



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:09 AM UTC

PDB ID : 5UKB / pdb_00005ukb
Title : VSV N PROTEIN IN COMPLEX WITH INHIBITORY NANOBODY 1004
Authors : Hanke, L.; Knockenhauer, K.E.; Ploegh, H.L.; Schwartz, T.U.
Deposited on : 2017-01-20
Resolution : 5.47 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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

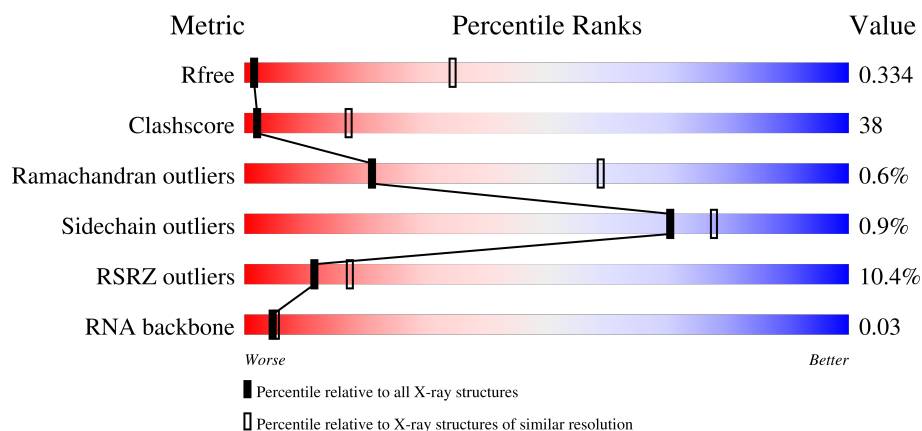
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 5.47 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}	180053	1066 (6.92-4.00)
Clashscore	190562	1123 (6.92-4.00)
Ramachandran outliers	187476	1048 (7.00-3.96)
Sidechain outliers	187428	1018 (7.00-3.96)
RSRZ outliers	180081	1059 (6.92-4.00)
RNA backbone	3983	1052 (7.80-3.10)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	a	138	3% 40% 44% 12%
1	b	138	5% 38% 46% 12%
1	c	138	% 38% 46% 12%
1	d	138	39% 45% 12%

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Mol	Chain	Length	Quality of chain
1	e	138	4% 40% 44% 12%
2	A	423	14% 72% 27%
2	B	423	12% 71% 27% ..
2	C	423	13% 73% 26% .
2	D	423	12% 72% 26% .
2	E	423	12% 74% 24% ..
3	R	45	7% 18% 64% 11%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 22210 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 Anti-vesicular stomatitis virus N VHH.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	d	122	Total	C	N	O	S	0	0	0
			946	596	166	181	3			
1	c	122	Total	C	N	O	S	0	0	0
			946	596	166	181	3			
1	b	122	Total	C	N	O	S	0	0	0
			946	596	166	181	3			
1	a	122	Total	C	N	O	S	0	0	0
			946	596	166	181	3			
1	e	122	Total	C	N	O	S	0	0	0
			946	596	166	181	3			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
d	1	GLN	-	expression tag	UNP A0A192B6J5
d	2	VAL	-	expression tag	UNP A0A192B6J5
d	125	GLY	-	expression tag	UNP A0A192B6J5
d	126	GLY	-	expression tag	UNP A0A192B6J5
d	127	LEU	-	expression tag	UNP A0A192B6J5
d	128	PRO	-	expression tag	UNP A0A192B6J5
d	129	GLU	-	expression tag	UNP A0A192B6J5
d	130	THR	-	expression tag	UNP A0A192B6J5
d	131	GLY	-	expression tag	UNP A0A192B6J5
d	132	GLY	-	expression tag	UNP A0A192B6J5
d	133	HIS	-	expression tag	UNP A0A192B6J5
d	134	HIS	-	expression tag	UNP A0A192B6J5
d	135	HIS	-	expression tag	UNP A0A192B6J5
d	136	HIS	-	expression tag	UNP A0A192B6J5
d	137	HIS	-	expression tag	UNP A0A192B6J5
d	138	HIS	-	expression tag	UNP A0A192B6J5
c	1	GLN	-	expression tag	UNP A0A192B6J5
c	2	VAL	-	expression tag	UNP A0A192B6J5
c	125	GLY	-	expression tag	UNP A0A192B6J5

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Chain	Residue	Modelled	Actual	Comment	Reference
c	126	GLY	-	expression tag	UNP A0A192B6J5
c	127	LEU	-	expression tag	UNP A0A192B6J5
c	128	PRO	-	expression tag	UNP A0A192B6J5
c	129	GLU	-	expression tag	UNP A0A192B6J5
c	130	THR	-	expression tag	UNP A0A192B6J5
c	131	GLY	-	expression tag	UNP A0A192B6J5
c	132	GLY	-	expression tag	UNP A0A192B6J5
c	133	HIS	-	expression tag	UNP A0A192B6J5
c	134	HIS	-	expression tag	UNP A0A192B6J5
c	135	HIS	-	expression tag	UNP A0A192B6J5
c	136	HIS	-	expression tag	UNP A0A192B6J5
c	137	HIS	-	expression tag	UNP A0A192B6J5
c	138	HIS	-	expression tag	UNP A0A192B6J5
b	1	GLN	-	expression tag	UNP A0A192B6J5
b	2	VAL	-	expression tag	UNP A0A192B6J5
b	125	GLY	-	expression tag	UNP A0A192B6J5
b	126	GLY	-	expression tag	UNP A0A192B6J5
b	127	LEU	-	expression tag	UNP A0A192B6J5
b	128	PRO	-	expression tag	UNP A0A192B6J5
b	129	GLU	-	expression tag	UNP A0A192B6J5
b	130	THR	-	expression tag	UNP A0A192B6J5
b	131	GLY	-	expression tag	UNP A0A192B6J5
b	132	GLY	-	expression tag	UNP A0A192B6J5
b	133	HIS	-	expression tag	UNP A0A192B6J5
b	134	HIS	-	expression tag	UNP A0A192B6J5
b	135	HIS	-	expression tag	UNP A0A192B6J5
b	136	HIS	-	expression tag	UNP A0A192B6J5
b	137	HIS	-	expression tag	UNP A0A192B6J5
b	138	HIS	-	expression tag	UNP A0A192B6J5
a	1	GLN	-	expression tag	UNP A0A192B6J5
a	2	VAL	-	expression tag	UNP A0A192B6J5
a	125	GLY	-	expression tag	UNP A0A192B6J5
a	126	GLY	-	expression tag	UNP A0A192B6J5
a	127	LEU	-	expression tag	UNP A0A192B6J5
a	128	PRO	-	expression tag	UNP A0A192B6J5
a	129	GLU	-	expression tag	UNP A0A192B6J5
a	130	THR	-	expression tag	UNP A0A192B6J5
a	131	GLY	-	expression tag	UNP A0A192B6J5
a	132	GLY	-	expression tag	UNP A0A192B6J5
a	133	HIS	-	expression tag	UNP A0A192B6J5
a	134	HIS	-	expression tag	UNP A0A192B6J5
a	135	HIS	-	expression tag	UNP A0A192B6J5

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Chain	Residue	Modelled	Actual	Comment	Reference
a	136	HIS	-	expression tag	UNP A0A192B6J5
a	137	HIS	-	expression tag	UNP A0A192B6J5
a	138	HIS	-	expression tag	UNP A0A192B6J5
e	1	GLN	-	expression tag	UNP A0A192B6J5
e	2	VAL	-	expression tag	UNP A0A192B6J5
e	125	GLY	-	expression tag	UNP A0A192B6J5
e	126	GLY	-	expression tag	UNP A0A192B6J5
e	127	LEU	-	expression tag	UNP A0A192B6J5
e	128	PRO	-	expression tag	UNP A0A192B6J5
e	129	GLU	-	expression tag	UNP A0A192B6J5
e	130	THR	-	expression tag	UNP A0A192B6J5
e	131	GLY	-	expression tag	UNP A0A192B6J5
e	132	GLY	-	expression tag	UNP A0A192B6J5
e	133	HIS	-	expression tag	UNP A0A192B6J5
e	134	HIS	-	expression tag	UNP A0A192B6J5
e	135	HIS	-	expression tag	UNP A0A192B6J5
e	136	HIS	-	expression tag	UNP A0A192B6J5
e	137	HIS	-	expression tag	UNP A0A192B6J5
e	138	HIS	-	expression tag	UNP A0A192B6J5

- Molecule 2 is a protein called Nucleocapsid.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	419	Total	C	N	O	S	0	0	0
			3316	2111	556	631	18			
2	C	419	Total	C	N	O	S	0	0	0
			3316	2111	556	631	18			
2	B	419	Total	C	N	O	S	0	0	0
			3316	2111	556	631	18			
2	A	419	Total	C	N	O	S	0	0	0
			3316	2111	556	631	18			
2	E	419	Total	C	N	O	S	0	0	0
			3316	2111	556	631	18			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	0	MET	-	expression tag	UNP A6H4P1
D	1	ALA	-	expression tag	UNP A6H4P1
C	0	MET	-	expression tag	UNP A6H4P1
C	1	ALA	-	expression tag	UNP A6H4P1
B	0	MET	-	expression tag	UNP A6H4P1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1	ALA	-	expression tag	UNP A6H4P1
A	0	MET	-	expression tag	UNP A6H4P1
A	1	ALA	-	expression tag	UNP A6H4P1
E	0	MET	-	expression tag	UNP A6H4P1
E	1	ALA	-	expression tag	UNP A6H4P1

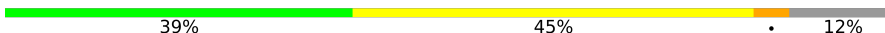
- Molecule 3 is a RNA chain called RNA (45-MER).

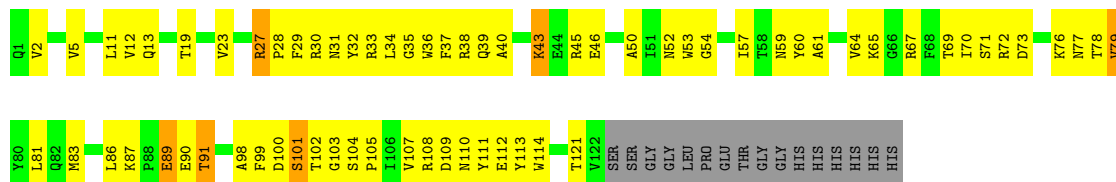
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	R	45	Total	C	N	O	P	0	0	0
			900	405	90	360	45			

3 Residue-property plots

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.

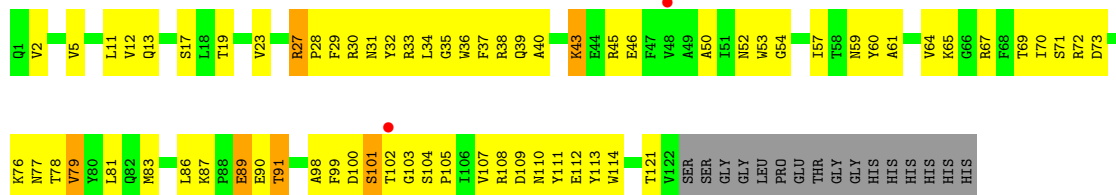
• Molecule 1: Anti-vesicular stomatitis virus N VHH

Chain d: 

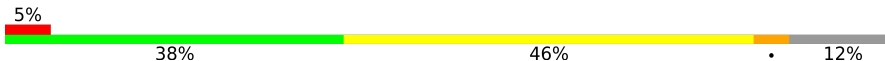


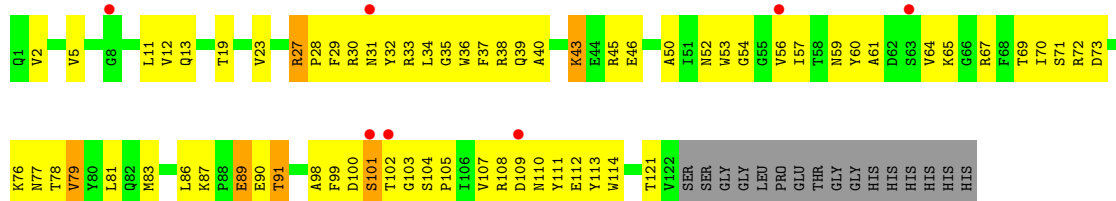
• Molecule 1: Anti-vesicular stomatitis virus N VHH

Chain c: 



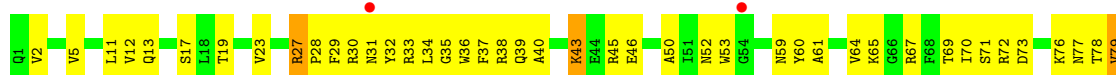
• Molecule 1: Anti-vesicular stomatitis virus N VHH

Chain b: 

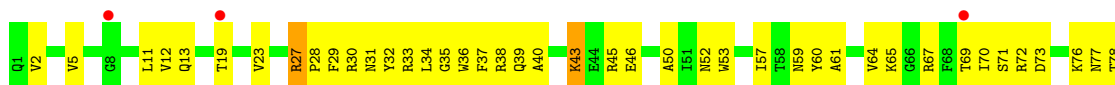


• Molecule 1: Anti-vesicular stomatitis virus N VHH

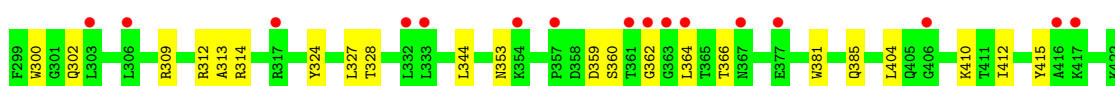
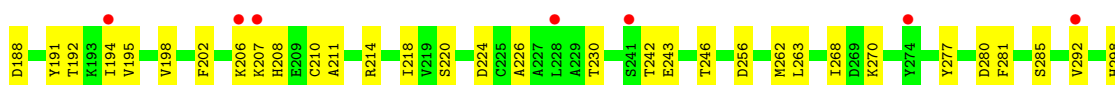
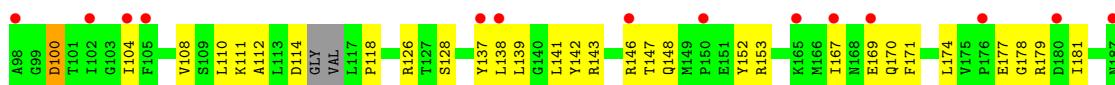
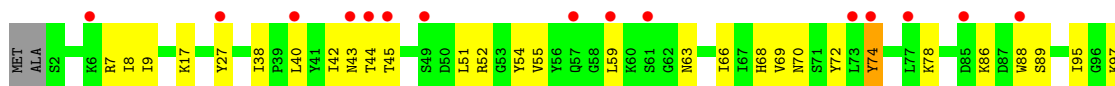
Chain a: 



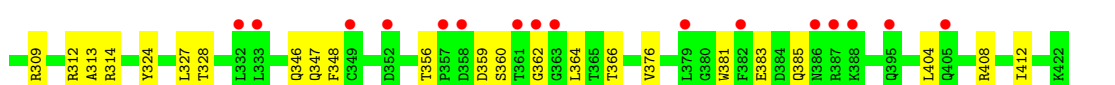
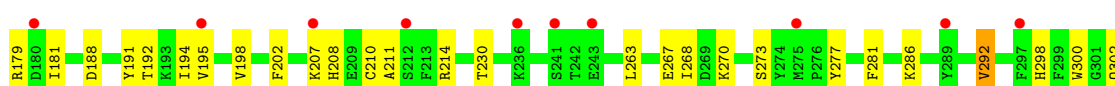
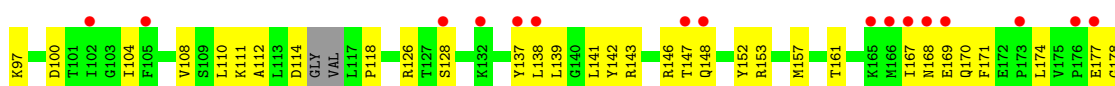
Chain e: 4% 40% 44% 12%



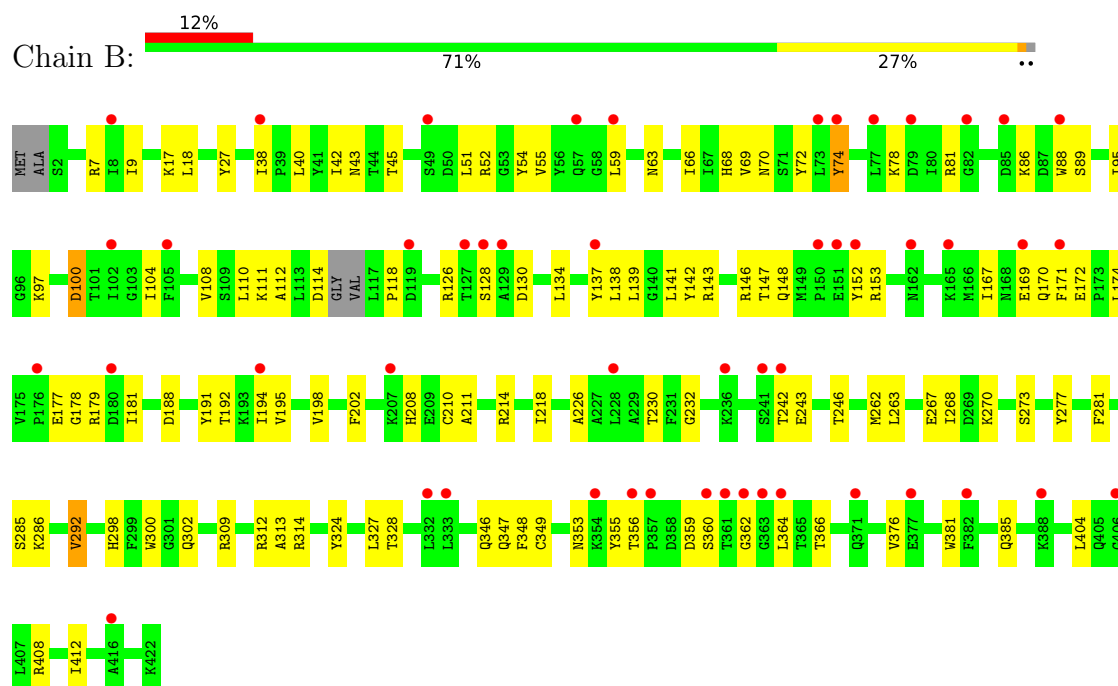
Chain D: 12% 72% 26%



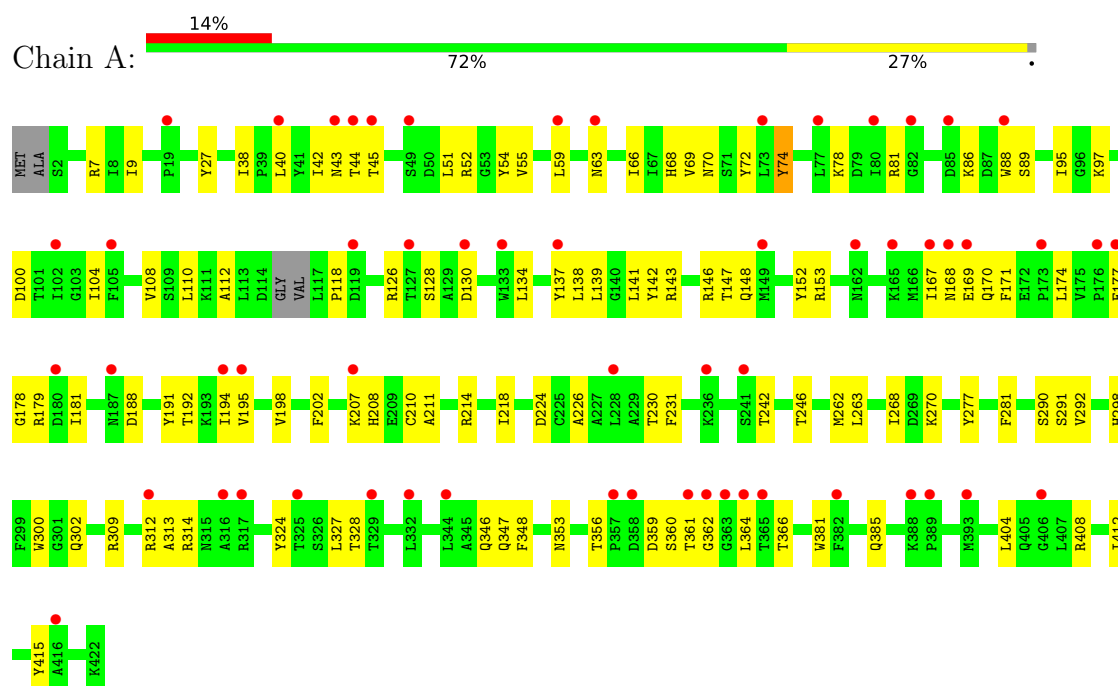
Chain C: 13% 73% 26%



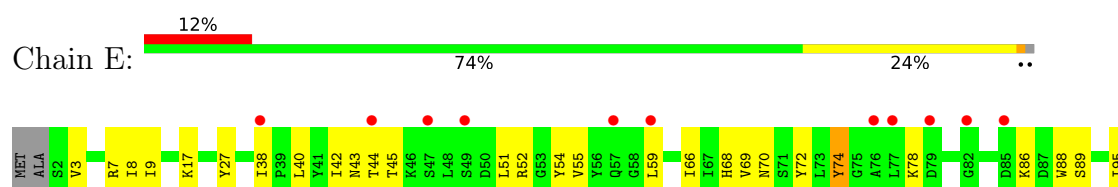
- Molecule 2: Nucleocapsid

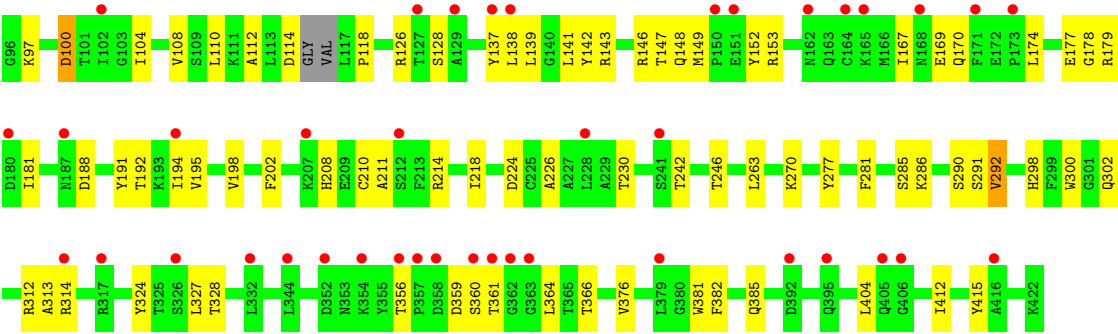


- Molecule 2: Nucleocapsid



- Molecule 2: Nucleocapsid





● Molecule 3: RNA (45-MER)



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	240.12Å 335.50Å 75.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	137.51 – 5.47 137.51 – 5.47	Depositor EDS
% Data completeness (in resolution range)	97.4 (137.51-5.47) 97.4 (137.51-5.47)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.17	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.24 (at 5.42Å)	Xtriage
Refinement program	PHENIX (1.11.1 _2575: ???)	Depositor
R, R_{free}	0.336 , 0.338 0.331 , 0.334	Depositor DCC
R_{free} test set	2000 reflections (9.46%)	wwPDB-VP
Wilson B-factor (Å ²)	292.7	Xtriage
Anisotropy	0.275	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 251.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	22210	wwPDB-VP
Average B, all atoms (Å ²)	309.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.78% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	a	0.33	0/967	0.82	3/1312 (0.2%)
1	b	0.33	0/967	0.82	3/1312 (0.2%)
1	c	0.33	0/967	0.82	3/1312 (0.2%)
1	d	0.33	0/967	0.82	3/1312 (0.2%)
1	e	0.33	0/967	0.82	3/1312 (0.2%)
2	A	0.13	0/3391	0.35	1/4589 (0.0%)
2	B	0.13	0/3391	0.35	1/4589 (0.0%)
2	C	0.13	0/3391	0.35	1/4589 (0.0%)
2	D	0.13	0/3391	0.35	1/4589 (0.0%)
2	E	0.13	0/3391	0.35	1/4589 (0.0%)
3	R	0.80	0/989	1.26	6/1526 (0.4%)
All	All	0.25	0/22779	0.56	26/31031 (0.1%)

There are no bond length outliers.

