wwPDB EM Map/Model Validation Report (i)

Apr 10, 2016 – 01:39 PM BST

PDB ID	:	3BO1
EMDB ID:	:	EMD-1484
Title	:	Ribosome-SecY complex
Authors	:	Akey, C.W.; Menetret, J.F.
Deposited on	:	2007-12-15
Resolution	:	9.60 Å(reported)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could
stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/EMValidationReportHelp

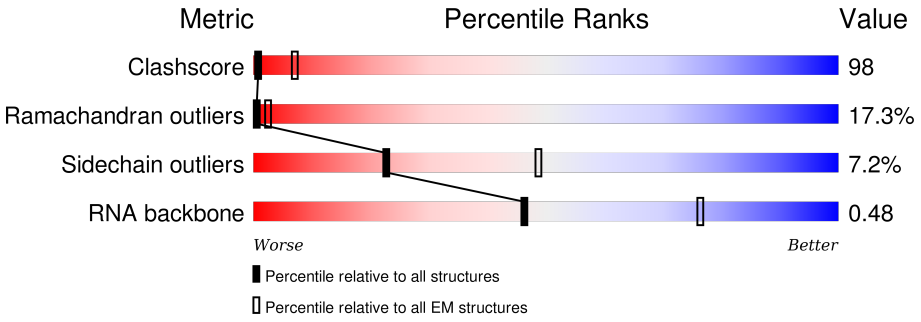
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk27241

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 9.60 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)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686
RNA backbone	3027	244

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

Mol	Chain	Length	Quality of chain
1	D	27	33% 44% 22%
2	E	27	44% 41% 15%
3	F	19	42% 47% 5% 5%
4	G	32	34% 53% 13%
5	A	442	22% 56% 20% •
6	B	65	25% 60% 15%
7	C	32	41% 56% •

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 6432 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 23S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	D	27	579	259	106	187	27	0	0

- Molecule 2 is a RNA chain called 23S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	E	27	592	264	122	179	27	0	0

- Molecule 3 is a RNA chain called 23S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	F	19	401	180	68	134	19	0	0

- Molecule 4 is a RNA chain called 23S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
4	G	32	691	308	131	220	32	0	0

- Molecule 5 is a protein called PREPROTEIN TRANSLOCASE SecY SUBUNIT.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	A	442	3407	2266	547	576	18	0	0

- Molecule 6 is a protein called PREPROTEIN TRANSLOCASE SecE SUBUNIT.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
6	B	65	505	332	88	85	0	0

- Molecule 7 is a protein called Preprotein translocase secG subunit.

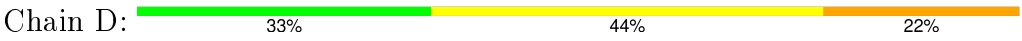
Mol	Chain	Residues	Atoms				AltConf	Trace
7	C	32	Total	C	N	O	0	0
			257	172	42	43		

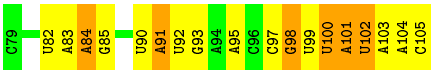
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: 23S RIBOSOMAL RNA

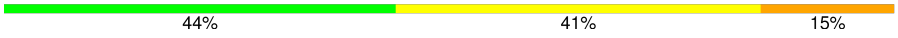
Chain D:

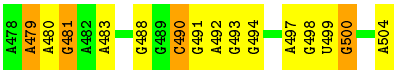




- Molecule 2: 23S RIBOSOMAL RNA

Chain E:





- Molecule 3: 23S RIBOSOMAL RNA

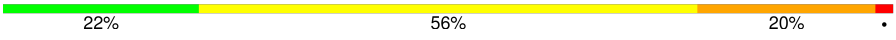
Chain F:

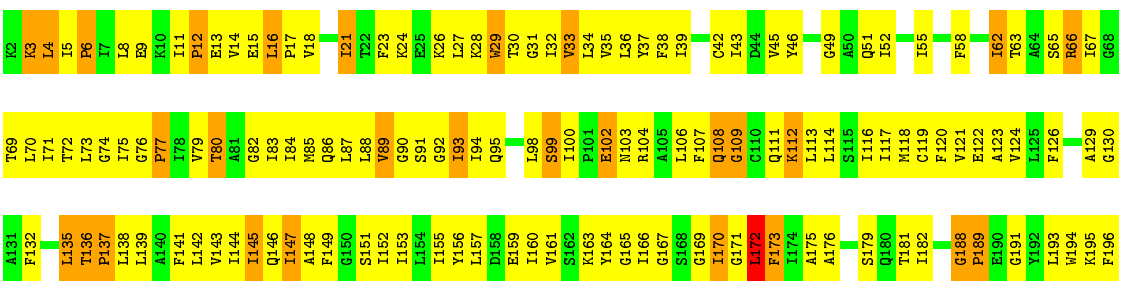
- Molecule 4: 23S RIBOSOMAL RNA

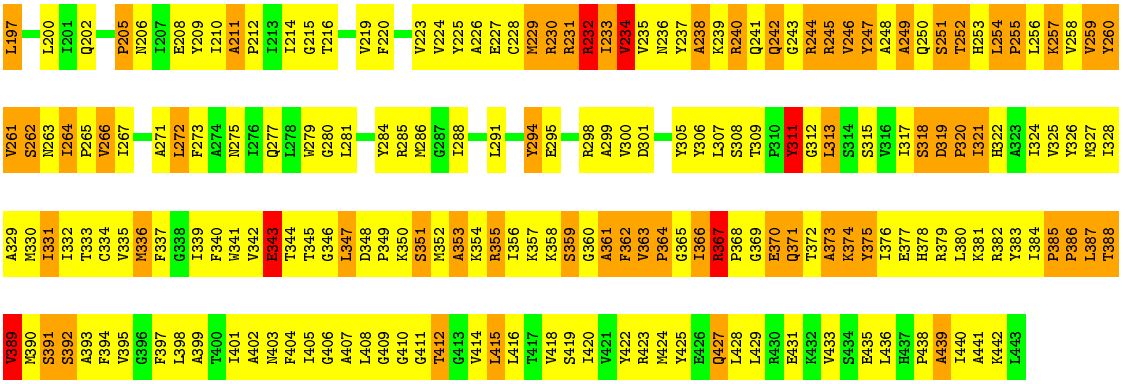
Chain G:

- Molecule 5: PREPROTEIN TRANSLOCASE SecY SUBUNIT

Chain A:

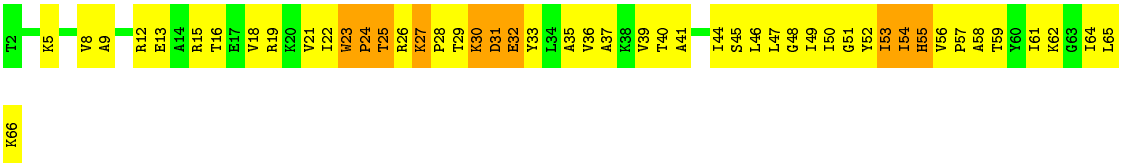






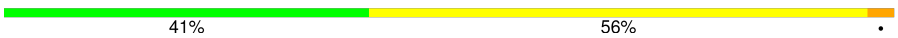
- Molecule 6: PREPROTEIN TRANSLOCASE SecE SUBUNIT

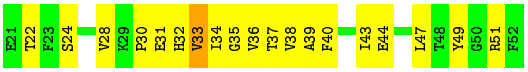
Chain B:



- Molecule 7: Preprotein translocase secG subunit

Chain C:





