



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 22, 2016 – 10:41 PM EST

PDB ID : 1U63
Title : THE STRUCTURE OF A RIBOSOMAL PROTEIN L1-mRNA COMPLEX
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Nikulin, A.; Garber, M.; Nikonov, S.; Piendl, W.
Deposited on : 2004-07-29
Resolution : 3.40 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

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

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : unknown
Xtriage (Phenix) : 1.9-1692
EDS : rb-20028320
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20028320

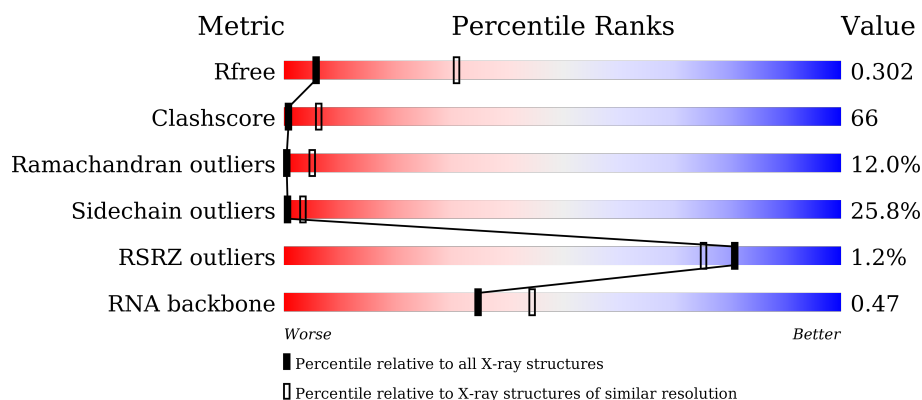
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1476 (3.50-3.30)
Clashscore	102246	1611 (3.50-3.30)
Ramachandran outliers	100387	1571 (3.50-3.30)
Sidechain outliers	100360	1571 (3.50-3.30)
RSRZ outliers	91569	1485 (3.50-3.30)
RNA backbone	2183	1041 (4.00-2.80)

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 on the lower 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 $\leq 5\%$. 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 chain
1	B	49	
1	D	49	
2	A	219	
2	C	219	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5510 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.

- Molecule 1 is a RNA chain called 49 NT FRAGMENT OF MRNA FOR L1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	49	Total	C	N	O	P	0	0	0
			1055	470	199	337	49			
1	D	49	Total	C	N	O	P	0	0	0
			1055	470	199	337	49			

- Molecule 2 is a protein called 50S ribosomal protein L1P.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	A	214	Total	C	N	O	S	Se	0	0	0
			1700	1088	303	302	1	6			
2	C	214	Total	C	N	O	S	Se	0	0	0
			1700	1088	303	302	1	6			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	37	MSE	MET	MODIFIED RESIDUE	UNP P54050
A	112	MSE	MET	MODIFIED RESIDUE	UNP P54050
A	119	MSE	MET	MODIFIED RESIDUE	UNP P54050
A	129	MSE	MET	MODIFIED RESIDUE	UNP P54050
A	169	MSE	MET	MODIFIED RESIDUE	UNP P54050
A	205	MSE	MET	MODIFIED RESIDUE	UNP P54050
C	37	MSE	MET	MODIFIED RESIDUE	UNP P54050
C	112	MSE	MET	MODIFIED RESIDUE	UNP P54050
C	119	MSE	MET	MODIFIED RESIDUE	UNP P54050
C	129	MSE	MET	MODIFIED RESIDUE	UNP P54050
C	169	MSE	MET	MODIFIED RESIDUE	UNP P54050
C	205	MSE	MET	MODIFIED RESIDUE	UNP P54050

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 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: 49 NT FRAGMENT OF MRNA FOR L1

Chain B: 

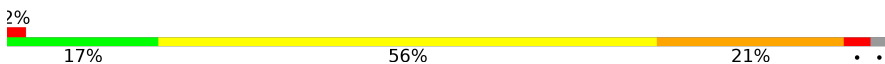


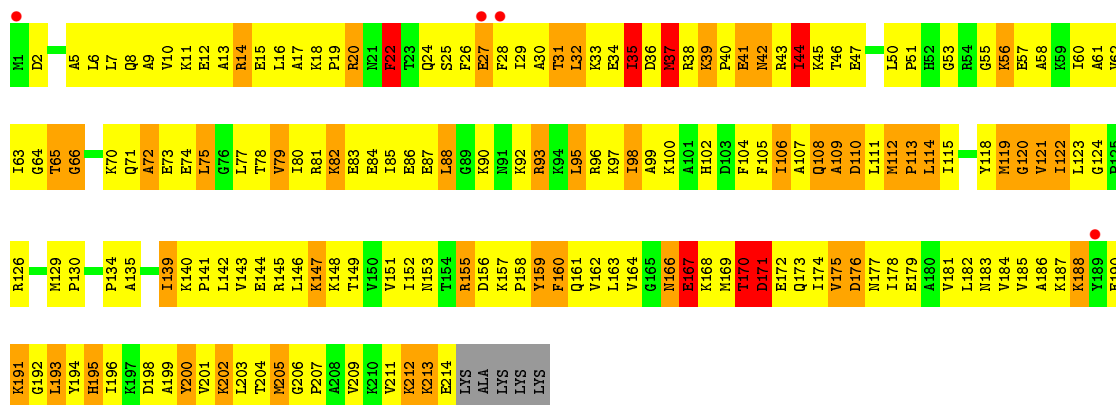
- Molecule 1: 49 NT FRAGMENT OF MRNA FOR L1

Chain D: 

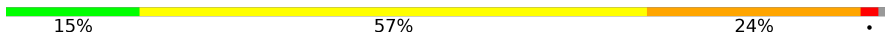


- Molecule 2: 50S ribosomal protein L1P

Chain A: 



- Molecule 2: 50S ribosomal protein L1P

Chain C: 



V62	M129	H102	D103
I63	P130	F104	F105
G64	K131	F106	I106
T65	P132	A107	A107
G66	V133	Q108	A109
	P134	D110	D110
A69	A135	L111	L111
K70	M136	M112	M112
Q71	A137	P113	P113
A72	N138	L114	L114
E73	I139	I115	I115
E74	K140	D116	D116
L75	P141	R117	R117
G76	L142	A118	A118
L77	V143	V121	V121
T78	E144	I122	I122
V79	R145	L123	L123
I80	L146	G124	G124
R81	K147	P125	P125
K82	R148	A126	A126
E83	T149	K127	K127
E84	V150		
I85	V151		
E86	I152		
E87	M153		
L88	T154		
G89	R155		
K90	D156		
	K157		
X91	P158		
R92	Y159		
R93	F160		
I94	Q161		
L95	V162		
R96	L163		
K97	V164		
	G165		
	M166		
	E167		
	K168		
	M169		
	T170		
	D171		
	E172		
	Q173		
	I174		
	V175		
	D176		
	M177		
	I178		
	E179		
	A180		
	V181		
	L182		
	M183		
	V184		
	V185		
	A186		
	K187		
K188			
Y189			
E190			
K191			
G192			
L193			
Y194			
H195			
I196			
K197			
D198			
A199			
Y200			
V201			
K202			
L203			
T204			
N205			
G206			
P207			
A208			
V209			
K210			
V211			
K212			
L213			
E214			
LYS			
ALA			
LYS			
LYS			
LYS			

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	212.29 Å 68.90 Å 115.87 Å 90.00° 122.99° 90.00°	Depositor
Resolution (Å)	8.00 – 3.40 28.97 – 3.40	Depositor EDS
% Data completeness (in resolution range)	92.7 (8.00-3.40) 92.5 (28.97-3.40)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.06 (at 3.39 Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.276 , 0.302 0.278 , 0.302	Depositor DCC
R_{free} test set	941 reflections (5.61%)	DCC
Wilson B-factor (Å ²)	95.0	Xtriage
Anisotropy	0.638	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 54.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.399 for -h-2*k,l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	5510	wwPDB-VP
Average B, all atoms (Å ²)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.95% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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.