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	R	20	U	P-O3'-C3'	6.82	130.44	120.20
1	b	89	GLU	N-CA-C	-6.42	104.93	112.89
1	c	89	GLU	N-CA-C	-6.42	104.93	112.89
1	a	89	GLU	N-CA-C	-6.41	104.94	112.89
1	e	89	GLU	N-CA-C	-6.38	104.97	112.89
1	d	89	GLU	N-CA-C	-6.38	104.98	112.89
2	E	292	VAL	N-CA-C	-6.22	106.74	112.96
2	B	292	VAL	N-CA-C	-6.20	106.76	112.96
2	C	292	VAL	N-CA-C	-6.16	106.80	112.96
2	A	292	VAL	N-CA-C	-6.16	106.80	112.96
2	D	292	VAL	N-CA-C	-6.13	106.83	112.96
3	R	9	U	O4'-C4'-C3'	-6.11	97.89	104.00
3	R	15	U	N1-C1'-C2'	5.53	120.29	112.00
1	b	91	THR	N-CA-C	5.33	116.83	109.15
1	d	91	THR	N-CA-C	5.29	116.77	109.15
1	c	91	THR	N-CA-C	5.28	116.76	109.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	e	91	THR	N-CA-C	5.28	116.75	109.15
1	a	91	THR	N-CA-C	5.27	116.74	109.15
3	R	20	U	C2'-C3'-O3'	5.20	121.50	113.70
1	a	64	VAL	CB-CA-C	-5.16	102.82	111.29
1	e	64	VAL	CB-CA-C	-5.16	102.82	111.29
3	R	26	U	C4'-C3'-O3'	-5.16	105.27	113.00
1	b	64	VAL	CB-CA-C	-5.15	102.84	111.29
1	c	64	VAL	CB-CA-C	-5.14	102.85	111.29
1	d	64	VAL	CB-CA-C	-5.14	102.87	111.29
3	R	30	U	C4'-C3'-C2'	-5.06	97.54	102.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	a	946	0	909	209	2
1	b	946	0	908	222	0
1	c	946	0	908	217	2
1	d	946	0	908	218	0
1	e	946	0	908	226	0
2	A	3316	0	3272	143	16
2	B	3316	0	3272	187	12
2	C	3316	0	3272	173	16
2	D	3316	0	3273	178	11
2	E	3316	0	3272	177	16
3	R	900	0	451	138	5
All	All	22210	0	21353	1634	56

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 38.

All (1634) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:d:32:TYR:CE2	1:d:53:TRP:HZ3	1.16	1.63
1:b:32:TYR:CE2	1:b:53:TRP:HZ3	1.16	1.63
1:a:32:TYR:CE2	1:a:53:TRP:HZ3	1.16	1.61
1:b:52:ASN:HD22	2:B:112:ALA:CB	1.11	1.61
1:e:32:TYR:CE2	1:e:53:TRP:HZ3	1.16	1.59
1:c:32:TYR:CE2	1:c:53:TRP:HZ3	1.16	1.57
1:e:102:THR:HG21	2:E:42:ILE:CG2	1.37	1.55
1:e:32:TYR:CE2	1:e:53:TRP:CZ3	1.95	1.54
1:a:34:LEU:CD1	1:a:79:VAL:HG21	1.37	1.53
1:d:32:TYR:CE2	1:d:53:TRP:CZ3	1.95	1.52
1:c:34:LEU:CD1	1:c:79:VAL:HG21	1.36	1.51
1:b:34:LEU:CD1	1:b:79:VAL:HG21	1.37	1.51
1:e:34:LEU:CD1	1:e:79:VAL:HG21	1.36	1.50
1:c:32:TYR:CE2	1:c:53:TRP:CZ3	1.96	1.50
1:a:32:TYR:CE2	1:a:53:TRP:CZ3	1.95	1.50
1:d:34:LEU:CD1	1:d:79:VAL:HG21	1.37	1.49
1:b:32:TYR:CE2	1:b:53:TRP:CZ3	1.95	1.49
1:b:102:THR:HG23	2:B:74:TYR:CE2	1.44	1.47
2:D:214:ARG:NH2	3:R:37:U:C5'	1.78	1.44
1:c:52:ASN:HD22	2:C:112:ALA:CB	1.31	1.44
1:c:33:ARG:CD	1:c:103:GLY:O	1.65	1.43
1:e:33:ARG:CD	1:e:103:GLY:O	1.65	1.43
2:D:206:LYS:CE	3:R:38:U:OP1	1.65	1.42
1:c:33:ARG:CG	1:c:103:GLY:O	1.68	1.42
1:b:33:ARG:CD	1:b:103:GLY:O	1.65	1.42
1:a:33:ARG:CD	1:a:103:GLY:O	1.65	1.41
1:d:33:ARG:CD	1:d:103:GLY:O	1.65	1.41
1:b:33:ARG:CG	1:b:103:GLY:O	1.68	1.41
1:e:102:THR:N	2:E:44:THR:CG2	1.80	1.41
1:d:102:THR:OG1	2:D:44:THR:CG2	1.65	1.40
1:d:33:ARG:CG	1:d:103:GLY:O	1.68	1.40
2:D:214:ARG:HH22	3:R:37:U:C5'	1.30	1.39
1:a:33:ARG:CG	1:a:103:GLY:O	1.68	1.39
1:e:33:ARG:CG	1:e:103:GLY:O	1.68	1.39
1:b:52:ASN:ND2	2:B:112:ALA:HB3	1.23	1.38
1:d:105:PRO:CG	1:d:110:ASN:CG	1.97	1.37
1:c:105:PRO:CG	1:c:110:ASN:CG	1.97	1.38
1:a:105:PRO:CG	1:a:110:ASN:CG	1.97	1.37
1:e:102:THR:OG1	2:E:44:THR:CG2	1.71	1.36
1:a:31:ASN:CG	2:A:74:TYR:OH	1.67	1.36
1:b:105:PRO:CG	1:b:110:ASN:CG	1.97	1.35
1:b:52:ASN:ND2	2:B:112:ALA:CB	1.78	1.35

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:c:102:THR:HG23	2:C:74:TYR:CE2	1.61	1.35
1:d:102:THR:N	2:D:44:THR:HG21	1.37	1.34
1:e:105:PRO:CG	1:e:110:ASN:CG	1.97	1.34
1:c:52:ASN:ND2	2:C:112:ALA:HB3	1.43	1.33
1:c:37:PHE:HE1	1:c:111:TYR:CE2	1.47	1.33
1:a:37:PHE:HE1	1:a:111:TYR:CE2	1.47	1.32
2:B:152:TYR:HE1	3:R:17:U:OP1	0.99	1.32
1:e:37:PHE:HE1	1:e:111:TYR:CE2	1.47	1.32
1:b:37:PHE:HE1	1:b:111:TYR:CE2	1.47	1.31
1:d:37:PHE:HE1	1:d:111:TYR:CE2	1.47	1.30
1:a:31:ASN:CB	2:A:74:TYR:OH	1.78	1.30
2:B:152:TYR:CE1	3:R:17:U:OP1	1.85	1.29
1:c:105:PRO:CG	1:c:110:ASN:OD1	1.81	1.29
1:a:105:PRO:CG	1:a:110:ASN:OD1	1.81	1.28
1:b:105:PRO:CG	1:b:110:ASN:OD1	1.81	1.28
1:e:31:ASN:HB3	2:E:110:LEU:CG	1.62	1.28
1:a:102:THR:HG23	2:A:74:TYR:CE2	1.69	1.28
2:D:206:LYS:NZ	3:R:38:U:OP1	1.64	1.28
2:A:290:SER:HB2	3:R:4:U:OP2	1.24	1.27
1:d:37:PHE:CE1	1:d:111:TYR:CE2	2.22	1.27
1:e:100:ASP:OD2	2:E:78:LYS:HE2	1.27	1.27
1:a:37:PHE:CE1	1:a:111:TYR:CE2	2.22	1.26
1:e:37:PHE:CE1	1:e:111:TYR:CE2	2.22	1.26
1:d:105:PRO:CG	1:d:110:ASN:OD1	1.81	1.26
1:b:37:PHE:CE1	1:b:111:TYR:CE2	2.22	1.26
1:e:105:PRO:CG	1:e:110:ASN:OD1	1.81	1.26
1:c:37:PHE:CE1	1:c:111:TYR:CE2	2.22	1.26
2:D:214:ARG:NH2	3:R:37:U:H5'	0.92	1.25
1:c:102:THR:N	2:C:44:THR:HG21	1.11	1.25
1:a:34:LEU:HD13	1:a:79:VAL:CG2	1.67	1.25
1:d:34:LEU:CD1	1:d:79:VAL:CG2	2.14	1.24
1:c:34:LEU:HD13	1:c:79:VAL:CG2	1.67	1.24
1:c:102:THR:N	2:C:44:THR:CG2	1.96	1.24
1:a:34:LEU:CD1	1:a:79:VAL:CG2	2.14	1.24
1:e:34:LEU:CD1	1:e:79:VAL:CG2	2.14	1.24
1:c:34:LEU:CD1	1:c:79:VAL:CG2	2.14	1.24
1:e:34:LEU:HD13	1:e:79:VAL:CG2	1.67	1.24
1:b:34:LEU:CD1	1:b:79:VAL:CG2	2.14	1.23
1:e:102:THR:H	2:E:44:THR:CG2	1.41	1.23
2:E:286:LYS:HD3	3:R:39:U:OP2	1.37	1.23
1:e:102:THR:CA	2:E:44:THR:HG21	1.69	1.22