4 Experimental information (i)

Property	Value	Source
Reconstruction method	Not provided	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	EMAN- phase flipping of particles form the same micrograph	Depositor
Microscope	TF20	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	1500	Depositor
Minimum defocus (nm)	-700	Depositor
Maximum defocus (nm)	-3000	Depositor
Magnification	50000	Depositor
Image detector	Not provided	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>2$	RMSZ	#$\|Z\|>2$
1	D	0.27	0/648	0.69	0/1008
2	E	0.21	0/666	0.70	0/1039
3	F	0.20	0/447	0.76	1/693 (0.1%)
4	G	0.24	0/774	0.71	0/1206
5	A	0.37	0/3483	0.60	0/4732
6	B	0.37	0/514	0.60	0/694
7	C	0.38	0/262	0.55	0/354
All	All	0.33	0/6794	0.64	1/9726 (0.0%)

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	E	0	1
4	G	0	1
5	A	3	0
All	All	3	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	1397	U	C5'-C4'-C3'	-5.62	107.01	116.00

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	A	238	ALA	CA
5	A	244	ARG	CA
5	A	373	ALA	CA

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	E	500	G	Sidechain
4	G	1546	G	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	D	579	0	291	19	0
2	E	592	0	297	17	0
3	F	401	0	203	16	0
4	G	691	0	348	24	0
5	A	3407	0	3619	937	0
6	B	505	0	557	262	0
7	C	257	0	272	31	0
All	All	6432	0	5587	1178	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 98.

All (1178) 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)
5:A:233:ILE:CG1	5:A:254:LEU:HB2	1.23	1.58
5:A:261:VAL:CG2	5:A:388:THR:HG22	1.32	1.52
6:B:26:ARG:CB	6:B:29:THR:HA	1.39	1.52
5:A:366:ILE:HG13	5:A:368:PRO:CD	1.37	1.50
6:B:26:ARG:CZ	6:B:30:LYS:HB2	1.39	1.50
5:A:239:LYS:HB2	5:A:240:ARG:CZ	1.41	1.50
5:A:234:VAL:CG1	5:A:235:VAL:HA	1.35	1.49
5:A:230:ARG:HG2	5:A:255:PRO:CG	1.42	1.49
5:A:389:VAL:HB	5:A:390:MET:CB	1.44	1.48
5:A:233:ILE:HG12	5:A:254:LEU:CB	1.38	1.47
5:A:389:VAL:CG1	5:A:390:MET:HA	1.44	1.46
5:A:261:VAL:HG21	5:A:388:THR:CG2	1.46	1.45
5:A:230:ARG:CG	5:A:255:PRO:HG2	1.48	1.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:331:ILE:CD1	5:A:393:ALA:HA	1.51	1.41
5:A:236:ASN:HB2	5:A:251:SER:CB	1.46	1.40
6:B:26:ARG:C	6:B:27:LYS:HD3	1.38	1.40
5:A:389:VAL:CG1	5:A:391:SER:HB3	1.50	1.40
5:A:393:ALA:O	5:A:397:PHE:CB	1.72	1.37
5:A:389:VAL:HG12	5:A:391:SER:CB	1.55	1.35
5:A:254:LEU:HB3	5:A:255:PRO:CA	1.53	1.35
6:B:26:ARG:HB3	6:B:29:THR:CA	1.57	1.34
5:A:366:ILE:CG1	5:A:368:PRO:HD3	1.56	1.33
5:A:239:LYS:O	5:A:366:ILE:CD1	1.75	1.31
5:A:234:VAL:CB	5:A:235:VAL:HA	1.53	1.31
5:A:241:GLN:HB2	5:A:246:VAL:O	1.13	1.29
5:A:228:CYS:CB	6:B:33:TYR:HD2	1.46	1.29
5:A:331:ILE:O	5:A:392:SER:HB2	1.30	1.29
5:A:254:LEU:CB	5:A:255:PRO:HA	1.49	1.28
5:A:232:ARG:HA	5:A:233:ILE:CB	1.61	1.28
5:A:236:ASN:CB	5:A:251:SER:HB2	1.61	1.27
5:A:363:VAL:HG22	5:A:364:PRO:CD	1.64	1.27
5:A:331:ILE:HD12	5:A:393:ALA:CA	1.62	1.27
5:A:38:PHE:CE1	6:B:50:ILE:HG23	1.70	1.25
5:A:365:GLY:O	5:A:366:ILE:HG12	1.30	1.25
5:A:360:GLY:CA	5:A:370:GLU:OE2	1.82	1.25
5:A:390:MET:HG2	6:B:15:ARG:NH1	1.49	1.24
5:A:232:ARG:CA	5:A:233:ILE:HB	1.68	1.24
5:A:176:ALA:N	6:B:47:LEU:HD21	1.51	1.23
5:A:241:GLN:HB3	5:A:247:TYR:C	1.56	1.23
5:A:335:VAL:HG23	5:A:392:SER:OG	1.38	1.23
5:A:389:VAL:CB	5:A:390:MET:HB3	1.67	1.23
6:B:26:ARG:HG2	6:B:30:LYS:N	1.51	1.23
5:A:335:VAL:CG2	5:A:392:SER:OG	1.87	1.22
5:A:260:TYR:HE1	5:A:423:ARG:CD	1.54	1.21
5:A:238:ALA:HB1	5:A:368:PRO:CA	1.70	1.21
5:A:230:ARG:CD	5:A:255:PRO:HG2	1.70	1.20
5:A:360:GLY:HA3	5:A:370:GLU:CD	1.60	1.20
5:A:240:ARG:HG2	5:A:367:ARG:N	1.57	1.18
5:A:261:VAL:HG11	5:A:388:THR:CB	1.73	1.18
5:A:360:GLY:HA3	5:A:370:GLU:OE2	1.04	1.18
5:A:388:THR:O	5:A:389:VAL:O	1.61	1.18
5:A:234:VAL:CG2	5:A:253:HIS:HA	1.73	1.18
6:B:26:ARG:HD2	6:B:27:LYS:NZ	1.59	1.18
4:G:1537:G:C8	5:A:375:TYR:HE2	1.62	1.18

