



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2026 – 11:29 PM UTC

PDB ID : 2BBV / pdb_00002bbv
Title : THE REFINED THREE-DIMENSIONAL STRUCTURE OF AN INSECT VIRUS AT 2.8 ANGSTROMS RESOLUTION
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Deposited on : 1994-06-06
Resolution : 2.80 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
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

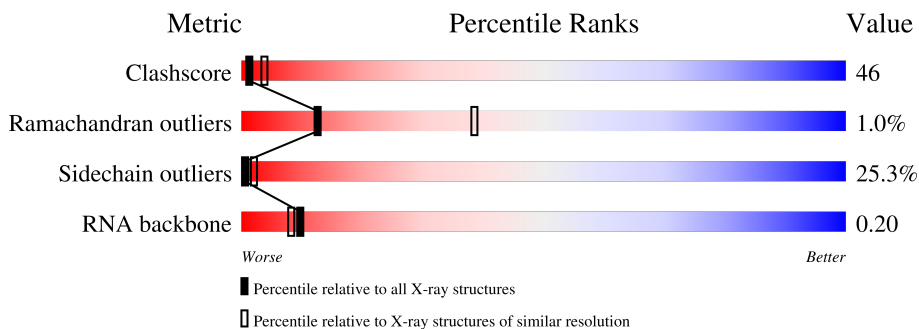
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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))
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RNA backbone	3983	1114 (3.00-2.60)


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 $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	N	10	50% (green), 40% (yellow), 10% (red)
2	A	363	34% (green), 33% (yellow), 17% (orange), 15% (grey)
2	B	363	35% (green), 35% (yellow), 14% (orange), 15% (grey)
2	C	363	33% (green), 38% (yellow), 15% (orange), 12% (grey)
3	D	44	7% (green), 14% (yellow), 14% (orange), 64% (grey)
3	E	44	11% (green), 9% (yellow), 14% (orange), 64% (grey)

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Mol	Chain	Length	Quality of chain
3	F	44	 9% 16% 9% . 64%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 7817 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called RNA (5'-R(*UP*CP*UP*UP*AP*UP*AP*UP*CP*U)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	N	10	201	92	28	72	9	0	0	0

- Molecule 2 is a protein called PROTEIN (BLACK BEETLE VIRUS CAPSID PROTEIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	A	308	2311	1478	385	438	10	0	0	0
2	B	308	2311	1478	385	438	10	0	0	0
2	C	321	2406	1536	402	458	10	0	0	0

- Molecule 3 is a protein called PROTEIN (BLACK BEETLE VIRUS CAPSID PROTEIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	D	16	125	80	22	22	1	0	0	0
3	E	16	125	80	22	22	1	0	0	0
3	F	16	125	80	22	22	1	0	0	0

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	2	Total Ca 2 2	0	0
4	B	1	Total Ca 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	2	Total 2	Ca 2	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	68	Total 68	O 68	0	0
5	D	1	Total 1	O 1	0	0
5	B	70	Total 70	O 70	0	0
5	C	65	Total 65	O 65	0	0
5	F	4	Total 4	O 4	0	0

Chain F:  9% 16% 9% . 64%

A364	S365	M366	V367	E368	R369	V370	K371	I372	I373	S376	S377	L378	A379	MET	ALA	SER	ASN	VAL	PRO	GLY	PRO	ILE	GLY	ILE	ALA	ALA	SER	GLY	LEU	SER	GLY	LEU	SER	ALA	LEU	PHE	GLU	GLY	PHE	GLY	PHE
------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 42 3 2	Depositor
Cell constants a, b, c, α , β , γ	362.00Å 362.00Å 362.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 2.80	Depositor
% Data completeness (in resolution range)	67.5 (6.00-2.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR, PROLSQ	Depositor
R, R_{free}	0.221 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	7817	wwPDB-VP
Average B, all atoms (Å ²)	12.0	wwPDB-VP

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: CA

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	N	0.90	0/222	1.18	1/342 (0.3%)
2	A	1.09	2/2372 (0.1%)	1.80	48/3249 (1.5%)
2	B	1.09	2/2372 (0.1%)	1.83	36/3249 (1.1%)
2	C	1.09	2/2469 (0.1%)	1.74	36/3384 (1.1%)
3	D	1.04	1/126 (0.8%)	1.56	3/167 (1.8%)
3	E	1.06	1/126 (0.8%)	1.53	3/167 (1.8%)
3	F	1.19	2/126 (1.6%)	1.85	2/167 (1.2%)
All	All	1.09	10/7813 (0.1%)	1.77	129/10725 (1.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	363	ASN	CA-C	-10.53	1.30	1.52
3	F	364	ALA	CA-CB	8.02	1.79	1.52
2	C	316	TRP	NE1-CE2	-5.65	1.31	1.37
2	A	316	TRP	NE1-CE2	-5.59	1.31	1.37
2	B	191	TRP	NE1-CE2	-5.58	1.31	1.37
3	E	367	TRP	NE1-CE2	-5.56	1.31	1.37
3	D	367	TRP	NE1-CE2	-5.54	1.31	1.37
2	A	124	TRP	NE1-CE2	-5.49	1.31	1.37
2	B	291	TRP	NE1-CE2	-5.43	1.31	1.37
3	F	367	TRP	NE1-CE2	-5.35	1.31	1.37

All (129) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	364	ALA	N-CA-CB	-12.46	91.71	110.40
2	B	144	ASN	CA-CB-CG	10.74	123.34	112.60
2	B	101	GLN	OE1-CD-NE2	9.13	131.73	122.60
2	B	145	PHE	CA-CB-CG	8.99	122.79	113.80
2	C	55	ALA	O-C-N	8.63	136.81	123.00
2	A	58	ARG	O-C-N	8.17	130.59	121.93
2	C	55	ALA	CB-CA-C	-8.08	98.38	110.50
2	A	352	ARG	CD-NE-CZ	7.90	135.46	124.40
2	A	332	PHE	CA-CB-CG	7.82	121.62	113.80
2	A	229	ASP	CA-C-O	-7.82	112.79	120.92
2	B	309	ASN	CA-CB-CG	7.78	120.38	112.60
3	D	364	ALA	O-C-N	7.55	135.07	123.00
2	C	335	ASP	CA-CB-CG	7.39	119.99	112.60
2	C	309	ASN	CA-CB-CG	7.38	119.98	112.60
2	B	145	PHE	N-CA-C	-7.33	100.53	110.36
2	A	86	ASP	CA-CB-CG	7.26	119.86	112.60
2	A	229	ASP	CA-CB-CG	7.14	119.74	112.60
2	C	208	PRO	N-CA-C	-7.14	104.55	113.84
2	B	154	ASN	CA-CB-CG	-7.14	105.46	112.60
2	C	229	ASP	CA-CB-CG	7.04	119.64	112.60
2	C	291	TRP	CB-CA-C	7.01	120.61	111.42
2	C	267	VAL	CA-C-O	-6.96	113.36	120.25
2	A	335	ASP	CA-C-O	-6.96	113.01	121.36
2	C	348	ARG	NE-CZ-NH2	6.95	125.45	119.20
2	B	285	VAL	CB-CA-C	6.94	117.97	111.30
2	C	84	ILE	CA-C-O	6.90	122.98	119.12
2	A	320	GLU	CA-C-O	-6.83	112.99	120.30
2	A	58	ARG	N-CA-C	-6.80	104.30	114.64
2	B	63	GLY	N-CA-C	-6.77	104.60	112.73
2	B	210	THR	O-C-N	6.71	130.42	121.83
2	A	104	ASN	OD1-CG-ND2	6.70	129.30	122.60
2	A	87	ARG	CD-NE-CZ	-6.65	115.09	124.40
2	C	145	PHE	N-CA-C	-6.63	101.14	110.29
2	C	207	THR	O-C-N	-6.63	113.69	121.32
2	C	56	LEU	N-CA-C	-6.59	102.47	111.56
2	B	66	PHE	CA-CB-CG	6.52	120.32	113.80
2	B	332	PHE	N-CA-C	-6.50	104.59	113.30
2	A	262	LEU	O-C-N	-6.44	112.55	121.12
2	C	137	THR	CA-CB-OG1	-6.38	100.03	109.60
2	A	193	CYS	O-C-N	6.37	127.28	121.80
2	B	308	VAL	CB-CA-C	6.34	118.95	111.59
2	B	334	HIS	CA-CB-CG	6.31	120.11	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	92	VAL	N-CA-CB	-6.31	100.83	111.23
2	C	262	LEU	O-C-N	-6.28	114.10	121.32
2	C	145	PHE	CA-CB-CG	6.23	120.03	113.80
2	B	128	VAL	O-C-N	6.20	126.06	121.72
2	B	128	VAL	N-CA-CB	-6.16	105.10	111.87
2	C	267	VAL	O-C-N	6.10	129.31	123.03
2	C	144	ASN	CA-CB-CG	6.06	118.66	112.60
2	C	163	VAL	N-CA-CB	-6.06	102.67	111.52
2	B	208	PRO	N-CA-C	-6.03	106.01	113.84
2	C	88	PHE	CA-CB-CG	5.92	119.72	113.80
2	A	79	ASP	O-C-N	5.87	128.07	121.32
2	C	26	PRO	O-C-N	5.87	129.38	122.98
2	A	191	TRP	CA-CB-CG	5.84	124.69	113.60
2	C	255	ILE	N-CA-C	-5.82	102.07	109.58
2	C	159	ARG	N-CA-C	5.81	119.46	112.38
2	B	90	GLY	O-C-N	5.80	128.57	122.59
2	A	154	ASN	CA-CB-CG	-5.80	106.80	112.60
2	B	168	TYR	O-C-N	5.77	129.86	123.16
2	B	200	VAL	O-C-N	5.76	129.42	123.20
2	C	208	PRO	O-C-N	5.75	129.95	122.24
2	A	337	PRO	O-C-N	5.74	123.95	121.31
2	B	184	PHE	CA-CB-CG	-5.74	108.06	113.80
2	B	169	ALA	N-CA-C	-5.73	106.92	114.31
2	A	93	VAL	N-CA-C	-5.71	100.26	108.48
2	A	153	GLY	O-C-N	5.69	128.31	122.90
2	B	178	THR	N-CA-CB	-5.69	103.47	110.98
2	B	111	THR	O-C-N	5.65	129.66	123.22
2	B	208	PRO	O-C-N	5.64	129.80	122.24
2	C	106	THR	CA-CB-OG1	-5.62	101.16	109.60
2	A	215	HIS	CA-CB-CG	5.62	119.42	113.80
2	A	208	PRO	N-CA-C	-5.60	106.76	113.98
2	B	187	SER	O-C-N	5.58	129.51	123.10
2	A	115	ILE	CB-CA-C	5.58	119.45	111.81
2	C	195	VAL	CA-C-O	-5.57	114.21	120.95
2	A	233	GLU	CB-CG-CD	5.55	122.04	112.60
2	B	312	ILE	N-CA-CB	5.52	118.31	111.41
2	C	95	ARG	NE-CZ-NH2	5.52	124.17	119.20
2	C	102	SER	CA-C-O	-5.51	114.76	121.05
2	B	154	ASN	OD1-CG-ND2	5.51	128.11	122.60
2	A	233	GLU	CA-CB-CG	5.49	125.09	114.10
2	A	104	ASN	CA-C-O	-5.48	114.59	120.46
2	B	261	THR	O-C-N	5.47	129.61	123.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	358	VAL	O-C-N	5.43	129.19	123.00
2	A	58	ARG	NE-CZ-NH2	5.42	124.07	119.20
3	E	378	LEU	N-CA-C	-5.39	105.33	112.94
2	B	109	ARG	NE-CZ-NH2	5.39	124.05	119.20
2	B	332	PHE	CA-CB-CG	5.38	119.18	113.80
2	A	355	PRO	CA-C-O	-5.37	115.20	122.08
3	D	369	ARG	NE-CZ-NH2	5.37	124.03	119.20
3	E	369	ARG	NE-CZ-NH2	5.36	124.02	119.20
2	A	337	PRO	CA-C-N	5.33	125.31	120.03
2	A	337	PRO	C-N-CA	5.33	125.31	120.03
2	C	312	ILE	N-CA-CB	5.33	117.44	111.21
2	B	243	SER	N-CA-C	-5.32	102.03	109.69
3	F	369	ARG	NE-CZ-NH2	5.31	123.98	119.20
2	B	200	VAL	CA-C-O	-5.29	114.75	120.36
2	B	98	VAL	O-C-N	5.26	128.73	123.10
2	B	322	ARG	NE-CZ-NH2	5.25	123.93	119.20
2	C	191	TRP	CA-CB-CG	5.25	123.57	113.60
2	C	352	ARG	NE-CZ-NH2	5.24	123.92	119.20
2	A	280	ALA	N-CA-C	-5.24	105.63	112.23
2	A	187	SER	N-CA-C	5.22	115.94	108.74
2	A	179	SER	N-CA-C	-5.19	104.03	110.41
2	A	82	LYS	CA-C-O	-5.17	115.82	121.20
2	A	352	ARG	CA-C-O	-5.14	114.97	120.42
2	C	22	THR	O-C-N	5.14	129.08	123.01
2	A	320	GLU	O-C-N	5.13	129.23	123.27
2	A	332	PHE	N-CA-C	-5.13	107.05	113.72
3	E	378	LEU	O-C-N	5.13	128.40	122.19
2	C	149	ASN	O-C-N	5.12	128.21	122.22
2	A	356	VAL	O-C-N	5.11	127.03	121.87
2	A	268	THR	N-CA-CB	5.10	117.53	109.83
2	A	359	ILE	N-CA-C	-5.10	104.44	110.21
2	A	362	GLN	CB-CA-C	-5.09	102.75	111.46
2	C	180	ASN	CB-CA-C	5.09	118.74	109.83
2	A	336	SER	N-CA-C	-5.09	103.37	109.83
2	A	312	ILE	N-CA-C	-5.08	100.43	107.80
2	A	112	PHE	O-C-N	5.08	129.26	123.27
3	D	364	ALA	N-CA-C	5.07	125.19	111.00
2	C	58	ARG	NE-CZ-NH2	5.06	123.76	119.20
2	A	208	PRO	O-C-N	5.06	129.61	122.37
1	N	7	A	C1'-C2'-O2'	5.04	115.96	108.40
2	A	87	ARG	NE-CZ-NH1	-5.04	116.46	121.50
2	C	109	ARG	NE-CZ-NH2	5.02	123.72	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	116	ALA	CA-C-O	-5.00	115.32	120.87
2	B	337	PRO	CA-C-N	5.00	125.27	119.92
2	B	337	PRO	C-N-CA	5.00	125.27	119.92

