Full wwPDB X-ray Structure Validation Report ⓘ

Aug 23, 2023 – 12:39 AM EDT

PDB ID	:	3E3J
Title	:	Crystal Structure of an Intermediate Complex of T7 RNAP and 8nt of RNA
Authors	:	Durniak, K.J.; Bailey, S.; Steitz, T.A.
Deposited on	:	2008-08-07
Resolution	:	6.70 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:

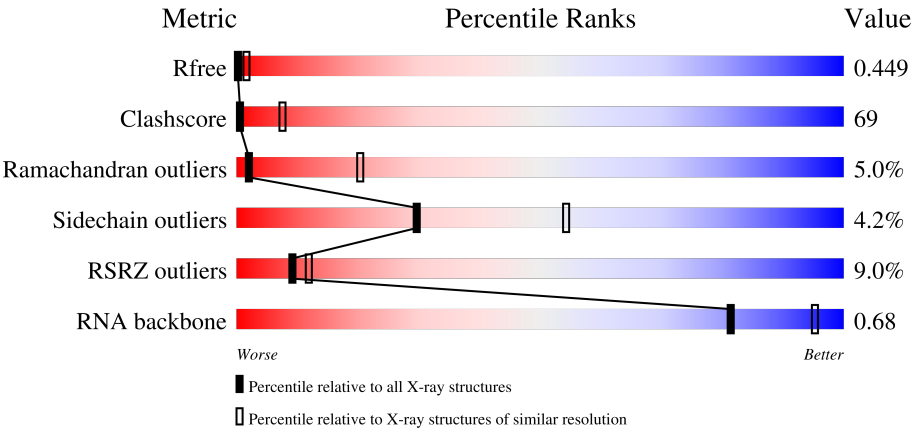
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 6.70 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}	130704	1002 (9.50-3.90)
Clashscore	141614	1066 (9.50-3.90)
Ramachandran outliers	138981	1000 (9.50-3.90)
Sidechain outliers	138945	1000 (9.50-3.86)
RSRZ outliers	127900	1004 (9.50-3.80)
RNA backbone	3102	1078 (10.00-3.00)

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	889	8% 52% 35% 6% • 6%
1	C	889	7% 57% 32% 5% 6%
2	T	32	9% 19% 47% 22% 12%
2	X	32	16% 6% 81% 12%

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Mol	Chain	Length	Quality of chain
3	N	32	25% 28% 9% 38%
3	Y	32	12% 38% 12% 38%
4	R	8	75% 12% 88%
4	Z	8	62% 12% 88%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 15406 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 DNA-directed RNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	833	Total	C	N	O	S	0	0	0
			6567	4191	1133	1207	36			
1	B	833	Total	C	N	O	S	0	0	0
			6545	4176	1126	1206	37			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-5	HIS	-	expression tag	UNP P00573
C	-4	HIS	-	expression tag	UNP P00573
C	-3	HIS	-	expression tag	UNP P00573
C	-2	HIS	-	expression tag	UNP P00573
C	-1	HIS	-	expression tag	UNP P00573
C	0	HIS	-	expression tag	UNP P00573
C	266	LEU	PRO	engineered mutation	UNP P00573
B	-5	HIS	-	expression tag	UNP P00573
B	-4	HIS	-	expression tag	UNP P00573
B	-3	HIS	-	expression tag	UNP P00573
B	-2	HIS	-	expression tag	UNP P00573
B	-1	HIS	-	expression tag	UNP P00573
B	0	HIS	-	expression tag	UNP P00573
B	266	LEU	PRO	engineered mutation	UNP P00573

- Molecule 2 is a DNA chain called DNA (28-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	T	28	Total	C	N	O	P	0	0	0
			569	273	93	175	28			
2	X	28	Total	C	N	O	P	0	0	0
			569	273	93	175	28			

- Molecule 3 is a DNA chain called DNA (5'-D(*DTP*DAP*DAP*DTP*DAP*DCP*DGP*DAP*DCP*DTP*DCP*DAP*DCP*DTP*DAP*DTP*DAP*DTP*DTP*DTP*DCP*DTP*

DGP*DCP*DCP*DAP*DAP*DAP*DCP*DGP*DGP*DC)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	N	20	Total	C	N	O	P	0	0	0
			404	194	79	112	19			
3	Y	20	Total	C	N	O	P	0	0	0
			404	194	79	112	19			

- Molecule 4 is a RNA chain called RNA (5'-R(*GP*GP*GP*AP*GP*UP*AP*A)-3').

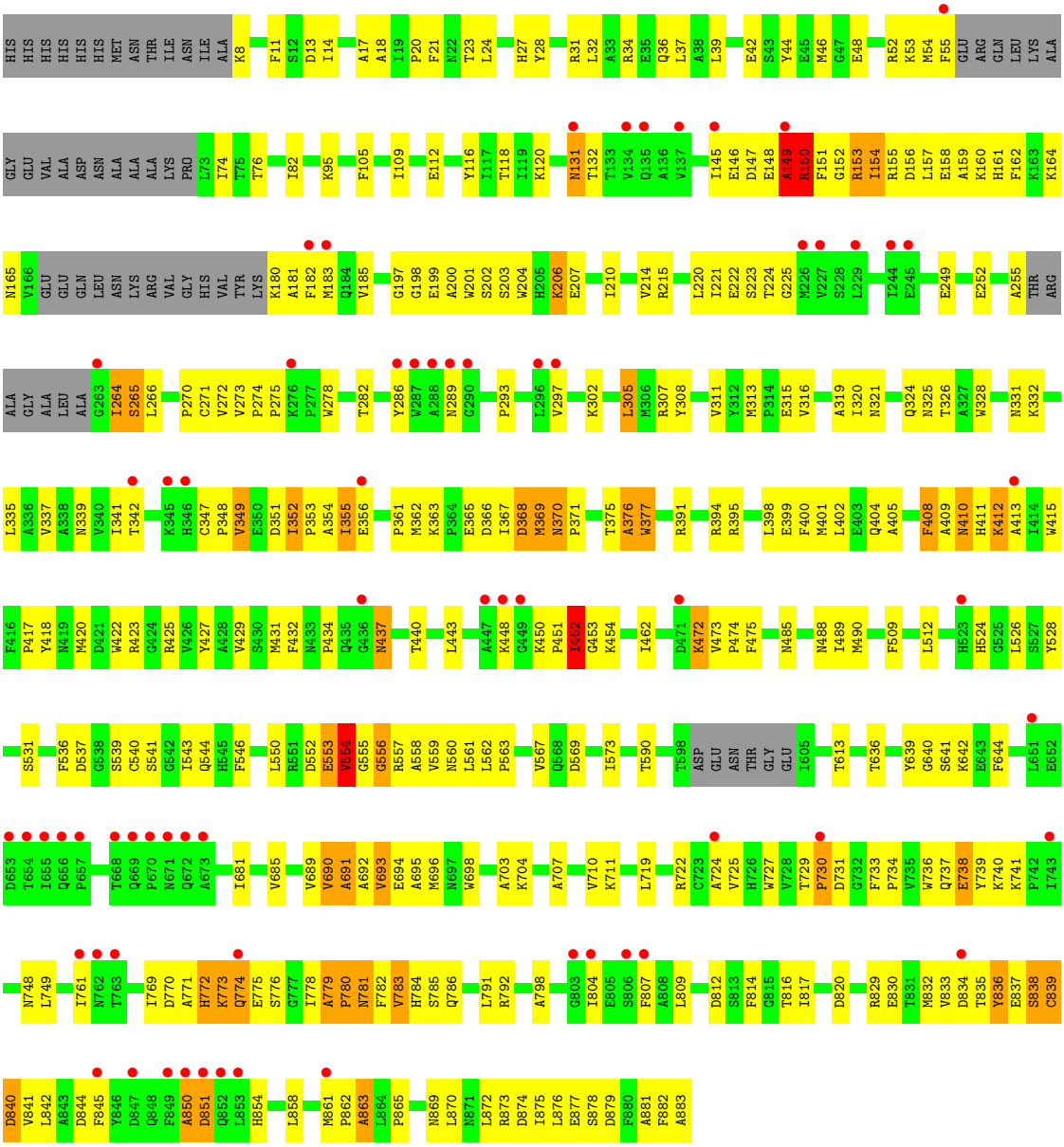
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	R	8	Total	C	N	O	P	0	0	0
			174	79	37	51	7			
4	Z	8	Total	C	N	O	P	0	0	0
			174	79	37	51	7			

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: DNA-directed RNA polymerase

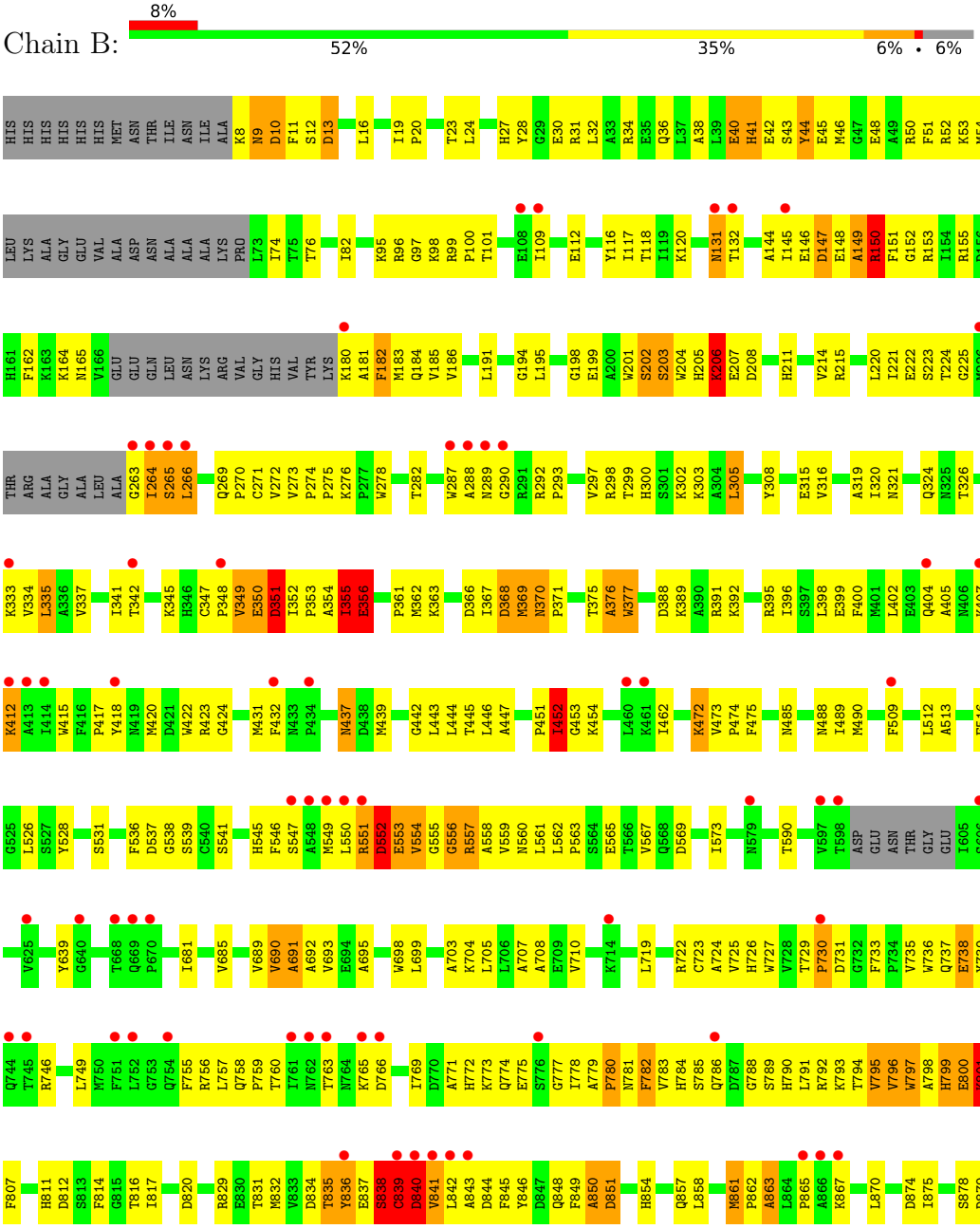
Chain C:



WORLDWIDE PDB PROTEIN DATA BANK

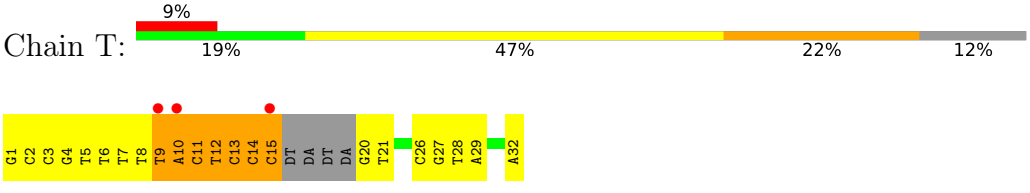
• Molecule 1: DNA-directed RNA polymerase

Chain B:



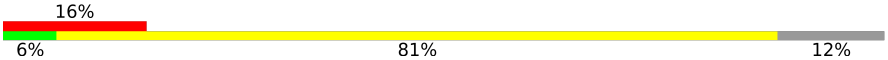
• Molecule 2: DNA (28-MER)

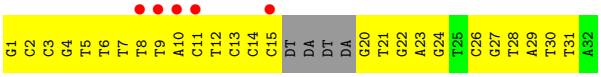
Chain T:



• Molecule 2: DNA (28-MER)

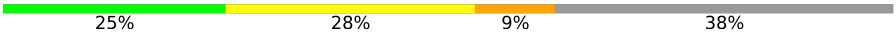
Chain X:

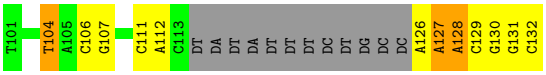




• Molecule 3: DNA (5'-D(*DTP*DAP*DAP*DTP*DAP*DCP*DGP*DAP*DCP*DTP*DCP*DAP*DCP*DTP*DAP*DTP*DAP*DTP*DTP*DTP*DCP*DTP*DGP*DCP*DCP*DAP*DAP*DAP*DCP*DGP*DGP*DC)-3')

Chain N:



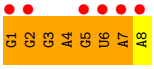


• Molecule 3: DNA (5'-D(*DTP*DAP*DAP*DTP*DAP*DCP*DGP*DAP*DCP*DTP*DCP*DAP*DCP*DTP*DAP*DTP*DAP*DTP*DTP*DTP*DCP*DTP*DGP*DCP*DCP*DAP*DAP*DAP*DCP*DGP*DGP*DC)-3')

Chain Y:

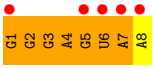
• Molecule 4: RNA (5'-R(*GP*GP*GP*AP*GP*UP*AP*A)-3')

Chain R:



• Molecule 4: RNA (5'-R(*GP*GP*GP*AP*GP*UP*AP*A)-3')

Chain Z:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	99.22Å 180.60Å 198.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.81 – 6.70 49.82 – 6.70	Depositor EDS
% Data completeness (in resolution range)	87.2 (49.81-6.70) 88.3 (49.82-6.70)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.50 (at 6.68Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.392 , 0.454 0.390 , 0.449	Depositor DCC
R_{free} test set	274 reflections (4.56%)	wwPDB-VP
Wilson B-factor (Å^2)	305.5	Xtriage
Anisotropy	0.170	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.25 , 44.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.76	EDS
Total number of atoms	15406	wwPDB-VP
Average B, all atoms (Å^2)	94.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.00% 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

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	B	0.34	0/6694	0.54	0/9055
1	C	0.34	0/6716	0.53	0/9082
2	T	1.10	6/633 (0.9%)	1.46	15/972 (1.5%)
2	X	0.74	0/633	1.10	0/972
3	N	0.88	2/453 (0.4%)	1.10	1/694 (0.1%)
3	Y	0.88	3/453 (0.7%)	1.11	1/694 (0.1%)
4	R	1.03	1/196 (0.5%)	2.15	14/306 (4.6%)
4	Z	1.02	1/196 (0.5%)	2.15	14/306 (4.6%)
All	All	0.49	13/15974 (0.1%)	0.76	45/22081 (0.2%)

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	C	0	2
All	All	0	3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	R	6	U	C1'-N1	6.94	1.59	1.48
2	T	15	DC	C1'-N1	6.93	1.58	1.49
2	T	11	DC	C1'-N1	6.91	1.58	1.49
2	T	13	DC	C1'-N1	6.91	1.58	1.49
2	T	14	DC	C1'-N1	6.90	1.58	1.49
2	T	12	DT	C1'-N1	6.89	1.58	1.49
2	T	9	DT	C1'-N1	6.79	1.58	1.49
4	Z	6	U	C1'-N1	6.79	1.58	1.48
3	N	127	DA	C1'-N9	-5.38	1.39	1.47
3	Y	126	DA	C1'-N9	-5.30	1.39	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	N	128	DA	C1'-N9	-5.25	1.40	1.47
3	Y	128	DA	C1'-N9	-5.16	1.40	1.47
3	Y	127	DA	C1'-N9	-5.13	1.40	1.47

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	Z	1	G	OP2-P-O3'	7.38	121.44	105.20
2	T	13	DC	OP2-P-O3'	7.25	121.16	105.20
4	Z	2	G	OP2-P-O3'	7.23	121.12	105.20
2	T	10	DA	OP2-P-O3'	7.23	121.11	105.20
4	R	6	U	OP2-P-O3'	7.22	121.09	105.20
2	T	9	DT	OP2-P-O3'	7.22	121.08	105.20
4	R	2	G	OP2-P-O3'	7.22	121.08	105.20
4	R	7	A	OP2-P-O3'	7.22	121.08	105.20
4	R	4	A	OP2-P-O3'	7.21	121.07	105.20
4	R	3	G	OP2-P-O3'	7.21	121.07	105.20
4	R	1	G	OP2-P-O3'	7.21	121.06	105.20
4	Z	3	G	OP2-P-O3'	7.20	121.05	105.20
4	Z	5	G	OP2-P-O3'	7.20	121.05	105.20
4	R	5	G	OP2-P-O3'	7.20	121.04	105.20
2	T	11	DC	OP2-P-O3'	7.20	121.04	105.20
4	Z	6	U	OP2-P-O3'	7.20	121.03	105.20
2	T	12	DT	OP2-P-O3'	7.19	121.02	105.20
4	Z	7	A	OP2-P-O3'	7.18	121.00	105.20
4	Z	4	A	OP2-P-O3'	7.17	120.97	105.20
2	T	14	DC	OP2-P-O3'	7.17	120.97	105.20
4	R	5	G	O3'-P-O5'	-6.81	91.07	104.00
4	R	1	G	O3'-P-O5'	-6.80	91.07	104.00
2	T	10	DA	O3'-P-O5'	-6.80	91.08	104.00
2	T	12	DT	O3'-P-O5'	-6.79	91.09	104.00
2	T	13	DC	O3'-P-O5'	-6.79	91.11	104.00
4	Z	7	A	O3'-P-O5'	-6.79	91.11	104.00
4	R	6	U	O3'-P-O5'	-6.78	91.11	104.00
4	Z	3	G	O3'-P-O5'	-6.78	91.11	104.00
4	Z	1	G	O3'-P-O5'	-6.78	91.12	104.00
4	R	2	G	O3'-P-O5'	-6.77	91.13	104.00
4	Z	4	A	O3'-P-O5'	-6.77	91.13	104.00
4	Z	5	G	O3'-P-O5'	-6.77	91.13	104.00
4	Z	6	U	O3'-P-O5'	-6.77	91.13	104.00
2	T	9	DT	O3'-P-O5'	-6.77	91.13	104.00
4	R	4	A	O3'-P-O5'	-6.77	91.14	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	R	3	G	O3'-P-O5'	-6.77	91.14	104.00
2	T	14	DC	O3'-P-O5'	-6.76	91.15	104.00
4	R	7	A	O3'-P-O5'	-6.76	91.15	104.00
2	T	11	DC	O3'-P-O5'	-6.76	91.16	104.00
4	Z	2	G	O3'-P-O5'	-6.75	91.18	104.00
2	T	9	DT	O4'-C1'-N1	5.71	112.00	108.00
3	Y	104	DT	C1'-O4'-C4'	-5.32	104.78	110.10
2	T	12	DT	O4'-C1'-N1	5.16	111.61	108.00
2	T	10	DA	O4'-C1'-N9	5.16	111.61	108.00
3	N	104	DT	C1'-O4'-C4'	-5.12	104.98	110.10

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	40	GLU	Mainchain
1	C	149	ALA	Peptide
1	C	150	ARG	Peptide

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	6545	0	6473	1142	1
1	C	6567	0	6519	776	2
2	T	569	0	321	126	6
2	X	569	0	321	96	7
3	N	404	0	223	28	4
3	Y	404	0	223	106	4
4	R	174	0	85	42	0
4	Z	174	0	86	21	0
All	All	15406	0	14251	2057	12

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 69.

All (2057) 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:B:28:TYR:CE1	1:B:182:PHE:HA	1.31	1.66
1:B:28:TYR:CD1	1:B:182:PHE:CB	1.77	1.64
1:C:724:ALA:CB	1:C:738:GLU:HB3	1.17	1.64
1:C:54:MET:CA	1:C:255:ALA:HB2	1.21	1.62
1:C:553:GLU:HB3	1:C:554:VAL:CG1	1.14	1.62
1:C:644:PHE:HB2	3:N:126:DA:C2	1.29	1.61
1:B:28:TYR:CD1	1:B:182:PHE:HB2	1.08	1.61
1:B:551:ARG:HD2	1:B:867:LYS:CG	1.19	1.60
1:B:28:TYR:CE1	1:B:182:PHE:CA	1.83	1.60
1:C:54:MET:CA	1:C:255:ALA:CB	1.77	1.59
1:C:727:TRP:CD1	1:C:782:PHE:CE1	1.90	1.59
1:B:707:ALA:CB	1:B:774:GLN:HB3	1.28	1.58
1:B:474:PRO:CA	1:B:880:PHE:CZ	1.85	1.58
1:B:474:PRO:HA	1:B:880:PHE:CZ	1.06	1.57
1:C:553:GLU:HB2	1:C:554:VAL:CG2	1.33	1.53
1:B:474:PRO:HA	1:B:880:PHE:CE1	1.04	1.53
1:C:727:TRP:CE2	1:C:782:PHE:CD1	1.92	1.53
1:C:722:ARG:CD	1:C:771:ALA:N	1.73	1.51
1:C:727:TRP:CG	1:C:782:PHE:HE1	1.28	1.51
1:B:553:GLU:HB3	1:B:554:VAL:CB	1.35	1.51
1:B:562:LEU:HD21	1:B:870:LEU:CD1	1.42	1.50
1:C:553:GLU:CA	1:C:554:VAL:HG22	1.35	1.49
1:B:28:TYR:HD1	1:B:182:PHE:CB	1.12	1.49
1:B:793:LYS:NZ	1:B:835:THR:HG23	1.21	1.49
1:B:735:VAL:CG1	1:B:785:SER:CB	1.87	1.48
1:C:553:GLU:N	1:C:554:VAL:HG22	1.17	1.47
1:C:722:ARG:NE	1:C:771:ALA:CB	1.76	1.47
1:B:96:ARG:NH1	3:Y:102:DA:C1'	1.75	1.47
1:B:698:TRP:CD1	1:B:861:MET:HE1	1.51	1.46
1:C:812:ASP:CG	4:R:8:A:H4'	1.29	1.46
1:B:44:TYR:CZ	1:B:155:ARG:HD2	1.46	1.46
1:C:780:PRO:HA	1:C:783:VAL:CG2	1.47	1.45
1:C:553:GLU:N	1:C:554:VAL:CG2	1.79	1.44
1:C:722:ARG:CG	1:C:771:ALA:HB2	1.48	1.44
1:C:639:TYR:CG	2:T:8:DT:C2	2.05	1.42
1:C:722:ARG:HD3	1:C:771:ALA:CA	1.46	1.42
2:T:6:DT:C2'	2:T:7:DT:H71	1.48	1.42
1:C:727:TRP:NE1	1:C:782:PHE:CE1	1.88	1.42
1:C:553:GLU:CB	1:C:554:VAL:CG2	1.95	1.41
1:B:475:PHE:CZ	1:B:879:ASP:O	1.72	1.41
1:B:793:LYS:NZ	1:B:835:THR:CG2	1.80	1.41
1:C:553:GLU:CB	1:C:554:VAL:HG22	1.49	1.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:735:VAL:HG11	1:B:785:SER:CB	0.92	1.40
1:B:562:LEU:CD2	1:B:870:LEU:CD1	1.97	1.40
1:C:781:ASN:HD21	2:T:9:DT:C4'	1.31	1.39
1:B:474:PRO:CA	1:B:880:PHE:CE1	1.91	1.39
1:C:21:PHE:CD1	1:C:161:HIS:HB3	1.58	1.39
1:B:146:GLU:N	1:B:148:GLU:HG3	1.37	1.39
1:C:776:SER:CB	2:T:7:DT:P	2.11	1.38
1:C:781:ASN:ND2	2:T:9:DT:H4'	1.33	1.38
1:B:705:LEU:HB3	1:B:857:GLN:NE2	1.38	1.38
1:B:354:ALA:HB1	1:B:355:ILE:C	1.38	1.38
1:B:145:ILE:C	1:B:148:GLU:HG3	1.43	1.38
1:B:147:ASP:HA	1:B:150:ARG:CB	1.54	1.37
1:B:698:TRP:CD1	1:B:861:MET:CE	2.07	1.37
1:C:776:SER:CB	2:T:7:DT:OP1	1.70	1.37
1:C:553:GLU:CB	1:C:554:VAL:CG1	2.01	1.37
1:B:793:LYS:HZ2	1:B:835:THR:CG2	1.37	1.36
1:C:836:TYR:C	1:C:872:LEU:HD13	1.41	1.36
1:B:562:LEU:CG	1:B:870:LEU:HD11	1.53	1.36
1:C:21:PHE:CD2	1:C:161:HIS:CD2	2.14	1.36
1:C:639:TYR:CZ	4:R:8:A:C2	2.13	1.35
1:B:772:HIS:NE2	3:Y:130:DG:H5"	1.39	1.35
1:B:96:ARG:NH1	3:Y:102:DA:H1'	1.02	1.34
1:B:727:TRP:CE2	1:B:782:PHE:HA	1.63	1.34
1:B:146:GLU:C	1:B:148:GLU:HB2	1.45	1.34
1:C:727:TRP:CE2	1:C:782:PHE:CE1	2.15	1.34
1:B:562:LEU:CG	1:B:870:LEU:CD1	2.04	1.33
1:C:722:ARG:CD	1:C:771:ALA:HB2	1.58	1.33
1:C:644:PHE:CB	3:N:126:DA:C2	2.12	1.33
1:B:551:ARG:CD	1:B:867:LYS:CG	2.04	1.33
1:B:729:THR:CG2	1:B:789:SER:HB3	1.56	1.33
1:B:704:LYS:O	1:B:775:GLU:CG	1.74	1.33
1:C:553:GLU:H	1:C:554:VAL:CG2	1.39	1.32
1:C:722:ARG:CD	1:C:771:ALA:CB	2.06	1.32
1:B:96:ARG:CG	3:Y:103:DA:H1'	1.59	1.32
1:B:475:PHE:CE2	1:B:879:ASP:O	1.79	1.32
1:B:149:ALA:N	1:B:150:ARG:HB2	1.41	1.32
1:C:553:GLU:CB	1:C:554:VAL:HG13	1.58	1.31
1:B:28:TYR:CE1	1:B:182:PHE:O	1.83	1.31
1:B:149:ALA:HB3	1:B:150:ARG:CB	1.58	1.30
1:B:551:ARG:CD	1:B:867:LYS:HG2	1.58	1.30
1:B:727:TRP:CZ2	1:B:782:PHE:CA	2.14	1.30