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:d:34:LEU:HD13	1:d:79:VAL:CG2	1.67	1.21
1:b:34:LEU:HD13	1:b:79:VAL:CG2	1.67	1.21
1:a:32:TYR:CD2	1:a:53:TRP:HZ3	1.59	1.21
1:b:32:TYR:CD2	1:b:53:TRP:HZ3	1.59	1.20
1:d:32:TYR:CD2	1:d:53:TRP:HZ3	1.59	1.20
1:d:102:THR:OG1	2:D:44:THR:HG23	1.08	1.20
1:d:52:ASN:HD22	2:D:112:ALA:CB	1.53	1.20
1:a:37:PHE:CE1	1:a:111:TYR:HE2	1.59	1.19
1:e:37:PHE:CE1	1:e:111:TYR:HE2	1.59	1.19
1:e:102:THR:CB	2:E:44:THR:HG23	1.70	1.19
1:c:32:TYR:CD2	1:c:53:TRP:HZ3	1.59	1.19
1:e:102:THR:N	2:E:44:THR:HG21	0.86	1.19
1:c:32:TYR:CD2	1:c:53:TRP:CZ3	2.31	1.19
1:b:32:TYR:CD2	1:b:53:TRP:CZ3	2.31	1.19
1:a:32:TYR:CD2	1:a:53:TRP:CZ3	2.31	1.19
1:e:32:TYR:CD2	1:e:53:TRP:HZ3	1.58	1.19
1:c:33:ARG:HG2	1:c:103:GLY:O	1.27	1.17
1:d:37:PHE:CE1	1:d:111:TYR:HE2	1.60	1.17
1:e:32:TYR:CD2	1:e:53:TRP:CZ3	2.31	1.17
1:d:102:THR:CA	2:D:44:THR:HG21	1.75	1.17
1:a:33:ARG:HG2	1:a:103:GLY:O	1.27	1.17
1:d:103:GLY:CA	2:D:44:THR:OG1	1.92	1.16
1:d:103:GLY:N	2:D:44:THR:OG1	1.78	1.16
1:b:37:PHE:CE1	1:b:111:TYR:HE2	1.59	1.16
1:b:33:ARG:HG2	1:b:103:GLY:O	1.27	1.16
1:b:105:PRO:HG3	1:b:110:ASN:OD1	1.46	1.16
1:d:33:ARG:HG2	1:d:103:GLY:O	1.27	1.15
2:D:206:LYS:HE2	3:R:38:U:OP1	1.47	1.15
1:c:105:PRO:HG2	1:c:110:ASN:OD1	1.46	1.15
1:e:102:THR:CG2	2:E:42:ILE:CG2	2.25	1.15
1:d:32:TYR:CD2	1:d:53:TRP:CZ3	2.31	1.13
1:b:100:ASP:O	2:B:78:LYS:HE3	1.46	1.13
1:a:105:PRO:HG2	1:a:110:ASN:OD1	1.46	1.13
1:e:102:THR:CA	2:E:44:THR:CG2	2.25	1.13
1:d:103:GLY:HA3	2:D:44:THR:OG1	1.45	1.13
1:c:105:PRO:HG3	1:c:110:ASN:OD1	1.46	1.12
1:e:99:PHE:HB2	1:e:111:TYR:HA	1.16	1.12
1:a:105:PRO:HG3	1:a:110:ASN:OD1	1.46	1.12
1:d:105:PRO:HG3	1:d:110:ASN:OD1	1.46	1.11
1:d:52:ASN:ND2	2:D:112:ALA:HB3	1.64	1.11
1:e:105:PRO:HG3	1:e:110:ASN:OD1	1.46	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:b:102:THR:CG2	2:B:74:TYR:CE2	2.31	1.11
1:e:105:PRO:HB2	1:e:110:ASN:ND2	1.65	1.11
1:b:99:PHE:HB2	1:b:111:TYR:HA	1.16	1.11
1:a:105:PRO:HB2	1:a:110:ASN:ND2	1.66	1.11
2:C:17:LYS:HG3	2:B:268:ILE:HD11	1.30	1.10
1:b:102:THR:HG21	2:B:42:ILE:HG21	1.17	1.10
1:e:31:ASN:HB3	2:E:110:LEU:HG	1.15	1.10
1:c:99:PHE:HB2	1:c:111:TYR:HA	1.16	1.10
1:b:105:PRO:HB2	1:b:110:ASN:ND2	1.66	1.10
1:b:31:ASN:HD21	2:B:78:LYS:HD2	1.03	1.10
2:E:143:ARG:NH2	3:R:44:U:H5''	1.65	1.10
1:d:105:PRO:HB2	1:d:110:ASN:ND2	1.66	1.10
1:c:105:PRO:HB2	1:c:110:ASN:ND2	1.66	1.10
1:d:99:PHE:HB2	1:d:111:TYR:HA	1.16	1.10
1:c:37:PHE:CE1	1:c:111:TYR:HE2	1.60	1.10
1:a:31:ASN:ND2	2:A:74:TYR:OH	1.85	1.09
1:a:99:PHE:HB2	1:a:111:TYR:HA	1.16	1.09
1:e:100:ASP:OD2	2:E:78:LYS:CE	2.00	1.09
1:c:52:ASN:ND2	2:C:112:ALA:CB	2.07	1.09
1:b:105:PRO:HG2	1:b:110:ASN:OD1	1.46	1.09
1:e:105:PRO:HG2	1:e:110:ASN:OD1	1.46	1.09
1:a:52:ASN:HD22	2:A:112:ALA:CB	1.66	1.08
1:d:105:PRO:HG3	1:d:110:ASN:CG	1.73	1.08
1:d:105:PRO:HG2	1:d:110:ASN:OD1	1.46	1.08
1:a:31:ASN:HB3	2:A:74:TYR:OH	1.50	1.07
2:E:290:SER:HB2	3:R:40:U:OP2	1.54	1.07
1:e:33:ARG:HG2	1:e:103:GLY:O	1.27	1.07
1:c:52:ASN:HD22	2:C:112:ALA:HB3	0.95	1.06
1:a:105:PRO:HG3	1:a:110:ASN:CG	1.73	1.06
1:c:102:THR:HG21	2:C:42:ILE:HG21	1.32	1.06
1:a:102:THR:CG2	2:A:74:TYR:CE2	2.39	1.06
1:d:57:ILE:HD11	2:D:114:ASP:HB3	1.32	1.06
1:c:105:PRO:HG3	1:c:110:ASN:CG	1.73	1.06
1:b:105:PRO:HG3	1:b:110:ASN:CG	1.73	1.06
1:e:33:ARG:HD2	1:e:103:GLY:O	1.56	1.06
1:d:34:LEU:HD12	1:d:79:VAL:HG21	1.39	1.05
1:d:100:ASP:O	2:D:78:LYS:HE3	1.55	1.05
2:C:348:PHE:CD1	2:E:7:ARG:HA	1.89	1.05
1:b:52:ASN:HD22	2:B:112:ALA:HB1	1.21	1.05
1:a:52:ASN:ND2	2:A:112:ALA:CB	2.20	1.05
1:c:34:LEU:HD12	1:c:79:VAL:HG21	1.39	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:e:34:LEU:HD12	1:e:79:VAL:HG21	1.39	1.05
1:d:33:ARG:HD2	1:d:103:GLY:O	1.56	1.04
1:b:31:ASN:HB3	2:B:110:LEU:HG	1.38	1.04
1:d:99:PHE:CD1	1:d:112:GLU:HG3	1.93	1.04
1:c:27:ARG:HH22	2:C:81:ARG:CZ	1.71	1.04
1:a:102:THR:HG23	2:A:74:TYR:HE2	0.91	1.04
1:c:99:PHE:CD1	1:c:112:GLU:HG3	1.93	1.03
1:e:99:PHE:CD1	1:e:112:GLU:HG3	1.93	1.03
1:e:105:PRO:HG3	1:e:110:ASN:CG	1.73	1.03
1:c:99:PHE:CG	1:c:110:ASN:O	2.11	1.03
1:b:99:PHE:CD1	1:b:112:GLU:HG3	1.93	1.03
1:b:99:PHE:CG	1:b:110:ASN:O	2.11	1.03
1:e:99:PHE:CG	1:e:110:ASN:O	2.11	1.03
1:e:102:THR:CB	2:E:44:THR:CG2	2.33	1.03
2:E:143:ARG:HH22	3:R:44:U:H5''	1.21	1.03
1:c:33:ARG:HD2	1:c:103:GLY:O	1.56	1.03
1:b:102:THR:HG21	2:B:42:ILE:CG2	1.88	1.03
1:b:34:LEU:HD12	1:b:79:VAL:HG21	1.39	1.03
1:e:31:ASN:CB	2:E:110:LEU:HG	1.87	1.03
1:d:102:THR:HG23	2:D:74:TYR:CE2	1.93	1.02
1:a:102:THR:CG2	2:A:74:TYR:HE2	1.72	1.02
1:e:102:THR:HG21	2:E:42:ILE:HG21	1.10	1.02
1:c:69:THR:O	1:c:81:LEU:HD12	1.59	1.02
1:d:99:PHE:CG	1:d:110:ASN:O	2.11	1.02
1:a:33:ARG:HD2	1:a:103:GLY:O	1.56	1.02
1:d:69:THR:O	1:d:81:LEU:HD12	1.59	1.02
1:a:99:PHE:CG	1:a:110:ASN:O	2.11	1.02
1:b:69:THR:O	1:b:81:LEU:HD12	1.59	1.02
1:e:99:PHE:CD1	1:e:110:ASN:O	2.13	1.02
1:c:102:THR:CG2	2:C:74:TYR:CE2	2.43	1.01
1:a:34:LEU:HD12	1:a:79:VAL:HG21	1.39	1.01
1:a:99:PHE:CD1	1:a:112:GLU:HG3	1.93	1.01
1:e:69:THR:O	1:e:81:LEU:HD12	1.59	1.01
1:c:31:ASN:HD21	2:C:78:LYS:HD2	1.22	1.01
2:C:348:PHE:CE1	2:E:7:ARG:HB2	1.96	1.01
1:a:27:ARG:HH22	2:A:81:ARG:CZ	1.74	1.01
1:a:69:THR:O	1:a:81:LEU:HD12	1.59	1.01
1:c:102:THR:HG23	2:C:74:TYR:HE2	0.90	1.01
1:c:31:ASN:HB2	1:c:101:SER:O	1.61	1.01
1:c:57:ILE:HD11	2:C:114:ASP:HB3	1.40	1.01
1:c:99:PHE:CD1	1:c:110:ASN:O	2.13	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:348:PHE:HE1	2:E:7:ARG:HB2	1.24	1.01
1:b:33:ARG:HD2	1:b:103:GLY:O	1.56	1.01
1:d:31:ASN:HB2	1:d:101:SER:O	1.61	1.00
1:d:52:ASN:HD22	2:D:112:ALA:HB3	0.90	1.00
1:d:99:PHE:CD1	1:d:110:ASN:O	2.13	1.00
1:a:99:PHE:CD1	1:a:110:ASN:O	2.13	1.00
1:b:99:PHE:CD1	1:b:110:ASN:O	2.13	1.00
1:b:31:ASN:HB2	1:b:101:SER:O	1.61	1.00
1:a:105:PRO:HG2	1:a:110:ASN:CG	1.81	1.00
1:e:102:THR:HG21	2:E:42:ILE:HG23	1.42	1.00
2:A:224:ASP:OD2	3:R:3:U:P	2.20	0.99
2:E:218:ILE:HD12	3:R:45:U:H3'	1.42	0.99
1:a:31:ASN:HB2	1:a:101:SER:O	1.61	0.99
1:e:100:ASP:O	2:E:78:LYS:HE3	1.63	0.99
2:D:202:PHE:HB3	2:D:214:ARG:HD3	1.45	0.99
2:D:214:ARG:HH21	3:R:37:U:H5'	1.17	0.99
2:E:202:PHE:HB3	2:E:214:ARG:HD3	1.45	0.98
1:d:33:ARG:NE	1:d:105:PRO:HD3	1.77	0.98
1:d:99:PHE:HD1	1:d:112:GLU:HG3	1.27	0.98
1:e:52:ASN:HD22	2:E:112:ALA:HB3	1.25	0.98
1:d:105:PRO:CB	1:d:110:ASN:CG	2.37	0.98
1:c:105:PRO:HG2	1:c:110:ASN:CG	1.81	0.98
1:d:32:TYR:CE2	1:d:53:TRP:CH2	2.52	0.98
1:c:33:ARG:NE	1:c:105:PRO:HD3	1.77	0.98
1:a:31:ASN:HD21	2:A:78:LYS:HD2	1.25	0.98
1:c:32:TYR:CE2	1:c:53:TRP:CH2	2.52	0.98
2:A:202:PHE:HB3	2:A:214:ARG:HD3	1.45	0.98
1:a:33:ARG:NE	1:a:105:PRO:HD3	1.77	0.98
1:e:33:ARG:NE	1:e:105:PRO:HD3	1.77	0.98
1:e:105:PRO:CB	1:e:110:ASN:CG	2.37	0.98
1:c:105:PRO:CB	1:c:110:ASN:CG	2.37	0.97
1:e:102:THR:OG1	2:E:44:THR:HG23	0.81	0.97
1:b:32:TYR:CE2	1:b:53:TRP:CH2	2.52	0.97
1:b:33:ARG:NE	1:b:105:PRO:HD3	1.77	0.97
1:a:31:ASN:ND2	2:A:74:TYR:CZ	2.32	0.97
1:e:32:TYR:CE2	1:e:53:TRP:CH2	2.52	0.97
2:A:290:SER:CB	3:R:4:U:OP2	2.12	0.97
1:b:57:ILE:HD11	2:B:114:ASP:HB3	1.45	0.97
1:b:105:PRO:CB	1:b:110:ASN:CG	2.37	0.97
1:e:102:THR:CB	2:E:42:ILE:HG23	1.94	0.97
1:e:31:ASN:HB2	1:e:101:SER:O	1.61	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:c:102:THR:HG21	2:C:42:ILE:CG2	1.95	0.97
2:C:348:PHE:CE1	2:E:7:ARG:CB	2.48	0.97
2:B:202:PHE:HB3	2:B:214:ARG:HD3	1.45	0.97
1:a:32:TYR:CE2	1:a:53:TRP:CH2	2.52	0.97
1:a:105:PRO:CB	1:a:110:ASN:CG	2.37	0.97
1:e:37:PHE:CZ	1:e:111:TYR:HE2	1.83	0.97
2:E:286:LYS:CD	3:R:39:U:OP2	2.13	0.96
1:b:37:PHE:CZ	1:b:111:TYR:HE2	1.83	0.96
2:B:408:ARG:NH2	3:R:15:U:H3'	1.81	0.96
2:A:224:ASP:OD2	3:R:3:U:OP2	1.84	0.96
2:C:202:PHE:HB3	2:C:214:ARG:HD3	1.45	0.96
1:b:99:PHE:HD1	1:b:112:GLU:HG3	1.26	0.96
1:a:37:PHE:CZ	1:a:111:TYR:HE2	1.83	0.96
1:d:102:THR:HG21	2:D:42:ILE:HG21	1.45	0.96
2:B:312:ARG:HD2	3:R:14:U:C4	2.00	0.96
1:e:105:PRO:HG2	1:e:110:ASN:CG	1.81	0.96
1:c:37:PHE:CZ	1:c:111:TYR:HE2	1.83	0.96
1:c:99:PHE:HD1	1:c:112:GLU:HG3	1.27	0.96
2:D:214:ARG:HH22	3:R:37:U:H5''	1.28	0.96
1:a:52:ASN:ND2	2:A:112:ALA:HB3	1.80	0.96
1:d:37:PHE:CZ	1:d:111:TYR:HE2	1.83	0.95
2:E:143:ARG:HH22	3:R:44:U:C5'	1.79	0.95
1:d:108:ARG:HG3	1:d:114:TRP:CH2	2.02	0.94
1:e:102:THR:CG2	2:E:42:ILE:HG23	1.95	0.94
1:a:99:PHE:HD1	1:a:112:GLU:HG3	1.27	0.94
1:e:101:SER:C	2:E:44:THR:HG21	1.92	0.94
1:a:108:ARG:HG3	1:a:114:TRP:CH2	2.03	0.94
1:c:108:ARG:HG3	1:c:114:TRP:CH2	2.03	0.94
1:e:102:THR:H	2:E:44:THR:CB	1.78	0.94
2:A:291:SER:OG	3:R:4:U:H5''	1.67	0.94
2:C:348:PHE:CE1	2:E:7:ARG:HG3	2.03	0.94
1:b:31:ASN:ND2	2:B:78:LYS:HD2	1.82	0.94
1:d:60:TYR:HB2	1:d:65:LYS:CD	1.99	0.93
1:e:60:TYR:HB2	1:e:65:LYS:CD	1.99	0.93
1:e:52:ASN:ND2	2:E:112:ALA:HB3	1.82	0.93
2:D:218:ILE:HD11	3:R:36:U:C6	2.03	0.93
1:e:33:ARG:CD	1:e:103:GLY:C	2.41	0.93
1:a:60:TYR:HB2	1:a:65:LYS:CD	1.99	0.93
1:c:60:TYR:HB2	1:c:65:LYS:CD	1.99	0.93
1:b:108:ARG:HG3	1:b:114:TRP:CH2	2.03	0.93
1:a:33:ARG:CD	1:a:103:GLY:C	2.41	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:e:108:ARG:HG3	1:e:114:TRP:CH2	2.02	0.93
1:c:33:ARG:CD	1:c:103:GLY:C	2.42	0.92
1:e:99:PHE:HD1	1:e:112:GLU:HG3	1.27	0.92
1:d:33:ARG:CD	1:d:103:GLY:C	2.42	0.92
2:D:268:ILE:HD11	2:E:17:LYS:HG3	1.49	0.92
1:b:33:ARG:CD	1:b:103:GLY:C	2.41	0.92
1:c:102:THR:H	2:C:44:THR:CG2	1.76	0.92
1:b:60:TYR:HB2	1:b:65:LYS:CD	1.99	0.92
1:c:32:TYR:CZ	1:c:53:TRP:HZ3	1.88	0.91
1:a:32:TYR:CZ	1:a:53:TRP:HZ3	1.88	0.91
2:C:348:PHE:CE1	2:E:7:ARG:CG	2.53	0.91
1:a:31:ASN:HD21	2:A:78:LYS:CD	1.82	0.91
1:d:32:TYR:CZ	1:d:53:TRP:HZ3	1.88	0.91
2:C:17:LYS:HE2	2:B:268:ILE:HG12	1.51	0.91
2:C:17:LYS:HG3	2:B:268:ILE:CD1	2.00	0.90
1:e:32:TYR:CZ	1:e:53:TRP:HZ3	1.88	0.90
2:A:312:ARG:HD2	3:R:5:U:C4	2.05	0.90
1:d:33:ARG:HD2	1:d:104:SER:HA	1.52	0.90
1:a:72:ARG:HB3	1:a:79:VAL:HG22	1.54	0.90
1:e:52:ASN:HD22	2:E:112:ALA:CB	1.84	0.90
1:e:33:ARG:HD2	1:e:104:SER:HA	1.52	0.90
1:b:72:ARG:HB3	1:b:79:VAL:HG22	1.53	0.90
1:c:72:ARG:HB3	1:c:79:VAL:HG22	1.54	0.90
1:b:31:ASN:HD21	2:B:78:LYS:CD	1.84	0.90
1:b:38:ARG:NH1	1:b:90:GLU:OE1	2.05	0.89
1:a:38:ARG:NH1	1:a:90:GLU:OE1	2.05	0.89
1:d:31:ASN:HB3	2:D:110:LEU:HD23	1.53	0.89
1:d:72:ARG:HB3	1:d:79:VAL:HG22	1.53	0.89
1:c:33:ARG:HD2	1:c:104:SER:HA	1.52	0.89
1:b:33:ARG:HD2	1:b:104:SER:HA	1.52	0.89
1:c:38:ARG:NH1	1:c:90:GLU:OE1	2.05	0.89
1:e:38:ARG:NH1	1:e:90:GLU:OE1	2.05	0.89
1:b:32:TYR:CZ	1:b:53:TRP:HZ3	1.88	0.89
1:d:102:THR:HG23	2:D:74:TYR:HE2	1.37	0.89
1:a:31:ASN:ND2	2:A:78:LYS:HD2	1.88	0.89
1:d:103:GLY:HA3	2:D:44:THR:HG1	1.32	0.89
2:C:17:LYS:CG	2:B:268:ILE:HD11	2.02	0.88
1:b:102:THR:CB	2:B:42:ILE:HG23	2.03	0.88
1:d:102:THR:H	2:D:44:THR:CG2	1.85	0.88
1:a:33:ARG:HD2	1:a:104:SER:HA	1.52	0.88
1:d:38:ARG:NH1	1:d:90:GLU:OE1	2.05	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:312:ARG:HD2	3:R:14:U:C5	2.08	0.88
1:d:33:ARG:HD3	1:d:103:GLY:O	1.74	0.88
2:C:312:ARG:HD2	3:R:23:U:C4	2.09	0.88
1:e:33:ARG:HD3	1:e:103:GLY:O	1.74	0.88
1:c:33:ARG:HD3	1:c:103:GLY:O	1.74	0.88
1:b:33:ARG:HD3	1:b:103:GLY:O	1.74	0.88
1:d:35:GLY:HA3	1:d:111:TYR:OH	1.74	0.87
1:e:35:GLY:HA3	1:e:111:TYR:OH	1.74	0.87
1:d:105:PRO:CB	1:d:110:ASN:ND2	2.37	0.87
1:e:105:PRO:CB	1:e:110:ASN:ND2	2.37	0.87
1:b:52:ASN:ND2	2:B:112:ALA:HB2	1.89	0.87
1:d:105:PRO:HG2	1:d:110:ASN:CG	1.81	0.87
1:d:107:VAL:HG12	1:d:108:ARG:N	1.90	0.87
1:c:31:ASN:HB3	2:C:110:LEU:HG	1.56	0.87
1:c:35:GLY:HA3	1:c:111:TYR:OH	1.74	0.87
1:b:105:PRO:CB	1:b:110:ASN:ND2	2.37	0.87
1:a:33:ARG:HD3	1:a:103:GLY:O	1.74	0.87
1:e:72:ARG:HB3	1:e:79:VAL:HG22	1.53	0.87
1:b:35:GLY:HA3	1:b:111:TYR:OH	1.74	0.87
1:b:107:VAL:HG12	1:b:108:ARG:N	1.89	0.87
1:a:35:GLY:HA3	1:a:111:TYR:OH	1.74	0.87
1:c:50:ALA:HB1	1:c:104:SER:HB2	1.57	0.87
1:a:87:LYS:HG2	1:a:90:GLU:HG2	1.57	0.87
1:b:50:ALA:HB1	1:b:104:SER:HB2	1.57	0.86
1:e:34:LEU:HD13	1:e:79:VAL:HG21	0.88	0.86
2:D:218:ILE:HD11	3:R:36:U:H6	1.40	0.86
2:C:346:GLN:O	2:E:8:ILE:HD11	1.75	0.86
1:d:50:ALA:HB1	1:d:104:SER:HB2	1.57	0.86
1:d:102:THR:H	2:D:44:THR:HG21	1.05	0.86
1:d:102:THR:CB	2:D:44:THR:CG2	2.53	0.86
1:a:105:PRO:CB	1:a:110:ASN:ND2	2.37	0.86
1:b:52:ASN:HD21	2:B:112:ALA:HB3	1.34	0.86
1:a:107:VAL:HG12	1:a:108:ARG:N	1.90	0.86
1:c:105:PRO:CB	1:c:110:ASN:ND2	2.37	0.86
1:a:34:LEU:HD13	1:a:79:VAL:HG21	0.88	0.86
1:d:34:LEU:HD13	1:d:79:VAL:HG21	0.88	0.86
1:b:87:LYS:HG2	1:b:90:GLU:HG2	1.57	0.86
1:e:50:ALA:HB1	1:e:104:SER:HB2	1.57	0.86
1:c:34:LEU:HD13	1:c:79:VAL:HG21	0.87	0.85
2:C:348:PHE:CD1	2:E:7:ARG:CA	2.58	0.85
1:b:34:LEU:HD13	1:b:79:VAL:HG21	0.88	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:50:ALA:HB1	1:a:104:SER:HB2	1.57	0.85
2:D:7:ARG:HG3	2:B:348:PHE:CE1	2.11	0.85
1:d:102:THR:CA	2:D:44:THR:CG2	2.53	0.85
2:B:408:ARG:NH2	3:R:16:U:OP1	2.08	0.85
1:e:102:THR:HG1	2:E:44:THR:HG23	1.37	0.85
1:c:107:VAL:HG12	1:c:108:ARG:N	1.90	0.85
1:e:107:VAL:HG12	1:e:108:ARG:N	1.90	0.85
1:c:87:LYS:HZ2	1:c:89:GLU:HB2	1.40	0.85
1:b:105:PRO:HG2	1:b:110:ASN:CG	1.81	0.85
1:c:87:LYS:HG2	1:c:90:GLU:HG2	1.57	0.84
1:d:102:THR:HG21	2:D:42:ILE:CG2	2.07	0.84
1:b:102:THR:HB	2:B:42:ILE:HG23	1.58	0.84
2:D:300:TRP:HB2	2:D:327:LEU:HD12	1.59	0.84
2:C:300:TRP:HB2	2:C:327:LEU:HD12	1.59	0.84
1:b:27:ARG:HH22	2:B:81:ARG:CZ	1.91	0.84
2:E:149:MET:HE3	3:R:42:U:C6	2.11	0.84
1:d:87:LYS:HG2	1:d:90:GLU:HG2	1.57	0.84
1:e:31:ASN:HB3	2:E:110:LEU:CB	2.08	0.84
1:a:107:VAL:HG12	1:a:109:ASP:H	1.43	0.83
1:e:107:VAL:HG12	1:e:109:ASP:H	1.43	0.83
2:E:300:TRP:HB2	2:E:327:LEU:HD12	1.59	0.83
1:c:100:ASP:O	2:C:78:LYS:HE3	1.78	0.83
2:A:300:TRP:HB2	2:A:327:LEU:HD12	1.59	0.83
1:e:87:LYS:HG2	1:e:90:GLU:HG2	1.57	0.83
2:B:300:TRP:HB2	2:B:327:LEU:HD12	1.59	0.83
1:d:31:ASN:HB3	2:D:110:LEU:CD2	2.09	0.83
2:D:7:ARG:HA	2:B:348:PHE:CD1	2.13	0.83
1:b:107:VAL:HG12	1:b:109:ASP:H	1.44	0.83
1:d:102:THR:HG22	2:D:110:LEU:HB3	1.60	0.83
1:b:31:ASN:HB3	2:B:110:LEU:CG	2.07	0.83
2:E:143:ARG:NH2	3:R:44:U:C5'	2.38	0.82
2:B:17:LYS:HG3	2:A:268:ILE:HD11	1.58	0.82
1:d:102:THR:C	2:D:44:THR:OG1	2.22	0.82
1:d:107:VAL:HG12	1:d:109:ASP:H	1.43	0.82
1:c:107:VAL:HG12	1:c:109:ASP:H	1.43	0.82
1:d:102:THR:N	2:D:44:THR:CG2	2.34	0.82
1:c:27:ARG:HH22	2:C:81:ARG:NH2	1.77	0.82
1:a:31:ASN:HB3	2:A:110:LEU:HG	1.60	0.82
3:R:11:U:H3'	3:R:12:U:H5''	1.62	0.81
1:c:31:ASN:HD21	2:C:78:LYS:CD	1.93	0.81
1:b:102:THR:CG2	2:B:42:ILE:CG2	2.58	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:b:102:THR:CG2	2:B:74:TYR:HE2	1.82	0.81
1:d:32:TYR:HE2	1:d:53:TRP:CH2	1.99	0.81
1:e:31:ASN:HB3	2:E:110:LEU:CD2	2.09	0.81
1:b:32:TYR:CZ	1:b:53:TRP:CZ3	2.66	0.81
1:a:32:TYR:CZ	1:a:53:TRP:CZ3	2.66	0.81
1:c:102:THR:H	2:C:44:THR:CB	1.94	0.81
1:d:102:THR:OG1	2:D:42:ILE:HG23	1.81	0.80
1:c:31:ASN:ND2	2:C:78:LYS:HD2	1.94	0.80
1:d:102:THR:HG21	2:D:110:LEU:HD12	1.63	0.80
1:c:32:TYR:CZ	1:c:53:TRP:CZ3	2.66	0.80
1:e:87:LYS:HZ2	1:e:89:GLU:HB2	1.47	0.80
1:d:34:LEU:HD12	1:d:79:VAL:CG2	2.02	0.80
2:D:214:ARG:CZ	3:R:37:U:H5'	2.07	0.80
1:c:32:TYR:HE2	1:c:53:TRP:CH2	1.99	0.80
1:c:30:ARG:O	1:c:32:TYR:HD2	1.65	0.80
1:b:30:ARG:O	1:b:32:TYR:HD2	1.65	0.80
1:b:100:ASP:O	2:B:78:LYS:CE	2.26	0.79
1:b:102:THR:HG23	2:B:74:TYR:CD2	2.15	0.79
1:a:27:ARG:HH22	2:A:81:ARG:NH2	1.79	0.79
1:d:30:ARG:O	1:d:32:TYR:HD2	1.65	0.79
1:e:30:ARG:O	1:e:32:TYR:HD2	1.65	0.79
1:a:30:ARG:O	1:a:32:TYR:HD2	1.65	0.79
1:a:102:THR:HG21	2:A:42:ILE:HG21	1.65	0.79
1:e:67:ARG:NH2	1:e:90:GLU:OE2	2.15	0.79
1:b:32:TYR:HE2	1:b:53:TRP:CH2	1.99	0.78
1:d:32:TYR:CZ	1:d:53:TRP:CZ3	2.66	0.78
2:C:7:ARG:HB2	2:A:348:PHE:CE1	2.19	0.78
1:a:67:ARG:NH2	1:a:90:GLU:OE2	2.15	0.78
2:D:312:ARG:HD2	3:R:32:U:C4	2.19	0.78
1:b:67:ARG:NH2	1:b:90:GLU:OE2	2.15	0.78
1:e:32:TYR:CZ	1:e:53:TRP:CZ3	2.66	0.78
2:D:268:ILE:HG12	2:E:17:LYS:HE2	1.66	0.78
1:a:32:TYR:HE2	1:a:53:TRP:CH2	1.99	0.78
2:D:7:ARG:HB2	2:B:348:PHE:HE1	1.49	0.78
2:C:348:PHE:HD1	2:E:7:ARG:HA	1.45	0.78
1:b:102:THR:CG2	2:B:42:ILE:HG21	2.06	0.78
1:a:108:ARG:HG3	1:a:114:TRP:CZ2	2.19	0.78
1:a:34:LEU:HD12	1:a:79:VAL:CG2	2.02	0.77
1:b:108:ARG:HG3	1:b:114:TRP:CZ2	2.19	0.77
1:c:27:ARG:NH2	2:C:81:ARG:CZ	2.47	0.77
1:c:34:LEU:HD12	1:c:79:VAL:CG2	2.02	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:e:108:ARG:HG3	1:e:114:TRP:CZ2	2.19	0.77
2:D:7:ARG:CG	2:B:348:PHE:CE1	2.67	0.77
1:b:100:ASP:C	2:B:78:LYS:HE3	2.09	0.77
2:D:7:ARG:HB2	2:B:348:PHE:CE1	2.19	0.77
1:a:87:LYS:NZ	1:a:89:GLU:HB2	2.00	0.77
1:c:108:ARG:HG3	1:c:114:TRP:CZ2	2.19	0.77
1:c:67:ARG:NH2	1:c:90:GLU:OE2	2.15	0.77
2:E:218:ILE:HD13	3:R:45:U:H5'	1.65	0.77
1:b:87:LYS:NZ	1:b:89:GLU:HB2	2.00	0.77
1:a:37:PHE:CZ	1:a:111:TYR:CE2	2.67	0.77
1:e:87:LYS:NZ	1:e:89:GLU:HB2	2.00	0.77
1:c:87:LYS:CG	1:c:90:GLU:HG2	2.15	0.77
1:c:87:LYS:NZ	1:c:89:GLU:HB2	2.00	0.77
1:b:87:LYS:CG	1:b:90:GLU:HG2	2.15	0.77
1:e:102:THR:CG2	2:E:42:ILE:HG21	2.02	0.77
2:B:312:ARG:CD	3:R:14:U:C4	2.68	0.77
1:e:32:TYR:HE2	1:e:53:TRP:CH2	1.99	0.77
1:a:87:LYS:CG	1:a:90:GLU:HG2	2.15	0.76
1:e:60:TYR:HB2	1:e:65:LYS:NZ	2.00	0.76
1:e:87:LYS:CG	1:e:90:GLU:HG2	2.15	0.76
1:b:33:ARG:CD	1:b:105:PRO:HD3	2.16	0.76
2:E:218:ILE:HD12	3:R:45:U:C3'	2.15	0.76
1:b:34:LEU:HD12	1:b:79:VAL:CG2	2.02	0.76
1:e:34:LEU:HD12	1:e:79:VAL:CG2	2.02	0.76
1:b:100:ASP:OD2	2:B:78:LYS:HE2	1.86	0.76
1:d:108:ARG:HG3	1:d:114:TRP:CZ2	2.19	0.76
1:d:67:ARG:NH2	1:d:90:GLU:OE2	2.15	0.76
1:b:31:ASN:CB	2:B:110:LEU:HG	2.13	0.76
1:d:87:LYS:CG	1:d:90:GLU:HG2	2.15	0.76
1:b:33:ARG:HE	1:b:105:PRO:HD3	1.50	0.76
1:d:60:TYR:HB2	1:d:65:LYS:NZ	2.00	0.76
1:d:102:THR:CB	2:D:44:THR:HG21	2.15	0.76
1:b:107:VAL:HG12	1:b:108:ARG:H	1.49	0.76
1:d:87:LYS:NZ	1:d:89:GLU:HB2	2.00	0.75
1:b:37:PHE:CZ	1:b:111:TYR:CE2	2.67	0.75
1:c:33:ARG:CD	1:c:105:PRO:HD3	2.16	0.75
1:a:102:THR:HG21	2:A:42:ILE:CG2	2.15	0.75
1:e:33:ARG:CD	1:e:105:PRO:HD3	2.16	0.75
1:d:33:ARG:CD	1:d:105:PRO:HD3	2.16	0.75
1:d:33:ARG:HE	1:d:105:PRO:HD3	1.50	0.75
1:d:87:LYS:HZ2	1:d:89:GLU:HB2	1.51	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:d:107:VAL:HG12	1:d:108:ARG:H	1.49	0.75
1:c:60:TYR:HB2	1:c:65:LYS:NZ	2.00	0.75
1:e:107:VAL:HG12	1:e:108:ARG:H	1.49	0.75
2:C:286:LYS:HD3	3:R:21:U:OP2	1.86	0.75
1:b:60:TYR:HB2	1:b:65:LYS:NZ	2.00	0.75
1:a:33:ARG:CD	1:a:105:PRO:HD3	2.16	0.75
1:e:105:PRO:HB2	1:e:110:ASN:CG	2.09	0.75
1:a:105:PRO:CG	1:a:110:ASN:ND2	2.50	0.75
1:d:100:ASP:OD2	2:D:78:LYS:HE2	1.87	0.75
1:b:105:PRO:CG	1:b:110:ASN:ND2	2.50	0.75
2:B:292:VAL:HG21	3:R:12:U:H5'	1.67	0.75
1:c:33:ARG:HE	1:c:105:PRO:HD3	1.50	0.74
1:c:37:PHE:CZ	1:c:111:TYR:CE2	2.67	0.74
1:e:33:ARG:HE	1:e:105:PRO:HD3	1.50	0.74
2:E:202:PHE:HB3	2:E:214:ARG:CD	2.17	0.74
1:d:12:VAL:HG13	1:d:13:GLN:OE1	1.86	0.74
1:a:33:ARG:HE	1:a:105:PRO:HD3	1.50	0.74
1:a:72:ARG:CB	1:a:79:VAL:HG22	2.17	0.74
1:c:72:ARG:CB	1:c:79:VAL:HG22	2.17	0.74
1:a:60:TYR:HB2	1:a:65:LYS:NZ	2.00	0.74
1:a:12:VAL:HG13	1:a:13:GLN:OE1	1.87	0.74
1:c:105:PRO:CG	1:c:110:ASN:ND2	2.50	0.74
1:b:12:VAL:HG13	1:b:13:GLN:OE1	1.87	0.74
2:D:202:PHE:HB3	2:D:214:ARG:CD	2.17	0.74
1:a:33:ARG:HD3	1:a:103:GLY:C	2.10	0.74
1:e:105:PRO:CG	1:e:110:ASN:ND2	2.50	0.74
2:D:7:ARG:CB	2:B:348:PHE:CE1	2.71	0.74
1:a:107:VAL:HG12	1:a:108:ARG:H	1.50	0.74
1:d:105:PRO:CG	1:d:110:ASN:ND2	2.50	0.73
1:b:72:ARG:CB	1:b:79:VAL:HG22	2.17	0.73
1:e:72:ARG:CB	1:e:79:VAL:HG22	2.17	0.73
3:R:3:U:H2'	3:R:4:U:H4'	1.70	0.73
1:d:37:PHE:CZ	1:d:111:TYR:CE2	2.67	0.73
1:c:107:VAL:HG12	1:c:108:ARG:H	1.50	0.73
1:a:52:ASN:HD22	2:A:112:ALA:HB1	1.50	0.73
1:e:33:ARG:HD3	1:e:103:GLY:C	2.10	0.73
1:b:33:ARG:HD2	1:b:103:GLY:C	2.11	0.73
1:e:12:VAL:HG13	1:e:13:GLN:OE1	1.87	0.73
1:e:37:PHE:CZ	1:e:111:TYR:CE2	2.67	0.73
2:A:291:SER:OG	3:R:4:U:C5'	2.37	0.73
1:e:33:ARG:HD2	1:e:103:GLY:C	2.11	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:218:ILE:HD11	3:R:45:U:H2'	1.68	0.73
1:d:33:ARG:HD3	1:d:103:GLY:C	2.10	0.73
1:c:12:VAL:HG13	1:c:13:GLN:OE1	1.87	0.73
1:e:69:THR:C	1:e:81:LEU:HD12	2.14	0.73
1:d:33:ARG:HD2	1:d:103:GLY:C	2.11	0.73
1:d:72:ARG:CB	1:d:79:VAL:HG22	2.17	0.73
1:c:33:ARG:HD2	1:c:103:GLY:C	2.11	0.73
2:C:17:LYS:HE2	2:B:268:ILE:CG1	2.18	0.72
2:C:7:ARG:HB2	2:A:348:PHE:HE1	1.54	0.72
2:C:202:PHE:HB3	2:C:214:ARG:CD	2.17	0.72
1:a:107:VAL:CG1	1:a:108:ARG:H	2.03	0.72
2:B:408:ARG:NH1	3:R:15:U:H5'	2.05	0.72
1:e:100:ASP:CG	2:E:78:LYS:HE2	2.12	0.72
1:c:107:VAL:CG1	1:c:108:ARG:H	2.03	0.72
1:c:102:THR:H	2:C:44:THR:HG21	1.29	0.72
1:a:30:ARG:HH22	1:a:100:ASP:HB2	1.55	0.72
2:A:202:PHE:HB3	2:A:214:ARG:CD	2.18	0.72
3:R:38:U:H3'	3:R:39:U:H5''	1.69	0.72
1:d:107:VAL:CG1	1:d:108:ARG:H	2.03	0.72
1:c:102:THR:CB	2:C:42:ILE:HG23	2.19	0.72
1:a:31:ASN:HD21	2:A:78:LYS:CE	2.01	0.72
1:e:100:ASP:CG	2:E:78:LYS:CE	2.63	0.72
2:D:268:ILE:CD1	2:E:17:LYS:HG3	2.19	0.72
1:b:30:ARG:HH22	1:b:100:ASP:HB2	1.55	0.72
2:E:291:SER:OG	3:R:40:U:C6	2.42	0.72
1:d:102:THR:CB	2:D:44:THR:HG23	2.16	0.72
2:B:143:ARG:NH2	3:R:17:U:H5''	2.05	0.72
2:B:202:PHE:HB3	2:B:214:ARG:CD	2.17	0.72
1:e:101:SER:OG	2:E:44:THR:CG2	2.38	0.72
1:e:107:VAL:CG1	1:e:108:ARG:H	2.03	0.72
1:c:33:ARG:HD3	1:c:103:GLY:C	2.10	0.72
1:e:102:THR:OG1	2:E:42:ILE:HG23	1.88	0.72
2:E:218:ILE:CD1	3:R:45:U:H5'	2.19	0.72
1:d:69:THR:C	1:d:81:LEU:HD12	2.14	0.71
2:A:218:ILE:HD11	3:R:9:U:H6	1.54	0.71
1:d:102:THR:CB	2:D:42:ILE:HG23	2.20	0.71
1:c:30:ARG:HH22	1:c:100:ASP:HB2	1.55	0.71
1:a:69:THR:C	1:a:81:LEU:HD12	2.14	0.71
1:e:30:ARG:HH22	1:e:100:ASP:HB2	1.55	0.71
1:b:107:VAL:CG1	1:b:108:ARG:H	2.02	0.71
1:b:33:ARG:HD3	1:b:103:GLY:C	2.10	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:b:57:ILE:HD11	2:B:114:ASP:CB	2.18	0.71
1:a:87:LYS:HZ2	1:a:89:GLU:HB2	1.53	0.71
1:d:31:ASN:HB3	2:D:110:LEU:CG	2.20	0.71
1:b:69:THR:C	1:b:81:LEU:HD12	2.14	0.71
1:c:69:THR:C	1:c:81:LEU:HD12	2.14	0.71
2:B:143:ARG:HH22	3:R:17:U:H3'	1.55	0.71
1:d:102:THR:CG2	2:D:110:LEU:HD12	2.21	0.70
1:d:107:VAL:CG1	1:d:108:ARG:N	2.54	0.70
1:b:102:THR:HG23	2:B:74:TYR:HE2	0.87	0.70
2:B:214:ARG:NH2	3:R:19:U:H5'	2.06	0.70
1:a:27:ARG:NH2	2:A:81:ARG:CZ	2.52	0.70
2:D:206:LYS:NZ	3:R:38:U:P	2.65	0.70
2:C:3:VAL:HG12	2:B:243:GLU:HG3	1.72	0.70
1:d:30:ARG:HH22	1:d:100:ASP:HB2	1.55	0.70
1:c:107:VAL:CG1	1:c:108:ARG:N	2.54	0.70
1:d:52:ASN:ND2	2:D:112:ALA:CB	2.37	0.70
1:b:87:LYS:HZ2	1:b:89:GLU:HB2	1.53	0.69
2:B:302:GLN:OE1	2:B:312:ARG:NH1	2.25	0.69
1:d:102:THR:C	2:D:44:THR:CG2	2.66	0.69
1:e:107:VAL:CG1	1:e:108:ARG:N	2.54	0.69
2:D:17:LYS:HG3	2:C:268:ILE:HD11	1.75	0.69
1:e:60:TYR:CB	1:e:65:LYS:HD2	2.23	0.69