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	58	ARG	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	N	201	0	106	34	0
2	A	2311	0	2262	217	0
2	B	2311	0	2262	197	0
2	C	2406	0	2357	249	0
3	D	125	0	135	20	0
3	E	125	0	135	19	0
3	F	125	0	135	12	0
4	A	2	0	0	0	0
4	B	1	0	0	0	0
4	C	2	0	0	0	0
5	A	68	0	0	7	0
5	B	70	0	0	12	0
5	C	65	0	0	13	0
5	D	1	0	0	0	0
5	F	4	0	0	0	0
All	All	7817	0	7392	695	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 46.

All (695) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:364:ALA:CB	3:F:364:ALA:CA	1.79	1.58
2:B:207:THR:CG2	2:B:208:PRO:HD3	1.36	1.52
2:C:21:GLN:HG3	2:C:181:LEU:CD1	1.40	1.48
2:C:21:GLN:CG	2:C:181:LEU:HD11	1.54	1.36
2:C:264:PRO:O	2:C:267:VAL:HG13	1.22	1.32
5:B:429:HOH:O	2:C:215:HIS:HE1	0.97	1.30
2:B:279:ALA:HB1	5:B:414:HOH:O	1.27	1.26
1:N:4:U:O2'	1:N:5:A:C5'	1.87	1.23
2:A:129:PRO:O	2:A:132:THR:HG23	1.07	1.22
2:B:207:THR:HG23	2:B:208:PRO:CD	1.70	1.22
2:B:207:THR:CG2	2:B:208:PRO:CD	2.19	1.21
2:C:206:THR:O	2:C:209:ALA:HA	1.44	1.16
3:E:368:GLU:OE2	3:E:371:LYS:NZ	1.80	1.15
2:C:20:THR:C	2:C:21:GLN:NE2	2.06	1.13
2:C:207:THR:HG22	2:C:208:PRO:HD3	1.22	1.13
2:B:159:ARG:HG3	2:B:289:VAL:HG12	1.30	1.13
1:N:2:C:N3	1:N:3:U:C5	2.15	1.12
2:B:207:THR:HG22	2:B:208:PRO:HD3	1.27	1.13
1:N:2:C:C2	1:N:3:U:C5	2.36	1.12
2:B:254:ASP:OD2	5:B:366:HOH:O	1.63	1.12
3:E:368:GLU:CD	3:E:371:LYS:NZ	2.08	1.11
3:E:368:GLU:OE1	3:E:371:LYS:NZ	1.84	1.11
2:A:129:PRO:HB2	2:A:132:THR:HG21	1.19	1.10
1:N:4:U:O2'	1:N:5:A:H5'	0.91	1.09
2:C:20:THR:HA	2:C:21:GLN:NE2	1.66	1.09
2:C:25:VAL:CG1	2:C:27:GLN:NE2	2.16	1.08
1:N:2:C:O2	1:N:3:U:C6	2.07	1.08
2:A:217:LEU:HD22	2:A:262:LEU:HD23	1.36	1.08
2:C:100:ASN:ND2	2:C:314:LYS:HE2	1.68	1.08
2:C:25:VAL:HG13	2:C:27:GLN:NE2	1.70	1.07
2:C:206:THR:O	2:C:209:ALA:CA	2.01	1.06
2:C:20:THR:CA	2:C:21:GLN:NE2	2.20	1.05
2:C:21:GLN:CG	2:C:181:LEU:CD1	2.23	1.04
2:A:129:PRO:O	2:A:132:THR:CG2	2.04	1.04
3:E:368:GLU:CD	3:E:371:LYS:HZ2	1.62	1.04
1:N:2:C:C2	1:N:3:U:C6	2.46	1.04
2:C:264:PRO:O	2:C:267:VAL:CG1	2.04	1.03
2:B:245:CYS:HA	2:B:294:MET:HE2	1.37	1.02
1:N:5:A:C2'	1:N:6:U:H5'	1.90	1.02
2:A:57:THR:HG23	2:A:57:THR:O	1.58	1.01
3:E:368:GLU:OE1	3:E:368:GLU:HA	1.59	1.01
2:C:21:GLN:HE21	2:C:21:GLN:N	1.57	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:204:VAL:HG22	2:B:210:THR:OG1	1.59	1.01
2:A:129:PRO:HB2	2:A:132:THR:CG2	1.91	1.00
2:C:20:THR:C	2:C:21:GLN:HE21	1.66	0.99
2:C:362:GLN:O	5:C:430:HOH:O	1.80	0.99
2:C:25:VAL:CG1	2:C:27:GLN:HE22	1.76	0.98
5:B:429:HOH:O	2:C:215:HIS:CE1	1.83	0.97
2:A:207:THR:HB	2:A:208:PRO:HD3	1.45	0.97
2:A:129:PRO:C	2:A:132:THR:HG23	1.89	0.97
2:B:264:PRO:O	2:B:267:VAL:HG13	1.67	0.95
2:A:122:ALA:HB1	2:A:315:THR:HG21	1.48	0.94
2:A:75:ASP:OD1	2:A:363:ASN:OXT	1.84	0.94
2:B:207:THR:HG23	2:B:208:PRO:HD3	0.98	0.94
2:A:61:GLN:NE2	2:A:62:PRO:HD3	1.83	0.94
2:A:217:LEU:CD2	2:A:262:LEU:HD23	1.98	0.93
2:B:167:ARG:HD2	2:B:252:PHE:CE1	2.03	0.93
2:A:354:LEU:CD2	3:D:366:MET:HE1	1.98	0.93
2:C:82:LYS:O	2:C:94:THR:HG21	1.68	0.93
2:B:263:PRO:HD2	2:B:277:ASN:HB2	1.48	0.92
2:C:362:GLN:HB3	5:C:430:HOH:O	1.67	0.92
2:A:354:LEU:HD22	3:D:366:MET:HE1	1.51	0.92
2:C:21:GLN:HG3	2:C:181:LEU:HD11	0.93	0.92
2:C:207:THR:HG22	2:C:208:PRO:CD	2.01	0.91
2:C:115:ILE:HG12	2:C:173:VAL:CG1	2.00	0.91
2:B:324:ASN:HB3	2:B:326:ASN:ND2	1.86	0.89
1:N:4:U:HO2'	1:N:5:A:H5'	1.25	0.89
3:F:364:ALA:CB	3:F:364:ALA:N	2.35	0.89
2:C:100:ASN:ND2	2:C:314:LYS:CE	2.36	0.89
2:A:353:SER:HB2	3:D:373:ILE:HD13	1.54	0.89
2:A:56:LEU:HD12	2:A:56:LEU:N	1.86	0.89
2:B:63:GLY:HA3	2:B:340:ASP:OD2	1.73	0.89
2:C:170:SER:HA	5:C:372:HOH:O	1.73	0.89
2:B:279:ALA:CB	5:B:414:HOH:O	1.97	0.88
2:C:154:ASN:HD22	2:C:154:ASN:H	1.18	0.88
2:A:57:THR:O	2:A:57:THR:CG2	2.18	0.88
2:B:245:CYS:HA	2:B:294:MET:CE	2.03	0.87
2:C:21:GLN:HG3	2:C:181:LEU:HD13	1.50	0.87
2:A:61:GLN:HB2	2:A:62:PRO:HD3	1.53	0.87
2:B:324:ASN:HB3	2:B:326:ASN:HD21	1.40	0.87
1:N:4:U:C2'	1:N:5:A:H5'	2.05	0.87
2:C:82:LYS:HE3	2:C:334:HIS:ND1	1.89	0.87
2:B:268:THR:HG22	2:B:271:THR:H	1.39	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:339:CYS:SG	5:A:421:HOH:O	2.33	0.86
2:A:56:LEU:O	2:A:58:ARG:N	2.06	0.86
2:B:57:THR:O	2:B:57:THR:HG22	1.75	0.85
2:C:98:VAL:HG13	2:C:316:TRP:CD1	2.12	0.85
2:B:352:ARG:NH2	5:B:433:HOH:O	2.09	0.85
2:A:162:GLN:HE21	2:A:327:ALA:CB	1.89	0.84
2:C:68:LYS:HD3	2:C:76:PHE:CZ	2.12	0.84
2:C:108:ASN:HB2	2:C:305:THR:HG22	1.59	0.84
1:N:5:A:H2'	1:N:6:U:H5'	1.57	0.84
2:C:160:SER:HB3	2:C:255:ILE:HG21	1.59	0.84
3:D:367:TRP:NE1	3:D:371:LYS:HD2	1.93	0.84
2:C:206:THR:O	2:C:209:ALA:N	2.10	0.84
2:A:61:GLN:HE21	2:A:62:PRO:HD3	1.40	0.83
2:B:213:LEU:HD23	2:C:213:LEU:HD23	1.61	0.82
2:C:20:THR:HA	2:C:21:GLN:HE22	1.39	0.82
2:C:68:LYS:HD3	2:C:76:PHE:CE1	2.14	0.82
3:E:368:GLU:OE1	3:E:371:LYS:CE	2.27	0.82
2:B:217:LEU:HD22	2:B:262:LEU:HD23	1.61	0.82
2:B:229:ASP:OD2	2:C:91:LYS:HE2	1.78	0.81
2:A:87:ARG:HH11	2:C:345:GLN:NE2	1.79	0.81
2:A:228:PRO:HG2	2:B:330:TYR:CD1	2.17	0.80
2:C:282:ALA:HB3	2:C:285:VAL:HG23	1.64	0.80
2:A:204:VAL:HG22	2:A:205:ALA:H	1.45	0.79
2:A:207:THR:HB	2:A:208:PRO:CD	2.11	0.79
2:A:99:LEU:HB3	2:A:315:THR:HG22	1.64	0.79
2:B:207:THR:HG22	2:B:208:PRO:CD	1.96	0.79
2:C:337:PRO:O	5:C:377:HOH:O	2.02	0.78
2:B:314:LYS:HE2	2:B:316:TRP:CZ2	2.18	0.78
2:A:183:GLN:HB2	2:A:308:VAL:HB	1.64	0.78
2:B:93:VAL:HG12	2:B:333:GLY:HA2	1.66	0.78
2:B:247:GLU:O	2:B:348:ARG:NH2	2.18	0.77
2:A:326:ASN:H	2:A:326:ASN:HD22	1.33	0.77
2:B:57:THR:O	2:B:57:THR:CG2	2.32	0.76
2:B:179:SER:HB3	2:B:183:GLN:HG3	1.67	0.76
2:C:21:GLN:CB	2:C:181:LEU:HD11	2.15	0.76
1:N:8:U:O2'	1:N:9:C:H5'	1.85	0.76
1:N:5:A:O2'	1:N:6:U:H5'	1.86	0.75
2:C:25:VAL:HG12	2:C:27:GLN:NE2	1.99	0.75
2:A:172:ASN:ND2	2:A:242:GLN:HB3	2.02	0.75
2:A:61:GLN:NE2	5:A:367:HOH:O	2.20	0.75
2:B:60:SER:HB2	2:B:62:PRO:HD2	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:233:GLU:HG3	2:B:237:LYS:HD2	1.67	0.75
2:A:109:ARG:HH21	2:A:128:VAL:HA	1.51	0.74
1:N:3:U:H2'	1:N:3:U:O2	1.88	0.74
2:A:182:MET:O	2:A:182:MET:HG3	1.85	0.74
2:C:68:LYS:CD	2:C:76:PHE:CZ	2.70	0.74
2:A:105:PHE:CE2	2:A:301:VAL:HG21	2.22	0.74
3:F:369:ARG:O	3:F:373:ILE:HG13	1.87	0.74
2:A:324:ASN:HB3	2:A:326:ASN:HD21	1.52	0.74
