A:804:C:C6	6:E:148:THR:HG21	2.21	0.62
4:C:4:LYS:C	4:C:5:SER:O	2.36	0.62
6:E:130:LYS:CB	6:E:141:TYR:CE1	2.82	0.62
2:F:1604:G:O4'	4:C:26:TYR:CD2	2.52	0.62
5:D:62:LYS:HG2	5:D:64:LYS:NZ	2.15	0.62
3:B:686:U:O2'	3:B:687:A:H8	1.82	0.62
3:B:667:G:N2	6:E:101:HIS:NE2	2.48	0.62
4:C:49:PRO:CG	5:D:41:PHE:CG	2.50	0.62
4:C:19:SER:HG	4:C:20:GLY:N	1.97	0.62
2:F:1591:A:N6	4:C:24:LEU:HD21	1.88	0.62
6:E:80:LEU:C	6:E:82:PRO:HD3	2.20	0.62
5:D:47:VAL:HG22	5:D:57:CYS:SG	2.40	0.61
4:C:67:HIS:NE2	4:C:103:THR:O	2.32	0.61
6:E:91:LEU:HD11	6:E:121:ARG:HH11	1.65	0.61
6:E:127:ARG:HH22	6:E:141:TYR:CA	1.80	0.61
5:D:62:LYS:HG2	5:D:64:LYS:HZ3	1.63	0.61
3:B:728:A:H61	6:E:110:ASP:HA	1.65	0.61
4:C:31:LYS:NZ	4:C:35:SER:OG	2.33	0.61
4:C:8:ASN:CG	4:C:8:ASN:C	2.59	0.61
4:C:24:LEU:N	4:C:24:LEU:HD13	2.16	0.61
5:D:37:TYR:HB2	5:D:47:VAL:HB	1.82	0.61
4:C:32:THR:HG21	4:C:92:LEU:HD23	1.83	0.61
4:C:71:GLY:C	4:C:72:ASN:CG	2.58	0.60
6:E:133:LYS:CG	6:E:133:LYS:CB	2.79	0.60
4:C:53:SER:O	4:C:57:TYR:CD1	2.55	0.60
2:F:1605:G:C5	4:C:27:LYS:HB2	2.31	0.60
1:A:796:A:H62	1:A:817:G:H1'	1.64	0.60
4:C:94:PRO:HG3	4:C:100:ILE:CG2	2.31	0.60
4:C:31:LYS:HE2	4:C:31:LYS:C	2.21	0.60
3:B:750:G:O4'	6:E:83:GLU:OE1	2.20	0.60
4:C:20:GLY:C	4:C:22:TYR:CD2	2.74	0.60
6:E:84:ILE:HB	6:E:86:GLU:CD	2.22	0.60
5:D:50:LYS:HA	5:D:50:LYS:HE3	1.83	0.60
4:C:67:HIS:CA	4:C:104:THR:HG21	2.20	0.60
5:D:36:LYS:NZ	5:D:36:LYS:HA	2.17	0.60
3:B:740:U:O4'	6:E:101:HIS:NE2	2.33	0.60
4:C:71:GLY:O	4:C:72:ASN:ND2	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:75:ASP:CA	4:C:83:TYR:CZ	2.84	0.59
5:D:57:CYS:SG	5:D:62:LYS:CD	2.90	0.59
4:C:4:LYS:C	4:C:5:SER:HA	2.23	0.59
5:D:38:PHE:HB3	5:D:45:PHE:CE2	2.37	0.59
5:D:22:LEU:O	5:D:26:ILE:HG12	2.02	0.59
4:C:40:LEU:CD2	4:C:67:HIS:CE1	2.86	0.58
1:A:807:A:H2'	1:A:808:A:O4'	2.03	0.58
4:C:20:GLY:O	4:C:22:TYR:HD2	1.86	0.58
5:D:62:LYS:CG	5:D:64:LYS:NZ	2.66	0.58
1:A:806:A:OP2	6:E:147:SER:HA	2.03	0.58
4:C:49:PRO:C	4:C:51:ARG:H	2.07	0.58
3:B:736:C:H2'	3:B:737:A:C8	2.39	0.58
4:C:42:ILE:CG2	4:C:70:HIS:CD2	2.69	0.57
6:E:88:LEU:CD1	6:E:122:ILE:HG23	2.33	0.57
