



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:41 AM GMT

PDB ID : 2BBV
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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

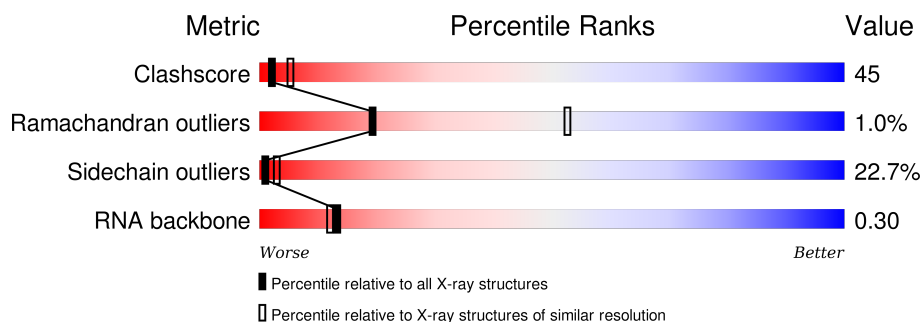
1 Overall quality at a glance

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	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RNA backbone	2183	1091 (3.20-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	N	10	
2	A	363	
2	B	363	
2	C	363	
3	D	44	
3	E	44	

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Mol	Chain	Length	Quality of chain
3	F	44	<div><div></div><div>11%14%9%•64%</div></div>

2 Entry composition

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
1	N	10	Total	C	N	O	P	0	0	0
			201	92	28	72	9			

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

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

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

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

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

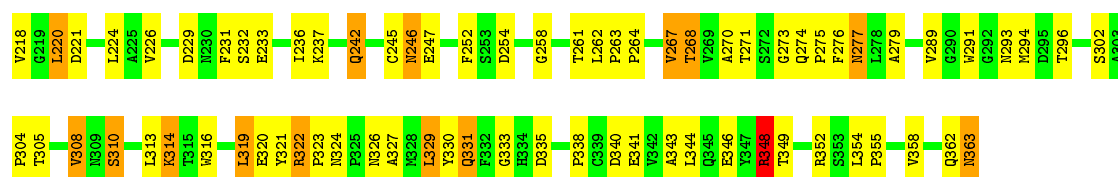
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	2	Total	Ca	0	0
			2	2		

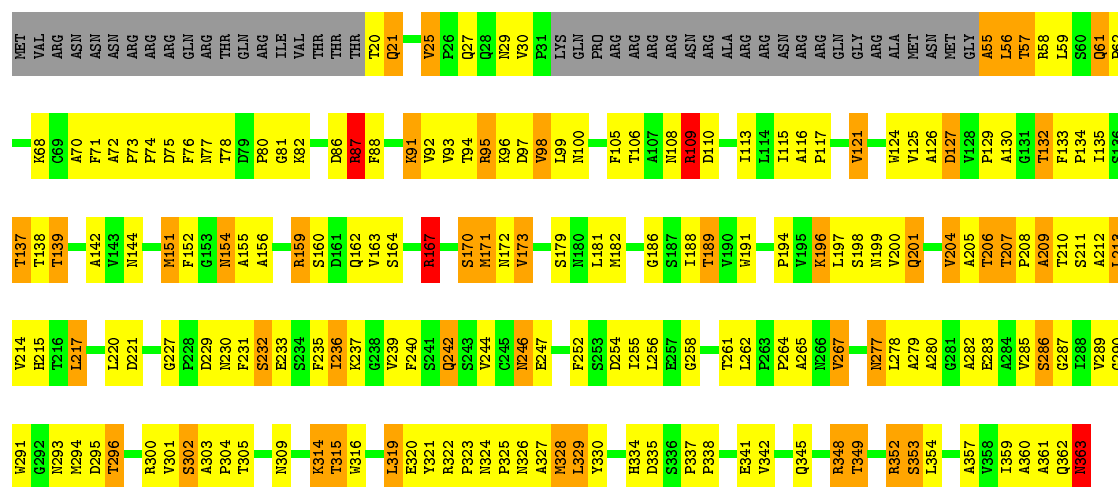
- Molecule 5 is water.

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



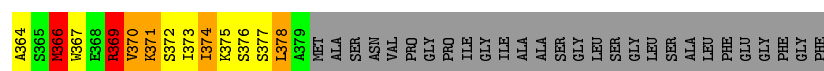
• Molecule 2: PROTEIN (BLACK BEETLE VIRUS CAPSID PROTEIN)

Chain C: 36% 38% 13% 12%



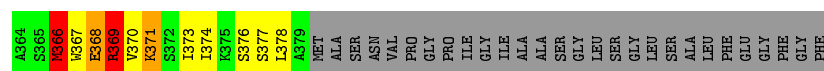
• Molecule 3: PROTEIN (BLACK BEETLE VIRUS CAPSID PROTEIN)

Chain D: 7% 16% 9% 5% 64%



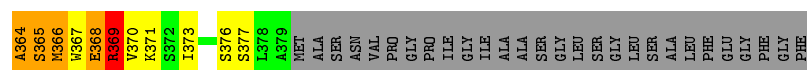
• Molecule 3: PROTEIN (BLACK BEETLE VIRUS CAPSID PROTEIN)

Chain E: 11% 16% 5% 5% 64%



• Molecule 3: PROTEIN (BLACK BEETLE VIRUS CAPSID PROTEIN)

