Full wwPDB X-ray Structure Validation Report ⓘ

Oct 21, 2024 – 11:31 AM EDT

PDB ID	:	1U63
Title	:	THE STRUCTURE OF A RIBOSOMAL PROTEIN L1-mRNA COMPLEX
Authors	:	Nevskaya, N.; Tishchenko, S.; Gabdoulkhakov, A.; Nikonova, E.; Nikonov, O.; 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

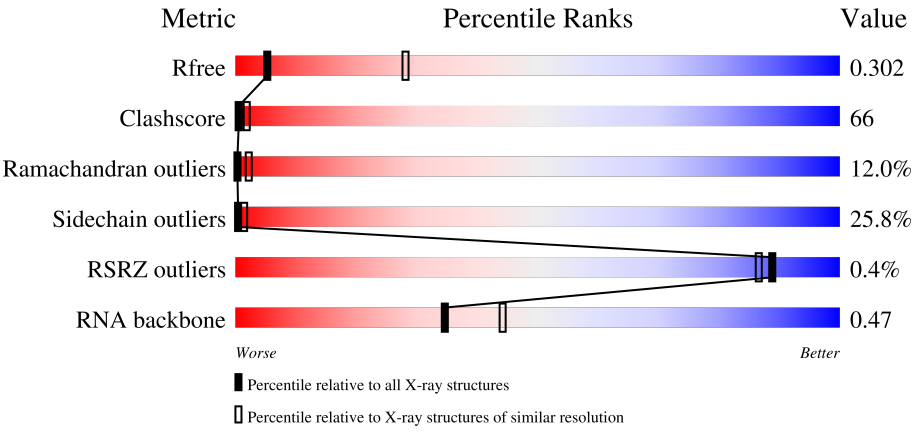
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance (i)

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}	164625	1140 (3.46-3.34)
Clashscore	180529	1172 (3.46-3.34)
Ramachandran outliers	177936	1172 (3.46-3.34)
Sidechain outliers	177891	1172 (3.46-3.34)
RSRZ outliers	164620	1140 (3.46-3.34)
RNA backbone	3690	1033 (3.80-3.00)

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

Mol	Chain	Length	Quality of chain
1	B	49	2% 12% 45% 33% 10%
1	D	49	2% 20% 41% 29% 10%
2	A	219	17% 56% 21%
2	C	219	15% 57% 24%

2 Entry composition (i)

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:

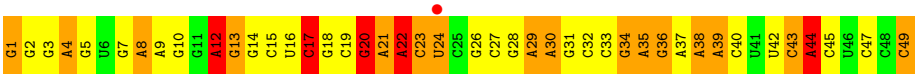
Chain	Residue	Modelled	Actual	Comment	Reference
A	37	MSE	MET	modified residue	UNP P54050
A	112	MSE	MET	modified residue	UNP P54050
A	119	MSE	MET	modified residue	UNP P54050
A	129	MSE	MET	modified residue	UNP P54050
A	169	MSE	MET	modified residue	UNP P54050
A	205	MSE	MET	modified residue	UNP P54050
C	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 (i)

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

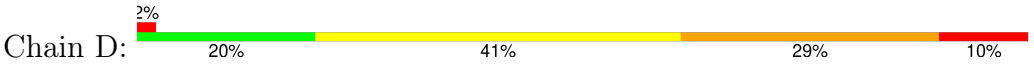
• Molecule 1: 49 NT FRAGMENT OF MRNA FOR L1

Chain B:



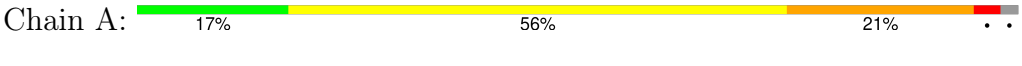
• Molecule 1: 49 NT FRAGMENT OF MRNA FOR L1

