Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 03:49 PM GMT

PDB ID	:	4D8J
Title	:	Structure of E. coli MatP-mats complex
Authors	:	Dupaigne, P.; Tonthat, N.K.; Espeli, O.; Whitfill, T.; Boccard, F.; Schumacher, M.A.
Deposited on	:	2012-01-10
Resolution	:	3.55 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 ①) were used in the production of this report:

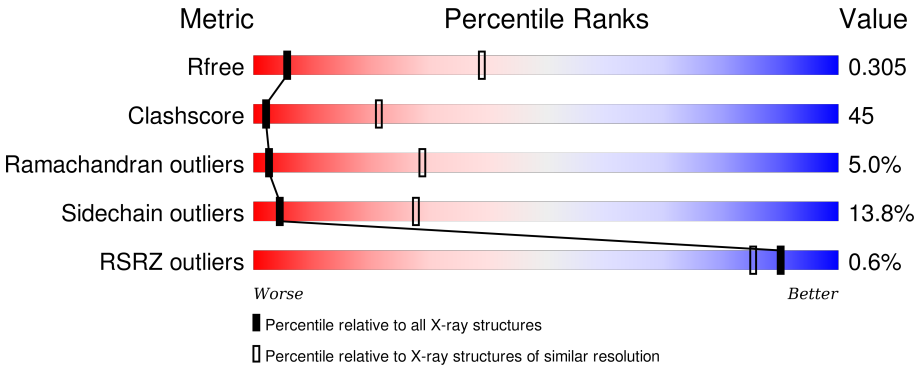
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 3.55 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	1240 (3.72-3.40)
Clashscore	102246	1057 (3.70-3.42)
Ramachandran outliers	100387	1017 (3.70-3.42)
Sidechain outliers	100360	1017 (3.70-3.42)
RSRZ outliers	91569	1247 (3.72-3.40)

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 <=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	A	150	29% 56% 13%
1	B	150	29% 57% 13%
1	C	150	42% 47% 9%
1	D	150	39% 48% 12%
1	G	150	37% 49% 12%

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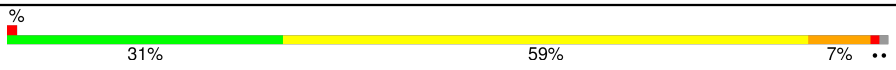
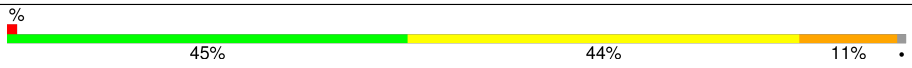
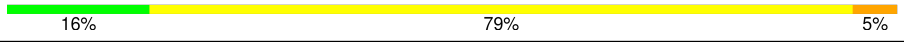
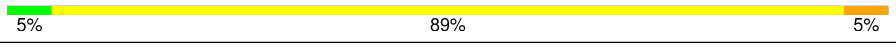
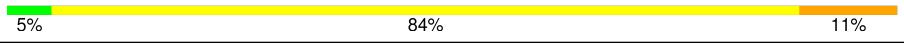
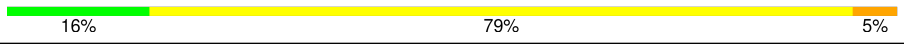
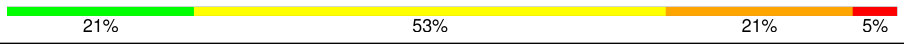
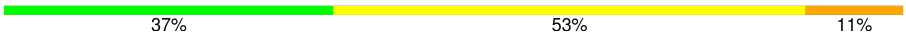
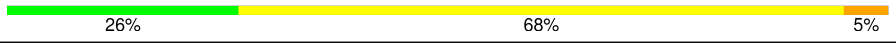
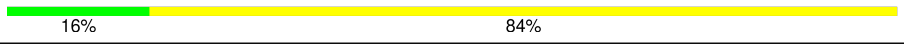
Mol	Chain	Length	Quality of chain
1	H	150	
1	K	150	
1	L	150	
2	F	19	
2	J	19	
2	N	19	
2	P	19	
3	E	19	
3	I	19	
3	M	19	
3	O	19	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12904 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 protein called Macrodomain Ter protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	148	Total	C	N	O	S	0	0	0
			1224	770	228	222	4			
1	A	149	Total	C	N	O	S	0	0	0
			1233	776	230	223	4			
1	D	149	Total	C	N	O	S	0	0	0
			1229	773	229	223	4			
1	C	148	Total	C	N	O	S	0	0	0
			1220	767	227	222	4			
1	H	148	Total	C	N	O	S	0	0	0
			1224	770	228	222	4			
1	G	148	Total	C	N	O	S	0	0	0
			1223	770	229	221	3			
1	L	149	Total	C	N	O	S	0	0	0
			1234	777	230	223	4			
1	K	148	Total	C	N	O	S	0	0	0
			1225	771	228	222	4			

- Molecule 2 is a DNA chain called 5'-D(*TP*TP*CP*GP*TP*GP*AP*CP*AP*TP*TP*GP*TP*CP*AP*CP*GP*AP*A)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	N	19	Total	C	N	O	P	0	0	0
			386	186	69	113	18			
2	F	19	Total	C	N	O	P	0	0	0
			386	186	69	113	18			
2	J	19	Total	C	N	O	P	0	0	0
			386	186	69	113	18			
2	P	19	Total	C	N	O	P	0	0	0
			386	186	69	113	18			

- Molecule 3 is a DNA chain called 5'-D(*TP*TP*CP*GP*TP*GP*AP*CP*AP*AP*TP*GP*TP*CP*AP*CP*GP*AP*A)-3'.

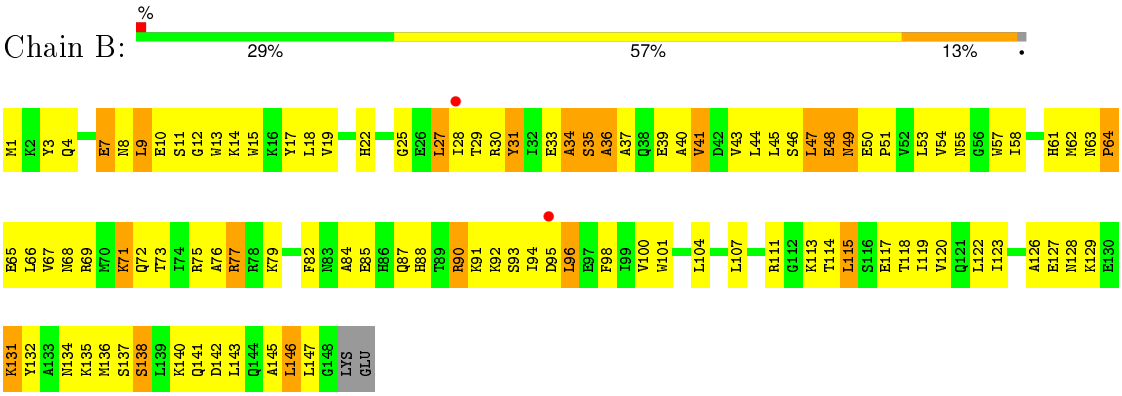
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	19	Total	C	N	O	P	0	0	0
			387	186	72	111	18			
3	E	19	Total	C	N	O	P	0	0	0
			387	186	72	111	18			
3	I	19	Total	C	N	O	P	0	0	0
			387	186	72	111	18			
3	O	19	Total	C	N	O	P	0	0	0
			387	186	72	111	18			

3 Residue-property plots (i)

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

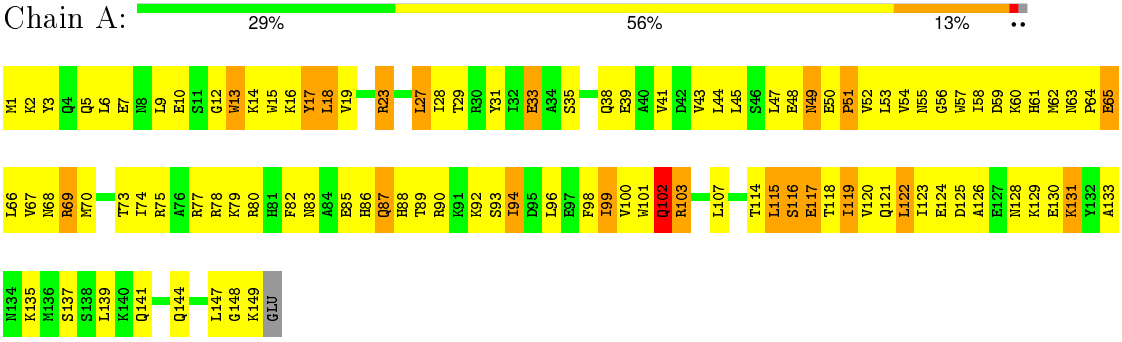
- Molecule 1: Macrodomain Ter protein

Chain B:



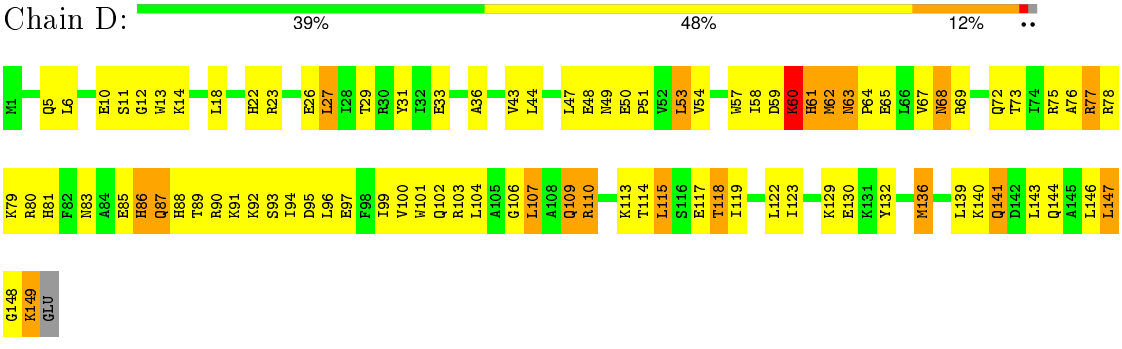
- Molecule 1: Macrodomain Ter protein

Chain A:



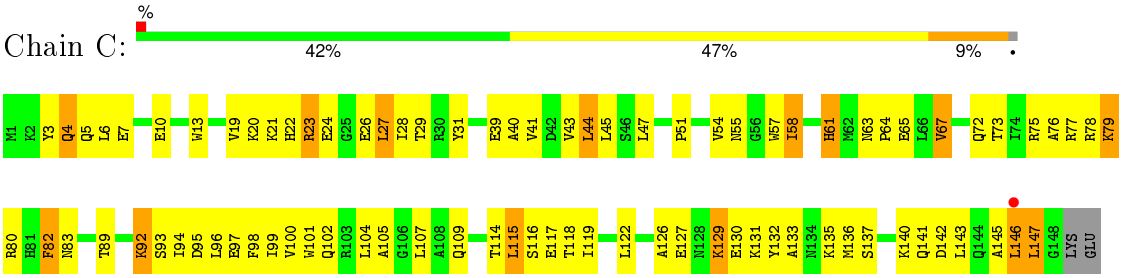
- Molecule 1: Macrodomain Ter protein

Chain D:



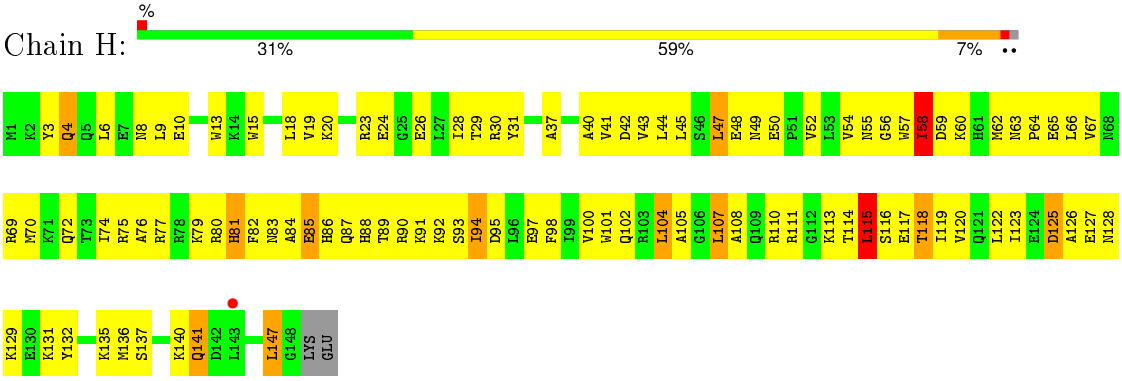
• Molecule 1: Macrodomain Ter protein

Chain C:



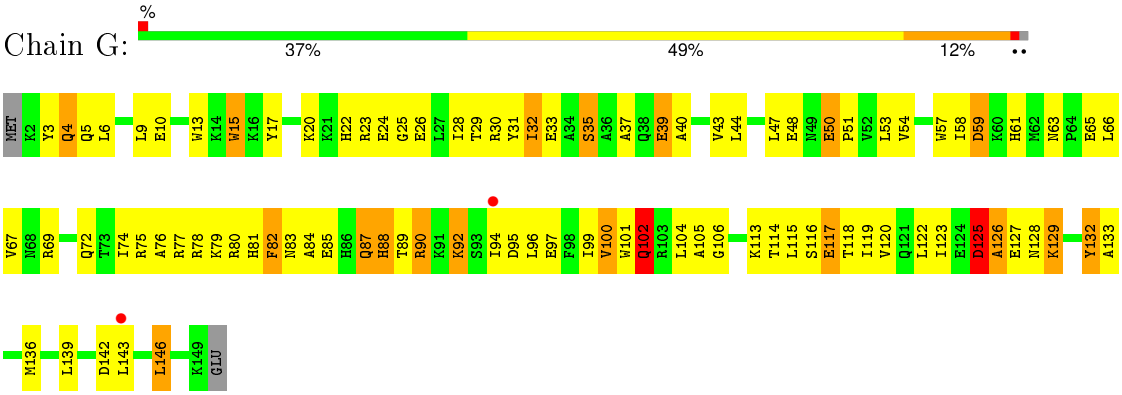
• Molecule 1: Macrodomain Ter protein

Chain H:



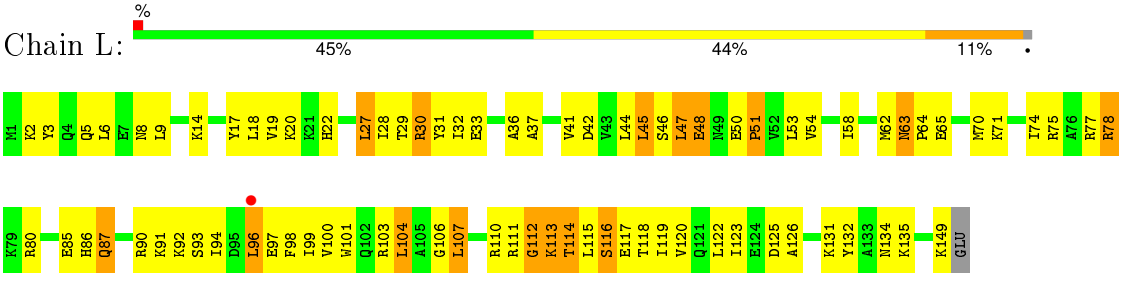
• Molecule 1: Macrodomain Ter protein

Chain G:



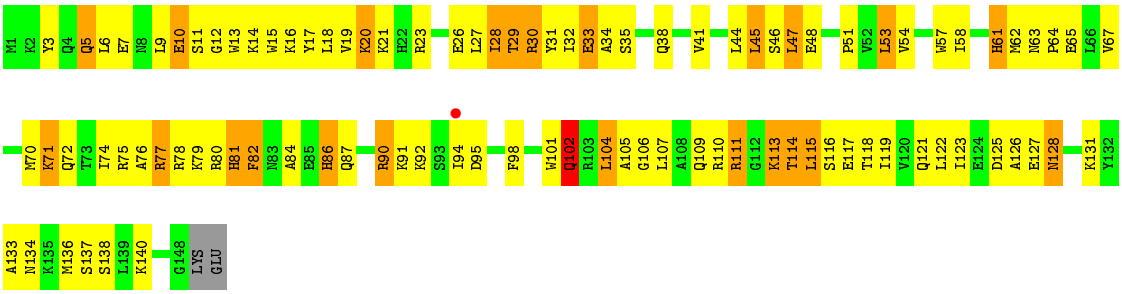
• Molecule 1: Macrodomain Ter protein

Chain L:



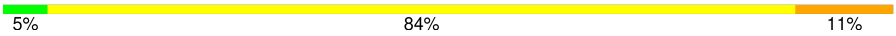
• Molecule 1: Macrodomain Ter protein

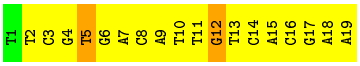
Chain K:



• Molecule 2: 5'-D(*TP*TP*CP*GP*TP*GP*AP*CP*AP*TP*TP*GP*TP*CP*AP*CP*GP*AP*A)-3'

Chain N:



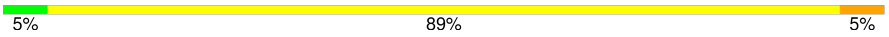


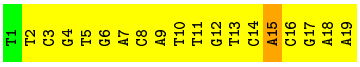
• Molecule 2: 5'-D(*TP*TP*CP*GP*TP*GP*AP*CP*AP*TP*TP*GP*TP*CP*AP*CP*GP*AP*A)-3'

Chain F:

• Molecule 2: 5'-D(*TP*TP*CP*GP*TP*GP*AP*CP*AP*TP*TP*GP*TP*CP*AP*CP*GP*AP*A)-3'

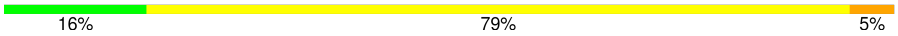
Chain J:

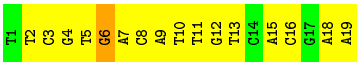




• Molecule 2: 5'-D(*TP*TP*CP*GP*TP*GP*AP*CP*AP*TP*TP*GP*TP*CP*AP*CP*GP*AP*A)-3'

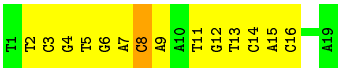
Chain P:





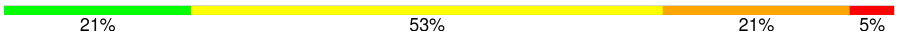
• Molecule 3: 5'-D(*TP*TP*CP*GP*TP*GP*AP*CP*AP*AP*TP*GP*TP*CP*AP*CP*GP*AP*A)-3'

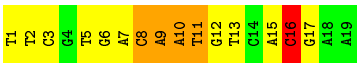
Chain M:



• Molecule 3: 5'-D(*TP*TP*CP*GP*TP*GP*AP*CP*AP*AP*TP*GP*TP*CP*AP*CP*GP*AP*A)-3'

Chain E:





• Molecule 3: 5'-D(*TP*TP*CP*GP*TP*GP*AP*CP*AP*AP*TP*GP*TP*CP*AP*CP*GP*AP*A)-3'

Chain I:

• Molecule 3: 5'-D(*TP*TP*CP*GP*TP*GP*AP*CP*AP*AP*TP*GP*TP*CP*AP*CP*GP*AP*A)-3'

Chain O:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	114.87Å 180.10Å 184.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	97.58 – 3.55 97.58 – 3.50	Depositor EDS
% Data completeness (in resolution range)	87.8 (97.58-3.55) 87.9 (97.58-3.50)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	2.08 (at 3.49Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.299 , 0.313 0.312 , 0.305	Depositor DCC
R_{free} test set	4189 reflections (10.14%)	DCC
Wilson B-factor (Å^2)	102.4	Xtriage
Anisotropy	0.779	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.23 , 47.5	EDS
Estimated twinning fraction	0.059 for -h,l,k	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.36$, $< L^2 > = 0.19$	Xtriage
Outliers	2 of 43221 reflections (0.005%)	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	12904	wwPDB-VP
Average B, all atoms (Å^2)	145.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.48% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	A	0.51	0/1253	0.61	0/1680
1	B	0.60	0/1244	0.72	0/1669
1	C	0.58	0/1240	0.63	0/1665
1	D	0.55	0/1249	0.65	1/1676 (0.1%)
1	G	0.51	1/1243 (0.1%)	0.89	3/1667 (0.2%)
1	H	0.51	0/1244	0.62	1/1669 (0.1%)
1	K	0.45	0/1245	0.63	0/1670
1	L	0.52	0/1254	0.61	0/1681
2	F	0.87	1/432 (0.2%)	0.85	2/665 (0.3%)
2	J	0.84	1/432 (0.2%)	0.79	1/665 (0.2%)
2	N	0.91	1/432 (0.2%)	0.85	1/665 (0.2%)
2	P	0.77	0/432	0.91	1/665 (0.2%)
3	E	1.08	4/434 (0.9%)	1.21	7/668 (1.0%)
3	I	0.71	0/434	0.86	2/668 (0.3%)
3	M	0.78	1/434 (0.2%)	0.73	0/668
3	O	0.60	0/434	0.72	0/668
All	All	0.62	9/13436 (0.1%)	0.74	19/18709 (0.1%)

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	0	1
1	G	0	1
3	E	0	1
All	All	0	3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	9	DA	C5-C6	-11.67	1.30	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	15	DA	O3'-P	-10.22	1.48	1.61
2	N	12	DG	C5-C6	-9.07	1.33	1.42
1	G	125	ASP	C-N	8.15	1.52	1.34
3	E	11	DT	C4-O4	-6.45	1.17	1.23
3	E	8	DC	O3'-P	-6.37	1.53	1.61
3	E	11	DT	C2-O2	5.65	1.26	1.22
3	E	9	DA	C2-N3	-5.59	1.28	1.33
3	M	8	DC	C4-N4	-5.48	1.29	1.33

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	125	ASP	O-C-N	-21.99	87.52	122.70
1	G	125	ASP	CA-C-N	-15.21	83.75	117.20
1	G	125	ASP	C-N-CA	-7.52	102.91	121.70
3	E	9	DA	O4'-C1'-N9	6.87	112.81	108.00
2	F	9	DA	N1-C6-N6	6.59	122.55	118.60
3	E	11	DT	C1'-O4'-C4'	-6.51	103.59	110.10
3	E	11	DT	C5-C4-O4	-6.29	120.50	124.90
3	I	11	DT	C2'-C3'-O3'	-6.21	92.10	112.60
3	E	11	DT	C3'-C2'-C1'	-6.04	95.25	102.50
3	E	11	DT	O4'-C1'-C2'	-5.82	101.24	105.90
3	E	16	DC	N1-C1'-C2'	5.62	123.28	112.60
1	D	147	LEU	N-CA-C	5.60	126.11	111.00
3	E	10	DA	O5'-P-OP1	-5.59	100.67	105.70
2	P	6	DG	O5'-P-OP2	5.50	117.30	110.70
1	H	141	GLN	N-CA-CB	-5.34	100.99	110.60
2	N	5	DT	N1-C1'-C2'	5.30	122.68	112.60
3	I	12	DG	O5'-P-OP1	5.25	117.00	110.70
2	J	16	DC	O5'-P-OP1	5.20	116.94	110.70
2	F	9	DA	C5-C6-N6	-5.15	119.58	123.70

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	31	TYR	Sidechain
3	E	16	DC	Sidechain
1	G	125	ASP	Mainchain

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1233	0	1262	131	0
1	B	1224	0	1249	168	0
1	C	1220	0	1238	98	0
1	D	1229	0	1251	122	0
1	G	1223	0	1245	122	0
1	H	1224	0	1249	112	0
1	K	1225	0	1251	158	0
1	L	1234	0	1264	101	0
2	F	386	0	217	30	0
2	J	386	0	217	34	0
2	N	386	0	217	48	0
2	P	386	0	217	42	0
3	E	387	0	216	41	0
3	I	387	0	216	30	0
3	M	387	0	214	34	0
3	O	387	0	216	35	0
All	All	12904	0	11739	1099	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 45.