Chain F: 11% 14% 9% 64%



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 4 ₂ 3 2	Depositor
Cell constants a, b, c, α , β , γ	362.00 Å 362.00 Å 362.00 Å 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.	Xtriage
Total number of atoms	7817	wwPDB-VP
Average B, all atoms (Å ²)	12.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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	1.31	1/222 (0.5%)	1.59	3/342 (0.9%)
2	A	0.89	0/2372	1.41	15/3249 (0.5%)
2	B	0.88	0/2372	1.43	15/3249 (0.5%)
2	C	0.88	1/2469 (0.0%)	1.41	22/3384 (0.7%)
3	D	1.01	0/126	1.57	5/167 (3.0%)
3	E	1.02	0/126	1.43	2/167 (1.2%)
3	F	1.48	1/126 (0.8%)	1.75	3/167 (1.8%)
All	All	0.92	3/7813 (0.0%)	1.43	65/10725 (0.6%)

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 (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	364	ALA	CA-CB	12.65	1.79	1.52
1	N	7	A	N9-C4	-10.46	1.31	1.37
2	C	363	ASN	CA-C	-8.50	1.30	1.52

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	364	ALA	N-CA-CB	-13.14	91.71	110.10
2	A	352	ARG	NE-CZ-NH1	11.89	126.24	120.30
2	C	348	ARG	NE-CZ-NH2	10.31	125.45	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	87	ARG	NE-CZ-NH1	9.61	125.11	120.30
2	C	55	ALA	O-C-N	8.82	136.81	122.70
2	A	229	ASP	CB-CG-OD2	8.74	126.16	118.30
2	C	221	ASP	CB-CG-OD2	8.54	125.99	118.30
2	A	352	ARG	CD-NE-CZ	8.47	135.46	123.60
2	C	87	ARG	NE-CZ-NH2	-8.27	116.16	120.30
2	C	55	ALA	CB-CA-C	-7.81	98.38	110.10
3	D	364	ALA	O-C-N	7.74	135.07	122.70
2	C	95	ARG	NE-CZ-NH2	7.73	124.17	120.30
2	B	221	ASP	CB-CG-OD2	7.68	125.21	118.30
2	A	87	ARG	NE-CZ-NH1	-7.68	116.46	120.30
2	A	58	ARG	NE-CZ-NH2	7.55	124.07	120.30
2	B	109	ARG	NE-CZ-NH2	7.50	124.05	120.30
3	D	369	ARG	NE-CZ-NH2	7.47	124.03	120.30
3	E	369	ARG	NE-CZ-NH2	7.45	124.02	120.30
3	F	369	ARG	NE-CZ-NH2	7.36	123.98	120.30
2	B	322	ARG	NE-CZ-NH2	7.26	123.93	120.30
2	C	352	ARG	NE-CZ-NH2	7.23	123.92	120.30
2	C	87	ARG	NE-CZ-NH1	7.20	123.90	120.30
1	N	7	A	C8-N9-C4	7.00	108.60	105.80
2	C	58	ARG	NE-CZ-NH2	6.91	123.76	120.30
2	C	109	ARG	NE-CZ-NH2	6.83	123.72	120.30
2	C	127	ASP	CB-CG-OD1	6.83	124.44	118.30
2	C	55	ALA	CA-C-N	-6.63	102.60	117.20
2	C	335	ASP	CB-CG-OD2	6.62	124.25	118.30
2	B	87	ARG	NE-CZ-NH2	-6.57	117.01	120.30
2	A	182	MET	CG-SD-CE	6.35	110.36	100.20
3	F	366	MET	CG-SD-CE	6.30	110.28	100.20
2	B	348	ARG	NE-CZ-NH1	-6.28	117.16	120.30
3	D	366	MET	CG-SD-CE	6.27	110.23	100.20
2	A	109	ARG	NE-CZ-NH2	6.25	123.43	120.30
2	C	171	MET	CG-SD-CE	6.23	110.17	100.20
2	A	300	ARG	NE-CZ-NH2	6.17	123.39	120.30
3	E	366	MET	CG-SD-CE	6.12	110.00	100.20
2	A	87	ARG	CD-NE-CZ	-6.08	115.09	123.60
3	D	364	ALA	CA-C-N	-6.08	103.83	117.20
1	N	7	A	C4-C5-C6	-6.06	113.97	117.00
2	C	167	ARG	NE-CZ-NH1	6.04	123.32	120.30
2	B	95	ARG	NE-CZ-NH2	5.98	123.29	120.30
2	B	159	ARG	NE-CZ-NH2	5.89	123.25	120.30
2	B	348	ARG	NE-CZ-NH2	5.79	123.19	120.30
2	A	191	TRP	CA-CB-CG	5.79	124.69	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	127	ASP	CB-CG-OD2	-5.70	113.17	118.30
2	B	97	ASP	CB-CG-OD1	-5.70	113.17	118.30
2	A	343	ALA	CB-CA-C	5.59	118.49	110.10
2	B	182	MET	CG-SD-CE	5.56	109.10	100.20
2	C	167	ARG	CD-NE-CZ	5.47	131.26	123.60
2	A	300	ARG	NE-CZ-NH1	-5.46	117.57	120.30
2	C	97	ASP	CB-CG-OD1	-5.46	113.38	118.30
1	N	7	A	N9-C1'-C2'	-5.41	106.05	112.00
2	A	157	ALA	N-CA-CB	5.40	117.66	110.10
2	A	340	ASP	CB-CG-OD2	5.38	123.14	118.30
2	C	279	ALA	N-CA-CB	5.36	117.60	110.10
2	B	185	ALA	N-CA-CB	5.33	117.56	110.10
2	A	233	GLU	CA-CB-CG	5.31	125.09	113.40
3	D	364	ALA	N-CA-C	5.25	125.19	111.00
2	B	221	ASP	CB-CG-OD1	-5.25	113.57	118.30
2	C	191	TRP	CA-CB-CG	5.19	123.57	113.70
2	B	335	ASP	CB-CG-OD1	-5.18	113.64	118.30
2	C	300	ARG	NE-CZ-NH2	5.12	122.86	120.30
2	B	58	ARG	NE-CZ-NH1	5.11	122.86	120.30
2	C	291	TRP	CB-CA-C	5.10	120.61	110.40

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	209	0
2	B	2311	0	2262	190	0
2	C	2406	0	2357	242	0
3	D	125	0	135	18	0
3	E	125	0	135	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	674	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 45.