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 > 5$	RMSZ	# $ Z > 5$
1	B	0.63	2/1181 (0.2%)	1.31	16/1839 (0.9%)
1	D	0.70	2/1181 (0.2%)	1.47	23/1839 (1.3%)
2	A	0.70	1/1718 (0.1%)	0.97	2/2294 (0.1%)
2	C	0.66	1/1718 (0.1%)	0.97	3/2294 (0.1%)
All	All	0.68	6/5798 (0.1%)	1.18	44/8266 (0.5%)

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	B	3	2
1	D	9	3
All	All	12	5

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1	G	OP3-P	-6.92	1.52	1.61
1	D	1	G	OP3-P	-6.75	1.53	1.61
2	A	169	MSE	CG-SE	-5.76	1.75	1.95
2	C	169	MSE	CG-SE	-5.73	1.75	1.95
1	D	43	C	C4'-C3'	-5.57	1.47	1.52
1	B	1	G	P-O5'	5.06	1.64	1.59

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	20	G	N9-C1'-C2'	22.85	143.71	114.00
1	D	43	C	N1-C1'-C2'	21.21	141.57	114.00
1	D	11	G	N9-C1'-C2'	19.49	139.34	114.00
1	B	8	A	O5'-P-OP2	-17.98	89.12	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	43	C	O4'-C1'-N1	-16.60	94.92	108.20
1	D	12	A	N9-C1'-C2'	15.03	133.53	114.00
1	B	20	G	O4'-C1'-N9	-13.44	97.45	108.20
1	D	43	C	C5'-C4'-O4'	13.38	125.15	109.10
1	B	1	G	O5'-P-OP2	13.32	126.68	110.70
1	D	11	G	O4'-C1'-N9	-11.95	98.64	108.20
1	D	11	G	C5'-C4'-O4'	11.31	122.67	109.10
1	B	44	A	N9-C1'-C2'	10.07	127.09	114.00
1	B	20	G	C5'-C4'-O4'	10.06	121.17	109.10
1	D	12	A	C8-N9-C1'	-9.84	109.99	127.70
1	D	12	A	C4-N9-C1'	9.03	142.55	126.30
1	B	17	C	O5'-P-OP2	-8.61	97.95	105.70
1	B	20	G	C2'-C3'-O3'	8.45	128.09	109.50
1	D	12	A	C2'-C3'-O3'	8.43	128.05	109.50
1	D	43	C	C2'-C3'-O3'	8.33	127.83	109.50
1	D	10	G	O5'-P-OP1	-8.31	98.22	105.70
1	D	11	G	C2'-C3'-O3'	7.97	127.04	109.50
1	B	1	G	O5'-P-OP1	-7.49	98.96	105.70
2	C	192	GLY	N-CA-C	7.41	131.62	113.10
1	D	11	G	OP2-P-O3'	7.18	120.99	105.20
1	D	12	A	OP2-P-O3'	7.10	120.81	105.20
1	D	10	G	OP2-P-O3'	7.09	120.80	105.20
1	D	43	C	OP2-P-O3'	6.83	120.22	105.20
2	A	212	LYS	N-CA-C	6.60	128.81	111.00
1	D	11	G	O5'-P-OP2	-6.52	99.84	105.70
1	B	12	A	N9-C1'-C2'	6.39	122.31	114.00
1	D	12	A	C5'-C4'-O4'	6.04	116.34	109.10
1	B	20	G	OP2-P-O3'	5.67	117.67	105.20
2	C	170	THR	N-CA-C	5.66	126.29	111.00
1	B	17	C	C5'-C4'-C3'	5.66	125.06	116.00
1	D	36	G	OP1-P-O3'	5.65	117.63	105.20
1	D	11	G	C8-N9-C1'	-5.63	119.68	127.00
1	B	22	A	N9-C1'-C2'	5.57	121.24	114.00
1	B	8	A	C5'-C4'-C3'	5.45	124.72	116.00
1	D	42	U	O5'-P-OP2	5.37	117.14	110.70
1	B	36	G	N9-C1'-C2'	5.31	120.90	114.00
2	A	170	THR	N-CA-C	5.30	125.30	111.00
2	C	136	ASN	N-CA-C	-5.28	96.74	111.00
1	B	44	A	O5'-P-OP2	5.12	116.84	110.70
1	D	1	G	OP1-P-OP2	-5.04	112.04	119.60

All (12) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	20	G	C4',C3',C1'
1	D	11	G	C4',C3',C1'
1	D	12	A	C4',C3',C1'
1	D	43	C	C4',C3',C1'

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	20	G	Sidechain
1	B	44	A	Sidechain
1	D	11	G	Sidechain
1	D	12	A	Sidechain
1	D	43	C	Sidechain

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	B	1055	0	534	94	0
1	D	1055	0	534	75	0
2	A	1700	0	1824	256	0
2	C	1700	0	1824	287	0
All	All	5510	0	4716	678	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 66.