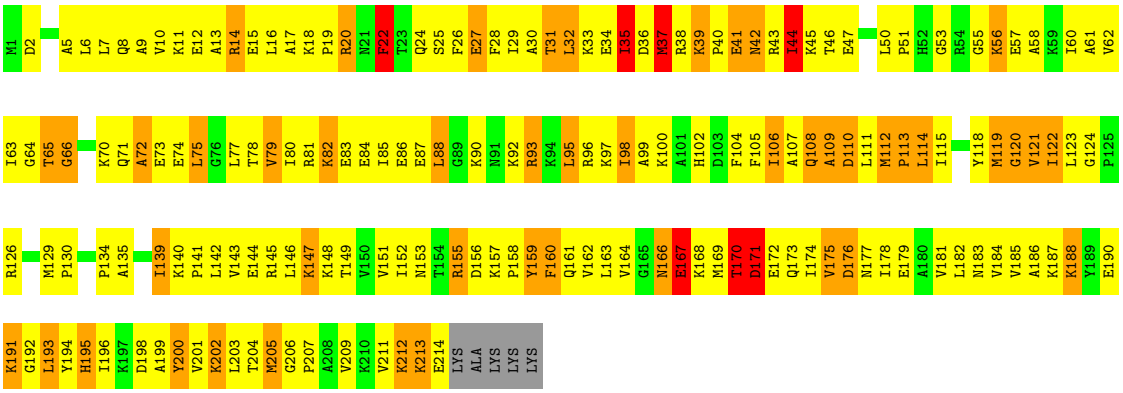
Chain D:



• Molecule 2: 50S ribosomal protein L1P

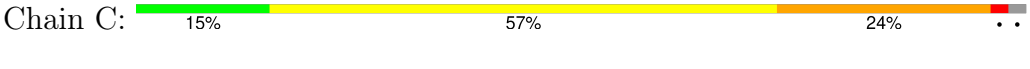
Chain A:

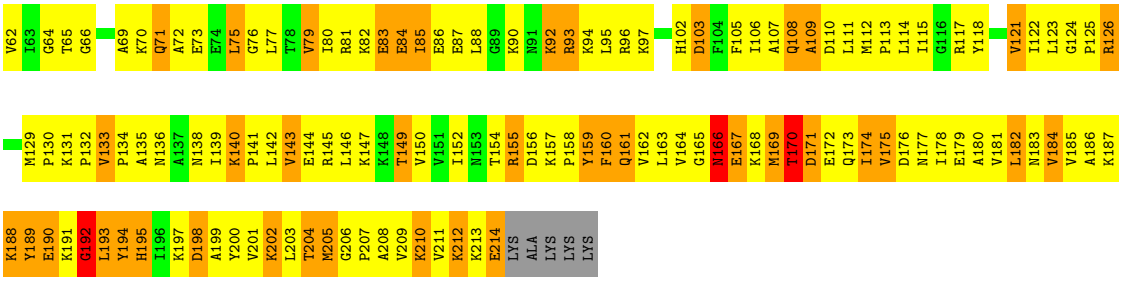




• Molecule 2: 50S ribosomal protein L1P

Chain C:




V62 I63 G64 T65 G66 A69 K70 Q71 A72 E73 E74 L75 G76 L77 T78 V79 I80 R81 K82 E83 E84 I85 E86 E87 L88 G89 K90 N91 K92 R93 K94 L95 R96 K97 H102 D103 F104 F105 I106 A107 Q108 A109 D110 L111 M112 P113 L114 I115 G116 R117 Y118 V121 I122 L123 G124 P125 R126
M129 P130 K131 P132 V133 P134 A135 N136 A137 N138 I139 K140 P141 L142 V143 E144 R145 L146 K147 K148 T149 V150 V151 I152 N153 T154 R155 D156 K157 P158 Y159 F160 Q161 V162 L163 V164 G165 N166 E167 K168 M169 T170 D171 E172 Q173 I174 V175 D176 N177 I178 E179 A180 V181 L182 N183 V184 V185 A186 K187
K188 Y189 E190 K191 G192 L193 Y194 H195 T196 K197 D198 A199 Y200 V201 K202 L203 T204 M205 G206 P207 A208 V209 K210 V211 K212 K213 E214 LYS ALA LYS LYS LYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	212.29Å 68.90Å 115.87Å 90.00° 122.99° 90.00°	Depositor
Resolution (Å)	8.00 – 3.40 8.00 – 3.40	Depositor EDS
% Data completeness (in resolution range)	92.7 (8.00-3.40) 93.1 (8.00-3.40)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	2.06 (at 3.39Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.276 , 0.302 0.278 , 0.302	Depositor DCC
R_{free} test set	2388 reflections (6.54%)	wwPDB-VP
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 , 107.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	0.399 for -h-2*l,-k,l	Xtriage
F_o,F_c correlation	0.94	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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	#$\|Z\|$ >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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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 (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	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:32:LEU:HD12	2:C:158:PRO:HA	1.30	1.05
2:C:44:ILE:HD12	2:C:44:ILE:H	1.15	1.05
1:B:1:G:C8	1:B:1:G:H5"	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:HB2	2:A:14:ARG:HH11	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
1:D:12:A:H2'	1:D:13:G:O4'	1.67	0.94
2:C:22:PHE:H	2:C:22:PHE:HD2	1.13	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:HG2	2:A:20:ARG:HH11	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:33:LYS:HB2	2:A:195:HIS:O	1.77	0.84
2:A:108:GLN:HG2	2:A:110:ASP:OD1	1.78	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:HB2	2:C:202:LYS:NZ	1.93	0.83
2:A:57:GLU:HB2	2:A:147:LYS:HE2	1.60	0.83
2:A:195:HIS:O	2:A:195:HIS:ND1	2.11	0.83
2:C:86:GLU:HG3	2:C:87:GLU:N	1.94	0.83
2:A:145:ARG:HG2	2:A:145:ARG:HH11	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:HB2	2:C:202:LYS:HZ3	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:HB2	2:A:14:ARG:NH1	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:HD13	2:C:174:ILE:H	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:80:ILE:N	2:A:80:ILE:HD12	1.97	0.78
2:A:123:LEU:HD21	2:A:130:PRO:HD3	1.65	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:79:VAL:O	2:C:80:ILE:HD13	1.84	0.77
2:C:186:ALA:HB1	2:C:192:GLY:O	1.84	0.77
2:C:62:VAL:HG21	2:C:72:ALA:CB	2.14	0.77
2:C:92:LYS:O	2:C:96:ARG:HG2	1.84	0.76
2:C:200:TYR:CD2	2:C:210:LYS:HA	2.20	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:16:LEU:N	2:C:16:LEU:HD12	2.02	0.75
2:C:57:GLU:CB	2:C:147:LYS:HE2	2.16	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:63:ILE:HG21	2:A:115:ILE:HD11	1.70	0.73