2:C:29:ASN:N	2:C:77:ASN:OD1	2.20	0.74
2:B:206:THR:HG23	2:B:208:PRO:HD2	1.67	0.74
2:C:99:LEU:O	2:C:314:LYS:HA	1.87	0.73
2:A:106:THR:CG2	2:A:109:ARG:HG3	2.18	0.73
2:C:154:ASN:H	2:C:154:ASN:ND2	1.86	0.73
2:A:56:LEU:N	2:A:56:LEU:CD1	2.51	0.73
2:A:84:ILE:HD12	2:A:167:ARG:HD3	1.71	0.73
2:C:108:ASN:CB	2:C:305:THR:HG22	2.19	0.73
2:A:201:GLN:NE2	2:B:264:PRO:HB3	2.04	0.72
2:C:20:THR:O	2:C:181:LEU:HD13	1.90	0.72
2:C:108:ASN:CG	2:C:305:THR:HG22	2.14	0.72
2:A:159:ARG:HD3	2:A:289:VAL:HG12	1.71	0.72
2:B:61:GLN:HA	2:B:61:GLN:NE2	2.02	0.72
2:A:156:ALA:HB1	2:A:258:GLY:HA2	1.71	0.72
2:C:20:THR:C	2:C:21:GLN:CD	2.58	0.72
2:B:199:ASN:OD1	5:B:429:HOH:O	2.08	0.71
2:C:72:ALA:HB1	2:C:75:ASP:OD2	1.89	0.71
2:A:162:GLN:HE21	2:A:327:ALA:HB1	1.56	0.70
2:A:169:ALA:O	5:A:420:HOH:O	2.08	0.70
2:C:25:VAL:HG13	2:C:27:GLN:HE22	1.38	0.70
3:F:366:MET:O	3:F:370:VAL:HG23	1.90	0.70
2:A:87:ARG:NH1	2:C:345:GLN:NE2	2.39	0.70
2:C:286:SER:OG	2:C:287:GLY:N	2.23	0.70
2:A:207:THR:C	2:A:209:ALA:H	1.96	0.70
3:D:367:TRP:CE2	3:D:371:LYS:HD2	2.26	0.70
2:C:135:ILE:HG13	2:C:137:THR:H	1.56	0.70
1:N:3:U:N3	1:N:4:U:C5	2.60	0.70
2:A:200:VAL:HG12	2:A:214:VAL:HG12	1.73	0.70
2:B:206:THR:HG23	2:B:207:THR:H	1.56	0.70
3:E:368:GLU:OE1	3:E:371:LYS:HE3	1.90	0.70
2:B:206:THR:CG2	2:B:208:PRO:HD2	2.21	0.70
2:C:55:ALA:N	2:C:57:THR:HB	2.07	0.70
2:C:160:SER:HB3	2:C:255:ILE:CG2	2.21	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:377:SER:O	3:D:378:LEU:HD23	1.92	0.69
2:A:106:THR:HG22	2:A:109:ARG:HG3	1.72	0.69
2:A:322:ARG:HH22	2:C:295:ASP:CG	1.99	0.69
2:A:324:ASN:HB3	2:A:326:ASN:ND2	2.08	0.69
2:A:163:VAL:HG11	2:A:321:TYR:CD1	2.27	0.69
2:C:25:VAL:CG1	2:C:27:GLN:HE21	2.02	0.69
2:B:246:ASN:HD22	2:B:247:GLU:HG2	1.58	0.69
2:B:341:GLU:OE1	2:B:341:GLU:HA	1.93	0.69
2:C:231:PHE:CG	2:C:357:ALA:HB3	2.29	0.68
2:B:163:VAL:HG11	2:B:321:TYR:CD1	2.28	0.68
2:A:331:GLN:CA	2:A:331:GLN:HE21	2.05	0.68
2:A:207:THR:C	2:A:209:ALA:N	2.48	0.68
2:C:167:ARG:NH1	2:C:320:GLU:OE1	2.25	0.68
2:B:85:PRO:HB2	2:B:340:ASP:HB3	1.76	0.68
2:B:207:THR:HG23	2:B:208:PRO:N	2.08	0.68
2:C:156:ALA:HB1	2:C:258:GLY:HA2	1.76	0.68
2:C:115:ILE:HG12	2:C:173:VAL:HG13	1.77	0.67
2:A:204:VAL:HG22	2:A:205:ALA:N	2.09	0.67
3:D:367:TRP:HE1	3:D:371:LYS:NZ	1.92	0.67
2:C:115:ILE:HG12	2:C:173:VAL:HG11	1.77	0.67
2:A:165:SER:OG	2:C:196:LYS:HE3	1.95	0.67
2:B:206:THR:HG23	2:B:207:THR:N	2.10	0.67
2:B:246:ASN:HD22	2:B:246:ASN:C	2.02	0.67
2:B:340:ASP:C	2:B:340:ASP:OD1	2.36	0.67
2:A:208:PRO:CG	2:B:206:THR:HA	2.26	0.66
2:A:61:GLN:HB2	2:A:62:PRO:CD	2.24	0.66
2:C:135:ILE:CG1	2:C:137:THR:HB	2.25	0.66
1:N:2:C:O2	1:N:3:U:H6	1.77	0.66
2:B:56:LEU:HD23	3:E:374:ILE:HG21	1.76	0.66
3:E:374:ILE:O	3:E:378:LEU:HB2	1.95	0.66
2:C:88:PHE:O	5:C:377:HOH:O	2.12	0.66
2:C:139:THR:HG21	5:C:416:HOH:O	1.95	0.66
2:B:217:LEU:HB3	2:B:220:LEU:HD22	1.78	0.65
3:F:365:SER:OG	3:F:368:GLU:HB2	1.96	0.65
2:A:354:LEU:HD22	3:D:366:MET:CE	2.27	0.65
2:A:246:ASN:C	2:A:246:ASN:HD22	2.03	0.65
2:A:155:ALA:HA	2:A:283:GLU:HG3	1.79	0.65
2:C:82:LYS:HE3	2:C:334:HIS:CE1	2.31	0.65
2:A:313:LEU:C	2:A:313:LEU:HD23	2.23	0.64
3:E:367:TRP:O	3:E:371:LYS:HB2	1.97	0.64
2:C:172:ASN:HD22	2:C:242:GLN:HB3	1.61	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:124:TRP:CZ3	2:C:142:ALA:HB2	2.32	0.64
2:C:265:ALA:O	2:C:267:VAL:HG12	1.98	0.64
2:B:84:ILE:CD1	2:B:167:ARG:HG3	2.28	0.64
2:A:61:GLN:NE2	2:A:62:PRO:CD	2.59	0.64
2:A:295:ASP:CG	2:B:322:ARG:HH22	2.05	0.64
3:E:366:MET:HE1	3:E:369:ARG:HD2	1.78	0.64
2:C:20:THR:CA	2:C:21:GLN:HE21	1.98	0.64
2:C:256:LEU:HD12	2:C:290:GLY:HA2	1.79	0.64
2:C:108:ASN:CG	2:C:305:THR:CG2	2.71	0.63
2:B:293:ASN:O	2:B:294:MET:HE2	1.97	0.63
2:C:25:VAL:HG12	2:C:27:GLN:HE21	1.59	0.63
2:C:100:ASN:CG	2:C:314:LYS:HE2	2.22	0.63
2:A:167:ARG:HD2	2:A:320:GLU:OE1	1.99	0.63
2:C:329:LEU:HD12	2:C:330:TYR:N	2.13	0.63
2:A:331:GLN:HE21	2:A:331:GLN:N	1.97	0.63
2:B:183:GLN:HB2	2:B:308:VAL:HG13	1.80	0.63
2:B:327:ALA:HB1	2:B:329:LEU:HD22	1.81	0.63
2:C:282:ALA:HB3	2:C:285:VAL:CG2	2.28	0.63
2:C:207:THR:C	2:C:209:ALA:N	2.55	0.63
2:C:303:ALA:HB2	2:C:309:ASN:ND2	2.14	0.63
2:A:264:PRO:O	2:A:267:VAL:HG13	1.98	0.62
2:C:246:ASN:HD22	2:C:247:GLU:HG2	1.64	0.62
2:C:135:ILE:HG13	2:C:137:THR:HB	1.80	0.62
2:A:109:ARG:HH21	2:A:128:VAL:CA	2.12	0.62
2:B:245:CYS:CA	2:B:294:MET:CE	2.76	0.62
2:A:162:GLN:HG3	2:A:329:LEU:HD13	1.82	0.62
2:C:61:GLN:HB2	2:C:62:PRO:HD3	1.81	0.62
2:B:124:TRP:CZ3	2:B:142:ALA:HB2	2.35	0.62
2:A:185:ALA:H	2:A:309:ASN:HD21	1.46	0.62
2:A:264:PRO:HG2	2:A:267:VAL:HG11	1.82	0.62
1:N:2:C:N3	1:N:3:U:C4	2.68	0.61
2:A:206:THR:HG22	2:C:208:PRO:HG2	1.82	0.61
2:A:106:THR:HG22	2:A:109:ARG:CG	2.30	0.61
2:C:154:ASN:HD22	2:C:154:ASN:N	1.83	0.61
2:A:206:THR:O	2:A:209:ALA:HA	2.00	0.61
2:A:104:ASN:ND2	2:A:310:SER:HB3	2.14	0.61
3:D:367:TRP:HA	3:D:370:VAL:HG13	1.81	0.61
2:B:65:ALA:CB	2:B:82:LYS:HD3	2.31	0.61
2:B:206:THR:CG2	2:B:207:THR:N	2.63	0.61
2:B:321:TYR:O	2:B:323:PRO:HD3	2.00	0.61
2:B:204:VAL:CG2	2:B:210:THR:OG1	2.43	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:80:PRO:O	2:B:81:GLY:O	2.18	0.61
2:C:81:GLY:O	2:C:96:LYS:NZ	2.33	0.60
1:N:5:A:H2'	1:N:6:U:C5'	2.29	0.60
2:A:326:ASN:H	2:A:326:ASN:ND2	1.98	0.60
2:C:345:GLN:O	2:C:349:THR:HG23	2.01	0.60
2:B:263:PRO:CD	2:B:277:ASN:HB2	2.26	0.60
2:A:358:VAL:HG22	2:A:362:GLN:OE1	2.01	0.60
2:A:67:LEU:HD13	3:D:374:ILE:HD11	1.84	0.60
2:A:259:ILE:HG22	2:A:288:ILE:HB	1.82	0.60
2:B:80:PRO:O	2:B:81:GLY:C	2.44	0.60
2:B:93:VAL:HG13	2:B:323:PRO:HG3	1.84	0.60
2:B:172:ASN:OD1	2:B:242:GLN:CG	2.50	0.60
2:B:224:LEU:HD11	2:B:275:PRO:HB3	1.84	0.60
2:A:359:ILE:HD11	2:A:362:GLN:HG3	1.83	0.60
3:E:366:MET:O	3:E:370:VAL:HG23	2.01	0.60
2:C:135:ILE:HD11	2:C:137:THR:HB	1.82	0.60
2:A:200:VAL:CG1	2:A:214:VAL:HG12	2.31	0.60
2:B:326:ASN:H	2:B:326:ASN:HD22	1.49	0.60
2:C:21:GLN:NE2	2:C:21:GLN:N	2.34	0.60
2:A:329:LEU:HD23	2:A:329:LEU:C	2.27	0.59
1:N:7:A:H2'	1:N:8:U:H5'	1.84	0.59
2:A:61:GLN:CB	2:A:62:PRO:HD3	2.28	0.59
2:A:123:TYR:CE2	2:A:125:VAL:HG22	2.37	0.59
1:N:2:C:H2'	1:N:3:U:H6	1.68	0.59
2:B:104:ASN:OD1	2:B:310:SER:HB3	2.02	0.59
2:A:331:GLN:N	2:A:331:GLN:NE2	2.50	0.59
2:A:121:VAL:HA	2:A:144:ASN:HA	1.82	0.59