All (678) 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)
1:D:23:C:H3'	1:D:24:U:H5''	1.28	1.13
1:D:43:C:H4'	1:D:44:A:OP2	1.41	1.10
1:B:34:G:H2'	1:B:35:A:H5''	1.31	1.09
2:A:62:VAL:HG12	2:A:106:ILE:HG13	1.26	1.09
2:C:44:ILE:HD12	2:C:44:ILE:H	1.15	1.05
2:C:32:LEU:HD12	2:C:158:PRO:HA	1.30	1.05
1:B:1:G:H5''	1:B:1:G:C8	1.90	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:112:MSE:HE1	2:A:130:PRO:HG2	1.40	1.04
2:A:14:ARG:HH11	2:A:14:ARG:HB2	1.19	1.01
1:B:20:G:H4'	1:B:21:A:OP2	1.61	1.00
2:A:32:LEU:HD12	2:A:158:PRO:HA	1.43	0.99
2:C:45:LYS:HE2	2:C:45:LYS:O	1.63	0.98
2:A:166:ASN:HD21	2:A:168:LYS:HB2	1.24	0.98
2:C:75:LEU:HB3	2:C:77:LEU:HD13	1.40	0.97
2:A:204:THR:HG22	2:A:205:MSE:HE3	1.45	0.97
2:C:22:PHE:HD2	2:C:22:PHE:H	1.13	0.94
1:D:12:A:H2'	1:D:13:G:O4'	1.67	0.94
2:A:177:ASN:O	2:A:181:VAL:HG23	1.68	0.93
1:D:11:G:H4'	1:D:12:A:OP2	1.69	0.93
2:A:170:THR:HG22	2:A:173:GLN:HG3	1.50	0.93
2:C:10:VAL:HG22	2:C:201:VAL:HG11	1.51	0.92
2:A:20:ARG:HH11	2:A:20:ARG:HG2	1.33	0.91
1:D:34:G:H2'	1:D:35:A:H5''	1.51	0.90
1:D:23:C:C3'	1:D:24:U:H5''	2.02	0.90
2:A:122:ILE:O	2:A:122:ILE:HG13	1.69	0.90
1:D:23:C:H3'	1:D:24:U:C5'	2.00	0.90
1:D:40:C:O2	2:C:205:MSE:HE2	1.73	0.89
2:A:105:PHE:HB3	2:A:130:PRO:HB3	1.54	0.89
2:C:171:ASP:O	2:C:174:ILE:HG12	1.71	0.89
2:A:85:ILE:HA	2:A:119:MSE:HE3	1.53	0.88
2:C:26:PHE:O	2:C:163:LEU:HD12	1.73	0.88
2:A:62:VAL:HG12	2:A:106:ILE:CG1	2.03	0.87
2:A:50:LEU:HD22	2:A:177:ASN:OD1	1.74	0.87
2:A:73:GLU:N	2:A:73:GLU:OE1	2.08	0.86
2:C:7:LEU:HD11	2:C:172:GLU:HG3	1.59	0.85
2:A:7:LEU:CD2	2:A:11:LYS:HE3	2.06	0.85
1:B:12:A:H4'	1:B:13:G:O5'	1.76	0.85
1:B:33:C:H3'	1:B:34:G:H5''	1.59	0.84
1:B:20:G:C6	1:B:22:A:H1'	2.11	0.84
2:A:108:GLN:HG2	2:A:110:ASP:OD1	1.78	0.84
2:A:33:LYS:HB2	2:A:195:HIS:O	1.77	0.84
2:A:26:PHE:O	2:A:163:LEU:HD12	1.77	0.83
1:B:24:U:H4'	1:B:24:U:OP1	1.78	0.83
2:C:202:LYS:NZ	2:C:202:LYS:HB2	1.93	0.83
2:A:195:HIS:ND1	2:A:195:HIS:O	2.11	0.83
2:A:57:GLU:HB2	2:A:147:LYS:HE2	1.60	0.83
2:C:86:GLU:HG3	2:C:87:GLU:N	1.94	0.83
2:A:145:ARG:HH11	2:A:145:ARG:HG2	1.44	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:204:THR:HG22	2:A:205:MSE:CE	2.08	0.82
2:A:96:ARG:HG2	2:A:122:ILE:HD11	1.59	0.82
2:C:152:ILE:HG22	2:C:162:VAL:HB	1.62	0.82
2:C:202:LYS:HZ3	2:C:202:LYS:HB2	1.43	0.82
2:A:82:LYS:O	2:A:85:ILE:HG22	1.80	0.82
2:C:139:ILE:HG22	2:C:143:VAL:HG23	1.62	0.82
2:A:50:LEU:HB3	2:A:53:GLY:HA2	1.61	0.81
2:C:108:GLN:HG2	2:C:110:ASP:OD1	1.81	0.81
2:A:14:ARG:NH1	2:A:14:ARG:HB2	1.96	0.81
1:B:1:G:H5''	1:B:1:G:H8	1.44	0.81
2:C:93:ARG:O	2:C:97:LYS:HG3	1.81	0.80
2:C:174:ILE:H	2:C:174:ILE:HD13	1.47	0.80
2:C:174:ILE:O	2:C:178:ILE:HG13	1.80	0.80
2:C:16:LEU:O	2:C:207:PRO:HD3	1.81	0.80
2:A:28:PHE:HA	2:A:201:VAL:HG12	1.62	0.80
2:C:57:GLU:HB3	2:C:147:LYS:HE2	1.64	0.79
2:A:146:LEU:O	2:A:149:THR:HG22	1.82	0.79
2:A:20:ARG:NH2	2:A:205:MSE:HG2	1.99	0.78
2:A:123:LEU:HD21	2:A:130:PRO:HD3	1.65	0.78
2:A:80:ILE:HD12	2:A:80:ILE:N	1.97	0.78
2:C:175:VAL:HA	2:C:178:ILE:HD12	1.66	0.77
2:A:93:ARG:O	2:A:97:LYS:HG3	1.83	0.77
2:C:186:ALA:HB1	2:C:192:GLY:O	1.84	0.77
2:C:79:VAL:O	2:C:80:ILE:HD13	1.84	0.77
2:C:62:VAL:HG21	2:C:72:ALA:CB	2.14	0.77
2:C:200:TYR:CD2	2:C:210:LYS:HA	2.20	0.76
2:C:92:LYS:O	2:C:96:ARG:HG2	1.84	0.76
2:C:5:ALA:HB2	2:C:213:LYS:HG2	1.67	0.76
1:D:10:G:H2'	2:C:204:THR:HG22	1.68	0.76
1:D:8:A:H5''	2:C:155:ARG:NH2	2.01	0.76
1:B:23:C:H3'	1:B:24:U:H5''	1.68	0.75
1:B:33:C:C3'	1:B:34:G:H5''	2.15	0.75
1:B:14:G:H5''	2:A:20:ARG:HE	1.51	0.75
2:C:57:GLU:CB	2:C:147:LYS:HE2	2.16	0.75
2:C:16:LEU:HD12	2:C:16:LEU:N	2.02	0.75
2:C:86:GLU:HG3	2:C:87:GLU:H	1.50	0.75
2:A:46:THR:O	2:A:152:ILE:HG22	1.86	0.75
2:A:166:ASN:ND2	2:A:168:LYS:HB2	2.00	0.75
2:C:182:LEU:O	2:C:185:VAL:HB	1.86	0.75
2:C:112:MSE:HE2	2:C:132:PRO:HG3	1.68	0.74
2:A:121:VAL:HG23	2:A:122:ILE:H	1.50	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:146:LEU:O	2:C:149:THR:HG22	1.87	0.74
1:B:21:A:H4'	1:B:22:A:N7	2.03	0.74
2:C:174:ILE:HD13	2:C:174:ILE:N	2.02	0.74
2:C:59:LYS:H	2:C:103:ASP:HB2	1.52	0.74
1:B:34:G:C2'	1:B:35:A:H5''	2.14	0.73
2:A:170:THR:HG23	2:A:172:GLU:OE1	1.88	0.73
2:A:63:ILE:HG21	2:A:115:ILE:HD11	1.70	0.73
2:A:85:ILE:HG21	2:A:114:LEU:HD23	1.70	0.73
2:C:43:ARG:HG2	2:C:154:THR:HG23	1.70	0.73
2:C:50:LEU:HB3	2:C:177:ASN:OD1	1.88	0.73
2:C:181:VAL:O	2:C:184:VAL:HG23	1.88	0.73
2:A:42:ASN:CG	2:A:188:LYS:HG2	2.09	0.73
2:A:143:VAL:HG12	2:A:144:GLU:N	2.04	0.73
1:D:26:G:OP1	2:A:90:LYS:HG3	1.88	0.73
1:B:27:C:H2'	1:B:28:G:H5'	1.71	0.72
2:C:55:GLY:HA3	2:C:166:ASN:ND2	2.04	0.72
2:C:154:THR:HG23	2:C:154:THR:O	1.90	0.72
2:C:32:LEU:HD22	2:C:35:ILE:HD13	1.72	0.71
2:A:20:ARG:CZ	2:A:205:MSE:HG2	2.21	0.71
2:A:24:GLN:CB	2:A:203:LEU:HD13	2.21	0.71
2:C:186:ALA:HB2	2:C:193:LEU:HA	1.71	0.71
2:C:37:MSE:HE2	2:C:37:MSE:HA	1.71	0.71
1:D:42:U:H2'	1:D:43:C:C6	2.26	0.70
1:B:44:A:H2'	1:B:45:C:C6	2.26	0.70
2:C:112:MSE:O	2:C:115:ILE:HB	1.91	0.70
1:B:42:U:H2'	1:B:43:C:C6	2.27	0.70
2:C:44:ILE:HD12	2:C:44:ILE:N	1.99	0.70
1:D:2:G:H2'	1:D:3:G:H8	1.55	0.70
1:D:13:G:C5	1:D:34:G:C2	2.80	0.70
1:B:37:A:C8	1:B:38:A:C2	2.80	0.69
2:C:150:VAL:HG11	2:C:162:VAL:HG23	1.73	0.69
2:A:15:GLU:O	2:A:15:GLU:OE1	2.11	0.69
2:C:71:GLN:OE1	2:C:139:ILE:HG12	1.92	0.69
2:C:8:GLN:HA	2:C:11:LYS:HE2	1.75	0.69
2:C:152:ILE:HG13	2:C:152:ILE:O	1.91	0.69
2:A:7:LEU:HD21	2:A:11:LYS:HE3	1.75	0.68
2:A:29:ILE:HG23	2:A:161:GLN:HG2	1.75	0.68
2:C:113:PRO:HG2	2:C:114:LEU:HD12	1.75	0.68
1:D:37:A:C8	1:D:38:A:C2	2.81	0.68
2:A:12:GLU:O	2:A:16:LEU:HB2	1.92	0.68
2:A:202:LYS:HG2	2:A:203:LEU:N	2.09	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:44:ILE:H	2:C:44:ILE:CD1	1.99	0.68
1:D:34:G:C2'	1:D:35:A:H5''	2.23	0.68
2:C:141:PRO:O	2:C:145:ARG:HG2	1.94	0.67
2:C:178:ILE:O	2:C:182:LEU:HD23	1.93	0.67
2:C:20:ARG:HH11	2:C:20:ARG:HG2	1.59	0.67
2:C:20:ARG:NH2	2:C:205:MSE:HG2	2.08	0.67
1:B:20:G:H5'	1:B:22:A:N6	2.08	0.67
2:A:84:GLU:HG3	2:A:87:GLU:OE1	1.94	0.67
2:C:8:GLN:HA	2:C:11:LYS:CE	2.25	0.67
1:D:24:U:OP1	1:D:25:C:C6	2.48	0.67
2:C:90:LYS:O	2:C:90:LYS:HG2	1.95	0.67
2:C:200:TYR:HD2	2:C:210:LYS:HA	1.59	0.67
2:A:112:MSE:N	2:A:113:PRO:HD2	2.10	0.66
2:A:39:LYS:HE2	2:A:39:LYS:HA	1.77	0.66
2:A:33:LYS:HB2	2:A:195:HIS:ND1	2.10	0.66
1:B:29:A:H5''	1:B:29:A:H8	1.61	0.66
2:C:172:GLU:HA	2:C:175:VAL:HG23	1.77	0.66
2:A:33:LYS:HD3	2:A:195:HIS:HA	1.77	0.66
2:A:7:LEU:HD23	2:A:11:LYS:HE3	1.77	0.66
1:D:43:C:C4'	1:D:44:A:OP2	2.31	0.66
1:D:10:G:C2'	2:C:204:THR:HG22	2.25	0.66
2:A:105:PHE:CB	2:A:130:PRO:HB3	2.24	0.66
1:B:37:A:H5''	1:B:38:A:OP2	1.96	0.66
2:A:24:GLN:HB3	2:A:203:LEU:HB2	1.78	0.66
2:C:124:GLY:C	2:C:126:ARG:H	1.99	0.65
2:A:200:TYR:CD1	2:A:200:TYR:N	2.65	0.65
2:A:211:VAL:HG22	2:A:212:LYS:HD3	1.79	0.65
2:C:7:LEU:O	2:C:11:LYS:HG2	1.97	0.65
1:D:12:A:H2'	1:D:13:G:O5'	1.96	0.65
2:A:174:ILE:O	2:A:177:ASN:HB2	1.97	0.64
1:B:29:A:C2	1:D:38:A:C2	2.85	0.64
2:A:85:ILE:HD11	2:A:115:ILE:HA	1.79	0.64
2:C:55:GLY:C	2:C:56:LYS:HE3	2.18	0.64
2:C:61:ALA:HB2	2:C:102:HIS:CD2	2.31	0.64
2:A:32:LEU:HA	2:A:196:ILE:HG22	1.79	0.64
2:A:36:ASP:O	2:A:38:ARG:HG3	1.97	0.64
2:C:129:MSE:SE	2:C:130:PRO:HD2	2.48	0.64