2:A:170:THR:HG23	2:A:172:GLU:OE1	1.88	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
1:D:26:G:OP1	2:A:90:LYS:HG3	1.88	0.73
2:A:143:VAL:HG12	2:A:144:GLU:N	2.04	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:37:MSE:HA	2:C:37:MSE:HE2	1.71	0.71
2:C:186:ALA:HB2	2:C:193:LEU: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
1:D:2:G:H2'	1:D:3:G:H8	1.55	0.70
2:C:44:ILE:HD12	2:C:44:ILE:N	1.99	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:OE1	2:A:15:GLU:O	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:O	2:C:152:ILE:HG13	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:20:ARG:HH11	2:C:20:ARG:HG2	1.59	0.67
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: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
1:B:29:A:H8	1:B:29:A:H5"	1.61	0.66
2:A:33:LYS:HB2	2:A:195:HIS:ND1	2.10	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
1:D:43:C:C4'	1:D:44:A:OP2	2.31	0.66
2:A:7:LEU:HD23	2:A:11:LYS:HE3	1.77	0.66
1:D:10:G:C2'	2:C:204:THR:HG22	2.25	0.66
1:B:37:A:H5"	1:B:38:A:OP2	1.96	0.66
2:A:105:PHE:CB	2:A:130:PRO:HB3	2.24	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
1:D:12:A:H2'	1:D:13:G:O5'	1.96	0.65
2:A:200:TYR:N	2:A:200:TYR:CD1	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:B:29:A:C2	1:D:38:A:C2	2.85	0.64
2:A:174:ILE:O	2:A:177:ASN:HB2	1.97	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:CD2	2:C:182:LEU:H	2.12	0.63
1:B:21:A:OP2	1:B:22:A:N7	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:45:LYS:HA	2:A:153:ASN:HD22	1.61	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:32:LEU:HD22	2:C:35:ILE:CD1	2.29	0.62
2:C:123:LEU:O	2:C:126:ARG:N	2.32	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:55:GLY:HA3	2:C:166:ASN:HD21	1.66	0.60
2:C:174:ILE:H	2:C:174:ILE:CD1	2.04	0.60
1:B:1:G:C8	1:B:1:G:C5'	2.77	0.60
2:A:172:GLU:O	2:A:175:VAL:HG23	2.02	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:7:LEU:CD1	2:C:172:GLU:HG3	2.29	0.60
2:C:113:PRO:C	2:C:115:ILE:H	2.03	0.60
2:C:47:GLU:O	2:C:47:GLU:HG2	2.03	0.59
2:C:200:TYR:HA	2:C:211:VAL:HG23	1.85	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
1:B:20:G:C4'	1:B:21:A:OP2	2.44	0.59
2:A:92:LYS:O	2:A:96:ARG:HG3	2.02	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:OP2	1:D:21:A:H4'	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
1:D:10:G:O2'	2:C:204:THR:HG22	2.04	0.58
2:A:37:MSE:HE3	2:A:37:MSE:HA	1.84	0.58
2:A:109:ALA:C	2:A:111:LEU:H	2.05	0.58
2:A:176:ASP:OD2	2:A:176:ASP:N	2.34	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:20:ARG:HH11	2:A:20:ARG:CG	2.13	0.58
2:A:172:GLU:HA	2:A:175:VAL:CG2	2.33	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:66:GLY:O	2:A:70:LYS:N	2.37	0.58
2:A:190:GLU:O	2:A:190:GLU:HG3	2.02	0.58
2:C:123:LEU:O	2:C:126:ARG:HB2	2.03	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:24:GLN:CG	2:A:203:LEU:HD13	2.32	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
1:B:44:A:H5"	2:A:31:THR:CG2	2.34	0.57
2:A:108:GLN:O	2:A:111:LEU:N	2.36	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:HD3	2:C:45:LYS:N	2.20	0.57
1:B:13:G:C5	1:B:34:G:C2	2.93	0.56
1:D:20:G:H1'	1:D:26:G:N2	2.20	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:B:17:C:H2'	1:B:17:C:O2	2.05	0.56
1:B:20:G:O4'	1:B:22:A:N7	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:62:VAL:HG21	2:C:72:ALA:HB2	1.84	0.56
1:B:44:A:H5"	2:A:31:THR:HG21	1.87	0.56
2:C:81:ARG:HG3	2:C:81:ARG:HH11	1.71	0.56