All (1099) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:7:DA:H2"	3:I:8:DC:H5"	1.18	1.17
1:B:96:LEU:HD21	1:A:94:ILE:HD11	1.29	1.15
2:F:9:DA:N6	3:E:11:DT:O4	1.81	1.13
2:F:7:DA:H2"	2:F:8:DC:H5"	1.20	1.12
1:A:18:LEU:H	1:A:18:LEU:HD12	1.09	1.11
3:M:7:DA:H2"	3:M:8:DC:H5"	1.30	1.09
1:A:10:GLU:HG2	1:A:13:TRP:CH2	1.91	1.06
2:P:7:DA:H2"	2:P:8:DC:H5"	1.37	1.06
2:N:12:DG:O6	3:M:8:DC:N4	1.89	1.05
1:L:44:LEU:HA	1:L:47:LEU:HD13	1.40	1.03
1:A:18:LEU:HB3	1:A:28:ILE:HG21	1.41	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:2:DT:H2"	3:I:3:DC:H5"	1.38	1.03
1:D:144:GLN:O	1:D:147:LEU:HG	1.57	1.02
2:F:7:DA:C2'	2:F:8:DC:H5"	1.91	1.00
3:O:7:DA:H2"	3:O:8:DC:H5"	1.41	1.00
2:F:4:DG:O6	3:E:16:DC:N4	1.95	1.00
1:H:129:LYS:HD2	1:G:128:ASN:CB	1.92	0.99
1:B:71:LYS:NZ	2:N:3:DC:OP2	1.95	0.99
1:H:92:LYS:NZ	3:I:9:DA:OP1	2.00	0.95
1:H:94:ILE:HG21	1:G:115:LEU:HD12	1.48	0.95
1:K:27:LEU:HD23	1:K:29:THR:HG23	1.49	0.94
2:N:7:DA:H2"	2:N:8:DC:H5"	1.46	0.94
3:I:7:DA:C2'	3:I:8:DC:H5"	1.98	0.93
2:J:12:DG:H2"	2:J:13:DT:H5"	1.52	0.92
1:B:87:GLN:HB2	1:B:90:ARG:HH21	1.35	0.92
2:J:7:DA:H2"	2:J:8:DC:H5"	1.51	0.91
3:M:12:DG:H2"	3:M:13:DT:H5"	1.54	0.90
3:E:7:DA:H1'	3:E:8:DC:H5"	1.52	0.89
2:F:9:DA:N1	3:E:11:DT:N3	2.20	0.89
2:F:18:DA:H2"	2:F:19:DA:H5"	1.55	0.88
1:K:110:ARG:HB2	1:K:110:ARG:NH1	1.89	0.88
2:P:7:DA:H2"	2:P:8:DC:C5'	2.04	0.88
2:N:8:DC:H3'	1:A:92:LYS:HE3	1.54	0.87
1:B:96:LEU:H	1:B:96:LEU:HD12	1.38	0.86
1:G:125:ASP:C	1:G:127:GLU:N	2.28	0.86
3:E:7:DA:H1'	3:E:8:DC:C5'	2.05	0.86
1:H:129:LYS:HD2	1:G:128:ASN:HB2	1.56	0.85
1:A:87:GLN:HG3	1:A:88:HIS:H	1.41	0.85
1:K:63:ASN:HD21	1:K:65:GLU:HB2	1.42	0.85
1:L:126:ALA:HB2	1:K:126:ALA:HB2	1.58	0.84
1:K:19:VAL:HG12	1:K:23:ARG:HH11	1.42	0.84
1:G:33:GLU:HG2	1:G:35:SER:H	1.41	0.83
1:B:7:GLU:OE1	1:B:8:ASN:N	2.11	0.83
1:H:129:LYS:HD2	1:G:128:ASN:HB3	1.55	0.83
1:H:108:ALA:HA	1:H:118:THR:HG21	1.61	0.83
1:B:63:ASN:HD21	1:B:65:GLU:HB2	1.42	0.83
1:A:18:LEU:HD12	1:A:18:LEU:N	1.93	0.83
1:G:125:ASP:C	1:G:127:GLU:H	1.83	0.82
3:M:7:DA:C2'	3:M:8:DC:H5"	2.09	0.82
1:H:119:ILE:HA	1:H:122:LEU:HD12	1.61	0.82
1:A:52:VAL:HA	1:A:55:ASN:HD22	1.44	0.82
1:D:87:GLN:NE2	1:D:90:ARG:HE	1.77	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:9:LEU:HD12	1:B:10:GLU:H	1.43	0.82
1:K:29:THR:O	1:K:63:ASN:HB2	1.79	0.82
3:E:7:DA:P	1:C:115:LEU:HB2	2.20	0.81
2:P:7:DA:C2'	2:P:8:DC:H5"	2.09	0.81
1:D:63:ASN:HD22	1:D:64:PRO:HD2	1.44	0.81
3:M:4:DG:H4'	1:A:2:LYS:HD3	1.62	0.81
2:F:12:DG:H2"	2:F:13:DT:H5"	1.62	0.81
1:A:27:LEU:H	1:A:27:LEU:HD22	1.45	0.81
1:L:71:LYS:O	1:L:75:ARG:HG3	1.80	0.80
1:D:104:LEU:HD22	1:D:115:LEU:CD2	2.11	0.80
1:D:144:GLN:HA	1:D:147:LEU:HD23	1.64	0.80
2:P:2:DT:H2"	2:P:3:DC:H5"	1.62	0.80
1:D:139:LEU:O	1:D:143:LEU:HG	1.82	0.79
1:A:87:GLN:HG3	1:A:88:HIS:N	1.96	0.79
3:M:4:DG:H1'	3:M:5:DT:H5'	1.65	0.79
3:O:12:DG:H2"	3:O:13:DT:H5"	1.65	0.79
3:E:10:DA:H1'	3:E:11:DT:H5'	1.65	0.79
3:O:7:DA:C2'	3:O:8:DC:H5"	2.12	0.79
1:B:33:GLU:HG3	1:B:36:ALA:HB3	1.63	0.79
1:B:44:LEU:HA	1:B:47:LEU:HD13	1.65	0.79
1:A:18:LEU:CD1	1:A:18:LEU:H	1.87	0.79
3:I:2:DT:C2'	3:I:3:DC:H5"	2.13	0.79
2:P:12:DG:H2"	2:P:13:DT:C5'	2.13	0.79
1:B:50:GLU:HB3	1:B:53:LEU:HB2	1.64	0.78
1:H:47:LEU:HB3	1:H:54:VAL:HG22	1.64	0.78
1:L:87:GLN:HG2	1:K:98:PHE:CZ	2.18	0.78
2:F:7:DA:H2"	2:F:8:DC:C5'	2.09	0.78
3:M:5:DT:OP2	1:A:79:LYS:HE2	1.85	0.77
1:B:75:ARG:NH2	2:N:4:DG:N7	2.32	0.77
1:H:125:ASP:OD1	1:G:129:LYS:HG3	1.85	0.77
1:C:19:VAL:HG12	1:C:23:ARG:HD3	1.67	0.76
1:D:143:LEU:HD12	1:D:144:GLN:N	2.00	0.76
3:E:2:DT:H2"	3:E:3:DC:H5'	1.67	0.76
1:C:119:ILE:HA	1:C:122:LEU:HD12	1.68	0.75
1:K:119:ILE:HD12	1:K:119:ILE:H	1.51	0.75
1:K:110:ARG:HB2	1:K:110:ARG:CZ	2.16	0.75
1:K:14:LYS:O	1:K:17:TYR:HB3	1.86	0.75
2:P:18:DA:H2"	2:P:19:DA:H5'	1.66	0.75
2:N:9:DA:H2"	2:N:10:DT:C5'	2.17	0.75
1:A:9:LEU:O	1:A:12:GLY:N	2.18	0.75
1:A:87:GLN:HA	1:A:90:ARG:HD3	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:142:ASP:O	1:G:146:LEU:HB2	1.88	0.74
1:A:66:LEU:HD23	1:A:69:ARG:HD2	1.70	0.74
1:A:10:GLU:HG2	1:A:13:TRP:CZ2	2.23	0.74
3:E:7:DA:H2"	3:E:8:DC:H5'	1.70	0.74
1:L:92:LYS:HG3	1:K:101:TRP:CZ3	2.23	0.73
1:D:47:LEU:HD21	1:D:53:LEU:HD12	1.70	0.73
1:K:74:ILE:HG23	1:K:75:ARG:H	1.51	0.73
1:B:90:ARG:HH11	1:G:90:ARG:NH1	1.86	0.73
2:F:9:DA:C6	3:E:11:DT:O4	2.41	0.73
1:D:104:LEU:HD11	1:C:119:ILE:HD13	1.70	0.73
2:F:14:DC:H42	3:E:6:DG:H1	1.36	0.73
1:H:91:LYS:HG3	1:G:97:GLU:HA	1.71	0.72
1:K:119:ILE:HD12	1:K:119:ILE:N	2.04	0.72
1:G:58:ILE:HG13	1:G:59:ASP:H	1.52	0.72
3:E:12:DG:H2"	3:E:13:DT:H5'	1.71	0.72
3:E:7:DA:H2"	3:E:8:DC:OP2	1.89	0.72
3:O:7:DA:OP1	1:K:115:LEU:HB2	1.89	0.72
2:P:18:DA:H2"	2:P:19:DA:C5'	2.18	0.72
2:P:12:DG:H2"	2:P:13:DT:H5'	1.71	0.72
1:K:28:ILE:H	1:K:28:ILE:HD13	1.55	0.72
1:C:114:THR:HB	1:C:117:GLU:CB	2.20	0.71
3:I:3:DC:H2'	1:G:75:ARG:HD2	1.70	0.71
1:L:92:LYS:HD2	3:O:9:DA:P	2.31	0.71
2:N:9:DA:OP2	1:A:92:LYS:HB2	1.90	0.71
1:C:114:THR:HB	1:C:117:GLU:HB3	1.71	0.71
1:K:63:ASN:ND2	1:K:65:GLU:HB2	2.05	0.71
1:D:23:ARG:HE	1:C:23:ARG:HB2	1.54	0.71
1:L:77:ARG:HA	1:L:80:ARG:HD2	1.72	0.71
1:B:115:LEU:HB2	2:N:7:DA:OP1	1.90	0.71
1:B:64:PRO:O	1:B:67:VAL:HG23	1.91	0.70
1:D:119:ILE:HD11	1:C:96:LEU:HD22	1.72	0.70
1:L:113:LYS:HD3	1:L:117:GLU:HG3	1.72	0.70
2:P:6:DG:H1	3:O:14:DC:H42	1.40	0.70
1:G:69:ARG:HH11	1:G:69:ARG:HG3	1.55	0.70
1:H:15:TRP:O	1:H:19:VAL:HG23	1.92	0.70
1:C:13:TRP:CZ3	1:C:77:ARG:HB3	2.26	0.70
1:A:116:SER:HA	1:A:119:ILE:HD11	1.73	0.70
1:B:75:ARG:NH2	2:N:4:DG:O6	2.25	0.69
2:P:12:DG:C2	2:P:13:DT:C2	2.81	0.69
1:L:20:LYS:HD3	3:O:12:DG:OP1	1.92	0.69
1:B:33:GLU:HG3	1:B:36:ALA:CB	2.21	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:63:ASN:H	1:G:66:LEU:HD12	1.57	0.69
3:I:8:DC:P	1:G:101:TRP:HE1	2.16	0.69
1:B:58:ILE:HG23	1:B:62:MET:SD	2.33	0.69
2:J:12:DG:C2'	2:J:13:DT:H5"	2.23	0.69
1:K:47:LEU:HD12	1:K:47:LEU:H	1.58	0.69
1:K:113:LYS:HB3	1:K:117:GLU:HG3	1.73	0.69
1:K:74:ILE:HG23	1:K:75:ARG:N	2.07	0.68
1:K:28:ILE:HD13	1:K:28:ILE:N	2.07	0.68
1:G:28:ILE:HG22	1:G:28:ILE:O	1.93	0.68
2:N:7:DA:C2'	2:N:8:DC:H5"	2.23	0.68
1:L:51:PRO:O	1:L:54:VAL:HG23	1.94	0.68
1:C:97:GLU:HB2	1:C:100:VAL:HG23	1.76	0.68
1:L:91:LYS:O	1:L:92:LYS:HD3	1.93	0.68
1:L:77:ARG:NH1	1:L:77:ARG:HB2	2.08	0.68
1:G:113:LYS:HD2	1:G:117:GLU:HG3	1.76	0.68
1:H:129:LYS:CD	1:G:128:ASN:HB2	2.25	0.67
1:K:123:ILE:O	1:K:127:GLU:HB2	1.94	0.67
3:I:7:DA:H2"	3:I:8:DC:C5'	2.10	0.67
1:K:114:THR:CB	1:K:117:GLU:HG2	2.24	0.67
1:B:15:TRP:O	1:B:19:VAL:HG23	1.94	0.67
1:C:99:ILE:O	1:C:102:GLN:HB3	1.94	0.67
1:D:72:GLN:HA	1:D:75:ARG:HG3	1.77	0.67
1:K:86:HIS:O	1:K:90:ARG:HG3	1.94	0.67
1:H:44:LEU:HD13	1:H:44:LEU:O	1.95	0.67
1:D:99:ILE:O	1:D:102:GLN:HB3	1.95	0.67
1:B:94:ILE:HD11	1:A:96:LEU:HD12	1.74	0.67
1:K:70:MET:O	1:K:74:ILE:HG22	1.95	0.67
1:L:113:LYS:HA	1:L:113:LYS:HE2	1.76	0.67
2:N:15:DA:H2"	2:N:16:DC:OP2	1.95	0.67
1:B:63:ASN:OD1	1:B:64:PRO:HD2	1.94	0.67
1:D:104:LEU:HD22	1:D:115:LEU:HD21	1.76	0.67
1:B:4:GLN:HE22	1:G:9:LEU:HD11	1.60	0.67
3:M:7:DA:OP1	1:A:115:LEU:HB2	1.95	0.67
1:L:92:LYS:HD2	3:O:9:DA:OP1	1.94	0.67
1:D:96:LEU:HA	1:C:116:SER:OG	1.95	0.67
1:B:33:GLU:CG	1:B:36:ALA:HB3	2.24	0.67
1:K:41:VAL:O	1:K:45:LEU:HB2	1.95	0.67
2:P:12:DG:C2'	2:P:13:DT:H5"	2.24	0.66
1:H:65:GLU:O	1:H:69:ARG:HG3	1.96	0.66
1:A:47:LEU:HD22	1:A:53:LEU:HD13	1.77	0.66
1:L:18:LEU:HD12	1:L:28:ILE:HG23	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:9:DA:H2"	2:N:10:DT:H5'	1.77	0.66
2:N:12:DG:H2"	2:N:13:DT:H5"	1.77	0.66
3:I:11:DT:H2"	3:I:12:DG:OP2	1.94	0.66
2:J:8:DC:H2"	2:J:9:DA:C8	2.31	0.66
2:P:2:DT:C2'	2:P:3:DC:H5"	2.25	0.66
1:L:101:TRP:HZ2	2:P:8:DC:OP1	1.79	0.66
1:D:106:GLY:O	1:D:110:ARG:HG2	1.96	0.66
2:P:4:DG:H1'	2:P:5:DT:H5'	1.77	0.66
1:G:94:ILE:HG22	1:G:95:ASP:H	1.61	0.66
1:A:14:LYS:HE2	1:A:70:MET:CE	2.25	0.65
1:H:75:ARG:HD3	2:J:4:DG:N7	2.10	0.65
1:B:96:LEU:N	1:B:96:LEU:HD12	2.11	0.65
3:E:9:DA:H2"	3:E:10:DA:C8	2.32	0.65
1:B:143:LEU:O	1:B:147:LEU:HB2	1.96	0.65
2:P:2:DT:H2"	2:P:3:DC:C5'	2.26	0.65
2:P:15:DA:H61	3:O:5:DT:H3	1.44	0.65
1:B:44:LEU:HD22	1:B:47:LEU:HD13	1.79	0.65
2:N:16:DC:H4'	1:H:110:ARG:NH2	2.11	0.65
2:J:7:DA:C2'	2:J:8:DC:H5"	2.26	0.65
1:A:47:LEU:HD13	1:A:53:LEU:HD22	1.78	0.65
1:B:91:LYS:O	1:B:92:LYS:HD3	1.97	0.65
1:A:70:MET:O	1:A:74:ILE:HG22	1.96	0.64
1:C:22:HIS:HB2	1:C:28:ILE:HD11	1.79	0.64
3:E:9:DA:C2'	3:E:10:DA:C8	2.81	0.64
2:P:12:DG:H2"	2:P:13:DT:H5"	1.78	0.64
2:P:9:DA:H2"	2:P:10:DT:H5"	1.78	0.64
1:B:119:ILE:HG22	1:B:123:ILE:HD11	1.79	0.64
2:N:16:DC:H2"	2:N:17:DG:C8	2.32	0.64
1:H:116:SER:HB3	1:G:100:VAL:HG21	1.80	0.64
1:H:79:LYS:NZ	1:H:83:ASN:HD21	1.95	0.64
1:B:90:ARG:HD2	1:G:90:ARG:HH12	1.63	0.64
1:A:14:LYS:HE2	1:A:70:MET:SD	2.38	0.63
1:B:63:ASN:HD21	1:B:65:GLU:CB	2.09	0.63
1:H:63:ASN:CG	1:H:64:PRO:HD2	2.18	0.63
1:A:9:LEU:HG	1:A:13:TRP:HE1	1.63	0.63
1:L:115:LEU:O	1:L:119:ILE:HG13	1.97	0.63
1:B:65:GLU:O	1:B:66:LEU:HD12	1.97	0.63
1:B:87:GLN:CB	1:B:90:ARG:HH21	2.07	0.63
1:B:145:ALA:HB3	1:B:146:LEU:HD23	1.78	0.63
1:C:21:LYS:O	1:C:26:GLU:HB2	1.99	0.63
1:D:64:PRO:HA	1:D:67:VAL:HG23	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:91:LYS:HE3	1:C:97:GLU:HG2	1.81	0.63
1:K:57:TRP:O	1:K:61:HIS:HB2	1.98	0.63
1:B:92:LYS:HD2	3:M:9:DA:P	2.38	0.63
1:G:44:LEU:HB2	1:G:57:TRP:CE2	2.33	0.63
1:G:79:LYS:HD3	1:G:79:LYS:O	1.98	0.63
2:F:7:DA:C3'	2:F:8:DC:H5"	2.24	0.63
1:L:126:ALA:HA	1:K:126:ALA:HA	1.81	0.63
1:K:47:LEU:HD12	1:K:47:LEU:N	2.14	0.63
1:G:114:THR:O	1:G:117:GLU:HB2	1.99	0.63
1:L:122:LEU:HD11	1:K:123:ILE:CG1	2.28	0.63
1:H:104:LEU:HD13	1:H:115:LEU:CD2	2.29	0.62
3:M:12:DG:C2'	3:M:13:DT:H5"	2.27	0.62
1:K:44:LEU:HD23	1:K:57:TRP:CG	2.34	0.62
1:C:82:PHE:N	1:C:82:PHE:CD1	2.66	0.62
1:H:57:TRP:HE3	1:H:58:ILE:HD13	1.64	0.62
1:C:82:PHE:N	1:C:82:PHE:HD1	1.97	0.62
2:J:17:DG:H1	3:I:3:DC:H42	1.46	0.62
1:K:13:TRP:HA	1:K:16:LYS:HG3	1.82	0.62
3:E:7:DA:H1'	3:E:8:DC:H5'	1.82	0.62
1:A:62:MET:HG2	1:A:63:ASN:N	2.15	0.62
1:B:100:VAL:HG11	1:A:119:ILE:HD12	1.82	0.62
1:C:10:GLU:OE1	1:C:78:ARG:HD3	2.00	0.62
1:A:18:LEU:HB3	1:A:28:ILE:CG2	2.23	0.61
1:A:64:PRO:HA	1:A:67:VAL:HG23	1.81	0.61
1:H:123:ILE:O	1:H:127:GLU:HB2	2.00	0.61
1:D:119:ILE:HD12	1:C:100:VAL:HG11	1.82	0.61
2:F:9:DA:N1	3:E:11:DT:C4	2.69	0.61
1:L:75:ARG:NH2	2:P:4:DG:O6	2.34	0.61
1:G:13:TRP:CH2	1:G:77:ARG:HG2	2.35	0.61
1:D:87:GLN:HE21	1:D:87:GLN:HA	1.65	0.61
1:A:10:GLU:O	1:A:14:LYS:HB2	2.00	0.61
1:L:116:SER:HA	1:L:119:ILE:HD12	1.83	0.61
1:G:113:LYS:HB3	1:G:117:GLU:HB3	1.83	0.61
1:D:107:LEU:CD1	1:D:110:ARG:HH21	2.14	0.61
1:B:33:GLU:CG	1:B:36:ALA:CB	2.78	0.61
1:H:63:ASN:O	1:H:67:VAL:HG23	2.00	0.61
1:B:54:VAL:O	1:B:57:TRP:HB3	2.00	0.61
1:A:52:VAL:HA	1:A:55:ASN:ND2	2.15	0.61
1:B:123:ILE:HA	1:A:122:LEU:HD21	1.82	0.60
1:B:35:SER:O	1:B:37:ALA:N	2.34	0.60
1:A:103:ARG:O	1:A:107:LEU:HG	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:70:MET:O	1:H:74:ILE:HG12	2.01	0.60
1:B:69:ARG:HH11	1:B:69:ARG:HG3	1.65	0.60
1:K:10:GLU:OE1	1:K:13:TRP:HZ3	1.83	0.60
1:K:48:GLU:O	1:K:51:PRO:HD3	2.01	0.60
1:G:80:ARG:O	1:G:83:ASN:N	2.34	0.60
1:C:127:GLU:HA	1:C:130:GLU:OE1	2.01	0.60
1:K:19:VAL:HG12	1:K:23:ARG:NH1	2.14	0.60
1:K:35:SER:O	1:K:38:GLN:HB3	2.00	0.60
1:D:10:GLU:C	1:D:12:GLY:H	2.04	0.60
1:G:139:LEU:HG	1:G:143:LEU:HD11	1.83	0.60
1:B:47:LEU:HD23	1:B:50:GLU:HB2	1.82	0.60
1:B:39:GLU:O	1:B:43:VAL:HG23	2.01	0.60
3:M:3:DC:H4'	1:A:1:MET:HB3	1.83	0.60
1:L:96:LEU:HD11	1:K:94:ILE:HD11	1.81	0.60
3:O:6:DG:H2"	3:O:7:DA:C8	2.36	0.60
1:D:27:LEU:HD12	1:D:63:ASN:OD1	2.02	0.60