All (674) 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:CA	3:F:364:ALA:CB	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: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
2:B:207:THR:HG22	2:B:208:PRO:HD3	1.27	1.13
1:N:2:C:N3	1:N:3:U:C5	2.15	1.12
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: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:B:245:CYS:HA	2:B:294:MET:HE2	1.24	1.09
2:C:20:THR:HA	2:C:21:GLN:NE2	1.66	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:20:THR:C	2:C:21:GLN:NE2	2.06	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
3:E:368:GLU:CD	3:E:371:LYS:NZ	2.08	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
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
1:N:5:A:C2'	1:N:6:U:H5'	1.90	1.02
2:A:57:THR:O	2:A:57:THR:HG23	1.58	1.01
2:C:21:GLN:HE21	2:C:21:GLN:N	1.57	1.01
3:E:368:GLU:OE1	3:E:368:GLU:HA	1.59	1.01
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: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:B:264:PRO:O	2:B:267:VAL:HG13	1.67	0.95
2:C:20:THR:C	2:C:21:GLN:HE21	1.66	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:C:82:LYS:O	2:C:94:THR:HG21	1.68	0.93
2:A:129:PRO:C	2:A:132:THR:HG23	1.89	0.92
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: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
3:D:367:TRP:HE1	3:D:371:LYS:HZ3	1.11	0.90
2:B:324:ASN:HB3	2:B:326:ASN:ND2	1.86	0.89
3:F:364:ALA:N	3:F:364:ALA:CB	2.35	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:4:U:HO2'	1:N:5:A:H5'	1.25	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:C:170:SER:HA	5:C:372:HOH:O	1.73	0.89
2:B:63:GLY:HA3	2:B:340:ASP:OD2	1.73	0.89
2:B:279:ALA:CB	5:B:414:HOH:O	1.97	0.88
2:C:154:ASN:H	2:C:154:ASN:HD22	1.18	0.88
2:A:57:THR:O	2:A:57:THR:CG2	2.18	0.88
2:C:21:GLN:HG3	2:C:181:LEU:HD13	1.50	0.87
2:B:245:CYS:HA	2:B:294:MET:CE	2.03	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
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:C:68:LYS:HD3	2:C:76:PHE:CZ	2.12	0.84
2:A:162:GLN:HE21	2:A:327:ALA:CB	1.89	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
2:C:206:THR:O	2:C:209:ALA:N	2.10	0.84
3:E:368:GLU:CD	3:E:371:LYS:HZ1	1.70	0.84
3:D:367:TRP:NE1	3:D:371:LYS:HD2	1.93	0.84
2:B:245:CYS:CA	2:B:294:MET:HE2	2.08	0.83
2:A:61:GLN:HE21	2:A:62:PRO:HD3	1.40	0.83
2:C:20:THR:HA	2:C:21:GLN:HE22	1.39	0.82
2:B:213:LEU:HD23	2:C:213:LEU:HD23	1.61	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:207:THR:HB	2:A:208:PRO:CD	2.11	0.79
2:B:207:THR:HG22	2:B:208:PRO:CD	1.96	0.79
2:A:99:LEU:HB3	2:A:315:THR:HG22	1.64	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:B:93:VAL:HG12	2:B:333:GLY:HA2	1.66	0.78
2:A:183:GLN:HB2	2:A:308:VAL:HB	1.64	0.78
2:B:247:GLU:O	2:B:348:ARG:NH2	2.18	0.77
2:A:326:ASN:HD22	2:A:326:ASN:H	1.33	0.77
2:B:57:THR:CG2	2:B:57:THR:O	2.32	0.76
2:C:21:GLN:CB	2:C:181:LEU:HD11	2.15	0.76
2:B:179:SER:HB3	2:B:183:GLN:HG3	1.67	0.76
1:N:8:U:O2'	1:N:9:C:H5'	1.85	0.76
2:A:182:MET:O	2:A:182:MET:HG3	1.85	0.75
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
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:C:68:LYS:CD	2:C:76:PHE:CZ	2.70	0.74
3:F:369:ARG:O	3:F:373:ILE:HG13	1.87	0.74
2:A:105:PHE:CE2	2:A:301:VAL:HG21	2.22	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:CD1	2:A:56:LEU:N	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:C:20:THR:O	2:C:181:LEU:HD13	1.90	0.72
2:A:201:GLN:NE2	2:B:264:PRO:HB3	2.04	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
3:E:368:GLU:CD	3:E:371:LYS:HZ2	1.79	0.71
2:B:199:ASN:OD1	5:B:429:HOH:O	2.08	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:286:SER:OG	2:C:287:GLY:N	2.23	0.71
2:C:72:ALA:HB1	2:C:75:ASP:OD2	1.89	0.71
2:C:25:VAL:HG13	2:C:27:GLN:HE22	1.38	0.70
2:A:162:GLN:HE21	2:A:327:ALA:HB1	1.56	0.70
3:F:366:MET:O	3:F:370:VAL:HG23	1.90	0.70
2:A:169:ALA:O	5:A:420:HOH:O	2.08	0.70
2:A:87:ARG:NH1	2:C:345:GLN:NE2	2.39	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
2:B:206:THR:HG23	2:B:207: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
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:160:SER:HB3	2:C:255:ILE:CG2	2.21	0.70
2:C:55:ALA:N	2:C:57:THR:HB	2.07	0.70
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:C:20:THR:CA	2:C:21:GLN:HE21	1.98	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:C:167:ARG:NH1	2:C:320:GLU:OE1	2.25	0.68
2:C:108:ASN:CG	2:C:305:THR:HG22	2.14	0.68
2:B:207:THR:HG23	2:B:208:PRO:N	2.08	0.68
2:B:85:PRO:HB2	2:B:340:ASP:HB3	1.76	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:B:206:THR:HG23	2:B:207:THR:N	2.10	0.67
2:A:165:SER:OG	2:C:196:LYS:HE3	1.95	0.67
2:A:207:THR:C	2:A:209:ALA:N	2.48	0.66
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:207:THR:C	2:A:209:ALA:H	1.96	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:A:354:LEU:HD22	3:D:366:MET:HE3	1.77	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: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
3:E:367:TRP:O	3:E:371:LYS:HB2	1.97	0.64
2:A:322:ARG:HH22	2:C:295:ASP:CG	1.99	0.64
2:C:172:ASN:HD22	2:C:242:GLN:HB3	1.61	0.64
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:B:340:ASP:C	2:B:340:ASP:OD1	2.36	0.64
2:C:256:LEU:HD12	2:C:290:GLY:HA2	1.79	0.64
2:C:154:ASN:N	2:C:154:ASN:ND2	2.46	0.63