1:a:60:TYR:CB	1:a:65:LYS:HD2	2.23	0.69
2:A:302:GLN:OE1	2:A:312:ARG:NH1	2.25	0.69
2:D:302:GLN:OE1	2:D:312:ARG:NH1	2.26	0.69
1:c:57:ILE:HD11	2:C:114:ASP:CB	2.21	0.69
1:c:100:ASP:OD2	2:C:78:LYS:NZ	2.26	0.69
1:c:102:THR:CG2	2:C:42:ILE:CG2	2.71	0.69
2:C:302:GLN:OE1	2:C:312:ARG:NH1	2.25	0.69
1:b:60:TYR:CB	1:b:65:LYS:HD2	2.23	0.69
2:E:292:VAL:HG21	3:R:39:U:H5'	1.74	0.69
2:E:302:GLN:OE1	2:E:312:ARG:NH1	2.25	0.69
2:D:218:ILE:CD1	3:R:36:U:H6	2.06	0.68
2:C:152:TYR:HE1	3:R:26:U:OP1	1.75	0.68
1:d:60:TYR:CB	1:d:65:LYS:HD2	2.23	0.68
2:D:143:ARG:HH22	3:R:35:U:H5''	1.58	0.68
1:a:60:TYR:HB2	1:a:65:LYS:HD2	1.74	0.68
2:D:206:LYS:HE3	3:R:38:U:OP1	1.86	0.68
1:b:33:ARG:O	1:b:98:ALA:HA	1.93	0.68
1:e:33:ARG:HD2	1:e:104:SER:CA	2.24	0.68
1:d:100:ASP:O	2:D:78:LYS:CE	2.38	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:c:52:ASN:HD22	2:C:112:ALA:HB2	1.49	0.68
1:a:33:ARG:HD2	1:a:103:GLY:C	2.11	0.68
1:c:33:ARG:O	1:c:98:ALA:HA	1.93	0.68
1:d:33:ARG:O	1:d:98:ALA:HA	1.93	0.68
2:C:7:ARG:HA	2:A:348:PHE:CD1	2.29	0.68
1:c:60:TYR:HB2	1:c:65:LYS:HD2	1.74	0.68
1:e:31:ASN:CB	2:E:110:LEU:CG	2.54	0.68
1:a:33:ARG:O	1:a:98:ALA:HA	1.93	0.68
1:c:60:TYR:CB	1:c:65:LYS:HD2	2.23	0.68
1:e:33:ARG:O	1:e:98:ALA:HA	1.93	0.68
1:e:101:SER:OG	2:E:44:THR:HB	1.93	0.68
1:b:100:ASP:OD2	2:B:78:LYS:NZ	2.27	0.67
2:C:17:LYS:O	2:B:262:MET:HE1	1.95	0.67
2:A:230:THR:HG22	2:A:312:ARG:HH12	1.59	0.67
1:b:100:ASP:OD2	2:B:78:LYS:CE	2.41	0.67
1:a:33:ARG:HD2	1:a:104:SER:CA	2.24	0.67
2:A:208:HIS:CD2	2:A:210:CYS:H	2.13	0.67
2:B:208:HIS:CD2	2:B:210:CYS:H	2.13	0.67
1:d:33:ARG:HD2	1:d:104:SER:CA	2.24	0.67
2:C:208:HIS:CD2	2:C:210:CYS:H	2.13	0.67
1:e:69:THR:O	1:e:81:LEU:HA	1.95	0.67
2:E:230:THR:HG22	2:E:312:ARG:HH12	1.59	0.67
3:R:44:U:C2'	3:R:45:U:H5''	2.25	0.67
1:c:69:THR:O	1:c:81:LEU:HA	1.95	0.67
1:b:33:ARG:HD2	1:b:104:SER:CA	2.24	0.67
1:a:60:TYR:CB	1:a:65:LYS:CD	2.73	0.67
1:a:69:THR:O	1:a:81:LEU:HA	1.95	0.67
1:d:60:TYR:HB2	1:d:65:LYS:HD2	1.74	0.67
1:d:69:THR:O	1:d:81:LEU:HA	1.95	0.67
2:B:230:THR:HG22	2:B:312:ARG:HH12	1.59	0.67
2:C:143:ARG:NH2	3:R:26:U:H5''	2.11	0.66
1:b:31:ASN:HB3	2:B:110:LEU:CD2	2.25	0.66
1:b:59:ASN:OD1	1:b:60:TYR:N	2.29	0.66
1:a:59:ASN:OD1	1:a:60:TYR:N	2.29	0.66
1:e:73:ASP:HB3	1:e:76:LYS:HG2	1.77	0.66
1:c:27:ARG:NH1	1:c:30:ARG:NE	2.43	0.66
1:c:59:ASN:OD1	1:c:60:TYR:N	2.29	0.66
1:c:105:PRO:HB2	1:c:110:ASN:CG	2.09	0.66
1:b:105:PRO:HG2	1:b:110:ASN:ND2	2.11	0.66
1:a:5:VAL:HB	1:a:23:VAL:HG12	1.77	0.66
1:e:30:ARG:O	1:e:32:TYR:CD2	2.49	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:e:32:TYR:HA	1:e:100:ASP:HA	1.77	0.66
1:e:60:TYR:HB2	1:e:65:LYS:HD2	1.74	0.66
1:d:27:ARG:NH1	1:d:30:ARG:NE	2.43	0.66
2:C:230:THR:HG22	2:C:312:ARG:HH12	1.59	0.66
1:d:59:ASN:OD1	1:d:60:TYR:N	2.29	0.66
1:c:5:VAL:HB	1:c:23:VAL:HG12	1.77	0.66
2:C:348:PHE:CD1	2:E:7:ARG:CB	2.79	0.66
1:e:102:THR:HG21	2:E:42:ILE:HG22	1.65	0.66
2:E:208:HIS:CD2	2:E:210:CYS:H	2.13	0.66
2:D:208:HIS:CD2	2:D:210:CYS:H	2.13	0.66
2:D:214:ARG:CZ	3:R:37:U:C5'	2.71	0.66
1:b:69:THR:O	1:b:81:LEU:HA	1.95	0.66
1:e:27:ARG:NH1	1:e:30:ARG:NE	2.43	0.66
2:D:230:THR:HG22	2:D:312:ARG:HH12	1.59	0.66
1:b:5:VAL:HB	1:b:23:VAL:HG12	1.77	0.66
1:b:107:VAL:CG1	1:b:108:ARG:N	2.54	0.66
1:a:27:ARG:NH1	1:a:30:ARG:NE	2.43	0.66
1:d:5:VAL:HB	1:d:23:VAL:CG1	2.26	0.66
1:d:32:TYR:HA	1:d:100:ASP:HA	1.77	0.66
1:c:33:ARG:HD2	1:c:104:SER:CA	2.24	0.66
2:C:292:VAL:HG21	3:R:21:U:H5'	1.77	0.66
2:C:348:PHE:HD1	2:E:7:ARG:CA	2.01	0.66
1:a:30:ARG:O	1:a:32:TYR:CD2	2.49	0.66
1:e:5:VAL:HB	1:e:23:VAL:CG1	2.26	0.66
1:e:59:ASN:OD1	1:e:60:TYR:N	2.29	0.66
1:d:60:TYR:CB	1:d:65:LYS:CD	2.73	0.66
1:d:73:ASP:HB3	1:d:76:LYS:HG2	1.77	0.66
1:c:105:PRO:HG2	1:c:110:ASN:ND2	2.11	0.66
1:b:27:ARG:NH1	1:b:30:ARG:NE	2.43	0.66
1:d:5:VAL:HB	1:d:23:VAL:HG12	1.77	0.66
1:e:102:THR:H	2:E:44:THR:HG21	0.83	0.65
1:c:5:VAL:HB	1:c:23:VAL:CG1	2.26	0.65
2:B:286:LYS:HD3	3:R:12:U:OP2	1.96	0.65
1:b:30:ARG:O	1:b:32:TYR:CD2	2.49	0.65
1:e:107:VAL:O	1:e:110:ASN:ND2	2.30	0.65
1:b:52:ASN:HB2	2:B:112:ALA:HB2	1.79	0.65
2:B:17:LYS:O	2:A:262:MET:HE1	1.96	0.65
1:a:32:TYR:HA	1:a:100:ASP:HA	1.77	0.65
1:e:5:VAL:HB	1:e:23:VAL:HG12	1.77	0.65
1:e:60:TYR:CB	1:e:65:LYS:CD	2.73	0.65
1:e:108:ARG:HG3	1:e:114:TRP:HH2	1.60	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:7:ARG:HA	2:B:348:PHE:HD1	1.62	0.65
2:D:313:ALA:HB1	2:D:412:ILE:HD11	1.78	0.65
1:a:5:VAL:HB	1:a:23:VAL:CG1	2.26	0.65
2:E:291:SER:OG	3:R:40:U:C5	2.49	0.65
1:d:60:TYR:HB2	1:d:65:LYS:HD3	1.79	0.65
1:c:73:ASP:HB3	1:c:76:LYS:HG2	1.77	0.65
2:A:313:ALA:HB1	2:A:412:ILE:HD11	1.78	0.65
1:d:105:PRO:HG2	1:d:110:ASN:ND2	2.11	0.65
1:c:30:ARG:O	1:c:32:TYR:CD2	2.49	0.65
1:c:32:TYR:HA	1:c:100:ASP:HA	1.77	0.65
1:c:107:VAL:O	1:c:110:ASN:ND2	2.30	0.65
2:C:313:ALA:HB1	2:C:412:ILE:HD11	1.78	0.65
1:b:73:ASP:HB3	1:b:76:LYS:HG2	1.78	0.65
1:b:107:VAL:O	1:b:110:ASN:ND2	2.30	0.65
1:b:60:TYR:HB2	1:b:65:LYS:HD2	1.74	0.65
1:b:60:TYR:HB2	1:b:65:LYS:HD3	1.79	0.65
1:a:73:ASP:HB3	1:a:76:LYS:HG2	1.78	0.65
1:e:30:ARG:HH22	1:e:100:ASP:CB	2.10	0.65
1:e:105:PRO:HG2	1:e:110:ASN:ND2	2.11	0.65
2:E:313:ALA:HB1	2:E:412:ILE:HD11	1.78	0.65
3:R:44:U:C3'	3:R:45:U:H5''	2.27	0.65
1:d:107:VAL:O	1:d:110:ASN:ND2	2.30	0.65
2:E:218:ILE:CD1	3:R:45:U:H2'	2.26	0.65
2:C:137:TYR:O	2:C:141:LEU:HD22	1.97	0.64
2:C:178:GLY:HA2	2:C:181:ILE:HG12	1.79	0.64
1:b:30:ARG:HH22	1:b:100:ASP:CB	2.10	0.64
1:b:32:TYR:HA	1:b:100:ASP:HA	1.77	0.64
2:B:214:ARG:CZ	3:R:19:U:H5'	2.28	0.64
1:d:30:ARG:HH22	1:d:100:ASP:CB	2.10	0.64
2:D:137:TYR:O	2:D:141:LEU:HD22	1.97	0.64
1:b:5:VAL:HB	1:b:23:VAL:CG1	2.26	0.64
1:a:107:VAL:O	1:a:110:ASN:ND2	2.30	0.64
2:C:17:LYS:CE	2:B:268:ILE:HG12	2.27	0.64
2:B:313:ALA:HB1	2:B:412:ILE:HD11	1.78	0.64
1:a:60:TYR:HB2	1:a:65:LYS:HD3	1.79	0.64
2:A:42:ILE:CD1	2:A:74:TYR:HB2	2.27	0.64
1:c:33:ARG:NH1	1:c:101:SER:HB3	2.13	0.64
2:B:42:ILE:CD1	2:B:74:TYR:HB2	2.27	0.64
2:A:137:TYR:O	2:A:141:LEU:HD22	1.97	0.64
1:d:33:ARG:NH1	1:d:101:SER:HB3	2.13	0.64
1:b:54:GLY:CA	2:B:111:LYS:HG3	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:137:TYR:O	2:E:141:LEU:HD22	1.97	0.64
2:D:178:GLY:HA2	2:D:181:ILE:HG12	1.79	0.64
2:C:104:ILE:HD11	2:C:198:VAL:HG22	1.79	0.64
2:B:137:TYR:O	2:B:141:LEU:HD22	1.97	0.64
1:a:30:ARG:HH22	1:a:100:ASP:CB	2.10	0.64
1:a:100:ASP:O	2:A:78:LYS:HE3	1.98	0.64
2:D:104:ILE:HD11	2:D:198:VAL:HG22	1.79	0.64
1:b:45:ARG:HD2	1:b:108:ARG:HD2	1.79	0.64
2:E:42:ILE:CD1	2:E:74:TYR:HB2	2.28	0.64
1:d:33:ARG:HE	1:d:105:PRO:CD	2.11	0.64
1:c:37:PHE:CE1	1:c:111:TYR:CD2	2.85	0.64
2:C:42:ILE:CD1	2:C:74:TYR:HB2	2.27	0.64
2:C:347:GLN:O	2:E:8:ILE:HG12	1.98	0.64
2:B:104:ILE:HD11	2:B:198:VAL:HG22	1.79	0.64
1:e:33:ARG:HE	1:e:105:PRO:CD	2.11	0.64
1:d:57:ILE:HD11	2:D:114:ASP:CB	2.17	0.64
2:D:42:ILE:CD1	2:D:74:TYR:HB2	2.28	0.64
1:b:33:ARG:NH1	1:b:101:SER:HB3	2.13	0.64
1:e:28:PRO:HB2	1:e:77:ASN:CG	2.23	0.64
3:R:6:U:H5"	3:R:6:U:C6	2.32	0.64
1:d:45:ARG:HD2	1:d:108:ARG:HD2	1.79	0.63
2:D:312:ARG:HD2	3:R:32:U:C5	2.33	0.63
1:b:28:PRO:HB2	1:b:77:ASN:CG	2.23	0.63
1:d:30:ARG:O	1:d:32:TYR:CD2	2.49	0.63
1:c:60:TYR:HB2	1:c:65:LYS:HD3	1.79	0.63
2:B:178:GLY:HA2	2:B:181:ILE:HG12	1.79	0.63
1:e:33:ARG:NH1	1:e:101:SER:HB3	2.13	0.63
2:E:104:ILE:HD11	2:E:198:VAL:HG22	1.79	0.63
1:c:45:ARG:HD2	1:c:108:ARG:HD2	1.79	0.63
1:c:60:TYR:CB	1:c:65:LYS:CD	2.73	0.63
2:C:348:PHE:HA	2:E:8:ILE:HG23	1.81	0.63
1:b:60:TYR:CB	1:b:65:LYS:CD	2.73	0.63
2:A:104:ILE:HD11	2:A:198:VAL:HG22	1.79	0.63
1:e:102:THR:HG23	2:E:74:TYR:CE2	2.33	0.63
1:d:31:ASN:HB3	2:D:110:LEU:HG	1.80	0.63
1:d:33:ARG:HH11	1:d:101:SER:HB3	1.63	0.63
1:d:39:GLN:HG3	1:d:43:LYS:O	1.98	0.63
1:c:30:ARG:HH22	1:c:100:ASP:CB	2.10	0.63
1:a:33:ARG:NH1	1:a:101:SER:HB3	2.12	0.63
1:a:45:ARG:HD2	1:a:108:ARG:HD2	1.79	0.63
1:a:28:PRO:HB2	1:a:77:ASN:CG	2.23	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:d:28:PRO:HB2	1:d:77:ASN:CG	2.23	0.63
1:c:33:ARG:HE	1:c:105:PRO:CD	2.11	0.63
1:c:33:ARG:HH11	1:c:101:SER:HB3	1.63	0.63
1:e:45:ARG:HD2	1:e:108:ARG:HD2	1.79	0.63
2:E:178:GLY:HA2	2:E:181:ILE:HG12	1.79	0.63
1:a:33:ARG:HE	1:a:105:PRO:CD	2.11	0.63
1:d:35:GLY:HA3	1:d:111:TYR:HH	1.64	0.63
1:b:39:GLN:HG3	1:b:43:LYS:O	1.98	0.63
2:A:178:GLY:HA2	2:A:181:ILE:HG12	1.79	0.63
3:R:2:U:H3'	3:R:3:U:H5''	1.79	0.63
1:c:28:PRO:HB2	1:c:77:ASN:CG	2.23	0.62
1:c:39:GLN:HG3	1:c:43:LYS:O	1.98	0.62
2:C:8:ILE:HD11	2:A:346:GLN:O	1.99	0.62
1:a:105:PRO:HG2	1:a:110:ASN:ND2	2.11	0.62
2:D:268:ILE:HD11	2:E:17:LYS:CG	2.26	0.62
1:c:31:ASN:HB3	2:C:110:LEU:CG	2.27	0.62
1:a:33:ARG:HH11	1:a:101:SER:HB3	1.63	0.62
1:a:39:GLN:HG3	1:a:43:LYS:O	1.98	0.62
1:e:105:PRO:HG3	1:e:110:ASN:CB	2.30	0.62
1:d:105:PRO:HG3	1:d:110:ASN:CB	2.30	0.62
1:b:37:PHE:CE1	1:b:111:TYR:CD2	2.85	0.62
1:e:39:GLN:HG3	1:e:43:LYS:O	1.98	0.62
1:b:67:ARG:HH12	1:b:87:LYS:HG2	1.65	0.62
1:e:57:ILE:HD11	2:E:114:ASP:HB3	1.80	0.62
2:C:17:LYS:HE2	2:B:268:ILE:CD1	2.29	0.62
1:d:67:ARG:HH12	1:d:87:LYS:HG2	1.65	0.62
1:c:27:ARG:NH2	2:C:81:ARG:NH2	2.47	0.62
1:b:33:ARG:HH11	1:b:101:SER:HB3	1.63	0.62
2:B:208:HIS:CD2	2:B:210:CYS:HB2	2.35	0.62
1:e:37:PHE:CE1	1:e:111:TYR:CD2	2.85	0.62
1:b:33:ARG:HE	1:b:105:PRO:CD	2.11	0.62
2:C:347:GLN:O	2:E:8:ILE:HG23	2.00	0.62
2:A:291:SER:HG	3:R:4:U:C5'	2.12	0.62
1:e:33:ARG:HH11	1:e:101:SER:HB3	1.63	0.62
1:c:105:PRO:HG3	1:c:110:ASN:CB	2.30	0.62
1:a:108:ARG:HG3	1:a:114:TRP:HH2	1.61	0.62
1:e:67:ARG:HH12	1:e:87:LYS:HG2	1.65	0.62
1:a:67:ARG:HH12	1:a:87:LYS:HG2	1.65	0.61
1:d:102:THR:C	2:D:44:THR:HG21	2.24	0.61
2:C:7:ARG:CB	2:A:348:PHE:CE1	2.83	0.61
2:C:208:HIS:CD2	2:C:210:CYS:HB2	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:100:ASP:OD2	2:A:78:LYS:NZ	2.31	0.61
2:A:208:HIS:CD2	2:A:210:CYS:HB2	2.35	0.61
1:d:31:ASN:HD21	2:D:78:LYS:HD2	1.66	0.61
1:a:105:PRO:HB2	1:a:110:ASN:CG	2.09	0.61
1:e:60:TYR:HB2	1:e:65:LYS:HD3	1.79	0.61
3:R:44:U:H2'	3:R:45:U:H5''	1.82	0.61
2:E:208:HIS:CD2	2:E:210:CYS:HB2	2.35	0.61
1:d:37:PHE:CE1	1:d:111:TYR:CD2	2.85	0.61
2:D:138:LEU:O	2:D:191:TYR:OH	2.19	0.61
1:a:105:PRO:HG3	1:a:110:ASN:CB	2.30	0.61
1:c:67:ARG:HH12	1:c:87:LYS:HG2	1.65	0.61
2:C:138:LEU:O	2:C:191:TYR:OH	2.19	0.61
2:C:202:PHE:CB	2:C:214:ARG:HD3	2.28	0.61
2:A:51:LEU:HB3	2:A:72:TYR:HB2	1.82	0.61
2:D:208:HIS:CD2	2:D:210:CYS:HB2	2.35	0.61
1:b:105:PRO:HG3	1:b:110:ASN:CB	2.30	0.61
1:c:102:THR:H	2:C:44:THR:HB	1.66	0.61
2:E:138:LEU:O	2:E:191:TYR:OH	2.19	0.61
2:B:138:LEU:O	2:B:191:TYR:OH	2.19	0.61
1:c:34:LEU:CD1	1:c:79:VAL:HG23	2.28	0.60
1:b:54:GLY:HA2	2:B:111:LYS:HG3	1.81	0.60
1:e:28:PRO:HB2	1:e:77:ASN:OD1	2.01	0.60
1:d:102:THR:CB	2:D:42:ILE:CG2	2.80	0.60
2:D:51:LEU:HB3	2:D:72:TYR:HB2	1.82	0.60
2:E:51:LEU:HB3	2:E:72:TYR:HB2	1.82	0.60
2:B:51:LEU:HB3	2:B:72:TYR:HB2	1.82	0.60
2:A:138:LEU:O	2:A:191:TYR:OH	2.19	0.60
2:E:291:SER:HG	3:R:40:U:H5	1.41	0.60
1:d:27:ARG:NH1	1:d:30:ARG:HE	1.99	0.60
2:D:7:ARG:CA	2:B:348:PHE:CD1	2.83	0.60
1:c:100:ASP:OD2	2:C:78:LYS:CE	2.49	0.60
1:c:102:THR:HB	2:C:42:ILE:HG23	1.82	0.60
1:a:37:PHE:CE1	1:a:111:TYR:CD2	2.85	0.60
1:a:28:PRO:HB2	1:a:77:ASN:OD1	2.01	0.60
1:a:107:VAL:CG1	1:a:108:ARG:N	2.54	0.60
1:c:28:PRO:HB2	1:c:77:ASN:OD1	2.01	0.60
1:b:28:PRO:HB2	1:b:77:ASN:OD1	2.01	0.60
2:C:40:LEU:HD12	2:C:108:VAL:HG21	1.84	0.60
1:d:30:ARG:NH2	1:d:100:ASP:HB2	2.17	0.60
1:b:27:ARG:NH1	1:b:30:ARG:HE	1.99	0.60
2:B:40:LEU:HD12	2:B:108:VAL:HG21	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:30:ARG:NH2	1:a:100:ASP:HB2	2.17	0.60
2:C:376:VAL:HG21	2:B:353:ASN:ND2	2.17	0.60
1:c:33:ARG:HD2	1:c:105:PRO:HD3	1.84	0.59
1:d:33:ARG:HD2	1:d:105:PRO:HD3	1.84	0.59
1:c:30:ARG:NH2	1:c:100:ASP:HB2	2.17	0.59
1:e:27:ARG:NH1	1:e:30:ARG:HE	1.99	0.59
1:d:28:PRO:HB2	1:d:77:ASN:OD1	2.01	0.59
2:C:51:LEU:HB3	2:C:72:TYR:HB2	1.82	0.59
1:b:108:ARG:HG3	1:b:114:TRP:HH2	1.61	0.59
2:A:40:LEU:HD12	2:A:108:VAL:HG21	1.84	0.59
1:e:30:ARG:NH2	1:e:100:ASP:HB2	2.17	0.59
1:e:102:THR:C	2:E:44:THR:CG2	2.75	0.59
1:a:34:LEU:CD1	1:a:79:VAL:HG23	2.28	0.59
2:D:40:LEU:HD12	2:D:108:VAL:HG21	1.84	0.59
1:c:27:ARG:NH1	1:c:30:ARG:HE	1.99	0.59
1:d:27:ARG:HH11	1:d:30:ARG:HE	1.51	0.59
1:e:27:ARG:HH11	1:e:30:ARG:HE	1.51	0.59
1:e:101:SER:OG	2:E:44:THR:HG22	2.02	0.59
1:c:52:ASN:ND2	2:C:112:ALA:HB2	2.10	0.59
2:C:42:ILE:HD11	2:C:74:TYR:HB2	1.85	0.59
1:b:27:ARG:HH11	1:b:30:ARG:HE	1.51	0.59
1:b:102:THR:CG2	2:B:74:TYR:CD2	2.81	0.59
1:a:33:ARG:HD2	1:a:105:PRO:HD3	1.84	0.59
1:e:101:SER:OG	2:E:44:THR:CB	2.51	0.59
2:D:42:ILE:HD11	2:D:74:TYR:HB2	1.85	0.59
1:c:27:ARG:HH11	1:c:30:ARG:HE	1.51	0.59
1:b:27:ARG:CD	1:b:30:ARG:HE	2.16	0.59
1:d:108:ARG:HG3	1:d:114:TRP:HH2	1.60	0.59
1:c:100:ASP:OD2	2:C:78:LYS:HE2	2.02	0.58
1:b:30:ARG:NH2	1:b:100:ASP:HB2	2.17	0.58
1:b:33:ARG:HD2	1:b:105:PRO:HD3	1.83	0.58
1:a:27:ARG:CD	1:a:30:ARG:HE	2.16	0.58
2:A:312:ARG:HD2	3:R:5:U:N3	2.18	0.58
2:E:42:ILE:HD11	2:E:74:TYR:HB2	1.85	0.58
1:c:27:ARG:CD	1:c:30:ARG:HE	2.16	0.58
1:c:108:ARG:HG3	1:c:114:TRP:HH2	1.61	0.58
2:B:408:ARG:CZ	3:R:15:U:H3'	2.33	0.58
1:a:27:ARG:HH11	1:a:30:ARG:HE	1.51	0.58
1:b:105:PRO:HB2	1:b:110:ASN:HD22	1.66	0.58
1:e:33:ARG:HD2	1:e:105:PRO:HD3	1.84	0.58
2:C:18:LEU:CD1	2:B:232:GLY:HA2	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:286:LYS:CD	3:R:21:U:OP2	2.51	0.58
1:b:105:PRO:HB2	1:b:110:ASN:CG	2.09	0.58
2:A:153:ARG:NH2	2:A:179:ARG:O	2.36	0.58
2:D:153:ARG:NH2	2:D:179:ARG:O	2.36	0.58
2:C:153:ARG:NH2	2:C:179:ARG:O	2.36	0.58
2:C:348:PHE:CA	2:E:8:ILE:HG23	2.33	0.58
1:e:27:ARG:CD	1:e:30:ARG:HE	2.16	0.58
3:R:17:U:H2'	3:R:18:U:H5''	1.85	0.58
1:d:27:ARG:CD	1:d:30:ARG:HE	2.16	0.58
1:a:27:ARG:NH1	1:a:30:ARG:HE	1.99	0.58
2:E:153:ARG:NH2	2:E:179:ARG:O	2.36	0.58
2:B:202:PHE:CB	2:B:214:ARG:HD3	2.28	0.58
2:E:40:LEU:HD12	2:E:108:VAL:HG21	1.84	0.58
1:d:102:THR:CG2	2:D:42:ILE:CG2	2.79	0.58
2:B:42:ILE:HD11	2:B:74:TYR:HB2	1.85	0.58
1:e:100:ASP:OD2	2:E:78:LYS:NZ	2.36	0.58
2:E:291:SER:O	3:R:40:U:C5	2.57	0.58
1:d:54:GLY:HA2	2:D:111:LYS:HE3	1.86	0.57
2:C:8:ILE:HG23	2:A:347:GLN:O	2.04	0.57
1:e:31:ASN:CB	2:E:110:LEU:CB	2.80	0.57
2:C:346:GLN:O	2:E:8:ILE:CD1	2.49	0.57
2:C:347:GLN:O	2:E:8:ILE:N	2.32	0.57
1:a:27:ARG:NH2	2:A:81:ARG:NH2	2.51	0.57
2:B:153:ARG:NH2	2:B:179:ARG:O	2.36	0.57
1:a:105:PRO:HB2	1:a:110:ASN:HD22	1.66	0.57
2:D:324:TYR:O	2:D:328:THR:OG1	2.19	0.57
1:a:45:ARG:HD2	1:a:108:ARG:CD	2.35	0.57
2:A:42:ILE:HD11	2:A:74:TYR:HB2	1.85	0.57
2:A:143:ARG:NH2	3:R:9:U:OP2	2.38	0.57
2:B:324:TYR:O	2:B:328:THR:OG1	2.19	0.57
1:d:67:ARG:HH22	1:d:87:LYS:HE3	1.70	0.57
2:D:152:TYR:CG	3:R:33:U:H4'	2.39	0.57
2:B:143:ARG:HH21	3:R:17:U:H5''	1.69	0.57
2:A:139:LEU:HD22	2:A:195:VAL:HG12	1.87	0.57
1:e:31:ASN:HB3	2:E:110:LEU:HD23	1.85	0.57
2:B:139:LEU:HD22	2:B:195:VAL:HG12	1.87	0.57
2:C:139:LEU:HD22	2:C:195:VAL:HG12	1.87	0.56
2:E:139:LEU:HD22	2:E:195:VAL:HG12	1.87	0.56
2:D:88:TRP:CG	2:D:95:ILE:HD11	2.40	0.56
2:D:202:PHE:CB	2:D:214:ARG:HD3	2.28	0.56
1:c:67:ARG:HH22	1:c:90:GLU:CD	2.13	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:b:45:ARG:HD2	1:b:108:ARG:CD	2.35	0.56
2:D:139:LEU:HD22	2:D:195:VAL:HG12	1.87	0.56
2:B:408:ARG:HH22	3:R:15:U:H3'	1.65	0.56
1:d:60:TYR:HB2	1:d:65:LYS:HZ2	1.69	0.56
2:B:88:TRP:CG	2:B:95:ILE:HD11	2.40	0.56
1:a:67:ARG:HH22	1:a:87:LYS:HE3	1.70	0.56
2:D:224:ASP:OD2	3:R:30:U:O5'	2.24	0.56
1:e:67:ARG:HH22	1:e:87:LYS:HE3	1.70	0.56
1:c:43:LYS:HE2	1:c:46:GLU:OE2	2.06	0.56
2:C:88:TRP:CG	2:C:95:ILE:HD11	2.40	0.56
2:C:348:PHE:CZ	2:E:7:ARG:HG3	2.41	0.56
1:a:67:ARG:HH22	1:a:90:GLU:CD	2.13	0.56
3:R:24:U:H6	3:R:24:U:H5'	1.70	0.56
1:d:43:LYS:HE2	1:d:46:GLU:OE2	2.06	0.56
1:d:105:PRO:HB2	1:d:110:ASN:CG	2.09	0.56
1:c:67:ARG:HH22	1:c:87:LYS:HE3	1.70	0.56
1:b:43:LYS:HE2	1:b:46:GLU:OE2	2.06	0.56
1:a:43:LYS:HE2	1:a:46:GLU:OE2	2.06	0.56
1:d:34:LEU:CD1	1:d:79:VAL:HG23	2.28	0.56
1:c:45:ARG:HD2	1:c:108:ARG:CD	2.35	0.56
2:B:7:ARG:HG2	2:B:9:ILE:HG22	1.88	0.56
2:D:181:ILE:HD11	2:C:168:ASN:ND2	2.20	0.56
2:C:7:ARG:HG2	2:C:9:ILE:HG22	1.88	0.56
1:e:45:ARG:HD2	1:e:108:ARG:CD	2.35	0.56
1:d:45:ARG:HD2	1:d:108:ARG:CD	2.35	0.55
1:d:67:ARG:HH22	1:d:90:GLU:CD	2.13	0.55
1:e:19:THR:HG23	1:e:19:THR:O	2.06	0.55
2:C:324:TYR:HB2	2:B:309:ARG:HB2	1.88	0.55
1:b:67:ARG:HH22	1:b:87:LYS:HE3	1.70	0.55
2:E:202:PHE:CB	2:E:214:ARG:HD3	2.28	0.55
2:D:243:GLU:HG3	2:E:3:VAL:HG12	1.88	0.55
2:C:89:SER:O	2:C:270:LYS:NZ	2.40	0.55
2:B:89:SER:O	2:B:270:LYS:NZ	2.39	0.55
2:E:88:TRP:CG	2:E:95:ILE:HD11	2.40	0.55
2:E:89:SER:O	2:E:270:LYS:NZ	2.39	0.55
2:E:291:SER:OG	3:R:40:U:H6	1.88	0.55
2:A:88:TRP:CG	2:A:95:ILE:HD11	2.40	0.55
2:E:7:ARG:HG2	2:E:9:ILE:HG22	1.88	0.55
2:E:324:TYR:O	2:E:328:THR:OG1	2.19	0.55
1:b:53:TRP:CD1	2:B:110:LEU:CB	2.90	0.55
1:e:31:ASN:H	2:E:110:LEU:HD23	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:e:43:LYS:HE2	1:e:46:GLU:OE2	2.06	0.55
1:c:31:ASN:ND2	1:c:101:SER:HA	2.22	0.55
2:A:7:ARG:HG2	2:A:9:ILE:HG22	1.88	0.55
2:B:218:ILE:HD12	3:R:18:U:H3'	1.89	0.55
2:A:174:LEU:HG	2:A:178:GLY:HA3	1.89	0.55
2:D:89:SER:O	2:D:270:LYS:NZ	2.39	0.55
1:c:31:ASN:CB	2:C:110:LEU:HG	2.35	0.55
1:b:31:ASN:ND2	1:b:101:SER:HA	2.22	0.55
1:a:33:ARG:NH1	1:a:101:SER:CB	2.70	0.55
2:A:89:SER:O	2:A:270:LYS:NZ	2.40	0.55
1:d:102:THR:HG22	2:D:110:LEU:CB	2.33	0.55
2:D:7:ARG:HG2	2:D:9:ILE:HG22	1.88	0.55
1:c:19:THR:HG23	1:c:19:THR:O	2.06	0.55
2:C:143:ARG:HH22	3:R:26:U:H3'	1.72	0.55
1:e:31:ASN:ND2	1:e:101:SER:HA	2.22	0.55
1:b:33:ARG:NH1	1:b:101:SER:CB	2.71	0.54
1:b:67:ARG:HH22	1:b:90:GLU:CD	2.13	0.54
2:B:174:LEU:HG	2:B:178:GLY:HA3	1.89	0.54
2:E:174:LEU:HG	2:E:178:GLY:HA3	1.89	0.54
1:a:19:THR:HG23	1:a:19:THR:O	2.06	0.54
1:a:102:THR:CG2	2:A:74:TYR:CD2	2.89	0.54
1:d:102:THR:OG1	2:D:44:THR:HG22	1.91	0.54
1:a:31:ASN:ND2	1:a:101:SER:HA	2.22	0.54
1:b:57:ILE:CD1	2:B:114:ASP:HB3	2.30	0.54
1:e:99:PHE:HB2	1:e:111:TYR:CA	2.11	0.54
1:d:19:THR:HG23	1:d:19:THR:O	2.06	0.54
2:D:174:LEU:HG	2:D:178:GLY:HA3	1.89	0.54
1:c:33:ARG:NH1	1:c:101:SER:CB	2.71	0.54
1:a:99:PHE:HB2	1:a:111:TYR:CA	2.11	0.54
1:a:102:THR:HG23	2:A:74:TYR:CD2	2.35	0.54
1:b:60:TYR:HB2	1:b:65:LYS:HZ3	1.72	0.54
2:B:285:SER:HB2	2:A:207:LYS:HD3	1.88	0.54
1:e:52:ASN:HB2	2:E:112:ALA:HB2	1.89	0.54
1:e:33:ARG:NH1	1:e:101:SER:CB	2.70	0.54
3:R:18:U:H4'	3:R:18:U:OP1	2.08	0.54
1:d:31:ASN:ND2	1:d:101:SER:HA	2.22	0.54
1:d:33:ARG:NH1	1:d:101:SER:CB	2.71	0.54
2:D:27:TYR:CZ	2:D:263:LEU:HD22	2.43	0.54
2:D:88:TRP:CD1	2:D:95:ILE:HD11	2.43	0.54
2:C:88:TRP:CD1	2:C:95:ILE:HD11	2.43	0.54
1:b:99:PHE:HB2	1:b:111:TYR:CA	2.11	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:88:TRP:CD1	2:E:95:ILE:HD11	2.43	0.54
2:E:143:ARG:HH22	3:R:44:U:H5'	1.69	0.54
2:C:27:TYR:CZ	2:C:263:LEU:HD22	2.43	0.54
2:A:88:TRP:CD1	2:A:95:ILE:HD11	2.43	0.54
2:B:181:ILE:HD11	2:A:168:ASN:ND2	2.23	0.53
1:d:73:ASP:HB3	1:d:76:LYS:CG	2.39	0.53
2:D:55:VAL:O	2:D:59:LEU:HB2	2.08	0.53
1:b:19:THR:O	1:b:19:THR:HG23	2.06	0.53
2:B:27:TYR:CZ	2:B:263:LEU:HD22	2.43	0.53
1:b:73:ASP:HB3	1:b:76:LYS:CG	2.39	0.53
2:B:88:TRP:CD1	2:B:95:ILE:HD11	2.43	0.53
2:D:206:LYS:HZ3	3:R:38:U:P	2.31	0.53
2:A:27:TYR:CZ	2:A:263:LEU:HD22	2.43	0.53
2:E:55:VAL:O	2:E:59:LEU:HB2	2.08	0.53
3:R:6:U:H5''	3:R:6:U:H6	1.72	0.53
1:d:105:PRO:HB2	1:d:110:ASN:HD22	1.66	0.53
2:C:174:LEU:HG	2:C:178:GLY:HA3	1.89	0.53
2:D:8:ILE:HD11	2:B:346:GLN:O	2.09	0.53
2:B:312:ARG:HG3	3:R:14:U:C2	2.43	0.53
2:B:408:ARG:HH12	3:R:15:U:H5'	1.74	0.53
1:e:12:VAL:HG12	1:e:13:GLN:N	2.24	0.53
1:d:11:LEU:HG	1:d:121:THR:HB	1.90	0.53
1:a:67:ARG:NH2	1:a:87:LYS:HE3	2.24	0.53
2:E:27:TYR:CZ	2:E:263:LEU:HD22	2.43	0.53
1:c:11:LEU:HG	1:c:121:THR:HB	1.90	0.53
1:c:12:VAL:HG12	1:c:13:GLN:N	2.24	0.53
3:R:30:U:H2'	3:R:31:U:O4'	2.09	0.53
2:C:55:VAL:O	2:C:59:LEU:HB2	2.09	0.53
1:b:11:LEU:HG	1:b:121:THR:HB	1.90	0.53
2:B:55:VAL:O	2:B:59:LEU:HB2	2.09	0.53
1:e:38:ARG:HH12	1:e:90:GLU:CD	2.13	0.53
1:d:12:VAL:HG12	1:d:13:GLN:N	2.24	0.53
1:c:60:TYR:HB2	1:c:65:LYS:CE	2.39	0.53
1:b:12:VAL:HG12	1:b:13:GLN:N	2.24	0.53
1:a:11:LEU:HG	1:a:121:THR:HB	1.90	0.53
1:a:73:ASP:HB3	1:a:76:LYS:CG	2.39	0.53
2:A:55:VAL:O	2:A:59:LEU:HB2	2.08	0.53
2:E:211:ALA:HB1	2:E:214:ARG:NH2	2.24	0.53
1:d:31:ASN:CB	2:D:110:LEU:HG	2.39	0.52
1:c:73:ASP:HB3	1:c:76:LYS:CG	2.39	0.52
1:b:60:TYR:HB2	1:b:65:LYS:CE	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:e:105:PRO:HB2	1:e:110:ASN:HD22	1.66	0.52
1:d:60:TYR:HB2	1:d:65:LYS:CE	2.39	0.52
1:d:105:PRO:CB	1:d:110:ASN:CB	2.88	0.52
2:D:211:ALA:HB1	2:D:214:ARG:NH2	2.25	0.52
1:c:67:ARG:NH2	1:c:87:LYS:HE3	2.24	0.52
1:c:105:PRO:CB	1:c:110:ASN:CB	2.88	0.52
1:a:31:ASN:HD21	2:A:78:LYS:HE3	1.72	0.52
2:A:51:LEU:HA	2:A:54:TYR:HB2	1.91	0.52
2:E:51:LEU:HA	2:E:54:TYR:HB2	1.91	0.52
2:E:291:SER:O	3:R:40:U:H5	1.93	0.52
1:b:67:ARG:NH2	1:b:87:LYS:HE3	2.24	0.52
2:A:202:PHE:CB	2:A:214:ARG:HD3	2.28	0.52
2:D:51:LEU:HA	2:D:54:TYR:HB2	1.91	0.52
1:c:87:LYS:O	1:c:90:GLU:HB2	2.10	0.52
2:C:3:VAL:CG1	2:B:243:GLU:HG3	2.39	0.52
1:b:71:SER:O	1:b:79:VAL:HG13	2.10	0.52
2:A:211:ALA:HB1	2:A:214:ARG:NH2	2.24	0.52
2:C:18:LEU:HD21	2:B:232:GLY:N	2.24	0.52
1:b:105:PRO:CB	1:b:110:ASN:CB	2.88	0.52
1:a:12:VAL:HG12	1:a:13:GLN:N	2.24	0.52
1:e:73:ASP:HB3	1:e:76:LYS:CG	2.39	0.52
1:d:33:ARG:N	1:d:99:PHE:O	2.27	0.52
1:d:71:SER:O	1:d:79:VAL:HG13	2.10	0.52
2:D:324:TYR:HB2	2:C:309:ARG:HB2	1.92	0.52
2:D:353:ASN:ND2	2:E:376:VAL:HG21	2.24	0.52
2:C:347:GLN:C	2:E:8:ILE:HG23	2.35	0.52
1:b:34:LEU:CD1	1:b:79:VAL:HG23	2.28	0.52
2:A:208:HIS:HD2	2:A:210:CYS:HB2	1.74	0.52
1:e:11:LEU:HG	1:e:121:THR:HB	1.90	0.52
1:d:87:LYS:O	1:d:90:GLU:HB2	2.10	0.52
2:D:152:TYR:CD1	3:R:33:U:H4'	2.45	0.52
1:c:54:GLY:HA3	2:C:111:LYS:HG3	1.91	0.52
2:B:218:ILE:CD1	3:R:18:U:H3'	2.39	0.52
1:a:105:PRO:CB	1:a:110:ASN:CB	2.88	0.52
1:c:38:ARG:HH12	1:c:90:GLU:CD	2.13	0.52
1:e:70:ILE:HB	1:e:81:LEU:HD13	1.91	0.52
1:e:105:PRO:CB	1:e:110:ASN:CB	2.87	0.52
3:R:3:U:C2'	3:R:4:U:H4'	2.36	0.52
1:d:67:ARG:NH2	1:d:87:LYS:HE3	2.24	0.52
1:b:87:LYS:O	1:b:90:GLU:HB2	2.10	0.52
2:B:211:ALA:HB1	2:B:214:ARG:NH2	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:e:67:ARG:HH22	1:e:90:GLU:CD	2.13	0.52
1:e:73:ASP:OD2	1:e:76:LYS:HE3	2.10	0.52
2:D:208:HIS:HD2	2:D:210:CYS:HB2	1.74	0.52
2:C:51:LEU:HA	2:C:54:TYR:HB2	1.91	0.52
2:C:312:ARG:HD2	3:R:23:U:C5	2.45	0.52
1:b:2:VAL:HB	1:b:113:TYR:CD2	2.45	0.52
2:B:51:LEU:HA	2:B:54:TYR:HB2	1.91	0.52