1:A:803:C:O2'	1:A:804:C:H5'	2.03	0.57
1:A:805:G:C8	6:E:147:SER:O	2.57	0.57
1:A:806:A:P	6:E:147:SER:H	2.25	0.57
4:C:69:PHE:HD2	4:C:70:HIS:HA	1.66	0.57
2:F:1605:G:N7	4:C:27:LYS:CG	2.68	0.57
1:A:795:G:C2'	1:A:817:G:N2	2.64	0.57
6:E:80:LEU:C	6:E:82:PRO:CD	2.73	0.57
4:C:49:PRO:HD2	5:D:41:PHE:O	2.04	0.57
4:C:72:ASN:HB3	4:C:83:TYR:CE2	2.39	0.57
4:C:29:VAL:HG23	4:C:41:ILE:HD12	1.87	0.57
5:D:69:TYR:CD1	5:D:70:THR:HG23	2.40	0.57
4:C:79:ALA:O	4:C:80:CYS:O	2.23	0.57
5:D:60:CYS:HB2	5:D:62:LYS:HE3	1.86	0.57
4:C:46:ASN:OD1	4:C:47:CYS:N	2.38	0.57
6:E:130:LYS:N	6:E:140:LYS:NZ	2.50	0.57
4:C:51:ARG:HD3	4:C:51:ARG:O	2.05	0.57
1:A:817:G:HO2'	1:A:818:A:H8	1.53	0.57
4:C:66:VAL:O	4:C:66:VAL:HG13	2.04	0.57
4:C:83:TYR:O	4:C:84:TYR:HA	2.05	0.56
5:D:60:CYS:HB2	5:D:62:LYS:CE	2.35	0.56
4:C:47:CYS:CB	4:C:87:CYS:SG	2.92	0.56
4:C:49:PRO:HG2	5:D:41:PHE:CD2	2.28	0.56
4:C:73:ASN:OD1	4:C:84:TYR:N	2.38	0.56
6:E:133:LYS:O	6:E:137:PRO:CG	2.52	0.56
4:C:73:ASN:C	4:C:83:TYR:CE2	2.76	0.56
6:E:83:GLU:CB	6:E:84:ILE:HG13	2.36	0.56
1:A:795:G:C2'	1:A:817:G:H22	2.08	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1586:G:O2'	2:F:1587:U:H5'	2.06	0.56
3:B:743:U:H2'	3:B:744:C:C6	2.42	0.55
3:B:739:C:O2	6:E:101:HIS:NE2	2.39	0.55
4:C:26:TYR:OH	4:C:54:GLU:HB2	2.05	0.55
1:A:817:G:O2'	1:A:818:A:H8	1.90	0.55
1:A:806:A:C8	6:E:123:HIS:ND1	2.71	0.55
4:C:66:VAL:C	4:C:104:THR:HG21	2.27	0.55
4:C:4:LYS:C	4:C:5:SER:CA	2.75	0.55
5:D:39:CYS:SG	5:D:47:VAL:HG23	2.47	0.55
6:E:133:LYS:HB3	6:E:136:PRO:CD	2.24	0.54
4:C:20:GLY:CA	4:C:22:TYR:CE2	2.87	0.54
4:C:32:THR:CG2	4:C:38:GLY:N	2.70	0.54
3:B:741:G:O2'	6:E:114:ARG:CD	2.55	0.54
6:E:130:LYS:NZ	6:E:137:PRO:CG	2.68	0.54
2:F:1603:A:H5'	2:F:1605:G:O4'	2.07	0.54
1:A:819:A:C4'	5:D:13:LYS:HB2	2.38	0.54
4:C:20:GLY:C	4:C:22:TYR:HD2	2.10	0.54
4:C:32:THR:HG22	4:C:38:GLY:CA	2.38	0.54
6:E:75:LEU:CA	6:E:80:LEU:CD2	2.45	0.54
1:A:805:G:O5'	6:E:147:SER:O	2.25	0.53
2:F:1588:G:C6	2:F:1589:G:N1	2.77	0.53
4:C:33:LEU:HD23	4:C:64:ILE:HG13	1.89	0.53
4:C:89:LEU:HD23	4:C:90:SER:H	1.73	0.53
5:D:62:LYS:N	5:D:62:LYS:HD2	2.09	0.53