2:C:25:VAL:HG12	2:C:27:GLN:HE21	1.59	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: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:B:183:GLN:HB2	2:B:308:VAL:HG13	1.80	0.63
2:A:331:GLN:N	2:A:331:GLN:HE21	1.97	0.63
2:C:303:ALA:HB2	2:C:309:ASN:ND2	2.14	0.63
2:C:246:ASN:HD22	2:C:247:GLU:HG2	1.64	0.62
2:A:264:PRO:O	2:A:267:VAL:HG13	1.98	0.62
2:C:20:THR:C	2:C:21:GLN:CD	2.58	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:A:162:GLN:HG3	2:A:329:LEU:HD13	1.82	0.62
2:B:246:ASN:HD22	2:B:246:ASN:C	2.02	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:246:ASN:C	2:A:246:ASN:HD22	2.03	0.62
2:A:264:PRO:HG2	2:A:267:VAL:HG11	1.82	0.62
2:A:206:THR:HG22	2:C:208:PRO:HG2	1.82	0.61
1:N:2:C:N3	1:N:3:U:C4	2.68	0.61
2:A:106:THR:HG22	2:A:109:ARG:CG	2.30	0.61
2:C:154:ASN:N	2:C:154:ASN:HD22	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: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:65:ALA:CB	2:B:82:LYS:HD3	2.31	0.61
2:B:204:VAL:CG2	2:B:210:THR:OG1	2.43	0.61
2:B:80:PRO:O	2:B:81:GLY:O	2.18	0.61
1:N:5:A:H2'	1:N:6:U:C5'	2.29	0.60
2:C:345:GLN:O	2:C:349:THR:HG23	2.01	0.60
2:A:326:ASN:ND2	2:A:326:ASN:H	1.98	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: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: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:A:359:ILE:HD11	2:A:362:GLN:HG3	1.83	0.60
2:C:135:ILE:HD11	2:C:137:THR:HB	1.82	0.60
3:E:366:MET:O	3:E:370:VAL:HG23	2.01	0.60
2:B:326:ASN:HD22	2:B:326:ASN:H	1.49	0.60
2:A:200:VAL:CG1	2:A:214:VAL:HG12	2.31	0.60
2:A:313:LEU:C	2:A:313:LEU:HD23	2.23	0.60
2:C:21:GLN:NE2	2:C:21:GLN:N	2.34	0.60
2:A:61:GLN:CB	2:A:62:PRO:HD3	2.28	0.59
1:N:7:A:H2'	1:N:8:U:H5'	1.84	0.59
2:A:123:TYR:CE2	2:A:125:VAL:HG22	2.37	0.59
2:A:295:ASP:CG	2:B:322:ARG:HH22	2.05	0.59
1:N:2:C:H2'	1:N:3:U:H6	1.68	0.59
2:A:215:HIS:NE2	5:A:433:HOH:O	2.31	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:232:SER:O	2:A:233:GLU:HB2	2.01	0.59
2:A:121:VAL:HA	2:A:144:ASN:HA	1.82	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:108:ASN:CG	2:C:305:THR:CG2	2.71	0.59
1:N:1:U:O2	1:N:1:U:H2'	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: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:C:100:ASN:CG	2:C:314:LYS:HE2	2.22	0.58
2:C:135:ILE:CD1	2:C:137:THR:HB	2.33	0.58
2:A:68:LYS:HD2	2:A:76:PHE:CZ	2.38	0.58
2:C:200:VAL:HG12	2:C:214:VAL:CG2	2.33	0.58
2:C:363:ASN:O	3:F:365:SER:HA	2.03	0.58
2:B:75:ASP:OD1	2:B:363:ASN:O	2.21	0.58
2:C:207:THR:C	2:C:209:ALA:N	2.55	0.58
2:C:73:PRO:N	2:C:74:PRO:CD	2.66	0.58
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: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:182:MET:HG3	2:B:182:MET:O	2.02	0.57
2:C:117:PRO:HB3	2:C:171:MET:HE1	1.85	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:C:108:ASN:O	2:C:109:ARG:HG2	2.04	0.57
2:B:108:ASN:HB2	2:B:305:THR:OG1	2.03	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: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:C:206:THR:HG22	2:C:210:THR:N	2.21	0.56
2:A:99:LEU:HB3	2:A:315:THR:CG2	2.35	0.56
2:C:82:LYS:HE3	2:C:334:HIS:HD1	1.66	0.56
2:A:104:ASN:HD22	2:A:310:SER:HB3	1.71	0.56
2:C:197:LEU:CD1	2:C:217:LEU:HD13	2.35	0.56
2:A:217:LEU:HB3	2:A:220:LEU:HD22	1.88	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:C:206:THR:HG22	2:C:209:ALA:CA	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:68:LYS:CD	2:C:76:PHE:CE1	2.88	0.56
2:B:109:ARG:HD2	2:B:128:VAL:O	2.06	0.56
2:A:87:ARG:NH1	2:C:345:GLN:HE21	2.04	0.56
2:C:117:PRO:HA	2:C:171:MET:HE2	1.87	0.56
2:C:82:LYS:O	2:C:334:HIS:CE1	2.59	0.55
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:B:80:PRO:O	2:B:81:GLY:C	2.44	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:B:167:ARG:HD2	2:B:252:PHE:CZ	2.41	0.55
2:A:144:ASN:N	2:A:144:ASN:HD22	2.05	0.55
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:A:329:LEU:C	2:A:329:LEU:HD23	2.27	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:C:73:PRO:N	2:C:74:PRO:HD2	2.22	0.55
2:B:125:VAL:HG22	2:B:126:ALA:N	2.22	0.55
2:A:91:LYS:NZ	2:C:229:ASP:OD2	2.34	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:360:ALA:O	2:A:363:ASN:ND2	2.38	0.54
2:C:197:LEU:HD13	2:C:217:LEU:CD1	2.37	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:360:ALA:O	2:C:362:GLN:N	2.41	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:A:181:LEU:HD12	2:A:236:ILE:HG12	1.89	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:B:245:CYS:CA	2:B:294:MET:CE	2.76	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:C:61:GLN:CB	2:C:62:PRO:HD3	2.37	0.54
2:A:136:SER:HA	2:A:275:PRO:O	2.08	0.54
2:A:81:GLY:O	2:A:96:LYS:HE3	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:348:ARG:HG2	2:C:87:ARG:O	2.08	0.54
2:B:67:LEU:HD13	3:E:374:ILE:HD11	1.90	0.54
2:A:359:ILE:CD1	2:A:362:GLN:HG3	2.38	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:B:340:ASP:OD2	2:B:343:ALA:HB2	2.09	0.53
3:D:366:MET:O	3:D:369:ARG:HB3	2.08	0.53
2:A:96:LYS:HD3	2:A:318:CYS:SG	2.48	0.53
2:C:70:ALA:HA	2:C:170:SER:HB2	1.89	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: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:236:ILE:HG13	2:C:236:ILE:O	2.09	0.53
2:B:94:THR:HG22	2:B:320:GLU:HG2	1.91	0.53
2:C:181:LEU:CD2	2:C:236:ILE:HG12	2.38	0.52
2:B:61:GLN:N	2:B:62:PRO:CD	2.71	0.52
2:C:280:ALA:CB	2:C:287:GLY:HA2	2.39	0.52
2:A:173:VAL:HG11	2:A:299:ILE:HD11	1.91	0.52