2:C:38:ARG:HG3	2:C:38:ARG:HH11	1.63	0.64
2:C:20:ARG:HH21	2:C:205:MSE:HG2	1.61	0.64
2:C:182:LEU:H	2:C:182:LEU:CD2	2.12	0.63
2:A:45:LYS:HA	2:A:153:ASN:HD22	1.61	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:21:A:OP2	1:B:22:A:N7	2.31	0.63
2:C:20:ARG:CZ	2:C:205:MSE:HB3	2.28	0.63
2:C:22:PHE:HD2	2:C:22:PHE:N	1.91	0.63
2:C:47:GLU:HB2	2:C:149:THR:OG1	1.99	0.63
1:B:21:A:H4'	1:B:22:A:C8	2.33	0.63
1:B:29:A:H2	1:D:38:A:C2	2.16	0.63
2:A:96:ARG:HE	2:A:122:ILE:CD1	2.12	0.62
2:A:146:LEU:HG	2:A:149:THR:HG21	1.80	0.62
2:C:16:LEU:N	2:C:16:LEU:CD1	2.62	0.62
2:A:41:GLU:OE2	2:A:42:ASN:ND2	2.32	0.62
2:C:123:LEU:O	2:C:126:ARG:N	2.32	0.62
2:C:32:LEU:HD22	2:C:35:ILE:CD1	2.29	0.62
1:D:13:G:C8	1:D:34:G:N2	2.68	0.62
2:A:199:ALA:H	2:A:211:VAL:HB	1.65	0.61
2:C:156:ASP:OD2	2:C:157:LYS:HD2	2.00	0.61
2:C:17:ALA:HB2	2:C:206:GLY:HA3	1.81	0.61
2:C:39:LYS:HG2	2:C:41:GLU:HG3	1.80	0.61
2:A:60:ILE:HG22	2:A:61:ALA:N	2.15	0.61
2:A:102:HIS:HB2	2:A:105:PHE:CE1	2.36	0.61
2:C:83:GLU:HG3	2:C:84:GLU:H	1.64	0.61
1:B:37:A:N7	1:B:38:A:C2	2.69	0.60
2:C:43:ARG:HG2	2:C:154:THR:CG2	2.31	0.60
2:C:163:LEU:HG	2:C:164:VAL:N	2.15	0.60
2:C:107:ALA:O	2:C:109:ALA:N	2.34	0.60
2:C:150:VAL:CG1	2:C:162:VAL:HG23	2.31	0.60
2:C:174:ILE:CD1	2:C:174:ILE:H	2.04	0.60
2:C:55:GLY:HA3	2:C:166:ASN:HD21	1.66	0.60
1:B:1:G:C5'	1:B:1:G:C8	2.77	0.60
2:A:172:GLU:O	2:A:175:VAL:HG23	2.02	0.60
2:C:113:PRO:C	2:C:115:ILE:H	2.03	0.60
2:C:7:LEU:CD1	2:C:172:GLU:HG3	2.29	0.60
1:D:12:A:H2'	1:D:13:G:C4'	2.32	0.60
1:D:20:G:O6	1:D:22:A:H1'	2.01	0.60
2:C:200:TYR:HA	2:C:211:VAL:HG23	1.85	0.59
2:C:47:GLU:HG2	2:C:47:GLU:O	2.03	0.59
2:A:96:ARG:HE	2:A:122:ILE:HD11	1.67	0.59
2:A:25:SER:HB2	2:A:163:LEU:HD11	1.83	0.59
2:A:50:LEU:HD22	2:A:177:ASN:CG	2.22	0.59
2:A:92:LYS:O	2:A:96:ARG:HG3	2.02	0.59
1:B:20:G:C4'	1:B:21:A:OP2	2.44	0.59
2:C:139:ILE:C	2:C:141:PRO:HD2	2.21	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:178:ILE:HG22	2:C:182:LEU:HD21	1.84	0.59
1:D:21:A:H4'	1:D:21:A:OP2	2.01	0.59
2:C:106:ILE:HG22	2:C:133:VAL:HG22	1.85	0.59
2:A:20:ARG:HG2	2:A:20:ARG:NH1	2.10	0.59
2:A:63:ILE:N	2:A:63:ILE:HD12	2.18	0.59
2:A:176:ASP:HA	2:A:179:GLU:HB2	1.84	0.58
2:A:109:ALA:C	2:A:111:LEU:H	2.05	0.58
2:A:176:ASP:N	2:A:176:ASP:OD2	2.34	0.58
2:A:37:MSE:HE3	2:A:37:MSE:HA	1.84	0.58
1:D:10:G:O2'	2:C:204:THR:HG22	2.04	0.58
1:B:29:A:C5	1:D:37:A:N6	2.71	0.58
2:C:57:GLU:CD	2:C:57:GLU:H	2.06	0.58
2:A:172:GLU:HA	2:A:175:VAL:CG2	2.33	0.58
2:A:20:ARG:CG	2:A:20:ARG:HH11	2.13	0.58
2:A:57:GLU:HB2	2:A:147:LYS:CE	2.33	0.58
1:D:9:A:H1'	2:C:161:GLN:HG2	1.84	0.58
2:A:190:GLU:HG3	2:A:190:GLU:O	2.02	0.58
2:A:66:GLY:O	2:A:70:LYS:N	2.37	0.58
2:C:123:LEU:O	2:C:126:ARG:HB2	2.03	0.58
2:A:24:GLN:CG	2:A:203:LEU:HD13	2.32	0.58
1:B:27:C:C2'	1:B:28:G:H5'	2.34	0.58
1:D:9:A:O2'	2:C:161:GLN:HB3	2.03	0.58
2:A:200:TYR:HB3	2:A:209:VAL:O	2.04	0.58
2:C:112:MSE:N	2:C:113:PRO:HD2	2.19	0.58
2:C:170:THR:O	2:C:173:GLN:N	2.37	0.58
2:A:108:GLN:O	2:A:111:LEU:N	2.36	0.57
1:B:44:A:H5''	2:A:31:THR:CG2	2.34	0.57
2:A:55:GLY:HA3	2:A:166:ASN:ND2	2.19	0.57
2:A:174:ILE:O	2:A:178:ILE:HG13	2.04	0.57
2:C:172:GLU:HA	2:C:175:VAL:CG2	2.33	0.57
2:A:202:LYS:HG3	2:A:206:GLY:O	2.05	0.57
1:B:49:C:H4'	1:B:49:C:OP1	2.05	0.57
2:C:15:GLU:O	2:C:15:GLU:HG3	2.05	0.57
2:C:10:VAL:CG2	2:C:201:VAL:HG11	2.31	0.57
2:C:45:LYS:N	2:C:45:LYS:HD3	2.20	0.57
1:B:13:G:C5	1:B:34:G:C2	2.93	0.56
2:A:107:ALA:O	2:A:109:ALA:N	2.38	0.56
2:C:33:LYS:O	2:C:35:ILE:HD12	2.04	0.56
1:D:20:G:H1'	1:D:26:G:N2	2.20	0.56
1:B:17:C:O2	1:B:17:C:H2'	2.05	0.56
2:C:62:VAL:HG21	2:C:72:ALA:HB2	1.84	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:20:G:O4'	1:B:22:A:N7	2.38	0.56
1:B:44:A:H5''	2:A:31:THR:HG21	1.87	0.56
2:C:81:ARG:HH11	2:C:81:ARG:HG3	1.71	0.56
2:A:98:ILE:HG22	2:A:99:ALA:N	2.20	0.56
2:C:118:TYR:CD1	2:C:118:TYR:N	2.74	0.56
2:C:174:ILE:C	2:C:178:ILE:HG13	2.25	0.56
2:C:94:LYS:HA	2:C:97:LYS:HB2	1.88	0.56
1:D:31:G:H2'	1:D:32:C:H6	1.71	0.56
2:A:186:ALA:HA	2:A:191:LYS:O	2.05	0.56
1:B:34:G:H2'	1:B:35:A:C5'	2.21	0.56
1:B:35:A:OP1	1:B:36:G:C8	2.59	0.56
2:C:43:ARG:CD	2:C:156:ASP:HA	2.36	0.56
2:A:146:LEU:O	2:A:148:LYS:N	2.38	0.56
2:A:171:ASP:OD2	2:A:172:GLU:OE1	2.24	0.56
2:C:34:GLU:HB2	2:C:195:HIS:CE1	2.40	0.56
2:A:121:VAL:HG23	2:A:122:ILE:HG22	1.88	0.55
2:A:170:THR:O	2:A:173:GLN:HB2	2.05	0.55
2:A:172:GLU:HA	2:A:175:VAL:HG23	1.87	0.55
1:B:14:G:H5''	2:A:20:ARG:NE	2.20	0.55
1:B:29:A:C2	1:D:38:A:H2	2.25	0.55
2:C:155:ARG:HB2	2:C:155:ARG:NH1	2.21	0.55
1:D:18:G:O2'	1:D:19:C:H5'	2.05	0.55
2:A:146:LEU:C	2:A:148:LYS:N	2.60	0.55
2:C:146:LEU:HA	2:C:149:THR:HG22	1.88	0.55
2:A:146:LEU:C	2:A:148:LYS:H	2.10	0.55
2:A:25:SER:HA	2:A:166:ASN:HA	1.88	0.55
2:C:108:GLN:HB3	2:C:111:LEU:HD12	1.88	0.55
2:C:202:LYS:C	2:C:203:LEU:HD12	2.26	0.55
2:C:141:PRO:HG2	2:C:142:LEU:H	1.72	0.55
1:B:12:A:H5'	2:A:22:PHE:CD1	2.42	0.55
1:B:4:A:O2'	1:B:5:G:H5'	2.06	0.55
2:A:96:ARG:HG2	2:A:122:ILE:CD1	2.32	0.55
1:D:10:G:H1'	2:C:27:GLU:OE1	2.07	0.55
2:A:174:ILE:HG22	2:A:178:ILE:HD11	1.89	0.54
2:A:34:GLU:O	2:A:195:HIS:NE2	2.39	0.54
2:C:138:ASN:HD21	2:C:141:PRO:HD3	1.72	0.54
1:D:13:G:C4	1:D:34:G:C2	2.95	0.54
2:A:18:LYS:HD2	2:A:19:PRO:HD2	1.90	0.54
2:A:199:ALA:O	2:A:211:VAL:HA	2.08	0.54
1:D:12:A:C2'	1:D:13:G:O4'	2.50	0.54
1:D:23:C:C3'	1:D:24:U:C5'	2.74	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:85:ILE:HG23	2:A:86:GLU:N	2.23	0.54
1:D:8:A:H5''	2:C:155:ARG:HH21	1.73	0.54
2:A:129:MSE:SE	2:A:130:PRO:HD2	2.57	0.54
2:A:111:LEU:O	2:A:115:ILE:HG12	2.08	0.54
1:B:9:A:O4'	2:A:161:GLN:NE2	2.41	0.54
2:C:170:THR:C	2:C:174:ILE:HD11	2.28	0.54
2:A:65:THR:N	2:A:108:GLN:OE1	2.41	0.53
2:A:156:ASP:O	2:A:157:LYS:HD3	2.08	0.53
2:C:32:LEU:N	2:C:158:PRO:O	2.41	0.53
2:A:200:TYR:HD1	2:A:200:TYR:N	2.07	0.53
1:B:14:G:OP1	2:A:20:ARG:CD	2.56	0.53
1:B:27:C:H2'	1:B:28:G:C5'	2.38	0.53
2:A:142:LEU:O	2:A:145:ARG:HB3	2.08	0.53
2:C:10:VAL:HG12	2:C:11:LYS:N	2.23	0.53
2:C:32:LEU:HB2	2:C:158:PRO:HB2	1.90	0.53
2:C:188:LYS:HG3	2:C:189:TYR:H	1.74	0.53
2:C:5:ALA:HB1	2:C:213:LYS:H	1.72	0.53
2:A:64:GLY:HA2	2:A:108:GLN:HB2	1.91	0.53
2:A:152:ILE:O	2:A:152:ILE:HG23	2.09	0.53
1:B:13:G:N2	1:B:39:A:H1'	2.24	0.53
2:C:26:PHE:HE1	2:C:167:GLU:HA	1.74	0.53
1:D:28:G:N2	1:D:30:A:C5	2.76	0.53
2:A:112:MSE:O	2:A:115:ILE:N	2.42	0.53
1:B:20:G:H8	1:B:20:G:H5''	1.74	0.53
2:C:37:MSE:HG3	2:C:158:PRO:HD3	1.91	0.53
2:C:194:TYR:O	2:C:195:HIS:HB2	2.09	0.53
2:A:145:ARG:CG	2:A:145:ARG:HH11	2.18	0.53
1:B:43:C:N4	1:B:44:A:H62	2.06	0.53
1:D:2:G:H2'	1:D:3:G:C8	2.41	0.53
1:B:38:A:N1	1:D:29:A:N3	2.56	0.52
1:B:20:G:C8	1:B:20:G:H5''	2.43	0.52
1:B:44:A:H2'	1:B:45:C:H6	1.71	0.52
2:C:106:ILE:HG22	2:C:133:VAL:CG2	2.39	0.52
2:C:139:ILE:CG2	2:C:143:VAL:HG23	2.35	0.52
2:C:112:MSE:O	2:C:115:ILE:N	2.43	0.52
2:C:88:LEU:C	2:C:90:LYS:H	2.13	0.52
2:A:62:VAL:HG12	2:A:106:ILE:CD1	2.39	0.52
2:C:203:LEU:HD12	2:C:203:LEU:N	2.25	0.52
2:C:43:ARG:HD2	2:C:156:ASP:HA	1.90	0.52
2:A:18:LYS:HB2	2:A:20:ARG:HH12	1.74	0.52
2:C:138:ASN:ND2	2:C:141:PRO:HD3	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:154:THR:CG2	2:C:154:THR:O	2.56	0.51
2:C:25:SER:HA	2:C:166:ASN:HA	1.92	0.51
2:A:126:ARG:O	2:A:126:ARG:HG2	2.10	0.51