1:e:2:VAL:HB	1:e:113:TYR:CD2	2.45	0.52
1:d:73:ASP:OD2	1:d:76:LYS:HE3	2.10	0.51
2:C:211:ALA:HB1	2:C:214:ARG:NH2	2.24	0.51
1:a:60:TYR:HB2	1:a:65:LYS:CE	2.39	0.51
2:A:214:ARG:HH22	3:R:10:U:H4'	1.76	0.51
1:e:67:ARG:NH2	1:e:87:LYS:HE3	2.24	0.51
1:d:2:VAL:HB	1:d:113:TYR:CD2	2.45	0.51
1:d:70:ILE:HB	1:d:81:LEU:HD13	1.91	0.51
1:c:73:ASP:OD2	1:c:76:LYS:HE3	2.10	0.51
1:b:38:ARG:HH12	1:b:90:GLU:CD	2.13	0.51
2:C:70:ASN:ND2	2:C:188:ASP:OD2	2.41	0.51
1:b:73:ASP:OD2	1:b:76:LYS:HE3	2.10	0.51
1:a:87:LYS:O	1:a:90:GLU:HB2	2.10	0.51
1:e:57:ILE:HD11	2:E:114:ASP:CB	2.40	0.51
1:e:60:TYR:HB2	1:e:65:LYS:CE	2.39	0.51
1:d:38:ARG:HH12	1:d:90:GLU:CD	2.13	0.51
2:C:312:ARG:HD2	3:R:23:U:O4	2.10	0.51
1:d:54:GLY:HA3	2:D:111:LYS:HG3	1.92	0.51
1:c:2:VAL:HB	1:c:113:TYR:CD2	2.45	0.51
1:b:32:TYR:HE2	1:b:53:TRP:HH2	1.55	0.51
1:b:52:ASN:CG	2:B:112:ALA:CB	2.74	0.51
1:c:70:ILE:HB	1:c:81:LEU:HD13	1.91	0.51
2:C:314:ARG:HE	2:C:404:LEU:HD22	1.76	0.51
1:a:36:TRP:CD1	1:a:81:LEU:HD22	2.46	0.51
1:a:73:ASP:OD2	1:a:76:LYS:HE3	2.10	0.51
1:c:36:TRP:CD1	1:c:81:LEU:HD22	2.46	0.51
2:C:208:HIS:HD2	2:C:210:CYS:HB2	1.74	0.51
2:C:348:PHE:HE1	2:E:7:ARG:CB	1.98	0.51
1:b:52:ASN:CB	2:B:112:ALA:HB2	2.39	0.51
2:B:314:ARG:HE	2:B:404:LEU:HD22	1.76	0.51
1:a:52:ASN:ND2	2:A:112:ALA:HB2	2.19	0.51
1:e:87:LYS:O	1:e:90:GLU:HB2	2.10	0.51
1:e:61:ALA:O	1:e:65:LYS:HG2	2.11	0.51
2:E:208:HIS:HD2	2:E:210:CYS:HB2	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:c:71:SER:O	1:c:79:VAL:HG13	2.10	0.51
1:a:38:ARG:HH12	1:a:90:GLU:CD	2.13	0.51
1:a:70:ILE:HB	1:a:81:LEU:HD13	1.91	0.51
1:a:71:SER:O	1:a:79:VAL:HG13	2.10	0.51
2:A:242:THR:O	2:A:246:THR:OG1	2.27	0.51
2:E:314:ARG:HE	2:E:404:LEU:HD22	1.76	0.51
2:D:218:ILE:HD11	3:R:36:U:C5	2.44	0.50
2:D:312:ARG:HG3	3:R:32:U:C2	2.46	0.50
2:D:314:ARG:HE	2:D:404:LEU:HD22	1.76	0.50
1:c:32:TYR:HE2	1:c:53:TRP:HH2	1.55	0.50
1:a:2:VAL:HB	1:a:113:TYR:CD2	2.45	0.50
1:d:61:ALA:O	1:d:65:LYS:HG2	2.11	0.50
2:D:242:THR:O	2:D:246:THR:OG1	2.27	0.50
1:b:70:ILE:HB	1:b:81:LEU:HD13	1.91	0.50
1:e:34:LEU:CD1	1:e:79:VAL:HG23	2.28	0.50
1:e:71:SER:O	1:e:79:VAL:HG13	2.10	0.50
1:e:102:THR:HG23	2:E:74:TYR:HE2	1.73	0.50
1:d:60:TYR:HB3	1:d:65:LYS:HD2	1.94	0.50
1:c:54:GLY:CA	2:C:111:LYS:HG3	2.41	0.50
1:b:60:TYR:HB3	1:b:65:LYS:HD2	1.94	0.50
2:C:143:ARG:HH22	3:R:26:U:H5''	1.76	0.50
1:b:61:ALA:O	1:b:65:LYS:HG2	2.11	0.50
1:b:102:THR:CG2	2:B:42:ILE:HG23	2.35	0.50
2:B:218:ILE:HD13	3:R:18:U:H5'	1.91	0.50
2:B:364:LEU:HG	2:B:366:THR:HG23	1.94	0.50
2:D:70:ASN:ND2	2:D:188:ASP:OD2	2.41	0.50
2:B:376:VAL:HG21	2:A:353:ASN:ND2	2.27	0.50
1:e:60:TYR:HB3	1:e:65:LYS:HD2	1.93	0.50
1:d:36:TRP:CD1	1:d:81:LEU:HD22	2.46	0.50
1:c:52:ASN:HB2	2:C:112:ALA:HB2	1.92	0.50
1:c:61:ALA:O	1:c:65:LYS:HG2	2.11	0.50
2:C:7:ARG:CA	2:A:348:PHE:CD1	2.94	0.50
2:B:208:HIS:HD2	2:B:210:CYS:HB2	1.74	0.50
1:c:27:ARG:HH11	1:c:30:ARG:NE	2.09	0.50
1:b:102:THR:CB	2:B:42:ILE:CG2	2.77	0.50
1:a:32:TYR:HE2	1:a:53:TRP:HH2	1.55	0.50
1:a:33:ARG:N	1:a:99:PHE:O	2.27	0.50
2:A:214:ARG:NH2	3:R:10:U:H4'	2.27	0.50
2:E:364:LEU:HG	2:E:366:THR:HG23	1.94	0.50
1:d:99:PHE:HB2	1:d:111:TYR:CA	2.11	0.50
1:b:36:TRP:CD1	1:b:81:LEU:HD22	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:102:THR:HG21	2:A:42:ILE:HG23	1.91	0.50
2:A:364:LEU:HG	2:A:366:THR:HG23	1.94	0.50
2:E:43:ASN:OD1	2:E:45:THR:OG1	2.22	0.50
2:E:70:ASN:ND2	2:E:188:ASP:OD2	2.41	0.50
2:D:43:ASN:OD1	2:D:45:THR:OG1	2.22	0.49
2:D:143:ARG:NH2	3:R:35:U:H5''	2.25	0.49
2:A:314:ARG:HE	2:A:404:LEU:HD22	1.76	0.49
1:e:36:TRP:CD1	1:e:81:LEU:HD22	2.46	0.49
1:e:52:ASN:ND2	2:E:112:ALA:CB	2.56	0.49
2:D:364:LEU:HG	2:D:366:THR:HG23	1.94	0.49
1:c:100:ASP:C	2:C:78:LYS:HE3	2.37	0.49
1:a:61:ALA:O	1:a:65:LYS:HG2	2.11	0.49
2:A:214:ARG:NH2	3:R:10:U:C4'	2.75	0.49
2:C:364:LEU:HG	2:C:366:THR:HG23	1.94	0.49
1:b:100:ASP:CG	2:B:78:LYS:CE	2.86	0.49
1:b:101:SER:C	2:B:74:TYR:HE2	2.19	0.49
2:E:202:PHE:CB	2:E:214:ARG:CG	2.91	0.49
1:c:105:PRO:HB2	1:c:110:ASN:HD22	1.66	0.49
2:D:8:ILE:HG12	2:B:347:GLN:O	2.13	0.49
1:c:31:ASN:HD21	2:C:78:LYS:CE	2.24	0.49
1:b:28:PRO:HB2	1:b:77:ASN:ND2	2.28	0.49
1:b:53:TRP:NE1	2:B:110:LEU:N	2.60	0.49
1:a:27:ARG:HH11	1:a:30:ARG:NE	2.09	0.49
1:d:28:PRO:HB2	1:d:77:ASN:ND2	2.28	0.49
2:D:202:PHE:CB	2:D:214:ARG:CG	2.91	0.49
1:d:102:THR:CG2	2:D:74:TYR:CE2	2.80	0.49
1:c:27:ARG:HD3	1:c:30:ARG:CB	2.43	0.49
2:C:312:ARG:CD	3:R:23:U:C4	2.91	0.49
1:b:27:ARG:HD3	1:b:30:ARG:CB	2.43	0.49
1:a:27:ARG:HD3	1:a:30:ARG:CB	2.43	0.49
2:A:43:ASN:OD1	2:A:45:THR:OG1	2.22	0.49
2:A:202:PHE:CB	2:A:214:ARG:CG	2.91	0.49
1:c:28:PRO:CB	1:c:77:ASN:ND2	2.76	0.49
1:b:52:ASN:CG	2:B:112:ALA:HB2	2.37	0.49
1:e:28:PRO:HB2	1:e:77:ASN:ND2	2.28	0.49
1:d:27:ARG:HD3	1:d:30:ARG:CB	2.43	0.49
1:d:32:TYR:HE2	1:d:53:TRP:HH2	1.55	0.48
2:C:88:TRP:CD2	2:C:95:ILE:HD11	2.48	0.48
1:b:54:GLY:HA3	2:B:111:LYS:HG3	1.94	0.48
1:a:28:PRO:CB	1:a:77:ASN:ND2	2.76	0.48
1:e:28:PRO:CB	1:e:77:ASN:ND2	2.76	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:202:PHE:CB	2:B:214:ARG:CG	2.91	0.48
2:B:181:ILE:HD11	2:A:168:ASN:CG	2.39	0.48
2:B:242:THR:O	2:B:246:THR:OG1	2.27	0.48
2:B:267:GLU:OE1	2:B:273:SER:OG	2.30	0.48
1:e:27:ARG:HD3	1:e:30:ARG:CB	2.43	0.48
2:D:312:ARG:CD	3:R:32:U:C4	2.94	0.48
1:c:102:THR:CG2	2:C:42:ILE:HG23	2.43	0.48
2:C:267:GLU:OE1	2:C:273:SER:OG	2.30	0.48
2:A:214:ARG:CZ	3:R:10:U:H5'	2.43	0.48
1:e:83:MET:HE2	1:e:86:LEU:HD21	1.95	0.48
2:D:88:TRP:CD2	2:D:95:ILE:HD11	2.48	0.48
1:a:27:ARG:NH2	2:A:81:ARG:NE	2.62	0.48
1:a:83:MET:HE2	1:a:86:LEU:HD21	1.95	0.48
2:D:214:ARG:CZ	3:R:37:U:P	3.02	0.48
2:C:202:PHE:CB	2:C:214:ARG:CG	2.91	0.48
1:b:28:PRO:CB	1:b:77:ASN:ND2	2.76	0.48
1:e:39:GLN:CG	1:e:43:LYS:O	2.62	0.48
1:d:28:PRO:CB	1:d:77:ASN:ND2	2.76	0.48
1:d:52:ASN:HB2	2:D:112:ALA:HB2	1.96	0.48
2:B:88:TRP:CD2	2:B:95:ILE:HD11	2.48	0.48
2:A:167:ILE:HG23	2:A:170:GLN:HB2	1.96	0.48
1:d:83:MET:HE2	1:d:86:LEU:HD21	1.95	0.48
2:C:167:ILE:HG23	2:C:170:GLN:HB2	1.96	0.48
2:B:42:ILE:HD13	2:B:74:TYR:HB2	1.96	0.48
2:E:88:TRP:CD2	2:E:95:ILE:HD11	2.48	0.48
2:D:17:LYS:HE2	2:C:268:ILE:HG12	1.95	0.48
2:D:167:ILE:HG23	2:D:170:GLN:HB2	1.96	0.48
2:C:202:PHE:HB3	2:C:214:ARG:CG	2.44	0.48
2:B:202:PHE:HB3	2:B:214:ARG:CG	2.44	0.48
1:c:28:PRO:HB2	1:c:77:ASN:ND2	2.28	0.48
2:C:42:ILE:HD13	2:C:74:TYR:HB2	1.96	0.48
1:b:33:ARG:HD2	1:b:105:PRO:CD	2.44	0.48
1:a:28:PRO:HB2	1:a:77:ASN:ND2	2.28	0.48
1:d:100:ASP:OD2	2:D:78:LYS:CE	2.60	0.47
2:D:7:ARG:CB	2:B:348:PHE:CD1	2.97	0.47
2:D:7:ARG:CA	2:B:348:PHE:HD1	2.23	0.47
1:c:39:GLN:CG	1:c:43:LYS:O	2.62	0.47
2:B:167:ILE:HG23	2:B:170:GLN:HB2	1.96	0.47
1:a:39:GLN:CG	1:a:43:LYS:O	2.62	0.47
2:A:66:ILE:H	2:A:66:ILE:HD12	1.79	0.47
2:A:88:TRP:CD2	2:A:95:ILE:HD11	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:143:ARG:HH21	3:R:44:U:H5''	1.71	0.47
2:E:218:ILE:CD1	3:R:45:U:C2'	2.93	0.47
2:D:202:PHE:HB3	2:D:214:ARG:CG	2.44	0.47
1:c:33:ARG:HD2	1:c:105:PRO:CD	2.44	0.47
1:b:35:GLY:HA3	1:b:111:TYR:HH	1.74	0.47
1:b:39:GLN:CG	1:b:43:LYS:O	2.62	0.47
1:d:32:TYR:CE1	1:d:72:ARG:NH2	2.83	0.47
2:D:42:ILE:HD13	2:D:74:TYR:HB2	1.96	0.47
1:c:52:ASN:HD21	2:C:112:ALA:HB3	1.62	0.47
2:C:157:MET:O	2:C:161:THR:OG1	2.30	0.47
1:b:32:TYR:CE1	1:b:72:ARG:NH2	2.83	0.47
1:e:100:ASP:OD1	1:e:112:GLU:OE1	2.33	0.47
2:E:167:ILE:HG23	2:E:170:GLN:HB2	1.96	0.47
1:d:39:GLN:CG	1:d:43:LYS:O	2.61	0.47
2:D:8:ILE:HG22	2:B:349:CYS:SG	2.54	0.47
1:c:32:TYR:CE1	1:c:72:ARG:NH2	2.83	0.47
1:c:60:TYR:HB3	1:c:65:LYS:HD2	1.94	0.47
2:A:202:PHE:HB3	2:A:214:ARG:CG	2.44	0.47
2:D:66:ILE:HD12	2:D:66:ILE:H	1.79	0.47
1:b:56:VAL:HG11	2:B:114:ASP:OD2	2.14	0.47
1:b:83:MET:HE2	1:b:86:LEU:HD21	1.95	0.47
1:a:32:TYR:CE1	1:a:72:ARG:NH2	2.83	0.47
1:a:33:ARG:HD2	1:a:105:PRO:CD	2.44	0.47
2:A:192:THR:HA	2:A:195:VAL:HG22	1.96	0.47
1:c:99:PHE:HB2	1:c:111:TYR:CA	2.11	0.47
2:C:43:ASN:OD1	2:C:45:THR:OG1	2.22	0.47
1:a:28:PRO:CB	1:a:77:ASN:CG	2.87	0.47
1:e:31:ASN:HB3	2:E:110:LEU:HB2	1.92	0.47
1:e:33:ARG:HD2	1:e:105:PRO:CD	2.44	0.47
1:d:87:LYS:O	1:d:90:GLU:N	2.42	0.47
1:c:83:MET:HE2	1:c:86:LEU:HD21	1.95	0.47
1:b:27:ARG:HH22	2:B:81:ARG:NE	2.11	0.47
1:a:60:TYR:HB3	1:a:65:LYS:HD2	1.94	0.47
2:A:218:ILE:HD13	3:R:9:U:H5''	1.96	0.47
1:e:28:PRO:CB	1:e:77:ASN:CG	2.87	0.47
2:E:66:ILE:HD12	2:E:66:ILE:H	1.80	0.47
2:E:202:PHE:HB3	2:E:214:ARG:CG	2.44	0.47
3:R:27:U:O2'	3:R:29:U:OP2	2.32	0.47
1:d:100:ASP:OD1	1:d:112:GLU:OE1	2.33	0.47
1:d:108:ARG:CG	1:d:114:TRP:CZ2	2.96	0.47
1:c:100:ASP:OD1	1:c:112:GLU:OE1	2.33	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:b:100:ASP:CG	2:B:78:LYS:HE2	2.39	0.47
1:b:100:ASP:OD1	1:b:112:GLU:OE1	2.33	0.47
1:b:105:PRO:CG	1:b:110:ASN:CB	2.87	0.47
2:E:86:LYS:HD3	2:E:86:LYS:HA	1.79	0.47
1:c:28:PRO:CB	1:c:77:ASN:CG	2.87	0.47
1:c:33:ARG:N	1:c:99:PHE:O	2.27	0.47
1:e:32:TYR:HE2	1:e:53:TRP:HH2	1.55	0.47
2:E:218:ILE:CD1	3:R:45:U:C3'	2.91	0.47
1:d:33:ARG:HD2	1:d:105:PRO:CD	2.44	0.47
1:d:102:THR:HG22	2:D:110:LEU:CG	2.45	0.47
2:C:66:ILE:HD12	2:C:66:ILE:H	1.79	0.47
1:b:28:PRO:CB	1:b:77:ASN:CG	2.87	0.46
1:a:60:TYR:HD1	1:a:65:LYS:HZ2	1.62	0.46
1:a:100:ASP:OD1	1:a:112:GLU:OE1	2.33	0.46
2:D:8:ILE:HG23	2:B:348:PHE:HA	1.97	0.46
2:C:7:ARG:HG3	2:A:348:PHE:CE1	2.51	0.46
1:b:53:TRP:HE1	2:B:110:LEU:N	2.14	0.46
2:B:192:THR:HA	2:B:195:VAL:HG22	1.97	0.46
2:A:218:ILE:HD13	3:R:9:U:C5'	2.45	0.46
1:e:32:TYR:CE1	1:e:72:ARG:NH2	2.83	0.46
1:d:28:PRO:CB	1:d:77:ASN:CG	2.87	0.46
2:D:38:ILE:HG23	2:D:108:VAL:HG12	1.97	0.46
1:b:27:ARG:HH22	2:B:81:ARG:NH2	2.13	0.46
1:a:87:LYS:O	1:a:90:GLU:N	2.42	0.46
2:E:242:THR:O	2:E:246:THR:OG1	2.27	0.46
1:c:33:ARG:NE	1:c:105:PRO:CD	2.62	0.46
1:a:100:ASP:OD2	2:A:78:LYS:CE	2.64	0.46
1:e:78:THR:C	1:e:79:VAL:HG23	2.41	0.46
2:E:42:ILE:HD13	2:E:74:TYR:HB2	1.96	0.46
1:d:33:ARG:NE	1:d:105:PRO:CD	2.62	0.46
2:E:38:ILE:HG23	2:E:108:VAL:HG12	1.97	0.46
2:E:126:ARG:HA	2:E:126:ARG:HD3	1.67	0.46
2:E:290:SER:CB	3:R:40:U:OP2	2.45	0.46
2:E:381:TRP:O	2:E:385:GLN:HG2	2.16	0.46
1:d:12:VAL:CG1	1:d:13:GLN:OE1	2.60	0.46
2:D:262:MET:HE1	2:E:17:LYS:O	2.15	0.46
2:D:381:TRP:O	2:D:385:GLN:HG2	2.16	0.46
2:C:17:LYS:HG3	2:B:268:ILE:CG1	2.44	0.46
1:b:12:VAL:CG1	1:b:13:GLN:N	2.79	0.46
2:B:66:ILE:HD12	2:B:66:ILE:H	1.80	0.46
1:a:53:TRP:CD1	2:A:110:LEU:CB	2.99	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:83:MET:HB3	1:a:86:LEU:HD21	1.98	0.46
2:A:42:ILE:HD13	2:A:74:TYR:HB2	1.96	0.46
1:d:78:THR:C	1:d:79:VAL:HG23	2.41	0.46
1:c:83:MET:HB3	1:c:86:LEU:HD21	1.98	0.46
2:C:126:ARG:HD3	2:C:126:ARG:HA	1.67	0.46
2:E:192:THR:HA	2:E:195:VAL:HG22	1.97	0.46
1:d:83:MET:HB3	1:d:86:LEU:HD21	1.98	0.46
2:C:38:ILE:HG23	2:C:108:VAL:HG12	1.98	0.46
1:b:87:LYS:O	1:b:90:GLU:N	2.42	0.46
1:c:78:THR:C	1:c:79:VAL:HG23	2.41	0.46
1:c:78:THR:O	1:c:79:VAL:HG23	2.16	0.46
1:c:87:LYS:HG3	1:c:90:GLU:HG2	1.96	0.46
1:b:83:MET:HB3	1:b:86:LEU:HD21	1.98	0.46
1:c:31:ASN:HB3	2:C:110:LEU:CD2	2.45	0.45
2:C:8:ILE:CD1	2:A:346:GLN:O	2.62	0.45
2:C:147:THR:HG21	2:C:152:TYR:CE2	2.51	0.45
2:C:192:THR:HA	2:C:195:VAL:HG22	1.96	0.45
2:C:381:TRP:O	2:C:385:GLN:HG2	2.16	0.45
1:a:12:VAL:CG1	1:a:13:GLN:N	2.79	0.45
1:d:78:THR:O	1:d:79:VAL:HG23	2.16	0.45
2:A:147:THR:HG21	2:A:152:TYR:CE2	2.51	0.45
1:e:60:TYR:HB2	1:e:65:LYS:HZ3	1.79	0.45
2:C:18:LEU:HD11	2:B:232:GLY:HA2	1.97	0.45
2:C:383:GLU:HG3	2:B:355:TYR:OH	2.17	0.45
2:B:18:LEU:HD21	2:A:231:PHE:CD2	2.51	0.45
2:B:381:TRP:O	2:B:385:GLN:HG2	2.16	0.45
1:a:78:THR:C	1:a:79:VAL:HG23	2.41	0.45
2:A:38:ILE:HG23	2:A:108:VAL:HG12	1.97	0.45
2:D:192:THR:HA	2:D:195:VAL:HG22	1.97	0.45
1:c:12:VAL:CG1	1:c:13:GLN:N	2.79	0.45
2:C:7:ARG:CG	2:A:348:PHE:CE1	2.99	0.45
1:e:83:MET:HB3	1:e:86:LEU:HD21	1.98	0.45
3:R:11:U:H3'	3:R:12:U:C5'	2.41	0.45
2:D:268:ILE:CG1	2:E:17:LYS:HG3	2.46	0.45
2:C:408:ARG:HH22	3:R:25:U:P	2.40	0.45
1:b:87:LYS:HG3	1:b:90:GLU:HG2	1.96	0.45
2:B:38:ILE:HG23	2:B:108:VAL:HG12	1.97	0.45
2:B:43:ASN:OD1	2:B:45:THR:OG1	2.22	0.45
1:a:78:THR:O	1:a:79:VAL:HG23	2.16	0.45
2:A:381:TRP:O	2:A:385:GLN:HG2	2.16	0.45
1:b:78:THR:C	1:b:79:VAL:HG23	2.41	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:b:108:ARG:CG	1:b:114:TRP:CZ2	2.96	0.45
1:a:108:ARG:CG	1:a:114:TRP:CZ2	2.96	0.45
1:e:40:ALA:HB3	1:e:43:LYS:HD3	1.98	0.45
1:d:40:ALA:HB3	1:d:43:LYS:HD3	1.98	0.45
2:D:147:THR:HG21	2:D:152:TYR:CE2	2.51	0.45
2:B:147:THR:HG21	2:B:152:TYR:CE2	2.51	0.45
1:a:12:VAL:CG1	1:a:13:GLN:OE1	2.60	0.45
1:a:52:ASN:HD21	2:A:112:ALA:HB3	1.74	0.45
1:e:60:TYR:HD1	1:e:65:LYS:HZ2	1.62	0.45
1:c:27:ARG:NH2	2:C:81:ARG:NE	2.64	0.45
1:c:40:ALA:HB3	1:c:43:LYS:HD3	1.98	0.45
2:C:202:PHE:HE1	2:C:208:HIS:CD2	2.35	0.45
1:a:40:ALA:HB3	1:a:43:LYS:HD3	1.98	0.45
2:A:142:TYR:O	2:A:146:ARG:HG3	2.17	0.45
2:A:202:PHE:HE1	2:A:208:HIS:CD2	2.35	0.45
2:E:142:TYR:O	2:E:146:ARG:HG3	2.17	0.45
1:d:12:VAL:CG1	1:d:13:GLN:N	2.79	0.45
2:C:152:TYR:CE1	3:R:26:U:OP1	2.64	0.45
1:b:40:ALA:HB3	1:b:43:LYS:HD3	1.98	0.45
1:b:78:THR:O	1:b:79:VAL:HG23	2.16	0.45
2:B:142:TYR:O	2:B:146:ARG:HG3	2.17	0.45
1:e:78:THR:O	1:e:79:VAL:HG23	2.17	0.45
1:e:87:LYS:HG2	1:e:90:GLU:CG	2.38	0.45
2:E:147:THR:HG21	2:E:152:TYR:CE2	2.51	0.45
2:E:194:ILE:O	2:E:198:VAL:HG23	2.17	0.45
2:B:70:ASN:ND2	2:B:188:ASP:OD2	2.41	0.45
1:d:87:LYS:HG2	1:d:90:GLU:CG	2.38	0.44
2:D:8:ILE:HG23	2:B:347:GLN:O	2.17	0.44
1:b:87:LYS:HZ3	1:b:89:GLU:HB2	1.81	0.44
2:B:202:PHE:HE1	2:B:208:HIS:CD2	2.35	0.44
2:B:324:TYR:HB2	2:A:309:ARG:HB2	1.99	0.44
1:a:60:TYR:HB2	1:a:65:LYS:HZ2	1.76	0.44
1:e:12:VAL:CG1	1:e:13:GLN:N	2.79	0.44
1:e:12:VAL:CG1	1:e:13:GLN:OE1	2.60	0.44
2:D:194:ILE:O	2:D:198:VAL:HG23	2.17	0.44
2:D:220:SER:OG	2:D:280:ASP:OD2	2.34	0.44
2:C:142:TYR:O	2:C:146:ARG:HG3	2.17	0.44
2:D:268:ILE:CG1	2:E:17:LYS:HE2	2.42	0.44
1:c:12:VAL:CG1	1:c:13:GLN:OE1	2.60	0.44
1:d:27:ARG:HH11	1:d:30:ARG:NE	2.09	0.44
2:C:194:ILE:O	2:C:198:VAL:HG23	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:194:ILE:O	2:B:198:VAL:HG23	2.17	0.44
1:e:108:ARG:CG	1:e:114:TRP:CZ2	2.96	0.44
2:E:202:PHE:HE1	2:E:208:HIS:CD2	2.35	0.44
1:c:60:TYR:HB2	1:c:65:LYS:HZ2	1.78	0.44
1:c:91:THR:HG23	1:c:121:THR:HA	2.00	0.44
1:c:102:THR:HG23	2:C:74:TYR:CD2	2.39	0.44
2:A:194:ILE:O	2:A:198:VAL:HG23	2.17	0.44
1:e:27:ARG:HD3	1:e:30:ARG:HB3	1.99	0.44
1:c:27:ARG:HD3	1:c:30:ARG:HB3	1.99	0.44
1:b:91:THR:HG23	1:b:121:THR:HA	2.00	0.44
1:e:105:PRO:CG	1:e:110:ASN:CB	2.87	0.44
1:a:27:ARG:HD3	1:a:30:ARG:HB3	1.99	0.44
1:e:87:LYS:HG3	1:e:90:GLU:HG2	1.97	0.44
1:d:27:ARG:HD3	1:d:30:ARG:HB3	1.99	0.44
1:d:87:LYS:NZ	1:d:89:GLU:CB	2.78	0.44
1:d:87:LYS:HG3	1:d:90:GLU:HG2	1.96	0.43
2:D:202:PHE:HE1	2:D:208:HIS:CD2	2.35	0.43
2:D:256:ASP:OD1	2:E:7:ARG:NH2	2.30	0.43
1:b:27:ARG:NH2	2:B:81:ARG:NE	2.66	0.43
1:a:91:THR:HG23	1:a:121:THR:HA	2.00	0.43
1:a:99:PHE:CE1	1:a:112:GLU:HG3	2.50	0.43
1:d:19:THR:O	1:d:19:THR:CG2	2.66	0.43
1:c:78:THR:O	1:c:79:VAL:CG2	2.66	0.43
1:c:108:ARG:CG	1:c:114:TRP:CZ2	2.96	0.43
1:b:102:THR:HB	2:B:42:ILE:CG2	2.39	0.43
1:e:27:ARG:HH11	1:e:30:ARG:NE	2.09	0.43
1:e:78:THR:O	1:e:79:VAL:CG2	2.66	0.43
1:b:12:VAL:CG1	1:b:13:GLN:OE1	2.60	0.43
1:b:78:THR:O	1:b:79:VAL:CG2	2.66	0.43
2:B:286:LYS:CD	3:R:12:U:OP2	2.65	0.43
2:A:270:LYS:HE2	2:A:270:LYS:HB3	1.93	0.43
1:d:78:THR:O	1:d:79:VAL:CG2	2.66	0.43
1:d:91:THR:HG23	1:d:121:THR:HA	2.00	0.43
1:c:19:THR:O	1:c:19:THR:CG2	2.66	0.43
2:B:126:ARG:HA	2:B:126:ARG:HD3	1.67	0.43
1:e:87:LYS:O	1:e:90:GLU:N	2.42	0.43
2:A:70:ASN:ND2	2:A:188:ASP:OD2	2.41	0.43
2:D:142:TYR:O	2:D:146:ARG:HG3	2.17	0.43
1:c:67:ARG:NH2	1:c:90:GLU:CD	2.75	0.43
1:b:27:ARG:HD3	1:b:30:ARG:HB3	1.99	0.43
1:b:105:PRO:HG3	1:b:110:ASN:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:87:LYS:HG3	1:a:90:GLU:HG2	1.96	0.43
1:e:19:THR:O	1:e:19:THR:CG2	2.66	0.43
1:e:73:ASP:CB	1:e:76:LYS:HG2	2.48	0.43
1:e:91:THR:HG23	1:e:121:THR:HA	2.00	0.43
2:E:277:TYR:O	2:E:281:PHE:HB2	2.19	0.43
1:c:87:LYS:HG2	1:c:90:GLU:CG	2.38	0.43
2:D:207:LYS:HD3	2:E:285:SER:HB2	2.00	0.43
1:c:100:ASP:O	2:C:78:LYS:CE	2.59	0.43
2:A:202:PHE:HB2	2:A:214:ARG:HG2	2.01	0.43
2:A:214:ARG:CZ	3:R:10:U:C5'	2.97	0.43
1:c:105:PRO:CG	1:c:110:ASN:CB	2.87	0.43
1:b:33:ARG:N	1:b:99:PHE:O	2.27	0.43
2:B:152:TYR:HH	3:R:17:U:P	2.42	0.43
1:a:19:THR:O	1:a:19:THR:CG2	2.66	0.43
1:e:87:LYS:NZ	1:e:90:GLU:OE2	2.52	0.43
3:R:2:U:H3'	3:R:3:U:C5'	2.46	0.43
1:b:19:THR:O	1:b:19:THR:CG2	2.66	0.43
2:B:202:PHE:HB2	2:B:214:ARG:HG2	2.01	0.43
1:a:78:THR:O	1:a:79:VAL:CG2	2.66	0.43
1:a:87:LYS:NZ	1:a:90:GLU:OE2	2.52	0.43
2:A:277:TYR:O	2:A:281:PHE:HB2	2.19	0.43
1:e:60:TYR:CD1	1:e:65:LYS:NZ	2.85	0.43
2:C:277:TYR:O	2:C:281:PHE:HB2	2.19	0.42
1:b:87:LYS:HG2	1:b:90:GLU:CG	2.38	0.42
2:E:286:LYS:HD3	3:R:39:U:P	2.51	0.42
3:R:27:U:H4'	3:R:29:U:C5	2.54	0.42
2:D:86:LYS:HD3	2:D:86:LYS:HA	1.79	0.42
2:D:277:TYR:O	2:D:281:PHE:HB2	2.19	0.42
1:b:50:ALA:CB	1:b:104:SER:HB2	2.40	0.42
1:b:87:LYS:NZ	1:b:90:GLU:OE2	2.52	0.42
1:a:100:ASP:C	2:A:78:LYS:HE3	2.43	0.42
1:e:33:ARG:N	1:e:99:PHE:O	2.27	0.42
2:D:230:THR:HG21	2:D:298:HIS:ND1	2.35	0.42
1:a:87:LYS:NZ	1:a:89:GLU:CB	2.78	0.42
2:D:309:ARG:HB2	2:E:324:TYR:HB2	2.02	0.42
2:C:202:PHE:HB2	2:C:214:ARG:HG2	2.01	0.42
1:b:27:ARG:HH11	1:b:30:ARG:NE	2.09	0.42
1:a:100:ASP:OD2	2:A:78:LYS:HE2	2.20	0.42
1:e:87:LYS:NZ	1:e:89:GLU:CB	2.78	0.42
2:A:66:ILE:HA	2:A:69:VAL:HG22	2.01	0.42
1:d:28:PRO:HD2	1:d:29:PHE:CE2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:d:87:LYS:NZ	1:d:90:GLU:OE2	2.52	0.42
2:D:100:ASP:OD1	2:D:100:ASP:N	2.53	0.42
2:A:86:LYS:HA	2:A:86:LYS:HD3	1.79	0.42
1:c:87:LYS:NZ	1:c:90:GLU:OE2	2.52	0.42
2:B:230:THR:HG21	2:B:298:HIS:ND1	2.35	0.42
1:e:50:ALA:CB	1:e:104:SER:HB2	2.40	0.42
2:D:52:ARG:NH1	2:D:128:SER:HA	2.35	0.42
2:C:52:ARG:NH1	2:C:128:SER:HA	2.35	0.42
2:C:230:THR:HG21	2:C:298:HIS:ND1	2.35	0.42
1:a:28:PRO:HD2	1:a:29:PHE:CE2	2.55	0.42
2:C:88:TRP:CD2	2:C:95:ILE:CD1	3.03	0.42
1:a:60:TYR:HB2	1:a:65:LYS:HZ3	1.83	0.42
1:e:67:ARG:NH2	1:e:90:GLU:CD	2.75	0.42
1:d:67:ARG:NH2	1:d:90:GLU:CD	2.75	0.41
1:c:28:PRO:HD2	1:c:29:PHE:CE2	2.55	0.41
1:c:87:LYS:O	1:c:90:GLU:N	2.42	0.41
2:B:66:ILE:HA	2:B:69:VAL:HG22	2.01	0.41
1:e:28:PRO:HD2	1:e:29:PHE:CE2	2.55	0.41
2:E:52:ARG:NH1	2:E:128:SER:HA	2.35	0.41
2:E:202:PHE:HB2	2:E:214:ARG:HG2	2.01	0.41
2:D:66:ILE:HA	2:D:69:VAL:HG22	2.01	0.41
1:c:32:TYR:CZ	1:c:72:ARG:NH2	2.88	0.41
1:c:60:TYR:CB	1:c:65:LYS:HD3	2.48	0.41
2:C:66:ILE:HA	2:C:69:VAL:HG22	2.01	0.41
2:C:148:GLN:OE1	2:C:153:ARG:NH1	2.54	0.41
2:C:211:ALA:HB1	2:C:214:ARG:CZ	2.50	0.41
1:b:28:PRO:HD2	1:b:29:PHE:CE2	2.55	0.41
2:B:277:TYR:O	2:B:281:PHE:HB2	2.19	0.41
1:a:35:GLY:HA3	1:a:111:TYR:HH	1.81	0.41
1:a:87:LYS:HG2	1:a:90:GLU:CG	2.38	0.41
1:e:32:TYR:CZ	1:e:72:ARG:NH2	2.88	0.41
1:e:99:PHE:CE1	1:e:112:GLU:HG3	2.50	0.41
2:D:202:PHE:HB2	2:D:214:ARG:HG2	2.01	0.41
2:D:211:ALA:HB1	2:D:214:ARG:CZ	2.50	0.41
1:a:102:THR:CG2	2:A:42:ILE:CG2	2.93	0.41
1:e:60:TYR:HB2	1:e:65:LYS:HZ2	1.80	0.41
2:E:148:GLN:OE1	2:E:153:ARG:NH1	2.54	0.41
2:E:230:THR:HG21	2:E:298:HIS:ND1	2.35	0.41
2:E:412:ILE:HA	2:E:415:TYR:HB3	2.02	0.41
2:D:126:ARG:HA	2:D:126:ARG:HD3	1.67	0.41
2:C:408:ARG:NH2	3:R:24:U:H2'	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:32:TYR:CZ	1:a:72:ARG:NH2	2.88	0.41
1:d:32:TYR:CZ	1:d:72:ARG:NH2	2.88	0.41
2:D:224:ASP:OD1	3:R:30:U:H4'	2.20	0.41
2:B:52:ARG:NH1	2:B:128:SER:HA	2.35	0.41
2:B:88:TRP:CD2	2:B:95:ILE:CD1	3.03	0.41
2:A:68:HIS:NE2	2:A:118:PRO:HG2	2.36	0.41
2:A:324:TYR:O	2:A:328:THR:OG1	2.19	0.41
2:A:408:ARG:NH2	3:R:7:U:OP1	2.49	0.41
1:c:60:TYR:CD1	1:c:65:LYS:NZ	2.84	0.41
2:A:226:ALA:O	2:A:230:THR:HG23	2.21	0.41
2:D:88:TRP:CD2	2:D:95:ILE:CD1	3.03	0.41
2:D:344:LEU:HD12	2:E:382:PHE:CE2	2.55	0.41
2:B:86:LYS:HD3	2:B:86:LYS:HA	1.79	0.41
2:B:211:ALA:HB1	2:B:214:ARG:CZ	2.50	0.41
1:a:105:PRO:HG3	1:a:110:ASN:HB2	2.01	0.41
3:R:23:U:H2'	3:R:25:U:H5''	2.02	0.41
2:D:412:ILE:HA	2:D:415:TYR:HB3	2.02	0.41
1:b:60:TYR:HD1	1:b:65:LYS:HZ2	1.64	0.41
2:B:148:GLN:OE1	2:B:153:ARG:NH1	2.54	0.41
2:A:52:ARG:NH1	2:A:128:SER:HA	2.35	0.41
1:e:101:SER:CB	2:E:44:THR:HB	2.51	0.41
1:c:105:PRO:HG3	1:c:110:ASN:HB2	2.00	0.41
1:b:32:TYR:CZ	1:b:72:ARG:NH2	2.88	0.41
2:B:152:TYR:OH	3:R:17:U:OP2	2.36	0.41
1:a:102:THR:CG2	2:A:42:ILE:HG23	2.50	0.41
2:A:88:TRP:CD2	2:A:95:ILE:CD1	3.03	0.41
2:A:230:THR:HG21	2:A:298:HIS:ND1	2.35	0.41
1:e:31:ASN:CB	2:E:110:LEU:HB2	2.49	0.41
2:E:68:HIS:NE2	2:E:118:PRO:HG2	2.36	0.41
2:E:88:TRP:CD2	2:E:95:ILE:CD1	3.03	0.41
2:E:100:ASP:OD1	2:E:100:ASP:N	2.53	0.41
2:E:211:ALA:HB1	2:E:214:ARG:CZ	2.50	0.41
2:E:226:ALA:O	2:E:230:THR:HG23	2.21	0.41
2:D:148:GLN:OE1	2:D:153:ARG:NH1	2.54	0.41
2:D:226:ALA:O	2:D:230:THR:HG23	2.21	0.41
2:B:68:HIS:NE2	2:B:118:PRO:HG2	2.36	0.41
2:B:100:ASP:OD1	2:B:100:ASP:N	2.53	0.41
1:a:31:ASN:HD22	1:a:101:SER:HA	1.86	0.41
2:A:110:LEU:HD13	2:A:110:LEU:HA	1.93	0.41
2:A:143:ARG:NH1	3:R:9:U:OP2	2.53	0.41
1:e:35:GLY:HA3	1:e:111:TYR:HH	1.80	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:66:ILE:HA	2:E:69:VAL:HG22	2.01	0.41
2:D:270:LYS:HE2	2:D:270:LYS:HB3	1.93	0.40
1:c:60:TYR:HD1	1:c:65:LYS:HZ2	1.62	0.40
2:C:68:HIS:NE2	2:C:118:PRO:HG2	2.36	0.40
2:C:324:TYR:O	2:C:328:THR:OG1	2.19	0.40
2:C:359:ASP:OD1	2:C:359:ASP:N	2.50	0.40
1:a:105:PRO:CG	1:a:110:ASN:CB	2.87	0.40
2:A:412:ILE:HA	2:A:415:TYR:HB3	2.02	0.40
1:d:37:PHE:HZ	1:d:107:VAL:O	2.05	0.40
2:B:226:ALA:O	2:B:230:THR:HG23	2.21	0.40
2:B:312:ARG:HG3	3:R:14:U:N3	2.37	0.40
2:A:126:ARG:HA	2:A:126:ARG:HD3	1.67	0.40
3:R:20:U:H2'	3:R:21:U:O4'	2.21	0.40
1:d:76:LYS:O	1:d:78:THR:HG23	2.22	0.40
2:D:285:SER:HB2	2:C:207:LYS:HD3	2.04	0.40
1:c:35:GLY:HA3	1:c:111:TYR:HH	1.80	0.40
2:B:130:ASP:O	2:B:134:LEU:HB2	2.22	0.40
3:R:13:U:H5'	3:R:14:U:OP2	2.21	0.40
2:D:410:LYS:HE3	2:D:410:LYS:HB3	1.92	0.40
1:c:76:LYS:O	1:c:78:THR:HG23	2.22	0.40
1:b:37:PHE:HZ	1:b:107:VAL:O	2.05	0.40
2:B:172:GLU:H	2:B:172:GLU:CD	2.28	0.40
2:B:285:SER:HB3	2:A:207:LYS:NZ	2.36	0.40
1:a:76:LYS:O	1:a:78:THR:HG23	2.22	0.40
1:a:102:THR:H	2:A:44:THR:HB	1.37	0.40
2:A:130:ASP:O	2:A:134:LEU:HB2	2.22	0.40
1:e:76:LYS:O	1:e:78:THR:HG23	2.22	0.40
1:e:105:PRO:HG3	1:e:110:ASN:HB2	2.00	0.40
2:E:224:ASP:HA	3:R:40:U:OP1	2.22	0.40
2:D:68:HIS:NE2	2:D:118:PRO:HG2	2.36	0.40
1:c:50:ALA:CB	1:c:104:SER:HB2	2.40	0.40
2:B:143:ARG:HH22	3:R:17:U:C3'	2.30	0.40
2:A:148:GLN:OE1	2:A:153:ARG:NH1	2.54	0.40
2:A:211:ALA:HB1	2:A:214:ARG:CZ	2.50	0.40