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:241:GLN:HB2	5:A:246:VAL:C	1.63	1.17
5:A:349:PRO:HG3	5:A:384:ILE:HD12	1.23	1.17
5:A:261:VAL:HG11	5:A:388:THR:CG2	1.74	1.17
5:A:228:CYS:HB3	6:B:33:TYR:CD2	1.79	1.17
5:A:62:ILE:H	5:A:62:ILE:HD12	1.10	1.16
5:A:349:PRO:HG3	5:A:384:ILE:CD1	1.74	1.16
5:A:228:CYS:CB	6:B:33:TYR:CD2	2.28	1.16
5:A:176:ALA:CA	6:B:47:LEU:HD21	1.75	1.16
4:G:1537:G:H8	5:A:375:TYR:CE2	1.63	1.16
6:B:26:ARG:CG	6:B:29:THR:HA	1.75	1.16
5:A:261:VAL:CG1	5:A:388:THR:HB	1.76	1.16
6:B:26:ARG:O	6:B:27:LYS:HD3	1.43	1.15
5:A:389:VAL:HG12	5:A:390:MET:CA	1.76	1.15
5:A:362:PHE:O	5:A:363:VAL:HG12	1.44	1.14
5:A:38:PHE:CB	6:B:54:ILE:HD13	1.76	1.14
5:A:344:THR:HG23	5:A:345:THR:H	1.09	1.14
5:A:385:PRO:HB2	5:A:386:PRO:CD	1.77	1.14
5:A:257:LYS:HG2	5:A:258:VAL:H	1.00	1.13
5:A:260:TYR:HE1	5:A:423:ARG:HD3	1.04	1.13
5:A:393:ALA:O	5:A:397:PHE:HB3	1.43	1.13
5:A:234:VAL:HG12	5:A:235:VAL:CA	1.78	1.12
5:A:335:VAL:N	5:A:392:SER:HB3	1.64	1.12
5:A:260:TYR:CE1	5:A:423:ARG:HD3	1.82	1.12
5:A:393:ALA:O	5:A:397:PHE:HB2	1.39	1.12
5:A:335:VAL:HG23	5:A:392:SER:CB	1.79	1.12
5:A:230:ARG:NE	5:A:255:PRO:HG2	1.65	1.11
5:A:365:GLY:O	5:A:366:ILE:CG1	1.97	1.11
5:A:38:PHE:HB3	6:B:54:ILE:HD13	1.26	1.11
6:B:15:ARG:O	6:B:18:VAL:HG12	1.50	1.11
5:A:230:ARG:HG2	5:A:255:PRO:HG3	1.14	1.11
5:A:239:LYS:O	5:A:366:ILE:HD12	0.93	1.11
5:A:334:CYS:HB2	5:A:392:SER:HA	1.33	1.10
5:A:239:LYS:C	5:A:366:ILE:HD12	1.72	1.10
5:A:230:ARG:CG	5:A:255:PRO:CG	2.14	1.10
5:A:334:CYS:CB	5:A:392:SER:HA	1.80	1.10
5:A:390:MET:HA	5:A:391:SER:HB3	1.14	1.10
5:A:234:VAL:CG1	5:A:235:VAL:CA	2.30	1.10
5:A:389:VAL:CB	5:A:390:MET:CA	2.30	1.10
6:B:26:ARG:HD2	6:B:27:LYS:HZ3	0.94	1.09
5:A:227:GLU:HB3	5:A:257:LYS:HE3	1.34	1.09
5:A:236:ASN:ND2	5:A:359:SER:OG	1.86	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:260:TYR:CE1	5:A:423:ARG:CD	2.35	1.09
5:A:239:LYS:HB2	5:A:240:ARG:NH1	1.68	1.08
5:A:241:GLN:CB	5:A:247:TYR:HB2	1.84	1.08
5:A:363:VAL:HG22	5:A:364:PRO:HD2	1.09	1.07
6:B:26:ARG:CZ	6:B:30:LYS:CB	2.30	1.07
5:A:234:VAL:CB	5:A:235:VAL:CA	2.30	1.07
5:A:84:ILE:HD12	5:A:114:LEU:HD21	1.31	1.07
5:A:240:ARG:CG	5:A:367:ARG:H	1.68	1.07
5:A:381:LYS:O	5:A:385:PRO:HD3	1.53	1.07
5:A:234:VAL:HB	5:A:235:VAL:CA	1.84	1.07
5:A:239:LYS:CB	5:A:240:ARG:CZ	2.32	1.06
6:B:26:ARG:HH22	6:B:30:LYS:CD	1.68	1.06
6:B:26:ARG:NH2	6:B:30:LYS:HB2	1.69	1.06
5:A:389:VAL:CG1	5:A:390:MET:CA	2.30	1.06
6:B:26:ARG:HG2	6:B:30:LYS:H	0.96	1.06
5:A:234:VAL:HG12	5:A:235:VAL:HA	1.07	1.06
5:A:236:ASN:CB	5:A:251:SER:CB	2.24	1.06
5:A:242:GLN:O	5:A:244:ARG:N	1.89	1.05
6:B:26:ARG:NH2	6:B:30:LYS:HD2	1.69	1.05
5:A:386:PRO:HB3	6:B:15:ARG:HH11	1.20	1.04
5:A:390:MET:CG	6:B:15:ARG:NH1	2.19	1.04
5:A:175:ALA:C	6:B:47:LEU:HD21	1.76	1.04
5:A:246:VAL:HG22	5:A:247:TYR:H	1.18	1.04
5:A:38:PHE:HE1	6:B:50:ILE:CG2	1.69	1.04
5:A:235:VAL:HG22	5:A:236:ASN:H	1.17	1.03
5:A:220:PHE:O	5:A:224:VAL:HG23	1.59	1.03
5:A:389:VAL:HB	5:A:390:MET:CA	1.86	1.03
5:A:227:GLU:CB	5:A:257:LYS:HE3	1.90	1.02
5:A:38:PHE:HE1	6:B:50:ILE:HG23	0.91	1.02
5:A:241:GLN:CB	5:A:246:VAL:O	2.07	1.02
5:A:239:LYS:HA	5:A:248:ALA:O	1.57	1.01
5:A:176:ALA:HA	6:B:47:LEU:HD21	1.43	1.01
6:B:23:TRP:CE2	6:B:27:LYS:HB3	1.94	1.01
5:A:258:VAL:O	5:A:259:VAL:HG22	1.61	1.01
6:B:54:ILE:HG23	6:B:55:HIS:H	1.22	1.01
5:A:382:ARG:O	5:A:385:PRO:HD2	1.59	1.01
5:A:386:PRO:O	5:A:389:VAL:HG23	1.58	1.01
5:A:234:VAL:HG21	5:A:253:HIS:CA	1.90	1.01
5:A:334:CYS:HB2	5:A:392:SER:CA	1.91	1.01
5:A:34:LEU:CD2	6:B:50:ILE:HD13	1.91	1.01
5:A:227:GLU:CB	6:B:36:VAL:HG21	1.91	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:258:VAL:O	5:A:259:VAL:HG13	1.61	1.00
5:A:385:PRO:CB	5:A:386:PRO:HD3	1.91	1.00
5:A:233:ILE:HD11	5:A:254:LEU:HD12	1.42	1.00
5:A:233:ILE:HD11	5:A:254:LEU:CD1	1.89	1.00
5:A:237:TYR:HA	5:A:250:GLN:O	1.62	1.00
5:A:261:VAL:HG11	5:A:388:THR:HG21	1.44	0.99
5:A:389:VAL:CB	5:A:390:MET:CB	2.30	0.99
5:A:238:ALA:HB3	5:A:369:GLY:H	1.25	0.99
5:A:389:VAL:CB	5:A:390:MET:HA	1.85	0.99
6:B:26:ARG:HH22	6:B:30:LYS:HD2	0.85	0.99
5:A:238:ALA:HB1	5:A:368:PRO:HA	1.01	0.99