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:727:TRP:CZ2	1:B:782:PHE:HA	1.64	1.30
1:B:475:PHE:CD2	1:B:879:ASP:HB3	1.64	1.30
1:B:562:LEU:CD2	1:B:870:LEU:HD11	1.60	1.30
1:B:28:TYR:HE1	1:B:182:PHE:C	1.32	1.29
1:B:354:ALA:HA	1:B:355:ILE:CG1	1.62	1.29
1:B:727:TRP:NE1	1:B:785:SER:OG	1.64	1.29
1:B:850:ALA:CB	1:B:851:ASP:HB2	1.63	1.29
1:C:307:ARG:HB3	1:C:736:TRP:CH2	1.67	1.28
1:C:639:TYR:O	2:T:8:DT:H5"	1.24	1.28
1:B:707:ALA:HB2	1:B:774:GLN:C	1.50	1.28
1:C:639:TYR:CD2	2:T:8:DT:N3	2.00	1.27
1:C:850:ALA:CB	1:C:851:ASP:HB2	1.63	1.27
1:B:707:ALA:CB	1:B:774:GLN:CB	2.11	1.27
1:C:563:PRO:HD3	1:C:874:ASP:O	1.29	1.27
1:B:270:PRO:HD2	1:B:408:PHE:CE1	1.69	1.27
1:C:703:ALA:CB	1:C:778:ILE:HD13	1.62	1.26
1:C:836:TYR:O	1:C:872:LEU:HD13	1.29	1.26
1:B:28:TYR:CE1	1:B:182:PHE:C	2.07	1.26
1:B:723:CYS:O	1:B:774:GLN:CG	1.76	1.26
1:C:54:MET:N	1:C:255:ALA:CB	1.98	1.26
1:C:812:ASP:CG	4:R:8:A:C4'	2.04	1.26
1:C:812:ASP:OD2	4:R:8:A:O3'	1.55	1.25
1:C:722:ARG:HD3	1:C:771:ALA:N	0.94	1.25
1:C:812:ASP:OD1	4:R:8:A:C5'	1.83	1.25
1:B:55:PHE:CE1	1:B:74:ILE:HG21	1.71	1.25
1:B:704:LYS:O	1:B:775:GLU:HG2	1.23	1.25
1:C:724:ALA:CB	1:C:738:GLU:CB	2.14	1.25
1:B:28:TYR:HE1	1:B:182:PHE:CA	1.28	1.25
1:C:776:SER:HB3	2:T:7:DT:O5'	1.16	1.24
1:B:149:ALA:CA	1:B:150:ARG:HB2	1.65	1.24
1:C:639:TYR:OH	4:R:8:A:C2	1.87	1.24
1:B:109:ILE:CD1	1:B:148:GLU:OE2	1.85	1.24
1:C:556:GLY:HA2	1:C:558:ALA:N	1.53	1.23
1:B:424:GLY:CA	1:B:792:ARG:NH1	2.01	1.23
1:C:316:VAL:HG22	1:C:731:ASP:OD2	1.31	1.23
1:C:307:ARG:HD3	1:C:736:TRP:CE2	1.71	1.23
1:B:28:TYR:CD1	1:B:182:PHE:HA	1.71	1.22
1:C:552:ASP:HB3	1:C:555:GLY:N	1.53	1.22
1:B:28:TYR:CD1	1:B:182:PHE:CA	2.08	1.22
1:B:424:GLY:CA	1:B:792:ARG:HH12	1.52	1.22
1:B:97:GLY:HA3	3:Y:104:DT:O2	1.34	1.22