All (56) 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)
2:C:169:GLU:CB	2:C:359:ASP:CB[1_554]	0.90	1.30

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:171:PHE:CZ	2:A:362:GLY:CA[1_554]	1.11	1.09
2:C:171:PHE:CZ	2:C:362:GLY:CA[1_554]	1.13	1.07
2:C:171:PHE:CE2	2:C:362:GLY:CA[1_554]	1.32	0.88
2:D:169:GLU:CB	2:D:359:ASP:CB[1_554]	1.39	0.81
2:A:169:GLU:CB	2:A:359:ASP:CB[1_554]	1.40	0.80
1:c:13:GLN:NE2	1:a:17:SER:O[4_477]	1.59	0.61
3:R:1:U:P	3:R:45:U:O3'[2_675]	1.60	0.60
2:D:360:SER:OG	2:E:177:GLU:OE1[1_556]	1.63	0.57
2:B:177:GLU:CD	2:A:360:SER:O[1_554]	1.67	0.53
2:B:169:GLU:CB	2:B:359:ASP:CB[1_554]	1.70	0.50
2:E:169:GLU:CB	2:E:359:ASP:CB[1_554]	1.71	0.49
2:E:214:ARG:CZ	3:R:1:U:O5'[2_675]	1.74	0.46
2:C:63:ASN:ND2	2:B:356:THR:CG2[1_554]	1.75	0.45
2:A:177:GLU:CD	2:E:360:SER:O[2_674]	1.75	0.45
2:A:63:ASN:ND2	2:E:356:THR:CG2[2_674]	1.76	0.44
2:D:169:GLU:N	2:D:359:ASP:OD2[1_554]	1.78	0.42
2:A:177:GLU:OE1	2:E:360:SER:O[2_674]	1.78	0.42
2:A:171:PHE:CE2	2:A:362:GLY:CA[1_554]	1.79	0.41
2:E:169:GLU:N	2:E:359:ASP:OD2[1_554]	1.79	0.41
2:E:214:ARG:NH2	3:R:1:U:O5'[2_675]	1.82	0.38
2:D:360:SER:O	2:E:177:GLU:CD[1_556]	1.86	0.34
2:C:171:PHE:CZ	2:C:362:GLY:N[1_554]	1.87	0.33
2:B:177:GLU:OE1	2:A:360:SER:O[1_554]	1.87	0.33
2:D:169:GLU:CG	2:D:359:ASP:CB[1_554]	1.92	0.28
2:C:169:GLU:CB	2:C:359:ASP:CA[1_554]	1.92	0.28
2:C:169:GLU:CG	2:C:359:ASP:CB[1_554]	1.92	0.28
2:B:177:GLU:OE1	2:A:360:SER:C[1_554]	1.94	0.26
2:E:169:GLU:CG	2:E:359:ASP:CB[1_554]	1.96	0.24
2:C:169:GLU:N	2:C:359:ASP:OD2[1_554]	1.97	0.23
2:C:171:PHE:CE2	2:C:362:GLY:C[1_554]	1.99	0.21
2:C:177:GLU:OE1	2:B:360:SER:O[1_554]	2.00	0.20
2:B:177:GLU:OE2	2:A:361:THR:CA[1_554]	2.01	0.19
2:A:177:GLU:OE1	2:E:360:SER:C[2_674]	2.01	0.19
2:C:169:GLU:CB	2:C:359:ASP:CG[1_554]	2.02	0.18
2:D:171:PHE:CZ	2:D:362:GLY:CA[1_554]	2.04	0.16
2:C:169:GLU:CG	2:C:359:ASP:CA[1_554]	2.04	0.16
2:E:169:GLU:CB	2:E:359:ASP:OD2[1_554]	2.05	0.15
1:c:17:SER:O	1:a:13:GLN:NE2[4_477]	2.07	0.13
2:B:171:PHE:CZ	2:B:362:GLY:CA[1_554]	2.07	0.13
2:A:171:PHE:CE2	2:A:362:GLY:O[1_554]	2.07	0.13
2:D:171:PHE:CE2	2:D:362:GLY:CA[1_554]	2.08	0.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:169:GLU:N	2:B:359:ASP:OD2[1_554]	2.09	0.11
2:D:169:GLU:CB	2:D:359:ASP:CG[1_554]	2.11	0.09
2:C:177:GLU:CD	2:B:360:SER:O[1_554]	2.11	0.09
2:E:214:ARG:NH1	3:R:1:U:O5'[2_675]	2.11	0.09
3:R:1:U:OP1	3:R:45:U:O3'[2_675]	2.11	0.09
2:A:171:PHE:CE2	2:A:362:GLY:C[1_554]	2.13	0.07
2:D:63:ASN:ND2	2:C:356:THR:CG2[1_554]	2.14	0.06
2:B:177:GLU:CG	2:A:360:SER:O[1_554]	2.14	0.06
2:A:177:GLU:OE2	2:E:361:THR:CA[2_674]	2.16	0.04
2:D:177:GLU:CD	2:C:360:SER:O[1_554]	2.17	0.03
2:C:171:PHE:CE2	2:C:362:GLY:O[1_554]	2.17	0.03
2:D:360:SER:O	2:E:177:GLU:OE2[1_556]	2.18	0.02
2:E:169:GLU:CB	2:E:359:ASP:CG[1_554]	2.18	0.02
2:B:63:ASN:ND2	2:A:356:THR:CG2[1_554]	2.19	0.01