2:A:98:ILE:HG22	2:A:99:ALA:N	2.20	0.56
2:C:118:TYR:N	2:C:118:TYR:CD1	2.74	0.56
2:C:174:ILE:C	2:C:178:ILE:HG13	2.25	0.56
1:D:31:G:H2'	1:D:32:C:H6	1.71	0.56
2:C:94:LYS:HA	2:C:97:LYS:HB2	1.88	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:A:186:ALA:HA	2:A:191:LYS:O	2.05	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
1:B:14:G:H5"	2:A:20:ARG:NE	2.20	0.55
2:A:172:GLU:HA	2:A:175:VAL:HG23	1.87	0.55
1:B:29:A:C2	1:D:38:A:H2	2.25	0.55
1:D:18:G:O2'	1:D:19:C:H5'	2.05	0.55
2:C:155:ARG:HB2	2:C:155:ARG:NH1	2.21	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:25:SER:HA	2:A:166:ASN:HA	1.88	0.55
2:A:146:LEU:C	2:A:148:LYS:H	2.10	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:4:A:O2'	1:B:5:G:H5'	2.06	0.55
1:B:12:A:H5'	2:A:22:PHE:CD1	2.42	0.55
1:D:10:G:H1'	2:C:27:GLU:OE1	2.07	0.55
2:A:96:ARG:HG2	2:A:122:ILE:CD1	2.32	0.55
2:A:34:GLU:O	2:A:195:HIS:NE2	2.39	0.54
2:A:174:ILE:HG22	2:A:178:ILE:HD11	1.89	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:8:A:H5"	2:C:155:ARG:HH21	1.73	0.54
2:A:85:ILE:HG23	2:A:86:GLU:N	2.23	0.54
2:A:129:MSE:SE	2:A:130:PRO:HD2	2.57	0.54
1:B:9:A:O4'	2:A:161:GLN:NE2	2.41	0.54
2:A:111:LEU:O	2:A:115:ILE:HG12	2.08	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
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:200:TYR:N	2:A:200:TYR:HD1	2.07	0.53
2:A:142:LEU:O	2:A:145:ARG:HB3	2.08	0.53
2:C:5:ALA:HB1	2:C:213:LYS:H	1.72	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:A:64:GLY:HA2	2:A:108:GLN:HB2	1.91	0.53
2:A:152:ILE:HG23	2:A:152:ILE:O	2.09	0.53
1:B:13:G:N2	1:B:39:A:H1'	2.24	0.53
1:D:28:G:N2	1:D:30:A:C5	2.76	0.53
2:C:26:PHE:HE1	2:C:167:GLU:HA	1.74	0.53
1:B:20:G:H5"	1:B:20:G:H8	1.74	0.53
2:A:112:MSE:O	2:A:115:ILE:N	2.42	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
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
2:A:145:ARG:HH11	2:A:145:ARG:CG	2.18	0.53
1:B:38:A:N1	1:D:29:A:N3	2.56	0.52
1:B:20:G:H5"	1:B:20:G:C8	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:88:LEU:C	2:C:90:LYS:H	2.13	0.52
2:C:112:MSE:O	2:C:115:ILE:N	2.43	0.52
2:A:62:VAL:HG12	2:A:106:ILE:CD1	2.39	0.52
2:C:43:ARG:HD2	2:C:156:ASP:HA	1.90	0.52
2:C:203:LEU:HD12	2:C:203:LEU:N	2.25	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:25:SER:HA	2:C:166:ASN:HA	1.92	0.51
2:C:154:THR:O	2:C:154:THR:CG2	2.56	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:A:126:ARG:O	2:A:126:ARG:HG2	2.10	0.51
2:C:166:ASN:C	2:C:166:ASN:OD1	2.48	0.51
1:B:38:A:C2	1:D:29:A:N3	2.78	0.51
2:A:60:ILE:CG2	2:A:61:ALA:N	2.73	0.51
2:C:20:ARG:HB3	2:C:22:PHE:CE2	2.46	0.51
2:C:46:THR:O	2:C:152:ILE:HG12	2.11	0.51
2:C:54:ARG:NH2	2:C:149:THR:O	2.41	0.51
2:C:108:GLN:O	2:C:110:ASP:N	2.44	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:9:ALA:O	2:A:209:VAL:HG11	2.10	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:N	2:A:193:LEU:HD23	2.25	0.51
2:A:36:ASP:C	2:A:38:ARG:H	2.12	0.51
1:D:2:G:O2'	1:D:3:G:H5'	2.11	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
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
1:D:31:G:H2'	1:D:32:C:C6	2.46	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:B:3:G:H2'	1:B:4:A:H5"	1.93	0.51
2:A:55:GLY:HA3	2:A:166:ASN:HD22	1.76	0.51
2:A:85:ILE:CA	2:A:119:MSE:HE3	2.33	0.51
2:C:25:SER:HA	2:C:166:ASN:HB2	1.93	0.51
2:A:75:LEU:HG	2:A:77:LEU:HD13	1.92	0.50
2:A:202:LYS:HG2	2:A:203:LEU:O	2.10	0.50