1:B:31:G:O2'	1:B:32:C:H5'	2.10	0.51
1:B:35:A:OP1	1:B:36:G:N7	2.43	0.51
2:C:166:ASN:C	2:C:166:ASN:OD1	2.48	0.51
2:A:60:ILE:CG2	2:A:61:ALA:N	2.73	0.51
1:B:38:A:C2	1:D:29:A:N3	2.78	0.51
2:C:108:GLN:O	2:C:110:ASP:N	2.44	0.51
2:C:54:ARG:NH2	2:C:149:THR:O	2.41	0.51
2:C:46:THR:O	2:C:152:ILE:HG12	2.11	0.51
2:C:20:ARG:HB3	2:C:22:PHE:CE2	2.46	0.51
2:A:57:GLU:OE1	2:A:147:LYS:HE3	2.09	0.51
2:A:104:PHE:CE2	2:A:149:THR:HG23	2.45	0.51
2:A:193:LEU:HD23	2:A:193:LEU:N	2.25	0.51
2:A:9:ALA:O	2:A:209:VAL:HG11	2.10	0.51
1:B:14:G:OP1	2:A:20:ARG:HD2	2.10	0.51
1:D:37:A:C8	1:D:38:A:H2	2.26	0.51
2:A:36:ASP:C	2:A:38:ARG:H	2.12	0.51
2:A:30:ALA:O	2:A:159:TYR:HA	2.11	0.51
2:C:202:LYS:HB3	2:C:208:ALA:HA	1.92	0.51
1:D:2:G:O2'	1:D:3:G:H5'	2.11	0.51
2:C:32:LEU:HB3	2:C:35:ILE:HD13	1.93	0.51
2:C:39:LYS:HD3	2:C:41:GLU:HG2	1.93	0.51
2:A:104:PHE:C	2:A:105:PHE:HD1	2.14	0.51
2:C:37:MSE:O	2:C:43:ARG:NH1	2.44	0.51
2:C:43:ARG:O	2:C:45:LYS:HD3	2.11	0.51
1:D:31:G:H2'	1:D:32:C:C6	2.46	0.51
2:A:85:ILE:CA	2:A:119:MSE:HE3	2.33	0.51
2:A:55:GLY:HA3	2:A:166:ASN:HD22	1.76	0.51
1:B:3:G:H2'	1:B:4:A:H5''	1.93	0.51
2:C:25:SER:HA	2:C:166:ASN:HB2	1.93	0.51
2:A:202:LYS:HG2	2:A:203:LEU:O	2.10	0.50
2:A:75:LEU:HG	2:A:77:LEU:HD13	1.92	0.50
2:C:140:LYS:N	2:C:141:PRO:HD2	2.26	0.50
2:A:145:ARG:NH1	2:A:145:ARG:HG2	2.21	0.50
2:A:24:GLN:O	2:A:167:GLU:HB2	2.11	0.50
2:A:176:ASP:O	2:A:177:ASN:C	2.49	0.50
2:A:28:PHE:CA	2:A:201:VAL:HG12	2.37	0.50
2:A:16:LEU:HG	2:A:207:PRO:HG2	1.92	0.50
2:A:85:ILE:HG13	2:A:119:MSE:HE3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:141:PRO:O	2:A:145:ARG:HB2	2.10	0.50
1:D:41:U:H1'	2:C:204:THR:O	2.12	0.50
2:C:123:LEU:O	2:C:126:ARG:CB	2.60	0.50
1:D:36:G:O2'	1:D:37:A:OP1	2.22	0.50
2:A:112:MSE:O	2:A:114:LEU:N	2.44	0.50
1:D:1:G:OP2	1:D:1:G:H8	1.95	0.50
1:D:46:U:C2'	1:D:47:C:H5'	2.41	0.50
2:A:177:ASN:O	2:A:181:VAL:CG2	2.53	0.50
2:C:202:LYS:NZ	2:C:206:GLY:O	2.45	0.50
2:C:22:PHE:N	2:C:22:PHE:CD2	2.63	0.50
2:C:32:LEU:CD1	2:C:37:MSE:SE	3.10	0.50
2:C:50:LEU:HB2	2:C:53:GLY:HA2	1.94	0.50
2:A:172:GLU:OE1	2:A:172:GLU:N	2.43	0.49
1:B:23:C:C3'	1:B:24:U:H5''	2.39	0.49
2:C:20:ARG:HB3	2:C:22:PHE:HE2	1.77	0.49
2:A:109:ALA:O	2:A:111:LEU:N	2.45	0.49
2:A:43:ARG:C	2:A:44:ILE:HG13	2.32	0.49
2:A:75:LEU:HG	2:A:77:LEU:CD1	2.42	0.49
2:A:77:LEU:N	2:A:77:LEU:HD12	2.27	0.49
2:C:18:LYS:O	2:C:19:PRO:C	2.50	0.49
2:A:16:LEU:HD23	2:A:209:VAL:HG23	1.94	0.49
1:B:14:G:C2	1:B:33:C:N3	2.81	0.49
2:C:117:ARG:HG3	2:C:118:TYR:CD1	2.47	0.49
2:C:174:ILE:O	2:C:175:VAL:C	2.49	0.49
2:C:202:LYS:HZ3	2:C:202:LYS:CB	2.19	0.49
1:B:29:A:H4'	1:B:29:A:OP2	2.11	0.49
2:C:95:LEU:O	2:C:95:LEU:HG	2.13	0.49
2:A:20:ARG:HB3	2:A:22:PHE:CE2	2.47	0.49
2:C:211:VAL:O	2:C:212:LYS:HB2	2.12	0.49
2:A:202:LYS:HB2	2:A:207:PRO:O	2.12	0.49
1:D:38:A:H3'	1:D:38:A:C8	2.47	0.49
2:A:44:ILE:HG22	2:A:152:ILE:HG23	1.95	0.49
2:A:44:ILE:O	2:A:153:ASN:HA	2.12	0.49
2:A:62:VAL:C	2:A:63:ILE:HD12	2.33	0.49
2:C:59:LYS:N	2:C:103:ASP:HB2	2.26	0.49
2:C:81:ARG:H	2:C:84:GLU:HG3	1.78	0.49
2:C:8:GLN:HA	2:C:11:LYS:NZ	2.27	0.49
2:C:177:ASN:O	2:C:181:VAL:HG23	2.13	0.49
2:C:33:LYS:O	2:C:35:ILE:CD1	2.60	0.49
2:C:43:ARG:CG	2:C:154:THR:HG23	2.42	0.49
1:D:13:G:N9	1:D:34:G:N2	2.61	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:204:THR:C	2:A:205:MSE:HE3	2.33	0.48
2:C:112:MSE:HE1	2:C:130:PRO:HG2	1.94	0.48
2:C:39:LYS:HB3	2:C:41:GLU:OE1	2.13	0.48
2:A:190:GLU:O	2:A:190:GLU:CG	2.61	0.48
2:C:96:ARG:HG3	2:C:97:LYS:N	2.29	0.48
2:C:176:ASP:HA	2:C:179:GLU:HG3	1.95	0.48
2:C:37:MSE:HB3	2:C:156:ASP:O	2.14	0.48
2:C:45:LYS:N	2:C:45:LYS:CD	2.77	0.48
2:A:80:ILE:CD1	2:A:80:ILE:N	2.69	0.48
1:B:23:C:H3'	1:B:24:U:C5'	2.41	0.48
2:C:124:GLY:C	2:C:126:ARG:N	2.66	0.48
2:C:188:LYS:NZ	2:C:188:LYS:HB2	2.29	0.48
2:C:13:ALA:CB	2:C:209:VAL:HG21	2.43	0.48
2:A:15:GLU:C	2:A:17:ALA:H	2.17	0.48
2:C:146:LEU:HD12	2:C:149:THR:HG21	1.95	0.47
2:C:170:THR:HG22	2:C:173:GLN:HG3	1.95	0.47
2:A:170:THR:CG2	2:A:172:GLU:OE1	2.59	0.47
2:A:35:ILE:H	2:A:35:ILE:HD12	1.78	0.47
1:B:22:A:OP1	1:B:22:A:H8	1.97	0.47
1:B:26:G:OP1	2:C:90:LYS:HE3	2.13	0.47
2:C:122:ILE:HG13	2:C:126:ARG:NH1	2.29	0.47
2:C:142:LEU:O	2:C:142:LEU:HD12	2.13	0.47
2:A:15:GLU:C	2:A:17:ALA:N	2.67	0.47
2:A:41:GLU:HG3	2:A:41:GLU:O	2.13	0.47
2:A:85:ILE:HA	2:A:119:MSE:CE	2.34	0.47
2:A:140:LYS:O	2:A:144:GLU:HB3	2.15	0.47
2:C:113:PRO:C	2:C:115:ILE:N	2.67	0.47
2:C:70:LYS:O	2:C:71:GLN:C	2.53	0.47
2:C:57:GLU:HB2	2:C:147:LYS:HE2	1.96	0.47
2:C:94:LYS:O	2:C:97:LYS:N	2.48	0.47
1:D:46:U:O2'	1:D:47:C:H5'	2.13	0.47
2:A:109:ALA:C	2:A:111:LEU:N	2.68	0.47
2:A:37:MSE:HG3	2:A:157:LYS:CA	2.44	0.47
2:A:162:VAL:HG21	2:A:181:VAL:HG11	1.96	0.47
2:A:27:GLU:O	2:A:201:VAL:HA	2.14	0.47
2:C:194:TYR:CD1	2:C:194:TYR:C	2.88	0.47
2:C:166:ASN:O	2:C:168:LYS:N	2.47	0.47
2:C:202:LYS:NZ	2:C:202:LYS:CB	2.69	0.47
1:D:18:G:H2'	1:D:19:C:H6	1.80	0.47
1:D:13:G:C4	1:D:34:G:N2	2.82	0.47
2:A:182:LEU:O	2:A:185:VAL:HB	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:20:ARG:HB3	2:A:22:PHE:CD2	2.50	0.47
2:A:6:LEU:HA	2:A:9:ALA:HB3	1.97	0.47
1:B:33:C:C2'	1:B:34:G:H5''	2.44	0.47
2:A:108:GLN:O	2:A:109:ALA:C	2.53	0.47
1:B:28:G:C2	1:B:30:A:C5	3.03	0.47
2:C:15:GLU:C	2:C:16:LEU:HD12	2.35	0.47
2:C:5:ALA:HB2	2:C:213:LYS:CG	2.41	0.47
1:B:29:A:C4	1:D:37:A:N6	2.83	0.46
2:C:156:ASP:OD2	2:C:157:LYS:CD	2.62	0.46
1:D:26:G:H2'	1:D:27:C:O4'	2.15	0.46
2:C:172:GLU:CA	2:C:175:VAL:HG23	2.44	0.46
2:C:213:LYS:HB3	2:C:214:GLU:H	1.41	0.46
2:C:44:ILE:C	2:C:45:LYS:HD3	2.35	0.46
1:B:34:G:H8	1:B:34:G:H5'	1.81	0.46
2:C:160:PHE:C	2:C:160:PHE:CD1	2.89	0.46
2:C:182:LEU:CD2	2:C:182:LEU:N	2.77	0.46
2:C:77:LEU:CD1	2:C:77:LEU:N	2.78	0.46
2:A:174:ILE:O	2:A:175:VAL:C	2.54	0.46
2:A:86:GLU:HG2	2:A:87:GLU:N	2.30	0.46
2:C:13:ALA:HB2	2:C:209:VAL:HG21	1.97	0.46
2:C:26:PHE:HB2	2:C:165:GLY:CA	2.45	0.46
1:D:23:C:C2'	1:D:24:U:H5''	2.46	0.46
2:A:112:MSE:CE	2:A:130:PRO:HG2	2.27	0.46
2:C:115:ILE:HD13	2:C:130:PRO:HG3	1.98	0.46
1:D:20:G:C6	1:D:22:A:H1'	2.50	0.46
2:A:178:ILE:O	2:A:179:GLU:C	2.54	0.46
2:A:10:VAL:HG13	2:A:26:PHE:HE2	1.81	0.46
2:C:182:LEU:HA	2:C:185:VAL:HB	1.97	0.46
2:C:75:LEU:HB3	2:C:77:LEU:CD1	2.29	0.46
2:A:155:ARG:HH11	2:A:155:ARG:HB2	1.81	0.46
2:A:33:LYS:HD3	2:A:195:HIS:CA	2.46	0.46
2:C:69:ALA:O	2:C:70:LYS:C	2.55	0.46
2:C:59:LYS:C	2:C:60:ILE:HD13	2.36	0.45
2:A:102:HIS:HB2	2:A:105:PHE:HE1	1.82	0.45
1:B:18:G:H2'	1:B:19:C:C6	2.52	0.45
1:B:28:G:C2	1:B:30:A:N7	2.84	0.45
2:C:32:LEU:HB2	2:C:158:PRO:CB	2.45	0.45
2:C:190:GLU:O	2:C:191:LYS:HB2	2.16	0.45
2:A:96:ARG:O	2:A:99:ALA:N	2.49	0.45
2:A:120:GLY:O	2:A:121:VAL:C	2.53	0.45
2:A:140:LYS:N	2:A:141:PRO:HD2	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:24:GLN:HG2	2:A:203:LEU:HD13	1.99	0.45
1:B:13:G:N7	2:C:93:ARG:NH2	2.64	0.45
1:B:30:A:C2	1:B:31:G:C5	3.04	0.45
1:D:17:C:H2'	1:D:18:G:C8	2.52	0.45
2:A:139:ILE:HG23	2:A:143:VAL:HB	1.98	0.45
2:A:73:GLU:H	2:A:73:GLU:CD	2.02	0.45
2:A:92:LYS:CD	2:A:92:LYS:H	2.30	0.45
2:C:124:GLY:O	2:C:126:ARG:N	2.49	0.45
2:C:142:LEU:O	2:C:146:LEU:HB2	2.17	0.45
2:C:171:ASP:C	2:C:174:ILE:HG12	2.36	0.45
2:C:73:GLU:O	2:C:76:GLY:N	2.47	0.45
2:C:143:VAL:HG12	2:C:144:GLU:N	2.30	0.45