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	a	120/138 (87%)	110 (92%)	8 (7%)	2 (2%)	7	35
1	b	120/138 (87%)	110 (92%)	8 (7%)	2 (2%)	7	35
1	c	120/138 (87%)	110 (92%)	8 (7%)	2 (2%)	7	35
1	d	120/138 (87%)	110 (92%)	8 (7%)	2 (2%)	7	35
1	e	120/138 (87%)	110 (92%)	8 (7%)	2 (2%)	7	35
2	A	415/423 (98%)	395 (95%)	19 (5%)	1 (0%)	43	77
2	B	415/423 (98%)	395 (95%)	19 (5%)	1 (0%)	43	77
2	C	415/423 (98%)	395 (95%)	19 (5%)	1 (0%)	43	77
2	D	415/423 (98%)	395 (95%)	19 (5%)	1 (0%)	43	77
2	E	415/423 (98%)	395 (95%)	19 (5%)	1 (0%)	43	77
All	All	2675/2805 (95%)	2525 (94%)	135 (5%)	15 (1%)	21	59

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	d	101	SER
1	c	101	SER
1	b	101	SER
1	a	101	SER
1	e	101	SER
2	D	74	TYR
2	C	74	TYR
2	B	74	TYR
2	A	74	TYR
2	E	74	TYR
1	d	79	VAL
1	c	79	VAL
1	b	79	VAL
1	a	79	VAL
1	e	79	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	a	98/110 (89%)	96 (98%)	2 (2%)	48	66
1	b	98/110 (89%)	96 (98%)	2 (2%)	48	66
1	c	98/110 (89%)	96 (98%)	2 (2%)	48	66
1	d	98/110 (89%)	96 (98%)	2 (2%)	48	66
1	e	98/110 (89%)	96 (98%)	2 (2%)	48	66
2	A	361/363 (99%)	359 (99%)	2 (1%)	78	82
2	B	361/363 (99%)	359 (99%)	2 (1%)	78	82
2	C	361/363 (99%)	359 (99%)	2 (1%)	78	82
2	D	361/363 (99%)	359 (99%)	2 (1%)	78	82
2	E	361/363 (99%)	359 (99%)	2 (1%)	78	82
All	All	2295/2365 (97%)	2275 (99%)	20 (1%)	70	78