1:A:817:G:O2'	1:A:818:A:C8	2.62	0.53
6:E:123:HIS:HD2	6:E:144:THR:CB	2.21	0.53
4:C:79:ALA:HB1	6:E:99:ARG:HH22	1.73	0.53
5:D:62:LYS:CG	5:D:64:LYS:HZ2	2.21	0.53
4:C:43:LEU:O	4:C:70:HIS:N	2.42	0.53
5:D:39:CYS:CB	5:D:62:LYS:HZ2	2.20	0.53
2:F:1591:A:H4'	2:F:1592:G:O5'	2.09	0.53
4:C:23:THR:HG22	4:C:90:SER:HG	1.73	0.53
4:C:32:THR:HG21	4:C:92:LEU:CD2	2.38	0.53
4:C:27:LYS:HZ2	4:C:27:LYS:HA	1.73	0.53
1:A:806:A:N3	6:E:119:GLU:CG	2.72	0.52
4:C:44:ALA:C	4:C:70:HIS:C	2.66	0.52
2:F:1589:G:H22	2:F:1605:G:H2'	1.73	0.52
5:D:46:ALA:HB1	5:D:58:LYS:HG2	1.90	0.52
3:B:740:U:H5'	6:E:101:HIS:CB	2.40	0.52
1:A:804:C:C5	6:E:148:THR:CG2	2.79	0.52
5:D:10:ILE:HB	5:D:27:LYS:HG3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:42:ILE:O	4:C:88:CYS:HA	2.10	0.52
4:C:35:SER:O	4:C:36:SER:HB2	2.09	0.52
4:C:32:THR:CG2	4:C:92:LEU:CD2	2.88	0.52
1:A:805:G:H3'	6:E:147:SER:O	2.10	0.51
4:C:76:LEU:HD22	6:E:92:ILE:O	2.10	0.51
1:A:806:A:O2'	6:E:119:GLU:OE2	2.25	0.51
4:C:20:GLY:O	4:C:93:ASP:HB3	2.09	0.51
6:E:84:ILE:N	6:E:86:GLU:CG	2.74	0.51
3:B:728:A:N6	6:E:113:PHE:CE2	2.78	0.51
4:C:44:ALA:CB	4:C:70:HIS:HB2	2.20	0.51
4:C:14:GLN:HE22	4:C:74:VAL:HG22	1.76	0.51
3:B:740:U:C2'	6:E:101:HIS:ND1	2.73	0.51
3:B:746:A:O2'	3:B:747:C:H5'	2.10	0.51
4:C:26:TYR:C	4:C:29:VAL:HG12	2.25	0.51
6:E:130:LYS:HB3	6:E:141:TYR:OH	2.10	0.50
3:B:658:G:P	6:E:90:PHE:CE2	2.73	0.50
4:C:91:ILE:HG23	4:C:93:ASP:O	2.11	0.50
5:D:28:LYS:O	5:D:31:VAL:HG12	2.11	0.50
1:A:804:C:C1'	6:E:148:THR:CG2	2.89	0.50
6:E:84:ILE:H	6:E:86:GLU:CB	2.25	0.50
6:E:115:LEU:O	6:E:118:VAL:HG12	2.12	0.50
1:A:806:A:N3	6:E:119:GLU:HG2	2.26	0.50
4:C:44:ALA:HA	4:C:70:HIS:N	2.22	0.50
4:C:43:LEU:N	4:C:70:HIS:HD2	2.10	0.50
4:C:80:CYS:SG	6:E:143:SER:O	2.70	0.50
4:C:39:LYS:C	4:C:40:LEU:CD1	2.79	0.50
6:E:133:LYS:CB	6:E:136:PRO:HD2	2.26	0.50
6:E:84:ILE:CB	6:E:86:GLU:OE2	2.45	0.50
6:E:84:ILE:H	6:E:86:GLU:HB3	1.77	0.49
5:D:79:VAL:HG23	5:D:80:ARG:N	2.27	0.49
4:C:91:ILE:HG22	4:C:94:PRO:HD3	1.95	0.49
3:B:659:U:O2'	3:B:660:G:H5'	2.12	0.49
5:D:11:VAL:HG22	5:D:27:LYS:HD3	1.95	0.49
3:B:728:A:H62	6:E:110:ASP:HA	1.75	0.49