2:B:277:ASN:OD1	2:B:277:ASN:C	2.47	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:B:263:PRO:HD3	2:B:274:GLN:NE2	2.24	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: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:277:ASN:HD22	2:C:277:ASN:N	2.08	0.51
2:C:197:LEU:HD13	2:C:217:LEU:HD13	1.92	0.51
2:B:195:VAL:HG22	2:B:195:VAL:O	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:232:SER:O	2:B:233:GLU:HB2	2.10	0.51
2:C:144:ASN:OD1	2:C:286:SER:HB2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:199:ASN:CA	2:B:216:THR:HG22	2.41	0.51
2:C:235:PHE:C	2:C:237:LYS:H	2.14	0.51
3:E:366:MET:O	3:E:366:MET:SD	2.69	0.51
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: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:A:354:LEU:CD2	3:D:366:MET:HE1	2.41	0.51
2:A:354:LEU:CD2	3:D:366:MET:CE	2.89	0.50
2:C:71:PHE:O	2:C:242:GLN:NE2	2.44	0.50
2:B:341:GLU:CD	2:C:87:ARG:HH22	2.14	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
2:B:193:CYS:SG	2:C:325:PRO:HG2	2.51	0.50
2:B:189:THR:HA	2:B:231:PHE:O	2.10	0.50
2:B:233:GLU:CG	2:B:237:LYS:HD2	2.38	0.50
2:A:161:ASP:N	2:A:161:ASP:OD1	2.44	0.50
2:A:263:PRO:HD2	2:A:277:ASN:CG	2.31	0.50
2:C:324:ASN:HB3	2:C:326:ASN:OD1	2.12	0.50
2:A:116:ALA:HB2	2:A:296:THR:HG23	1.93	0.50
2:B:199:ASN:C	2:B:216:THR:HG22	2.32	0.50
2:A:322:ARG:NH2	2:C:295:ASP:OD1	2.45	0.50
2:B:99:LEU:O	2:B:314:LYS:HA	2.12	0.50
1:N:7:A:C2'	1:N:8:U:H5'	2.41	0.50
2:A:73:PRO:CB	2:A:74:PRO:HD3	2.42	0.50
2:B:92:VAL:HA	2:B:323:PRO:HD3	1.94	0.50
2:C:246:ASN:C	2:C:247:GLU:HG2	2.32	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:C:201:GLN:HA	2:C:212:ALA:O	2.11	0.50
2:C:21:GLN:HA	2:C:181:LEU:HD21	1.94	0.50
2:B:195:VAL:CG2	2:B:291:TRP:CZ2	2.94	0.50
2:A:208:PRO:HG2	2:B:206:THR:HA	1.94	0.49
3:F:367:TRP:CE2	3:F:371:LYS:HG3	2.46	0.49
2:C:81:GLY:O	2:C:96:LYS:NZ	2.33	0.49
2:C:81:GLY:C	2:C:96:LYS:HZ1	2.14	0.49
2:B:207:THR:C	2:B:209:ALA:N	2.64	0.49
2:A:73:PRO:CD	2:A:74:PRO:HD2	2.41	0.49
2:B:213:LEU:CD2	2:C:213:LEU:HD23	2.39	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
3:E:366:MET:HE1	3:E:369:ARG:HD2	1.93	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
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:C:264:PRO:C	2:C:267:VAL:HG13	2.21	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:A:156:ALA:O	2:A:258:GLY:N	2.38	0.49
2:B:355:PRO:HG2	2:B:358:VAL:HG12	1.95	0.49
2:B:341:GLU:OE1	2:C:87:ARG:NH2	2.46	0.48
2:B:73:PRO:CG	2:B:74:PRO:HD3	2.43	0.48
2:C:200:VAL:CG1	2:C:200:VAL:O	2.60	0.48
2:C:99:LEU:HB3	2:C:315:THR:HG23	1.94	0.48
2:B:341:GLU:CA	2:B:341:GLU:OE1	2.61	0.48
2:C:280:ALA:HB1	2:C:286:SER:OG	2.13	0.48
2:C:246:ASN:HD21	2:C:293:ASN:HB3	1.77	0.48
2:A:183:GLN:NE2	2:A:308:VAL:HG11	2.28	0.48
2:A:172:ASN:HD22	2:A:242:GLN:HB3	1.77	0.48
2:A:204:VAL:CG1	2:A:206:THR:HG23	2.42	0.48
2:A:181:LEU:CD1	2:A:236:ILE:HG12	2.43	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:C:20:THR:C	2:C:21:GLN:CG	2.82	0.48
2:B:65:ALA:CB	2:B:82:LYS:CD	2.92	0.48
2:A:201:GLN:OE1	2:B:264:PRO:HG3	2.14	0.48
2:A:144:ASN:H	2:A:144:ASN:HD22	1.61	0.48
2:C:59:LEU:CD2	2:C:342:VAL:HG12	2.44	0.48
2:B:233:GLU:CD	2:B:237:LYS:HZ3	2.17	0.48
2:C:319:LEU:CD2	2:C:319:LEU:N	2.77	0.48
2:C:133:PHE:HB3	2:C:134:PRO:HD2	1.95	0.48
2:C:256:LEU:CD1	2:C:290:GLY:HA2	2.42	0.48
2:C:61:GLN:HB2	2:C:62:PRO:CD	2.43	0.48
2:C:151:MET:HG2	2:C:152:PHE:CE2	2.48	0.48
2:A:244:VAL:C	2:A:294:MET:HE3	2.35	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:121:VAL:HA	2:B:144:ASN:HA	1.96	0.48
2:C:360:ALA:O	2:C:363:ASN:N	2.47	0.47
2:B:94:THR:HA	2:B:319:LEU:O	2.14	0.47
2:C:72:ALA:C	2:C:74:PRO:HD2	2.34	0.47
2:C:133:PHE:HB3	2:C:134:PRO:CD	2.43	0.47
2:B:201:GLN:HA	2:B:212:ALA:O	2.14	0.47
2:A:325:PRO:HB3	2:C:227:GLY:HA3	1.95	0.47
2:C:92:VAL:HA	2:C:321:TYR:O	2.14	0.47
2:A:160:SER:HA	2:A:163:VAL:O	2.15	0.47
2:C:277:ASN:ND2	2:C:277:ASN:N	2.62	0.47
2:A:117:PRO:HB2	2:A:292:GLY:HA3	1.94	0.47
2:C:121:VAL:HA	2:C:144:ASN:HA	1.96	0.47
2:B:210:THR:HB	2:B:211:SER:H	1.49	0.47
2:A:165:SER:OG	2:C:196:LYS:CE	2.62	0.47
2:A:145:PHE:CE1	2:A:315:THR:O	2.68	0.47
2:C:91:LYS:HE3	2:C:330:TYR:CZ	2.50	0.47
2:C:264:PRO:HG2	2:C:267:VAL:HG11	1.97	0.47
2:B:326:ASN:ND2	2:B:326:ASN:H	2.11	0.47
2:A:264:PRO:CG	2:A:267:VAL:HG11	2.45	0.47
2:C:159:ARG:HD3	2:C:289:VAL:HG12	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: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:207:THR:O	2:C:208:PRO:C	2.52	0.46
2:A:73:PRO:HD2	2:A:74:PRO:HD2	1.97	0.46
2:B:63:GLY:O	2:B:66:PHE:HB3	2.15	0.46
2:A:94:THR:CG2	2:A:319:LEU:O	2.63	0.46
2:C:21:GLN:HG2	2:C:181:LEU:CD1	2.35	0.46
2:B:329:LEU:C	2:B:329:LEU:HD23	2.35	0.46
2:A:105:PHE:CZ	2:A:301:VAL:HG21	2.50	0.46
2:C:96:LYS:CE	5:C:373:HOH:O	2.61	0.46
2:C:264:PRO:CG	2:C:267:VAL:HG11	2.45	0.46
2:A:73:PRO:HG2	2:A:74:PRO:HD3	1.97	0.46
2:C:264:PRO:C	2:C:267:VAL:CG1	2.80	0.46
2:A:128:VAL:HB	2:A:129:PRO:HD2	1.96	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:C:68:LYS:HG2	2:C:76:PHE:CZ	2.51	0.46
2:A:162:GLN:NE2	2:A:327:ALA:CB	2.70	0.46
2:A:264:PRO:C	2:A:267:VAL:HG13	2.36	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:188:ILE:O	2:A:232:SER:HA	2.15	0.46
2:C:129:PRO:O	2:C:132:THR:HG23	2.15	0.46
2:B:202:PHE:CD1	2:B:202:PHE:N	2.84	0.46
2:A:223:VAL:HG12	2:A:223:VAL:O	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:322:ARG:NH2	2:C:295:ASP:CG	2.67	0.46