3:E:6:DG:C5	3:E:7:DA:N6	2.70	0.59
1:K:47:LEU:CD1	1:K:47:LEU:H	2.14	0.59
1:H:92:LYS:NZ	3:I:9:DA:P	2.74	0.59
2:N:14:DC:H42	3:M:6:DG:H1	1.49	0.59
1:B:126:ALA:CB	1:A:122:LEU:HD23	2.32	0.59
3:M:16:DC:H6	3:M:16:DC:H5'	1.66	0.59
2:J:4:DG:H1'	2:J:5:DT:H5'	1.83	0.59
1:L:114:THR:HG23	1:L:117:GLU:CD	2.22	0.59
1:G:39:GLU:O	1:G:43:VAL:HG23	2.02	0.59
1:A:14:LYS:HE2	1:A:70:MET:HE1	1.84	0.59
1:A:23:ARG:HB3	1:A:23:ARG:HH11	1.65	0.59
1:K:44:LEU:HA	1:K:47:LEU:HD13	1.83	0.59
1:K:46:SER:C	1:K:48:GLU:H	2.04	0.59
3:I:12:DG:H2"	3:I:13:DT:H5"	1.85	0.59
1:L:30:ARG:HA	1:L:63:ASN:HD22	1.66	0.59
2:J:9:DA:H2"	2:J:10:DT:H5"	1.84	0.59
1:H:79:LYS:HZ1	1:H:83:ASN:HD21	1.48	0.59
1:D:96:LEU:HD21	1:C:119:ILE:CD1	2.33	0.59
1:D:101:TRP:CD2	1:C:92:LYS:HE3	2.38	0.59
1:G:104:LEU:HG	1:G:115:LEU:HD21	1.85	0.59
2:J:12:DG:OP2	1:G:77:ARG:NH2	2.36	0.59
3:M:15:DA:H1'	3:M:16:DC:H5"	1.86	0.58
1:K:114:THR:H	1:K:117:GLU:HG2	1.68	0.58
1:K:113:LYS:HB3	1:K:117:GLU:CG	2.33	0.58
1:H:76:ALA:O	1:H:79:LYS:N	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:58:ILE:HG23	1:K:62:MET:SD	2.42	0.58
1:C:44:LEU:O	1:C:44:LEU:HD13	2.03	0.58
1:H:116:SER:O	1:H:120:VAL:HG23	2.03	0.58
1:A:90:ARG:HD2	1:D:90:ARG:NH1	2.18	0.58
1:K:122:LEU:O	1:K:126:ALA:HB3	2.03	0.58
1:L:125:ASP:O	1:K:126:ALA:HA	2.03	0.58
3:O:7:DA:H2"	3:O:8:DC:C5'	2.25	0.58
1:G:119:ILE:O	1:G:123:ILE:HG13	2.04	0.58
1:K:28:ILE:CD1	1:K:28:ILE:H	2.15	0.58
3:I:2:DT:H2"	3:I:3:DC:C5'	2.22	0.58
1:L:92:LYS:HZ2	1:K:101:TRP:HZ3	1.51	0.58
1:G:50:GLU:HB2	1:G:53:LEU:HD23	1.86	0.58
1:D:48:GLU:HG3	1:D:49:ASN:OD1	2.03	0.58
2:F:2:DT:H1'	2:F:3:DC:H5"	1.86	0.58
3:I:7:DA:C2	3:I:8:DC:C2	2.91	0.58
1:C:94:ILE:HG22	1:C:95:ASP:N	2.18	0.58
1:D:104:LEU:HD22	1:D:115:LEU:HD23	1.85	0.58
3:E:7:DA:C2'	3:E:8:DC:H5'	2.33	0.57
1:A:29:THR:O	1:A:63:ASN:HB2	2.04	0.57
3:O:8:DC:P	1:K:101:TRP:HZ2	2.27	0.57
1:G:113:LYS:HB3	1:G:117:GLU:CB	2.33	0.57
1:D:107:LEU:HD12	1:D:110:ARG:HH21	1.68	0.57
1:K:87:GLN:HA	1:K:90:ARG:CD	2.34	0.57
3:M:3:DC:H2'	1:A:75:ARG:HD2	1.85	0.57
3:M:2:DT:H2"	3:M:3:DC:C5'	2.34	0.57
2:P:6:DG:H1	3:O:14:DC:N4	2.02	0.57
2:J:17:DG:H1	3:I:3:DC:N4	2.02	0.57
1:H:50:GLU:O	1:H:54:VAL:HG23	2.04	0.57
1:H:95:ASP:HA	1:G:92:LYS:O	2.03	0.57
3:M:12:DG:H2"	3:M:13:DT:C5'	2.32	0.57
3:E:9:DA:H2'	3:E:10:DA:N7	2.20	0.57
1:B:94:ILE:O	1:A:93:SER:HA	2.05	0.57
1:C:143:LEU:O	1:C:147:LEU:HB2	2.03	0.57
1:D:104:LEU:HB3	1:D:115:LEU:HD21	1.85	0.57
1:L:115:LEU:HB2	2:P:7:DA:OP1	2.04	0.57
1:H:55:ASN:HA	1:H:58:ILE:HG12	1.85	0.57
2:P:9:DA:OP2	1:K:92:LYS:HD2	2.04	0.57
1:L:94:ILE:HD12	1:K:115:LEU:HD11	1.87	0.57
1:G:128:ASN:O	1:G:132:TYR:HB2	2.04	0.57
1:B:46:SER:C	1:B:48:GLU:H	2.07	0.57
3:M:14:DC:H2"	3:M:15:DA:C8	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:119:ILE:O	1:L:123:ILE:HG13	2.05	0.57
1:B:50:GLU:HB3	1:B:53:LEU:HD12	1.86	0.57
1:K:33:GLU:C	1:K:35:SER:H	2.08	0.57
1:K:80:ARG:HH11	1:K:80:ARG:HG3	1.70	0.57
1:A:86:HIS:HB2	1:A:89:THR:OG1	2.04	0.57
1:C:63:ASN:ND2	1:C:65:GLU:HB2	2.20	0.57
1:H:137:SER:HA	1:H:140:LYS:HE2	1.87	0.57
1:D:119:ILE:CD1	1:C:96:LEU:HD22	2.34	0.57
1:B:122:LEU:HD21	1:A:123:ILE:HA	1.85	0.57
1:D:93:SER:C	1:D:94:ILE:HD13	2.25	0.57
1:D:83:ASN:HB3	1:D:89:THR:OG1	2.05	0.57
2:P:9:DA:H2"	2:P:10:DT:C5'	2.35	0.56
1:A:41:VAL:O	1:A:45:LEU:HD12	2.06	0.56
2:J:14:DC:H2"	2:J:15:DA:C8	2.40	0.56
3:E:10:DA:H2"	3:E:11:DT:O5'	2.05	0.56
1:D:43:VAL:O	1:D:47:LEU:HD13	2.04	0.56
1:B:128:ASN:O	1:B:132:TYR:N	2.31	0.56
1:B:94:ILE:CD1	1:A:96:LEU:HD12	2.34	0.56
1:L:122:LEU:HD21	1:K:123:ILE:HA	1.88	0.56
1:D:106:GLY:O	1:D:110:ARG:CG	2.54	0.56
1:D:144:GLN:HA	1:D:147:LEU:CD2	2.33	0.56
1:G:58:ILE:HG13	1:G:59:ASP:N	2.21	0.56
3:M:2:DT:H2"	3:M:3:DC:H5'	1.88	0.56
1:D:64:PRO:HA	1:D:67:VAL:CG2	2.34	0.56
1:D:96:LEU:HD22	1:C:94:ILE:HD11	1.85	0.56
1:L:87:GLN:HE21	1:K:98:PHE:HZ	1.52	0.56
1:B:39:GLU:O	1:B:43:VAL:HB	2.06	0.56
1:G:94:ILE:HG22	1:G:95:ASP:N	2.20	0.56
3:E:9:DA:H2'	3:E:10:DA:C8	2.41	0.56
1:H:47:LEU:HD23	1:H:54:VAL:HA	1.88	0.56
1:K:64:PRO:HA	1:K:67:VAL:HG23	1.87	0.56
3:O:5:DT:H2"	3:O:6:DG:C8	2.41	0.56
1:B:90:ARG:NH1	1:G:90:ARG:NH1	2.53	0.56
2:J:4:DG:H2"	2:J:5:DT:O5'	2.06	0.56
1:A:130:GLU:HA	1:A:133:ALA:HB3	1.87	0.56
1:H:92:LYS:O	1:G:95:ASP:HA	2.06	0.56
2:N:9:DA:H1'	2:N:10:DT:H5"	1.87	0.56
1:K:15:TRP:CZ3	1:K:19:VAL:HG21	2.41	0.56
1:A:52:VAL:O	1:A:55:ASN:HB2	2.06	0.56
1:L:63:ASN:ND2	1:L:64:PRO:HD2	2.21	0.56
1:K:87:GLN:HA	1:K:90:ARG:HD3	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:ASN:HD21	1:A:65:GLU:HB3	1.71	0.55
1:L:44:LEU:HD23	1:L:47:LEU:HD22	1.87	0.55
1:D:107:LEU:HG	1:D:110:ARG:HE	1.71	0.55
1:A:117:GLU:HA	1:A:120:VAL:CG2	2.35	0.55
1:B:39:GLU:OE1	1:B:43:VAL:HG21	2.06	0.55
1:H:115:LEU:O	1:H:118:THR:OG1	2.21	0.55
2:P:3:DC:H42	3:O:16:DC:N4	2.04	0.55
3:O:4:DG:H1'	3:O:5:DT:H5'	1.88	0.55
1:L:77:ARG:HB2	1:L:77:ARG:HH11	1.70	0.55
1:A:144:GLN:NE2	1:A:147:LEU:HD21	2.20	0.55
1:B:1:MET:N	2:N:3:DC:O3'	2.38	0.55
1:D:96:LEU:HD22	1:C:94:ILE:CD1	2.37	0.55
1:A:99:ILE:O	1:A:102:GLN:HB2	2.07	0.55
1:H:9:LEU:HD12	1:H:10:GLU:N	2.22	0.55
3:I:8:DC:H2"	3:I:9:DA:C8	2.41	0.55
1:A:17:TYR:CE2	1:A:70:MET:HA	2.41	0.55
1:D:136:MET:HG3	1:C:136:MET:HB2	1.88	0.55
1:A:116:SER:HA	1:A:119:ILE:CD1	2.36	0.55
2:N:8:DC:H3'	1:A:92:LYS:CE	2.31	0.55
1:C:31:TYR:OH	1:C:61:HIS:HB3	2.07	0.55
1:B:50:GLU:CB	1:B:53:LEU:HB2	2.36	0.55
2:N:7:DA:C4	2:N:8:DC:C5	2.95	0.55
1:B:7:GLU:CD	1:B:8:ASN:H	2.10	0.55
1:C:83:ASN:HB3	1:C:89:THR:O	2.05	0.55
2:J:2:DT:H2"	2:J:3:DC:H5'	1.89	0.55
1:B:75:ARG:NH2	2:N:4:DG:C6	2.75	0.55
1:L:44:LEU:CA	1:L:47:LEU:HD13	2.26	0.55
1:H:29:THR:HG21	1:H:37:ALA:HB1	1.89	0.55
2:N:18:DA:H2"	2:N:19:DA:OP2	2.07	0.55
1:D:96:LEU:HD21	1:C:119:ILE:HD12	1.88	0.54
2:F:14:DC:N4	3:E:6:DG:H1	2.02	0.54
1:B:94:ILE:CG2	1:A:115:LEU:HD13	2.37	0.54
1:H:93:SER:O	3:I:8:DC:H2'	2.07	0.54
1:D:119:ILE:O	1:D:123:ILE:HG13	2.07	0.54
1:D:94:ILE:HG22	1:D:95:ASP:H	1.72	0.54
1:C:40:ALA:HB1	1:C:57:TRP:CH2	2.42	0.54
1:H:90:ARG:NH1	1:K:90:ARG:NE	2.55	0.54
1:L:104:LEU:HD12	1:K:119:ILE:HG21	1.89	0.54
2:N:9:DA:H2"	2:N:10:DT:H5"	1.88	0.54
1:K:70:MET:O	1:K:72:GLN:N	2.40	0.54
2:P:9:DA:C2'	2:P:10:DT:H5"	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:17:DG:C6	2:F:18:DA:N6	2.75	0.54
1:K:44:LEU:O	1:K:46:SER:N	2.36	0.54
1:B:92:LYS:HD2	3:M:9:DA:OP1	2.08	0.54
1:G:92:LYS:HB3	1:G:92:LYS:HZ3	1.72	0.54
1:C:114:THR:HB	1:C:117:GLU:HB2	1.89	0.54
1:D:114:THR:HG23	1:D:117:GLU:H	1.72	0.54
1:B:58:ILE:HD12	1:B:62:MET:SD	2.48	0.54
1:K:114:THR:OG1	1:K:117:GLU:HG2	2.08	0.54
1:D:103:ARG:O	1:D:107:LEU:N	2.35	0.54
1:G:44:LEU:O	1:G:44:LEU:HD13	2.06	0.54
1:B:98:PHE:HE2	1:A:87:GLN:HB2	1.72	0.54
1:H:55:ASN:HB3	1:H:59:ASP:OD2	2.08	0.54
1:L:44:LEU:CD2	1:L:47:LEU:HD22	2.38	0.54
1:B:33:GLU:CD	1:B:36:ALA:HB2	2.28	0.54
3:E:7:DA:OP1	1:C:115:LEU:HB2	2.06	0.54
1:A:77:ARG:O	1:A:78:ARG:C	2.45	0.54
1:B:40:ALA:HB1	1:B:57:TRP:CZ2	2.43	0.54
1:G:31:TYR:HE1	1:G:61:HIS:CD2	2.26	0.54
1:B:66:LEU:HA	1:B:69:ARG:HG3	1.89	0.53
1:H:43:VAL:O	1:H:47:LEU:HD13	2.08	0.53
1:B:39:GLU:O	1:B:43:VAL:CG2	2.56	0.53
1:D:141:GLN:H	1:D:141:GLN:HE21	1.56	0.53
3:O:3:DC:H2'	1:K:75:ARG:HD2	1.91	0.53
1:L:92:LYS:NZ	1:K:101:TRP:HZ3	2.06	0.53
1:C:107:LEU:HD23	1:C:107:LEU:C	2.29	0.53
1:A:135:LYS:O	1:A:139:LEU:HB2	2.09	0.53
1:D:104:LEU:CD1	1:C:119:ILE:HD13	2.38	0.53
1:B:50:GLU:O	1:B:54:VAL:HG23	2.09	0.53
1:B:92:LYS:HB3	3:M:9:DA:OP2	2.08	0.53
2:J:18:DA:H1'	2:J:19:DA:H5"	1.89	0.53
1:G:23:ARG:HH11	1:G:23:ARG:HG2	1.73	0.53
1:B:75:ARG:CD	2:N:3:DC:H2'	2.38	0.53
1:L:87:GLN:HG2	1:K:98:PHE:CE1	2.43	0.53
1:B:93:SER:HA	1:A:94:ILE:O	2.09	0.53
3:O:12:DG:C2'	3:O:13:DT:H5"	2.36	0.53
1:D:10:GLU:OE1	1:D:78:ARG:HD3	2.08	0.53
1:A:39:GLU:O	1:A:43:VAL:HG23	2.08	0.53
1:L:126:ALA:CB	1:K:126:ALA:HB2	2.35	0.53
1:D:63:ASN:ND2	1:D:65:GLU:HG3	2.23	0.53
1:A:116:SER:O	1:A:120:VAL:HG23	2.09	0.53
1:L:5:GLN:O	1:L:6:LEU:HD23	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:115:LEU:O	1:G:116:SER:C	2.46	0.53
1:B:98:PHE:CE2	1:A:87:GLN:HB2	2.44	0.53
1:A:115:LEU:O	1:A:118:THR:HB	2.08	0.53
1:K:44:LEU:C	1:K:46:SER:H	2.13	0.53
1:G:48:GLU:O	1:G:51:PRO:HD3	2.09	0.53
1:H:94:ILE:CG2	1:G:115:LEU:HD12	2.32	0.52
1:L:93:SER:O	1:L:94:ILE:HD13	2.09	0.52
3:O:7:DA:C2	3:O:8:DC:N3	2.77	0.52
1:B:7:GLU:N	1:B:7:GLU:CD	2.62	0.52
1:C:77:ARG:HA	1:C:80:ARG:HB2	1.91	0.52
1:C:22:HIS:C	1:C:24:GLU:H	2.12	0.52
1:H:107:LEU:HD23	1:H:111:ARG:HG2	1.91	0.52
1:B:75:ARG:NH1	2:N:3:DC:C5	2.78	0.52
1:D:113:LYS:HD3	1:D:117:GLU:HB3	1.91	0.52
1:D:118:THR:O	1:D:122:LEU:HG	2.09	0.52
1:L:80:ARG:HH12	3:O:11:DT:H2"	1.74	0.52
3:E:6:DG:H2"	3:E:7:DA:C8	2.45	0.52
1:D:140:LYS:HA	1:D:143:LEU:HD11	1.91	0.52
1:K:27:LEU:HD23	1:K:29:THR:CG2	2.31	0.52
1:H:40:ALA:HB1	1:H:57:TRP:HZ2	1.73	0.52
1:D:44:LEU:O	1:D:47:LEU:HB2	2.10	0.52
1:D:5:GLN:O	1:D:6:LEU:HD23	2.09	0.52
1:A:19:VAL:HG12	1:A:23:ARG:HH22	1.75	0.52
1:D:83:ASN:N	1:D:83:ASN:HD22	2.06	0.52
1:B:113:LYS:HE3	1:B:117:GLU:HB3	1.90	0.52
1:L:44:LEU:HD22	1:L:47:LEU:HB2	1.90	0.52
1:L:50:GLU:OE1	1:L:53:LEU:HD13	2.09	0.52
1:B:12:GLY:O	1:B:15:TRP:HB3	2.10	0.52
1:C:44:LEU:HA	1:C:47:LEU:HD13	1.91	0.52
1:C:51:PRO:HA	1:C:54:VAL:CG2	2.39	0.52
1:A:58:ILE:HG23	1:A:62:MET:SD	2.50	0.52
1:K:119:ILE:CD1	1:K:119:ILE:H	2.20	0.52
2:J:3:DC:N4	3:I:17:DG:H1	2.07	0.52
1:L:106:GLY:O	1:L:110:ARG:HB2	2.10	0.52
1:H:100:VAL:O	1:H:102:GLN:N	2.42	0.52
1:G:13:TRP:CZ2	1:G:77:ARG:HG2	2.44	0.52
1:A:44:LEU:HD23	1:A:57:TRP:CE2	2.45	0.52
1:K:51:PRO:C	1:K:53:LEU:H	2.13	0.52
1:G:81:HIS:C	1:G:83:ASN:H	2.13	0.52
1:B:39:GLU:O	1:B:43:VAL:CB	2.58	0.52
1:H:131:LYS:O	1:H:135:LYS:HG3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:123:ILE:O	1:H:127:GLU:N	2.42	0.52
1:D:87:GLN:HE22	1:D:90:ARG:HE	1.52	0.52
1:K:13:TRP:CA	1:K:16:LYS:HG3	2.40	0.52
1:C:94:ILE:HG22	1:C:95:ASP:H	1.75	0.52
2:F:19:DA:H2	3:E:2:DT:H3	1.57	0.52
1:G:113:LYS:HD2	1:G:117:GLU:CG	2.40	0.52
1:H:30:ARG:HB3	1:H:62:MET:O	2.10	0.52
1:L:22:HIS:NE2	1:L:41:VAL:HG13	2.25	0.52
1:B:75:ARG:HD2	2:N:3:DC:H2'	1.91	0.51
1:D:144:GLN:O	1:D:147:LEU:CG	2.44	0.51
1:L:14:LYS:O	1:L:17:TYR:HB3	2.10	0.51
1:G:22:HIS:C	1:G:24:GLU:H	2.14	0.51
2:N:14:DC:N4	3:M:6:DG:H1	2.07	0.51
1:K:74:ILE:CG2	1:K:75:ARG:H	2.20	0.51
1:B:35:SER:C	1:B:37:ALA:N	2.61	0.51
1:G:39:GLU:HG3	1:G:40:ALA:N	2.25	0.51
1:D:115:LEU:O	1:D:118:THR:N	2.42	0.51
1:L:123:ILE:HG12	1:K:122:LEU:CD1	2.40	0.51
1:K:27:LEU:HD21	1:K:31:TYR:O	2.10	0.51
2:J:11:DT:H3'	1:G:77:ARG:NH2	2.25	0.51
1:B:47:LEU:O	1:B:49:ASN:N	2.42	0.51
1:G:40:ALA:HB1	1:G:57:TRP:CZ2	2.45	0.51
1:H:115:LEU:HB2	2:J:7:DA:OP1	2.09	0.51
2:J:9:DA:C2'	2:J:10:DT:H5"	2.40	0.51
1:B:126:ALA:HB2	1:A:126:ALA:HB2	1.93	0.51
2:N:12:DG:C6	3:M:8:DC:N4	2.73	0.51
1:B:50:GLU:HB3	1:B:53:LEU:CB	2.36	0.51
2:P:9:DA:H61	3:O:11:DT:H3	1.58	0.51
1:L:85:GLU:O	1:L:86:HIS:ND1	2.43	0.51
1:G:84:ALA:O	1:G:90:ARG:HD2	2.10	0.51
1:G:3:TYR:HE2	1:G:79:LYS:HG2	1.75	0.51
1:H:84:ALA:O	1:H:85:GLU:C	2.48	0.51
1:A:15:TRP:O	1:A:19:VAL:HG23	2.10	0.51
1:K:65:GLU:OE1	1:K:65:GLU:HA	2.10	0.51
1:K:51:PRO:HA	1:K:54:VAL:HG23	1.92	0.51
1:K:114:THR:N	1:K:117:GLU:HG2	2.25	0.51
1:B:4:GLN:HE22	1:G:9:LEU:CD1	2.23	0.51
1:L:131:LYS:O	1:L:135:LYS:HB2	2.10	0.51
1:B:126:ALA:HB2	1:A:122:LEU:HD23	1.92	0.51
3:E:6:DG:C6	3:E:7:DA:N6	2.78	0.51
3:O:5:DT:OP2	1:K:79:LYS:HE2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:81:HIS:O	1:K:84:ALA:N	2.43	0.51
2:N:6:DG:H2"	2:N:7:DA:H8	1.75	0.51
1:D:94:ILE:HG23	1:C:115:LEU:HD13	1.93	0.51
3:E:7:DA:C1'	3:E:8:DC:H5'	2.41	0.51
1:A:10:GLU:CG	1:A:13:TRP:CH2	2.81	0.51