2:C:140:LYS:N	2:C:141:PRO:HD2	2.26	0.50
2:A:16:LEU:HG	2:A:207:PRO:HG2	1.92	0.50
2:A:24:GLN:O	2:A:167:GLU:HB2	2.11	0.50
2:A:28:PHE:CA	2:A:201:VAL:HG12	2.37	0.50
2:A:145:ARG:HG2	2:A:145:ARG:NH1	2.21	0.50
2:A:176:ASP:O	2:A:177:ASN:C	2.49	0.50
1:D:41:U:H1'	2:C:204:THR:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:85:ILE:HG13	2:A:119:MSE:HE3	1.93	0.50
2:A:141:PRO:O	2:A:145:ARG:HB2	2.10	0.50
1:D:36:G:O2'	1:D:37:A:OP1	2.22	0.50
2:C:123:LEU:O	2:C:126:ARG:CB	2.60	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:112:MSE:O	2:A:114:LEU:N	2.44	0.50
2:A:177:ASN:O	2:A:181:VAL:CG2	2.53	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:C:202:LYS:NZ	2:C:206:GLY:O	2.45	0.50
1:B:23:C:C3'	1:B:24:U:H5"	2.39	0.49
2:A:172:GLU:OE1	2:A:172:GLU:N	2.43	0.49
2:C:20:ARG:HB3	2:C:22:PHE:HE2	1.77	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:HD12	2:A:77:LEU:N	2.27	0.49
2:A:109:ALA:O	2:A:111:LEU:N	2.45	0.49
2:C:18:LYS:O	2:C:19:PRO:C	2.50	0.49
1:B:14:G:C2	1:B:33:C:N3	2.81	0.49
2:A:16:LEU:HD23	2:A:209:VAL:HG23	1.94	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
1:D:38:A:C8	1:D:38:A:H3'	2.47	0.49
2:A:202:LYS:HB2	2:A:207:PRO:O	2.12	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:8:GLN:HA	2:C:11:LYS:NZ	2.27	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:33:LYS:O	2:C:35:ILE:CD1	2.60	0.49
2:C:177:ASN:O	2:C:181:VAL:HG23	2.13	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
1:B:23:C:H3'	1:B:24:U:C5'	2.41	0.48
2:A:80:ILE:N	2:A:80:ILE:CD1	2.69	0.48
2:C:124:GLY:C	2:C:126:ARG:N	2.66	0.48
2:C:188:LYS:HB2	2:C:188:LYS:NZ	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
1:B:22:A:H8	1:B:22:A:OP1	1.97	0.47
1:B:26:G:OP1	2:C:90:LYS:HE3	2.13	0.47
2:A:35:ILE:HD12	2:A:35:ILE:H	1.78	0.47
2:A:170:THR:CG2	2:A:172:GLU:OE1	2.59	0.47
2:C:122:ILE:HG13	2:C:126:ARG:NH1	2.29	0.47
2:C:142:LEU:HD12	2:C:142:LEU:O	2.13	0.47
2:A:15:GLU:C	2:A:17:ALA:N	2.67	0.47
2:A:41:GLU:O	2:A:41:GLU:HG3	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:70:LYS:O	2:C:71:GLN:C	2.53	0.47
2:C:113:PRO:C	2:C:115:ILE:N	2.67	0.47
1:D:46:U:O2'	1:D:47:C:H5'	2.13	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
2:A:27:GLU:O	2:A:201:VAL:HA	2.14	0.47
2:A:37:MSE:HG3	2:A:157:LYS:CA	2.44	0.47
2:A:109:ALA:C	2:A:111:LEU:N	2.68	0.47
2:A:162:VAL:HG21	2:A:181:VAL:HG11	1.96	0.47
2:C:194:TYR:CD1	2:C:194:TYR:C	2.88	0.47
1:D:13:G:C4	1:D:34:G:N2	2.82	0.47
1:D:18:G:H2'	1:D:19:C:H6	1.80	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:B:33:C:C2'	1:B:34:G:H5"	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:6:LEU:HA	2:A:9:ALA:HB3	1.97	0.47
2:A:20:ARG:HB3	2:A:22:PHE:CD2	2.50	0.47
2:A:182:LEU:O	2:A:185:VAL:HB	2.14	0.47
1:B:28:G:C2	1:B:30:A:C5	3.03	0.47
2:A:108:GLN:O	2:A:109:ALA:C	2.53	0.47
2:C:5:ALA:HB2	2:C:213:LYS:CG	2.41	0.47
2:C:15:GLU:C	2:C:16:LEU:HD12	2.35	0.47
1:B:29:A:C4	1:D:37:A:N6	2.83	0.46
1:D:26:G:H2'	1:D:27:C:O4'	2.15	0.46
2:C:156:ASP:OD2	2:C:157:LYS:CD	2.62	0.46
2:C:44:ILE:C	2:C:45:LYS:HD3	2.35	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
1:B:34:G:H5'	1:B:34:G:H8	1.81	0.46
2:C:77:LEU:CD1	2:C:77:LEU:N	2.78	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:A:174:ILE:O	2:A:175:VAL:C	2.54	0.46
1:D:23:C:C2'	1:D:24:U:H5"	2.46	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:20:G:C6	1:D:22:A:H1'	2.50	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