2:C:175:VAL:HA	2:C:178:ILE:CD1	2.43	0.45
2:C:199:ALA:O	2:C:211:VAL:HG23	2.17	0.45
1:B:38:A:C2	1:D:29:A:C2	3.05	0.45
1:B:13:G:C4	1:B:34:G:C2	3.04	0.45
2:A:139:ILE:C	2:A:141:PRO:HD2	2.37	0.45
2:A:41:GLU:O	2:A:42:ASN:C	2.55	0.45
2:A:20:ARG:CG	2:A:20:ARG:NH1	2.75	0.45
2:A:36:ASP:O	2:A:38:ARG:N	2.50	0.45
2:C:142:LEU:HA	2:C:145:ARG:HG2	1.98	0.45
1:D:28:G:C2	1:D:30:A:N7	2.85	0.45
2:A:175:VAL:O	2:A:178:ILE:HB	2.17	0.45
2:A:183:ASN:HB3	2:A:187:LYS:NZ	2.32	0.45
1:B:13:G:C8	1:B:34:G:N2	2.85	0.45
1:B:13:G:H21	1:B:39:A:H1'	1.82	0.45
2:C:50:LEU:HD11	2:C:150:VAL:HG21	1.98	0.45
2:A:10:VAL:HG22	2:A:201:VAL:HG21	1.98	0.44
2:A:111:LEU:HD12	2:A:111:LEU:HA	1.65	0.44
2:A:160:PHE:CD1	2:A:160:PHE:C	2.90	0.44
2:A:172:GLU:CA	2:A:175:VAL:HG23	2.47	0.44
2:A:33:LYS:HB3	2:A:34:GLU:H	1.51	0.44
1:B:29:A:C8	1:B:29:A:H5''	2.48	0.44
1:D:43:C:C4'	1:D:43:C:C6	3.00	0.44
2:A:175:VAL:O	2:A:178:ILE:N	2.50	0.44
2:A:33:LYS:HD3	2:A:195:HIS:C	2.37	0.44
1:B:30:A:H2'	1:B:31:G:H8	1.83	0.44
2:C:163:LEU:HD11	2:C:165:GLY:O	2.18	0.44
2:A:203:LEU:H	2:A:203:LEU:HG	1.55	0.44
2:A:35:ILE:C	2:A:35:ILE:CD1	2.86	0.44
2:C:7:LEU:O	2:C:11:LYS:N	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:184:VAL:O	2:A:188:LYS:NZ	2.46	0.44
2:A:212:LYS:HB3	2:A:213:LYS:H	1.58	0.44
2:A:13:ALA:HA	2:A:16:LEU:HB3	1.98	0.44
2:C:159:TYR:C	2:C:159:TYR:CD2	2.87	0.44
2:C:166:ASN:OD1	2:C:166:ASN:O	2.35	0.44
2:C:41:GLU:HG3	2:C:41:GLU:H	1.18	0.44
2:C:66:GLY:O	2:C:69:ALA:HB3	2.17	0.44
2:A:40:PRO:O	2:A:41:GLU:C	2.56	0.44
2:A:78:THR:HG22	2:A:79:VAL:N	2.33	0.44
2:C:33:LYS:HG2	2:C:34:GLU:HG3	1.99	0.44
2:A:104:PHE:C	2:A:105:PHE:CD1	2.90	0.44
2:A:84:GLU:HA	2:A:87:GLU:HB3	2.00	0.44
1:B:44:A:C2'	1:B:45:C:C6	2.99	0.44
2:C:182:LEU:HD22	2:C:182:LEU:N	2.32	0.44
1:D:31:G:O2'	1:D:32:C:H5'	2.17	0.44
2:A:179:GLU:O	2:A:182:LEU:HB2	2.18	0.44
2:A:202:LYS:HE3	2:A:202:LYS:N	2.32	0.44
2:C:111:LEU:O	2:C:115:ILE:HG13	2.17	0.44
2:C:57:GLU:HB3	2:C:147:LYS:HB3	1.99	0.44
1:D:7:G:C2	1:D:44:A:C2	3.06	0.44
1:B:16:U:C2	1:B:31:G:C2	3.06	0.43
2:C:154:THR:O	2:C:155:ARG:C	2.57	0.43
2:C:39:LYS:HG2	2:C:41:GLU:CG	2.45	0.43
2:C:47:GLU:N	2:C:47:GLU:OE2	2.50	0.43
1:B:10:G:N2	2:A:205:MSE:CE	2.81	0.43
1:B:14:G:OP1	2:A:20:ARG:HD3	2.17	0.43
2:A:80:ILE:H	2:A:80:ILE:HD12	1.75	0.43
2:A:88:LEU:HB3	2:A:95:LEU:HD22	2.00	0.43
1:B:3:G:H2'	1:B:4:A:C5'	2.48	0.43
2:C:182:LEU:H	2:C:182:LEU:HD22	1.82	0.43
2:C:28:PHE:CE2	2:C:30:ALA:HB2	2.53	0.43
2:A:85:ILE:CG2	2:A:86:GLU:N	2.81	0.43
1:B:18:G:H2'	1:B:19:C:H6	1.84	0.43
2:C:182:LEU:H	2:C:182:LEU:HD23	1.83	0.43
2:C:20:ARG:NH1	2:C:20:ARG:HG2	2.28	0.43
2:A:174:ILE:O	2:A:177:ASN:CB	2.66	0.43
2:A:16:LEU:HD23	2:A:209:VAL:CG2	2.48	0.43
2:C:122:ILE:CD1	2:C:126:ARG:HH12	2.31	0.43
2:A:112:MSE:N	2:A:113:PRO:CD	2.81	0.43
2:A:200:TYR:HD1	2:A:200:TYR:H	1.66	0.43
2:C:47:GLU:HA	2:C:150:VAL:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:42:ASN:OD1	2:A:188:LYS:HG2	2.18	0.43
2:A:22:PHE:N	2:A:22:PHE:CD2	2.87	0.43
2:A:39:LYS:C	2:A:41:GLU:N	2.70	0.43
1:D:38:A:H3'	1:D:38:A:H8	1.82	0.43
2:A:8:GLN:HA	2:A:11:LYS:HG3	2.00	0.43
2:A:176:ASP:HA	2:A:179:GLU:CG	2.49	0.43
2:A:36:ASP:C	2:A:38:ARG:N	2.71	0.43
2:C:142:LEU:HD11	2:C:146:LEU:HD13	2.00	0.43
2:C:180:ALA:O	2:C:183:ASN:HB3	2.19	0.43
2:C:182:LEU:O	2:C:185:VAL:N	2.52	0.43
2:C:183:ASN:OD1	2:C:187:LYS:HE2	2.19	0.43
2:C:194:TYR:O	2:C:194:TYR:CD1	2.72	0.43
1:D:43:C:C5'	1:D:43:C:C6	3.01	0.43
2:A:202:LYS:HE2	2:A:202:LYS:HB3	1.77	0.43
2:A:35:ILE:HD12	2:A:35:ILE:N	2.34	0.43
2:C:115:ILE:C	2:C:117:ARG:N	2.72	0.43
2:A:16:LEU:HA	2:A:16:LEU:HD12	1.78	0.42
2:C:118:TYR:N	2:C:118:TYR:HD1	2.17	0.42
1:B:40:C:O5'	1:B:40:C:H6	2.01	0.42
2:C:210:LYS:H	2:C:210:LYS:HG3	1.54	0.42
2:A:27:GLU:OE1	2:A:202:LYS:HD2	2.19	0.42
2:A:57:GLU:C	2:A:58:ALA:O	2.56	0.42
1:B:17:C:C2'	1:B:17:C:O2	2.66	0.42
2:C:188:LYS:CG	2:C:189:TYR:H	2.29	0.42
2:A:72:ALA:HB3	2:A:73:GLU:OE1	2.20	0.42
2:C:197:LYS:HB3	2:C:198:ASP:H	1.63	0.42
2:C:46:THR:HA	2:C:47:GLU:OE2	2.19	0.42
2:C:77:LEU:N	2:C:77:LEU:HD12	2.35	0.42
2:C:93:ARG:O	2:C:96:ARG:HG3	2.20	0.42
1:D:17:C:H2'	1:D:18:G:H8	1.82	0.42
1:D:26:G:OP1	2:A:90:LYS:CG	2.63	0.42
1:D:41:U:O2'	2:C:206:GLY:O	2.37	0.42
2:A:112:MSE:C	2:A:114:LEU:H	2.23	0.42
2:C:65:THR:N	2:C:108:GLN:OE1	2.49	0.42
2:C:172:GLU:H	2:C:172:GLU:CD	2.22	0.42
2:C:56:LYS:N	2:C:56:LYS:HE3	2.34	0.42
2:A:92:LYS:H	2:A:92:LYS:HD2	1.85	0.42
1:B:12:A:H5'	2:A:22:PHE:HD1	1.85	0.42
1:B:37:A:C8	1:B:38:A:N3	2.87	0.42
2:A:178:ILE:O	2:A:181:VAL:N	2.53	0.42
2:C:142:LEU:HA	2:C:145:ARG:CG	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:112:MSE:O	2:A:115:ILE:HB	2.19	0.42
1:B:14:G:O2'	1:B:40:C:H4'	2.18	0.42
2:C:178:ILE:O	2:C:181:VAL:N	2.50	0.42
2:C:33:LYS:CG	2:C:34:GLU:HG3	2.50	0.42
1:D:7:G:O2'	1:D:8:A:H5'	2.20	0.42
2:A:140:LYS:O	2:A:144:GLU:CB	2.68	0.42
2:A:22:PHE:N	2:A:22:PHE:HD2	2.18	0.42
2:C:115:ILE:C	2:C:117:ARG:H	2.22	0.42
2:C:64:GLY:HA2	2:C:108:GLN:HB2	2.02	0.42
1:D:28:G:N2	1:D:30:A:N7	2.68	0.42
2:A:114:LEU:O	2:A:118:TYR:HB2	2.18	0.41
2:C:16:LEU:HB3	2:C:207:PRO:HG2	2.01	0.41
2:C:20:ARG:NH1	2:C:20:ARG:CG	2.83	0.41
2:C:83:GLU:HG3	2:C:84:GLU:N	2.33	0.41
2:C:172:GLU:OE2	2:C:172:GLU:N	2.40	0.41
2:C:57:GLU:O	2:C:58:ALA:C	2.58	0.41
2:C:152:ILE:CG2	2:C:162:VAL:HB	2.42	0.41
2:C:95:LEU:O	2:C:95:LEU:CG	2.68	0.41
2:A:56:LYS:HD3	2:A:56:LYS:HA	1.63	0.41
2:A:71:GLN:O	2:A:75:LEU:HB2	2.21	0.41
2:C:32:LEU:HD12	2:C:37:MSE:SE	2.70	0.41
2:C:39:LYS:HA	2:C:40:PRO:HD3	1.82	0.41
2:C:43:ARG:NE	2:C:156:ASP:HA	2.36	0.41
1:B:33:C:H2'	1:B:34:G:H5''	2.01	0.41
2:C:105:PHE:O	2:C:131:LYS:N	2.52	0.41
2:C:172:GLU:O	2:C:173:GLN:C	2.58	0.41
2:A:88:LEU:CD2	2:A:119:MSE:HE1	2.50	0.41
1:B:14:G:C2'	1:B:15:C:H5'	2.51	0.41
2:C:88:LEU:O	2:C:90:LYS:N	2.52	0.41
1:D:36:G:HO2'	1:D:37:A:P	2.40	0.41
1:B:1:G:C5'	1:B:1:G:H8	2.23	0.41
2:C:114:LEU:HD12	2:C:114:LEU:N	2.36	0.41
2:C:123:LEU:O	2:C:124:GLY:C	2.58	0.41
2:C:48:VAL:O	2:C:49:VAL:C	2.59	0.41
2:A:96:ARG:O	2:A:97:LYS:C	2.59	0.41
2:C:160:PHE:C	2:C:160:PHE:HD1	2.23	0.41
1:B:44:A:H2'	1:B:45:C:C5	2.55	0.41
2:C:57:GLU:OE2	2:C:57:GLU:N	2.30	0.41
1:D:30:A:C2	1:D:31:G:C4	3.08	0.41
1:B:30:A:N3	1:B:31:G:C8	2.89	0.41
2:C:163:LEU:C	2:C:164:VAL:HG13	2.41	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:170:THR:O	2:C:173:GLN:HB2	2.20	0.40
2:C:65:THR:HG21	2:C:82:LYS:HB2	2.03	0.40
1:B:7:G:C6	1:B:44:A:N6	2.88	0.40
2:C:32:LEU:HB3	2:C:35:ILE:CD1	2.51	0.40
2:C:83:GLU:O	2:C:85:ILE:N	2.54	0.40
1:D:12:A:H2'	1:D:13:G:C5'	2.51	0.40
1:B:28:G:N2	1:B:30:A:C5	2.89	0.40
2:C:203:LEU:O	2:C:205:MSE:N	2.55	0.40
2:C:44:ILE:HG21	2:C:152:ILE:HD12	2.03	0.40
2:C:62:VAL:HG21	2:C:72:ALA:HB3	2.01	0.40
2:A:124:GLY:C	2:A:126:ARG:H	2.25	0.40
2:A:145:ARG:NH1	2:A:145:ARG:CG	2.80	0.40
1:B:43:C:H42	1:B:44:A:H62	1.68	0.40
2:A:206:GLY:HA2	2:A:207:PRO:HD3	1.88	0.40
2:C:165:GLY:HA2	2:C:169:MSE:CE	2.52	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 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	Percentiles	
2	A	212/219 (97%)	156 (74%)	29 (14%)	27 (13%)	0	4
2	C	212/219 (97%)	139 (66%)	49 (23%)	24 (11%)	0	6
All	All	424/438 (97%)	295 (70%)	78 (18%)	51 (12%)	0	5