1:C:44:LEU:HD23	1:C:57:TRP:CE2	2.46	0.51
1:K:32:ILE:HG23	1:K:33:GLU:H	1.74	0.51
1:K:90:ARG:O	1:K:91:LYS:HD3	2.10	0.50
1:B:75:ARG:NH2	2:N:4:DG:C5	2.77	0.50
3:I:11:DT:C2'	3:I:12:DG:OP2	2.57	0.50
1:D:147:LEU:HD12	1:D:148:GLY:N	2.26	0.50
1:G:114:THR:HG23	1:G:117:GLU:H	1.76	0.50
1:G:15:TRP:HE1	1:G:44:LEU:HD13	1.76	0.50
1:A:137:SER:O	1:A:141:GLN:HG3	2.12	0.50
1:D:76:ALA:O	1:D:79:LYS:N	2.44	0.50
1:H:115:LEU:HD12	2:J:7:DA:OP1	2.11	0.50
1:A:121:GLN:HA	1:A:124:GLU:OE1	2.12	0.50
1:K:101:TRP:O	1:K:105:ALA:N	2.45	0.50
1:B:90:ARG:HD2	1:G:90:ARG:HH22	1.77	0.50
3:E:3:DC:C5	1:C:75:ARG:NH1	2.79	0.50
1:A:6:LEU:HD12	1:A:13:TRP:HZ2	1.76	0.50
1:H:87:GLN:C	1:H:89:THR:H	2.14	0.50
1:H:119:ILE:CA	1:H:122:LEU:HD12	2.39	0.50
1:B:15:TRP:CE3	1:B:19:VAL:HG21	2.47	0.50
1:G:80:ARG:O	1:G:81:HIS:C	2.48	0.50
1:B:107:LEU:O	1:B:111:ARG:HG3	2.12	0.50
1:H:119:ILE:O	1:H:122:LEU:HB2	2.12	0.50
1:H:129:LYS:O	1:H:132:TYR:HB2	2.12	0.50
1:B:77:ARG:HH22	3:M:11:DT:H3'	1.77	0.50
1:K:9:LEU:O	1:K:12:GLY:N	2.44	0.50
1:D:69:ARG:HA	1:D:72:GLN:HG2	1.94	0.50
1:G:79:LYS:O	1:G:83:ASN:HB2	2.12	0.50
1:G:83:ASN:CG	1:G:89:THR:HB	2.32	0.50
1:A:50:GLU:O	1:A:54:VAL:HG23	2.11	0.50
1:A:7:GLU:CD	1:A:7:GLU:H	2.15	0.50
1:D:11:SER:HB2	1:D:51:PRO:HB2	1.94	0.50
1:A:117:GLU:O	1:A:120:VAL:HB	2.11	0.50
1:H:20:LYS:NZ	3:I:11:DT:O3'	2.44	0.50
1:L:122:LEU:O	1:L:122:LEU:HD23	2.12	0.50
1:H:80:ARG:NH2	3:I:12:DG:N7	2.59	0.50
1:H:28:ILE:HA	1:H:66:LEU:HD22	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:63:ASN:HD21	1:C:65:GLU:HB2	1.77	0.50
1:K:136:MET:O	1:K:140:LYS:HG3	2.12	0.50
1:C:20:LYS:O	1:C:24:GLU:HG3	2.12	0.49
2:F:2:DT:H2"	2:F:3:DC:C5'	2.42	0.49
1:D:94:ILE:CG2	1:C:115:LEU:HD13	2.42	0.49
1:K:76:ALA:C	1:K:78:ARG:N	2.66	0.49
1:H:80:ARG:O	1:H:81:HIS:C	2.50	0.49
3:E:5:DT:OP2	1:C:79:LYS:HE2	2.12	0.49
1:B:98:PHE:HE2	1:A:87:GLN:NE2	2.08	0.49
1:B:14:LYS:O	1:B:17:TYR:HB3	2.12	0.49
1:K:64:PRO:HA	1:K:67:VAL:CG2	2.42	0.49
1:H:107:LEU:HD23	1:H:111:ARG:CG	2.43	0.49
1:H:114:THR:HG22	1:H:117:GLU:OE2	2.13	0.49
1:G:72:GLN:HG3	1:G:75:ARG:NH2	2.27	0.49
1:B:66:LEU:HA	1:B:69:ARG:CG	2.42	0.49
1:A:119:ILE:O	1:A:123:ILE:HD12	2.13	0.49
2:N:4:DG:H2"	2:N:5:DT:O5'	2.11	0.49
1:D:94:ILE:HG22	1:D:95:ASP:N	2.26	0.49
2:P:12:DG:H1'	2:P:13:DT:H5"	1.95	0.49
1:A:33:GLU:HG3	1:A:35:SER:HB3	1.95	0.49
1:A:90:ARG:NE	1:D:90:ARG:CZ	2.76	0.49
1:A:17:TYR:HB3	1:A:18:LEU:HD12	1.94	0.49
1:B:137:SER:O	1:B:141:GLN:HB3	2.12	0.49
3:O:1:DT:H2"	3:O:2:DT:O5'	2.13	0.49
1:H:56:GLY:O	1:H:60:LYS:HD2	2.12	0.49
1:K:74:ILE:CG2	1:K:75:ARG:N	2.76	0.49
2:F:1:DT:H2"	2:F:2:DT:O5'	2.12	0.49
1:D:146:LEU:HD22	1:D:149:LYS:NZ	2.28	0.49
1:K:111:ARG:NH1	1:K:121:GLN:HG2	2.27	0.49
1:H:119:ILE:O	1:H:123:ILE:HG13	2.13	0.49
1:D:114:THR:HG1	2:F:7:DA:P	2.35	0.49
1:B:47:LEU:HG	1:B:50:GLU:HG3	1.94	0.49
1:K:13:TRP:O	1:K:14:LYS:C	2.51	0.49
1:D:83:ASN:ND2	1:D:83:ASN:N	2.60	0.49
1:K:107:LEU:CD2	1:K:111:ARG:HG3	2.43	0.49
1:L:97:GLU:HB2	1:L:100:VAL:HG23	1.94	0.49
3:O:4:DG:H2"	3:O:5:DT:O5'	2.13	0.49
1:D:33:GLU:HB2	1:D:36:ALA:HB3	1.94	0.49
1:B:3:TYR:HE1	1:B:79:LYS:HA	1.77	0.49
3:I:7:DA:C6	3:I:8:DC:C4	3.01	0.49
2:N:9:DA:C2'	2:N:10:DT:H5"	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:30:ARG:HD3	1:K:30:ARG:O	2.12	0.49
1:K:44:LEU:HA	1:K:47:LEU:CD1	2.42	0.49
1:K:33:GLU:O	1:K:35:SER:N	2.45	0.49
1:H:80:ARG:O	1:H:83:ASN:N	2.46	0.49
1:H:3:TYR:HB2	2:J:4:DG:OP1	2.12	0.49
3:M:3:DC:H2"	3:M:4:DG:C8	2.48	0.48
3:E:16:DC:H2"	3:E:17:DG:C8	2.48	0.48
1:B:50:GLU:CG	1:B:53:LEU:HD12	2.42	0.48
1:C:44:LEU:HD23	1:C:57:TRP:NE1	2.28	0.48
2:J:7:DA:C4	2:J:8:DC:C5	3.01	0.48
1:G:104:LEU:HG	1:G:115:LEU:CD2	2.43	0.48
1:B:131:LYS:O	1:B:134:ASN:HB2	2.12	0.48
1:C:142:ASP:O	1:C:146:LEU:HG	2.14	0.48
1:G:13:TRP:CZ3	1:G:77:ARG:HB3	2.48	0.48
1:K:123:ILE:O	1:K:127:GLU:CB	2.59	0.48
1:G:40:ALA:HB2	1:G:61:HIS:CD2	2.48	0.48
1:A:103:ARG:HD2	3:I:15:DA:H5"	1.95	0.48
1:H:31:TYR:HD1	1:H:37:ALA:HB2	1.78	0.48
1:B:96:LEU:HD12	1:A:92:LYS:O	2.13	0.48
1:C:119:ILE:CA	1:C:122:LEU:HD12	2.40	0.48
1:K:13:TRP:O	1:K:16:LYS:HG3	2.13	0.48
1:H:77:ARG:HD2	3:I:12:DG:OP2	2.12	0.48
1:L:107:LEU:O	1:L:111:ARG:HG3	2.13	0.48
1:K:131:LYS:O	1:K:134:ASN:HB2	2.13	0.48
3:M:8:DC:OP1	1:A:101:TRP:HZ2	1.96	0.48
1:B:27:LEU:C	1:B:28:ILE:HD13	2.33	0.48
1:B:3:TYR:CE1	1:B:79:LYS:HA	2.48	0.48
3:I:7:DA:C2	3:I:8:DC:N3	2.82	0.48
1:L:115:LEU:O	1:L:118:THR:HB	2.13	0.48
1:L:47:LEU:N	1:L:47:LEU:HD12	2.27	0.48
1:C:76:ALA:HB1	1:C:80:ARG:CZ	2.43	0.48
1:B:15:TRP:CZ3	1:B:19:VAL:HG21	2.49	0.48
1:A:131:LYS:O	1:A:135:LYS:HG2	2.13	0.48
1:D:146:LEU:CD2	1:D:149:LYS:NZ	2.77	0.48
2:F:10:DT:H73	1:C:93:SER:OG	2.14	0.48
2:F:12:DG:C2'	2:F:13:DT:H5"	2.41	0.48
2:P:12:DG:N2	2:P:13:DT:O2	2.46	0.48
2:P:10:DT:H5'	2:P:10:DT:H6	1.78	0.48
1:B:120:VAL:HG22	1:A:100:VAL:HG22	1.95	0.48
2:N:6:DG:H2"	2:N:7:DA:C8	2.49	0.48
1:D:95:ASP:HA	1:C:92:LYS:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:101:TRP:HE1	2:F:8:DC:P	2.36	0.48
1:B:13:TRP:CZ2	1:B:77:ARG:HG3	2.49	0.48
1:C:141:GLN:O	1:C:145:ALA:HB2	2.14	0.48
1:K:101:TRP:CD1	1:K:105:ALA:HB2	2.49	0.48
1:K:110:ARG:HH11	1:K:110:ARG:HB2	1.75	0.48
2:P:18:DA:H2"	2:P:19:DA:H5"	1.94	0.48
1:L:31:TYR:HD2	1:L:36:ALA:HB1	1.78	0.48
3:M:15:DA:H2"	3:M:16:DC:OP2	2.13	0.47
1:D:144:GLN:HG3	1:D:147:LEU:HD21	1.95	0.47
1:B:65:GLU:C	1:B:66:LEU:HD12	2.34	0.47
1:B:34:ALA:O	1:B:37:ALA:HB3	2.13	0.47
2:N:10:DT:OP1	1:D:87:GLN:HB2	2.14	0.47
1:B:68:ASN:CG	1:B:69:ARG:N	2.67	0.47
1:G:139:LEU:O	1:G:143:LEU:HG	2.14	0.47
1:D:76:ALA:O	1:D:79:LYS:HB3	2.14	0.47
1:D:97:GLU:HB2	1:D:100:VAL:HG23	1.97	0.47
3:I:9:DA:C2	3:I:10:DA:C2	3.02	0.47
1:K:106:GLY:O	1:K:109:GLN:HB2	2.13	0.47
1:D:69:ARG:O	1:D:73:THR:N	2.47	0.47
3:M:16:DC:C6	3:M:16:DC:H5'	2.49	0.47
1:H:18:LEU:HG	1:H:28:ILE:HD12	1.96	0.47
1:D:10:GLU:C	1:D:12:GLY:N	2.67	0.47
1:H:41:VAL:O	1:H:45:LEU:HG	2.14	0.47
1:D:14:LYS:O	1:D:18:LEU:HB2	2.14	0.47
1:H:93:SER:C	1:H:94:ILE:HD13	2.35	0.47
1:B:120:VAL:HA	1:B:123:ILE:HD12	1.96	0.47
1:B:63:ASN:ND2	1:B:65:GLU:HB2	2.20	0.47
1:B:68:ASN:O	1:B:69:ARG:C	2.53	0.47
1:C:55:ASN:HA	1:C:58:ILE:HD12	1.97	0.47
1:L:98:PHE:CE2	1:K:87:GLN:HG2	2.49	0.47
1:L:47:LEU:O	1:L:50:GLU:HB2	2.14	0.47
1:C:132:TYR:O	1:C:136:MET:HB3	2.15	0.47
1:G:123:ILE:HA	1:G:126:ALA:HB3	1.96	0.47
1:B:35:SER:O	1:B:36:ALA:C	2.51	0.47
1:G:87:GLN:O	1:G:89:THR:N	2.48	0.47
1:H:119:ILE:HG22	1:H:123:ILE:HD11	1.97	0.47
1:D:94:ILE:HD13	1:D:94:ILE:N	2.29	0.47
1:G:69:ARG:NH1	1:G:69:ARG:HG3	2.27	0.47
1:H:48:GLU:C	1:H:50:GLU:H	2.17	0.47
2:N:15:DA:H1'	2:N:16:DC:H5"	1.95	0.47
1:K:32:ILE:HG23	1:K:33:GLU:N	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:107:LEU:HA	1:D:110:ARG:HE	1.80	0.47
1:A:102:GLN:O	1:A:103:ARG:C	2.53	0.47
2:F:2:DT:H2"	2:F:3:DC:H5'	1.96	0.47
1:L:6:LEU:HD12	1:L:9:LEU:HD11	1.97	0.47
1:B:101:TRP:CD2	1:A:92:LYS:HD3	2.49	0.47
1:D:119:ILE:HG22	1:D:123:ILE:HD11	1.96	0.47
3:E:12:DG:H2"	3:E:13:DT:C5'	2.43	0.47
1:L:50:GLU:CD	1:L:53:LEU:HD13	2.34	0.47
1:G:69:ARG:O	1:G:72:GLN:N	2.46	0.47
1:C:129:LYS:HD3	1:C:130:GLU:N	2.30	0.47
1:B:132:TYR:O	1:B:136:MET:HG2	2.15	0.47
1:K:67:VAL:O	1:K:71:LYS:HG3	2.15	0.47
1:K:133:ALA:O	1:K:137:SER:HB2	2.15	0.47
1:A:13:TRP:CE3	1:A:77:ARG:HG2	2.49	0.47
1:B:18:LEU:HD12	1:B:28:ILE:CG2	2.45	0.47
1:B:37:ALA:O	1:B:41:VAL:HG23	2.14	0.47
1:D:115:LEU:HB2	2:F:7:DA:OP1	2.15	0.47
1:K:46:SER:O	1:K:48:GLU:N	2.48	0.47
1:K:64:PRO:O	1:K:67:VAL:HG23	2.15	0.47
1:G:99:ILE:H	1:G:99:ILE:HD12	1.80	0.47
1:H:92:LYS:HG3	1:G:101:TRP:CE3	2.50	0.46
3:E:11:DT:C2	3:E:12:DG:C5	3.03	0.46
3:O:14:DC:H2"	3:O:15:DA:C8	2.50	0.46
3:E:15:DA:H1'	3:E:16:DC:H5"	1.97	0.46
1:B:84:ALA:O	1:B:90:ARG:NH1	2.48	0.46
1:B:7:GLU:CD	1:B:8:ASN:N	2.68	0.46
3:O:8:DC:O5'	1:K:101:TRP:CZ2	2.68	0.46
1:L:92:LYS:HD2	3:O:9:DA:OP2	2.14	0.46
1:G:101:TRP:O	1:G:105:ALA:N	2.45	0.46
1:D:115:LEU:O	1:D:119:ILE:HG13	2.16	0.46
1:B:87:GLN:HG2	1:A:98:PHE:CD2	2.50	0.46
1:H:79:LYS:NZ	1:H:83:ASN:ND2	2.61	0.46
1:C:57:TRP:HA	1:C:61:HIS:CE1	2.51	0.46
1:B:3:TYR:HB3	1:B:82:PHE:CE1	2.51	0.46
1:G:104:LEU:C	1:G:106:GLY:N	2.67	0.46
2:N:9:DA:P	1:A:92:LYS:HB2	2.55	0.46
3:M:2:DT:H1'	3:M:3:DC:H5"	1.96	0.46
2:P:5:DT:H2"	2:P:6:DG:C8	2.50	0.46
1:K:76:ALA:C	1:K:78:ARG:H	2.19	0.46
1:B:10:GLU:O	1:B:13:TRP:HB2	2.15	0.46
1:B:9:LEU:HD12	1:B:10:GLU:N	2.21	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:13:TRP:CE3	1:C:77:ARG:HB3	2.51	0.46
1:G:15:TRP:C	1:G:17:TYR:H	2.17	0.46
1:G:87:GLN:C	1:G:89:THR:H	2.19	0.46
1:K:80:ARG:NH1	1:K:80:ARG:HG3	2.30	0.46
2:J:9:DA:H2"	2:J:10:DT:C5'	2.45	0.46
1:K:115:LEU:HD23	1:K:115:LEU:O	2.16	0.46
1:B:90:ARG:CD	1:G:90:ARG:HH12	2.27	0.46
1:K:10:GLU:HA	1:K:13:TRP:CE3	2.50	0.46
1:L:117:GLU:HA	1:L:120:VAL:CG2	2.46	0.46
1:L:3:TYR:CD2	1:L:3:TYR:N	2.84	0.46
1:B:44:LEU:HB2	1:B:57:TRP:CZ2	2.51	0.46
1:G:58:ILE:HG13	1:G:59:ASP:OD1	2.16	0.46
1:K:54:VAL:O	1:K:57:TRP:HB3	2.16	0.46
1:B:132:TYR:CE1	1:A:133:ALA:HA	2.50	0.46
1:G:5:GLN:HG2	1:G:78:ARG:NE	2.31	0.46
1:D:115:LEU:HA	1:D:118:THR:OG1	2.15	0.46
1:G:6:LEU:HD13	1:G:9:LEU:HB2	1.97	0.46
1:H:114:THR:O	1:H:115:LEU:C	2.55	0.46
1:B:123:ILE:HA	1:A:122:LEU:CD2	2.45	0.46
1:B:72:GLN:NE2	3:M:13:DT:H2'	2.31	0.46
1:L:75:ARG:NH2	2:P:5:DT:O4	2.48	0.46
1:L:93:SER:HA	1:K:94:ILE:O	2.16	0.46
3:O:7:DA:OP1	1:K:115:LEU:CB	2.61	0.46
1:K:3:TYR:HB3	1:K:82:PHE:CE2	2.51	0.46
2:J:7:DA:C2	2:J:8:DC:C2	3.04	0.46
1:B:44:LEU:HA	1:B:47:LEU:CD1	2.42	0.46
1:G:129:LYS:O	1:G:133:ALA:HB2	2.16	0.46
1:K:46:SER:C	1:K:48:GLU:N	2.69	0.46
1:L:30:ARG:HA	1:L:63:ASN:ND2	2.31	0.46
2:F:1:DT:H2'	2:F:2:DT:H71	1.97	0.46
1:A:75:ARG:HG3	1:A:78:ARG:NH2	2.31	0.45
1:B:87:GLN:HA	1:B:90:ARG:HE	1.80	0.45
1:H:105:ALA:O	1:H:108:ALA:HB3	2.16	0.45
2:N:7:DA:H2"	2:N:8:DC:C5'	2.33	0.45
1:K:26:GLU:HG3	1:K:27:LEU:N	2.30	0.45
1:A:27:LEU:CD2	1:A:27:LEU:H	2.23	0.45
1:D:60:LYS:HB3	1:D:61:HIS:ND1	2.31	0.45
1:L:115:LEU:O	1:L:116:SER:C	2.54	0.45
1:L:92:LYS:HG3	1:K:101:TRP:CE3	2.51	0.45
2:J:12:DG:C3'	2:J:13:DT:H5"	2.46	0.45
1:A:124:GLU:O	1:A:128:ASN:ND2	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:TRP:CD1	1:A:13:TRP:N	2.79	0.45
1:D:50:GLU:O	1:D:54:VAL:HG23	2.17	0.45
1:K:6:LEU:O	1:K:7:GLU:C	2.54	0.45
1:G:29:THR:OG1	1:G:37:ALA:HB1	2.16	0.45
1:K:114:THR:HB	1:K:117:GLU:HG2	1.98	0.45
1:G:32:ILE:O	1:G:32:ILE:HG12	2.17	0.45
1:A:15:TRP:CE3	1:A:19:VAL:HG21	2.52	0.45
1:K:70:MET:C	1:K:72:GLN:N	2.69	0.45
1:K:11:SER:HA	1:K:14:LYS:HZ3	1.82	0.45
1:L:122:LEU:HD11	1:K:123:ILE:HG12	1.99	0.45
1:L:63:ASN:HD22	1:L:63:ASN:HA	1.54	0.45
1:C:51:PRO:HA	1:C:54:VAL:HG23	1.98	0.45
1:A:56:GLY:HA2	1:A:59:ASP:OD2	2.16	0.45
1:C:104:LEU:O	1:C:105:ALA:C	2.55	0.45
3:E:7:DA:C1'	3:E:8:DC:C5'	2.87	0.45
1:K:110:ARG:NH1	1:K:110:ARG:CB	2.71	0.45
1:K:19:VAL:O	1:K:20:LYS:C	2.55	0.45
1:B:62:MET:HG2	1:B:63:ASN:N	2.32	0.45
1:K:92:LYS:HB3	1:K:92:LYS:HZ3	1.81	0.45
1:K:38:GLN:O	1:K:41:VAL:HB	2.16	0.45
1:A:47:LEU:HD22	1:A:53:LEU:CD1	2.44	0.45
1:B:129:LYS:HD3	1:A:125:ASP:O	2.17	0.45
1:D:114:THR:O	1:D:115:LEU:C	2.55	0.45
1:L:104:LEU:HD22	1:L:115:LEU:CD2	2.46	0.45
1:K:101:TRP:O	1:K:102:GLN:C	2.54	0.45
2:F:17:DG:C2	2:F:18:DA:C6	3.05	0.45
1:D:63:ASN:HD22	1:D:64:PRO:CD	2.22	0.45
1:K:13:TRP:N	1:K:16:LYS:HE3	2.32	0.45
1:D:29:THR:HB	1:D:31:TYR:CD1	2.52	0.45
1:B:71:LYS:HZ1	2:N:2:DT:C2'	2.30	0.45
1:L:58:ILE:HD12	1:L:62:MET:HE2	1.98	0.45
1:C:107:LEU:HD23	1:C:107:LEU:O	2.16	0.45
1:B:11:SER:HB3	1:B:55:ASN:ND2	2.32	0.45
1:H:126:ALA:C	1:H:128:ASN:N	2.69	0.45
1:B:115:LEU:HB2	2:N:7:DA:P	2.56	0.45
1:A:74:ILE:HG23	1:A:75:ARG:N	2.32	0.45
1:B:13:TRP:O	1:B:14:LYS:C	2.55	0.45