2:A:232:SER:O	2:A:233:GLU:HB2	2.01	0.59
1:N:1:U:H2'	1:N:1:U:O2	2.01	0.59
2:A:204:VAL:CG2	2:A:205:ALA:H	2.13	0.59
2:B:323:PRO:HB2	2:B:330:TYR:CD2	2.38	0.59
2:C:168:TYR:HB3	2:C:294:MET:HE2	1.85	0.59
3:F:364:ALA:CB	3:F:364:ALA:C	2.73	0.59
2:A:206:THR:HA	2:C:208:PRO:CG	2.32	0.58
2:A:246:ASN:HD22	2:A:247:GLU:HG2	1.68	0.58
2:A:68:LYS:HD2	2:A:76:PHE:CZ	2.38	0.58
2:C:135:ILE:CD1	2:C:137:THR:HB	2.33	0.58
2:C:200:VAL:HG12	2:C:214:VAL:CG2	2.33	0.58
2:B:75:ASP:OD1	2:B:363:ASN:O	2.21	0.58
2:C:363:ASN:O	3:F:365:SER:HA	2.03	0.58
2:C:73:PRO:N	2:C:74:PRO:CD	2.66	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:189:THR:HA	2:A:231:PHE:O	2.02	0.58
1:N:2:C:C2	1:N:3:U:H5	2.14	0.58
2:A:122:ALA:HB1	2:A:315:THR:CG2	2.27	0.58
2:B:185:ALA:O	2:B:304:PRO:HD2	2.04	0.58
2:B:182:MET:HG3	2:B:182:MET:O	2.02	0.57
2:C:20:THR:O	2:C:21:GLN:HG3	2.04	0.57
2:C:200:VAL:CG1	2:C:214:VAL:HG22	2.34	0.57
2:B:167:ARG:HD3	2:B:320:GLU:OE1	2.04	0.57
2:B:268:THR:HG22	2:B:271:THR:N	2.14	0.57
2:B:108:ASN:HB2	2:B:305:THR:OG1	2.03	0.57
2:C:108:ASN:O	2:C:109:ARG:HG2	2.04	0.57
2:C:189:THR:HA	2:C:231:PHE:O	2.05	0.57
2:C:231:PHE:CB	2:C:357:ALA:HB3	2.34	0.57
2:B:172:ASN:OD1	2:B:242:GLN:HG2	2.04	0.57
2:C:117:PRO:HB3	2:C:171:MET:HE1	1.85	0.57
2:C:115:ILE:CD1	2:C:173:VAL:HG11	2.35	0.57
1:N:2:C:C4	1:N:3:U:C5	2.92	0.56
3:D:367:TRP:NE1	3:D:371:LYS:CD	2.66	0.56
2:B:277:ASN:OD1	2:B:277:ASN:C	2.47	0.56
2:A:99:LEU:HB3	2:A:315:THR:CG2	2.35	0.56
2:A:104:ASN:HD22	2:A:310:SER:HB3	1.71	0.56
2:C:82:LYS:HE3	2:C:334:HIS:HD1	1.66	0.56
2:C:197:LEU:CD1	2:C:217:LEU:HD13	2.35	0.56
2:C:206:THR:HG22	2:C:210:THR:N	2.21	0.56
2:A:217:LEU:HB3	2:A:220:LEU:HD22	1.88	0.56
2:C:171:MET:HE3	2:C:294:MET:HG3	1.86	0.56
2:C:167:ARG:HD2	2:C:252:PHE:CE1	2.40	0.56
2:C:206:THR:HG21	2:C:210:THR:HG23	1.86	0.56
2:B:109:ARG:HD2	2:B:128:VAL:O	2.06	0.56
2:C:68:LYS:CD	2:C:76:PHE:CE1	2.88	0.56
2:C:206:THR:HG22	2:C:209:ALA:CA	2.35	0.56
2:C:235:PHE:C	2:C:237:LYS:H	2.14	0.56
2:A:87:ARG:NH1	2:C:345:GLN:HE21	2.04	0.56
2:A:353:SER:HB2	3:D:373:ILE:CD1	2.31	0.55
2:B:188:ILE:O	2:B:232:SER:HA	2.06	0.55
2:C:82:LYS:O	2:C:334:HIS:CE1	2.59	0.55
2:B:170:SER:OG	5:B:404:HOH:O	2.17	0.55
2:A:229:ASP:OD1	5:A:392:HOH:O	2.18	0.55
2:A:144:ASN:N	2:A:144:ASN:HD22	2.05	0.55
2:B:167:ARG:HD2	2:B:252:PHE:CZ	2.41	0.55
2:B:341:GLU:CD	2:C:87:ARG:HH22	2.14	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:73:PRO:CG	2:A:74:PRO:HD3	2.35	0.55
2:A:167:ARG:HG3	2:A:252:PHE:CE2	2.41	0.55
1:N:4:U:C2	1:N:5:A:C2	2.95	0.55
2:A:59:LEU:HD21	2:A:342:VAL:HG12	1.89	0.55
2:C:264:PRO:C	2:C:267:VAL:HG13	2.21	0.55
2:B:246:ASN:ND2	2:B:247:GLU:HG2	2.20	0.55
2:C:139:THR:HB	2:C:277:ASN:HB2	1.89	0.55
2:A:91:LYS:NZ	2:C:229:ASP:OD2	2.34	0.55
2:B:125:VAL:HG22	2:B:126:ALA:N	2.22	0.55
2:B:199:ASN:C	2:B:216:THR:HG22	2.32	0.55
3:E:368:GLU:CD	3:E:371:LYS:HZ1	1.87	0.55
2:C:73:PRO:N	2:C:74:PRO:HD2	2.22	0.55
2:C:246:ASN:C	2:C:247:GLU:HG2	2.32	0.55
2:A:204:VAL:HG13	2:A:206:THR:HG23	1.87	0.54
2:B:176:TYR:HE1	2:B:363:ASN:OD1	1.91	0.54
2:A:201:GLN:HA	2:A:212:ALA:O	2.08	0.54
2:A:263:PRO:HD2	2:A:277:ASN:CG	2.31	0.54
2:A:360:ALA:O	2:A:363:ASN:ND2	2.38	0.54
2:B:68:LYS:HE2	2:B:76:PHE:CE1	2.42	0.54
2:B:88:PHE:CZ	2:B:90:GLY:HA3	2.43	0.54
2:C:197:LEU:HD13	2:C:217:LEU:CD1	2.37	0.54
2:A:181:LEU:HD12	2:A:236:ILE:HG12	1.89	0.54
3:D:366:MET:O	3:D:369:ARG:N	2.36	0.54
2:C:246:ASN:ND2	2:C:293:ASN:HB3	2.23	0.54
2:C:360:ALA:O	2:C:362:GLN:N	2.41	0.54
2:B:196:LYS:O	2:B:218:VAL:HG22	2.08	0.54
2:C:125:VAL:HG22	2:C:126:ALA:N	2.21	0.54
2:C:154:ASN:ND2	2:C:154:ASN:N	2.46	0.54
3:F:367:TRP:NE1	3:F:371:LYS:HD3	2.22	0.54
1:N:3:U:N3	1:N:4:U:H5	2.06	0.54
2:A:81:GLY:O	2:A:96:LYS:HE3	2.08	0.54
2:A:136:SER:HA	2:A:275:PRO:O	2.08	0.54
2:B:207:THR:C	2:B:209:ALA:N	2.64	0.54
2:C:61:GLN:CB	2:C:62:PRO:HD3	2.37	0.54
2:A:244:VAL:C	2:A:294:MET:HE3	2.33	0.54
2:A:359:ILE:CD1	2:A:362:GLN:HG3	2.38	0.54
2:B:67:LEU:HD13	3:E:374:ILE:HD11	1.90	0.54
2:B:348:ARG:HG2	2:C:87:ARG:O	2.08	0.54
2:A:162:GLN:HA	2:A:162:GLN:NE2	2.23	0.53
2:A:58:ARG:HD3	3:D:378:LEU:HD13	1.90	0.53
2:A:96:LYS:HD3	2:A:318:CYS:SG	2.48	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:366:MET:O	3:D:369:ARG:HB3	2.08	0.53
2:B:340:ASP:OD2	2:B:343:ALA:HB2	2.09	0.53
2:A:235:PHE:CZ	2:A:309:ASN:HB3	2.44	0.53
2:B:136:SER:HA	2:B:275:PRO:O	2.08	0.53
2:C:70:ALA:HA	2:C:170:SER:HB2	1.89	0.53
2:A:322:ARG:NH2	2:C:295:ASP:CG	2.67	0.53
2:B:56:LEU:CD2	3:E:374:ILE:HG21	2.37	0.53
2:A:247:GLU:HB3	2:A:248:PRO:HD2	1.91	0.53
2:B:60:SER:OG	2:B:340:ASP:OD2	2.27	0.53
3:E:373:ILE:O	3:E:376:SER:HB3	2.08	0.53
2:C:20:THR:C	2:C:21:GLN:CG	2.82	0.53
2:B:94:THR:HG22	2:B:320:GLU:HG2	1.91	0.53
2:C:236:ILE:HG13	2:C:236:ILE:O	2.09	0.53
2:A:173:VAL:HG11	2:A:299:ILE:HD11	1.91	0.52
2:B:61:GLN:N	2:B:62:PRO:CD	2.71	0.52
2:C:181:LEU:CD2	2:C:236:ILE:HG12	2.38	0.52
2:C:280:ALA:CB	2:C:287:GLY:HA2	2.39	0.52
2:C:72:ALA:C	2:C:74:PRO:HD2	2.34	0.52
2:C:200:VAL:O	2:C:200:VAL:HG13	2.08	0.52
2:A:106:THR:HG21	2:A:109:ARG:HG3	1.92	0.52
2:A:145:PHE:HE1	2:A:315:THR:O	1.92	0.52
2:C:93:VAL:HG22	2:C:93:VAL:O	2.09	0.52
2:A:61:GLN:CB	2:A:62:PRO:CD	2.85	0.52
2:A:207:THR:O	2:A:209:ALA:N	2.43	0.52
2:A:163:VAL:HG11	2:A:321:TYR:HD1	1.75	0.52
2:A:194:PRO:HB3	2:B:322:ARG:CZ	2.40	0.52
2:B:263:PRO:HD3	2:B:274:GLN:NE2	2.24	0.52
2:C:200:VAL:HG12	2:C:214:VAL:HG22	1.92	0.52
2:A:180:ASN:OD1	2:A:183:GLN:HG2	2.11	0.51
2:C:197:LEU:HD13	2:C:217:LEU:HD13	1.92	0.51
2:C:277:ASN:HD22	2:C:277:ASN:N	2.08	0.51
2:B:195:VAL:O	2:B:195:VAL:HG22	2.10	0.51
2:C:132:THR:CB	5:C:387:HOH:O	2.43	0.51
3:D:367:TRP:HA	3:D:370:VAL:CG1	2.41	0.51
2:B:217:LEU:CD2	2:B:262:LEU:HD23	2.36	0.51
2:B:329:LEU:C	2:B:329:LEU:HD23	2.35	0.51
2:C:144:ASN:OD1	2:C:286:SER:HB2	2.10	0.51
2:B:199:ASN:CA	2:B:216:THR:HG22	2.41	0.51
2:A:354:LEU:HD21	3:D:366:MET:HE1	1.88	0.51
3:E:366:MET:O	3:E:366:MET:SD	2.69	0.51
2:C:264:PRO:C	2:C:267:VAL:CG1	2.80	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:5:A:H2'	1:N:6:U:O4'	2.11	0.51
2:A:162:GLN:NE2	2:A:327:ALA:HA	2.26	0.51
2:A:303:ALA:HB1	2:A:307:ALA:HB3	1.93	0.51
2:C:110:ASP:OD1	2:C:130:ALA:HA	2.11	0.51
2:A:264:PRO:C	2:A:267:VAL:HG13	2.36	0.51