6:E:109:LYS:H	6:E:109:LYS:HD2	1.77	0.49
4:C:48:PRO:HB2	4:C:51:ARG:CB	2.42	0.49
2:F:1604:G:P	4:C:51:ARG:HH21	2.36	0.49
3:B:657:G:O2'	3:B:658:G:H5'	2.12	0.49
4:C:31:LYS:NZ	4:C:37:LYS:HE3	2.28	0.49
3:B:666:G:H5'	3:B:726:C:H1'	1.94	0.49
5:D:11:VAL:HG13	5:D:27:LYS:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:134:LYS:CG	6:E:134:LYS:CA	2.90	0.49
2:F:1604:G:N3	4:C:51:ARG:HG3	2.26	0.49
5:D:11:VAL:HB	5:D:23:ARG:HB2	1.95	0.48
6:E:85:PRO:HG3	6:E:129:TYR:CZ	2.48	0.48
4:C:49:PRO:N	5:D:41:PHE:CE2	2.81	0.48
4:C:44:ALA:H	4:C:70:HIS:HB2	1.56	0.48
4:C:30:LEU:HD23	4:C:30:LEU:C	2.33	0.48
1:A:797:A:H4'	5:D:10:ILE:CG2	2.32	0.48
5:D:22:LEU:O	5:D:25:GLN:HG2	2.13	0.48
4:C:23:THR:HG23	4:C:90:SER:OG	2.10	0.48
3:B:722:A:H4'	3:B:723:U:C5	2.49	0.48
5:D:22:LEU:HD13	5:D:22:LEU:C	2.34	0.48
4:C:40:LEU:CD2	4:C:67:HIS:HE1	2.26	0.48
5:D:39:CYS:SG	5:D:47:VAL:CG2	3.01	0.48
6:E:83:GLU:HB2	6:E:84:ILE:HG13	1.95	0.48
4:C:48:PRO:HB2	4:C:51:ARG:HB3	1.94	0.48
4:C:49:PRO:HD2	5:D:41:PHE:C	2.35	0.48
3:B:728:A:N6	6:E:113:PHE:HD2	1.93	0.48
5:D:77:VAL:HA	5:D:80:ARG:HH11	1.79	0.48
3:B:740:U:H4'	6:E:101:HIS:HB2	1.95	0.47
4:C:30:LEU:CD2	4:C:34:ARG:NE	2.77	0.47
3:B:659:U:H2'	3:B:660:G:O4'	2.14	0.47
4:C:73:ASN:OD1	4:C:84:TYR:CA	2.62	0.47
3:B:743:U:H2'	3:B:744:C:H6	1.78	0.47
5:D:63:VAL:HG13	5:D:63:VAL:O	2.14	0.47
3:B:686:U:O4	3:B:703:G:H1'	2.14	0.47
3:B:740:U:C5'	6:E:101:HIS:CG	2.97	0.47
5:D:57:CYS:SG	5:D:62:LYS:CG	3.03	0.47
2:F:1607:A:H2'	2:F:1608:G:O4'	2.15	0.47
3:B:750:G:O2'	6:E:84:ILE:CG1	2.61	0.47
5:D:33:GLN:O	5:D:37:TYR:HE1	1.98	0.47
3:B:652:U:O4	3:B:752:G:O2'	2.29	0.46
5:D:48:LYS:HA	5:D:48:LYS:HE2	1.96	0.46
4:C:29:VAL:HG23	4:C:41:ILE:CD1	2.44	0.46
4:C:9:ILE:CG2	4:C:69:PHE:CZ	2.80	0.46
2:F:1605:G:C8	2:F:1605:G:H5''	2.50	0.46
6:E:133:LYS:CG	6:E:133:LYS:HA	2.45	0.46
4:C:29:VAL:HG13	4:C:30:LEU:N	2.30	0.46
4:C:94:PRO:CG	4:C:100:ILE:CG2	2.94	0.46
6:E:84:ILE:O	6:E:87:ASP:N	2.47	0.46
6:E:134:LYS:CG	6:E:134:LYS:O	2.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:72:ASN:O	5:D:72:ASN:ND2	2.48	0.46
3:B:740:U:C5'	6:E:101:HIS:CB	2.90	0.46