2:A:99:LEU:O	2:A:314:LYS:HA	2.16	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:A:246:ASN:ND2	2:A:247:GLU:HG2	2.30	0.46
2:C:200:VAL:HG12	2:C:214:VAL:HG23	1.97	0.46
2:B:86:ASP:HA	2:B:344:LEU:HD11	1.96	0.46
3:F:364:ALA:C	3:F:364:ALA:CB	2.73	0.46
2:B:293:ASN:O	2:B:294:MET:HE2	2.16	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:C:82:LYS:O	2:C:334:HIS:HE1	1.98	0.45
2:B:73:PRO:CD	2:B:74:PRO:HD2	2.46	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:B:273:GLY:C	5:B:416:HOH:O	2.54	0.45
2:C:98:VAL:CG1	2:C:316:TRP:CD1	2.93	0.45
2:C:188:ILE:O	2:C:232:SER:HA	2.16	0.45
2:B:96:LYS:HZ3	2:B:96:LYS:HG3	1.67	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:139:THR:CG2	5:C:416:HOH:O	2.62	0.45
2:A:247:GLU:O	2:A:348:ARG:NH2	2.48	0.45
2:B:208:PRO:O	2:B:209:ALA:HB3	2.16	0.45
2:A:358:VAL:HG13	2:A:359:ILE:O	2.17	0.45
2:A:331:GLN:H	2:A:331:GLN:NE2	2.15	0.44
2:A:194:PRO:HB3	2:B:322:ARG:NH2	2.31	0.44
2:C:186:GLY:HA3	2:C:302:SER:O	2.17	0.44
2:C:21:GLN:HG2	2:C:181:LEU:HD11	1.79	0.44
2:A:159:ARG:HD3	2:A:289:VAL:CG1	2.44	0.44
3:F:367:TRP:HE1	3:F:371:LYS:HD3	1.82	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
2:B:268:THR:CG2	2:B:270:ALA:HB3	2.47	0.44
2:A:113:ILE:HG12	2:A:125:VAL:HG13	1.99	0.44
2:A:94:THR:HA	2:A:319:LEU:O	2.18	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:C:113:ILE:HG22	2:C:115:ILE:HD12	2.00	0.44
2:B:73:PRO:CD	2:B:74:PRO:CD	2.96	0.44
2:C:171:MET:HE3	2:C:294:MET:HG3	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:C:93:VAL:CG2	2:C:93:VAL:O	2.65	0.44
2:B:207:THR:O	2:B:208:PRO:C	2.56	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:B:313:LEU:HD23	2:B:313:LEU:C	2.38	0.43
2:C:280:ALA:HB3	2:C:287:GLY:HA2	2.00	0.43
2:C:319:LEU:HD22	2:C:319:LEU:N	2.33	0.43
2:C:207:THR:CG2	2:C:208:PRO:CD	2.84	0.43
2:C:82:LYS:O	2:C:82:LYS:HG3	2.17	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:B:184:PHE:C	2:B:184:PHE:CD2	2.87	0.43
2:C:109:ARG:HD3	2:C:127:ASP:OD1	2.19	0.43
2:C:181:LEU:HD23	2:C:236:ILE:HG12	2.00	0.43
2:C:25:VAL:O	2:C:25:VAL:CG1	2.66	0.43
2:B:125:VAL:CG2	2:B:126:ALA:N	2.80	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:C:116:ALA:HA	2:C:296:THR:HB	2.01	0.43
2:B:191:TRP:CZ3	2:B:226:VAL:HG22	2.54	0.43
2:B:179:SER:HA	2:B:183:GLN:OE1	2.19	0.43
2:B:354:LEU:HB3	2:B:355:PRO:HD2	2.00	0.43
2:A:295:ASP:OD1	2:B:322:ARG:NH2	2.52	0.43
2:C:254:ASP:HB2	5:C:411:HOH:O	2.18	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:319:LEU:N	2:B:319:LEU:HD23	2.34	0.43
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:A:206:THR:CA	2:C:208:PRO:HG2	2.49	0.42
3:E:368:GLU:OE1	3:E:368:GLU:CA	2.44	0.42
2:C:134:PRO:HB3	2:C:138:THR:HG21	2.00	0.42
2:C:337:PRO:HA	2:C:338:PRO:HD3	1.90	0.42
1:N:8:U:O2'	1:N:9:C:C5'	2.63	0.42
2:C:135:ILE:N	2:C:138:THR:OG1	2.36	0.42
2:B:65:ALA:HB3	2:B:82:LYS:HD3	1.99	0.42
2:A:205:ALA:O	2:A:206:THR:C	2.56	0.42
2:B:67:LEU:HD23	2:B:67:LEU:HA	1.84	0.42
2:A:246:ASN:C	2:A:246:ASN:ND2	2.72	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: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:146:PRO:HG2	5:B:380:HOH:O	2.18	0.42
2:C:20:THR:O	2:C:21:GLN:CG	2.67	0.42
2:B:217:LEU:HA	2:B:217:LEU:HD12	1.86	0.42
2:A:261:THR:O	2:A:264:PRO:HA	2.20	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:B:354:LEU:HD22	3:E:366:MET:HE1	2.01	0.42
2:A:276:PHE:HB2	2:A:277:ASN:H	1.67	0.42
2:C:206:THR:HG22	2:C:209:ALA:C	2.40	0.42
2:B:267:VAL:O	2:B:267:VAL:HG22	2.20	0.42
2:B:167:ARG:HD2	2:B:252:PHE:CD1	2.52	0.42
2:A:215:HIS:CD2	2:A:259:ILE:HD11	2.54	0.42
2:B:167:ARG:HD3	2:B:167:ARG:HH11	1.71	0.42
2:A:183:GLN:NE2	2:A:308:VAL:CG1	2.83	0.42
2:A:159:ARG:HH12	2:A:260:GLN:HE22	1.67	0.42
2:B:128:VAL:HB	2:B:129:PRO:HD2	2.02	0.42
2:C:304:PRO:HG3	5:C:384:HOH:O	2.19	0.42
2:A:220:LEU:HD12	2:A:220:LEU:HA	1.79	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:A:275:PRO:HB2	2:A:276:PHE:CD1	2.55	0.41
2:B:181:LEU:HA	2:B:181:LEU:HD12	1.81	0.41
2:C:322:ARG:HA	2:C:322:ARG:HD2	1.83	0.41
3:E:371:LYS:HB2	3:E:371:LYS:HE3	1.66	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:91:LYS:O	2:C:322:ARG:HD2	2.20	0.41
2:A:295:ASP:CG	2:B:322:ARG:NH2	2.72	0.41
2:B:195:VAL:CG2	2:B:195:VAL:O	2.68	0.41
2:A:159:ARG:NH1	2:A:260:GLN:HE22	2.19	0.41
2:B:124:TRP:HA	2:B:141:ASN:O	2.20	0.41
2:A:259:ILE:HD11	5:A:433:HOH:O	2.21	0.41
2:C:68:LYS:CG	2:C:76:PHE:CZ	3.03	0.41
2:B:202:PHE:HE1	2:B:214:VAL:HG13	1.85	0.41
2:B:194:PRO:HB2	2:C:164:SER:OG	2.20	0.41
2:C:262:LEU:HA	2:C:262:LEU:HD12	1.95	0.41
2:A:167:ARG:CG	2:A:252:PHE:CE2	3.04	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
3:E:366:MET:CE	3:E:369:ARG:HD2	2.51	0.41
2:B:176:TYR:CE1	2:B:363:ASN:OD1	2.73	0.41
2:C:328:MET:HG2	2:C:328:MET:O	2.20	0.41
2:C:78:THR:O	2:C:80:PRO:HD3	2.21	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
2:A:206:THR:O	2:A:209:ALA:CA	2.65	0.40
2:C:204:VAL:CG2	2:C:206:THR:HB	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: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:360:ALA:C	2:C:362:GLN:N	2.74	0.40
2:B:163:VAL:CG2	2:B:321:TYR:HB3	2.51	0.40
1:N:10:U:H4'	2:C:55:ALA:CB	2.52	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%)	19	52
2	B	306/363 (84%)	278 (91%)	25 (8%)	3 (1%)	19	52
2	C	317/363 (87%)	296 (93%)	18 (6%)	3 (1%)	21	55
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	3
All	All	971/1221 (80%)	892 (92%)	69 (7%)	10 (1%)	19	52