2:B:61:GLN:N	2:B:62:PRO:HD3	2.25	0.51
2:C:115:ILE:CG1	2:C:173:VAL:HG11	2.39	0.51
2:C:71:PHE:O	2:C:242:GLN:NE2	2.44	0.50
2:B:73:PRO:N	2:B:74:PRO:HD2	2.27	0.50
2:A:72:ALA:HB1	2:A:75:ASP:OD2	2.11	0.50
3:D:367:TRP:HE1	3:D:371:LYS:HZ2	1.58	0.50
2:B:189:THR:HA	2:B:231:PHE:O	2.10	0.50
2:B:193:CYS:SG	2:C:325:PRO:HG2	2.51	0.50
2:B:245:CYS:CA	2:B:294:MET:HE1	2.41	0.50
2:A:161:ASP:N	2:A:161:ASP:OD1	2.44	0.50
2:B:233:GLU:CG	2:B:237:LYS:HD2	2.38	0.50
2:A:116:ALA:HB2	2:A:296:THR:HG23	1.93	0.50
2:C:324:ASN:HB3	2:C:326:ASN:OD1	2.12	0.50
2:A:322:ARG:NH2	2:C:295:ASP:OD1	2.45	0.50
2:B:232:SER:O	2:B:233:GLU:HB2	2.10	0.50
1:N:7:A:C2'	1:N:8:U:H5'	2.41	0.50
2:B:99:LEU:O	2:B:314:LYS:HA	2.12	0.50
2:A:73:PRO:CB	2:A:74:PRO:HD3	2.42	0.50
2:A:295:ASP:OD2	2:B:322:ARG:NH2	2.25	0.50
2:B:68:LYS:HE2	2:B:76:PHE:CZ	2.47	0.50
2:B:92:VAL:HA	2:B:323:PRO:HD3	1.94	0.50
2:C:201:GLN:HA	2:C:212:ALA:O	2.11	0.50
2:B:195:VAL:CG2	2:B:291:TRP:CZ2	2.94	0.50
2:C:21:GLN:HA	2:C:181:LEU:HD21	1.94	0.50
2:A:208:PRO:HG2	2:B:206:THR:HA	1.94	0.49
2:B:273:GLY:C	5:B:416:HOH:O	2.54	0.49
3:F:367:TRP:CE2	3:F:371:LYS:HG3	2.46	0.49
2:B:171:MET:HE2	2:B:243:SER:HB3	1.92	0.49
2:A:73:PRO:CD	2:A:74:PRO:HD2	2.41	0.49
2:B:73:PRO:N	2:B:74:PRO:CD	2.75	0.49
2:B:156:ALA:HB1	2:B:258:GLY:HA2	1.95	0.49
2:B:213:LEU:CD2	2:C:213:LEU:HD23	2.39	0.49
1:N:2:C:O2	1:N:2:C:H2'	2.11	0.49
2:A:314:LYS:HE3	2:A:316:TRP:CZ2	2.48	0.49
2:A:200:VAL:HG21	2:A:271:THR:O	2.12	0.49
2:B:167:ARG:HG2	2:B:320:GLU:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:200:VAL:CG1	2:C:214:VAL:CG2	2.90	0.49
2:B:163:VAL:HG11	2:B:321:TYR:HD1	1.72	0.49
2:C:61:GLN:CB	2:C:62:PRO:CD	2.90	0.49
2:A:156:ALA:O	2:A:258:GLY:N	2.38	0.49
2:A:208:PRO:HG3	2:B:206:THR:HA	1.95	0.49
2:B:84:ILE:HD12	2:B:167:ARG:HG3	1.94	0.49
2:B:355:PRO:HG2	2:B:358:VAL:HG12	1.95	0.49
2:B:73:PRO:CG	2:B:74:PRO:HD3	2.43	0.48
2:B:341:GLU:OE1	2:C:87:ARG:NH2	2.46	0.48
2:C:200:VAL:CG1	2:C:200:VAL:O	2.60	0.48
2:B:341:GLU:OE1	2:B:341:GLU:CA	2.61	0.48
2:C:99:LEU:HB3	2:C:315:THR:HG23	1.94	0.48
2:C:246:ASN:HD21	2:C:293:ASN:HB3	1.77	0.48
2:C:280:ALA:HB1	2:C:286:SER:OG	2.13	0.48
2:A:172:ASN:HD22	2:A:242:GLN:HB3	1.77	0.48
2:A:183:GLN:NE2	2:A:308:VAL:HG11	2.28	0.48
2:A:181:LEU:CD1	2:A:236:ILE:HG12	2.43	0.48
2:A:204:VAL:CG1	2:A:206:THR:HG23	2.42	0.48
2:B:313:LEU:HD23	2:B:313:LEU:C	2.38	0.48
2:C:93:VAL:CG1	2:C:323:PRO:HB3	2.44	0.48
1:N:7:A:N6	1:N:8:U:C4	2.81	0.48
2:A:79:ASP:OD1	2:A:96:LYS:HE2	2.13	0.48
2:B:184:PHE:C	2:B:184:PHE:CD2	2.87	0.48
2:B:65:ALA:CB	2:B:82:LYS:CD	2.92	0.48
2:A:144:ASN:HD22	2:A:144:ASN:H	1.61	0.48
2:A:201:GLN:OE1	2:B:264:PRO:HG3	2.14	0.48
2:C:59:LEU:CD2	2:C:342:VAL:HG12	2.44	0.48
2:C:319:LEU:N	2:C:319:LEU:CD2	2.77	0.48
2:B:121:VAL:HA	2:B:144:ASN:HA	1.96	0.48
2:C:61:GLN:HB2	2:C:62:PRO:CD	2.43	0.48
2:C:133:PHE:HB3	2:C:134:PRO:HD2	1.95	0.48
2:C:151:MET:HG2	2:C:152:PHE:CE2	2.48	0.48
2:C:256:LEU:CD1	2:C:290:GLY:HA2	2.42	0.48
2:A:325:PRO:HB3	2:C:227:GLY:HA3	1.95	0.47
2:B:94:THR:HA	2:B:319:LEU:O	2.14	0.47
2:B:201:GLN:HA	2:B:212:ALA:O	2.14	0.47
2:C:92:VAL:HA	2:C:321:TYR:O	2.14	0.47
2:C:133:PHE:HB3	2:C:134:PRO:CD	2.43	0.47
2:C:360:ALA:O	2:C:363:ASN:N	2.47	0.47
2:A:160:SER:HA	2:A:163:VAL:O	2.15	0.47
2:A:117:PRO:HB2	2:A:292:GLY:HA3	1.94	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:245:CYS:CA	2:B:294:MET:HE2	2.26	0.47
2:C:277:ASN:N	2:C:277:ASN:ND2	2.62	0.47
2:C:121:VAL:HA	2:C:144:ASN:HA	1.96	0.47
2:A:165:SER:OG	2:C:196:LYS:CE	2.62	0.47
2:B:210:THR:HB	2:B:211:SER:H	1.49	0.47
2:A:145:PHE:CE1	2:A:315:THR:O	2.68	0.47
2:A:205:ALA:O	2:A:206:THR:C	2.56	0.47
2:C:91:LYS:HE3	2:C:330:TYR:CZ	2.50	0.47
2:A:264:PRO:CG	2:A:267:VAL:HG11	2.45	0.47
2:B:326:ASN:ND2	2:B:326:ASN:H	2.11	0.47
2:C:159:ARG:HD3	2:C:289:VAL:HG12	1.97	0.47
2:C:264:PRO:HG2	2:C:267:VAL:HG11	1.97	0.47
2:A:204:VAL:CG2	2:A:205:ALA:N	2.74	0.47
2:A:259:ILE:CG2	2:A:288:ILE:HB	2.45	0.47
2:C:207:THR:O	2:C:208:PRO:C	2.52	0.47
2:C:239:VAL:HG22	2:C:240:PHE:H	1.80	0.47
2:C:197:LEU:CD1	2:C:217:LEU:CD1	2.93	0.47
2:C:206:THR:HG22	2:C:209:ALA:C	2.40	0.47
2:A:73:PRO:HD2	2:A:74:PRO:HD2	1.97	0.46
2:A:94:THR:CG2	2:A:319:LEU:O	2.63	0.46
2:B:63:GLY:O	2:B:66:PHE:HB3	2.15	0.46
2:A:105:PHE:CZ	2:A:301:VAL:HG21	2.50	0.46
2:C:21:GLN:HG2	2:C:181:LEU:CD1	2.35	0.46
2:C:96:LYS:CE	5:C:373:HOH:O	2.61	0.46
2:A:56:LEU:C	2:A:58:ARG:N	2.73	0.46
2:A:73:PRO:HG2	2:A:74:PRO:HD3	1.97	0.46
2:C:264:PRO:CG	2:C:267:VAL:HG11	2.45	0.46
2:A:128:VAL:HB	2:A:129:PRO:HD2	1.96	0.46
2:B:246:ASN:C	2:B:246:ASN:ND2	2.73	0.46
2:B:329:LEU:HD23	2:B:330:TYR:N	2.30	0.46
2:C:244:VAL:HG22	5:C:398:HOH:O	2.14	0.46
2:A:215:HIS:NE2	5:A:433:HOH:O	2.31	0.46
2:A:162:GLN:NE2	2:A:327:ALA:CB	2.70	0.46
2:A:188:ILE:O	2:A:232:SER:HA	2.15	0.46
2:B:202:PHE:CD1	2:B:202:PHE:N	2.84	0.46
2:C:68:LYS:HG2	2:C:76:PHE:CZ	2.51	0.46
2:C:129:PRO:O	2:C:132:THR:HG23	2.15	0.46
1:N:3:U:C2	1:N:4:U:C5	3.03	0.46
2:A:73:PRO:N	2:A:74:PRO:HD2	2.30	0.46
2:C:349:THR:O	2:C:353:SER:OG	2.33	0.46
2:A:99:LEU:O	2:A:314:LYS:HA	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:246:ASN:ND2	2:A:247:GLU:HG2	2.30	0.46
2:B:86:ASP:HA	2:B:344:LEU:HD11	1.96	0.46
2:B:313:LEU:HD23	2:B:314:LYS:N	2.31	0.46
5:B:376:HOH:O	2:C:87:ARG:HD3	2.15	0.46
2:C:200:VAL:HG12	2:C:214:VAL:HG23	1.97	0.46
2:A:295:ASP:CG	2:B:322:ARG:NH2	2.72	0.46
2:B:93:VAL:HG12	2:B:333:GLY:CA	2.42	0.46
2:B:275:PRO:HB2	2:B:276:PHE:CD1	2.50	0.46
2:B:73:PRO:CD	2:B:74:PRO:HD2	2.46	0.45
2:C:82:LYS:O	2:C:334:HIS:HE1	1.98	0.45
2:A:73:PRO:N	2:A:74:PRO:CD	2.79	0.45
2:A:263:PRO:HD2	2:A:277:ASN:OD1	2.16	0.45
2:B:78:THR:HG22	5:B:375:HOH:O	2.16	0.45
2:A:123:TYR:HE2	2:A:125:VAL:HG22	1.79	0.45
2:C:59:LEU:HD21	2:C:342:VAL:HG12	1.97	0.45
2:A:223:VAL:O	2:A:223:VAL:HG12	2.15	0.45
2:C:98:VAL:CG1	2:C:316:TRP:CD1	2.93	0.45
2:C:182:MET:C	2:C:183:GLN:HG2	2.41	0.45
2:C:188:ILE:O	2:C:232:SER:HA	2.16	0.45
2:B:171:MET:HE2	2:B:243:SER:CB	2.46	0.45
2:B:96:LYS:HZ3	2:B:96:LYS:HG3	1.67	0.45
2:C:81:GLY:C	2:C:96:LYS:HZ1	2.24	0.45
2:B:179:SER:HB3	2:B:183:GLN:CG	2.43	0.45
2:C:239:VAL:HG22	2:C:240:PHE:N	2.32	0.45
2:C:360:ALA:C	2:C:362:GLN:N	2.74	0.45
2:A:247:GLU:O	2:A:348:ARG:NH2	2.48	0.45
2:C:139:THR:CG2	5:C:416:HOH:O	2.62	0.45