6:E:127:ARG:HH12	6:E:146:ALA:HB3	1.80	0.46
4:C:42:ILE:CB	4:C:70:HIS:NE2	2.79	0.46
4:C:9:ILE:HG21	4:C:69:PHE:CZ	2.25	0.46
2:F:1603:A:H4'	2:F:1604:G:OP2	2.14	0.46
4:C:43:LEU:CA	4:C:70:HIS:HD2	2.28	0.46
4:C:45:ASN:HA	4:C:68:HIS:CE1	2.50	0.46
1:A:796:A:O2'	5:D:10:ILE:CD1	2.64	0.46
4:C:32:THR:CG2	4:C:38:GLY:CA	2.93	0.46
3:B:741:G:O4'	6:E:111:SER:HB2	2.16	0.46
1:A:795:G:H21	1:A:817:G:H2'	1.78	0.46
5:D:47:VAL:HG11	5:D:71:MET:SD	2.57	0.45
1:A:804:C:P	6:E:148:THR:HG22	2.55	0.45
2:F:1586:G:H2'	2:F:1587:U:O4'	2.16	0.45
4:C:85:ARG:O	4:C:85:ARG:CZ	2.64	0.45
4:C:26:TYR:HB2	4:C:51:ARG:HH21	1.80	0.45
1:A:819:A:H5'	5:D:13:LYS:HB2	1.98	0.45
3:B:740:U:C2'	6:E:101:HIS:CE1	2.87	0.45
1:A:804:C:O4'	6:E:148:THR:CG2	2.61	0.45
6:E:130:LYS:NZ	6:E:136:PRO:C	2.62	0.45
4:C:42:ILE:HB	4:C:70:HIS:NE2	2.31	0.45
3:B:740:U:O4'	6:E:101:HIS:CD2	2.70	0.45
3:B:740:U:C4'	6:E:101:HIS:CB	2.88	0.45
4:C:83:TYR:O	4:C:84:TYR:CD1	2.58	0.45
6:E:130:LYS:N	6:E:140:LYS:HZ2	2.14	0.45
1:A:816:G:C6	1:A:817:G:N1	2.85	0.45
5:D:49:ARG:HD2	5:D:52:VAL:HA	1.98	0.45
1:A:796:A:O2'	5:D:10:ILE:HD11	2.17	0.45
5:D:19:GLY:O	5:D:23:ARG:HG2	2.17	0.45
1:A:806:A:H1'	6:E:119:GLU:HG3	1.98	0.45
6:E:133:LYS:O	6:E:137:PRO:HG2	2.17	0.44
4:C:40:LEU:CG	4:C:65:SER:OG	2.59	0.44
4:C:91:ILE:HG21	4:C:94:PRO:HG3	1.99	0.44
3:B:735:C:O2'	3:B:736:C:H5'	2.17	0.44
3:B:740:U:H5'	6:E:101:HIS:CG	2.53	0.44
4:C:100:ILE:HG13	4:C:101:SER:H	1.81	0.44
6:E:84:ILE:C	6:E:86:GLU:CD	2.76	0.44
3:B:652:U:H2'	3:B:752:G:N1	2.32	0.44
1:A:804:C:C1'	6:E:148:THR:HG23	2.47	0.44
2:F:1587:U:C4	2:F:1588:G:C6	3.06	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:4:LYS:O	4:C:5:SER:C	2.56	0.44
3:B:690:G:H2'	3:B:691:G:O4'	2.18	0.44
4:C:43:LEU:HD21	4:C:55:ILE:HG21	1.99	0.44
3:B:742:G:H5'	6:E:114:ARG:HG3	1.93	0.44
4:C:77:GLY:C	4:C:82:LYS:HD2	2.39	0.44
4:C:26:TYR:CE1	4:C:55:ILE:HG13	2.53	0.43
4:C:76:LEU:HD21	6:E:96:VAL:CG1	2.48	0.43
3:B:740:U:C4'	6:E:101:HIS:HB2	2.48	0.43
4:C:20:GLY:C	4:C:22:TYR:CE2	2.91	0.43
2:F:1594:C:O2'	2:F:1595:G:H5'	2.19	0.43
4:C:55:ILE:O	4:C:59:ALA:HB2	2.18	0.43