All (51) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	35	ILE
2	A	82	LYS
2	A	121	VAL

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Mol	Chain	Res	Type
2	A	122	ILE
2	A	135	ALA
2	A	171	ASP
2	A	175	VAL
2	A	188	LYS
2	C	109	ALA
2	C	135	ALA
2	C	167	GLU
2	C	171	ASP
2	C	192	GLY
2	C	195	HIS
2	C	212	LYS
2	A	72	ALA
2	A	109	ALA
2	A	110	ASP
2	A	120	GLY
2	C	49	VAL
2	C	84	GLU
2	C	92	LYS
2	C	108	GLN
2	C	204	THR
2	A	37	MSE
2	A	42	ASN
2	A	113	PRO
2	A	147	LYS
2	A	164	VAL
2	A	193	LEU
2	C	11	LYS
2	C	58	ALA
2	C	134	PRO
2	A	167	GLU
2	A	195	HIS
2	C	85	ILE
2	A	5	ALA
2	A	44	ILE
2	A	108	GLN
2	C	125	PRO
2	C	166	ASN
2	A	22	PHE
2	A	32	LEU
2	C	33	LYS
2	C	44	ILE

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Mol	Chain	Res	Type
2	C	71	GLN
2	C	140	LYS
2	C	121	VAL
2	A	192	GLY
2	C	143	VAL
2	A	66	GLY