2:A:313:LEU:C	2:A:313:LEU:CD2	2.90	0.45
2:A:358:VAL:HG13	2:A:359:ILE:O	2.17	0.45
2:B:207:THR:O	2:B:208:PRO:C	2.56	0.45
2:B:208:PRO:O	2:B:209:ALA:HB3	2.16	0.45
2:A:194:PRO:HB3	2:B:322:ARG:NH2	2.31	0.44
2:A:331:GLN:NE2	2:A:331:GLN:H	2.15	0.44
2:C:108:ASN:C	2:C:109:ARG:HG2	2.42	0.44
2:C:186:GLY:HA3	2:C:302:SER:O	2.17	0.44
2:A:159:ARG:HD3	2:A:289:VAL:CG1	2.44	0.44
2:C:21:GLN:HG2	2:C:181:LEU:HD11	1.79	0.44
3:F:367:TRP:HE1	3:F:371:LYS:HD3	1.82	0.44
2:A:94:THR:HA	2:A:319:LEU:O	2.18	0.44
2:A:113:ILE:HG12	2:A:125:VAL:HG13	1.99	0.44
2:B:268:THR:CG2	2:B:270:ALA:HB3	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:25:VAL:O	2:C:27:GLN:NE2	2.49	0.44
1:N:4:U:C2'	1:N:5:A:C5'	2.81	0.44
2:B:186:GLY:HA3	2:B:302:SER:O	2.18	0.44
2:C:217:LEU:HB3	2:C:220:LEU:HD22	2.00	0.44
2:A:73:PRO:CD	2:A:74:PRO:CD	2.95	0.44
2:A:74:PRO:HG3	2:A:316:TRP:CH2	2.53	0.44
2:B:73:PRO:CD	2:B:74:PRO:CD	2.96	0.44
2:C:113:ILE:HG22	2:C:115:ILE:HD12	2.00	0.44
2:C:227:GLY:O	2:C:230:ASN:HB3	2.17	0.44
2:A:207:THR:CB	2:A:208:PRO:CD	2.87	0.44
2:B:109:ARG:HD2	2:B:128:VAL:C	2.42	0.44
2:C:93:VAL:O	2:C:93:VAL:CG2	2.65	0.44
2:A:233:GLU:OE2	5:A:394:HOH:O	2.21	0.44
2:A:217:LEU:HD22	2:A:262:LEU:CD2	2.26	0.43
2:C:280:ALA:HB3	2:C:287:GLY:HA2	2.00	0.43
2:C:319:LEU:N	2:C:319:LEU:HD22	2.33	0.43
2:A:222:GLY:HA2	2:B:326:ASN:HD22	1.83	0.43
2:C:142:ALA:O	5:C:393:HOH:O	2.21	0.43
2:C:207:THR:CG2	2:C:208:PRO:CD	2.84	0.43
2:B:127:ASP:C	2:B:128:VAL:HG13	2.43	0.43
2:C:109:ARG:HD3	2:C:127:ASP:OD1	2.19	0.43
2:A:129:PRO:C	2:A:132:THR:CG2	2.77	0.43
3:D:366:MET:O	3:D:367:TRP:C	2.62	0.43
2:B:125:VAL:CG2	2:B:126:ALA:N	2.80	0.43
2:C:25:VAL:CG1	2:C:25:VAL:O	2.66	0.43
2:C:117:PRO:CB	2:C:171:MET:HE1	2.47	0.43
2:C:181:LEU:HD23	2:C:236:ILE:HG12	2.00	0.43
2:A:208:PRO:HG2	2:B:206:THR:CA	2.47	0.43
2:B:56:LEU:HD23	3:E:374:ILE:CG2	2.44	0.43
2:B:65:ALA:HB2	2:B:82:LYS:HD3	1.99	0.43
2:B:191:TRP:CZ3	2:B:226:VAL:HG22	2.54	0.43
2:C:116:ALA:HA	2:C:296:THR:HB	2.01	0.43
2:B:179:SER:HA	2:B:183:GLN:OE1	2.19	0.43
2:A:295:ASP:OD1	2:B:322:ARG:NH2	2.52	0.43
2:B:354:LEU:HB3	2:B:355:PRO:HD2	2.00	0.43
2:C:254:ASP:HB2	5:C:411:HOH:O	2.18	0.43
2:A:329:LEU:C	2:A:329:LEU:CD2	2.92	0.43
2:B:319:LEU:N	2:B:319:LEU:HD23	2.34	0.43
2:C:204:VAL:HG23	2:C:205:ALA:N	2.32	0.43
2:C:206:THR:HG22	2:C:209:ALA:HA	2.00	0.43
2:A:184:PHE:CD1	2:A:184:PHE:C	2.96	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:206:THR:HA	2:C:208:PRO:HG3	1.99	0.43
2:C:73:PRO:CD	2:C:74:PRO:HD3	2.49	0.43
2:C:329:LEU:C	2:C:331:GLN:N	2.77	0.43
2:A:180:ASN:CG	2:A:183:GLN:HG2	2.44	0.42
2:A:206:THR:CA	2:C:208:PRO:HG2	2.49	0.42
2:A:246:ASN:C	2:A:246:ASN:ND2	2.72	0.42
2:C:134:PRO:HB3	2:C:138:THR:HG21	2.00	0.42
1:N:8:U:O2'	1:N:9:C:C5'	2.63	0.42
2:B:65:ALA:HB3	2:B:82:LYS:HD3	1.99	0.42
2:C:135:ILE:N	2:C:138:THR:OG1	2.36	0.42
2:C:337:PRO:HA	2:C:338:PRO:HD3	1.90	0.42
2:B:295:ASP:CG	2:C:322:ARG:HH22	2.24	0.42
2:A:149:ASN:ND2	2:A:153:GLY:O	2.53	0.42
2:A:157:ALA:HA	2:A:257:GLU:OE1	2.18	0.42
2:B:67:LEU:HA	2:B:67:LEU:HD23	1.84	0.42
2:B:146:PRO:HG2	5:B:380:HOH:O	2.18	0.42
2:C:125:VAL:CG2	2:C:126:ALA:N	2.80	0.42
2:C:162:GLN:HA	2:C:327:ALA:HB2	1.99	0.42
2:A:261:THR:O	2:A:264:PRO:HA	2.20	0.42
2:B:217:LEU:HD12	2:B:217:LEU:HA	1.86	0.42
2:C:20:THR:O	2:C:21:GLN:CG	2.67	0.42
2:C:68:LYS:HG2	2:C:76:PHE:HZ	1.85	0.42
2:C:105:PHE:CZ	2:C:301:VAL:HG21	2.55	0.42
2:A:276:PHE:HB2	2:A:277:ASN:H	1.67	0.42
2:B:129:PRO:O	2:B:130:ALA:C	2.62	0.42
2:A:215:HIS:CD2	2:A:259:ILE:HD11	2.54	0.42
2:B:167:ARG:HD2	2:B:252:PHE:CD1	2.52	0.42
2:B:267:VAL:O	2:B:267:VAL:HG22	2.20	0.42
2:A:159:ARG:HH12	2:A:260:GLN:HE22	1.67	0.42
2:A:183:GLN:NE2	2:A:308:VAL:CG1	2.83	0.42
2:B:128:VAL:HB	2:B:129:PRO:HD2	2.02	0.42
2:B:167:ARG:HD3	2:B:167:ARG:HH11	1.71	0.42
2:C:304:PRO:HG3	5:C:384:HOH:O	2.19	0.42
2:A:220:LEU:HA	2:A:220:LEU:HD12	1.79	0.41
2:A:275:PRO:HB2	2:A:276:PHE:CD1	2.55	0.41
2:B:181:LEU:HD12	2:B:181:LEU:HA	1.81	0.41
2:C:354:LEU:CD2	3:F:369:ARG:HD2	2.49	0.41
3:F:367:TRP:CE2	3:F:371:LYS:CG	3.03	0.41
2:C:246:ASN:HD22	2:C:246:ASN:C	2.28	0.41
2:C:322:ARG:HD2	2:C:322:ARG:HA	1.83	0.41
2:A:76:PHE:C	2:A:78:THR:H	2.28	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:318:CYS:C	2:B:319:LEU:HD23	2.45	0.41
3:E:371:LYS:HE3	3:E:371:LYS:HB2	1.66	0.41
2:A:68:LYS:CD	2:A:76:PHE:CZ	3.02	0.41
2:C:155:ALA:HA	2:C:283:GLU:HB3	2.01	0.41
1:N:5:A:C2'	1:N:6:U:C5'	2.80	0.41
2:A:303:ALA:HA	2:A:304:PRO:HD2	1.87	0.41
2:C:207:THR:C	2:C:209:ALA:H	2.22	0.41
2:B:195:VAL:O	2:B:195:VAL:CG2	2.68	0.41
2:C:91:LYS:O	2:C:322:ARG:HD2	2.20	0.41
2:A:159:ARG:NH1	2:A:260:GLN:HE22	2.19	0.41
2:A:259:ILE:HD11	5:A:433:HOH:O	2.21	0.41
2:B:124:TRP:HA	2:B:141:ASN:O	2.20	0.41
2:B:194:PRO:HB2	2:C:164:SER:OG	2.20	0.41
2:B:202:PHE:HE1	2:B:214:VAL:HG13	1.85	0.41
2:C:68:LYS:CG	2:C:76:PHE:CZ	3.03	0.41
2:C:262:LEU:HD12	2:C:262:LEU:HA	1.95	0.41
2:A:148:PHE:CD1	2:A:148:PHE:C	2.99	0.41
2:A:167:ARG:CG	2:A:252:PHE:CE2	3.04	0.41
3:D:367:TRP:HE1	3:D:371:LYS:HZ3	1.67	0.41
2:B:73:PRO:HG3	2:B:172:ASN:ND2	2.36	0.41
2:B:73:PRO:HD2	2:B:74:PRO:HD2	2.02	0.41
2:B:176:TYR:CE1	2:B:363:ASN:OD1	2.73	0.41
2:C:78:THR:O	2:C:80:PRO:HD3	2.21	0.41
2:C:135:ILE:C	2:C:137:THR:N	2.79	0.41
2:C:328:MET:O	2:C:328:MET:HG2	2.20	0.41
2:B:97:ASP:HB3	2:B:145:PHE:CG	2.56	0.41
2:A:206:THR:HA	2:C:208:PRO:HG2	2.01	0.40
2:C:56:LEU:CD2	2:C:59:LEU:HD12	2.51	0.40
1:N:5:A:C3'	1:N:6:U:H5'	2.45	0.40
2:A:122:ALA:HA	2:A:145:PHE:CE2	2.56	0.40
2:A:206:THR:O	2:A:209:ALA:CA	2.65	0.40
2:B:268:THR:HG23	2:B:270:ALA:H	1.86	0.40
2:B:331:GLN:HE21	2:B:331:GLN:HB3	1.47	0.40
2:C:204:VAL:CG2	2:C:206:THR:HB	2.51	0.40
1:N:10:U:H4'	2:C:55:ALA:CB	2.52	0.40
2:B:163:VAL:CG2	2:B:321:TYR:HB3	2.51	0.40
2:B:195:VAL:CG2	2:B:291:TRP:HZ2	2.33	0.40
2:A:162:GLN:HE21	2:A:327:ALA:HB2	1.81	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	A	306/363 (84%)	280 (92%)	23 (8%)	3 (1%)	12	38
2	B	306/363 (84%)	278 (91%)	25 (8%)	3 (1%)	12	38
2	C	317/363 (87%)	296 (93%)	18 (6%)	3 (1%)	14	41
3	D	14/44 (32%)	12 (86%)	2 (14%)	0	100	100
3	E	14/44 (32%)	13 (93%)	1 (7%)	0	100	100
3	F	14/44 (32%)	13 (93%)	0	1 (7%)	1	2
All	All	971/1221 (80%)	892 (92%)	69 (7%)	10 (1%)	12	38