5:A:241:GLN:CA	5:A:247:TYR:HB2	1.92	0.99
5:A:380:LEU:HB3	5:A:384:ILE:HD11	1.41	0.98
5:A:16:LEU:HD23	5:A:16:LEU:H	1.25	0.98
5:A:386:PRO:HB3	6:B:15:ARG:NH1	1.78	0.97
5:A:344:THR:HG23	5:A:345:THR:N	1.78	0.97
6:B:26:ARG:C	6:B:27:LYS:CD	2.33	0.97
5:A:294:TYR:HA	5:A:299:ALA:HA	1.46	0.97
5:A:386:PRO:CB	6:B:15:ARG:HD2	1.95	0.97
5:A:227:GLU:HB2	6:B:36:VAL:HG21	1.41	0.97
5:A:228:CYS:HB2	6:B:33:TYR:HD2	1.28	0.97
5:A:225:TYR:HA	6:B:33:TYR:HE2	1.26	0.96
6:B:33:TYR:O	6:B:36:VAL:HG12	1.63	0.96
6:B:26:ARG:CB	6:B:29:THR:CA	2.30	0.96
5:A:238:ALA:O	5:A:249:ALA:HB3	1.65	0.96
5:A:11:ILE:HD11	5:A:113:LEU:HD23	1.44	0.96
5:A:261:VAL:CG1	5:A:388:THR:CG2	2.43	0.96
5:A:231:ARG:O	5:A:232:ARG:HG3	1.66	0.96
5:A:227:GLU:HG2	5:A:257:LYS:HE2	1.47	0.96
5:A:238:ALA:CB	5:A:368:PRO:HA	1.96	0.95
5:A:234:VAL:HB	5:A:235:VAL:HA	1.42	0.95
5:A:238:ALA:HB3	5:A:369:GLY:N	1.80	0.95
5:A:385:PRO:HB2	5:A:386:PRO:HD3	0.96	0.95
5:A:98:LEU:HA	5:A:103:ASN:HB2	1.46	0.95
5:A:363:VAL:CG2	5:A:364:PRO:CD	2.44	0.95
5:A:227:GLU:HG2	5:A:257:LYS:CE	1.96	0.95
5:A:233:ILE:CD1	5:A:254:LEU:HB2	1.96	0.94
5:A:175:ALA:C	6:B:47:LEU:CD2	2.36	0.94
5:A:246:VAL:HG22	5:A:247:TYR:N	1.81	0.94
5:A:240:ARG:HG2	5:A:367:ARG:H	0.80	0.94
5:A:234:VAL:HB	5:A:235:VAL:CB	1.97	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:56:VAL:HG12	6:B:57:PRO:HD2	1.50	0.94
6:B:56:VAL:CG1	6:B:57:PRO:CD	2.46	0.94
5:A:225:TYR:O	5:A:228:CYS:SG	2.25	0.94
5:A:234:VAL:HG21	5:A:253:HIS:HA	0.95	0.94
5:A:241:GLN:HB2	5:A:247:TYR:HB2	1.49	0.94
5:A:389:VAL:CG1	5:A:391:SER:CB	2.30	0.93
5:A:436:LEU:O	5:A:438:PRO:HD3	1.67	0.93
6:B:26:ARG:NH1	6:B:30:LYS:CB	2.31	0.93
6:B:26:ARG:NH1	6:B:30:LYS:HB2	1.82	0.93
5:A:231:ARG:HG2	6:B:22:ILE:HD12	1.49	0.93
5:A:261:VAL:HG11	5:A:388:THR:HB	1.36	0.93
6:B:53:ILE:O	6:B:57:PRO:HD2	1.69	0.93
5:A:391:SER:N	5:A:394:PHE:HB3	1.83	0.93
5:A:253:HIS:O	5:A:254:LEU:HG	1.69	0.93
2:E:490:C:H42	5:A:358:LYS:NZ	1.65	0.92
5:A:124:VAL:HG22	5:A:144:ILE:HD13	1.51	0.92
5:A:67:ILE:HA	5:A:72:THR:HG23	1.49	0.92
5:A:257:LYS:HG2	5:A:258:VAL:N	1.81	0.92
5:A:176:ALA:HA	6:B:47:LEU:CD2	2.00	0.91
5:A:176:ALA:HA	6:B:47:LEU:CG	2.00	0.91
6:B:26:ARG:CG	6:B:29:THR:CA	2.46	0.91
5:A:239:LYS:HB2	5:A:240:ARG:NH2	1.83	0.91
5:A:157:LEU:HD23	5:A:160:ILE:HD12	1.52	0.91
5:A:238:ALA:CB	5:A:369:GLY:H	1.82	0.91
5:A:225:TYR:HA	6:B:33:TYR:CE2	2.06	0.91
6:B:56:VAL:HG13	6:B:57:PRO:CD	2.01	0.90
5:A:391:SER:N	5:A:394:PHE:CB	2.35	0.90
6:B:26:ARG:CG	6:B:30:LYS:N	2.35	0.90
5:A:262:SER:HB2	5:A:395:VAL:HG21	1.53	0.90
5:A:235:VAL:HG22	5:A:236:ASN:N	1.80	0.89
5:A:227:GLU:CB	5:A:257:LYS:CE	2.50	0.89
5:A:331:ILE:HA	5:A:392:SER:O	1.72	0.89
5:A:176:ALA:HA	6:B:47:LEU:HD11	1.55	0.89
5:A:227:GLU:CD	5:A:257:LYS:NZ	2.26	0.89
5:A:73:LEU:HD21	5:A:122:GLU:HB2	1.53	0.89
5:A:390:MET:SD	5:A:390:MET:O	2.30	0.88
5:A:241:GLN:HA	5:A:247:TYR:HB2	1.52	0.88
5:A:261:VAL:CB	5:A:388:THR:HB	2.02	0.88
5:A:335:VAL:N	5:A:392:SER:CB	2.36	0.88
3:F:1402:U:H5'	4:G:1521:G:O2'	1.72	0.88
5:A:344:THR:CG2	5:A:345:THR:H	1.85	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:390:MET:HA	5:A:391:SER:CB	1.98	0.88
5:A:227:GLU:CG	5:A:257:LYS:CE	2.52	0.88
5:A:363:VAL:CG2	5:A:364:PRO:HD2	2.01	0.88
5:A:82:GLY:HA2	5:A:111:GLN:HE21	1.38	0.88
5:A:82:GLY:HA2	5:A:111:GLN:NE2	1.88	0.88
5:A:13:GLU:HG3	5:A:14:VAL:H	1.36	0.88
6:B:23:TRP:H	6:B:24:PRO:HD2	1.37	0.88
6:B:26:ARG:HB3	6:B:29:THR:HA	0.89	0.87
6:B:29:THR:OG1	6:B:32:GLU:HB2	1.74	0.87
5:A:238:ALA:CB	5:A:369:GLY:N	2.38	0.87
5:A:354:LYS:O	5:A:355:ARG:HG3	1.75	0.87
5:A:195:LYS:HB3	5:A:209:TYR:CD2	2.09	0.87
5:A:227:GLU:HB3	5:A:257:LYS:CE	2.04	0.87
5:A:232:ARG:HD3	5:A:232:ARG:O	1.75	0.87
5:A:227:GLU:CG	5:A:257:LYS:NZ	2.38	0.87
5:A:34:LEU:HD21	6:B:50:ILE:HD13	1.56	0.87
5:A:386:PRO:HB3	6:B:15:ARG:HD2	1.55	0.87
6:B:56:VAL:HG13	6:B:57:PRO:HD3	1.56	0.87
5:A:80:THR:HG23	5:A:275:ASN:ND2	1.88	0.86
5:A:380:LEU:O	5:A:384:ILE:HG13	1.74	0.86
6:B:28:PRO:O	6:B:29:THR:HG23	1.75	0.86
5:A:235:VAL:CG2	5:A:236:ASN:H	1.88	0.86
5:A:335:VAL:H	5:A:392:SER:CB	1.89	0.86
5:A:46:TYR:HB3	5:A:146:GLN:HE22	1.37	0.86