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 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	Percentiles	
2	A	182/180 (101%)	134 (74%)	48 (26%)	0	3
2	C	182/180 (101%)	136 (75%)	46 (25%)	1	3
All	All	364/360 (101%)	270 (74%)	94 (26%)	0	3

All (94) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	2	ASP
2	A	14	ARG
2	A	20	ARG
2	A	22	PHE
2	A	27	GLU
2	A	31	THR
2	A	35	ILE
2	A	37	MSE
2	A	39	LYS
2	A	41	GLU
2	A	44	ILE
2	A	47	GLU
2	A	51	PRO
2	A	56	LYS
2	A	65	THR
2	A	74	GLU
2	A	75	LEU

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Mol	Chain	Res	Type
2	A	79	VAL
2	A	81	ARG
2	A	83	GLU
2	A	88	LEU
2	A	93	ARG
2	A	95	LEU
2	A	98	ILE
2	A	100	LYS
2	A	106	ILE
2	A	112	MSE
2	A	114	LEU
2	A	119	MSE
2	A	134	PRO
2	A	139	ILE
2	A	151	VAL
2	A	155	ARG
2	A	159	TYR
2	A	160	PHE
2	A	166	ASN
2	A	167	GLU
2	A	170	THR
2	A	171	ASP
2	A	176	ASP
2	A	191	LYS
2	A	194	TYR
2	A	198	ASP
2	A	200	TYR
2	A	202	LYS
2	A	205	MSE
2	A	213	LYS
2	A	214	GLU
2	C	1	MET
2	C	3	ARG
2	C	8	GLN
2	C	12	GLU
2	C	22	PHE
2	C	25	SER
2	C	29	ILE
2	C	31	THR
2	C	33	LYS
2	C	38	ARG
2	C	41	GLU

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Mol	Chain	Res	Type
2	C	42	ASN
2	C	44	ILE
2	C	45	LYS
2	C	46	THR
2	C	51	PRO
2	C	56	LYS
2	C	75	LEU
2	C	79	VAL
2	C	83	GLU
2	C	93	ARG
2	C	103	ASP
2	C	121	VAL
2	C	126	ARG
2	C	133	VAL
2	C	149	THR
2	C	155	ARG
2	C	159	TYR
2	C	160	PHE
2	C	161	GLN
2	C	166	ASN
2	C	170	THR
2	C	174	ILE
2	C	175	VAL
2	C	182	LEU
2	C	184	VAL
2	C	188	LYS
2	C	189	TYR
2	C	190	GLU
2	C	193	LEU
2	C	194	TYR
2	C	198	ASP
2	C	202	LYS
2	C	205	MSE
2	C	210	LYS
2	C	214	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	91	ASN
2	A	153	ASN
2	A	161	GLN

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Mol	Chain	Res	Type
2	A	166	ASN
2	A	173	GLN
2	A	183	ASN
2	C	21	ASN
2	C	91	ASN
2	C	161	GLN
2	C	195	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	B	48/49 (97%)	20 (41%)	3 (6%)
1	D	48/49 (97%)	17 (35%)	5 (10%)
All	All	96/98 (97%)	37 (38%)	8 (8%)

All (37) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	B	2	G
1	B	4	A
1	B	8	A
1	B	12	A
1	B	13	G
1	B	17	C
1	B	20	G
1	B	21	A
1	B	22	A
1	B	23	C
1	B	24	U
1	B	29	A
1	B	30	A
1	B	34	G
1	B	35	A
1	B	38	A
1	B	39	A
1	B	43	C
1	B	47	C
1	B	49	C
1	D	2	G
1	D	10	G
1	D	11	G

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Mol	Chain	Res	Type
1	D	12	A
1	D	13	G
1	D	21	A
1	D	22	A
1	D	23	C
1	D	24	U
1	D	25	C
1	D	30	A
1	D	35	A
1	D	37	A
1	D	38	A
1	D	39	A
1	D	43	C
1	D	44	A

All (8) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	B	12	A
1	B	20	G
1	B	44	A
1	D	11	G
1	D	12	A
1	D	36	G
1	D	38	A
1	D	43	C

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

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95th 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	OWAB(Å ²)	Q<0.9
1	B	49/49 (100%)	-0.56	0 100 100	56, 79, 117, 150	0
1	D	49/49 (100%)	-0.37	1 (2%) 68 62	53, 82, 139, 153	0
2	A	208/219 (94%)	-0.37	4 (1%) 70 64	9, 77, 134, 153	0
2	C	208/219 (94%)	-0.41	1 (0%) 91 89	21, 79, 132, 146	0
All	All	514/536 (95%)	-0.40	6 (1%) 81 75	9, 79, 134, 153	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	1	MET	4.7
2	C	1	MET	2.9
2	A	189	TYR	2.6
2	A	28	PHE	2.2
2	A	27	GLU	2.1
1	D	23	C	2.1

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 carbohydrates 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.