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:735:VAL:CG1	1:B:785:SER:HB3	1.56	1.22
2:T:6:DT:H2"	2:T:7:DT:C7	1.69	1.22
1:B:550:LEU:CD1	1:B:695:ALA:HB2	1.70	1.22
1:B:756:ARG:NH1	2:X:24:DG:N7	1.85	1.21
1:C:722:ARG:HD2	1:C:769:ILE:O	1.39	1.21
1:B:96:ARG:HD2	3:Y:103:DA:C1'	1.70	1.21
1:B:422:TRP:NE1	2:X:10:DA:OP1	1.73	1.21
1:B:563:PRO:CD	1:B:874:ASP:HB3	1.68	1.21
1:B:704:LYS:O	1:B:775:GLU:CD	1.78	1.21
1:B:349:VAL:CG2	1:B:352:ILE:HG12	1.71	1.20
1:C:14:ILE:HA	1:C:157:LEU:CD1	1.70	1.20
1:B:553:GLU:CB	1:B:554:VAL:HB	1.71	1.20
1:B:731:ASP:HB3	1:B:793:LYS:CG	1.70	1.20
1:C:727:TRP:CG	1:C:782:PHE:CE1	2.20	1.19
1:B:149:ALA:HB3	1:B:150:ARG:CD	1.70	1.19
1:B:562:LEU:CD2	1:B:870:LEU:HD12	1.65	1.19
1:B:703:ALA:O	1:B:775:GLU:HA	1.38	1.19
1:B:147:ASP:CB	1:B:150:ARG:HG3	1.71	1.19
1:B:158:GLU:OE1	1:B:290:GLY:HA3	1.41	1.19
1:B:782:PHE:CD1	1:B:845:PHE:CE1	2.21	1.19
1:C:400:PHE:CE1	1:C:431:MET:HB3	1.79	1.18
1:C:707:ALA:O	1:C:771:ALA:CA	1.92	1.18
1:C:776:SER:HB3	2:T:7:DT:P	1.79	1.18
1:B:707:ALA:CB	1:B:775:GLU:N	2.06	1.18
1:B:729:THR:CG2	1:B:789:SER:CB	2.22	1.18
2:T:6:DT:C2'	2:T:7:DT:C7	2.21	1.18
1:B:850:ALA:HB3	1:B:851:ASP:CB	1.74	1.18
1:C:724:ALA:HB2	1:C:738:GLU:CB	1.72	1.17
1:C:780:PRO:O	1:C:782:PHE:N	1.78	1.17
1:B:44:TYR:OH	1:B:155:ARG:CD	1.92	1.17
1:C:636:THR:HG22	2:T:8:DT:O4	1.41	1.17
1:C:639:TYR:HB3	2:T:8:DT:N1	1.59	1.17
1:C:722:ARG:NE	1:C:771:ALA:HB3	1.42	1.17
1:C:201:TRP:HE1	1:C:305:LEU:HD12	1.04	1.16
1:C:727:TRP:CD2	1:C:782:PHE:CE1	2.33	1.16
1:B:475:PHE:CE2	1:B:879:ASP:HB3	1.80	1.16
1:C:34:ARG:NH1	1:C:165:ASN:O	1.77	1.16
1:C:563:PRO:HB3	1:C:877:GLU:C	1.65	1.16
1:C:850:ALA:HB3	1:C:851:ASP:CB	1.74	1.16
1:B:549:MET:HB2	1:B:842:LEU:HD12	1.24	1.16
1:B:704:LYS:HA	1:B:775:GLU:CB	1.75	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:475:PHE:HE2	1:C:879:ASP:HB3	1.11	1.15
1:C:639:TYR:HB3	2:T:8:DT:C1'	1.77	1.15
1:B:707:ALA:HB1	1:B:774:GLN:HB3	1.20	1.15
1:C:727:TRP:CZ2	1:C:782:PHE:HD1	1.63	1.15
1:B:351:ASP:O	1:B:353:PRO:HD3	1.45	1.14
1:B:549:MET:HB3	1:B:841:VAL:HG21	1.18	1.14
1:B:424:GLY:HA3	1:B:792:ARG:NH1	1.58	1.14
1:C:21:PHE:CE1	1:C:161:HIS:HB3	1.80	1.14
1:C:727:TRP:CZ2	1:C:782:PHE:CD1	2.34	1.14
1:B:266:LEU:HD11	1:B:407:LYS:NZ	1.62	1.14
1:C:737:GLN:HE22	1:C:778:ILE:HA	1.07	1.13
1:B:729:THR:HG21	1:B:789:SER:CB	1.78	1.13
1:C:639:TYR:CD1	2:T:8:DT:O2	2.00	1.13
1:C:451:PRO:HA	1:C:452:ILE:HB	1.14	1.13
1:C:639:TYR:O	2:T:8:DT:C5'	1.95	1.13
1:C:703:ALA:HB1	1:C:778:ILE:CD1	1.77	1.13
1:C:776:SER:HB2	2:T:7:DT:OP1	0.96	1.13
1:B:149:ALA:HB1	1:B:150:ARG:CZ	1.76	1.13
1:B:201:TRP:CZ2	1:B:299:THR:O	2.02	1.13
2:X:6:DT:H2"	2:X:7:DT:OP2	1.31	1.12
1:C:554:VAL:N	1:C:555:GLY:HA2	1.65	1.12
1:B:95:LYS:HB3	3:Y:104:DT:C5'	1.79	1.12
1:B:862:PRO:HA	1:B:863:ALA:HB3	1.30	1.12
1:B:349:VAL:HG23	1:B:352:ILE:CG1	1.77	1.12
1:B:707:ALA:HB2	1:B:774:GLN:CB	1.74	1.12
1:B:840:ASP:HB3	1:B:843:ALA:HB3	1.32	1.12
1:C:14:ILE:CA	1:C:157:LEU:HD13	1.80	1.12
1:C:351:ASP:O	1:C:394:ARG:NH2	1.81	1.12
1:B:95:LYS:CG	3:Y:104:DT:H5"	1.80	1.11
1:B:264:ILE:CB	1:B:400:PHE:HE2	1.63	1.11
1:B:356:GLU:HA	1:B:356:GLU:OE2	1.49	1.11
1:B:410:ASN:O	1:B:411:HIS:HB2	1.47	1.11
1:B:707:ALA:CA	1:B:774:GLN:HB3	1.79	1.11
1:B:789:SER:HB3	1:B:792:ARG:NH2	1.65	1.11
1:C:862:PRO:HA	1:C:863:ALA:HB3	1.31	1.11
1:B:320:ILE:HD11	1:B:420:MET:SD	1.89	1.11
1:B:451:PRO:HA	1:B:452:ILE:HB	1.14	1.11
1:B:149:ALA:CB	1:B:150:ARG:HB2	1.79	1.11
1:B:551:ARG:CD	1:B:867:LYS:HG3	1.74	1.11
1:B:705:LEU:HD13	1:B:857:GLN:CG	1.79	1.11
2:X:9:DT:H1'	2:X:10:DA:C5'	1.81	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:408:PHE:HA	1:C:411:HIS:CD2	1.85	1.11
1:B:55:PHE:CE2	1:B:74:ILE:HG12	1.85	1.11
1:C:644:PHE:CB	3:N:126:DA:N1	2.14	1.11
1:C:727:TRP:CD1	1:C:782:PHE:HE1	1.40	1.11
1:B:474:PRO:CB	1:B:880:PHE:HZ	1.64	1.11
1:C:639:TYR:CD2	2:T:8:DT:C2	2.36	1.10
1:C:722:ARG:CD	1:C:771:ALA:CA	2.14	1.10
1:C:722:ARG:HG2	1:C:771:ALA:HB2	1.17	1.10
1:B:551:ARG:HB2	1:B:867:LYS:HG3	1.20	1.10
1:B:562:LEU:HG	1:B:870:LEU:HD11	1.12	1.10
1:B:789:SER:HA	1:B:792:ARG:CZ	1.81	1.10
1:C:24:LEU:HD11	1:C:273:VAL:HG21	1.27	1.10
1:B:475:PHE:HE2	1:B:879:ASP:CA	1.64	1.10
1:B:704:LYS:C	1:B:775:GLU:HG2	1.69	1.10
1:B:552:ASP:CG	1:B:555:GLY:H	1.54	1.10
1:B:149:ALA:CB	1:B:150:ARG:CB	2.30	1.10
1:B:475:PHE:CE2	1:B:879:ASP:C	2.23	1.10
1:C:722:ARG:CD	1:C:771:ALA:H	1.43	1.09
1:C:834:ASP:O	1:C:838:SER:CB	2.00	1.09
1:B:41:HIS:HE1	1:B:288:ALA:HB1	1.09	1.09
1:B:147:ASP:CB	1:B:150:ARG:CG	2.30	1.09
1:B:109:ILE:HD11	1:B:148:GLU:OE2	1.52	1.09
1:B:147:ASP:HA	1:B:150:ARG:CG	1.82	1.09
1:B:349:VAL:CG2	1:B:352:ILE:CG1	2.30	1.09
1:B:549:MET:CB	1:B:841:VAL:HG21	1.81	1.09
1:B:704:LYS:HA	1:B:775:GLU:HB3	1.13	1.09
1:B:354:ALA:HB1	1:B:355:ILE:O	1.51	1.09
1:B:550:LEU:HD22	1:B:865:PRO:HB2	1.30	1.09
1:C:739:TYR:HE2	1:C:770:ASP:OD2	1.34	1.09
1:C:812:ASP:OD1	4:R:8:A:H4'	1.53	1.09
1:B:149:ALA:CB	1:B:150:ARG:CD	2.30	1.08
1:B:707:ALA:HB2	1:B:774:GLN:HB3	1.32	1.08
1:C:553:GLU:HB2	1:C:554:VAL:HG21	1.10	1.08
1:B:549:MET:HG3	1:B:842:LEU:HD11	1.27	1.08
1:B:563:PRO:CG	1:B:874:ASP:HB3	1.81	1.08
1:B:811:HIS:ND1	4:Z:7:A:O2'	1.83	1.08
1:C:34:ARG:HG3	1:C:162:PHE:CA	1.82	1.08
1:C:563:PRO:HG3	1:C:877:GLU:HB2	1.19	1.08
1:B:109:ILE:HD13	1:B:148:GLU:OE2	1.50	1.08
1:B:354:ALA:CA	1:B:355:ILE:HG12	1.84	1.08
1:C:639:TYR:CE1	4:R:8:A:H2	1.72	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:707:ALA:O	1:C:771:ALA:CB	2.02	1.07
1:C:834:ASP:O	1:C:838:SER:HB3	1.52	1.07
1:B:735:VAL:HG11	1:B:785:SER:HB2	1.13	1.07
1:B:147:ASP:HA	1:B:150:ARG:HB3	1.08	1.07
1:B:264:ILE:HB	1:B:400:PHE:HE2	1.12	1.07
1:B:561:LEU:O	1:B:875:ILE:HG12	1.52	1.07
1:C:537:ASP:O	1:C:882:PHE:HB2	1.52	1.07
1:B:149:ALA:HB3	1:B:150:ARG:CA	1.84	1.07
1:B:475:PHE:HE2	1:B:879:ASP:C	1.54	1.07
1:C:727:TRP:CD2	1:C:782:PHE:HE1	1.69	1.07
1:B:147:ASP:CA	1:B:150:ARG:CG	2.33	1.07
1:B:423:ARG:HD2	1:B:784:HIS:HB3	1.28	1.07
1:B:789:SER:CA	1:B:792:ARG:NH2	2.17	1.07
1:C:354:ALA:HA	1:C:355:ILE:HG13	1.07	1.07
1:C:707:ALA:O	1:C:771:ALA:HA	1.54	1.07
1:B:54:MET:H	1:B:255:ALA:HB3	1.10	1.07
1:B:147:ASP:OD2	1:B:292:ARG:NH2	1.88	1.07
1:B:549:MET:HB2	1:B:841:VAL:HG23	1.37	1.07
1:B:553:GLU:HG2	1:B:554:VAL:CG2	1.83	1.07
1:B:44:TYR:OH	1:B:155:ARG:HD2	1.48	1.06
1:B:707:ALA:HB3	1:B:775:GLU:HG3	1.33	1.06
1:C:54:MET:N	1:C:255:ALA:HB1	1.64	1.06
1:C:201:TRP:HE1	1:C:305:LEU:CD1	1.65	1.06
1:C:249:GLU:OE1	1:B:30:GLU:OE2	1.72	1.06
1:B:131:ASN:HB3	1:B:132:THR:HA	1.07	1.06
2:X:9:DT:H1'	2:X:10:DA:H5'	1.07	1.06
1:C:553:GLU:CB	1:C:554:VAL:CB	2.34	1.06
1:B:553:GLU:HB3	1:B:554:VAL:CA	1.86	1.06
1:B:727:TRP:HH2	1:B:781:ASN:CB	1.69	1.06
1:B:36:GLN:NE2	1:B:272:VAL:HB	1.69	1.06
1:B:44:TYR:CZ	1:B:155:ARG:CD	2.39	1.06
1:B:549:MET:CB	1:B:841:VAL:CG2	2.33	1.06
1:B:731:ASP:CB	1:B:793:LYS:HG2	1.85	1.06
1:C:14:ILE:HD13	1:C:157:LEU:HD11	1.33	1.06
1:C:131:ASN:HB3	1:C:132:THR:HA	1.07	1.06
1:B:150:ARG:NE	1:B:150:ARG:HA	1.70	1.06
1:B:553:GLU:CB	1:B:554:VAL:CB	2.30	1.06
1:C:780:PRO:CA	1:C:783:VAL:CG2	2.34	1.05
1:C:17:ALA:HB1	1:C:158:GLU:N	1.70	1.05
1:C:642:LYS:CG	2:T:7:DT:H1'	1.86	1.05
1:B:730:PRO:HD2	1:B:786:GLN:OE1	1.56	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:54:MET:N	1:C:255:ALA:HB2	1.63	1.05
1:C:739:TYR:CE2	1:C:770:ASP:OD2	2.09	1.05
1:B:43:SER:HB3	1:B:44:TYR:HB2	1.35	1.05
1:B:147:ASP:HB3	1:B:150:ARG:HG3	1.08	1.05
1:B:315:GLU:HB2	1:B:731:ASP:O	1.57	1.05
1:C:537:ASP:C	1:C:882:PHE:HB2	1.77	1.05
1:B:829:ARG:HD2	1:B:875:ILE:HG22	1.38	1.05
1:C:21:PHE:CD1	1:C:161:HIS:CB	2.40	1.04
1:C:316:VAL:HG22	1:C:731:ASP:CG	1.77	1.04
1:C:639:TYR:CG	2:T:8:DT:O2	2.10	1.04
1:B:44:TYR:CE1	1:B:155:ARG:HD2	1.92	1.04
1:B:149:ALA:HB3	1:B:150:ARG:NE	1.73	1.04
1:C:544:GLN:HG2	1:C:561:LEU:CD1	1.86	1.04
1:B:707:ALA:HB2	1:B:774:GLN:CA	1.88	1.04
1:C:553:GLU:H	1:C:554:VAL:HG23	1.22	1.04
1:B:96:ARG:HG3	3:Y:103:DA:H1'	1.36	1.04
1:B:707:ALA:O	1:B:771:ALA:HB1	1.57	1.04
1:B:772:HIS:NE2	3:Y:130:DG:C5'	2.20	1.04
1:B:368:ASP:HA	1:B:369:MET:HB3	1.04	1.04
1:B:549:MET:HB2	1:B:842:LEU:CD1	1.88	1.04
1:B:96:ARG:CD	3:Y:103:DA:C1'	2.35	1.03
1:C:54:MET:CA	1:C:255:ALA:HB3	1.86	1.03
1:C:563:PRO:HB3	1:C:877:GLU:O	1.57	1.03
1:B:149:ALA:CB	1:B:150:ARG:CZ	2.36	1.03
1:B:551:ARG:HD2	1:B:867:LYS:HG2	1.06	1.03
1:C:812:ASP:OD1	4:R:8:A:H5'	1.53	1.03
1:B:147:ASP:CA	1:B:150:ARG:HB3	1.87	1.03
1:B:147:ASP:HB3	1:B:150:ARG:CG	1.88	1.03
1:C:552:ASP:HB3	1:C:555:GLY:H	1.13	1.03
1:C:639:TYR:CB	2:T:8:DT:N1	2.22	1.03
1:B:562:LEU:HG	1:B:870:LEU:CD1	1.79	1.03
1:B:735:VAL:CG1	1:B:785:SER:HB2	1.70	1.02
1:C:425:ARG:HH22	4:R:8:A:H1'	1.24	1.02
1:C:553:GLU:H	1:C:554:VAL:C	1.62	1.02
1:B:550:LEU:HD11	1:B:695:ALA:CB	1.90	1.02
1:B:705:LEU:HD13	1:B:857:GLN:HG2	1.41	1.02
1:B:423:ARG:HH11	1:B:784:HIS:CD2	1.78	1.02
1:B:731:ASP:OD1	1:B:789:SER:HB2	1.59	1.02
1:B:837:GLU:O	1:B:838:SER:HB2	1.57	1.02
1:C:722:ARG:HG2	1:C:771:ALA:CB	1.90	1.02
1:B:354:ALA:CA	1:B:355:ILE:CG1	2.38	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:707:ALA:HB3	1:B:775:GLU:N	1.72	1.02
1:B:789:SER:CB	1:B:792:ARG:NH2	2.22	1.01
1:B:147:ASP:N	1:B:148:GLU:HB2	1.72	1.01
1:B:704:LYS:HG2	1:B:775:GLU:OE1	1.60	1.01
1:B:707:ALA:CB	1:B:774:GLN:C	2.28	1.01
1:B:737:GLN:CA	1:B:781:ASN:HD22	1.72	1.01
1:C:544:GLN:CG	1:C:561:LEU:HD11	1.89	1.01
1:C:722:ARG:O	1:C:769:ILE:CD1	2.07	1.01
1:C:780:PRO:O	1:C:783:VAL:N	1.92	1.01
1:C:837:GLU:N	1:C:872:LEU:HD13	1.74	1.01
1:B:43:SER:HB3	1:B:44:TYR:CB	1.91	1.01
1:B:727:TRP:CH2	1:B:782:PHE:N	2.00	1.01
1:C:724:ALA:HB1	1:C:738:GLU:HB3	1.05	1.01
1:B:149:ALA:HB1	1:B:150:ARG:NH1	1.73	1.01
1:C:727:TRP:CD1	1:C:782:PHE:CZ	2.49	1.00
1:B:264:ILE:HG21	1:B:400:PHE:CE2	1.96	1.00
1:B:354:ALA:HA	1:B:355:ILE:HG12	1.01	1.00
1:C:544:GLN:CB	1:C:561:LEU:HD11	1.90	1.00
1:C:475:PHE:CE2	1:C:879:ASP:HB3	1.97	1.00
1:B:475:PHE:HD2	1:B:879:ASP:HB3	1.25	1.00
1:B:538:GLY:N	1:B:883:ALA:HB3	1.77	1.00
1:C:639:TYR:CB	2:T:8:DT:C2	2.43	1.00
1:B:698:TRP:CD1	1:B:861:MET:HE3	1.96	1.00
1:B:724:ALA:HB2	1:B:738:GLU:HB3	1.40	1.00
1:C:368:ASP:HA	1:C:369:MET:HB3	1.05	1.00
1:C:200:ALA:HA	1:C:293:PRO:HG2	1.40	1.00
1:C:316:VAL:CG2	1:C:731:ASP:OD2	2.10	0.99
1:C:780:PRO:HA	1:C:783:VAL:HG22	1.37	0.99
1:B:28:TYR:CZ	1:B:182:PHE:O	2.14	0.99
1:C:53:LYS:NZ	1:C:255:ALA:O	1.95	0.99
1:C:553:GLU:O	1:C:557:ARG:HG3	1.60	0.99
1:C:836:TYR:C	1:C:872:LEU:CD1	2.31	0.99
1:B:723:CYS:O	1:B:774:GLN:HG2	1.57	0.99
1:B:729:THR:OG1	1:B:789:SER:OG	1.78	0.99
1:B:146:GLU:O	1:B:150:ARG:HG2	1.59	0.99
1:B:158:GLU:OE1	1:B:290:GLY:CA	2.09	0.99
1:C:34:ARG:CG	1:C:162:PHE:HA	1.91	0.99
1:C:812:ASP:OD2	4:R:8:A:C4'	2.10	0.99
1:B:28:TYR:CG	1:B:182:PHE:HB2	1.96	0.99
1:B:96:ARG:HD2	3:Y:103:DA:O4'	1.59	0.99
1:B:96:ARG:HH12	3:Y:102:DA:C1'	1.53	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:148:GLU:C	1:B:150:ARG:CB	2.30	0.99
1:B:117:ILE:HD13	1:B:148:GLU:OE1	1.59	0.99
1:B:729:THR:HG21	1:B:789:SER:HB3	1.00	0.99
1:B:146:GLU:C	1:B:148:GLU:CB	2.30	0.99
1:B:474:PRO:CA	1:B:880:PHE:HE1	1.70	0.99
1:B:41:HIS:CE1	1:B:288:ALA:HB1	1.96	0.99
1:B:145:ILE:C	1:B:148:GLU:CG	2.30	0.99
1:C:544:GLN:CG	1:C:561:LEU:CD1	2.41	0.99
1:B:563:PRO:HD2	1:B:874:ASP:HB3	1.41	0.99
1:B:735:VAL:HG11	1:B:785:SER:OG	1.61	0.99
1:C:21:PHE:CG	1:C:161:HIS:CG	2.50	0.98
1:C:776:SER:CB	2:T:7:DT:O5'	2.08	0.98
1:C:131:ASN:CB	1:C:132:THR:HA	1.93	0.98
1:C:556:GLY:HA2	1:C:557:ARG:C	1.75	0.98
1:C:423:ARG:NH1	2:T:9:DT:H2"	1.77	0.98
1:B:149:ALA:HB3	1:B:150:ARG:CG	1.91	0.98
1:B:549:MET:HB2	1:B:841:VAL:CG2	1.92	0.98
1:B:551:ARG:CB	1:B:867:LYS:HG3	1.92	0.98
1:C:553:GLU:HB3	1:C:554:VAL:HG11	1.38	0.98
1:B:355:ILE:HG13	1:B:356:GLU:N	1.77	0.98
1:C:36:GLN:NE2	1:C:272:VAL:H	1.59	0.98
1:B:147:ASP:CA	1:B:150:ARG:HG2	1.94	0.98
1:C:21:PHE:CG	1:C:161:HIS:CD2	2.50	0.98
1:C:368:ASP:HA	1:C:369:MET:CB	1.91	0.98
1:B:44:TYR:OH	1:B:155:ARG:NE	1.97	0.98
1:B:95:LYS:CD	3:Y:104:DT:H5"	1.93	0.98
1:B:562:LEU:CD1	1:B:870:LEU:CD1	2.41	0.98
1:C:44:TYR:CE1	1:C:120:LYS:HE3	1.99	0.98
1:B:36:GLN:NE2	1:B:272:VAL:CB	2.27	0.98
1:B:772:HIS:HD2	3:Y:130:DG:H3'	1.29	0.98
1:B:760:THR:HB	2:X:20:DG:H5"	1.46	0.97
1:B:55:PHE:CZ	1:B:74:ILE:HG12	1.99	0.97
1:C:703:ALA:HB1	1:C:778:ILE:HD13	0.97	0.97
1:B:553:GLU:HG2	1:B:554:VAL:HG23	1.44	0.97
1:C:724:ALA:HB1	1:C:738:GLU:CB	1.82	0.97
1:C:812:ASP:OD1	4:R:8:A:C4'	2.06	0.97
1:B:98:LYS:HB2	2:X:29:DA:C2	1.99	0.97
1:B:131:ASN:CB	1:B:132:THR:HA	1.93	0.97
1:B:563:PRO:HD3	1:B:874:ASP:C	1.84	0.97
1:C:370:ASN:HB3	1:C:371:PRO:HD3	1.45	0.97
1:B:149:ALA:CB	1:B:150:ARG:HD2	1.92	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:149:ALA:HB2	1:B:150:ARG:HD2	1.46	0.97
1:C:698:TRP:HD1	1:C:863:ALA:N	1.63	0.97
1:B:95:LYS:HD3	3:Y:104:DT:H5"	1.47	0.97
1:B:811:HIS:CG	4:Z:7:A:O2'	2.17	0.97
1:B:148:GLU:C	1:B:150:ARG:HB2	1.85	0.97
1:B:264:ILE:CB	1:B:400:PHE:CE2	2.46	0.97
1:B:96:ARG:CG	3:Y:103:DA:C1'	2.42	0.96
1:C:563:PRO:HA	1:C:878:SER:HA	1.44	0.96
1:C:727:TRP:CE2	1:C:782:PHE:HD1	1.54	0.96
1:B:758:GLN:HE22	2:X:23:DA:H62	1.04	0.96
1:C:307:ARG:HB3	1:C:736:TRP:CZ2	1.98	0.96
1:B:698:TRP:HD1	1:B:861:MET:HE1	1.22	0.96
1:B:780:PRO:HB2	1:B:784:HIS:HE1	1.31	0.96
1:C:707:ALA:O	1:C:771:ALA:HB1	1.63	0.96
2:T:8:DT:H2'	2:T:9:DT:C6	2.00	0.96
1:C:375:THR:HB	1:C:376:ALA:HB3	1.48	0.96
1:C:201:TRP:NE1	1:C:305:LEU:HD12	1.79	0.96
1:C:554:VAL:HG23	1:C:554:VAL:O	1.66	0.96
1:B:729:THR:HG23	1:B:789:SER:CB	1.92	0.96
1:B:97:GLY:CA	3:Y:104:DT:O2	2.13	0.96
1:B:266:LEU:CD1	1:B:407:LYS:NZ	2.29	0.96
1:B:368:ASP:HA	1:B:369:MET:CB	1.91	0.96
1:B:354:ALA:CB	1:B:355:ILE:HG13	1.96	0.96
1:C:722:ARG:CG	1:C:771:ALA:CB	2.35	0.95
1:B:41:HIS:HE1	1:B:288:ALA:CB	1.79	0.95
1:C:34:ARG:HG3	1:C:162:PHE:HA	0.98	0.95
1:B:147:ASP:CA	1:B:150:ARG:CB	2.44	0.95
1:B:375:THR:HB	1:B:376:ALA:HB3	1.47	0.95
1:B:705:LEU:HB3	1:B:857:GLN:HE21	1.28	0.95
1:B:354:ALA:CB	1:B:355:ILE:C	2.32	0.95
1:C:639:TYR:CE1	4:R:8:A:C2	2.51	0.95
1:B:370:ASN:HB3	1:B:371:PRO:HD3	1.45	0.95
1:B:474:PRO:HA	1:B:880:PHE:HE1	1.20	0.95
1:B:98:LYS:HE2	3:Y:105:DA:N3	1.81	0.95
1:B:341:ILE:HD11	1:B:509:PHE:CZ	2.02	0.95
1:C:644:PHE:CG	3:N:126:DA:N1	2.30	0.95
1:B:782:PHE:HD1	1:B:845:PHE:CE1	1.53	0.95
1:C:724:ALA:HB2	1:C:738:GLU:HB3	0.96	0.95
1:B:100:PRO:HA	3:Y:105:DA:O3'	1.64	0.95
1:B:451:PRO:HA	1:B:452:ILE:CB	1.95	0.95
1:C:307:ARG:CD	1:C:736:TRP:CE2	2.49	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:474:PRO:HB3	1:B:880:PHE:HZ	1.30	0.95
1:B:549:MET:CG	1:B:842:LEU:HD11	1.97	0.95
1:C:544:GLN:HB3	1:C:561:LEU:HD11	1.47	0.94
1:C:737:GLN:NE2	1:C:778:ILE:HA	1.81	0.94
1:B:707:ALA:O	1:B:771:ALA:CB	2.14	0.94
1:B:789:SER:HB3	1:B:792:ARG:HH21	1.30	0.94
1:C:451:PRO:HA	1:C:452:ILE:CB	1.95	0.94
1:B:99:ARG:CZ	2:X:31:DT:H4'	1.97	0.94
1:B:423:ARG:NH1	1:B:784:HIS:HD2	1.66	0.94
1:B:424:GLY:HA3	1:B:792:ARG:HH12	0.80	0.94
1:C:780:PRO:HA	1:C:783:VAL:HG21	1.50	0.94
1:B:147:ASP:N	1:B:148:GLU:CB	2.30	0.94
1:B:55:PHE:CE1	1:B:74:ILE:CG2	2.50	0.94
1:B:829:ARG:CD	1:B:875:ILE:HG22	1.98	0.94
1:C:837:GLU:N	1:C:872:LEU:CD1	2.31	0.94
1:B:266:LEU:HD11	1:B:407:LYS:HZ3	1.26	0.94
1:B:550:LEU:CD1	1:B:695:ALA:CB	2.45	0.94
1:C:21:PHE:CD2	1:C:161:HIS:HD2	1.68	0.94
1:B:201:TRP:HZ2	1:B:299:THR:O	1.48	0.93
1:B:329:LYS:HD3	1:B:447:ALA:HA	1.50	0.93
1:B:475:PHE:CE2	1:B:879:ASP:CB	2.50	0.93
1:B:724:ALA:CB	1:B:738:GLU:HB3	1.97	0.93
1:B:149:ALA:N	1:B:150:ARG:CB	2.30	0.93
1:B:731:ASP:HB3	1:B:793:LYS:HG2	0.94	0.93
1:B:146:GLU:N	1:B:148:GLU:CG	2.30	0.93
1:B:562:LEU:HD11	1:B:870:LEU:CD1	1.98	0.93
1:B:780:PRO:HB2	1:B:784:HIS:CE1	2.04	0.93
1:C:36:GLN:HE22	1:C:272:VAL:H	0.94	0.93
1:B:149:ALA:CB	1:B:150:ARG:NE	2.30	0.93
1:B:405:ALA:HB1	1:B:443:LEU:HD13	1.48	0.93
1:B:793:LYS:HZ3	1:B:835:THR:CG2	1.63	0.93
1:C:722:ARG:O	1:C:769:ILE:HD13	1.69	0.93
1:C:727:TRP:NE1	1:C:782:PHE:CD1	2.23	0.93
1:C:131:ASN:HB3	1:C:132:THR:CA	1.99	0.93
1:C:563:PRO:CD	1:C:874:ASP:O	2.17	0.93
1:B:145:ILE:HA	1:B:148:GLU:CD	1.89	0.93
1:B:553:GLU:CG	1:B:554:VAL:HG23	1.98	0.93
1:C:553:GLU:N	1:C:554:VAL:C	2.23	0.92
1:B:329:LYS:HE2	1:B:446:LEU:O	1.66	0.92
1:B:737:GLN:CA	1:B:781:ASN:ND2	2.32	0.92
1:B:55:PHE:CZ	1:B:74:ILE:HG21	2.05	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:474:PRO:CB	1:B:880:PHE:CZ	2.44	0.92
1:C:780:PRO:HA	1:C:783:VAL:HG23	1.51	0.92
1:B:131:ASN:HB3	1:B:132:THR:CA	1.99	0.92
1:C:812:ASP:CG	4:R:8:A:C5'	2.34	0.92
2:T:8:DT:H2'	2:T:9:DT:H6	1.29	0.92
1:B:270:PRO:CD	1:B:408:PHE:CE1	2.52	0.92
1:B:551:ARG:HD3	1:B:867:LYS:HG2	1.48	0.92
1:C:14:ILE:HD13	1:C:157:LEU:CD1	2.00	0.92
1:C:727:TRP:CD2	1:C:782:PHE:CD1	2.56	0.92
1:B:36:GLN:HE22	1:B:272:VAL:HG23	1.35	0.92
1:B:147:ASP:N	1:B:148:GLU:CG	2.33	0.92
1:B:834:ASP:O	1:B:838:SER:CB	2.17	0.92
1:B:96:ARG:HD3	3:Y:102:DA:N3	1.84	0.92
1:B:551:ARG:HD2	1:B:867:LYS:HG3	0.98	0.92
1:B:786:GLN:NE2	1:B:841:VAL:CG1	2.33	0.92
1:B:789:SER:CA	1:B:792:ARG:CZ	2.48	0.92
1:C:812:ASP:OD2	4:R:8:A:C3'	2.18	0.92
1:C:722:ARG:NE	1:C:771:ALA:H	1.68	0.92
1:B:97:GLY:HA2	3:Y:103:DA:H2	1.34	0.92
1:C:836:TYR:O	1:C:872:LEU:CD1	2.19	0.91
1:B:550:LEU:HD11	1:B:695:ALA:HB2	1.45	0.91
1:B:97:GLY:HA3	3:Y:104:DT:C2	2.04	0.91
1:B:264:ILE:HA	1:B:265:SER:HB3	1.52	0.91
1:C:722:ARG:CZ	1:C:771:ALA:H	1.83	0.91
1:C:698:TRP:HD1	1:C:863:ALA:H	0.95	0.91
1:C:722:ARG:NH1	1:C:771:ALA:H	1.68	0.91
1:B:549:MET:O	1:B:842:LEU:HD13	1.70	0.91
1:C:544:GLN:HG2	1:C:561:LEU:HD13	1.52	0.91
1:B:562:LEU:HD21	1:B:870:LEU:HD12	0.93	0.91
1:C:776:SER:OG	2:T:6:DT:O3'	1.88	0.91
1:B:96:ARG:CD	3:Y:103:DA:O4'	2.18	0.91
1:B:264:ILE:CG2	1:B:400:PHE:CE2	2.53	0.91
1:C:307:ARG:CB	1:C:736:TRP:CH2	2.54	0.91
1:C:560:ASN:O	1:C:881:ALA:HB2	1.71	0.90
1:B:144:ALA:O	1:B:148:GLU:OE1	1.89	0.90
1:B:149:ALA:CB	1:B:150:ARG:NH1	2.34	0.90
1:B:201:TRP:CH2	1:B:299:THR:O	2.23	0.90
1:B:474:PRO:C	1:B:880:PHE:HE1	1.73	0.90
1:B:735:VAL:CB	1:B:785:SER:HB3	2.02	0.90
1:C:776:SER:HG	2:T:7:DT:P	1.95	0.90
1:B:347:CYS:SG	1:B:348:PRO:HD2	2.11	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:549:MET:CB	1:B:842:LEU:CD1	2.49	0.90
1:B:553:GLU:HB3	1:B:554:VAL:HB	0.91	0.90
1:B:705:LEU:HD13	1:B:857:GLN:HG3	1.53	0.90
1:B:707:ALA:O	1:B:771:ALA:CA	2.20	0.90
1:B:97:GLY:HA2	2:X:30:DT:O2	1.71	0.90
1:B:560:ASN:O	1:B:881:ALA:HB2	1.70	0.90
1:C:541:SER:HB3	4:R:8:A:O3'	1.71	0.90
1:B:36:GLN:HE22	1:B:272:VAL:CG2	1.83	0.90
1:B:758:GLN:NE2	2:X:23:DA:H62	1.69	0.90
1:B:563:PRO:CD	1:B:874:ASP:CB	2.47	0.90
1:B:730:PRO:HB3	1:B:835:THR:HG22	1.53	0.90
1:C:264:ILE:HA	1:C:265:SER:HB3	1.52	0.89
1:C:722:ARG:NE	1:C:771:ALA:HB2	1.61	0.89
1:B:96:ARG:HG2	3:Y:103:DA:H1'	1.53	0.89
1:B:146:GLU:O	1:B:148:GLU:HB2	1.71	0.89
1:C:537:ASP:O	1:C:882:PHE:HD2	1.56	0.89
1:B:199:GLU:OE2	1:B:302:LYS:NZ	2.05	0.89
1:C:784:HIS:CE1	2:T:9:DT:H1'	2.08	0.89
1:B:475:PHE:HZ	1:B:879:ASP:O	1.39	0.89
1:B:727:TRP:CH2	1:B:781:ASN:CB	2.55	0.89
1:C:704:LYS:HE2	1:C:775:GLU:OE2	1.73	0.89
1:C:639:TYR:CZ	4:R:8:A:N1	2.40	0.89
1:C:722:ARG:CZ	1:C:771:ALA:HB3	2.02	0.89
1:B:264:ILE:HB	1:B:400:PHE:CE2	2.05	0.89
1:B:266:LEU:HD21	1:B:407:LYS:HZ3	1.38	0.89
1:B:801:LYS:HD2	1:B:802:TYR:CD2	2.08	0.89
1:B:146:GLU:C	1:B:150:ARG:HG2	1.93	0.89
1:B:758:GLN:N	2:X:22:DG:OP2	2.05	0.89
1:C:722:ARG:HE	1:C:771:ALA:CB	1.65	0.88
1:C:642:LYS:CB	2:T:7:DT:H1'	2.01	0.88
1:C:316:VAL:CG2	1:C:731:ASP:CG	2.41	0.88
1:B:315:GLU:CB	1:B:731:ASP:O	2.22	0.88
1:B:723:CYS:O	1:B:774:GLN:HG3	1.72	0.88
1:C:537:ASP:O	1:C:882:PHE:CD2	2.27	0.87
1:B:205:HIS:O	1:B:207:GLU:N	2.07	0.87
1:C:722:ARG:HD3	1:C:770:ASP:C	1.94	0.87
1:C:552:ASP:HB3	1:C:554:VAL:C	1.94	0.87
1:C:400:PHE:CE1	1:C:431:MET:CB	2.57	0.87
1:B:475:PHE:CE2	1:B:879:ASP:CA	2.56	0.87
1:C:400:PHE:HE1	1:C:431:MET:HB3	1.31	0.87
1:C:368:ASP:CA	1:C:369:MET:HB3	2.00	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:703:ALA:CB	1:C:778:ILE:CD1	2.45	0.87
1:B:36:GLN:HE22	1:B:272:VAL:CB	1.84	0.87
1:C:642:LYS:HB2	2:T:7:DT:H1'	1.55	0.86
2:X:9:DT:C1'	2:X:10:DA:H5'	2.01	0.86
1:C:354:ALA:HA	1:C:355:ILE:CG1	2.00	0.86
1:B:639:TYR:O	2:X:8:DT:H1'	1.76	0.86
1:B:424:GLY:HA2	1:B:792:ARG:NH1	1.90	0.86
1:B:211:HIS:NE2	3:Y:107:DG:OP1	2.09	0.86
1:B:801:LYS:NZ	1:B:802:TYR:CZ	2.42	0.86
1:B:98:LYS:HB2	2:X:29:DA:H2	1.41	0.86
1:B:729:THR:OG1	1:B:786:GLN:HA	1.75	0.86
1:B:95:LYS:CB	3:Y:104:DT:C5'	2.53	0.86
1:C:829:ARG:HD2	1:C:875:ILE:O	1.76	0.86
1:C:44:TYR:OH	1:C:48:GLU:OE2	1.94	0.85
1:C:354:ALA:CA	1:C:355:ILE:HG13	2.00	0.85
1:B:36:GLN:HE21	1:B:272:VAL:HB	1.39	0.85
1:B:95:LYS:HB3	3:Y:104:DT:H4'	1.58	0.85
1:B:9:ASN:O	1:B:10:ASP:HB2	1.76	0.85
1:B:96:ARG:HD2	3:Y:103:DA:N9	1.91	0.85
1:B:43:SER:HA	1:B:266:LEU:O	1.76	0.85
1:B:145:ILE:HA	1:B:148:GLU:OE1	1.76	0.85
1:B:707:ALA:HB3	1:B:775:GLU:CG	2.05	0.85
1:B:553:GLU:N	1:B:554:VAL:C	2.30	0.85
1:C:252:GLU:OE1	1:B:165:ASN:CG	2.15	0.85
1:B:95:LYS:CB	3:Y:104:DT:H5"	2.05	0.85
1:C:200:ALA:CA	1:C:293:PRO:HG2	2.05	0.85
1:C:408:PHE:CA	1:C:411:HIS:CD2	2.58	0.85
1:B:96:ARG:CZ	3:Y:102:DA:H1'	2.06	0.85
1:B:148:GLU:C	1:B:150:ARG:HB3	1.96	0.85
1:B:149:ALA:HB3	1:B:150:ARG:HA	1.58	0.85
1:B:349:VAL:CB	1:B:352:ILE:HG12	2.07	0.85
1:B:738:GLU:O	1:B:739:TYR:CD2	2.30	0.85
1:B:538:GLY:CA	1:B:883:ALA:HB3	2.06	0.84
1:B:738:GLU:O	1:B:739:TYR:CG	2.30	0.84
1:C:563:PRO:CG	1:C:877:GLU:HB2	2.06	0.84
1:B:54:MET:N	1:B:255:ALA:HB3	1.92	0.84
1:C:18:ALA:HA	1:C:161:HIS:CE1	2.11	0.84
1:B:354:ALA:HA	1:B:355:ILE:CB	2.06	0.84
1:B:793:LYS:HZ2	1:B:835:THR:HG21	1.38	0.84
1:B:563:PRO:HD3	1:B:874:ASP:O	1.77	0.84
1:B:36:GLN:NE2	1:B:272:VAL:CG2	2.38	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:549:MET:C	1:B:842:LEU:HD13	1.97	0.84
1:C:552:ASP:OD2	1:C:691:ALA:HB3	1.78	0.84
1:C:644:PHE:CG	3:N:126:DA:C2	2.66	0.84
1:B:149:ALA:CB	1:B:150:ARG:CA	2.54	0.84
1:B:834:ASP:O	1:B:838:SER:HB2	1.78	0.84
1:C:42:GLU:OE2	1:C:46:MET:SD	2.36	0.83
2:X:6:DT:C2'	2:X:7:DT:OP2	2.20	0.83
1:C:639:TYR:HB3	2:T:8:DT:O4'	1.77	0.83
1:B:551:ARG:HB2	1:B:867:LYS:CG	2.07	0.83
1:B:735:VAL:HG11	1:B:785:SER:HB3	0.85	0.83
1:B:839:CYS:O	1:B:844:ASP:HB2	1.78	0.83
1:B:97:GLY:HA2	3:Y:103:DA:C2	2.13	0.83
1:B:97:GLY:CA	3:Y:103:DA:C2	2.61	0.83
1:B:117:ILE:CD1	1:B:148:GLU:OE1	2.25	0.83
1:B:553:GLU:CG	1:B:554:VAL:CG2	2.55	0.83
1:B:758:GLN:OE1	2:X:22:DG:N7	2.11	0.83
1:C:779:ALA:HB3	1:C:780:PRO:CD	2.08	0.83
1:B:266:LEU:CD1	1:B:407:LYS:HZ3	1.89	0.83
1:B:553:GLU:HB3	1:B:554:VAL:CG2	2.07	0.83
2:T:8:DT:C2'	2:T:9:DT:H6	1.91	0.83
1:B:205:HIS:O	1:B:208:ASP:N	2.10	0.83
1:B:758:GLN:HE22	2:X:23:DA:N6	1.77	0.83
1:C:829:ARG:CB	1:C:876:LEU:HD23	2.09	0.83
1:B:28:TYR:CE1	1:B:182:PHE:CB	2.41	0.83
1:B:96:ARG:HG3	3:Y:103:DA:N3	1.93	0.83
1:C:252:GLU:CD	1:B:165:ASN:O	2.17	0.82
1:C:779:ALA:HB3	1:C:780:PRO:HD3	1.60	0.82
1:B:349:VAL:CG2	1:B:352:ILE:HG13	2.10	0.82
1:B:264:ILE:HG12	1:B:400:PHE:CD2	2.14	0.82
1:B:96:ARG:CD	3:Y:103:DA:H1'	2.05	0.82
1:B:12:SER:O	1:B:13:ASP:CG	2.18	0.82
1:B:145:ILE:HG22	1:B:145:ILE:O	1.80	0.82
1:B:354:ALA:HB3	1:B:391:ARG:HE	1.45	0.82
1:C:722:ARG:HH11	1:C:770:ASP:HA	1.45	0.82
1:B:698:TRP:CG	1:B:861:MET:HE3	2.14	0.82
1:B:801:LYS:HD2	1:B:802:TYR:CG	2.15	0.82
1:C:776:SER:OG	2:T:7:DT:P	2.37	0.82
1:B:772:HIS:CD2	3:Y:130:DG:H3'	2.15	0.82
1:B:793:LYS:NZ	1:B:835:THR:HG22	1.94	0.82
1:C:552:ASP:CB	1:C:554:VAL:O	2.28	0.81
2:T:6:DT:H2'	2:T:7:DT:C7	2.09	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:354:ALA:HB3	1:C:391:ARG:HE	1.46	0.81
1:C:639:TYR:O	2:T:8:DT:O4'	1.97	0.81
1:B:100:PRO:HA	3:Y:106:DC:P	2.20	0.81
1:B:349:VAL:O	1:B:352:ILE:HB	1.81	0.81
1:B:707:ALA:CB	1:B:774:GLN:CA	2.53	0.81
1:B:801:LYS:C	1:B:801:LYS:HD3	2.01	0.81
1:C:14:ILE:HA	1:C:157:LEU:HD13	0.87	0.81
1:C:36:GLN:HE22	1:C:272:VAL:N	1.77	0.81
1:C:401:MET:SD	1:C:440:THR:CG2	2.68	0.81
2:T:8:DT:H2'	2:T:9:DT:H71	1.62	0.81
1:B:782:PHE:CD1	1:B:845:PHE:CZ	2.67	0.81
1:C:31:ARG:HG3	1:C:32:LEU:H	1.46	0.81
1:C:563:PRO:CA	1:C:878:SER:HA	2.10	0.81
1:B:562:LEU:HD11	1:B:870:LEU:HD13	1.61	0.81
1:B:707:ALA:HB1	1:B:771:ALA:O	1.81	0.81
1:B:836:TYR:HE1	1:B:841:VAL:CG1	1.93	0.81
1:B:354:ALA:CB	1:B:355:ILE:CG1	2.56	0.81
1:B:388:ASP:OD1	1:B:391:ARG:NH1	2.13	0.81
1:B:789:SER:HA	1:B:792:ARG:NH2	1.88	0.81
1:C:536:PHE:C	1:C:882:PHE:HB3	2.02	0.81
1:C:539:SER:OG	1:C:560:ASN:HB2	1.81	0.81
1:C:556:GLY:CA	1:C:558:ALA:N	2.41	0.81
1:B:699:LEU:HD23	1:B:845:PHE:HE2	1.45	0.81
2:X:10:DA:H1'	2:X:11:DC:H5'	1.63	0.81
1:C:408:PHE:HA	1:C:411:HIS:NE2	1.96	0.80
1:B:36:GLN:NE2	1:B:272:VAL:HG23	1.96	0.80
1:B:147:ASP:N	1:B:148:GLU:HG2	1.95	0.80
1:B:474:PRO:C	1:B:880:PHE:CE1	2.52	0.80
1:C:367:ILE:HG13	1:B:345:LYS:NZ	1.95	0.80
1:B:95:LYS:HB3	3:Y:104:DT:C4'	2.10	0.80
1:C:698:TRP:CD1	1:C:863:ALA:N	2.43	0.80
1:C:776:SER:HB3	2:T:7:DT:C5'	2.12	0.80
1:B:759:PRO:HA	2:X:21:DT:P	2.21	0.80
1:C:773:LYS:O	1:C:774:GLN:HB2	1.79	0.80
1:B:266:LEU:HD21	1:B:407:LYS:NZ	1.96	0.80
1:B:349:VAL:HG23	1:B:352:ILE:HG12	1.42	0.80
1:B:349:VAL:HG23	1:B:352:ILE:HG13	1.63	0.80
1:B:549:MET:HG3	1:B:842:LEU:CD1	2.10	0.80
1:C:252:GLU:OE1	1:B:165:ASN:ND2	2.13	0.80
1:C:355:ILE:HD12	1:C:356:GLU:H	1.45	0.80
1:C:780:PRO:CA	1:C:783:VAL:HG23	2.06	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:329:LYS:CD	1:B:447:ALA:HA	2.12	0.80
1:B:347:CYS:HB3	1:B:352:ILE:HG21	1.62	0.80
1:C:20:PRO:HG2	1:C:158:GLU:OE2	1.82	0.80
1:B:55:PHE:CD1	1:B:74:ILE:HG21	2.17	0.80
1:B:97:GLY:CA	3:Y:103:DA:H2	1.93	0.80
1:B:368:ASP:CA	1:B:369:MET:HB3	2.00	0.80
1:B:707:ALA:HA	1:B:774:GLN:HB3	1.64	0.80
1:B:316:VAL:HG22	1:B:733:PHE:HB2	1.64	0.79
1:B:549:MET:CG	1:B:842:LEU:CD1	2.60	0.79
1:B:475:PHE:N	1:B:880:PHE:HE1	1.81	0.79
1:C:400:PHE:CZ	1:C:431:MET:HB3	2.16	0.79
1:C:537:ASP:O	1:C:882:PHE:CB	2.29	0.79
1:B:96:ARG:HD3	3:Y:102:DA:C2	2.17	0.79
1:B:786:GLN:NE2	1:B:841:VAL:HG12	1.97	0.79
1:C:44:TYR:CE2	1:C:48:GLU:CG	2.65	0.79
1:C:252:GLU:OE1	1:B:165:ASN:CB	2.30	0.79
1:C:44:TYR:CZ	1:C:120:LYS:HE3	2.17	0.79
1:C:423:ARG:HH12	2:T:9:DT:H2"	1.42	0.79
1:B:96:ARG:HH11	3:Y:102:DA:H1'	1.05	0.79
1:B:707:ALA:CB	1:B:775:GLU:HG3	2.13	0.79
1:B:194:GLY:O	1:B:289:ASN:OD1	2.00	0.79
1:B:270:PRO:HD2	1:B:408:PHE:CD1	2.17	0.79
1:B:146:GLU:O	1:B:150:ARG:CG	2.30	0.79
1:B:150:ARG:HA	1:B:150:ARG:HE	1.48	0.79
1:B:746:ARG:CZ	2:X:21:DT:C7	2.60	0.79
1:C:252:GLU:OE1	1:B:165:ASN:HB2	1.83	0.79
1:B:52:ARG:HA	1:B:55:PHE:HB2	1.63	0.79
1:B:553:GLU:CB	1:B:554:VAL:O	2.30	0.79
1:C:537:ASP:N	1:C:882:PHE:CB	2.46	0.79
1:C:862:PRO:HA	1:C:863:ALA:CB	2.10	0.79
1:B:31:ARG:HG3	1:B:32:LEU:H	1.46	0.79
1:B:95:LYS:HB3	3:Y:104:DT:H5"	1.62	0.79
1:C:553:GLU:CA	1:C:554:VAL:CG2	2.21	0.78
1:C:725:VAL:HG21	1:C:778:ILE:HD11	1.65	0.78
1:B:42:GLU:O	1:B:266:LEU:HB2	1.82	0.78
1:B:547:SER:HA	1:B:552:ASP:HB2	1.66	0.78
1:B:789:SER:CB	1:B:792:ARG:HH21	1.92	0.78
1:B:836:TYR:HE1	1:B:841:VAL:HG11	1.48	0.78
1:C:553:GLU:N	1:C:554:VAL:HG23	1.84	0.78
1:C:554:VAL:H	1:C:555:GLY:HA2	1.44	0.78
1:C:722:ARG:O	1:C:769:ILE:HD12	1.83	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:264:ILE:CG1	1:B:400:PHE:CE2	2.67	0.78
1:B:563:PRO:HD2	1:B:874:ASP:CB	2.12	0.78
1:B:9:ASN:O	1:B:10:ASP:CB	2.31	0.78
1:B:699:LEU:HD23	1:B:845:PHE:CE2	2.17	0.78
1:B:405:ALA:CB	1:B:443:LEU:HD13	2.13	0.78
1:B:703:ALA:C	1:B:775:GLU:HA	2.03	0.78
1:C:308:TYR:CE2	1:C:734:PRO:O	2.37	0.78
1:C:781:ASN:ND2	2:T:9:DT:C4'	2.12	0.78
1:B:326:THR:HG21	1:B:807:PHE:O	1.82	0.78
1:B:705:LEU:CB	1:B:857:GLN:NE2	2.35	0.78
1:B:772:HIS:CD2	3:Y:130:DG:C3'	2.67	0.78
1:B:837:GLU:O	1:B:838:SER:CB	2.32	0.78
1:B:211:HIS:CE1	3:Y:107:DG:OP1	2.36	0.77
1:B:563:PRO:HA	1:B:878:SER:CB	2.13	0.77
1:C:644:PHE:HB2	3:N:126:DA:H2	1.42	0.77
1:B:698:TRP:NE1	1:B:861:MET:CE	2.45	0.77
1:B:850:ALA:HB3	1:B:851:ASP:HB2	0.81	0.77
1:B:549:MET:CB	1:B:842:LEU:HD12	2.08	0.77
1:B:563:PRO:CG	1:B:874:ASP:O	2.33	0.77
1:B:536:PHE:HB3	1:B:882:PHE:O	1.83	0.77
1:B:475:PHE:HE2	1:B:879:ASP:CB	1.92	0.77
1:C:182:PHE:HZ	1:C:413:ALA:HB3	1.50	0.77
1:C:182:PHE:CE2	1:C:415:TRP:HH2	2.02	0.77
1:C:722:ARG:CD	1:C:769:ILE:O	2.29	0.77
1:C:17:ALA:HB1	1:C:158:GLU:H	1.49	0.77