2:F:12:DG:OP2	1:C:77:ARG:NH2	2.51	0.45
1:D:23:ARG:NE	1:C:23:ARG:HB2	2.26	0.45
1:K:44:LEU:O	1:K:47:LEU:HD13	2.17	0.45
1:H:129:LYS:HD3	1:G:125:ASP:HA	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:122:LEU:HD21	1:K:123:ILE:CG1	2.47	0.44
1:G:10:GLU:OE1	1:G:78:ARG:HD3	2.17	0.44
3:I:10:DA:OP1	1:K:86:HIS:HA	2.17	0.44
1:B:47:LEU:O	1:B:48:GLU:C	2.56	0.44
1:B:122:LEU:O	1:B:122:LEU:HD23	2.17	0.44
1:H:3:TYR:CE1	2:J:4:DG:H3'	2.51	0.44
3:O:7:DA:C2	3:O:8:DC:C2	3.06	0.44
1:G:40:ALA:HB2	1:G:61:HIS:HD2	1.81	0.44
1:H:98:PHE:CZ	1:G:87:GLN:OE1	2.70	0.44
1:C:140:LYS:HA	1:C:143:LEU:CD1	2.48	0.44
1:L:29:THR:HG21	1:L:37:ALA:HA	2.00	0.44
1:H:116:SER:HA	1:H:119:ILE:HD12	1.99	0.44
1:A:6:LEU:HB2	1:A:10:GLU:HG3	1.98	0.44
2:J:19:DA:H5'	2:J:19:DA:C8	2.53	0.44
1:A:63:ASN:ND2	1:A:65:GLU:HB3	2.32	0.44
1:G:119:ILE:O	1:G:122:LEU:HB2	2.18	0.44
1:K:12:GLY:O	1:K:16:LYS:HG3	2.18	0.44
2:N:11:DT:H3	3:M:9:DA:H61	1.65	0.44
1:C:79:LYS:HD3	1:C:83:ASN:ND2	2.33	0.44
1:C:55:ASN:HA	1:C:58:ILE:CD1	2.47	0.44
1:B:115:LEU:O	1:B:118:THR:HB	2.18	0.44
1:C:119:ILE:HA	1:C:122:LEU:CD1	2.44	0.44
2:J:11:DT:H3'	1:G:77:ARG:HH22	1.83	0.44
1:B:69:ARG:NH1	1:B:69:ARG:HG3	2.33	0.44
1:A:47:LEU:CD1	1:A:53:LEU:HD22	2.45	0.44
1:H:98:PHE:CE1	1:G:87:GLN:NE2	2.85	0.44
1:B:132:TYR:HA	1:B:135:LYS:HE3	1.98	0.44
1:C:3:TYR:HE2	1:C:79:LYS:HG2	1.83	0.44
1:G:118:THR:O	1:G:122:LEU:HG	2.18	0.44
1:D:103:ARG:O	1:D:107:LEU:HB2	2.17	0.44
2:J:3:DC:H42	3:I:17:DG:H1	1.64	0.44
1:H:93:SER:HA	1:G:94:ILE:O	2.17	0.44
1:A:121:GLN:O	1:A:122:LEU:C	2.56	0.44
1:A:65:GLU:OE1	1:A:66:LEU:HG	2.17	0.44
1:K:122:LEU:O	1:K:126:ALA:CB	2.66	0.44
3:O:3:DC:H6	3:O:3:DC:H2'	1.62	0.44
1:L:17:TYR:C	1:L:19:VAL:H	2.21	0.44
1:C:126:ALA:O	1:C:129:LYS:HB3	2.17	0.44
1:L:30:ARG:HA	1:L:63:ASN:HA	2.00	0.44
1:D:13:TRP:CZ3	1:D:77:ARG:HB3	2.53	0.44
1:A:15:TRP:HE3	1:A:16:LYS:HD3	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:26:GLU:HG3	1:D:27:LEU:N	2.32	0.44
1:G:40:ALA:HB1	1:G:57:TRP:HZ2	1.82	0.44
1:C:133:ALA:O	1:C:137:SER:CB	2.66	0.44
1:L:46:SER:C	1:L:48:GLU:H	2.21	0.44
1:C:41:VAL:O	1:C:45:LEU:HG	2.17	0.44
3:M:3:DC:H2'	1:A:75:ARG:CD	2.48	0.43
1:K:51:PRO:C	1:K:53:LEU:N	2.71	0.43
1:K:114:THR:HB	1:K:117:GLU:H	1.83	0.43
1:B:101:TRP:CG	1:A:92:LYS:HD3	2.53	0.43
1:K:78:ARG:HG3	1:K:78:ARG:HH11	1.83	0.43
1:C:72:GLN:OE1	1:C:75:ARG:NH2	2.51	0.43
1:L:117:GLU:O	1:L:120:VAL:N	2.51	0.43
1:C:5:GLN:HG2	1:C:78:ARG:HD2	1.99	0.43
1:H:137:SER:HA	1:H:140:LYS:HB2	2.00	0.43
1:B:3:TYR:CD2	1:B:3:TYR:N	2.86	0.43
1:K:3:TYR:HB3	1:K:82:PHE:CD2	2.52	0.43
1:D:86:HIS:C	1:D:88:HIS:N	2.72	0.43
3:E:15:DA:C6	3:E:16:DC:N4	2.86	0.43
1:B:14:LYS:O	1:B:18:LEU:HD23	2.18	0.43
1:H:48:GLU:HA	1:H:48:GLU:OE1	2.19	0.43
1:B:19:VAL:O	1:B:22:HIS:HB3	2.17	0.43
1:K:35:SER:O	1:K:38:GLN:N	2.52	0.43
1:H:115:LEU:HD13	1:G:94:ILE:CG2	2.48	0.43
1:B:27:LEU:HD22	1:B:29:THR:H	1.83	0.43
1:L:14:LYS:HB3	1:L:70:MET:HE1	2.01	0.43
1:C:97:GLU:O	1:C:98:PHE:C	2.56	0.43
1:K:74:ILE:C	1:K:76:ALA:N	2.71	0.43
1:H:54:VAL:O	1:H:58:ILE:HG12	2.18	0.43
1:H:20:LYS:HA	1:H:23:ARG:HD2	2.01	0.43
2:J:14:DC:H2"	2:J:15:DA:N7	2.33	0.43
1:H:9:LEU:HD13	1:H:13:TRP:HE1	1.83	0.43
1:D:92:LYS:HE3	1:C:101:TRP:CZ3	2.53	0.43
2:J:7:DA:C2	2:J:8:DC:N3	2.86	0.43
1:B:119:ILE:O	1:B:123:ILE:HD12	2.19	0.43
1:G:4:GLN:O	1:G:82:PHE:HE1	2.00	0.43
1:L:94:ILE:HG23	1:K:115:LEU:HD13	2.00	0.43
1:D:146:LEU:HD23	1:D:146:LEU:HA	1.76	0.43
1:C:55:ASN:OD1	1:C:58:ILE:HD12	2.19	0.43
1:L:71:LYS:HE2	2:P:3:DC:OP2	2.19	0.43
1:B:35:SER:C	1:B:37:ALA:H	2.22	0.43
1:H:9:LEU:C	1:H:9:LEU:HD12	2.39	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:146:LEU:HD22	1:D:149:LYS:HZ2	1.83	0.43
2:N:7:DA:C2	2:N:8:DC:C4	3.07	0.43
2:F:14:DC:H2"	2:F:15:DA:C8	2.53	0.43
1:A:15:TRP:C	1:A:17:TYR:N	2.72	0.43
1:A:17:TYR:C	1:A:17:TYR:CD1	2.92	0.43
1:D:136:MET:HG2	1:C:136:MET:HG3	2.01	0.43
1:D:58:ILE:O	1:D:62:MET:HB3	2.19	0.43
1:A:15:TRP:O	1:A:17:TYR:N	2.52	0.43
1:B:128:ASN:HA	1:B:131:LYS:NZ	2.33	0.43
1:L:2:LYS:C	1:L:3:TYR:HD2	2.22	0.43
1:L:90:ARG:HH11	1:L:90:ARG:HG2	1.84	0.43
1:H:129:LYS:HD3	1:G:125:ASP:CA	2.49	0.42
2:N:16:DC:H4'	1:H:110:ARG:CZ	2.49	0.42
1:L:18:LEU:HD22	1:L:18:LEU:N	2.33	0.42
1:H:136:MET:O	1:H:140:LYS:HG3	2.19	0.42
2:J:7:DA:H2"	2:J:8:DC:C5'	2.36	0.42
3:E:7:DA:O5'	1:C:115:LEU:HD12	2.19	0.42
1:K:110:ARG:HH11	1:K:110:ARG:CB	2.32	0.42
1:B:9:LEU:CD1	1:B:10:GLU:H	2.21	0.42
1:L:117:GLU:HA	1:L:120:VAL:HG23	2.00	0.42
1:L:114:THR:HG23	1:L:117:GLU:OE2	2.19	0.42
1:D:146:LEU:CD2	1:D:149:LYS:HZ1	2.32	0.42
1:B:119:ILE:HG13	1:B:119:ILE:H	1.69	0.42
1:A:28:ILE:O	1:A:63:ASN:N	2.51	0.42
1:A:44:LEU:HD23	1:A:57:TRP:CD2	2.55	0.42
1:H:82:PHE:C	1:H:84:ALA:N	2.72	0.42
1:D:18:LEU:HD21	1:D:57:TRP:CZ3	2.54	0.42
1:H:119:ILE:HG22	1:H:123:ILE:CD1	2.49	0.42
1:A:15:TRP:CZ3	1:A:19:VAL:HG21	2.55	0.42
3:O:7:DA:C2	3:O:8:DC:C4	3.08	0.42
1:B:134:ASN:O	1:B:137:SER:N	2.52	0.42
1:L:110:ARG:HD2	1:L:110:ARG:O	2.19	0.42
1:H:4:GLN:OE1	1:H:6:LEU:HG	2.19	0.42
1:D:80:ARG:O	1:D:81:HIS:C	2.55	0.42
1:K:5:GLN:HB2	1:K:5:GLN:HE21	1.63	0.42
1:B:45:LEU:HD23	1:B:45:LEU:O	2.19	0.42
1:H:94:ILE:N	1:H:94:ILE:HD13	2.34	0.42
2:P:13:DT:OP1	1:K:21:LYS:HE3	2.20	0.42
1:H:28:ILE:O	1:H:63:ASN:HB2	2.20	0.42
1:B:29:THR:N	1:B:63:ASN:HB2	2.34	0.42
1:B:33:GLU:CG	1:B:36:ALA:HB2	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:23:ARG:HG2	1:G:23:ARG:NH1	2.33	0.42
1:C:64:PRO:O	1:C:67:VAL:HG23	2.19	0.42
1:G:116:SER:O	1:G:120:VAL:HG23	2.20	0.42
3:I:7:DA:C3'	3:I:8:DC:H5"	2.45	0.42
2:J:6:DG:C6	2:J:7:DA:C6	3.07	0.42
1:L:74:ILE:HD13	1:L:74:ILE:HA	1.88	0.42
3:O:7:DA:C6	3:O:8:DC:N4	2.88	0.42
1:B:46:SER:C	1:B:48:GLU:N	2.73	0.42
1:A:17:TYR:HE2	1:A:73:THR:HB	1.84	0.42
1:K:63:ASN:OD1	1:K:65:GLU:HG2	2.20	0.42
1:B:7:GLU:OE2	1:B:7:GLU:N	2.53	0.42
1:B:50:GLU:CB	1:B:53:LEU:HD12	2.50	0.42
1:K:12:GLY:C	1:K:16:LYS:HE3	2.40	0.42
1:D:107:LEU:HG	1:D:110:ARG:HH21	1.84	0.42
1:L:30:ARG:HB3	1:L:62:MET:C	2.39	0.42
1:C:40:ALA:HB1	1:C:57:TRP:HH2	1.84	0.42
1:C:3:TYR:OH	1:C:79:LYS:HE2	2.20	0.42
1:D:58:ILE:O	1:D:59:ASP:C	2.57	0.42
1:A:3:TYR:HB3	1:A:82:PHE:CE2	2.55	0.42
1:C:114:THR:O	1:C:115:LEU:C	2.58	0.42
1:K:105:ALA:O	1:K:106:GLY:C	2.57	0.42
3:E:3:DC:C2'	1:C:75:ARG:HD2	2.50	0.42
1:B:31:TYR:C	1:B:33:GLU:H	2.24	0.42
1:K:18:LEU:HD13	1:K:57:TRP:CZ3	2.55	0.42
1:H:3:TYR:CE2	1:H:79:LYS:HG3	2.55	0.42
1:G:51:PRO:O	1:G:54:VAL:HG23	2.20	0.42
1:C:4:GLN:H	1:C:4:GLN:HG3	1.69	0.42
1:L:32:ILE:HG23	1:L:33:GLU:N	2.35	0.42
1:G:122:LEU:O	1:G:126:ALA:N	2.47	0.42
1:D:109:GLN:O	1:D:110:ARG:C	2.58	0.42
1:G:47:LEU:HA	1:G:50:GLU:OE1	2.19	0.42
1:C:51:PRO:HA	1:C:54:VAL:HG21	2.01	0.42
1:H:4:GLN:HG3	1:H:82:PHE:CZ	2.55	0.42
1:D:118:THR:O	1:D:119:ILE:C	2.58	0.41
2:P:3:DC:N4	3:O:16:DC:N4	2.67	0.41
2:P:15:DA:H2"	2:P:16:DC:O5'	2.20	0.41
1:G:139:LEU:HG	1:G:143:LEU:CD1	2.47	0.41
1:A:48:GLU:HG3	1:A:49:ASN:OD1	2.20	0.41
1:L:42:ASP:HA	1:L:45:LEU:HB2	2.01	0.41
1:G:96:LEU:HD13	1:G:100:VAL:HG12	2.02	0.41
1:B:126:ALA:HA	1:A:126:ALA:HA	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:15:DA:C6	3:I:16:DC:N4	2.88	0.41
3:E:5:DT:OP2	1:C:79:LYS:CE	2.68	0.41
1:D:11:SER:HB2	1:D:51:PRO:CB	2.50	0.41
1:L:111:ARG:O	1:L:112:GLY:C	2.58	0.41
1:L:78:ARG:HH11	1:L:78:ARG:HG3	1.85	0.41
1:H:117:GLU:O	1:H:120:VAL:HB	2.21	0.41
1:A:87:GLN:CG	1:A:88:HIS:N	2.75	0.41
2:N:5:DT:H2"	2:N:6:DG:C8	2.55	0.41
3:M:7:DA:H2"	3:M:8:DC:C5'	2.22	0.41
3:O:3:DC:H2"	3:O:4:DG:O5'	2.20	0.41
1:K:30:ARG:HA	1:K:63:ASN:HA	2.02	0.41
1:B:10:GLU:HA	1:B:13:TRP:CE3	2.55	0.41
1:K:10:GLU:HA	1:K:13:TRP:CZ3	2.55	0.41
1:D:107:LEU:HA	1:D:110:ARG:NE	2.36	0.41
1:H:104:LEU:HD13	1:H:115:LEU:HD21	2.02	0.41
1:B:72:GLN:HA	1:B:75:ARG:HG3	2.01	0.41
1:D:77:ARG:NH1	3:E:12:DG:OP2	2.52	0.41
2:F:9:DA:H2"	2:F:10:DT:H5'	2.03	0.41
1:A:114:THR:HG22	1:A:115:LEU:N	2.35	0.41
1:L:18:LEU:H	1:L:18:LEU:HD22	1.85	0.41
1:C:22:HIS:HB2	1:C:28:ILE:CD1	2.49	0.41
1:B:127:GLU:O	1:B:131:LYS:N	2.54	0.41
1:K:77:ARG:O	1:K:77:ARG:HG3	2.21	0.41
1:G:104:LEU:O	1:G:106:GLY:N	2.54	0.41
2:N:9:DA:C1'	2:N:10:DT:H5"	2.51	0.41
2:N:13:DT:H2"	2:N:14:DC:O5'	2.21	0.41
1:D:136:MET:HA	1:D:139:LEU:HD13	2.02	0.41
1:G:63:ASN:O	1:G:67:VAL:HG23	2.21	0.41
1:G:87:GLN:HA	1:G:87:GLN:HE21	1.84	0.41
1:H:98:PHE:CE2	1:G:87:GLN:OE1	2.74	0.41
1:G:104:LEU:C	1:G:106:GLY:H	2.24	0.41
1:B:1:MET:O	1:B:1:MET:HG2	2.21	0.41
2:P:12:DG:C2	2:P:13:DT:O2	2.73	0.41
1:K:44:LEU:C	1:K:46:SER:N	2.74	0.41
1:G:17:TYR:O	1:G:20:LYS:HB3	2.21	0.41
1:L:31:TYR:CD1	1:L:31:TYR:N	2.88	0.41
1:D:129:LYS:HD3	1:D:130:GLU:N	2.36	0.41
1:B:138:SER:O	1:B:142:ASP:OD2	2.39	0.41
1:D:143:LEU:HD12	1:D:144:GLN:H	1.83	0.41
1:D:53:LEU:HD13	1:D:53:LEU:O	2.20	0.41
1:D:68:ASN:OD1	1:D:72:GLN:NE2	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:74:ILE:HG22	1:L:75:ARG:N	2.36	0.41
1:G:69:ARG:NH1	1:G:69:ARG:CG	2.81	0.41
1:H:137:SER:HA	1:H:140:LYS:CE	2.50	0.41
1:D:83:ASN:O	1:D:89:THR:OG1	2.38	0.41
1:H:115:LEU:O	1:H:116:SER:C	2.59	0.41
1:H:94:ILE:HG22	1:H:95:ASP:H	1.85	0.41
1:B:1:MET:N	2:N:4:DG:H5'	2.36	0.41
2:F:15:DA:C5	2:F:16:DC:N4	2.88	0.41
1:G:125:ASP:O	1:G:126:ALA:C	2.47	0.41
1:A:51:PRO:HG2	1:A:52:VAL:H	1.85	0.41
2:P:12:DG:C1'	2:P:13:DT:H5"	2.50	0.41
2:P:11:DT:H73	1:K:80:ARG:HD2	2.02	0.41
1:B:136:MET:O	1:B:140:LYS:HB2	2.21	0.41
1:B:114:THR:HG23	1:B:117:GLU:OE1	2.20	0.41
1:A:33:GLU:O	1:A:33:GLU:HG2	2.21	0.41
1:K:125:ASP:O	1:K:128:ASN:N	2.49	0.41
1:A:38:GLN:NE2	1:A:38:GLN:HA	2.35	0.41
1:D:94:ILE:HG23	1:C:115:LEU:CD1	2.50	0.41
1:K:74:ILE:O	1:K:76:ALA:N	2.54	0.41
1:B:118:THR:HG22	1:B:119:ILE:N	2.35	0.40
1:B:73:THR:O	1:B:76:ALA:HB3	2.22	0.40
1:B:73:THR:OG1	3:M:12:DG:C2'	2.69	0.40
1:D:114:THR:HG22	1:D:117:GLU:OE1	2.21	0.40
1:H:50:GLU:O	1:H:54:VAL:CG2	2.68	0.40
1:K:17:TYR:C	1:K:17:TYR:CD2	2.94	0.40
2:P:19:DA:C8	2:P:19:DA:H5'	2.56	0.40
1:L:14:LYS:O	1:L:18:LEU:HD22	2.21	0.40
1:K:104:LEU:CD1	1:K:118:THR:HG21	2.51	0.40
1:A:19:VAL:HG12	1:A:23:ARG:NH2	2.36	0.40
1:H:30:ARG:HA	1:H:63:ASN:HA	2.03	0.40
1:H:31:TYR:CD1	1:H:37:ALA:HB2	2.56	0.40
1:A:31:TYR:OH	1:A:61:HIS:HA	2.22	0.40
1:C:131:LYS:O	1:C:135:LYS:N	2.35	0.40
1:B:1:MET:H2	2:N:4:DG:H5'	1.86	0.40
2:N:7:DA:C6	2:N:8:DC:N4	2.90	0.40
1:L:126:ALA:CB	1:K:122:LEU:HD22	2.51	0.40
3:O:16:DC:H2"	3:O:17:DG:C8	2.57	0.40
1:C:73:THR:O	1:C:76:ALA:HB3	2.21	0.40
1:D:107:LEU:CG	1:D:110:ARG:HH21	2.34	0.40
1:G:76:ALA:O	1:G:79:LYS:N	2.54	0.40
1:A:147:LEU:HD12	1:A:148:GLY:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:107:LEU:O	1:L:111:ARG:HB2	2.22	0.40
1:K:86:HIS:O	1:K:90:ARG:CG	2.67	0.40
1:L:101:TRP:CZ2	2:P:8:DC:OP1	2.68	0.40
1:H:129:LYS:HG3	1:G:128:ASN:C	2.42	0.40
1:B:61:HIS:O	1:B:62:MET:HB2	2.20	0.40
1:B:44:LEU:O	1:B:47:LEU:HB2	2.22	0.40
1:G:28:ILE:CG2	1:G:28:ILE:O	2.63	0.40
1:B:15:TRP:CD2	1:B:19:VAL:HG21	2.57	0.40
1:A:129:LYS:O	1:A:133:ALA:HB2	2.21	0.40
1:C:79:LYS:HD3	1:C:83:ASN:HD21	1.85	0.40
1:C:27:LEU:HD22	1:C:29:THR:O	2.21	0.40
1:C:39:GLU:O	1:C:43:VAL:HG23	2.21	0.40
1:C:6:LEU:HA	1:C:6:LEU:HD23	1.94	0.40
1:G:102:GLN:C	1:G:104:LEU:N	2.75	0.40
1:G:102:GLN:O	1:G:104:LEU:N	2.55	0.40
2:J:9:DA:OP1	1:G:92:LYS:HD2	2.21	0.40
1:D:119:ILE:O	1:D:122:LEU:HB2	2.22	0.40
2:P:6:DG:H2"	2:P:7:DA:H8	1.86	0.40
3:E:1:DT:H2"	3:E:2:DT:O5'	2.21	0.40
1:H:63:ASN:OD1	1:H:64:PRO:HD2	2.21	0.40
1:G:87:GLN:C	1:G:89:THR:N	2.75	0.40
1:H:147:LEU:O	1:H:147:LEU:HD12	2.21	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
1	A	147/150 (98%)	110 (75%)	33 (22%)	4 (3%)	6 46
1	B	146/150 (97%)	107 (73%)	31 (21%)	8 (6%)	2 26
1	C	146/150 (97%)	116 (80%)	26 (18%)	4 (3%)	6 46