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	57	THR
2	A	209	ALA
2	B	81	GLY
2	B	206	THR
2	C	236	ILE
2	C	361	ALA
3	F	365	SER
2	C	209	ALA
2	A	181	LEU
2	B	209	ALA

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	A	251/301 (83%)	186 (74%)	65 (26%)	0	2
2	B	251/301 (83%)	198 (79%)	53 (21%)	1	4
2	C	263/301 (87%)	197 (75%)	66 (25%)	0	2
3	D	14/32 (44%)	5 (36%)	9 (64%)	0	0
3	E	14/32 (44%)	8 (57%)	6 (43%)	0	0
3	F	14/32 (44%)	9 (64%)	5 (36%)	0	0
All	All	807/999 (81%)	603 (75%)	204 (25%)	0	2

All (204) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	56	LEU
2	A	57	THR
2	A	61	GLN
2	A	77	ASN
2	A	78	THR
2	A	82	LYS
2	A	91	LYS
2	A	92	VAL
2	A	93	VAL
2	A	94	THR
2	A	95	ARG
2	A	96	LYS
2	A	102	SER
2	A	106	THR
2	A	121	VAL
2	A	125	VAL
2	A	132	THR
2	A	144	ASN
2	A	159	ARG
2	A	160	SER
2	A	161	ASP
2	A	162	GLN
2	A	163	VAL
2	A	167	ARG
2	A	175	ILE
2	A	181	LEU
2	A	182	MET
2	A	195	VAL
2	A	196	LYS
2	A	201	GLN