4:C:91:ILE:CG2	4:C:94:PRO:CD	2.94	0.43
6:E:127:ARG:NH2	6:E:141:TYR:CA	2.47	0.43
5:D:29:MET:O	5:D:33:GLN:HB2	2.19	0.43
5:D:11:VAL:CG1	5:D:27:LYS:HB2	2.49	0.43
6:E:84:ILE:O	6:E:85:PRO:O	2.35	0.43
4:C:91:ILE:HG23	4:C:94:PRO:CD	2.49	0.43
4:C:44:ALA:HB1	4:C:70:HIS:C	2.38	0.43
5:D:33:GLN:NE2	5:D:33:GLN:O	2.49	0.42
5:D:62:LYS:HG2	5:D:62:LYS:O	2.17	0.42
5:D:57:CYS:SG	5:D:64:LYS:NZ	2.92	0.42
4:C:76:LEU:CA	6:E:92:ILE:HG21	2.44	0.42
1:A:807:A:N1	1:A:808:A:C2	2.87	0.42
5:D:33:GLN:HE21	5:D:33:GLN:C	2.22	0.42
1:A:811:C:H2'	1:A:812:A:C8	2.55	0.42
3:B:730:G:C5	3:B:731:G:H1'	2.55	0.42
4:C:19:SER:C	4:C:20:GLY:CA	2.86	0.42
5:D:76:ALA:O	5:D:79:VAL:CG2	2.55	0.42
1:A:795:G:H22	1:A:817:G:H2'	1.82	0.42
3:B:665:A:H2'	3:B:725:G:N2	2.34	0.42
3:B:667:G:O2'	6:E:108:ASP:CB	2.67	0.42
4:C:76:LEU:CG	6:E:92:ILE:CG2	2.83	0.42
3:B:667:G:N2	6:E:101:HIS:CE1	2.88	0.42
2:F:1609:C:H2'	2:F:1610:G:H8	1.83	0.42
1:A:804:C:C5'	6:E:148:THR:CG2	2.63	0.42
4:C:49:PRO:O	4:C:51:ARG:N	2.53	0.42
2:F:1604:G:OP1	4:C:26:TYR:HB2	2.15	0.42
4:C:47:CYS:HB2	4:C:87:CYS:SG	2.60	0.42
4:C:49:PRO:C	4:C:51:ARG:N	2.72	0.42
6:E:106:ARG:H	6:E:106:ARG:HH11	1.67	0.42
2:F:1605:G:H8	4:C:27:LYS:HG3	1.75	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:49:PRO:O	5:D:41:PHE:CE2	2.72	0.41
5:D:41:PHE:HB3	5:D:62:LYS:HZ3	1.85	0.41
4:C:66:VAL:O	4:C:104:THR:CG2	2.60	0.41
4:C:13:LEU:HD23	4:C:13:LEU:C	2.38	0.41
4:C:46:ASN:O	4:C:47:CYS:O	2.38	0.41
1:A:819:A:H4'	5:D:13:LYS:HB2	2.02	0.41
5:D:30:GLU:HA	5:D:33:GLN:CB	2.51	0.41
5:D:32:SER:O	5:D:37:TYR:OH	2.38	0.41
5:D:34:HIS:O	5:D:34:HIS:CG	2.74	0.41
4:C:57:TYR:O	4:C:60:MET:HB2	2.20	0.41
4:C:76:LEU:HD21	6:E:96:VAL:HG11	2.03	0.41
4:C:16:VAL:HA	4:C:19:SER:OG	2.21	0.41
3:B:741:G:HO2'	6:E:114:ARG:CG	2.31	0.41
4:C:76:LEU:CA	6:E:92:ILE:CG2	2.97	0.41
3:B:723:U:O2	3:B:723:U:C2'	2.68	0.41
3:B:736:C:H2'	3:B:737:A:H8	1.83	0.41
5:D:49:ARG:HB2	5:D:55:TRP:CZ3	2.56	0.41
3:B:692:U:H1'	3:B:695:A:N7	2.36	0.41
5:D:36:LYS:HZ3	5:D:36:LYS:HA	1.84	0.40
6:E:133:LYS:CB	6:E:136:PRO:HG2	2.49	0.40
3:B:728:A:H2'	3:B:729:A:C8	2.56	0.40