5:A:246:VAL:O	5:A:247:TYR:HD1	1.56	0.86
7:C:44:GLU:HA	7:C:47:LEU:HB3	1.58	0.86
5:A:335:VAL:O	5:A:339:ILE:HG13	1.75	0.86
5:A:390:MET:CA	5:A:391:SER:HB3	2.02	0.86
5:A:223:VAL:HG11	5:A:415:LEU:HA	1.56	0.86
5:A:261:VAL:CG2	5:A:388:THR:CG2	2.25	0.86
5:A:390:MET:HG2	6:B:15:ARG:HH11	1.40	0.85
5:A:242:GLN:C	5:A:244:ARG:H	1.76	0.85
5:A:335:VAL:HG22	5:A:392:SER:OG	1.75	0.85
5:A:233:ILE:CD1	5:A:254:LEU:HD12	2.07	0.84
5:A:257:LYS:CG	5:A:258:VAL:H	1.83	0.84
5:A:334:CYS:HB3	5:A:392:SER:HA	1.59	0.84
5:A:234:VAL:HB	5:A:235:VAL:HB	1.57	0.84
5:A:246:VAL:O	5:A:247:TYR:CD1	2.30	0.84
5:A:335:VAL:CG2	5:A:392:SER:CB	2.51	0.84
5:A:349:PRO:CG	5:A:384:ILE:HD12	2.06	0.84
5:A:153:ILE:HD13	7:C:37:THR:HG23	1.59	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:240:ARG:HB2	5:A:368:PRO:HD3	1.61	0.83
5:A:176:ALA:HA	6:B:47:LEU:CD1	2.09	0.83
5:A:238:ALA:O	5:A:249:ALA:CB	2.27	0.83
5:A:260:TYR:OH	5:A:423:ARG:HD2	1.76	0.83
5:A:380:LEU:HB3	5:A:384:ILE:CD1	2.07	0.83
6:B:26:ARG:O	6:B:27:LYS:CD	2.24	0.83
5:A:390:MET:CG	6:B:15:ARG:HH12	1.91	0.83
5:A:230:ARG:HE	5:A:255:PRO:HG2	1.37	0.83
5:A:29:TRP:O	5:A:32:ILE:HG22	1.79	0.83
5:A:241:GLN:CB	5:A:247:TYR:CB	2.56	0.82
5:A:237:TYR:O	5:A:370:GLU:HG3	1.78	0.82
5:A:263:ASN:ND2	5:A:423:ARG:NH1	2.27	0.82
5:A:260:TYR:CE1	5:A:423:ARG:HD2	2.13	0.82
5:A:321:ILE:HD12	5:A:322:HIS:H	1.42	0.82
5:A:389:VAL:HG12	5:A:390:MET:HA	0.83	0.82
5:A:230:ARG:HE	5:A:255:PRO:CG	1.92	0.82
5:A:233:ILE:CG1	5:A:254:LEU:CB	2.17	0.82
5:A:239:LYS:CB	5:A:240:ARG:NH2	2.42	0.82
5:A:236:ASN:HB2	5:A:251:SER:HB2	0.83	0.82
5:A:236:ASN:CB	5:A:251:SER:HB3	2.08	0.82
5:A:34:LEU:CD2	6:B:50:ILE:CD1	2.58	0.82
5:A:391:SER:H	5:A:394:PHE:H	1.28	0.82
6:B:36:VAL:O	6:B:40:THR:HG23	1.79	0.81
5:A:227:GLU:CD	5:A:257:LYS:HZ1	1.84	0.81
6:B:29:THR:OG1	6:B:32:GLU:CB	2.28	0.81
5:A:366:ILE:HG13	5:A:368:PRO:CG	2.10	0.81
5:A:34:LEU:HD23	6:B:50:ILE:CD1	2.11	0.81
5:A:334:CYS:HB2	5:A:392:SER:CB	2.10	0.81
5:A:33:VAL:HG21	5:A:161:VAL:HG22	1.63	0.81
5:A:63:THR:HG23	5:A:76:GLY:H	1.46	0.80
6:B:53:ILE:O	6:B:57:PRO:CD	2.28	0.80
2:E:490:C:H42	5:A:358:LYS:HZ1	1.27	0.80
5:A:240:ARG:N	5:A:240:ARG:NE	2.30	0.80
5:A:258:VAL:O	5:A:259:VAL:CG2	2.30	0.80
5:A:253:HIS:O	5:A:254:LEU:CG	2.30	0.80
5:A:369:GLY:O	5:A:370:GLU:HG3	1.80	0.80
5:A:258:VAL:O	5:A:259:VAL:CG1	2.30	0.80
6:B:53:ILE:O	6:B:57:PRO:CG	2.30	0.80
5:A:381:LYS:O	5:A:385:PRO:CD	2.30	0.80
5:A:236:ASN:C	5:A:251:SER:CB	2.51	0.80
5:A:245:ARG:O	5:A:246:VAL:HG12	1.81	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:261:VAL:CB	5:A:388:THR:HG22	2.12	0.79
5:A:386:PRO:CB	6:B:15:ARG:NH1	2.45	0.79
5:A:231:ARG:O	5:A:232:ARG:CG	2.30	0.79
5:A:233:ILE:HG23	5:A:234:VAL:HG23	1.63	0.79
5:A:236:ASN:CA	5:A:251:SER:CB	2.59	0.79
5:A:38:PHE:HB2	6:B:54:ILE:HD13	1.62	0.79
5:A:236:ASN:HB2	5:A:251:SER:HB3	1.57	0.79
5:A:261:VAL:CG1	5:A:388:THR:CB	2.43	0.79
5:A:331:ILE:HD12	5:A:393:ALA:HA	0.80	0.79
5:A:389:VAL:HB	5:A:390:MET:HB3	0.80	0.79
6:B:15:ARG:O	6:B:18:VAL:CG1	2.30	0.79
6:B:18:VAL:O	6:B:21:VAL:HG12	1.82	0.79
5:A:232:ARG:CD	5:A:232:ARG:O	2.30	0.79
5:A:241:GLN:HB3	5:A:247:TYR:CA	2.11	0.79
5:A:233:ILE:HG12	5:A:254:LEU:CA	2.13	0.78
5:A:261:VAL:CB	5:A:388:THR:CB	2.60	0.78
5:A:354:LYS:O	5:A:355:ARG:CG	2.31	0.78
5:A:230:ARG:NE	5:A:255:PRO:CG	2.44	0.78
5:A:258:VAL:C	5:A:259:VAL:HG13	2.04	0.78
5:A:195:LYS:HD3	5:A:209:TYR:HE2	1.46	0.78
5:A:239:LYS:HD2	5:A:240:ARG:HH22	1.49	0.78
5:A:245:ARG:O	5:A:246:VAL:CG1	2.32	0.78
5:A:357:LYS:HD2	5:A:374:LYS:HA	1.64	0.78
6:B:28:PRO:HB2	6:B:32:GLU:OE1	1.82	0.78
5:A:382:ARG:O	5:A:385:PRO:CD	2.32	0.78
5:A:98:LEU:HA	5:A:103:ASN:CB	2.12	0.78
6:B:26:ARG:HB3	6:B:29:THR:N	1.97	0.77
5:A:157:LEU:O	5:A:161:VAL:HG23	1.84	0.77
5:A:260:TYR:O	5:A:263:ASN:HB2	1.84	0.77
5:A:369:GLY:O	5:A:370:GLU:CG	2.32	0.77
6:B:26:ARG:NH1	6:B:30:LYS:HB3	1.99	0.77
5:A:366:ILE:CG1	5:A:368:PRO:CD	2.34	0.77
6:B:28:PRO:O	6:B:29:THR:CG2	2.32	0.77
5:A:228:CYS:HB2	6:B:33:TYR:CD2	2.09	0.77
5:A:331:ILE:O	5:A:392:SER:CB	2.24	0.77
5:A:188:GLY:HA2	6:B:52:TYR:HE1	1.50	0.77
5:A:231:ARG:C	5:A:232:ARG:HG3	2.05	0.77