1:C:307:ARG:HD2	1:C:736:TRP:CD2	2.19	0.77
1:B:725:VAL:HG21	1:B:778:ILE:CA	2.13	0.77
1:C:183:MET:SD	1:C:448:LYS:HD3	2.25	0.77
1:B:266:LEU:CD1	1:B:407:LYS:HZ2	1.96	0.77
1:B:772:HIS:CD2	3:Y:130:DG:C4'	2.68	0.77
1:C:315:GLU:HB2	1:C:731:ASP:HB2	1.66	0.77
1:B:707:ALA:CB	1:B:775:GLU:H	1.98	0.77
1:B:354:ALA:HB1	1:B:356:GLU:N	1.99	0.77
1:B:354:ALA:CB	1:B:355:ILE:O	2.30	0.77
1:C:541:SER:CB	4:R:8:A:O3'	2.32	0.76
1:C:639:TYR:O	2:T:8:DT:C4'	2.33	0.76
1:C:812:ASP:OD2	4:R:8:A:H5"	1.85	0.76
1:B:266:LEU:CD2	1:B:407:LYS:HZ3	1.97	0.76
1:B:41:HIS:CE1	1:B:288:ALA:CB	2.63	0.76
1:B:812:ASP:OD1	4:Z:8:A:OP1	2.02	0.76
1:B:96:ARG:NH1	3:Y:102:DA:N3	2.32	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:337:VAL:HG21	1:B:512:LEU:HD21	1.66	0.76
1:B:201:TRP:HZ2	1:B:299:THR:C	1.89	0.76
1:B:347:CYS:SG	1:B:349:VAL:HG22	2.26	0.76
1:B:699:LEU:CD2	1:B:845:PHE:CE2	2.69	0.76
1:B:760:THR:N	2:X:21:DT:OP2	2.18	0.76
1:C:201:TRP:NE1	1:C:305:LEU:CD1	2.43	0.76
1:C:834:ASP:O	1:C:838:SER:HB2	1.86	0.76
1:C:642:LYS:CG	2:T:7:DT:C1'	2.62	0.76
1:B:51:PHE:CE1	1:B:120:LYS:HA	2.19	0.76
1:B:95:LYS:HB3	3:Y:104:DT:H5'	1.67	0.76
1:B:424:GLY:HA3	1:B:788:GLY:HA3	1.67	0.76
1:C:840:ASP:O	1:C:844:ASP:OD2	2.04	0.76
1:C:722:ARG:HH11	1:C:771:ALA:H	1.30	0.75
1:B:553:GLU:HG2	1:B:554:VAL:HG21	1.67	0.75
1:B:780:PRO:C	1:B:784:HIS:ND1	2.40	0.75
1:B:195:LEU:HD23	1:B:289:ASN:HD21	1.52	0.75
1:B:791:LEU:HD23	1:B:791:LEU:C	2.05	0.75
1:C:18:ALA:HA	1:C:161:HIS:HE1	1.51	0.75
1:B:546:PHE:CZ	1:B:783:VAL:HG11	2.22	0.75
1:C:342:THR:HG22	1:C:352:ILE:HG13	1.69	0.75
2:T:8:DT:C6	2:T:9:DT:H71	2.21	0.75
1:B:550:LEU:HD11	1:B:695:ALA:HB1	1.68	0.75
1:B:772:HIS:HD2	3:Y:130:DG:C3'	1.99	0.75
1:C:13:ASP:O	1:C:157:LEU:HD12	1.86	0.75
1:B:20:PRO:HG3	1:B:195:LEU:HD21	1.67	0.75
1:B:335:LEU:HD11	1:B:409:ALA:HB1	1.69	0.75
1:B:553:GLU:CB	1:B:554:VAL:CG2	2.65	0.75
1:C:53:LYS:C	1:C:255:ALA:HB1	2.06	0.75
1:B:553:GLU:H	1:B:555:GLY:N	1.85	0.75
1:C:781:ASN:HD21	2:T:9:DT:H4'	0.59	0.74
2:T:6:DT:H2"	2:T:7:DT:H71	0.78	0.74
1:B:98:LYS:CB	2:X:29:DA:H2	2.00	0.74
1:B:791:LEU:HD23	1:B:791:LEU:O	1.87	0.74
1:C:307:ARG:HD3	1:C:736:TRP:CZ2	2.21	0.74
1:B:565:GLU:O	1:B:880:PHE:HE2	1.70	0.74
1:B:777:GLY:O	1:B:780:PRO:HD2	1.87	0.74
1:C:313:MET:SD	1:C:733:PHE:HA	2.27	0.74
1:B:316:VAL:HG11	1:B:733:PHE:HD1	1.53	0.74
1:C:552:ASP:CB	1:C:555:GLY:H	1.95	0.74
1:B:316:VAL:HG21	1:B:733:PHE:HA	1.67	0.74
1:C:722:ARG:O	1:C:769:ILE:HG21	1.86	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:567:VAL:HG22	1:B:880:PHE:CG	2.21	0.74
1:C:21:PHE:CE2	1:C:161:HIS:HD2	2.06	0.74
1:B:95:LYS:HG2	3:Y:104:DT:H5"	1.69	0.74
1:B:474:PRO:CA	1:B:880:PHE:HZ	1.57	0.74
1:B:735:VAL:HG12	1:B:785:SER:HB2	1.67	0.74
1:C:152:GLY:O	1:C:154:ILE:N	2.19	0.74
1:C:411:HIS:O	1:C:413:ALA:N	2.21	0.74
1:C:812:ASP:OD2	4:R:8:A:C5'	2.34	0.74
1:C:833:VAL:HG22	1:C:872:LEU:O	1.88	0.74
1:B:16:LEU:HB3	1:B:289:ASN:OD1	1.87	0.74
1:B:201:TRP:CZ2	1:B:299:THR:C	2.61	0.74
1:B:707:ALA:HB1	1:B:774:GLN:CB	1.94	0.74
1:C:307:ARG:HD3	1:C:736:TRP:NE1	2.02	0.73
1:B:41:HIS:HE2	1:B:158:GLU:CD	1.91	0.73
1:C:722:ARG:NH1	1:C:771:ALA:N	2.36	0.73
1:B:404:GLN:HG3	1:B:432:PHE:HB2	1.70	0.73
1:B:704:LYS:CG	1:B:775:GLU:OE1	2.35	0.73
1:B:198:GLY:HA3	1:B:282:THR:OG1	1.88	0.73
1:C:347:CYS:SG	1:C:348:PRO:HD2	2.28	0.73
1:C:404:GLN:HG2	1:C:432:PHE:CB	2.18	0.73
1:C:722:ARG:NH1	1:C:741:LYS:NZ	2.37	0.73
1:B:349:VAL:HG21	1:B:352:ILE:CG1	2.17	0.73
1:B:563:PRO:CD	1:B:874:ASP:O	2.35	0.73
1:C:552:ASP:OD1	1:C:691:ALA:CB	2.35	0.73
1:C:850:ALA:HB3	1:C:851:ASP:HB2	0.81	0.73
1:C:339:ASN:OD1	1:C:402:LEU:HD22	1.89	0.73
1:B:28:TYR:HD1	1:B:182:PHE:HB3	1.41	0.73
1:B:780:PRO:CB	1:B:784:HIS:HE1	2.00	0.73
1:B:793:LYS:HZ3	1:B:835:THR:HG23	0.70	0.73
1:B:862:PRO:HA	1:B:863:ALA:CB	2.09	0.73
1:B:38:ALA:O	1:B:42:GLU:HB2	1.89	0.72
1:B:158:GLU:OE1	1:B:290:GLY:N	2.21	0.72
1:B:550:LEU:HD22	1:B:865:PRO:CB	2.16	0.72
1:C:182:PHE:CZ	1:C:413:ALA:HB3	2.24	0.72
1:C:642:LYS:HG2	2:T:7:DT:H1'	1.70	0.72
1:B:402:LEU:HD21	1:B:439:MET:SD	2.29	0.72
1:B:423:ARG:NH1	1:B:784:HIS:CD2	2.45	0.72
1:C:44:TYR:CZ	1:C:48:GLU:OE2	2.42	0.72
1:C:252:GLU:OE2	1:B:165:ASN:O	2.08	0.72
1:C:34:ARG:NH1	1:C:165:ASN:C	2.43	0.72
1:C:44:TYR:CE2	1:C:48:GLU:HG2	2.24	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:200:ALA:HB3	1:C:282:THR:HG21	1.70	0.72
1:B:698:TRP:CH2	1:B:849:PHE:HZ	2.07	0.72
1:C:562:LEU:CD2	1:C:874:ASP:HB2	2.20	0.72
1:B:563:PRO:HA	1:B:878:SER:HB2	1.69	0.72
1:B:562:LEU:CD1	1:B:870:LEU:HD13	2.15	0.72
1:B:563:PRO:CA	1:B:878:SER:HB2	2.19	0.72
1:B:698:TRP:NE1	1:B:861:MET:SD	2.63	0.72
1:C:554:VAL:N	1:C:555:GLY:CA	2.49	0.71
1:B:389:LYS:HA	1:B:392:LYS:HE3	1.72	0.71
1:B:727:TRP:CE2	1:B:782:PHE:CA	2.52	0.71
1:B:789:SER:N	1:B:792:ARG:NH2	2.37	0.71
1:C:722:ARG:HH11	1:C:771:ALA:N	1.88	0.71
1:B:475:PHE:N	1:B:880:PHE:CE1	2.57	0.71
1:C:553:GLU:O	1:C:557:ARG:CG	2.35	0.71
1:B:55:PHE:CZ	1:B:74:ILE:CG2	2.72	0.71
1:B:562:LEU:HD11	1:B:870:LEU:HD12	1.70	0.71
1:B:707:ALA:HB2	1:B:775:GLU:N	1.83	0.71
1:B:735:VAL:CG2	1:B:785:SER:HB3	2.21	0.71
1:C:307:ARG:CD	1:C:736:TRP:CD2	2.73	0.71
1:C:552:ASP:CG	1:C:554:VAL:O	2.29	0.71
1:C:832:MET:HE2	1:C:875:ILE:HG21	1.73	0.71
1:B:96:ARG:HH11	3:Y:102:DA:C1'	1.67	0.71
1:B:551:ARG:CG	1:B:867:LYS:HG3	2.19	0.71
1:C:21:PHE:CG	1:C:161:HIS:HB3	2.21	0.71
1:B:24:LEU:HD11	1:B:273:VAL:HG21	1.72	0.71
1:B:349:VAL:HB	1:B:352:ILE:HG12	1.70	0.71
1:B:726:HIS:CD2	1:B:736:TRP:NE1	2.58	0.71
1:C:55:PHE:CE2	1:C:74:ILE:HG21	2.25	0.71
1:C:308:TYR:CZ	1:C:734:PRO:O	2.43	0.71
1:B:772:HIS:NE2	3:Y:130:DG:C4'	2.54	0.71
1:B:801:LYS:CD	1:B:802:TYR:N	2.54	0.71
1:C:400:PHE:CE1	1:C:431:MET:CG	2.74	0.70
1:C:541:SER:HB3	4:R:8:A:C2'	2.21	0.70
1:C:553:GLU:HB3	1:C:554:VAL:HG13	0.71	0.70
1:B:704:LYS:O	1:B:775:GLU:OE1	2.10	0.70
1:C:17:ALA:O	1:C:158:GLU:HG3	1.91	0.70
1:C:642:LYS:HG2	2:T:7:DT:C1'	2.21	0.70
2:T:8:DT:H2'	2:T:9:DT:C7	2.21	0.70
2:T:11:DC:C4	2:T:12:DT:H73	2.27	0.70
1:B:12:SER:O	1:B:13:ASP:CB	2.39	0.70
1:B:195:LEU:HB3	1:B:276:LYS:NZ	2.06	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:324:GLN:HA	1:B:418:TYR:HD1	1.57	0.70
1:C:776:SER:HB2	2:T:7:DT:P	2.01	0.70
1:B:147:ASP:H	1:B:148:GLU:HG2	1.56	0.70
1:C:562:LEU:CD2	1:C:874:ASP:CB	2.69	0.70
1:C:722:ARG:HB2	1:C:769:ILE:HB	1.72	0.70
1:C:773:LYS:O	1:C:774:GLN:CB	2.38	0.70
1:B:553:GLU:H	1:B:554:VAL:C	1.95	0.70
1:C:224:THR:N	1:C:225:GLY:HA2	2.07	0.70
1:C:704:LYS:CE	1:C:775:GLU:OE2	2.38	0.70
1:B:423:ARG:HD2	1:B:784:HIS:CB	2.15	0.70
1:C:772:HIS:O	1:C:773:LYS:O	2.10	0.70
1:B:224:THR:N	1:B:225:GLY:HA2	2.07	0.70
1:B:422:TRP:HE1	2:X:10:DA:P	2.15	0.70
1:B:550:LEU:HD12	1:B:695:ALA:HB2	1.72	0.70
1:B:727:TRP:CH2	1:B:782:PHE:CA	2.59	0.70
1:C:722:ARG:HH12	1:C:741:LYS:HZ3	1.38	0.69
1:B:44:TYR:HE1	1:B:155:ARG:NH1	1.90	0.69
1:B:347:CYS:SG	1:B:349:VAL:CG2	2.80	0.69
1:B:727:TRP:CH2	1:B:782:PHE:HA	2.24	0.69
1:C:829:ARG:HB2	1:C:876:LEU:HD23	1.73	0.69
1:B:147:ASP:N	1:B:150:ARG:HG2	2.07	0.69
1:B:151:PHE:CZ	1:B:293:PRO:HD2	2.28	0.69
1:B:727:TRP:CH2	1:B:781:ASN:HB3	2.26	0.69
1:B:789:SER:HA	1:B:792:ARG:NE	2.07	0.69
1:B:811:HIS:HB2	4:Z:8:A:H5'	1.75	0.69
1:B:836:TYR:CE1	1:B:841:VAL:CG1	2.75	0.69
1:B:474:PRO:HB3	1:B:880:PHE:CZ	2.18	0.69
1:B:789:SER:N	1:B:792:ARG:CZ	2.55	0.69
1:C:14:ILE:CA	1:C:157:LEU:CD1	2.54	0.69
1:C:780:PRO:O	1:C:781:ASN:C	2.31	0.69
1:B:266:LEU:CD2	1:B:407:LYS:NZ	2.55	0.69
1:B:355:ILE:CG1	1:B:356:GLU:N	2.49	0.69
1:B:772:HIS:CD2	3:Y:130:DG:H5"	2.26	0.69
1:B:786:GLN:NE2	1:B:841:VAL:HG11	2.07	0.69
1:B:836:TYR:CE1	1:B:841:VAL:HG13	2.28	0.69
1:C:722:ARG:HE	1:C:771:ALA:HB3	1.27	0.69
1:C:737:GLN:HE22	1:C:778:ILE:CA	1.98	0.69
1:B:148:GLU:O	1:B:150:ARG:CB	2.40	0.69
1:B:269:GLN:HB3	1:B:408:PHE:CE1	2.28	0.69
1:B:347:CYS:CB	1:B:352:ILE:HG21	2.23	0.69
1:C:639:TYR:CB	2:T:8:DT:C6	2.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:96:ARG:O	3:Y:104:DT:H1'	1.93	0.69
1:B:345:LYS:O	1:B:355:ILE:HD13	1.93	0.69
1:B:729:THR:CG2	1:B:789:SER:OG	2.41	0.69
1:B:264:ILE:HG21	1:B:400:PHE:CZ	2.27	0.68
1:B:704:LYS:HA	1:B:775:GLU:CG	2.22	0.68
1:B:707:ALA:O	1:B:771:ALA:HA	1.92	0.68
1:C:401:MET:SD	1:C:440:THR:HG23	2.33	0.68
1:C:812:ASP:OD1	4:R:8:A:H5"	1.90	0.68
1:C:829:ARG:HB3	1:C:876:LEU:HD23	1.76	0.68
1:B:36:GLN:HE22	1:B:272:VAL:H	1.40	0.68
1:B:100:PRO:HA	3:Y:106:DC:OP1	1.94	0.68
1:B:735:VAL:HG21	1:B:785:SER:HB3	1.76	0.68
1:B:266:LEU:HD11	1:B:407:LYS:HZ2	1.52	0.68
1:C:367:ILE:O	1:B:345:LYS:HG2	1.93	0.68
1:B:552:ASP:CB	1:B:555:GLY:H	2.06	0.68
1:C:367:ILE:HG13	1:B:345:LYS:HZ1	1.56	0.68
2:T:6:DT:H2'	2:T:7:DT:H71	1.63	0.68
2:T:8:DT:C2'	2:T:9:DT:H71	2.24	0.68
1:B:95:LYS:CG	3:Y:104:DT:C5'	2.68	0.68
1:B:698:TRP:CH2	1:B:849:PHE:CZ	2.82	0.68
1:C:427:TYR:OH	2:T:10:DA:H1'	1.94	0.67
1:C:553:GLU:HB3	1:C:554:VAL:CB	2.00	0.67
1:C:812:ASP:CG	4:R:8:A:H5"	2.12	0.67
1:B:316:VAL:CG1	1:B:733:PHE:HD1	2.07	0.67
1:B:351:ASP:O	1:B:353:PRO:CD	2.35	0.67
1:B:553:GLU:CB	1:B:554:VAL:HG23	2.23	0.67
1:B:556:GLY:HA2	1:B:557:ARG:C	2.13	0.67
1:B:759:PRO:HA	2:X:21:DT:OP2	1.94	0.67
1:B:772:HIS:NE2	3:Y:130:DG:H4'	2.10	0.67
1:C:639:TYR:HB2	2:T:8:DT:C6	2.29	0.67
1:B:354:ALA:HA	1:B:355:ILE:CG2	2.24	0.67
1:B:524:HIS:HB2	1:B:528:TYR:HB2	1.75	0.67
1:B:730:PRO:CD	1:B:786:GLN:OE1	2.39	0.67
1:B:729:THR:HG21	1:B:792:ARG:NH2	2.09	0.67
1:B:746:ARG:NH1	2:X:21:DT:C4	2.62	0.67
1:B:151:PHE:O	1:B:155:ARG:HG3	1.93	0.67
1:C:324:GLN:HA	1:C:418:TYR:HD1	1.58	0.67
1:C:537:ASP:N	1:C:882:PHE:HB2	2.09	0.67
1:C:556:GLY:CA	1:C:557:ARG:C	2.58	0.67
1:B:145:ILE:CA	1:B:148:GLU:CD	2.63	0.67
1:B:689:VAL:HB	1:B:692:ALA:HB3	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:812:ASP:CB	4:R:8:A:H4'	2.23	0.67
1:B:42:GLU:O	1:B:266:LEU:CB	2.43	0.67
1:B:355:ILE:O	1:B:356:GLU:C	2.33	0.67
1:C:425:ARG:HH22	4:R:8:A:C1'	2.06	0.67
1:C:722:ARG:NH1	1:C:741:LYS:HZ3	1.93	0.67
1:C:722:ARG:C	1:C:769:ILE:HG21	2.15	0.67
1:C:34:ARG:CG	1:C:162:PHE:CA	2.62	0.67
1:C:552:ASP:O	1:C:870:LEU:HB2	1.95	0.67
1:C:704:LYS:HG3	1:C:775:GLU:OE2	1.95	0.67
1:B:95:LYS:HD3	3:Y:104:DT:C5'	2.24	0.67
1:B:264:ILE:CG1	1:B:400:PHE:CD2	2.78	0.67
1:C:639:TYR:CD2	2:T:8:DT:C4	2.83	0.66
1:B:264:ILE:HG12	1:B:400:PHE:CE2	2.30	0.66
1:B:746:ARG:CZ	2:X:21:DT:H71	2.25	0.66
1:C:311:VAL:HG21	1:C:734:PRO:HG3	1.76	0.66
1:B:738:GLU:C	1:B:739:TYR:CD2	2.69	0.66
1:C:554:VAL:CG2	1:C:554:VAL:O	2.39	0.66
1:B:402:LEU:CD2	1:B:439:MET:SD	2.84	0.66
1:C:722:ARG:NE	1:C:771:ALA:CA	2.47	0.66
1:C:722:ARG:HD3	1:C:771:ALA:HA	1.70	0.66
1:C:308:TYR:CE2	1:C:734:PRO:HD2	2.31	0.66
1:C:341:ILE:HD11	1:C:509:PHE:CZ	2.31	0.66
1:C:351:ASP:HA	1:C:394:ARG:NH2	2.10	0.66
1:C:639:TYR:HD2	2:T:8:DT:N3	1.91	0.66
1:C:644:PHE:HB2	3:N:126:DA:N3	2.03	0.66
2:T:6:DT:C2	2:T:7:DT:C4	2.84	0.66
1:B:100:PRO:HD3	3:Y:105:DA:C5'	2.26	0.66
1:C:636:THR:CG2	2:T:8:DT:O4	2.33	0.66
1:C:644:PHE:HB3	3:N:126:DA:N1	2.07	0.66
1:C:722:ARG:HH12	1:C:741:LYS:NZ	1.91	0.66
1:B:703:ALA:CB	1:B:778:ILE:CA	2.74	0.66
1:C:524:HIS:HB2	1:C:528:TYR:HB2	1.75	0.66
1:B:755:PHE:CD2	2:X:22:DG:H5"	2.31	0.66
1:B:791:LEU:HD12	1:B:811:HIS:O	1.96	0.66
1:C:537:ASP:N	1:C:882:PHE:HB3	2.11	0.66
1:B:55:PHE:CZ	1:B:74:ILE:CG1	2.77	0.66
1:B:195:LEU:HD23	1:B:289:ASN:ND2	2.11	0.66
1:B:756:ARG:N	2:X:23:DA:OP2	2.29	0.66
1:C:224:THR:H	1:C:225:GLY:HA2	1.59	0.66
1:B:43:SER:HB3	1:B:44:TYR:HB3	1.75	0.66
1:C:252:GLU:OE1	1:B:165:ASN:O	2.14	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:640:GLY:O	2:T:7:DT:O3'	2.14	0.66
2:T:8:DT:N1	2:T:9:DT:H71	2.11	0.66
1:B:28:TYR:OH	1:B:182:PHE:O	2.14	0.66
1:B:96:ARG:CD	3:Y:102:DA:N3	2.58	0.66
1:B:205:HIS:O	1:B:206:LYS:C	2.34	0.66
1:B:224:THR:H	1:B:225:GLY:HA2	1.60	0.66
1:B:474:PRO:N	1:B:880:PHE:CE1	2.62	0.66
1:C:553:GLU:H	1:C:554:VAL:CA	2.09	0.65
1:C:553:GLU:H	1:C:554:VAL:CB	2.08	0.65
2:T:8:DT:H2"	2:T:9:DT:O5'	1.96	0.65
1:B:475:PHE:CD2	1:B:879:ASP:CB	2.61	0.65
1:B:44:TYR:HE1	1:B:155:ARG:HH11	1.43	0.65
1:B:98:LYS:HB2	2:X:29:DA:N3	2.12	0.65
1:B:563:PRO:HG3	1:B:874:ASP:HB3	1.75	0.65
1:B:793:LYS:HZ2	1:B:835:THR:HG22	1.49	0.65
1:C:780:PRO:C	1:C:783:VAL:HG23	2.17	0.65
1:B:554:VAL:H	1:B:557:ARG:HB2	1.60	0.65
1:B:563:PRO:CD	1:B:874:ASP:C	2.64	0.65
1:B:145:ILE:O	1:B:145:ILE:CG2	2.45	0.65
1:B:326:THR:HG23	1:B:807:PHE:H	1.61	0.65
1:C:425:ARG:NH2	4:R:8:A:H1'	2.05	0.65
1:C:539:SER:HB2	1:C:559:VAL:O	1.97	0.65
1:C:562:LEU:HD23	1:C:874:ASP:HB2	1.77	0.65
1:B:147:ASP:O	1:B:152:GLY:N	2.30	0.65
1:B:703:ALA:HB2	1:B:778:ILE:CA	2.27	0.65
1:B:727:TRP:HH2	1:B:781:ASN:HB3	1.58	0.65
1:B:98:LYS:N	3:Y:104:DT:O2	2.30	0.65
1:B:150:ARG:CA	1:B:150:ARG:NE	2.54	0.65
1:B:545:HIS:HE1	1:B:790:HIS:CD2	2.15	0.65
1:B:563:PRO:CG	1:B:874:ASP:CB	2.69	0.65
1:B:704:LYS:CA	1:B:775:GLU:HG2	2.26	0.65
1:B:780:PRO:O	1:B:784:HIS:ND1	2.30	0.65
1:B:788:GLY:C	1:B:792:ARG:NH1	2.50	0.65
1:B:354:ALA:HB1	1:B:355:ILE:HG13	1.66	0.65
1:B:553:GLU:CB	1:B:554:VAL:C	2.65	0.65
1:C:411:HIS:O	1:C:412:LYS:C	2.35	0.65
1:C:639:TYR:HB3	2:T:8:DT:C2	2.20	0.65
1:B:350:GLU:O	1:B:352:ILE:N	2.30	0.65
1:C:639:TYR:OH	4:R:8:A:N3	2.24	0.65
1:C:737:GLN:NE2	1:C:778:ILE:HG13	2.11	0.65
1:B:54:MET:H	1:B:255:ALA:CB	1.98	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:729:THR:HG23	1:B:789:SER:HB3	1.56	0.65
1:B:730:PRO:CB	1:B:835:THR:HG22	2.25	0.65
1:B:731:ASP:CB	1:B:793:LYS:CG	2.60	0.65
1:C:639:TYR:CE1	2:T:8:DT:O2	2.50	0.64
1:B:553:GLU:HB3	1:B:554:VAL:C	2.17	0.64
1:B:563:PRO:HG3	1:B:874:ASP:O	1.97	0.64
1:B:707:ALA:CB	1:B:771:ALA:O	2.44	0.64
1:C:324:GLN:HE21	1:C:418:TYR:H	1.46	0.64
1:B:354:ALA:O	1:B:395:ARG:HD3	1.96	0.64
1:B:705:LEU:CD1	1:B:857:GLN:HG2	2.24	0.64
1:C:351:ASP:C	1:C:394:ARG:NH2	2.51	0.64
1:C:552:ASP:CB	1:C:555:GLY:N	2.46	0.64
1:B:148:GLU:O	1:B:150:ARG:HB3	1.97	0.64
1:C:146:GLU:OE1	1:C:202:SER:OG	2.16	0.64
1:B:424:GLY:C	1:B:792:ARG:NH1	2.50	0.64
1:C:690:VAL:O	1:C:693:VAL:N	2.30	0.64
1:B:52:ARG:HA	1:B:55:PHE:CB	2.26	0.64
1:B:147:ASP:HA	1:B:150:ARG:HG2	1.65	0.64
1:B:147:ASP:C	1:B:152:GLY:H	2.00	0.64
1:B:335:LEU:HD11	1:B:409:ALA:CB	2.27	0.64
1:B:698:TRP:CZ2	1:B:849:PHE:HZ	2.16	0.64
1:B:801:LYS:HD3	1:B:802:TYR:N	2.13	0.64
1:B:330:ILE:HD13	1:B:444:LEU:HD23	1.80	0.64
1:C:780:PRO:CA	1:C:783:VAL:HG22	2.15	0.64
1:B:553:GLU:HB2	1:B:554:VAL:O	1.98	0.64
1:B:562:LEU:HD21	1:B:870:LEU:CG	2.25	0.64
1:C:404:GLN:HG3	1:C:408:PHE:HE2	1.63	0.64
1:B:400:PHE:CZ	1:B:431:MET:HG2	2.32	0.64
1:B:538:GLY:HA2	1:B:883:ALA:HB3	1.79	0.64
1:B:560:ASN:O	1:B:881:ALA:CB	2.46	0.64
1:C:44:TYR:CE2	1:C:48:GLU:OE2	2.51	0.64
1:C:642:LYS:HB2	2:T:7:DT:O2	1.98	0.64
1:B:145:ILE:CA	1:B:148:GLU:HG3	2.26	0.64
1:B:195:LEU:HB3	1:B:276:LYS:HZ1	1.60	0.64
1:B:320:ILE:CD1	1:B:420:MET:SD	2.79	0.64
1:C:349:VAL:HG22	1:C:352:ILE:HB	1.79	0.63
1:B:422:TRP:CE2	2:X:10:DA:OP1	2.51	0.63
1:B:704:LYS:CA	1:B:775:GLU:CG	2.77	0.63
1:C:690:VAL:O	1:C:691:ALA:C	2.36	0.63
1:B:757:LEU:HD12	2:X:22:DG:OP1	1.98	0.63
1:B:840:ASP:HB3	1:B:843:ALA:CB	2.21	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:737:GLN:CD	1:C:778:ILE:HG13	2.18	0.63
1:C:774:GLN:HB3	1:C:778:ILE:HD12	1.81	0.63
2:T:3:DC:H2"	2:T:4:DG:OP2	1.98	0.63
1:B:146:GLU:CA	1:B:148:GLU:HG3	2.26	0.63
1:B:726:HIS:CD2	1:B:736:TRP:CD1	2.85	0.63
1:B:791:LEU:HD12	1:B:811:HIS:HA	1.81	0.63
1:C:351:ASP:C	1:C:394:ARG:HH22	1.99	0.63
1:C:553:GLU:OE2	1:C:869:ASN:HB2	1.98	0.63
1:C:850:ALA:CA	1:C:851:ASP:HB2	2.28	0.63
3:N:127:DA:H2"	3:N:128:DA:OP2	1.98	0.63
3:N:128:DA:H2"	3:N:129:DC:OP2	1.99	0.63
1:B:746:ARG:CZ	2:X:21:DT:C5	2.81	0.63
2:X:2:DC:H2"	2:X:3:DC:OP2	1.99	0.63
2:X:5:DT:H2"	2:X:6:DT:OP2	1.99	0.63
3:Y:129:DC:H2"	3:Y:130:DG:OP2	1.99	0.63
1:C:642:LYS:HG3	2:T:7:DT:H1'	1.80	0.63
2:T:4:DG:H2"	2:T:5:DT:OP2	1.99	0.63
3:N:126:DA:H2"	3:N:127:DA:OP2	1.98	0.63
3:N:131:DG:H2"	3:N:132:DC:OP2	1.98	0.63
1:B:404:GLN:CG	1:B:432:PHE:HB2	2.28	0.63
2:X:4:DG:H2"	2:X:5:DT:OP2	1.98	0.63
2:X:12:DT:H2"	2:X:13:DC:OP2	1.98	0.63
1:C:308:TYR:OH	1:C:734:PRO:O	2.15	0.63
1:B:201:TRP:CH2	1:B:300:HIS:C	2.72	0.63
3:Y:127:DA:H2"	3:Y:128:DA:OP2	1.99	0.63
1:C:366:ASP:C	1:C:368:ASP:HB2	2.19	0.63
2:T:5:DT:H2"	2:T:6:DT:OP2	1.98	0.63
1:B:43:SER:CB	1:B:44:TYR:HB2	2.21	0.63
1:B:727:TRP:CZ2	1:B:782:PHE:C	2.72	0.63
1:B:727:TRP:CD2	1:B:782:PHE:HA	2.29	0.63
3:N:130:DG:H2"	3:N:131:DG:OP2	1.99	0.62
1:B:551:ARG:HD2	1:B:867:LYS:CD	2.20	0.62
1:B:553:GLU:CA	1:B:554:VAL:C	2.66	0.62
1:C:14:ILE:CD1	1:C:157:LEU:HD11	2.22	0.62
1:C:829:ARG:HB3	1:C:876:LEU:HA	1.81	0.62
1:B:147:ASP:CA	1:B:148:GLU:HB2	2.29	0.62
1:B:565:GLU:O	1:B:880:PHE:CE2	2.52	0.62
1:C:550:LEU:HD11	1:C:695:ALA:HB2	1.81	0.62
1:B:100:PRO:CA	3:Y:106:DC:OP1	2.47	0.62
1:B:366:ASP:C	1:B:368:ASP:HB2	2.19	0.62
1:C:401:MET:SD	1:C:440:THR:HG21	2.37	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:722:ARG:CZ	1:C:771:ALA:N	2.58	0.62
1:B:567:VAL:HG22	1:B:880:PHE:CB	2.29	0.62
1:B:689:VAL:O	1:B:692:ALA:HB3	1.98	0.62
2:X:3:DC:H2"	2:X:4:DG:OP2	1.99	0.62
2:X:11:DC:H2"	2:X:12:DT:OP2	1.99	0.62
3:Y:128:DA:H2"	3:Y:129:DC:OP2	1.99	0.62
1:B:341:ILE:HD11	1:B:509:PHE:CE1	2.34	0.62
1:B:354:ALA:HA	1:B:355:ILE:HG23	1.81	0.62
1:B:553:GLU:N	1:B:554:VAL:O	2.31	0.62
1:C:541:SER:HB3	4:R:8:A:C3'	2.29	0.62
1:B:100:PRO:CA	3:Y:105:DA:O3'	2.44	0.62
1:B:759:PRO:HA	2:X:21:DT:OP1	1.99	0.62
2:X:13:DC:H2"	2:X:14:DC:OP2	1.99	0.62
2:X:14:DC:H2"	2:X:15:DC:OP2	1.99	0.62
1:C:182:PHE:CE2	1:C:415:TRP:CH2	2.85	0.62
1:C:553:GLU:N	1:C:554:VAL:O	2.26	0.62
1:B:562:LEU:CD1	1:B:870:LEU:HD12	2.19	0.62
1:B:698:TRP:HZ2	1:B:846:TYR:HD2	1.46	0.62
3:Y:126:DA:H2"	3:Y:127:DA:OP2	1.99	0.62
1:C:20:PRO:HB2	1:C:158:GLU:OE2	2.00	0.62
1:C:351:ASP:HA	1:C:394:ARG:HH21	1.64	0.62
1:C:780:PRO:C	1:C:782:PHE:N	2.52	0.62
1:B:147:ASP:CA	1:B:148:GLU:CB	2.77	0.62
2:T:2:DC:H2"	2:T:3:DC:OP2	1.98	0.61
2:T:6:DT:C2'	2:T:7:DT:H73	2.29	0.61
1:B:36:GLN:HE22	1:B:272:VAL:N	1.97	0.61
2:X:1:DG:H2"	2:X:2:DC:OP2	1.99	0.61
1:C:307:ARG:CB	1:C:736:TRP:CZ3	2.82	0.61
1:C:475:PHE:HE2	1:C:879:ASP:CB	2.00	0.61
1:B:772:HIS:CD2	3:Y:130:DG:H4'	2.33	0.61
1:C:153:ARG:O	1:C:155:ARG:N	2.33	0.61
1:C:221:ILE:O	1:C:221:ILE:HG22	2.00	0.61
1:C:401:MET:SD	1:C:440:THR:OG1	2.58	0.61
1:C:553:GLU:CA	1:C:554:VAL:HG13	2.27	0.61
1:C:816:THR:HG22	1:C:817:ILE:N	2.16	0.61
2:T:11:DC:N1	2:T:12:DT:H71	2.15	0.61
1:B:707:ALA:HB3	1:B:775:GLU:CA	2.30	0.61
3:Y:131:DG:H2"	3:Y:132:DC:OP2	1.98	0.61
1:C:423:ARG:HH12	2:T:9:DT:C2'	2.12	0.61
1:C:375:THR:H	1:C:376:ALA:C	2.04	0.61
2:T:1:DG:H2"	2:T:2:DC:OP2	1.98	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:841:VAL:HG23	1:B:842:LEU:HD12	1.83	0.61
1:C:563:PRO:HD2	1:C:874:ASP:HB3	1.82	0.61
3:N:129:DC:H2"	3:N:130:DG:OP2	1.98	0.61
1:C:20:PRO:CG	1:C:158:GLU:OE2	2.49	0.61
2:T:6:DT:H2'	2:T:7:DT:H73	1.82	0.61
1:B:537:ASP:C	1:B:883:ALA:HB3	2.21	0.61
1:C:8:LYS:HE2	1:C:289:ASN:OD1	1.99	0.61
1:C:17:ALA:HB1	1:C:158:GLU:CA	2.31	0.61
1:C:722:ARG:HB3	1:C:769:ILE:HG22	1.83	0.61
1:B:96:ARG:NE	3:Y:103:DA:O4'	2.34	0.61
1:B:850:ALA:CA	1:B:851:ASP:HB2	2.28	0.61
1:B:148:GLU:O	1:B:149:ALA:C	2.38	0.61
1:C:541:SER:HB3	4:R:8:A:O2'	2.01	0.61
1:B:97:GLY:CA	2:X:30:DT:O2	2.45	0.61
1:C:249:GLU:CD	1:B:30:GLU:OE2	2.39	0.60
1:C:553:GLU:N	1:C:554:VAL:CA	2.64	0.60
1:B:10:ASP:O	1:B:11:PHE:HB2	2.01	0.60
1:B:367:ILE:N	1:B:368:ASP:HB2	2.15	0.60
1:C:689:VAL:O	1:C:693:VAL:HG23	2.00	0.60
1:B:811:HIS:CG	4:Z:7:A:HO2'	2.04	0.60
3:Y:130:DG:H2"	3:Y:131:DG:OP2	1.98	0.60
1:B:375:THR:H	1:B:376:ALA:C	2.04	0.60
1:C:537:ASP:CA	1:C:882:PHE:HB2	2.31	0.60
1:B:552:ASP:OD1	1:B:691:ALA:HB3	2.01	0.60
1:B:746:ARG:NH2	2:X:21:DT:C5	2.69	0.60
1:C:146:GLU:CD	1:C:202:SER:OG	2.40	0.60
1:C:772:HIS:O	1:C:773:LYS:C	2.39	0.60
2:T:8:DT:H2'	2:T:9:DT:C5	2.36	0.60
1:B:707:ALA:HA	1:B:774:GLN:CB	2.30	0.60
1:C:21:PHE:CG	1:C:161:HIS:CB	2.73	0.60
1:C:297:VAL:CG2	1:C:733:PHE:HE1	2.14	0.60
1:B:221:ILE:HG22	1:B:221:ILE:O	2.01	0.60
1:B:735:VAL:CG1	1:B:785:SER:OG	2.34	0.60
1:B:816:THR:HG22	1:B:817:ILE:N	2.16	0.60
1:C:367:ILE:N	1:C:368:ASP:HB2	2.16	0.60
1:C:451:PRO:CA	1:C:452:ILE:HB	2.09	0.60
1:B:308:TYR:CE2	1:B:736:TRP:HZ3	2.20	0.60
1:B:556:GLY:HA2	1:B:558:ALA:N	2.17	0.60
1:C:342:THR:HG22	1:C:352:ILE:CD1	2.31	0.60
1:C:404:GLN:O	1:C:408:PHE:CD2	2.55	0.60
2:T:8:DT:C2'	2:T:9:DT:O5'	2.50	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:146:GLU:HG3	1:B:204:TRP:CE2	2.37	0.60
1:B:746:ARG:NH1	2:X:21:DT:H71	2.17	0.60
1:C:552:ASP:CB	1:C:554:VAL:C	2.66	0.60
1:C:695:ALA:HA	1:C:865:PRO:HG2	1.83	0.60
1:B:270:PRO:CD	1:B:408:PHE:CZ	2.85	0.60
1:C:544:GLN:O	1:C:561:LEU:HD21	2.02	0.60
1:B:45:GLU:OE1	1:B:162:PHE:HZ	1.84	0.59
1:B:422:TRP:HE1	2:X:10:DA:H5"	1.66	0.59
1:B:786:GLN:HE21	1:B:841:VAL:HG11	1.67	0.59
1:B:801:LYS:C	1:B:801:LYS:CD	2.70	0.59
1:C:556:GLY:N	1:C:557:ARG:HB2	2.17	0.59
1:C:707:ALA:O	1:C:771:ALA:C	2.39	0.59
1:C:832:MET:HE2	1:C:875:ILE:HD13	1.83	0.59
2:T:8:DT:C2'	2:T:9:DT:C6	2.73	0.59
1:B:147:ASP:CB	1:B:150:ARG:HG2	2.23	0.59
1:B:148:GLU:O	1:B:150:ARG:N	2.35	0.59
1:C:644:PHE:CD2	3:N:126:DA:N6	2.71	0.59
1:B:50:ARG:HA	1:B:53:LYS:HD3	1.84	0.59
1:B:704:LYS:C	1:B:775:GLU:CG	2.46	0.59
1:C:270:PRO:HD3	1:C:404:GLN:OE1	2.02	0.59
1:C:404:GLN:HG2	1:C:432:PHE:HB3	1.84	0.59
1:C:553:GLU:C	1:C:554:VAL:HG13	2.19	0.59
1:B:205:HIS:C	1:B:207:GLU:N	2.56	0.59
1:C:738:GLU:C	1:C:774:GLN:NE2	2.56	0.59
1:C:804:ILE:HG12	1:C:820:ASP:HB3	1.85	0.59
1:B:44:TYR:CE1	1:B:155:ARG:CD	2.75	0.59
1:B:278:TRP:H	1:B:321:ASN:HD21	1.51	0.59
1:B:730:PRO:CG	1:B:786:GLN:HE22	2.16	0.59
1:C:105:PHE:HB3	1:C:204:TRP:CZ2	2.37	0.59
1:C:308:TYR:CD2	1:C:734:PRO:HD2	2.38	0.59
1:C:319:ALA:CB	1:C:792:ARG:HB3	2.33	0.59
1:B:149:ALA:CB	1:B:150:ARG:HA	2.26	0.59
1:B:707:ALA:HA	1:B:774:GLN:HG2	1.84	0.59
1:B:777:GLY:C	1:B:780:PRO:HD2	2.23	0.59
1:B:804:ILE:HG12	1:B:820:ASP:HB3	1.84	0.59
1:B:341:ILE:HD11	1:B:509:PHE:HZ	1.64	0.59
1:B:424:GLY:C	1:B:792:ARG:HH11	2.06	0.59
1:C:105:PHE:HD2	1:C:204:TRP:CZ2	2.21	0.59
1:B:96:ARG:O	3:Y:104:DT:C1'	2.51	0.59
1:B:320:ILE:HD11	1:B:420:MET:CG	2.32	0.59
1:B:326:THR:CG2	1:B:807:PHE:H	2.15	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:730:PRO:CB	1:B:793:LYS:HZ2	2.15	0.59
1:B:730:PRO:HB2	1:B:793:LYS:HD2	1.83	0.59
1:C:39:LEU:HD21	1:C:408:PHE:CE1	2.38	0.58
1:B:31:ARG:HG3	1:B:32:LEU:N	2.17	0.58
1:B:41:HIS:NE2	1:B:158:GLU:CD	2.57	0.58
1:B:349:VAL:HG21	1:B:352:ILE:HG13	1.83	0.58
1:B:424:GLY:CA	1:B:792:ARG:HH11	2.12	0.58
1:B:552:ASP:CG	1:B:555:GLY:N	2.40	0.58
1:C:8:LYS:CE	1:C:289:ASN:OD1	2.52	0.58
1:C:342:THR:HG22	1:C:352:ILE:CG1	2.33	0.58
1:B:545:HIS:HE1	1:B:790:HIS:CG	2.21	0.58
1:C:557:ARG:HG2	1:C:562:LEU:HD12	1.85	0.58
1:B:44:TYR:OH	1:B:155:ARG:CB	2.52	0.58
1:B:707:ALA:O	1:B:771:ALA:O	2.22	0.58
1:B:41:HIS:NE2	1:B:158:GLU:OE1	2.27	0.58
1:B:772:HIS:CD2	3:Y:130:DG:C5'	2.83	0.58
1:C:105:PHE:CD2	1:C:204:TRP:CZ2	2.92	0.58
1:C:332:LYS:HE2	1:C:410:ASN:HD22	1.69	0.58
1:C:722:ARG:CB	1:C:769:ILE:HG22	2.33	0.58
1:C:400:PHE:CE1	1:C:431:MET:HG2	2.38	0.58
1:C:722:ARG:HH11	1:C:770:ASP:CA	2.16	0.58
1:C:814:PHE:HE1	1:C:883:ALA:HB1	1.68	0.58
1:B:96:ARG:NH1	3:Y:102:DA:N9	2.45	0.58
1:B:146:GLU:C	1:B:148:GLU:CG	2.71	0.58
1:B:451:PRO:CA	1:B:452:ILE:HB	2.09	0.58
1:C:52:ARG:HA	1:C:55:PHE:HB2	1.84	0.58
1:C:324:GLN:HA	1:C:418:TYR:CD1	2.37	0.58
1:C:552:ASP:CG	1:C:691:ALA:HB3	2.25	0.58
1:C:14:ILE:HD13	1:C:157:LEU:HD21	1.86	0.58
1:C:17:ALA:HB3	1:C:157:LEU:HB3	1.86	0.58
1:C:370:ASN:HB3	1:C:371:PRO:CD	2.29	0.58
1:C:748:ASN:HB3	3:N:106:DC:H2"	1.86	0.58
1:B:36:GLN:NE2	1:B:272:VAL:H	1.99	0.58
1:B:354:ALA:C	1:B:355:ILE:HG23	2.23	0.58
1:C:13:ASP:HA	1:C:154:ILE:HG12	1.86	0.58
1:B:354:ALA:HB2	1:B:355:ILE:HG13	1.86	0.58
1:B:756:ARG:NH2	2:X:24:DG:O6	2.25	0.58
1:C:562:LEU:HD23	1:C:874:ASP:CB	2.33	0.57
1:C:832:MET:CE	1:C:875:ILE:HD13	2.33	0.57
1:B:152:GLY:HA2	1:B:155:ARG:NE	2.19	0.57
1:B:324:GLN:HA	1:B:418:TYR:CD1	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:559:VAL:HG23	1:B:561:LEU:HD13	1.86	0.57
1:C:183:MET:SD	1:C:448:LYS:HB3	2.44	0.57
1:C:559:VAL:HG23	1:C:561:LEU:HD13	1.86	0.57
1:C:837:GLU:H	1:C:872:LEU:CD1	2.17	0.57
2:T:11:DC:C5	2:T:12:DT:H73	2.38	0.57
1:C:401:MET:HE2	1:C:432:PHE:HD1	1.69	0.57
2:T:11:DC:C2	2:T:12:DT:C7	2.87	0.57
1:C:39:LEU:CD2	1:C:408:PHE:HE1	2.16	0.57
1:C:544:GLN:CD	1:C:561:LEU:CD1	2.72	0.57
1:C:297:VAL:CG2	1:C:733:PHE:CE1	2.88	0.57
1:C:644:PHE:CD2	3:N:126:DA:C6	2.70	0.57
1:C:739:TYR:O	1:C:770:ASP:HB3	2.05	0.57
1:C:816:THR:HG22	1:C:817:ILE:H	1.69	0.57
1:B:147:ASP:CG	1:B:150:ARG:HG3	2.24	0.57
1:B:705:LEU:CB	1:B:857:GLN:HE21	2.09	0.57
1:C:722:ARG:HB2	1:C:769:ILE:CB	2.35	0.57
1:C:105:PHE:HB3	1:C:204:TRP:CH2	2.40	0.57
1:C:278:TRP:H	1:C:321:ASN:HD21	1.51	0.57
1:B:186:VAL:HB	1:B:287:TRP:HH2	1.69	0.57
1:B:330:ILE:HD13	1:B:444:LEU:CD2	2.35	0.57
1:C:21:PHE:CB	1:C:161:HIS:CG	2.88	0.57
1:C:544:GLN:CB	1:C:561:LEU:CD1	2.74	0.57
1:B:563:PRO:HB3	1:B:878:SER:N	2.19	0.57
2:X:10:DA:H1'	2:X:11:DC:C5'	2.34	0.57
1:C:639:TYR:CE2	4:R:8:A:N1	2.72	0.57
1:B:475:PHE:HE1	1:B:882:PHE:HE1	1.51	0.57
1:B:779:ALA:N	1:B:780:PRO:HD2	2.18	0.57
1:C:779:ALA:CB	1:C:780:PRO:CD	2.75	0.57
1:C:316:VAL:HG21	1:C:733:PHE:HB2	1.86	0.56
2:T:12:DT:H2'	2:T:13:DC:H6	1.71	0.56
1:C:307:ARG:O	1:C:736:TRP:HH2	1.87	0.56
1:C:727:TRP:HB3	1:C:845:PHE:CD1	2.39	0.56
2:T:10:DA:H2'	2:T:11:DC:H6	1.70	0.56
2:T:13:DC:H2'	2:T:14:DC:H6	1.71	0.56
1:B:100:PRO:CD	3:Y:105:DA:H4'	2.35	0.56
1:B:330:ILE:HG13	1:B:409:ALA:O	2.04	0.56
1:B:356:GLU:OE2	1:B:356:GLU:CA	2.34	0.56
1:C:34:ARG:HA	1:C:162:PHE:HB3	1.87	0.56
1:C:270:PRO:CD	1:C:404:GLN:OE1	2.53	0.56
1:C:326:THR:HG21	1:C:807:PHE:O	2.05	0.56
2:T:11:DC:C2	2:T:12:DT:C5	2.93	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:354:ALA:CA	1:B:355:ILE:HG23	2.35	0.56
1:B:400:PHE:CE1	1:B:431:MET:HG2	2.40	0.56
2:T:11:DC:C6	2:T:12:DT:H71	2.40	0.56
2:T:12:DT:C2	2:T:13:DC:C5	2.94	0.56
1:C:156:ASP:O	1:C:160:LYS:HG3	2.05	0.56
1:B:704:LYS:CA	1:B:775:GLU:HB3	2.09	0.56
1:B:816:THR:HG22	1:B:817:ILE:H	1.70	0.56
4:R:5:G:H2'	4:R:6:U:H6	1.71	0.56
1:C:31:ARG:HG3	1:C:32:LEU:N	2.17	0.56
1:B:147:ASP:N	1:B:147:ASP:OD1	2.38	0.56
1:B:791:LEU:C	1:B:791:LEU:CD2	2.72	0.56
1:C:105:PHE:CD2	1:C:204:TRP:CE2	2.94	0.56
1:C:544:GLN:CD	1:C:561:LEU:HD11	2.25	0.56
1:B:40:GLU:C	1:B:42:GLU:H	2.08	0.56
1:B:297:VAL:HG13	1:B:422:TRP:HA	1.88	0.56
1:B:396:ILE:HG22	2:X:14:DC:OP1	2.06	0.56
1:B:424:GLY:CA	1:B:788:GLY:HA3	2.35	0.56
1:B:731:ASP:OD1	1:B:789:SER:CB	2.46	0.56
1:B:801:LYS:HD2	1:B:802:TYR:N	2.21	0.56
1:C:180:LYS:HB3	1:C:181:ALA:HA	1.87	0.56
1:C:297:VAL:CG1	1:C:422:TRP:HA	2.36	0.56
1:C:400:PHE:HE1	1:C:431:MET:CB	2.10	0.56
1:C:739:TYR:CD2	1:C:770:ASP:HB3	2.40	0.56
1:C:832:MET:CE	1:C:875:ILE:HG21	2.36	0.56
1:B:556:GLY:HA3	1:B:559:VAL:HG22	1.88	0.56
1:B:829:ARG:NH2	1:B:881:ALA:O	2.38	0.56
4:Z:5:G:H2'	4:Z:6:U:H6	1.71	0.56
1:B:9:ASN:HD21	1:B:157:LEU:HD21	1.71	0.56
1:B:53:LYS:HB3	1:B:54:MET:HB2	1.88	0.56
1:B:704:LYS:CA	1:B:775:GLU:CB	2.67	0.56
1:B:779:ALA:N	1:B:780:PRO:CD	2.69	0.56
1:C:21:PHE:HD2	1:C:161:HIS:CD2	2.13	0.55
1:C:39:LEU:HD21	1:C:408:PHE:HE1	1.69	0.55
1:C:222:GLU:HB2	1:C:223:SER:OG	2.06	0.55
1:C:252:GLU:OE2	1:B:34:ARG:NH1	2.40	0.55
1:C:331:ASN:N	1:C:443:LEU:O	2.32	0.55
1:C:351:ASP:CA	1:C:394:ARG:NH2	2.70	0.55
1:C:367:ILE:HG13	1:B:345:LYS:HZ3	1.70	0.55
1:C:553:GLU:CB	1:C:554:VAL:HG11	2.10	0.55
1:C:739:TYR:CD2	1:C:770:ASP:OD2	2.59	0.55
1:B:180:LYS:HB3	1:B:181:ALA:HA	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:342:THR:HG21	1:B:402:LEU:HD21	1.88	0.55
1:C:20:PRO:CB	1:C:158:GLU:OE2	2.54	0.55
1:C:536:PHE:CA	1:C:882:PHE:HB3	2.36	0.55
4:R:5:G:C4	4:R:6:U:C5	2.95	0.55
2:T:14:DC:C2	2:T:15:DC:C5	2.94	0.55
1:B:151:PHE:CZ	1:B:293:PRO:CD	2.89	0.55
1:B:270:PRO:HD3	1:B:408:PHE:CZ	2.41	0.55
1:B:563:PRO:HG3	1:B:874:ASP:CB	2.36	0.55
1:B:794:THR:HG21	1:B:814:PHE:CE2	2.40	0.55
1:C:722:ARG:CZ	1:C:771:ALA:CB	2.72	0.55
1:B:146:GLU:HG3	1:B:204:TRP:CZ2	2.41	0.55
1:B:222:GLU:HB2	1:B:223:SER:OG	2.06	0.55
1:B:733:PHE:HB3	1:B:792:ARG:NH2	2.21	0.55