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	D	147/150 (98%)	121 (82%)	22 (15%)	4 (3%)	6 46
1	G	146/150 (97%)	105 (72%)	31 (21%)	10 (7%)	1 21
1	H	146/150 (97%)	108 (74%)	28 (19%)	10 (7%)	1 21
1	K	146/150 (97%)	103 (70%)	31 (21%)	12 (8%)	1 15
1	L	147/150 (98%)	112 (76%)	28 (19%)	7 (5%)	3 30
All	All	1171/1200 (98%)	882 (75%)	230 (20%)	59 (5%)	3 29

All (59) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	41	VAL
1	B	51	PRO
1	B	85	GLU
1	A	85	GLU
1	C	58	ILE
1	H	85	GLU
1	H	113	LYS
1	G	85	GLU
1	G	126	ALA
1	L	8	ASN
1	L	51	PRO
1	L	116	SER
1	K	34	ALA
1	K	113	LYS
1	B	36	ALA
1	B	48	GLU
1	A	51	PRO
1	A	102	GLN
1	D	60	LYS
1	D	86	HIS
1	C	147	LEU
1	H	47	LEU
1	H	101	TRP
1	G	25	GLY
1	G	35	SER
1	L	112	GLY
1	K	45	LEU
1	K	47	LEU
1	K	71	LYS
1	K	82	PHE