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	d	27	ARG
1	d	43	LYS
2	D	97	LYS
2	D	100	ASP
1	c	27	ARG
1	c	43	LYS
2	C	97	LYS
2	C	100	ASP
1	b	27	ARG
1	b	43	LYS
2	B	97	LYS
2	B	100	ASP
1	a	27	ARG
1	a	43	LYS
2	A	97	LYS
2	A	100	ASP
1	e	27	ARG
1	e	43	LYS
2	E	97	LYS
2	E	100	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	d	52	ASN
1	d	82	GLN
1	d	110	ASN
2	D	168	ASN
2	D	208	HIS
2	D	294	ASN
2	D	367	ASN
2	D	386	ASN
1	c	52	ASN
1	c	82	GLN
2	C	208	HIS
2	C	294	ASN
2	C	367	ASN
2	C	386	ASN
1	b	82	GLN
2	B	208	HIS
2	B	294	ASN

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Mol	Chain	Res	Type
2	B	367	ASN
2	B	386	ASN
1	a	31	ASN
1	a	82	GLN
1	a	110	ASN
2	A	208	HIS
2	A	294	ASN
2	A	367	ASN
1	e	82	GLN
1	e	110	ASN
2	E	208	HIS
2	E	294	ASN
2	E	315	ASN
2	E	367	ASN
2	E	386	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	R	44/45 (97%)	36 (81%)	8 (18%)

All (36) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	R	2	U
3	R	3	U
3	R	4	U
3	R	5	U
3	R	6	U
3	R	7	U
3	R	8	U
3	R	9	U
3	R	10	U
3	R	11	U
3	R	12	U
3	R	13	U
3	R	14	U
3	R	15	U
3	R	17	U
3	R	18	U
3	R	19	U

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Mol	Chain	Res	Type
3	R	21	U
3	R	23	U
3	R	24	U
3	R	25	U
3	R	26	U
3	R	27	U
3	R	28	U
3	R	29	U
3	R	30	U
3	R	32	U
3	R	33	U
3	R	36	U
3	R	37	U
3	R	38	U
3	R	39	U
3	R	40	U
3	R	41	U
3	R	42	U
3	R	45	U

All (8) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	R	4	U
3	R	5	U
3	R	6	U
3	R	12	U
3	R	14	U
3	R	20	U
3	R	32	U
3	R	39	U

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	a	122/138 (88%)	0.30	4 (3%) 49 43	303, 317, 325, 340	0
1	b	122/138 (88%)	0.42	7 (5%) 29 31	346, 363, 371, 373	0
1	c	122/138 (88%)	0.23	2 (1%) 70 58	311, 328, 337, 348	0
1	d	122/138 (88%)	0.10	0 100 100	371, 385, 392, 396	0
1	e	122/138 (88%)	0.49	6 (4%) 35 34	358, 378, 388, 390	0
2	A	419/423 (99%)	0.92	58 (13%) 6 13	236, 284, 336, 356	0
2	B	419/423 (99%)	0.86	50 (11%) 9 15	235, 288, 348, 365	0
2	C	419/423 (99%)	0.92	55 (13%) 7 13	242, 285, 342, 367	0
2	D	419/423 (99%)	0.79	52 (12%) 8 14	246, 309, 361, 377	0
2	E	419/423 (99%)	0.85	51 (12%) 8 15	247, 302, 355, 373	0
3	R	45/45 (100%)	0.32	0 100 100	289, 313, 332, 338	0
All	All	2750/2850 (96%)	0.73	285 (10%) 11 17	235, 311, 380, 396	0

All (285) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	362	GLY	9.7
2	A	363	GLY	7.1
2	E	362	GLY	6.8
2	A	85	ASP	6.6
2	B	363	GLY	6.1
2	C	82	GLY	5.9
2	D	85	ASP	5.7
2	A	137	TYR	5.3
2	E	361	THR	5.1
2	B	361	THR	5.1
2	E	85	ASP	5.0
2	D	363	GLY	4.9

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Mol	Chain	Res	Type	RSRZ
2	B	207	LYS	4.9
2	D	194	ILE	4.6
1	a	102	THR	4.6
2	C	102	ILE	4.5
2	D	207	LYS	4.4
2	C	207	LYS	4.4
2	D	49	SER	4.4
2	A	180	ASP	4.3
2	C	177	GLU	4.3
2	A	207	LYS	4.2
2	B	77	LEU	4.1
2	E	344	LEU	4.1
2	A	82	GLY	4.1
2	C	137	TYR	4.0
2	B	180	ASP	4.0
2	D	98	ALA	4.0
1	c	102	THR	3.9
2	E	137	TYR	3.9
2	B	49	SER	3.7
2	C	138	LEU	3.7
2	A	49	SER	3.7
2	D	138	LEU	3.7
2	B	119	ASP	3.7
2	C	361	THR	3.6
2	E	228	LEU	3.6
2	A	177	GLU	3.6
2	A	382	PHE	3.6
2	C	382	PHE	3.6
2	E	59	LEU	3.6
2	A	332	LEU	3.5
2	E	363	GLY	3.5
2	B	332	LEU	3.5
2	E	314	ARG	3.5
2	E	82	GLY	3.4
2	C	49	SER	3.4
2	B	85	ASP	3.4
2	D	176	PRO	3.4
2	B	171	PHE	3.4
2	A	73	LEU	3.4
2	A	364	LEU	3.3
2	A	325	THR	3.3
2	E	356	THR	3.3

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Mol	Chain	Res	Type	RSRZ
2	C	236	LYS	3.3
1	e	8	GLY	3.2
2	D	362	GLY	3.2
2	D	241	SER	3.2
2	D	73	LEU	3.2
2	E	138	LEU	3.1
1	b	31	ASN	3.1
2	C	88	TRP	3.1
2	D	333	LEU	3.1
2	A	362	GLY	3.1
2	D	102	ILE	3.1
2	E	360	SER	3.1
2	C	363	GLY	3.0
2	B	360	SER	3.0
2	E	241	SER	3.0
2	E	49	SER	3.0
2	A	361	THR	3.0
2	A	102	ILE	3.0
2	B	357	PRO	3.0
2	C	165	LYS	3.0
2	A	88	TRP	3.0
2	B	364	LEU	3.0
2	C	73	LEU	2.9
2	A	228	LEU	2.9
2	B	73	LEU	2.9
2	A	19	PRO	2.9
2	E	405	GLN	2.9
2	B	354	LYS	2.9
1	b	102	THR	2.9
2	C	105	PHE	2.9
2	D	150	PRO	2.9
2	D	364	LEU	2.9
2	E	207	LYS	2.9
2	A	133	TRP	2.9
2	E	77	LEU	2.9
2	E	354	LYS	2.8
2	B	382	PHE	2.8
2	E	332	LEU	2.8
2	E	162	ASN	2.8
2	C	167	ILE	2.8
2	A	43	ASN	2.8
2	A	317	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
2	A	77	LEU	2.8
2	A	44	THR	2.8
2	C	332	LEU	2.8
2	C	241	SER	2.8
2	C	395	GLN	2.7
2	E	151	GLU	2.7
2	D	74	TYR	2.7
2	A	416	ALA	2.7
2	A	45	THR	2.7
2	B	137	TYR	2.7
2	C	173	PRO	2.7
1	a	101	SER	2.7
2	B	241	SER	2.7
2	D	357	PRO	2.7
2	B	194	ILE	2.7
2	A	176	PRO	2.7
2	C	387	ARG	2.7
2	C	362	GLY	2.7
2	B	38	ILE	2.7
2	D	40	LEU	2.7
2	A	187	ASN	2.6
2	E	379	LEU	2.6
2	B	356	THR	2.6
2	A	194	ILE	2.6
2	D	187	ASN	2.6
2	E	57	GLN	2.6
2	A	105	PHE	2.6
2	E	392	ASP	2.6
2	C	43	ASN	2.6
2	E	212	SER	2.6
1	a	31	ASN	2.6
2	B	82	GLY	2.6
2	A	195	VAL	2.6
2	A	173	PRO	2.6
2	B	105	PHE	2.6
2	D	104	ILE	2.6
2	A	80	ILE	2.6
2	C	358	ASP	2.6
2	E	79	ASP	2.6
2	C	18	LEU	2.6
2	C	59	LEU	2.6
2	B	162	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
2	E	180	ASP	2.5
2	C	289	TYR	2.5
2	C	44	THR	2.5
2	D	361	THR	2.5
2	D	206	LYS	2.5
2	C	349	CYS	2.5
2	A	312	ARG	2.5
2	D	137	TYR	2.5
2	A	165	LYS	2.5
2	A	236	LYS	2.5
2	A	329	THR	2.5
2	E	326	SER	2.5
2	B	102	ILE	2.5
2	A	63	ASN	2.5
2	E	168	ASN	2.5
2	C	47	SER	2.5
2	C	333	LEU	2.5
2	A	169	GLU	2.5
2	D	317	ARG	2.5
2	B	129	ALA	2.5
2	D	44	THR	2.4
2	A	167	ILE	2.4
2	C	388	LYS	2.4
2	D	45	THR	2.4
2	B	74	TYR	2.4
2	C	212	SER	2.4
1	c	48	VAL	2.4
2	A	358	ASP	2.4
2	D	416	ALA	2.4
2	A	40	LEU	2.4
2	D	43	ASN	2.4
2	D	169	GLU	2.4
2	B	176	PRO	2.4
1	b	56	VAL	2.4
2	B	57	GLN	2.4
2	C	77	LEU	2.4
2	C	169	GLU	2.4
2	B	242	THR	2.4
2	A	388	LYS	2.4
2	D	77	LEU	2.4
2	D	306	LEU	2.4
2	E	416	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
2	C	352	ASP	2.4
2	D	228	LEU	2.4
2	B	150	PRO	2.4
2	B	371	GLN	2.4
2	C	128	SER	2.4
2	E	129	ALA	2.4
2	D	105	PHE	2.3
1	e	19	THR	2.3
2	A	241	SER	2.3
2	D	6	LYS	2.3
2	B	88	TRP	2.3
2	B	59	LEU	2.3
2	D	180	ASP	2.3
2	A	406	GLY	2.3
2	C	405	GLN	2.3
2	E	173	PRO	2.3
2	D	27	TYR	2.3
2	D	367	ASN	2.3
2	E	317	ARG	2.3
2	B	127	THR	2.3
2	E	44	THR	2.3
2	C	297	PHE	2.3
2	B	8	ILE	2.3
2	B	228	LEU	2.3
2	D	88	TRP	2.3
2	C	147	THR	2.3
2	C	176	PRO	2.3
2	B	388	LYS	2.3
2	D	59	LEU	2.3
2	B	236	LYS	2.2
2	C	379	LEU	2.2
2	C	180	ASP	2.2
2	A	59	LEU	2.2
2	A	316	ALA	2.2
1	b	109	ASP	2.2
2	C	79	ASP	2.2
2	B	151	GLU	2.2
2	E	395	GLN	2.2
2	C	132	LYS	2.2
2	C	357	PRO	2.2
2	B	406	GLY	2.2
2	D	354	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	165	LYS	2.2
2	E	357	PRO	2.2
2	A	365	THR	2.2
1	b	101	SER	2.2
2	B	152	TYR	2.2
2	A	149	MET	2.2
2	A	168	ASN	2.2
2	E	187	ASN	2.2
2	D	417	LYS	2.2
2	D	292	VAL	2.2
2	A	130	ASP	2.2
2	E	358	ASP	2.2
2	C	386	ASN	2.2
2	B	333	LEU	2.2
2	B	128	SER	2.2
2	C	243	GLU	2.2
2	A	119	ASP	2.1
2	D	332	LEU	2.1
2	C	168	ASN	2.1
2	E	38	ILE	2.1
2	E	165	LYS	2.1
2	D	57	GLN	2.1
2	E	352	ASP	2.1
2	A	344	LEU	2.1
1	b	63	SER	2.1
2	D	146	ARG	2.1
2	E	47	SER	2.1
1	b	8	GLY	2.1
2	B	169	GLU	2.1
2	B	416	ALA	2.1
2	D	167	ILE	2.1
2	B	377	GLU	2.1
2	E	406	GLY	2.1
2	C	95	ILE	2.1
2	E	171	PHE	2.1
2	E	164	CYS	2.1
2	C	275	MET	2.1
2	D	61	SER	2.1
1	e	69	THR	2.1
2	C	148	GLN	2.1
2	E	102	ILE	2.1
1	e	109	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
2	D	274	TYR	2.1
1	a	54	GLY	2.1
2	A	127	THR	2.1
2	A	162	ASN	2.1
1	e	101	SER	2.1
2	D	165	LYS	2.0
2	E	76	ALA	2.0
2	E	194	ILE	2.0
2	E	150	PRO	2.0
1	e	103	GLY	2.0
2	D	406	GLY	2.0
2	B	79	ASP	2.0
2	A	357	PRO	2.0
2	D	377	GLU	2.0
2	C	195	VAL	2.0
2	E	127	THR	2.0
2	A	393	MET	2.0
2	D	303	LEU	2.0
2	C	19	PRO	2.0
2	A	389	PRO	2.0
2	C	166	MET	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 oligosaccharides 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.