1:C:21:PHE:CE2	1:C:161:HIS:CD2	2.84	0.55
1:B:100:PRO:HD3	3:Y:105:DA:H4'	1.88	0.55
1:C:840:ASP:O	1:C:844:ASP:CG	2.44	0.55
2:T:10:DA:C4	2:T:11:DC:C5	2.94	0.55
1:B:150:ARG:CZ	1:B:150:ARG:HA	2.33	0.55
2:T:13:DC:C2	2:T:14:DC:C5	2.94	0.55
2:T:14:DC:H2'	2:T:15:DC:H6	1.70	0.55
1:B:40:GLU:C	1:B:42:GLU:N	2.58	0.55
1:B:703:ALA:O	1:B:775:GLU:CA	2.32	0.55
1:B:729:THR:CB	1:B:789:SER:OG	2.55	0.55
1:B:811:HIS:CE1	4:Z:7:A:O2'	2.57	0.55
2:X:7:DT:P	2:X:7:DT:H2'	2.47	0.55
1:B:731:ASP:HB3	1:B:793:LYS:CD	2.36	0.55
1:B:735:VAL:HG11	1:B:785:SER:HG	1.72	0.55
1:B:746:ARG:NH1	2:X:21:DT:C5	2.75	0.55
1:B:149:ALA:CB	1:B:150:ARG:HH11	2.19	0.55
1:B:727:TRP:CH2	1:B:781:ASN:HB2	2.39	0.55
1:C:780:PRO:C	1:C:783:VAL:CG2	2.73	0.55
1:B:729:THR:HG21	1:B:792:ARG:HH22	1.71	0.55
1:B:730:PRO:HB3	1:B:835:THR:CG2	2.33	0.55
1:C:200:ALA:CB	1:C:293:PRO:HG2	2.37	0.54
1:B:24:LEU:HD11	1:B:273:VAL:HG11	1.89	0.54
1:B:330:ILE:HG13	1:B:408:PHE:O	2.06	0.54
1:C:37:LEU:HB2	1:C:162:PHE:CD1	2.42	0.54
1:C:562:LEU:HD22	1:C:874:ASP:CB	2.37	0.54
1:C:707:ALA:O	1:C:771:ALA:O	2.25	0.54
1:C:722:ARG:HE	1:C:771:ALA:HB2	1.43	0.54
1:B:354:ALA:HB1	1:B:355:ILE:CA	2.32	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:370:ASN:HB3	1:B:371:PRO:CD	2.29	0.54
1:C:249:GLU:CG	1:B:30:GLU:OE2	2.55	0.54
1:C:307:ARG:HB2	1:C:736:TRP:CZ3	2.43	0.54
1:C:737:GLN:O	1:C:737:GLN:HG2	2.07	0.54
1:B:547:SER:CA	1:B:552:ASP:HB2	2.36	0.54
1:B:556:GLY:HA2	1:B:559:VAL:H	1.71	0.54
1:C:17:ALA:HB2	1:C:154:ILE:HG23	1.88	0.54
1:C:552:ASP:CA	1:C:554:VAL:O	2.55	0.54
1:B:44:TYR:OH	1:B:155:ARG:HB3	2.07	0.54
1:B:147:ASP:H	1:B:148:GLU:CG	2.15	0.54
1:B:264:ILE:CA	1:B:265:SER:HB3	2.33	0.54
1:B:266:LEU:CG	1:B:407:LYS:HZ3	2.19	0.54
4:Z:5:G:C4	4:Z:6:U:C5	2.95	0.54
1:C:375:THR:N	1:C:376:ALA:O	2.41	0.54
1:C:541:SER:CB	4:R:8:A:O2'	2.56	0.54
1:C:543:ILE:HB	1:C:559:VAL:HG11	1.88	0.54
1:B:48:GLU:OE1	1:B:120:LYS:HE3	2.07	0.54
1:B:147:ASP:HA	1:B:148:GLU:C	2.26	0.54
1:C:14:ILE:CD1	1:C:157:LEU:HD21	2.37	0.54
1:C:17:ALA:CB	1:C:157:LEU:HB2	2.38	0.54
1:C:307:ARG:HB3	1:C:736:TRP:CZ3	2.32	0.54
1:C:835:THR:O	1:C:836:TYR:CD1	2.60	0.54
2:T:6:DT:H2"	2:T:7:DT:OP2	2.08	0.54
1:B:729:THR:OG1	1:B:786:GLN:OE1	2.25	0.54
1:C:408:PHE:C	1:C:411:HIS:CD2	2.81	0.54
1:B:43:SER:CB	1:B:44:TYR:CB	2.76	0.54
1:B:266:LEU:HD11	1:B:407:LYS:CE	2.36	0.54
1:B:334:VAL:HG21	1:B:513:ALA:HB2	1.90	0.54
1:B:639:TYR:HB3	2:X:8:DT:O2	2.08	0.54
1:B:474:PRO:N	1:B:880:PHE:CZ	2.70	0.54
1:B:538:GLY:N	1:B:883:ALA:CB	2.60	0.54
1:C:13:ASP:C	1:C:157:LEU:HD12	2.28	0.54
1:B:51:PHE:CE2	1:B:120:LYS:HG2	2.43	0.54
1:B:98:LYS:O	3:Y:105:DA:O4'	2.25	0.54
1:B:375:THR:N	1:B:376:ALA:O	2.41	0.54
1:C:44:TYR:HE2	1:C:48:GLU:CG	2.20	0.53
1:B:316:VAL:HG11	1:B:733:PHE:CD1	2.38	0.53
1:B:333:LYS:HD3	1:B:516:PHE:HB3	1.90	0.53
1:B:698:TRP:CD1	1:B:863:ALA:N	2.76	0.53
1:B:780:PRO:CB	1:B:784:HIS:CE1	2.81	0.53
1:B:145:ILE:CA	1:B:148:GLU:CG	2.84	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:271:CYS:SG	1:B:417:PRO:HG3	2.48	0.53
1:B:342:THR:CB	1:B:402:LEU:HD11	2.38	0.53
1:B:561:LEU:O	1:B:875:ILE:CG1	2.42	0.53
1:B:727:TRP:CE2	1:B:785:SER:OG	2.27	0.53
1:C:185:VAL:HB	1:C:325:ASN:ND2	2.22	0.53
1:C:264:ILE:HA	1:C:265:SER:CB	2.34	0.53
1:C:264:ILE:CA	1:C:265:SER:HB3	2.33	0.53
1:C:784:HIS:ND1	2:T:9:DT:H1'	2.23	0.53
1:B:269:GLN:HB3	1:B:408:PHE:HE1	1.73	0.53
1:B:730:PRO:HB2	1:B:793:LYS:HZ2	1.74	0.53
1:B:755:PHE:HB2	2:X:22:DG:H3'	1.89	0.53
2:T:11:DC:H2'	2:T:12:DT:H6	1.74	0.53
1:C:337:VAL:HG21	1:C:512:LEU:HD21	1.91	0.53
1:C:563:PRO:HB3	1:C:878:SER:N	2.21	0.53
2:T:20:DG:H2'	2:T:21:DT:C6	2.44	0.53
1:B:729:THR:HG23	1:B:789:SER:HB2	1.87	0.53
1:C:639:TYR:HB3	2:T:8:DT:C6	2.37	0.53
1:C:489:ILE:HG22	1:C:490:MET:H	1.74	0.53
1:C:537:ASP:O	1:C:882:PHE:CG	2.62	0.53
1:C:452:ILE:HG23	1:C:453:GLY:N	2.23	0.53
1:B:19:ILE:HG22	1:B:195:LEU:HD11	1.91	0.53
1:C:200:ALA:HA	1:C:293:PRO:CG	2.26	0.53
1:C:639:TYR:HD2	2:T:8:DT:C4	2.25	0.53
1:B:422:TRP:HH2	1:B:781:ASN:OD1	1.92	0.53
1:B:144:ALA:O	1:B:148:GLU:CG	2.57	0.52
1:B:489:ILE:HG22	1:B:490:MET:H	1.74	0.52
1:B:707:ALA:HA	1:B:774:GLN:CG	2.37	0.52
1:C:14:ILE:HD13	1:C:157:LEU:CD2	2.39	0.52
1:B:335:LEU:HA	1:B:443:LEU:CD2	2.39	0.52
1:B:567:VAL:HG22	1:B:880:PHE:HB3	1.90	0.52
1:C:780:PRO:O	1:C:783:VAL:CG2	2.58	0.52
1:B:147:ASP:CG	1:B:150:ARG:CG	2.77	0.52
1:B:201:TRP:HH2	1:B:299:THR:O	1.89	0.52
1:B:264:ILE:HA	1:B:265:SER:CB	2.34	0.52
1:B:350:GLU:C	1:B:352:ILE:N	2.63	0.52
1:B:422:TRP:HH2	1:B:781:ASN:CG	2.12	0.52
1:C:55:PHE:CE2	1:C:74:ILE:CG2	2.93	0.52
1:C:563:PRO:HG3	1:C:877:GLU:CB	2.14	0.52
1:B:698:TRP:HD1	1:B:862:PRO:C	2.13	0.52
1:B:724:ALA:HB1	1:B:738:GLU:HB3	1.85	0.52
1:B:730:PRO:CB	1:B:835:THR:CG2	2.87	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:801:LYS:NZ	1:B:802:TYR:CE1	2.75	0.52
1:B:698:TRP:HZ3	1:B:845:PHE:CD2	2.27	0.52
1:C:798:ALA:HB1	1:C:804:ILE:HD12	1.91	0.52
1:B:48:GLU:CD	1:B:120:LYS:HE3	2.29	0.52
1:B:836:TYR:CE1	1:B:841:VAL:HG11	2.38	0.52
1:B:152:GLY:O	1:B:155:ARG:N	2.43	0.52
1:B:320:ILE:HD12	1:B:420:MET:HG3	1.91	0.52
1:C:200:ALA:HB3	1:C:282:THR:CG2	2.39	0.52
1:B:96:ARG:HD2	3:Y:103:DA:C4	2.45	0.52
1:B:552:ASP:CB	1:B:555:GLY:N	2.72	0.52
1:C:349:VAL:HG21	1:C:352:ILE:HG12	1.92	0.52
2:T:6:DT:C6	2:T:7:DT:H73	2.44	0.52
1:B:342:THR:HB	1:B:402:LEU:HD11	1.92	0.52
1:B:452:ILE:HG23	1:B:453:GLY:N	2.23	0.52
1:B:563:PRO:HG3	1:B:874:ASP:CA	2.39	0.52
1:B:738:GLU:C	1:B:739:TYR:CG	2.83	0.52
2:X:20:DG:H2'	2:X:21:DT:C6	2.44	0.52
1:C:531:SER:HA	1:C:817:ILE:HG22	1.91	0.51
1:C:17:ALA:HB3	1:C:157:LEU:CB	2.40	0.51
1:C:727:TRP:CH2	1:C:782:PHE:HD1	2.23	0.51
1:B:99:ARG:HD3	2:X:31:DT:H5'	1.91	0.51
1:B:531:SER:HA	1:B:817:ILE:HG22	1.92	0.51
1:B:563:PRO:HA	1:B:878:SER:CA	2.40	0.51
1:B:834:ASP:O	1:B:838:SER:HB3	2.05	0.51
1:B:100:PRO:N	3:Y:105:DA:H4'	2.26	0.51
1:B:475:PHE:CE1	1:B:882:PHE:HE1	2.27	0.51
1:B:841:VAL:HG23	1:B:842:LEU:H	1.75	0.51
1:C:562:LEU:CD2	1:C:874:ASP:HB3	2.40	0.51
1:C:727:TRP:HB3	1:C:845:PHE:HD1	1.74	0.51
1:B:191:LEU:HD21	1:B:287:TRP:CZ3	2.46	0.51
1:B:703:ALA:HB1	1:B:778:ILE:CA	2.39	0.51
1:B:707:ALA:HB3	1:B:775:GLU:CB	2.40	0.51
1:B:117:ILE:HG21	1:B:145:ILE:HG12	1.93	0.51
1:B:405:ALA:CB	1:B:443:LEU:CD1	2.85	0.51
1:B:829:ARG:HD3	1:B:875:ILE:HG22	1.90	0.51
1:B:840:ASP:CB	1:B:843:ALA:HB3	2.21	0.51
1:C:44:TYR:HE1	1:C:120:LYS:HE3	1.70	0.51
1:C:404:GLN:O	1:C:408:PHE:HD2	1.94	0.51
1:C:690:VAL:O	1:C:693:VAL:HG23	2.11	0.51
1:C:739:TYR:CD2	1:C:773:LYS:HB3	2.46	0.51
1:B:160:LYS:O	1:B:164:LYS:HG3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:13:ASP:O	1:C:157:LEU:CD1	2.57	0.51
1:C:308:TYR:CE2	1:C:733:PHE:CE1	2.99	0.51
1:C:316:VAL:HG23	1:C:731:ASP:CG	2.29	0.51
1:B:147:ASP:HB2	1:B:151:PHE:HB2	1.93	0.51
1:B:349:VAL:HG23	1:B:352:ILE:CB	2.40	0.51
1:B:472:LYS:HA	1:B:567:VAL:HG11	1.93	0.51
1:C:34:ARG:HG2	1:C:162:PHE:HB2	1.93	0.51
1:B:550:LEU:HD13	1:B:695:ALA:HB2	1.79	0.51
1:B:552:ASP:HB3	1:B:555:GLY:N	2.26	0.51
1:C:297:VAL:HG21	1:C:733:PHE:CE1	2.46	0.50
1:B:352:ILE:HD12	1:B:398:LEU:HD11	1.94	0.50
1:B:549:MET:C	1:B:842:LEU:CD1	2.76	0.50
1:B:735:VAL:CG1	1:B:785:SER:HG	2.25	0.50
1:B:221:ILE:HA	1:B:225:GLY:HA3	1.93	0.50
1:B:553:GLU:CB	1:B:554:VAL:CA	2.64	0.50
1:B:690:VAL:O	1:B:693:VAL:N	2.44	0.50
2:X:10:DA:H2"	2:X:11:DC:OP2	2.11	0.50
1:C:153:ARG:O	1:C:156:ASP:N	2.41	0.50
1:C:739:TYR:HD2	1:C:770:ASP:HB3	1.77	0.50
1:C:791:LEU:HD21	1:C:809:LEU:HD13	1.93	0.50
1:B:96:ARG:CG	3:Y:103:DA:N3	2.70	0.50
1:B:303:LYS:HD3	1:B:766:ASP:OD2	2.12	0.50
1:C:147:ASP:O	1:C:151:PHE:N	2.44	0.50
1:B:402:LEU:HD23	1:B:439:MET:CE	2.41	0.50
1:C:148:GLU:O	1:C:150:ARG:N	2.44	0.50
1:C:472:LYS:C	1:C:567:VAL:HG21	2.31	0.50
1:B:50:ARG:O	1:B:53:LYS:HB3	2.11	0.50
1:B:411:HIS:O	1:B:412:LYS:O	2.30	0.50
1:C:160:LYS:O	1:C:164:LYS:HG3	2.11	0.50
1:C:221:ILE:HA	1:C:225:GLY:HA3	1.94	0.50
1:B:563:PRO:HA	1:B:878:SER:HA	1.93	0.50
1:B:746:ARG:NH2	2:X:21:DT:C6	2.80	0.50
1:B:758:GLN:OE1	2:X:22:DG:C5	2.64	0.50
1:B:43:SER:HA	1:B:266:LEU:C	2.31	0.50
1:C:149:ALA:O	1:C:150:ARG:HB3	2.11	0.50
1:C:354:ALA:HB3	1:C:391:ARG:NE	2.20	0.49
1:B:553:GLU:HB3	1:B:554:VAL:O	2.05	0.49
1:B:791:LEU:CD1	1:B:811:HIS:HA	2.41	0.49
1:B:797:TRP:O	1:B:798:ALA:C	2.51	0.49
1:B:355:ILE:CG1	1:B:356:GLU:H	2.23	0.49
1:B:839:CYS:O	1:B:840:ASP:C	2.50	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:850:ALA:CB	1:B:851:ASP:CB	2.57	0.49
1:C:722:ARG:CB	1:C:769:ILE:CG2	2.90	0.49
1:B:730:PRO:HG2	1:B:786:GLN:HE22	1.77	0.49
1:B:758:GLN:OE1	2:X:22:DG:C8	2.64	0.49
1:C:44:TYR:CE2	1:C:48:GLU:HG3	2.47	0.49
1:C:207:GLU:HG3	1:C:761:ILE:HD11	1.95	0.49
1:C:563:PRO:CB	1:C:877:GLU:O	2.45	0.49
1:B:756:ARG:O	2:X:22:DG:H2'	2.12	0.49
1:C:17:ALA:CB	1:C:157:LEU:CB	2.90	0.49
1:B:101:THR:OG1	3:Y:106:DC:H5"	2.13	0.49
1:B:320:ILE:CD1	1:B:420:MET:CG	2.90	0.49
1:B:789:SER:HB3	1:B:792:ARG:HH22	1.67	0.49
2:X:9:DT:H2"	2:X:10:DA:O5'	2.11	0.49
1:C:681:ILE:O	1:C:685:VAL:HG12	2.13	0.49
1:C:722:ARG:NE	1:C:771:ALA:N	2.30	0.49
1:B:269:GLN:HB3	1:B:408:PHE:CZ	2.48	0.49
1:B:563:PRO:N	1:B:878:SER:HB2	2.27	0.49
1:C:544:GLN:OE1	1:C:561:LEU:HD12	2.13	0.49
1:C:779:ALA:N	1:C:780:PRO:HD2	2.28	0.49
1:C:850:ALA:CB	1:C:851:ASP:CB	2.57	0.49
3:N:106:DC:H2"	3:N:107:DG:C8	2.48	0.49
1:C:315:GLU:CB	1:C:731:ASP:HB2	2.39	0.49
1:C:451:PRO:CA	1:C:452:ILE:CB	2.82	0.49
1:C:707:ALA:HB1	1:C:771:ALA:O	2.13	0.49
1:B:144:ALA:O	1:B:148:GLU:HG2	2.13	0.49
1:B:214:VAL:HG11	1:B:749:LEU:HD13	1.94	0.49
1:B:681:ILE:O	1:B:685:VAL:HG12	2.13	0.49
1:C:214:VAL:HG11	1:C:749:LEU:HD13	1.94	0.49
1:C:724:ALA:HB2	1:C:738:GLU:HB2	1.83	0.49
1:B:97:GLY:C	3:Y:104:DT:O2	2.51	0.49
1:C:153:ARG:O	1:C:154:ILE:C	2.50	0.49
1:C:297:VAL:HG22	1:C:733:PHE:CE1	2.48	0.49
1:C:404:GLN:HG3	1:C:408:PHE:CE2	2.45	0.49
1:C:780:PRO:O	1:C:782:PHE:CA	2.58	0.49
1:B:334:VAL:HG11	1:B:442:GLY:C	2.34	0.49
1:B:829:ARG:CD	1:B:875:ILE:CG2	2.82	0.49
1:C:34:ARG:CG	1:C:162:PHE:CB	2.91	0.48
1:C:311:VAL:HG21	1:C:734:PRO:CG	2.43	0.48
1:C:704:LYS:CG	1:C:775:GLU:OE2	2.60	0.48
1:B:45:GLU:CD	1:B:162:PHE:CZ	2.86	0.48
1:B:409:ALA:O	1:B:410:ASN:O	2.30	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:562:LEU:C	1:C:878:SER:HB2	2.33	0.48
1:C:641:SER:HA	2:T:7:DT:H2"	1.95	0.48
3:Y:106:DC:H2"	3:Y:107:DG:C8	2.48	0.48
1:B:789:SER:N	1:B:792:ARG:NH1	2.60	0.48
2:T:10:DA:H2'	2:T:11:DC:C6	2.48	0.48
1:B:320:ILE:CD1	1:B:420:MET:HG3	2.42	0.48
1:C:738:GLU:C	1:C:774:GLN:HE22	2.16	0.48
1:C:791:LEU:HD11	1:C:809:LEU:HB3	1.94	0.48
2:T:13:DC:H2'	2:T:14:DC:C6	2.48	0.48
1:B:707:ALA:O	1:B:771:ALA:C	2.50	0.48
1:B:756:ARG:H	2:X:22:DG:H3'	1.78	0.48
1:C:17:ALA:HA	1:C:158:GLU:HB2	1.94	0.48
1:C:552:ASP:OD1	1:C:691:ALA:HB2	2.12	0.48
1:B:185:VAL:HA	1:B:274:PRO:HB2	1.95	0.48
1:B:264:ILE:CD1	1:B:400:PHE:CD2	2.97	0.48
1:B:266:LEU:HD13	1:B:407:LYS:HZ2	1.74	0.48
1:B:811:HIS:CB	4:Z:8:A:H5'	2.43	0.48
1:B:96:ARG:NH1	3:Y:102:DA:C4	2.65	0.48
1:B:100:PRO:HD3	3:Y:105:DA:H5"	1.93	0.48
1:B:454:LYS:H	1:B:526:LEU:HD22	1.79	0.48
1:B:758:GLN:CD	2:X:23:DA:H62	2.15	0.48
1:C:349:VAL:CG2	1:C:352:ILE:HB	2.44	0.48
1:C:562:LEU:HD22	1:C:874:ASP:HB3	1.96	0.48
1:B:100:PRO:HB3	3:Y:106:DC:OP1	2.14	0.48
1:B:730:PRO:CB	1:B:793:LYS:NZ	2.77	0.48
2:T:12:DT:H2'	2:T:13:DC:C6	2.48	0.48
1:B:36:GLN:HE22	1:B:272:VAL:CA	2.27	0.48
1:B:180:LYS:HA	1:B:182:PHE:N	2.29	0.48
1:B:850:ALA:CA	1:B:851:ASP:CB	2.90	0.48
1:C:32:LEU:HD13	1:C:272:VAL:HG12	1.96	0.47
1:C:722:ARG:NH1	1:C:741:LYS:HZ1	2.11	0.47
1:C:748:ASN:HB3	3:N:106:DC:C2'	2.43	0.47
1:B:201:TRP:CD1	1:B:305:LEU:HD12	2.49	0.47
1:B:264:ILE:CD1	1:B:400:PHE:HD2	2.27	0.47
1:B:551:ARG:HD2	1:B:867:LYS:CE	2.44	0.47
1:B:563:PRO:CB	1:B:874:ASP:O	2.62	0.47
1:C:180:LYS:HA	1:C:182:PHE:N	2.29	0.47
1:C:850:ALA:CA	1:C:851:ASP:CB	2.91	0.47
2:X:9:DT:H1'	2:X:10:DA:O5'	2.11	0.47
2:T:11:DC:C6	2:T:12:DT:C7	2.97	0.47
1:B:335:LEU:CD1	1:B:409:ALA:HB1	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:746:ARG:NH1	2:X:21:DT:C7	2.77	0.47
1:C:17:ALA:HB1	1:C:158:GLU:HB2	1.95	0.47
1:C:44:TYR:OH	1:C:120:LYS:HE3	2.13	0.47
1:C:541:SER:HB2	4:R:8:A:O3'	2.12	0.47
1:C:693:VAL:O	1:C:696:MET:N	2.48	0.47
1:C:829:ARG:CZ	1:C:878:SER:O	2.62	0.47
1:B:475:PHE:CE1	1:B:882:PHE:CE1	3.02	0.47
1:B:799:HIS:O	1:B:800:GLU:C	2.51	0.47
1:C:401:MET:CE	1:C:432:PHE:HA	2.45	0.47
1:B:437:ASN:C	1:B:437:ASN:HD22	2.18	0.47
1:C:105:PHE:HD2	1:C:204:TRP:CE2	2.30	0.47
1:C:405:ALA:O	1:C:409:ALA:CA	2.62	0.47
1:C:437:ASN:HD22	1:C:437:ASN:C	2.18	0.47
2:T:14:DC:H2'	2:T:15:DC:C6	2.48	0.47
1:B:95:LYS:HG2	3:Y:104:DT:C5'	2.43	0.47
1:B:316:VAL:CG2	1:B:733:PHE:HA	2.39	0.47
1:B:541:SER:HB3	4:Z:8:A:O3'	2.15	0.47
1:B:746:ARG:NH1	2:X:21:DT:O4	2.48	0.47
1:C:311:VAL:HG11	1:C:734:PRO:HD3	1.96	0.47
1:C:408:PHE:C	1:C:411:HIS:HD2	2.18	0.47
1:C:540:CYS:HB3	1:C:559:VAL:CG1	2.45	0.47
1:C:780:PRO:O	1:C:783:VAL:HG22	2.15	0.47
1:B:53:LYS:N	1:B:55:PHE:H	2.12	0.47
1:B:730:PRO:HB3	1:B:793:LYS:NZ	2.30	0.47
1:B:791:LEU:HD12	1:B:811:HIS:C	2.35	0.47
1:C:454:LYS:H	1:C:526:LEU:HD22	1.80	0.47
1:C:552:ASP:CG	1:C:691:ALA:CB	2.83	0.47
1:B:264:ILE:HD13	1:B:400:PHE:CD2	2.49	0.47
1:C:695:ALA:HA	1:C:865:PRO:CG	2.45	0.46
2:T:11:DC:H2'	2:T:12:DT:C6	2.51	0.46
4:R:5:G:H2'	4:R:6:U:C6	2.50	0.46
1:C:553:GLU:N	1:C:554:VAL:CB	2.65	0.46
1:C:830:GLU:HA	1:C:876:LEU:HD21	1.97	0.46
1:C:201:TRP:HE1	1:C:305:LEU:HD13	1.67	0.46
1:C:320:ILE:HD11	1:C:420:MET:SD	2.54	0.46
1:C:354:ALA:CB	1:C:391:ARG:HE	2.22	0.46
1:C:553:GLU:HB2	1:C:554:VAL:CB	2.15	0.46
1:C:561:LEU:O	1:C:875:ILE:HA	2.14	0.46
1:C:722:ARG:CG	1:C:771:ALA:CA	2.80	0.46
1:B:791:LEU:HD12	1:B:811:HIS:CA	2.44	0.46
1:B:799:HIS:O	1:B:802:TYR:O	2.32	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:408:PHE:O	1:C:409:ALA:C	2.53	0.46
2:T:6:DT:H2"	2:T:7:DT:C5	2.44	0.46
1:B:147:ASP:OD2	1:B:292:ARG:CZ	2.61	0.46
1:B:316:VAL:HG21	1:B:733:PHE:CA	2.42	0.46
1:C:722:ARG:HB2	1:C:769:ILE:CG2	2.46	0.46
1:C:833:VAL:HG11	1:C:873:ARG:HD3	1.96	0.46
1:B:99:ARG:NH2	2:X:31:DT:H4'	2.29	0.46
4:R:1:G:H2'	4:R:2:G:H8	1.81	0.46
4:Z:1:G:H2'	4:Z:2:G:H8	1.80	0.46
1:C:148:GLU:C	1:C:150:ARG:N	2.69	0.46
1:C:316:VAL:HG22	1:C:731:ASP:OD1	2.15	0.46
1:C:376:ALA:HA	1:C:377:TRP:HA	1.66	0.46
1:B:45:GLU:CD	1:B:162:PHE:HZ	2.19	0.46
1:B:316:VAL:CG2	1:B:733:PHE:CA	2.92	0.46
1:B:376:ALA:HA	1:B:377:TRP:HA	1.67	0.46
1:B:402:LEU:HD23	1:B:439:MET:SD	2.55	0.46
1:B:727:TRP:NE1	1:B:782:PHE:O	2.48	0.46
4:Z:5:G:H2'	4:Z:6:U:C6	2.50	0.46
1:C:82:ILE:HD13	1:C:112:GLU:HG3	1.97	0.46
1:C:278:TRP:H	1:C:321:ASN:ND2	2.13	0.46
1:C:781:ASN:HD21	2:T:9:DT:C5'	2.16	0.46
1:B:405:ALA:HA	1:B:432:PHE:CE1	2.51	0.46
1:C:146:GLU:OE2	1:C:202:SER:OG	2.33	0.46
1:C:307:ARG:O	1:C:736:TRP:CH2	2.69	0.46
1:C:722:ARG:O	1:C:769:ILE:CG2	2.59	0.46
1:B:149:ALA:HB2	1:B:150:ARG:HH11	1.79	0.46
1:B:183:MET:HB3	1:B:415:TRP:HH2	1.81	0.46
1:B:82:ILE:HD13	1:B:112:GLU:HG3	1.98	0.46
1:B:350:GLU:C	1:B:352:ILE:H	2.19	0.46
1:B:840:ASP:O	1:B:841:VAL:C	2.53	0.46
4:R:4:A:H2'	4:R:5:G:H8	1.81	0.46
4:Z:4:A:H2'	4:Z:5:G:H8	1.81	0.46
1:C:347:CYS:SG	1:C:352:ILE:HG21	2.56	0.46
2:T:5:DT:C6	2:T:6:DT:H72	2.51	0.45
2:T:8:DT:C6	2:T:9:DT:C7	2.95	0.45
1:C:556:GLY:CA	1:C:559:VAL:H	2.29	0.45
1:C:740:LYS:HA	1:C:770:ASP:H	1.81	0.45
1:B:410:ASN:O	1:B:411:HIS:CB	2.34	0.45
1:B:707:ALA:HB3	1:B:775:GLU:H	1.64	0.45
1:C:34:ARG:HG3	1:C:162:PHE:CB	2.46	0.45
1:C:404:GLN:HG2	1:C:432:PHE:HB2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:48:GLU:OE2	1:B:120:LYS:HE3	2.17	0.45
4:R:6:U:H2'	4:R:7:A:H8	1.81	0.45
4:Z:6:U:H2'	4:Z:7:A:H8	1.82	0.45
1:C:17:ALA:CB	1:C:158:GLU:HB2	2.45	0.45
1:B:722:ARG:O	1:B:769:ILE:HG21	2.17	0.45
4:Z:2:G:H2'	4:Z:3:G:H8	1.81	0.45
1:C:13:ASP:OD1	1:C:154:ILE:HD11	2.15	0.45
1:C:17:ALA:CA	1:C:158:GLU:HB2	2.47	0.45
1:B:329:LYS:O	1:B:445:THR:O	2.34	0.45
1:B:422:TRP:NE1	2:X:10:DA:H5"	2.31	0.45
1:B:473:VAL:CG2	1:B:474:PRO:HD2	2.46	0.45
1:B:698:TRP:CG	1:B:861:MET:CE	2.75	0.45
1:B:708:ALA:HB2	1:B:775:GLU:OE2	2.16	0.45
1:B:726:HIS:CD2	1:B:736:TRP:CE2	3.04	0.45
1:B:739:TYR:CD1	1:B:773:LYS:HD3	2.51	0.45
1:B:755:PHE:HB2	2:X:22:DG:C3'	2.47	0.45
2:X:5:DT:C6	2:X:6:DT:H72	2.51	0.45
1:C:367:ILE:CA	1:C:368:ASP:HB2	2.47	0.45
1:B:333:LYS:CD	1:B:516:PHE:HB3	2.47	0.45
1:B:537:ASP:C	1:B:883:ALA:CB	2.84	0.45
1:C:34:ARG:O	1:C:162:PHE:CB	2.64	0.45
2:T:11:DC:C2	2:T:12:DT:H71	2.52	0.45
1:B:272:VAL:O	1:B:415:TRP:CZ3	2.70	0.45
1:B:324:GLN:HG3	1:B:418:TYR:H	1.82	0.45
1:B:552:ASP:HB3	1:B:555:GLY:O	2.17	0.45
1:B:698:TRP:HD1	1:B:863:ALA:N	2.15	0.45
1:B:704:LYS:HA	1:B:775:GLU:CA	2.45	0.45
2:X:6:DT:H2"	2:X:7:DT:H71	1.98	0.45
4:R:2:G:H2'	4:R:3:G:H8	1.81	0.45
1:B:331:ASN:N	1:B:443:LEU:O	2.47	0.45
1:B:367:ILE:CA	1:B:368:ASP:HB2	2.46	0.45
1:B:590:THR:HB	1:B:613:THR:H	1.82	0.45
1:B:794:THR:HA	1:B:831:THR:HG21	1.98	0.45
1:C:361:PRO:HA	1:C:362:MET:HA	1.81	0.45
1:B:223:SER:HA	1:B:224:THR:HA	1.78	0.45
1:B:278:TRP:H	1:B:321:ASN:ND2	2.13	0.45
1:B:551:ARG:CB	1:B:867:LYS:CG	2.80	0.45
1:B:563:PRO:HB3	1:B:874:ASP:O	2.17	0.45
1:B:698:TRP:HZ3	1:B:845:PHE:HD2	1.65	0.45
4:R:7:A:H2'	4:R:8:A:H8	1.82	0.45
4:Z:7:A:H2'	4:Z:8:A:H8	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:159:ALA:HA	1:C:162:PHE:CE1	2.52	0.45
1:B:690:VAL:O	1:B:692:ALA:N	2.50	0.45
1:B:727:TRP:CZ2	1:B:782:PHE:O	2.70	0.45
2:X:11:DC:C6	2:X:12:DT:H72	2.51	0.45
1:C:349:VAL:CG2	1:C:352:ILE:H	2.30	0.44
1:B:202:SER:O	1:B:203:SER:O	2.35	0.44
1:B:274:PRO:HA	1:B:275:PRO:HD3	1.83	0.44
1:B:319:ALA:CB	1:B:792:ARG:HB3	2.47	0.44
1:B:730:PRO:HB2	1:B:793:LYS:CD	2.46	0.44
1:B:731:ASP:N	1:B:793:LYS:HD2	2.32	0.44
1:C:13:ASP:C	1:C:157:LEU:CD1	2.85	0.44
1:C:116:TYR:CE2	1:C:120:LYS:HD2	2.52	0.44
1:C:452:ILE:HG23	1:C:453:GLY:H	1.82	0.44
1:C:693:VAL:O	1:C:694:GLU:C	2.56	0.44
1:C:829:ARG:HD3	1:C:875:ILE:HG22	1.99	0.44
2:T:9:DT:H2'	2:T:10:DA:H8	1.81	0.44
1:B:159:ALA:HA	1:B:162:PHE:CE1	2.52	0.44
1:C:150:ARG:CG	1:C:150:ARG:O	2.63	0.44
1:C:153:ARG:C	1:C:155:ARG:N	2.70	0.44
1:C:590:THR:HB	1:C:613:THR:H	1.82	0.44
1:C:727:TRP:CD2	1:C:782:PHE:HD1	2.16	0.44
1:B:116:TYR:CE2	1:B:120:LYS:HD2	2.53	0.44
1:B:388:ASP:O	1:B:392:LYS:HG3	2.17	0.44
1:B:395:ARG:O	1:B:399:GLU:HG2	2.17	0.44
1:C:271:CYS:SG	1:C:417:PRO:HG3	2.58	0.44
1:C:349:VAL:HG23	1:C:352:ILE:H	1.83	0.44
1:C:694:GLU:OE2	1:C:865:PRO:HA	2.18	0.44
1:B:402:LEU:HD23	1:B:439:MET:HE3	2.00	0.44
1:B:562:LEU:CG	1:B:870:LEU:HD12	2.09	0.44
4:R:3:G:H2'	4:R:4:A:H8	1.82	0.44
1:C:355:ILE:CD1	1:C:356:GLU:H	2.25	0.44
1:C:395:ARG:O	1:C:399:GLU:HG2	2.17	0.44
1:C:841:VAL:HG23	1:C:842:LEU:HD12	1.98	0.44
1:B:12:SER:O	1:B:13:ASP:HB2	2.16	0.44
1:B:329:LYS:HG2	1:B:446:LEU:C	2.37	0.44
1:B:489:ILE:O	1:B:490:MET:HB2	2.18	0.44
1:B:547:SER:HB3	1:B:555:GLY:O	2.17	0.44
1:B:837:GLU:HG2	1:B:838:SER:N	2.32	0.44
1:C:14:ILE:N	1:C:157:LEU:CD1	2.81	0.44
1:C:21:PHE:CB	1:C:161:HIS:CD2	3.00	0.44
1:C:24:LEU:HD11	1:C:273:VAL:CG2	2.20	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:53:LYS:H	1:B:55:PHE:H	1.65	0.44
1:B:835:THR:C	1:B:837:GLU:O	2.56	0.44
1:C:546:PHE:HB3	1:C:692:ALA:CB	2.47	0.44
1:C:546:PHE:HB3	1:C:692:ALA:HB2	2.00	0.44
1:C:776:SER:OG	2:T:7:DT:OP1	2.28	0.44
1:C:489:ILE:O	1:C:490:MET:HB2	2.18	0.44
1:C:710:VAL:HG21	1:C:719:LEU:HB2	1.99	0.44
1:B:473:VAL:N	1:B:567:VAL:HG21	2.32	0.44
1:B:475:PHE:HE1	1:B:882:PHE:CE1	2.33	0.44
1:B:757:LEU:HA	2:X:22:DG:P	2.58	0.44
4:Z:3:G:H2'	4:Z:4:A:H8	1.82	0.44
1:B:144:ALA:O	1:B:148:GLU:CD	2.56	0.44
1:C:352:ILE:HD12	1:C:398:LEU:CD1	2.48	0.43
1:C:489:ILE:HG22	1:C:490:MET:N	2.32	0.43
1:B:96:ARG:CD	3:Y:103:DA:C4	3.01	0.43
1:B:99:ARG:NH1	2:X:31:DT:H4'	2.31	0.43
1:C:462:ILE:HD12	1:C:475:PHE:HD1	1.83	0.43
1:B:462:ILE:HD12	1:B:475:PHE:HD1	1.83	0.43
1:C:473:VAL:CG2	1:C:474:PRO:HD2	2.48	0.43
1:B:489:ILE:HG22	1:B:490:MET:N	2.32	0.43
1:B:550:LEU:HD12	1:B:695:ALA:CB	2.37	0.43
1:B:710:VAL:HG11	1:B:719:LEU:N	2.34	0.43
1:B:795:VAL:O	1:B:796:VAL:C	2.56	0.43
2:X:28:DT:H2"	2:X:29:DA:C8	2.53	0.43
1:C:274:PRO:HA	1:C:275:PRO:HD3	1.84	0.43
2:T:6:DT:C1'	2:T:7:DT:C7	2.93	0.43
2:T:28:DT:H2"	2:T:29:DA:C8	2.53	0.43
1:B:9:ASN:O	1:B:10:ASP:CG	2.56	0.43
1:B:183:MET:HB2	1:B:415:TRP:HZ2	1.83	0.43
1:B:191:LEU:CD2	1:B:287:TRP:HZ3	2.31	0.43
1:B:44:TYR:CE1	1:B:155:ARG:NH1	2.78	0.43
1:B:100:PRO:HD3	3:Y:105:DA:C4'	2.49	0.43
1:B:354:ALA:CB	1:B:355:ILE:CA	2.96	0.43
1:B:452:ILE:HG23	1:B:453:GLY:H	1.83	0.43
1:B:727:TRP:HA	1:B:848:GLN:HG3	1.99	0.43
1:B:829:ARG:HD3	1:B:875:ILE:CG2	2.48	0.43
1:C:829:ARG:CB	1:C:876:LEU:HA	2.47	0.43
1:B:388:ASP:O	1:B:392:LYS:N	2.41	0.43
1:B:431:MET:CE	2:X:13:DC:OP2	2.67	0.43
1:B:541:SER:HG	4:Z:8:A:HO3'	1.66	0.43
1:B:545:HIS:CE1	1:B:790:HIS:CD2	3.02	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:698:TRP:CZ2	1:B:849:PHE:CZ	3.02	0.43
1:C:198:GLY:O	1:C:199:GLU:HB3	2.19	0.43
1:C:691:ALA:O	1:C:692:ALA:C	2.55	0.43
1:B:183:MET:HB3	1:B:415:TRP:CH2	2.54	0.43
1:B:400:PHE:CE1	1:B:431:MET:CG	3.02	0.43
2:X:13:DC:H1'	2:X:14:DC:H5'	2.01	0.43
1:C:286:TYR:HE2	1:C:429:VAL:HG11	1.82	0.43
1:C:786:GLN:HE22	1:C:841:VAL:HG11	1.84	0.43
1:B:96:ARG:NE	3:Y:103:DA:C4'	2.82	0.43
1:B:98:LYS:CB	2:X:29:DA:C2	2.79	0.43
1:B:264:ILE:CG2	1:B:400:PHE:CZ	2.95	0.43
3:Y:131:DG:H1'	3:Y:132:DC:H5'	2.01	0.43
1:C:131:ASN:CB	1:C:132:THR:CA	2.76	0.43
2:T:26:DC:H2"	2:T:27:DG:C8	2.53	0.43
3:N:128:DA:H1'	3:N:129:DC:H5'	2.01	0.43
3:N:130:DG:H1'	3:N:131:DG:H5'	2.01	0.43
1:B:180:LYS:CB	1:B:181:ALA:HA	2.49	0.43
1:B:799:HIS:ND1	1:B:804:ILE:O	2.52	0.43
3:Y:129:DC:H1'	3:Y:130:DG:H5'	2.01	0.43
1:C:400:PHE:CZ	1:C:431:MET:CB	2.95	0.43
1:C:536:PHE:C	1:C:882:PHE:CB	2.76	0.43
1:C:556:GLY:HA3	1:C:559:VAL:HG22	2.01	0.43
1:C:710:VAL:HG11	1:C:719:LEU:N	2.34	0.43
3:N:126:DA:H1'	3:N:127:DA:H5'	2.01	0.43
3:N:129:DC:H1'	3:N:130:DG:H5'	2.01	0.43
2:X:3:DC:H1'	2:X:4:DG:H5'	2.01	0.43
1:C:150:ARG:O	1:C:150:ARG:HG2	2.19	0.42
3:N:131:DG:H1'	3:N:132:DC:H5'	2.01	0.42
1:B:710:VAL:HG21	1:B:719:LEU:HB2	2.00	0.42
2:X:9:DT:C2'	2:X:10:DA:O5'	2.67	0.42
1:C:95:LYS:HD3	3:N:104:DT:H5"	2.01	0.42
1:C:423:ARG:HB3	1:C:785:SER:HB3	2.00	0.42
2:T:4:DG:C8	2:T:5:DT:H72	2.53	0.42
2:T:6:DT:C1'	2:T:7:DT:C5	3.03	0.42
2:X:4:DG:C8	2:X:5:DT:H72	2.53	0.42
3:Y:130:DG:H1'	3:Y:131:DG:H5'	2.01	0.42
1:C:485:ASN:HB3	1:C:488:ASN:HB2	2.02	0.42
1:C:636:THR:HB	2:T:8:DT:H72	2.00	0.42
1:B:147:ASP:HB3	1:B:150:ARG:CB	2.47	0.42
1:B:730:PRO:HB3	1:B:793:LYS:HZ2	1.83	0.42
3:Y:111:DC:H2"	3:Y:112:DA:C8	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:44:TYR:CD2	1:C:48:GLU:HG2	2.54	0.42
1:C:109:ILE:HD11	1:C:145:ILE:O	2.19	0.42
1:C:182:PHE:HZ	1:C:413:ALA:CB	2.27	0.42
1:C:729:THR:OG1	1:C:730:PRO:HD2	2.19	0.42
1:C:836:TYR:HA	1:C:837:GLU:HA	1.56	0.42
1:B:149:ALA:HB2	1:B:150:ARG:NH1	2.28	0.42
1:B:729:THR:OG1	1:B:730:PRO:HD2	2.19	0.42
1:B:780:PRO:O	1:B:781:ASN:C	2.57	0.42
1:C:560:ASN:O	1:C:878:SER:OG	2.35	0.42
2:X:26:DC:H2"	2:X:27:DG:C8	2.54	0.42
1:C:401:MET:HE2	1:C:432:PHE:CD1	2.51	0.42
1:B:96:ARG:HG2	3:Y:103:DA:C1'	2.30	0.42
1:C:118:THR:HG22	1:C:220:LEU:HD22	2.01	0.42
1:C:707:ALA:CB	1:C:771:ALA:O	2.68	0.42
2:T:2:DC:H1'	2:T:3:DC:H5'	2.01	0.42
3:N:111:DC:H2"	3:N:112:DA:C8	2.54	0.42
1:B:97:GLY:HA3	3:Y:103:DA:C2	2.53	0.42
1:B:198:GLY:HA3	1:B:282:THR:CB	2.49	0.42
1:B:741:LYS:HA	1:B:742:PRO:HD3	1.88	0.42
1:C:8:LYS:HB2	1:C:197:GLY:HA3	2.01	0.42
1:C:341:ILE:HD11	1:C:509:PHE:HZ	1.81	0.42
1:C:816:THR:CG2	1:C:817:ILE:N	2.83	0.42
1:B:118:THR:HG22	1:B:220:LEU:HD22	2.01	0.42
1:B:836:TYR:CD1	1:B:841:VAL:HG13	2.54	0.42
2:X:1:DG:H1'	2:X:2:DC:H5'	2.01	0.42
2:X:4:DG:H1'	2:X:5:DT:H5'	2.01	0.42
1:C:703:ALA:HB2	1:C:778:ILE:CD1	2.44	0.42
2:T:4:DG:H1'	2:T:5:DT:H5'	2.01	0.42
1:B:552:ASP:HB3	1:B:553:GLU:H	1.59	0.42
1:C:28:TYR:CZ	1:C:274:PRO:HD2	2.54	0.42
1:C:311:VAL:CG2	1:C:734:PRO:HG3	2.48	0.42
1:B:97:GLY:C	2:X:30:DT:O2	2.58	0.42
1:B:100:PRO:HG3	3:Y:105:DA:H5"	2.01	0.42
1:B:329:LYS:CE	1:B:447:ALA:HA	2.50	0.42
1:B:763:THR:HG22	1:B:765:LYS:H	1.85	0.42
1:B:840:ASP:O	1:B:843:ALA:N	2.53	0.42
1:C:23:THR:O	1:C:27:HIS:HD2	2.03	0.41
1:C:556:GLY:HA2	1:C:559:VAL:H	1.85	0.41
1:B:97:GLY:N	3:Y:103:DA:C2	2.87	0.41
1:B:101:THR:N	3:Y:106:DC:OP1	2.53	0.41
1:B:263:GLY:HA3	1:B:264:ILE:HA	1.91	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:361:PRO:HA	1:B:362:MET:HA	1.81	0.41
1:B:539:SER:OG	1:B:560:ASN:HB2	2.20	0.41
1:B:550:LEU:HG	1:B:842:LEU:HD11	2.02	0.41
1:B:553:GLU:CG	1:B:554:VAL:HB	2.46	0.41
1:B:16:LEU:O	1:B:289:ASN:HB2	2.20	0.41
1:B:95:LYS:CB	3:Y:104:DT:H5'	2.35	0.41
1:B:297:VAL:CG1	1:B:422:TRP:HA	2.48	0.41
1:B:342:THR:HG21	1:B:402:LEU:HD11	2.01	0.41
1:C:36:GLN:NE2	1:C:272:VAL:N	2.44	0.41
1:C:74:ILE:C	1:C:76:THR:H	2.23	0.41
1:C:120:LYS:HB3	1:C:120:LYS:NZ	2.35	0.41
1:C:221:ILE:O	1:C:221:ILE:CG2	2.68	0.41
1:C:710:VAL:HG11	1:C:719:LEU:H	1.86	0.41
1:C:780:PRO:HG2	1:C:781:ASN:H	1.83	0.41
2:T:3:DC:H1'	2:T:4:DG:H5'	2.01	0.41
1:B:316:VAL:CG1	1:B:733:PHE:CD1	2.96	0.41
1:B:729:THR:HG22	1:B:733:PHE:HB3	2.01	0.41
2:X:5:DT:H1'	2:X:6:DT:H5'	2.01	0.41
1:C:838:SER:O	1:C:839:CYS:SG	2.79	0.41
1:B:74:ILE:C	1:B:76:THR:H	2.23	0.41
1:B:541:SER:CB	4:Z:8:A:O3'	2.67	0.41
2:T:5:DT:H1'	2:T:6:DT:H5'	2.01	0.41
3:N:127:DA:H1'	3:N:128:DA:H5'	2.01	0.41
1:B:100:PRO:CB	3:Y:106:DC:OP1	2.69	0.41
1:B:131:ASN:CB	1:B:132:THR:CA	2.77	0.41
1:B:689:VAL:O	1:B:690:VAL:C	2.58	0.41
2:X:11:DC:H1'	2:X:12:DT:H5'	2.01	0.41
2:X:14:DC:H1'	2:X:15:DC:H5'	2.01	0.41
3:Y:128:DA:H1'	3:Y:129:DC:H5'	2.01	0.41
1:C:563:PRO:N	1:C:878:SER:HB2	2.35	0.41
1:B:98:LYS:HE2	3:Y:105:DA:C2	2.51	0.41
1:B:298:ARG:HH11	2:X:11:DC:H3'	1.85	0.41
1:B:350:GLU:O	1:B:351:ASP:C	2.58	0.41
1:B:485:ASN:HB3	1:B:488:ASN:HB2	2.02	0.41
1:B:760:THR:HB	2:X:20:DG:C5'	2.32	0.41
1:B:816:THR:HG22	1:B:817:ILE:HG12	2.02	0.41
3:Y:127:DA:H1'	3:Y:128:DA:H5'	2.01	0.41
1:C:704:LYS:HG3	1:C:775:GLU:CD	2.41	0.41
1:C:729:THR:HG22	1:C:733:PHE:HB3	2.02	0.41
1:B:733:PHE:HB3	1:B:792:ARG:HH21	1.83	0.41
1:B:799:HIS:O	1:B:801:LYS:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:2:DC:H1'	2:X:3:DC:H5'	2.01	0.41
2:X:12:DT:H1'	2:X:13:DC:H5'	2.01	0.41
1:C:198:GLY:O	1:C:199:GLU:CB	2.67	0.41
1:C:569:ASP:O	1:C:573:ILE:HG12	2.21	0.41
1:C:738:GLU:HA	1:C:774:GLN:HE22	1.86	0.41
2:T:1:DG:H1'	2:T:2:DC:H5'	2.01	0.41
1:B:184:GLN:C	1:B:274:PRO:HG2	2.41	0.41
1:B:316:VAL:HG22	1:B:733:PHE:CB	2.44	0.41
2:X:7:DT:OP1	2:X:7:DT:H3'	2.21	0.41
2:X:20:DG:H2'	2:X:21:DT:H6	1.86	0.41
1:C:308:TYR:CE2	1:C:733:PHE:CZ	3.09	0.41
1:B:48:GLU:O	1:B:52:ARG:HG3	2.21	0.41
1:B:120:LYS:HB3	1:B:120:LYS:NZ	2.36	0.41
1:B:270:PRO:CD	1:B:408:PHE:CD1	2.93	0.41
1:B:832:MET:O	1:B:836:TYR:HD2	2.04	0.41
1:C:405:ALA:O	1:C:409:ALA:N	2.54	0.41
1:B:46:MET:O	1:B:50:ARG:HG3	2.20	0.41
1:C:541:SER:OG	4:R:8:A:O2'	2.33	0.40
2:T:8:DT:H2"	2:T:9:DT:C5'	2.50	0.40
2:T:8:DT:H5'	2:T:8:DT:H6	1.86	0.40
1:B:186:VAL:HB	1:B:287:TRP:CH2	2.54	0.40
1:B:569:ASP:O	1:B:573:ILE:HG12	2.21	0.40
1:B:710:VAL:HG11	1:B:719:LEU:H	1.86	0.40
1:C:351:ASP:CA	1:C:394:ARG:HH21	2.33	0.40
1:C:408:PHE:CD2	1:C:408:PHE:N	2.89	0.40
1:C:804:ILE:HG23	1:C:816:THR:HG21	2.03	0.40
1:B:316:VAL:CG2	1:B:733:PHE:HB2	2.41	0.40
1:B:400:PHE:HZ	1:B:431:MET:HG2	1.83	0.40
3:Y:129:DC:C2'	3:Y:130:DG:OP2	2.69	0.40
1:C:206:LYS:O	1:C:210:ILE:HG12	2.21	0.40
1:C:328:TRP:CH2	1:C:434:PRO:HB3	2.55	0.40
1:B:23:THR:O	1:B:27:HIS:HD2	2.03	0.40
1:B:95:LYS:HD3	3:Y:104:DT:O3'	2.22	0.40
1:B:541:SER:OG	4:Z:8:A:O3'	2.38	0.40
1:B:690:VAL:O	1:B:691:ALA:C	2.60	0.40
2:X:8:DT:C4	4:Z:8:A:N1	2.89	0.40
1:C:201:TRP:CE2	1:C:302:LYS:HA	2.55	0.40
1:C:450:LYS:HA	1:C:451:PRO:HD3	1.91	0.40
1:C:816:THR:HG22	1:C:817:ILE:HG12	2.02	0.40
1:B:96:ARG:HG3	3:Y:103:DA:C4	2.56	0.40
1:C:17:ALA:O	1:C:158:GLU:HA	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:642:LYS:HG3	2:T:7:DT:C1'	2.43	0.40
3:N:131:DG:C2'	3:N:132:DC:OP2	2.69	0.40
1:B:24:LEU:CD1	1:B:273:VAL:HG21	2.48	0.40
1:B:320:ILE:HG13	1:B:420:MET:CE	2.50	0.40
1:B:404:GLN:OE1	1:B:431:MET:HB3	2.21	0.40
1:B:722:ARG:O	1:B:769:ILE:HD13	2.22	0.40