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Mol	Chain	Res	Type
1	K	90	ARG
1	K	102	GLN
1	H	8	ASN
1	H	49	ASN
1	H	115	LEU
1	G	82	PHE
1	G	88	HIS
1	K	20	LYS
1	K	104	LEU
1	B	34	ALA
1	C	23	ARG
1	G	102	GLN
1	G	117	GLU
1	L	47	LEU
1	L	48	GLU
1	B	47	LEU
1	D	85	GLU
1	L	27	LEU
1	K	81	HIS
1	B	25	GLY
1	D	68	ASN
1	H	81	HIS
1	K	86	HIS
1	A	99	ILE
1	H	52	VAL
1	C	67	VAL
1	H	58	ILE
1	G	32	ILE
1	G	100	VAL

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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
1	A	131/133 (98%)	106 (81%)	25 (19%)	2 12
1	B	130/133 (98%)	112 (86%)	18 (14%)	4 28

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	C	129/133 (97%)	116 (90%)	13 (10%)	9 43
1	D	130/133 (98%)	112 (86%)	18 (14%)	4 28
1	G	129/133 (97%)	110 (85%)	19 (15%)	4 25
1	H	130/133 (98%)	113 (87%)	17 (13%)	5 29
1	K	130/133 (98%)	113 (87%)	17 (13%)	5 29
1	L	131/133 (98%)	114 (87%)	17 (13%)	5 30
All	All	1040/1064 (98%)	896 (86%)	144 (14%)	4 28

All (144) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	7	GLU
1	B	9	LEU
1	B	27	LEU
1	B	30	ARG
1	B	35	SER
1	B	49	ASN
1	B	64	PRO
1	B	71	LYS
1	B	77	ARG
1	B	88	HIS
1	B	90	ARG
1	B	95	ASP
1	B	96	LEU
1	B	104	LEU
1	B	115	LEU
1	B	131	LYS
1	B	138	SER
1	B	146	LEU
1	A	5	GLN
1	A	13	TRP
1	A	17	TYR
1	A	18	LEU
1	A	23	ARG
1	A	27	LEU
1	A	33	GLU
1	A	49	ASN
1	A	60	LYS
1	A	65	GLU
1	A	68	ASN

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Mol	Chain	Res	Type
1	A	69	ARG
1	A	80	ARG
1	A	83	ASN
1	A	87	GLN
1	A	94	ILE
1	A	102	GLN
1	A	103	ARG
1	A	115	LEU
1	A	116	SER
1	A	117	GLU
1	A	119	ILE
1	A	122	LEU
1	A	131	LYS
1	A	149	LYS
1	D	22	HIS
1	D	27	LEU
1	D	53	LEU
1	D	60	LYS
1	D	61	HIS
1	D	62	MET
1	D	63	ASN
1	D	77	ARG
1	D	87	GLN
1	D	107	LEU
1	D	109	GLN
1	D	110	ARG
1	D	115	LEU
1	D	118	THR
1	D	132	TYR
1	D	136	MET
1	D	141	GLN
1	D	149	LYS
1	C	4	GLN
1	C	7	GLU
1	C	27	LEU
1	C	44	LEU
1	C	61	HIS
1	C	79	LYS
1	C	82	PHE
1	C	92	LYS
1	C	109	GLN
1	C	115	LEU

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Mol	Chain	Res	Type
1	C	118	THR
1	C	129	LYS
1	C	146	LEU
1	H	4	GLN
1	H	24	GLU
1	H	26	GLU
1	H	42	ASP
1	H	58	ILE
1	H	72	GLN
1	H	86	HIS
1	H	88	HIS
1	H	94	ILE
1	H	97	GLU
1	H	104	LEU
1	H	107	LEU
1	H	115	LEU
1	H	118	THR
1	H	125	ASP
1	H	141	GLN
1	H	147	LEU
1	G	4	GLN
1	G	15	TRP
1	G	26	GLU
1	G	30	ARG
1	G	39	GLU
1	G	50	GLU
1	G	59	ASP
1	G	65	GLU
1	G	74	ILE
1	G	87	GLN
1	G	88	HIS
1	G	90	ARG
1	G	92	LYS
1	G	102	GLN
1	G	125	ASP
1	G	129	LYS
1	G	132	TYR
1	G	136	MET
1	G	146	LEU
1	L	27	LEU
1	L	30	ARG
1	L	45	LEU

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Mol	Chain	Res	Type
1	L	63	ASN
1	L	65	GLU
1	L	78	ARG
1	L	87	GLN
1	L	96	LEU
1	L	99	ILE
1	L	103	ARG
1	L	104	LEU
1	L	107	LEU
1	L	113	LYS
1	L	114	THR
1	L	132	TYR
1	L	134	ASN
1	L	149	LYS
1	K	5	GLN
1	K	10	GLU
1	K	28	ILE
1	K	29	THR
1	K	30	ARG
1	K	33	GLU
1	K	53	LEU
1	K	61	HIS
1	K	77	ARG
1	K	95	ASP
1	K	102	GLN
1	K	111	ARG
1	K	114	THR
1	K	115	LEU
1	K	116	SER
1	K	128	ASN
1	K	138	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	4	GLN
1	B	5	GLN
1	B	55	ASN
1	B	63	ASN
1	B	72	GLN
1	B	128	ASN
1	A	38	GLN

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Mol	Chain	Res	Type
1	A	55	ASN
1	A	72	GLN
1	A	81	HIS
1	A	86	HIS
1	A	87	GLN
1	A	102	GLN
1	A	128	ASN
1	A	134	ASN
1	A	141	GLN
1	A	144	GLN
1	D	5	GLN
1	D	38	GLN
1	D	63	ASN
1	D	72	GLN
1	D	87	GLN
1	D	141	GLN
1	C	4	GLN
1	C	5	GLN
1	C	63	ASN
1	C	134	ASN
1	H	38	GLN
1	H	87	GLN
1	H	141	GLN
1	G	4	GLN
1	G	5	GLN
1	G	38	GLN
1	G	68	ASN
1	G	83	ASN
1	G	109	GLN
1	G	121	GLN
1	G	141	GLN
1	L	38	GLN
1	L	63	ASN
1	L	72	GLN
1	L	109	GLN
1	L	141	GLN
1	K	4	GLN
1	K	5	GLN
1	K	38	GLN
1	K	72	GLN
1	K	81	HIS
1	K	83	ASN

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Mol	Chain	Res	Type
1	K	128	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

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

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	A	149/150 (99%)	-0.40	0 100 100	78, 144, 185, 200	0
1	B	148/150 (98%)	-0.31	2 (1%) 78 69	76, 133, 176, 189	0
1	C	148/150 (98%)	-0.33	1 (0%) 89 83	78, 155, 198, 200	0
1	D	149/150 (99%)	-0.29	0 100 100	86, 161, 200, 200	0
1	G	148/150 (98%)	-0.37	2 (1%) 78 69	96, 154, 193, 200	0
1	H	148/150 (98%)	-0.42	1 (0%) 89 83	95, 162, 199, 200	0
1	K	148/150 (98%)	-0.36	1 (0%) 89 83	76, 127, 173, 184	0
1	L	149/150 (99%)	-0.28	1 (0%) 89 83	85, 158, 199, 200	0
2	F	19/19 (100%)	-0.74	0 100 100	101, 127, 163, 175	0
2	J	19/19 (100%)	-0.67	0 100 100	97, 127, 172, 176	0
2	N	19/19 (100%)	-0.72	0 100 100	98, 128, 191, 196	0
2	P	19/19 (100%)	-0.68	0 100 100	106, 121, 186, 194	0
3	E	19/19 (100%)	-0.65	0 100 100	94, 136, 178, 189	0
3	I	19/19 (100%)	-0.71	0 100 100	98, 133, 176, 177	0
3	M	19/19 (100%)	-0.67	0 100 100	92, 127, 170, 193	0
3	O	19/19 (100%)	-0.74	0 100 100	91, 145, 199, 200	0
All	All	1339/1352 (99%)	-0.38	8 (0%) 90 85	76, 146, 198, 200	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	143	LEU	2.5
1	B	28	ILE	2.4
1	B	95	ASP	2.3
1	K	94	ILE	2.2
1	G	94	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	146	LEU	2.1
1	G	143	LEU	2.1
1	L	96	LEU	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.