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%)	196 (78%)	55 (22%)	1	3
2	B	251/301 (83%)	202 (80%)	49 (20%)	2	5
2	C	263/301 (87%)	202 (77%)	61 (23%)	1	3
3	D	14/32 (44%)	5 (36%)	9 (64%)	0	0
3	E	14/32 (44%)	9 (64%)	5 (36%)	0	0
3	F	14/32 (44%)	10 (71%)	4 (29%)	0	1
All	All	807/999 (81%)	624 (77%)	183 (23%)	1	3

All (183) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	56	LEU
2	A	57	THR
2	A	60	SER
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	94	THR
2	A	95	ARG
2	A	96	LYS
2	A	102	SER
2	A	109	ARG
2	A	125	VAL
2	A	132	THR
2	A	144	ASN
2	A	154	ASN
2	A	159	ARG
2	A	160	SER
2	A	161	ASP
2	A	162	GLN
2	A	167	ARG
2	A	175	ILE
2	A	181	LEU
2	A	182	MET
2	A	184	PHE
2	A	196	LYS
2	A	201	GLN
2	A	211	SER

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Mol	Chain	Res	Type
2	A	214	VAL
2	A	217	LEU
2	A	220	LEU
2	A	232	SER
2	A	234	SER
2	A	239	VAL
2	A	242	GLN
2	A	246	ASN
2	A	267	VAL
2	A	268	THR
2	A	271	THR
2	A	275	PRO
2	A	283	GLU
2	A	294	MET
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	353	SER
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
3	D	376	SER
3	D	378	LEU
2	B	57	THR
2	B	60	SER
2	B	61	GLN
2	B	78	THR
2	B	82	LYS
2	B	91	LYS
2	B	96	LYS
2	B	103	ILE