All (12) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:132:DC:N4	2:X:1:DG:N3[2_454]	1.48	0.72
1:C:873:ARG:NH2	1:B:801:LYS:CE[3_444]	1.68	0.52
1:C:711:LYS:NZ	2:X:2:DC:C2'[2_454]	1.69	0.51
3:N:132:DC:N4	2:X:1:DG:C4[2_454]	1.71	0.49
2:T:1:DG:O6	2:X:1:DG:N1[2_454]	1.79	0.41
3:N:132:DC:C4	2:X:1:DG:N3[2_454]	1.85	0.35
3:N:132:DC:N4	2:X:1:DG:C2[2_454]	1.87	0.33
2:T:1:DG:N7	3:Y:132:DC:N4[2_454]	2.05	0.15
2:T:32:DA:C2'	3:Y:101:DT:C4'[2_354]	2.10	0.10
2:T:1:DG:O6	2:X:1:DG:C6[2_454]	2.11	0.09
2:T:1:DG:N7	3:Y:132:DC:C4[2_454]	2.13	0.07
2:T:32:DA:C2'	3:Y:101:DT:C5'[2_354]	2.15	0.05

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	B	823/889 (93%)	684 (83%)	91 (11%)	48 (6%)	1	18
1	C	823/889 (93%)	704 (86%)	84 (10%)	35 (4%)	2	22
All	All	1646/1778 (93%)	1388 (84%)	175 (11%)	83 (5%)	2	20