2:A:10:VAL:HG13	2:A:26:PHE:HE2	1.81	0.46
2:A:178:ILE:O	2:A:179:GLU:C	2.54	0.46
2:C:75:LEU:HB3	2:C:77:LEU:CD1	2.29	0.46
2:C:182:LEU:HA	2:C:185:VAL:HB	1.97	0.46
2:A:33:LYS:HD3	2:A:195:HIS:CA	2.46	0.46
2:A:155:ARG:HH11	2:A:155:ARG:HB2	1.81	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
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:A:102:HIS:HB2	2:A:105:PHE:HE1	1.82	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:17:C:H2'	1:D:18:G:C8	2.52	0.45
2:A:24:GLN:HG2	2:A:203:LEU:HD13	1.99	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
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:A:139:ILE:HG23	2:A:143:VAL:HB	1.98	0.45
2:C:73:GLU:O	2:C:76:GLY:N	2.47	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
1:B:38:A:C2	1:D:29:A:C2	3.05	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:13:G:C4	1:B:34:G:C2	3.04	0.45
2:A:41:GLU:O	2:A:42:ASN:C	2.55	0.45
2:A:139:ILE:C	2:A:141:PRO:HD2	2.37	0.45
1:D:28:G:C2	1:D:30:A:N7	2.85	0.45
2:A:20:ARG:NH1	2:A:20:ARG:CG	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: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: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
2:C:50:LEU:HD11	2:C:150:VAL:HG21	1.98	0.45
1:B:29:A:H5"	1:B:29:A:C8	2.48	0.44
1:D:43:C:C6	1:D:43:C:C4'	3.00	0.44
2:A:10:VAL:HG22	2:A:201:VAL:HG21	1.98	0.44
2:A:33:LYS:HB3	2:A:34:GLU:H	1.51	0.44
2:A:111:LEU:HA	2:A:111:LEU:HD12	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
1:B:30:A:H2'	1:B:31:G:H8	1.83	0.44
2:A:33:LYS:HD3	2:A:195:HIS:C	2.37	0.44
2:A:175:VAL:O	2:A:178:ILE:N	2.50	0.44
2:C:163:LEU:HD11	2:C:165:GLY:O	2.18	0.44
2:A:35:ILE:CD1	2:A:35:ILE:C	2.86	0.44
2:A:203:LEU:H	2:A:203:LEU:HG	1.55	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: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:C:159:TYR:CD2	2:C:159:TYR:C	2.87	0.44
2:C:166:ASN:OD1	2:C:166:ASN:O	2.35	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
1:B:44:A:C2'	1:B:45:C:C6	2.99	0.44
1:D:31:G:O2'	1:D:32:C:H5'	2.17	0.44
2:A:84:GLU:HA	2:A:87:GLU:HB3	2.00	0.44
2:A:104:PHE:C	2:A:105:PHE:CD1	2.90	0.44
2:C:182:LEU:N	2:C:182:LEU:HD22	2.32	0.44
1:D:7:G:C2	1:D:44:A:C2	3.06	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:57:GLU:HB3	2:C:147:LYS:HB3	1.99	0.44
2:C:111:LEU:O	2:C:115:ILE:HG13	2.17	0.44
1:B:16:U:C2	1:B:31:G:C2	3.06	0.43
2:C:39:LYS:HG2	2:C:41:GLU:CG	2.45	0.43
2:C:47:GLU:OE2	2:C:47:GLU:N	2.50	0.43
2:C:154:THR:O	2:C:155:ARG:C	2.57	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
1:B:3:G:H2'	1:B:4:A:C5'	2.48	0.43
2:A:80:ILE:HD12	2:A:80:ILE:H	1.75	0.43
2:A:88:LEU:HB3	2:A:95:LEU:HD22	2.00	0.43
2:C:28:PHE:CE2	2:C:30:ALA:HB2	2.53	0.43
2:C:182:LEU:H	2:C:182:LEU:HD22	1.82	0.43
1:B:18:G:H2'	1:B:19:C:H6	1.84	0.43
2:A:85:ILE:CG2	2:A:86:GLU:N	2.81	0.43
2:C:20:ARG:HG2	2:C:20:ARG:NH1	2.28	0.43
2:C:182:LEU:HD23	2:C:182:LEU:H	1.83	0.43
2:A:16:LEU:HD23	2:A:209:VAL:CG2	2.48	0.43
2:A:174:ILE:O	2:A:177:ASN:CB	2.66	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)
1:D:38:A:H3'	1:D:38:A:H8	1.82	0.43
2:A:22:PHE:CD2	2:A:22:PHE:N	2.87	0.43
2:A:39:LYS:C	2:A:41:GLU:N	2.70	0.43
2:A:42:ASN:OD1	2:A:188:LYS:HG2	2.18	0.43
1:D:43:C:C6	1:D:43:C:C5'	3.01	0.43
2:A:8:GLN:HA	2:A:11:LYS:HG3	2.00	0.43
2:A:36:ASP:C	2:A:38:ARG:N	2.71	0.43
2:A:176:ASP:HA	2:A:179:GLU:CG	2.49	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