3:B:662:G:H2'	3:B:663:A:H8	1.78	0.40
4:C:26:TYR:OH	4:C:54:GLU:HB3	2.17	0.40
4:C:71:GLY:HA3	4:C:86:VAL:HG23	2.03	0.40
4:C:33:LEU:CD2	4:C:64:ILE:HG13	2.52	0.40
1:A:805:G:OP2	6:E:147:SER:CA	2.69	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	
4	C	92/104 (88%)	70 (76%)	12 (13%)	10 (11%)	0	11
5	D	71/73 (97%)	65 (92%)	5 (7%)	1 (1%)	14	58
6	E	77/84 (92%)	71 (92%)	3 (4%)	3 (4%)	4	36
All	All	240/261 (92%)	206 (86%)	20 (8%)	14 (6%)	4	27

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	C	47	CYS
4	C	72	ASN
4	C	79	ALA
4	C	80	CYS
4	C	102	THR
6	E	147	SER
4	C	74	VAL
4	C	101	SER
4	C	6	GLY
4	C	48	PRO
5	D	81	SER
6	E	138	THR
4	C	50	LEU
6	E	81	ALA

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	
4	C	91/91 (100%)	82 (90%)	9 (10%)	10	39
5	D	57/57 (100%)	50 (88%)	7 (12%)	6	30
6	E	76/76 (100%)	69 (91%)	7 (9%)	11	43
All	All	224/224 (100%)	201 (90%)	23 (10%)	13	37

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	C	18	LYS
4	C	24	LEU
4	C	27	LYS
4	C	31	LYS
4	C	51	ARG
4	C	63	LYS
4	C	85	ARG
4	C	92	LEU
4	C	93	ASP
5	D	10	ILE
5	D	33	GLN
5	D	36	LYS
5	D	48	LYS
5	D	50	LYS
5	D	62	LYS
5	D	72	ASN
6	E	73	ARG
6	E	76	LYS
6	E	100	LYS
6	E	106	ARG
6	E	107	LYS
6	E	109	LYS
6	E	129	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
4	C	10	ASN
4	C	67	HIS
4	C	70	HIS
5	D	25	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	27/28 (96%)	3 (11%)	1 (3%)
2	F	32/34 (94%)	5 (15%)	3 (9%)
3	B	100/101 (99%)	11 (11%)	3 (3%)
All	All	159/163 (97%)	19 (11%)	7 (4%)

All (19) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	809	G
1	A	817	G
1	A	818	A
2	F	1592	G
2	F	1593	C
2	F	1604	G
2	F	1605	G
2	F	1606	A
3	B	653	A
3	B	665	A
3	B	686	U
3	B	687	A
3	B	688	G
3	B	702	A
3	B	703	G
3	B	718	G
3	B	723	U
3	B	731	G
3	B	749	C

All (7) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	817	G
2	F	1591	A
2	F	1603	A
2	F	1605	G
3	B	687	A
3	B	701	C
3	B	748	C

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

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

5.5 Carbohydrates ⓘ

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.