All (83) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	150	ARG
1	C	153	ARG
1	C	265	SER
1	C	353	PRO
1	C	412	LYS
1	C	452	ILE
1	C	773	LYS
1	C	774	GLN
1	C	781	ASN
1	C	851	ASP
1	B	9	ASN
1	B	10	ASP
1	B	44	TYR
1	B	149	ALA
1	B	150	ARG
1	B	203	SER
1	B	206	LYS
1	B	265	SER
1	B	355	ILE
1	B	409	ALA
1	B	410	ASN
1	B	411	HIS
1	B	412	LYS
1	B	452	ILE
1	B	552	ASP
1	B	690	VAL
1	B	838	SER
1	B	851	ASP
1	C	11	PHE
1	C	149	ALA
1	C	154	ILE
1	C	266	LEU
1	C	355	ILE
1	C	369	MET
1	C	690	VAL
1	C	691	ALA
1	C	772	HIS
1	C	779	ALA
1	C	850	ALA
1	B	13	ASP
1	B	266	LEU
1	B	351	ASP

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Mol	Chain	Res	Type
1	B	356	GLU
1	B	369	MET
1	B	799	HIS
1	B	839	CYS
1	B	850	ALA
1	C	370	ASN
1	C	780	PRO
1	C	838	SER
1	C	839	CYS
1	B	41	HIS
1	B	370	ASN
1	B	796	VAL
1	B	797	TRP
1	B	801	LYS
1	C	376	ALA
1	C	854	HIS
1	C	863	ALA
1	B	376	ALA
1	B	557	ARG
1	B	691	ALA
1	B	840	ASP
1	B	854	HIS
1	B	863	ALA
1	C	365	GLU
1	B	202	SER
1	B	350	GLU
1	B	782	PHE
1	B	800	GLU
1	C	368	ASP
1	C	556	GLY
1	C	693	VAL
1	B	368	ASP
1	C	554	VAL
1	B	795	VAL
1	B	841	VAL
1	C	730	PRO
1	B	730	PRO
1	B	556	GLY
1	B	780	PRO
1	C	363	LYS
1	B	363	LYS