5:A:390:MET:C	5:A:394:PHE:HB2	2.04	0.77
6:B:46:LEU:O	6:B:49:ILE:HG22	1.85	0.76
5:A:354:LYS:O	5:A:355:ARG:CB	2.33	0.76
6:B:58:ALA:O	6:B:61:ILE:HG22	1.85	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:341:TRP:C	5:A:344:THR:HG22	2.06	0.76
5:A:403:ASN:HD21	5:A:412:THR:H	1.33	0.76
6:B:53:ILE:HG23	6:B:54:ILE:H	1.48	0.76
5:A:261:VAL:HB	5:A:388:THR:HB	1.68	0.76
6:B:26:ARG:CD	6:B:27:LYS:NZ	2.45	0.76
5:A:33:VAL:HG13	5:A:157:LEU:HD22	1.66	0.76
5:A:79:VAL:O	5:A:83:ILE:HG13	1.86	0.76
5:A:390:MET:O	5:A:390:MET:CE	2.33	0.76
6:B:5:LYS:O	6:B:8:VAL:HG12	1.86	0.76
5:A:39:ILE:N	6:B:54:ILE:HD11	2.00	0.75
5:A:362:PHE:O	5:A:363:VAL:CG1	2.30	0.75
5:A:391:SER:CA	5:A:394:PHE:HB3	2.16	0.75
5:A:75:ILE:HG22	5:A:79:VAL:HG23	1.68	0.75
6:B:23:TRP:H	6:B:24:PRO:CD	1.97	0.75
6:B:56:VAL:CG1	6:B:57:PRO:HD2	2.14	0.75
5:A:241:GLN:CB	5:A:247:TYR:CA	2.64	0.75
5:A:246:VAL:O	5:A:247:TYR:HB2	1.86	0.75
5:A:226:ALA:HB1	5:A:259:VAL:HG11	1.69	0.75
5:A:425:TYR:CG	6:B:39:VAL:HG21	2.21	0.75
1:D:90:U:H3'	1:D:91:A:H5"	1.68	0.75
5:A:229:MET:O	5:A:230:ARG:HB2	1.85	0.75
5:A:250:GLN:O	5:A:251:SER:CB	2.33	0.75
5:A:373:ALA:O	5:A:374:LYS:CB	2.33	0.75
6:B:23:TRP:CE2	6:B:27:LYS:CB	2.70	0.75
5:A:256:LEU:O	5:A:257:LYS:HB2	1.86	0.75
5:A:259:VAL:O	5:A:260:TYR:CB	2.35	0.75
5:A:261:VAL:CB	5:A:388:THR:CG2	2.63	0.75
5:A:389:VAL:HG12	5:A:391:SER:HB3	0.79	0.75
5:A:236:ASN:CA	5:A:251:SER:HB2	2.16	0.74
5:A:241:GLN:CB	5:A:246:VAL:C	2.49	0.74
5:A:367:ARG:N	5:A:368:PRO:CD	2.50	0.74
5:A:256:LEU:O	5:A:257:LYS:CB	2.36	0.74
5:A:241:GLN:HB2	5:A:247:TYR:CB	2.16	0.74
5:A:386:PRO:HB3	6:B:15:ARG:CD	2.16	0.74
5:A:103:ASN:HA	5:A:106:LEU:HD12	1.69	0.74
6:B:54:ILE:CG2	6:B:55:HIS:H	1.99	0.74
7:C:36:VAL:O	7:C:39:ALA:HB3	1.88	0.74
5:A:239:LYS:N	5:A:368:PRO:HB3	2.02	0.74
5:A:390:MET:HE1	5:A:390:MET:O	1.87	0.73
5:A:390:MET:C	5:A:394:PHE:CB	2.57	0.73
5:A:227:GLU:HB3	6:B:36:VAL:HG21	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:259:VAL:O	5:A:260:TYR:HB3	1.87	0.73
5:A:63:THR:HG23	5:A:76:GLY:N	2.03	0.73
5:A:245:ARG:N	5:A:247:TYR:HE1	1.85	0.73
5:A:236:ASN:C	5:A:251:SER:HB3	2.09	0.73
6:B:27:LYS:N	6:B:27:LYS:HD3	2.04	0.73
5:A:43:ILE:O	5:A:70:LEU:HD13	1.88	0.72
5:A:257:LYS:HD2	5:A:422:TYR:CE2	2.23	0.72
5:A:425:TYR:CD2	6:B:39:VAL:HG21	2.24	0.72
5:A:241:GLN:HB3	5:A:248:ALA:N	2.04	0.72
5:A:245:ARG:H	5:A:247:TYR:HE1	1.35	0.72
6:B:26:ARG:HG2	6:B:29:THR:C	2.10	0.72
2:E:480:A:H3'	2:E:481:G:H5"	1.70	0.72
5:A:175:ALA:O	6:B:47:LEU:HD23	1.90	0.72
5:A:260:TYR:CZ	5:A:423:ARG:HD2	2.23	0.72
5:A:175:ALA:O	6:B:47:LEU:CD2	2.37	0.72
5:A:62:ILE:N	5:A:62:ILE:HD12	1.95	0.72
5:A:86:GLN:O	5:A:340:PHE:HD2	1.73	0.72
5:A:357:LYS:HG2	5:A:373:ALA:HB1	1.70	0.72
5:A:335:VAL:CA	5:A:392:SER:HB3	2.20	0.72
6:B:54:ILE:HG23	6:B:55:HIS:N	2.03	0.72
5:A:102:GLU:O	5:A:106:LEU:HG	1.90	0.71
5:A:241:GLN:HA	5:A:247:TYR:CB	2.20	0.71
6:B:5:LYS:O	6:B:8:VAL:CG1	2.39	0.71
5:A:331:ILE:HD12	5:A:393:ALA:CB	2.20	0.71
5:A:349:PRO:HG3	5:A:384:ILE:HD13	1.71	0.71
6:B:50:ILE:O	6:B:53:ILE:HG22	1.90	0.71
5:A:241:GLN:OE1	5:A:241:GLN:C	2.30	0.70
5:A:39:ILE:HG12	6:B:54:ILE:HD11	1.71	0.70
5:A:281:LEU:O	5:A:284:TYR:HB3	1.91	0.70
5:A:234:VAL:CG2	5:A:253:HIS:CA	2.61	0.70
5:A:261:VAL:C	5:A:263:ASN:H	1.95	0.70
5:A:15:GLU:OE1	5:A:17:PRO:HG3	1.90	0.70
5:A:3:LYS:HA	5:A:3:LYS:HE3	1.74	0.70
6:B:25:THR:HG22	6:B:29:THR:HG22	1.72	0.70
5:A:152:ILE:HD13	5:A:155:ILE:HD12	1.72	0.70
5:A:335:VAL:HG23	5:A:392:SER:HG	1.57	0.70
5:A:237:TYR:N	5:A:251:SER:HB3	2.07	0.70
6:B:26:ARG:HB3	6:B:28:PRO:O	1.92	0.70
5:A:233:ILE:HD13	5:A:255:PRO:HB3	1.73	0.70
5:A:237:TYR:CA	5:A:250:GLN:O	2.39	0.70
6:B:26:ARG:HB3	6:B:28:PRO:C	2.12	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:220:PHE:O	5:A:224:VAL:CG2	2.40	0.69
5:A:246:VAL:O	5:A:247:TYR:CB	2.40	0.69
5:A:239:LYS:CA	5:A:248:ALA:O	2.37	0.69
6:B:23:TRP:NE1	6:B:27:LYS:HB2	2.06	0.69
5:A:195:LYS:HD3	5:A:209:TYR:CE2	2.26	0.69
5:A:262:SER:CB	5:A:395:VAL:HG21	2.22	0.69
5:A:366:ILE:HD11	5:A:368:PRO:HG3	1.72	0.69
6:B:26:ARG:NH2	6:B:30:LYS:CB	2.45	0.69
5:A:233:ILE:C	5:A:234:VAL:HG23	2.13	0.69