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Mol	Chain	Res	Type
2	B	109	ARG
2	B	137	THR
2	B	154	ASN
2	B	159	ARG
2	B	160	SER
2	B	164	SER
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	211	SER
2	B	214	VAL
2	B	217	LEU
2	B	220	LEU
2	B	236	ILE
2	B	242	GLN
2	B	246	ASN
2	B	261	THR
2	B	267	VAL
2	B	268	THR
2	B	277	ASN
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	338	PRO
2	B	346	GLU
2	B	348	ARG
2	B	349	THR
2	B	362	GLN
2	B	363	ASN
3	E	366	MET

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Mol	Chain	Res	Type
3	E	368	GLU
3	E	369	ARG
3	E	371	LYS
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	61	GLN
2	C	86	ASP
2	C	87	ARG
2	C	91	LYS
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	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

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Mol	Chain	Res	Type
2	C	232	SER
2	C	233	GLU
2	C	242	GLN
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	314	LYS
2	C	315	THR
2	C	319	LEU
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	359	ILE
2	C	363	ASN
3	F	368	GLU
3	F	369	ARG
3	F	376	SER
3	F	377	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	61	GLN
2	A	104	ASN
2	A	144	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

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Mol	Chain	Res	Type
2	A	331	GLN
2	B	61	GLN
2	B	154	ASN
2	B	201	GLN
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	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
2	C	242	GLN
2	C	246	ASN
2	C	277	ASN
2	C	331	GLN
2	C	345	GLN
2	C	362	GLN

5.3.3 RNA ⓘ

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 carbohydrates 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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.