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Mol	Chain	Res	Type
2	A	207	THR
2	A	211	SER
2	A	214	VAL
2	A	217	LEU
2	A	220	LEU
2	A	226	VAL
2	A	232	SER
2	A	234	SER
2	A	236	ILE
2	A	237	LYS
2	A	239	VAL
2	A	242	GLN
2	A	244	VAL
2	A	246	ASN
2	A	262	LEU
2	A	267	VAL
2	A	268	THR
2	A	269	VAL
2	A	271	THR
2	A	283	GLU
2	A	294	MET
2	A	299	ILE
2	A	305	THR
2	A	310	SER
2	A	314	LYS
2	A	326	ASN
2	A	329	LEU
2	A	331	GLN
2	A	345	GLN
2	A	348	ARG
2	A	349	THR
2	A	350	VAL
2	A	353	SER
2	A	356	VAL
2	A	358	VAL
3	D	366	MET
3	D	369	ARG
3	D	370	VAL
3	D	371	LYS
3	D	372	SER
3	D	374	ILE
3	D	375	LYS

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Mol	Chain	Res	Type
3	D	376	SER
3	D	378	LEU
2	B	57	THR
2	B	60	SER
2	B	61	GLN
2	B	64	LEU
2	B	78	THR
2	B	82	LYS
2	B	91	LYS
2	B	96	LYS
2	B	103	ILE
2	B	109	ARG
2	B	115	ILE
2	B	121	VAL
2	B	137	THR
2	B	154	ASN
2	B	159	ARG
2	B	160	SER
2	B	163	VAL
2	B	165	SER
2	B	167	ARG
2	B	170	SER
2	B	178	THR
2	B	181	LEU
2	B	182	MET
2	B	192	LYS
2	B	195	VAL
2	B	201	GLN
2	B	204	VAL
2	B	206	THR
2	B	214	VAL
2	B	217	LEU
2	B	220	LEU
2	B	236	ILE
2	B	242	GLN
2	B	244	VAL
2	B	246	ASN
2	B	261	THR
2	B	267	VAL
2	B	268	THR
2	B	277	ASN
2	B	285	VAL

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Mol	Chain	Res	Type
2	B	296	THR
2	B	308	VAL
2	B	310	SER
2	B	314	LYS
2	B	319	LEU
2	B	329	LEU
2	B	331	GLN
2	B	341	GLU
2	B	346	GLU
2	B	348	ARG
2	B	349	THR
2	B	362	GLN
2	B	363	ASN
3	E	366	MET
3	E	368	GLU
3	E	369	ARG
3	E	371	LYS
3	E	373	ILE
3	E	377	SER
2	C	21	GLN
2	C	25	VAL
2	C	30	VAL
2	C	56	LEU
2	C	57	THR
2	C	58	ARG
2	C	61	GLN
2	C	89	GLU
2	C	91	LYS
2	C	93	VAL
2	C	95	ARG
2	C	98	VAL
2	C	106	THR
2	C	109	ARG
2	C	121	VAL
2	C	132	THR
2	C	137	THR
2	C	139	THR
2	C	151	MET
2	C	154	ASN
2	C	159	ARG
2	C	163	VAL
2	C	165	SER

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Mol	Chain	Res	Type
2	C	167	ARG
2	C	170	SER
2	C	173	VAL
2	C	179	SER
2	C	182	MET
2	C	189	THR
2	C	194	PRO
2	C	196	LYS
2	C	198	SER
2	C	199	ASN
2	C	201	GLN
2	C	204	VAL
2	C	206	THR
2	C	207	THR
2	C	211	SER
2	C	213	LEU
2	C	217	LEU
2	C	220	LEU
2	C	232	SER
2	C	233	GLU
2	C	246	ASN
2	C	261	THR
2	C	267	VAL
2	C	277	ASN
2	C	278	LEU
2	C	286	SER
2	C	296	THR
2	C	302	SER
2	C	308	VAL
2	C	314	LYS
2	C	315	THR
2	C	319	LEU
2	C	320	GLU
2	C	328	MET
2	C	329	LEU
2	C	341	GLU
2	C	348	ARG
2	C	349	THR
2	C	352	ARG
2	C	353	SER
2	C	356	VAL
2	C	358	VAL

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Mol	Chain	Res	Type
2	C	359	ILE
3	F	368	GLU
3	F	369	ARG
3	F	376	SER
3	F	377	SER
3	F	378	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	61	GLN
2	A	104	ASN
2	A	144	ASN
2	A	149	ASN
2	A	162	GLN
2	A	172	ASN
2	A	242	GLN
2	A	246	ASN
2	A	260	GLN
2	A	293	ASN
2	A	309	ASN
2	A	326	ASN
2	A	331	GLN
2	B	61	GLN
2	B	100	ASN
2	B	154	ASN
2	B	201	GLN
2	B	215	HIS
2	B	242	GLN
2	B	246	ASN
2	B	293	ASN
2	B	324	ASN
2	B	326	ASN
2	B	331	GLN
2	B	363	ASN
2	C	21	GLN
2	C	27	GLN
2	C	61	GLN
2	C	100	ASN
2	C	154	ASN
2	C	172	ASN
2	C	215	HIS

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Mol	Chain	Res	Type
2	C	246	ASN
2	C	277	ASN
2	C	293	ASN
2	C	309	ASN
2	C	331	GLN
2	C	345	GLN
2	C	362	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	N	9/10 (90%)	5 (55%)	0

All (5) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	N	2	C
1	N	3	U
1	N	4	U
1	N	5	A
1	N	7	A

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 5 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.