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
1	B	684/735 (93%)	650 (95%)	34 (5%)	24 49
1	C	687/735 (94%)	663 (96%)	24 (4%)	36 59
All	All	1371/1470 (93%)	1313 (96%)	58 (4%)	30 54

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	131	ASN
1	C	150	ARG
1	C	203	SER
1	C	206	LYS
1	C	215	ARG
1	C	264	ILE
1	C	305	LEU
1	C	335	LEU
1	C	349	VAL
1	C	352	ILE
1	C	377	TRP
1	C	408	PHE
1	C	410	ASN
1	C	437	ASN
1	C	452	ILE
1	C	472	LYS
1	C	553	GLU
1	C	554	VAL
1	C	738	GLU
1	C	783	VAL
1	C	836	TYR
1	C	840	ASP
1	C	858	LEU
1	C	861	MET
1	B	8	LYS
1	B	131	ASN
1	B	147	ASP

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Mol	Chain	Res	Type
1	B	150	ARG
1	B	153	ARG
1	B	182	PHE
1	B	206	LYS
1	B	215	ARG
1	B	264	ILE
1	B	305	LEU
1	B	335	LEU
1	B	349	VAL
1	B	351	ASP
1	B	355	ILE
1	B	356	GLU
1	B	377	TRP
1	B	411	HIS
1	B	437	ASN
1	B	452	ILE
1	B	472	LYS
1	B	551	ARG
1	B	552	ASP
1	B	553	GLU
1	B	554	VAL
1	B	738	GLU
1	B	740	LYS
1	B	801	LYS
1	B	835	THR
1	B	836	TYR
1	B	838	SER
1	B	839	CYS
1	B	840	ASP
1	B	858	LEU
1	B	861	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (54) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	22	ASN
1	C	27	HIS
1	C	36	GLN
1	C	86	ASN
1	C	107	GLN
1	C	131	ASN
1	C	161	HIS

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Mol	Chain	Res	Type
1	C	239	GLN
1	C	269	GLN
1	C	321	ASN
1	C	324	GLN
1	C	410	ASN
1	C	411	HIS
1	C	419	ASN
1	C	433	ASN
1	C	435	GLN
1	C	437	ASN
1	C	619	GLN
1	C	649	GLN
1	C	737	GLN
1	C	744	GLN
1	C	764	ASN
1	C	774	GLN
1	C	781	ASN
1	C	786	GLN
1	C	823	ASN
1	B	9	ASN
1	B	22	ASN
1	B	27	HIS
1	B	36	GLN
1	B	86	ASN
1	B	107	GLN
1	B	131	ASN
1	B	239	GLN
1	B	321	ASN
1	B	324	GLN
1	B	406	ASN
1	B	419	ASN
1	B	433	ASN
1	B	435	GLN
1	B	437	ASN
1	B	544	GLN
1	B	545	HIS
1	B	619	GLN
1	B	649	GLN
1	B	697	ASN
1	B	726	HIS
1	B	744	GLN
1	B	758	GLN

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Mol	Chain	Res	Type
1	B	764	ASN
1	B	781	ASN
1	B	784	HIS
1	B	790	HIS
1	B	823	ASN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
4	R	7/8 (87%)	0	0
4	Z	7/8 (87%)	0	0
All	All	14/16 (87%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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 monosaccharides 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	B	833/889 (93%)	0.50	75 (9%) 9 12	20, 100, 100, 101	0
1	C	833/889 (93%)	0.47	66 (7%) 12 14	20, 100, 100, 101	0
2	T	28/32 (87%)	0.47	3 (10%) 6 9	20, 54, 100, 100	0
2	X	28/32 (87%)	0.57	5 (17%) 1 4	20, 20, 100, 100	0
3	N	20/32 (62%)	-0.29	0 100 100	20, 100, 100, 100	0
3	Y	20/32 (62%)	-0.28	0 100 100	20, 100, 100, 100	0
4	R	8/8 (100%)	2.58	6 (75%) 0 0	45, 50, 52, 55	0
4	Z	8/8 (100%)	2.69	5 (62%) 0 0	45, 50, 52, 55	0
All	All	1778/1922 (92%)	0.49	160 (8%) 9 12	20, 100, 100, 101	0

All (160) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	263	GLY	7.3
1	C	851	ASP	5.5
1	C	763	THR	5.1
1	B	413	ALA	5.1
1	B	288	ALA	4.9
1	C	670	PRO	4.8
1	C	671	ASN	4.8
1	B	867	LYS	4.4
1	C	183	MET	4.3
1	C	227	VAL	4.3
4	Z	7	A	4.2
1	B	263	GLY	4.2
2	X	8	DT	4.2
1	B	264	ILE	4.1
1	C	182	PHE	4.1
1	B	289	ASN	4.1

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Mol	Chain	Res	Type	RSRZ
1	C	226	MET	4.1
1	B	766	ASP	4.0
1	B	763	THR	3.9
1	C	850	ALA	3.8
4	Z	8	A	3.7
2	T	10	DA	3.7
4	Z	1	G	3.6
1	B	842	LEU	3.6
2	T	15	DC	3.5
1	B	242	GLU	3.5
1	B	598	THR	3.5
1	B	840	ASP	3.5
1	B	518	TYR	3.5
1	C	449	GLY	3.5
2	X	15	DC	3.5
1	C	290	GLY	3.5
1	B	330	ILE	3.5
4	R	7	A	3.4
4	R	6	U	3.4
1	C	669	GLN	3.4
1	C	657	PRO	3.4
1	C	345	LYS	3.4
1	C	297	VAL	3.4
1	C	448	LYS	3.4
1	B	836	TYR	3.3
1	B	432	PHE	3.3
1	C	471	ASP	3.3
1	C	654	THR	3.3
1	C	244	ILE	3.2
1	C	853	LEU	3.2
1	B	744	GLN	3.2
1	B	668	THR	3.2
1	B	404	GLN	3.2
1	B	625	VAL	3.2
4	Z	6	U	3.1
1	C	806	SER	3.1
1	C	656	GLN	3.1
4	R	1	G	3.0
1	B	551	ARG	3.0
1	B	408	PHE	3.0
1	B	841	VAL	3.0
2	X	9	DT	3.0

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Mol	Chain	Res	Type	RSRZ
4	R	5	G	3.0
1	B	745	THR	3.0
1	C	135	GLN	2.9
1	C	356	GLU	2.9
1	C	346	HIS	2.9
1	B	265	SER	2.9
1	B	342	THR	2.9
1	B	411	HIS	2.8
1	B	743	ILE	2.8
4	R	8	A	2.8
1	B	131	ASN	2.8
1	C	447	ALA	2.7
1	C	653	ASP	2.7
1	C	287	TRP	2.7
1	B	434	PRO	2.7
1	B	549	MET	2.7
1	B	550	LEU	2.7
2	T	9	DT	2.7
1	C	134	VAL	2.7
1	C	834	ASP	2.7
1	B	762	ASN	2.7
1	B	670	PRO	2.7
1	C	523	HIS	2.7
1	C	131	ASN	2.6
1	C	673	ALA	2.6
1	C	342	THR	2.6
1	B	226	MET	2.6
1	B	579	ASN	2.6
1	C	286	TYR	2.6
1	B	547	SER	2.6
1	B	606	SER	2.6
1	C	861	MET	2.6
1	B	180	LYS	2.5
1	C	762	ASN	2.5
1	B	145	ILE	2.5
1	C	730	PRO	2.5
1	B	730	PRO	2.5
4	Z	5	G	2.5
1	C	288	ALA	2.5
1	C	137	VAL	2.5
1	C	761	ILE	2.5
1	C	849	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	843	ALA	2.5
1	B	640	GLY	2.5
1	B	407	LYS	2.5
1	B	615	ALA	2.5
1	C	651	LEU	2.5
1	B	865	PRO	2.5
1	B	461	LYS	2.4
1	B	776	SER	2.4
1	B	765	LYS	2.4
1	B	597	VAL	2.4
1	C	672	GLN	2.4
1	C	743	ILE	2.4
1	C	245	GLU	2.4
1	C	229	LEU	2.4
1	B	669	GLN	2.4
1	B	754	GLN	2.3
1	C	724	ALA	2.3
1	B	266	LEU	2.3
1	B	109	ILE	2.3
1	C	413	ALA	2.3
1	C	655	ILE	2.3
1	C	436	GLY	2.2
1	B	290	GLY	2.2
1	B	132	THR	2.2
1	B	412	LYS	2.2
1	C	296	LEU	2.2
1	B	509	PHE	2.2
2	X	10	DA	2.2
1	B	839	CYS	2.2
1	C	276	LYS	2.2
1	B	751	PHE	2.2
1	B	331	ASN	2.2
4	R	2	G	2.2
1	C	289	ASN	2.2
1	C	804	ILE	2.2
1	B	866	ALA	2.2
1	C	145	ILE	2.2
1	B	108	GLU	2.2
1	C	668	THR	2.1
1	B	614	LYS	2.1
1	C	852	GLN	2.1
1	C	774	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	149	ALA	2.1
1	C	807	PHE	2.1
1	C	847	ASP	2.1
1	B	548	ALA	2.1
1	B	418	TYR	2.1
1	C	55	PHE	2.1
1	B	287	TRP	2.0
1	B	714	LYS	2.0
1	C	845	PHE	2.0
1	B	460	LEU	2.0
1	B	414	ILE	2.0
1	B	348	PRO	2.0
1	B	752	LEU	2.0
1	B	761	ILE	2.0
2	X	11	DC	2.0
1	B	333	LYS	2.0
1	B	786	GLN	2.0
1	C	803	GLY	2.0

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 monosaccharides 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.