5:A:416:LEU:O	5:A:420:ILE:HG13	1.92	0.69
6:B:26:ARG:HG2	6:B:29:THR:HA	1.68	0.69
5:A:264:ILE:HG22	5:A:265:PRO:HD3	1.74	0.69
4:G:1534:U:H2'	4:G:1536:C:N3	2.08	0.69
5:A:366:ILE:HG13	5:A:368:PRO:HD3	0.70	0.69
6:B:47:LEU:O	6:B:50:ILE:HG22	1.92	0.69
5:A:166:ILE:HD13	5:A:428:LEU:CD2	2.23	0.69
5:A:331:ILE:HD13	5:A:392:SER:O	1.93	0.69
5:A:239:LYS:HG2	5:A:248:ALA:O	1.93	0.69
5:A:234:VAL:HG12	5:A:235:VAL:C	2.13	0.68
6:B:23:TRP:NE1	6:B:27:LYS:CB	2.55	0.68
5:A:335:VAL:H	5:A:392:SER:HB2	1.58	0.68
5:A:280:GLY:HA2	5:A:291:LEU:HD12	1.74	0.68
5:A:232:ARG:HA	5:A:233:ILE:HB	0.76	0.68
6:B:54:ILE:O	6:B:57:PRO:HG2	1.92	0.68
5:A:85:MET:HE2	5:A:111:GLN:HB2	1.75	0.68
5:A:189:PRO:CG	6:B:56:VAL:HG23	2.23	0.68
5:A:253:HIS:O	5:A:254:LEU:CD2	2.42	0.68
5:A:363:VAL:HG13	5:A:364:PRO:N	2.08	0.68
5:A:227:GLU:CD	5:A:257:LYS:HZ3	1.96	0.67
5:A:231:ARG:O	5:A:232:ARG:CB	2.40	0.67
5:A:152:ILE:HA	5:A:155:ILE:HD12	1.76	0.67
5:A:280:GLY:CA	5:A:291:LEU:HD12	2.25	0.67
3:F:1386:C:H2'	3:F:1387:A:C8	2.29	0.67
5:A:366:ILE:CB	5:A:368:PRO:HD3	2.25	0.67
5:A:239:LYS:O	5:A:366:ILE:CG1	2.43	0.67
6:B:26:ARG:N	6:B:28:PRO:O	2.28	0.67
5:A:231:ARG:O	5:A:255:PRO:HG3	1.95	0.67
5:A:80:THR:HA	5:A:83:ILE:HD12	1.76	0.67
6:B:22:ILE:HG23	6:B:22:ILE:O	1.95	0.67
1:D:83:A:N6	1:D:101:A:H5'	2.09	0.66
5:A:365:GLY:O	5:A:366:ILE:CB	2.42	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:151:SER:O	5:A:155:ILE:HG13	1.95	0.66
5:A:215:GLY:O	5:A:219:VAL:HG23	1.95	0.66
5:A:13:GLU:HG3	5:A:14:VAL:N	2.10	0.66
5:A:239:LYS:O	5:A:368:PRO:HB3	1.95	0.66
5:A:242:GLN:O	5:A:244:ARG:HG3	1.96	0.66
5:A:239:LYS:CD	5:A:240:ARG:HH22	2.08	0.66
5:A:261:VAL:CG1	5:A:388:THR:HG21	2.18	0.66
5:A:317:ILE:O	5:A:320:PRO:HD3	1.96	0.66
5:A:277:GLN:NE2	5:A:308:SER:HB3	2.11	0.66
5:A:263:ASN:O	5:A:267:ILE:HG13	1.95	0.65
6:B:61:ILE:HA	6:B:64:ILE:HG22	1.78	0.65
5:A:350:LYS:O	5:A:351:SER:CB	2.43	0.65
5:A:227:GLU:CA	5:A:257:LYS:HE3	2.27	0.65
5:A:260:TYR:O	5:A:263:ASN:CB	2.43	0.65
5:A:369:GLY:O	5:A:370:GLU:CB	2.44	0.65
5:A:380:LEU:C	5:A:384:ILE:HG13	2.16	0.65
5:A:84:ILE:O	5:A:87:LEU:HB2	1.96	0.65
4:G:1536:C:H1'	4:G:1537:G:N2	2.12	0.65
5:A:373:ALA:O	5:A:374:LYS:HB3	1.95	0.65
4:G:1548:A:H2'	4:G:1549:A:C8	2.32	0.65
1:D:90:U:H3'	1:D:91:A:C5'	2.26	0.65
5:A:239:LYS:O	5:A:240:ARG:HB2	1.95	0.65
6:B:23:TRP:CZ2	6:B:27:LYS:HB3	2.31	0.65
5:A:391:SER:HA	5:A:394:PHE:HB3	1.77	0.65
5:A:65:SER:O	5:A:66:ARG:HB2	1.96	0.65
5:A:250:GLN:O	5:A:251:SER:HB3	1.95	0.65
5:A:256:LEU:HD23	5:A:256:LEU:N	2.11	0.65
5:A:275:ASN:O	5:A:279:TRP:HB2	1.95	0.65
5:A:232:ARG:O	5:A:232:ARG:NE	2.30	0.65
5:A:341:TRP:O	5:A:344:THR:CG2	2.44	0.65
6:B:27:LYS:N	6:B:28:PRO:HA	2.12	0.65
5:A:324:ILE:O	5:A:328:ILE:HG13	1.97	0.65
5:A:227:GLU:HG2	5:A:257:LYS:NZ	2.10	0.64
5:A:226:ALA:O	5:A:258:VAL:HG13	1.97	0.64
5:A:341:TRP:O	5:A:344:THR:HG22	1.95	0.64
6:B:23:TRP:N	6:B:24:PRO:CD	2.56	0.64
6:B:56:VAL:CG1	6:B:57:PRO:HD3	2.21	0.64
5:A:261:VAL:O	5:A:263:ASN:N	2.31	0.64
5:A:334:CYS:HB2	5:A:392:SER:HB2	1.80	0.64
5:A:29:TRP:NE1	5:A:164:TYR:HD2	1.94	0.64
5:A:354:LYS:O	5:A:355:ARG:HB2	1.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:166:ILE:HD13	5:A:428:LEU:HD21	1.80	0.64
5:A:38:PHE:HB2	6:B:54:ILE:CD1	2.27	0.64
5:A:401:ILE:O	5:A:405:ILE:HG22	1.98	0.64
5:A:327:MET:O	5:A:331:ILE:HG12	1.98	0.64
5:A:240:ARG:C	5:A:366:ILE:HD13	2.17	0.64
3:F:1395:A:H4'	3:F:1397:U:C5	2.33	0.63
5:A:365:GLY:O	5:A:366:ILE:HG23	1.99	0.63
5:A:62:ILE:H	5:A:62:ILE:CD1	1.87	0.63
6:B:23:TRP:O	6:B:24:PRO:C	2.36	0.63
4:G:1537:G:C8	5:A:375:TYR:CE2	2.54	0.63
5:A:260:TYR:O	5:A:263:ASN:N	2.31	0.63
6:B:29:THR:O	6:B:31:ASP:N	2.30	0.63
5:A:229:MET:O	5:A:230:ARG:CB	2.47	0.63
5:A:258:VAL:O	5:A:259:VAL:CB	2.46	0.63
5:A:341:TRP:CA	5:A:344:THR:HG22	2.29	0.63
6:B:26:ARG:CG	6:B:29:THR:C	2.67	0.63
5:A:389:VAL:CG1	5:A:390:MET:CB	2.70	0.63
6:B:24:PRO:O	6:B:25:THR:C	2.37	0.63
6:B:29:THR:HG1	6:B:32:GLU:HB2	1.63	0.63
5:A:176:ALA:CA	6:B:47:LEU:HD11	2.26	0.63
5:A:149:PHE:HD2	7:C:40:PHE:HZ	1.45	0.62
5:A:254:LEU:CB	5:A:255:PRO:CA	2.31	0.62
6:B:30:LYS:O	6:B:30:LYS:HG2	1.98	0.62