2:A:35:ILE:HD12	2:A:35:ILE:N	2.34	0.43
2:A:202:LYS:HE2	2:A:202:LYS:HB3	1.77	0.43
2:C:115:ILE:C	2:C:117:ARG:N	2.72	0.43
2:A:16:LEU:HD12	2:A:16:LEU:HA	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
1:B:17:C:O2	1:B:17:C:C2'	2.66	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
2:C:188:LYS:CG	2:C:189:TYR:H	2.29	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:72:ALA:HB3	2:A:73:GLU:OE1	2.20	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
2:C:197:LYS:HB3	2:C:198:ASP:H	1.63	0.42
2:A:112:MSE:C	2:A:114:LEU:H	2.23	0.42
2:C:56:LYS:HE3	2:C:56:LYS:N	2.34	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
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:92:LYS:H	2:A:92:LYS:HD2	1.85	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)
1:B:14:G:O2'	1:B:40:C:H4'	2.18	0.42
1:D:7:G:O2'	1:D:8:A:H5'	2.20	0.42
2:A:112:MSE:O	2:A:115:ILE:HB	2.19	0.42
2:C:33:LYS:CG	2:C:34:GLU:HG3	2.50	0.42
2:C:178:ILE:O	2:C:181:VAL:N	2.50	0.42
1:D:28:G:N2	1:D:30:A:N7	2.68	0.42
2:A:22:PHE:N	2:A:22:PHE:HD2	2.18	0.42
2:A:140:LYS:O	2:A:144:GLU:CB	2.68	0.42
2:C:64:GLY:HA2	2:C:108:GLN:HB2	2.02	0.42
2:C:115:ILE:C	2:C:117:ARG:H	2.22	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:57:GLU:O	2:C:58:ALA:C	2.58	0.41
2:C:172:GLU:OE2	2:C:172:GLU:N	2.40	0.41
2:C:95:LEU:O	2:C:95:LEU:CG	2.68	0.41
2:C:152:ILE:CG2	2:C:162:VAL:HB	2.42	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
1:B:14:G:C2'	1:B:15:C:H5'	2.51	0.41
1:D:36:G:HO2'	1:D:37:A:P	2.40	0.41
2:A:88:LEU:CD2	2:A:119:MSE:HE1	2.50	0.41
2:C:88:LEU:O	2:C:90:LYS:N	2.52	0.41
1:B:1:G:H8	1:B:1:G:C5'	2.23	0.41
2:C:48:VAL:O	2:C:49:VAL:C	2.59	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: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:30:A:N3	1:B:31:G:C8	2.89	0.41
1:B:44:A:H2'	1:B:45:C:C5	2.55	0.41
1:D:30:A:C2	1:D:31:G:C4	3.08	0.41
2:C:57:GLU:OE2	2:C:57:GLU:N	2.30	0.41
2:C:65:THR:HG21	2:C:82:LYS:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:163:LEU:C	2:C:164:VAL:HG13	2.41	0.40
2:C:170:THR:O	2:C:173:GLN:HB2	2.20	0.40
1:B:7:G:C6	1:B:44:A:N6	2.88	0.40
1:D:12:A:H2'	1:D:13:G:C5'	2.51	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:B:28:G:N2	1:B:30:A:C5	2.89	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:C:203:LEU:O	2:C:205:MSE:N	2.55	0.40
1:B:43:C:H42	1:B:44:A:H62	1.68	0.40
2:A:124:GLY:C	2:A:126:ARG:H	2.25	0.40
2:A:145:ARG:CG	2:A:145:ARG:NH1	2.80	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	1
2	C	212/219 (97%)	139 (66%)	49 (23%)	24 (11%)	0	2
All	All	424/438 (97%)	295 (70%)	78 (18%)	51 (12%)	0	2

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 (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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

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

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

Sometimes 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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	B	49/49 (100%)	-0.88	1 (2%) 64 55	56, 79, 117, 150	0
1	D	49/49 (100%)	-0.76	1 (2%) 64 55	53, 82, 139, 153	0
2	A	208/219 (94%)	-0.92	0 100 100	9, 77, 134, 153	0
2	C	208/219 (94%)	-0.93	0 100 100	21, 79, 132, 146	0
All	All	514/536 (95%)	-0.91	2 (0%) 89 86	9, 79, 134, 153	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	23	C	3.4
1	B	24	U	2.7

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.