6:B:50:ILE:O	6:B:53:ILE:CG2	2.46	0.62
5:A:288:ILE:HD12	5:A:288:ILE:N	2.15	0.62
5:A:238:ALA:CB	5:A:368:PRO:CA	2.64	0.62
5:A:164:TYR:CE1	7:C:30:PRO:HG2	2.35	0.62
5:A:241:GLN:HB2	5:A:247:TYR:N	2.14	0.62
5:A:366:ILE:CD1	5:A:368:PRO:HG3	2.29	0.62
5:A:75:ILE:HG22	5:A:79:VAL:CG2	2.30	0.62
5:A:129:ALA:HB1	5:A:281:LEU:HD12	1.82	0.62
5:A:356:ILE:HG22	5:A:356:ILE:O	2.00	0.62
5:A:245:ARG:O	5:A:247:TYR:CE1	2.53	0.62
5:A:245:ARG:O	5:A:247:TYR:CD1	2.53	0.62
5:A:52:ILE:HG23	5:A:132:PHE:HA	1.80	0.62
5:A:365:GLY:C	5:A:366:ILE:HG12	2.11	0.62
5:A:5:ILE:N	5:A:6:PRO:HD2	2.15	0.62
5:A:384:ILE:O	5:A:385:PRO:C	2.38	0.61
5:A:136:THR:HB	5:A:139:LEU:HB3	1.82	0.61
6:B:53:ILE:O	6:B:57:PRO:HG2	1.99	0.61
5:A:88:LEU:C	5:A:90:GLY:H	2.03	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:402:ALA:O	5:A:405:ILE:HG23	1.99	0.61
6:B:12:ARG:O	6:B:16:THR:HG23	2.01	0.61
5:A:341:TRP:HA	5:A:344:THR:HG22	1.83	0.61
4:G:1532:A:H2'	4:G:1533:C:C6	2.36	0.61
5:A:245:ARG:C	5:A:246:VAL:HG12	2.20	0.61
5:A:253:HIS:O	5:A:254:LEU:HD23	2.00	0.61
6:B:53:ILE:O	6:B:54:ILE:C	2.39	0.61
5:A:371:GLN:O	5:A:373:ALA:O	2.19	0.61
5:A:175:ALA:C	6:B:47:LEU:HD23	2.20	0.60
4:G:1526:C:H2'	4:G:1527:G:O4'	2.00	0.60
5:A:23:PHE:HE1	5:A:431:GLU:HB2	1.65	0.60
5:A:246:VAL:CG2	5:A:247:TYR:N	2.53	0.60
6:B:27:LYS:N	6:B:28:PRO:CA	2.64	0.60
5:A:16:LEU:HD23	5:A:16:LEU:N	2.05	0.60
5:A:11:ILE:HD11	5:A:113:LEU:CD2	2.27	0.60
5:A:100:ILE:HG22	5:A:102:GLU:H	1.67	0.60
5:A:157:LEU:HA	5:A:160:ILE:HD12	1.84	0.60
5:A:5:ILE:HG22	5:A:9:GLU:CD	2.22	0.60
5:A:341:TRP:HA	5:A:344:THR:CG2	2.31	0.60
5:A:391:SER:N	5:A:394:PHE:HB2	2.13	0.60
5:A:43:ILE:HB	5:A:70:LEU:HD22	1.84	0.60
5:A:261:VAL:HB	5:A:388:THR:CB	2.28	0.60
6:B:28:PRO:C	6:B:29:THR:HG23	2.21	0.60
5:A:332:ILE:HG13	5:A:333:THR:N	2.17	0.60
6:B:26:ARG:NH2	6:B:30:LYS:CD	2.45	0.60
5:A:241:GLN:O	5:A:242:GLN:HB2	2.02	0.60
5:A:38:PHE:HB3	6:B:54:ILE:HG21	1.84	0.60
6:B:46:LEU:O	6:B:49:ILE:CG2	2.49	0.60
5:A:361:ALA:N	5:A:370:GLU:OE1	2.33	0.59
5:A:391:SER:O	5:A:393:ALA:N	2.34	0.59
5:A:38:PHE:CE1	6:B:50:ILE:CG2	2.57	0.59
2:E:492:A:H2'	2:E:493:G:O4'	2.01	0.59
5:A:240:ARG:C	5:A:366:ILE:CD1	2.70	0.59
5:A:415:LEU:O	5:A:416:LEU:C	2.41	0.59
5:A:83:ILE:HG21	5:A:272:LEU:HD23	1.84	0.59
6:B:26:ARG:NH2	6:B:30:LYS:CG	2.65	0.59
5:A:152:ILE:HA	5:A:155:ILE:CD1	2.33	0.59
5:A:135:LEU:HD12	5:A:135:LEU:H	1.68	0.59
5:A:260:TYR:CE1	5:A:423:ARG:CB	2.86	0.59
6:B:61:ILE:HG23	6:B:62:LYS:N	2.18	0.59
5:A:264:ILE:HG22	5:A:265:PRO:CD	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:88:LEU:O	5:A:90:GLY:N	2.36	0.59
5:A:264:ILE:HG21	5:A:341:TRP:CH2	2.37	0.59
5:A:55:ILE:HG22	5:A:67:ILE:HD12	1.84	0.59
5:A:93:ILE:HG22	5:A:94:ILE:HG13	1.84	0.59
5:A:200:LEU:HD23	5:A:205:PRO:HG3	1.85	0.59
5:A:391:SER:N	5:A:394:PHE:H	1.99	0.59
6:B:36:VAL:HG13	6:B:37:ALA:N	2.17	0.59
5:A:3:LYS:C	5:A:5:ILE:H	2.06	0.59
2:E:490:C:N4	5:A:358:LYS:NZ	2.45	0.58
6:B:26:ARG:HG2	6:B:29:THR:CA	2.23	0.58
5:A:211:ALA:HB3	5:A:212:PRO:CD	2.33	0.58
1:D:100:U:OP1	1:D:100:U:H2'	2.03	0.58
5:A:236:ASN:C	5:A:251:SER:OG	2.41	0.58
5:A:83:ILE:HG23	5:A:337:PHE:CZ	2.38	0.58
5:A:380:LEU:O	5:A:384:ILE:CG1	2.48	0.58
6:B:5:LYS:C	6:B:8:VAL:HG12	2.23	0.58
5:A:391:SER:O	5:A:394:PHE:N	2.36	0.58
5:A:52:ILE:N	5:A:52:ILE:HD12	2.19	0.58
5:A:335:VAL:HG12	5:A:339:ILE:HD11	1.86	0.58
5:A:34:LEU:O	5:A:37:TYR:HB3	2.04	0.58
5:A:353:ALA:C	5:A:357:LYS:HE2	2.24	0.58
5:A:403:ASN:HD21	5:A:412:THR:HG22	1.68	0.58
5:A:246:VAL:C	5:A:247:TYR:CD1	2.77	0.58
5:A:235:VAL:HG22	5:A:251:SER:OG	2.04	0.58
5:A:241:GLN:CB	5:A:247:TYR:C	2.49	0.58
5:A:386:PRO:O	5:A:387:LEU:C	2.40	0.58
5:A:388:THR:O	5:A:389:VAL:C	2.40	0.58
5:A:87:LEU:HD21	5:A:336:MET:HE1	1.85	0.58
5:A:306:TYR:C	5:A:307:LEU:HD23	2.24	0.58
4:G:1544:A:H2'	4:G:1545:A:C8	2.39	0.57
5:A:238:ALA:HB1	5:A:368:PRO:C	2.21	0.57
5:A:176:ALA:CA	6:B:47:LEU:CD2	2.60	0.57
5:A:254:LEU:HB3	5:A:255:PRO:HA	0.67	0.57
5:A:226:ALA:O	5:A:258:VAL:CG1	2.52	0.57
5:A:16:LEU:CD2	5:A:16:LEU:H	2.07	0.57
5:A:363:VAL:HG22	5:A:364:PRO:N	2.18	0.57
7:C:30:PRO:O	7:C:34:ILE:HG12	2.03	0.57
3:F:1395:A:H4'	3:F:1397:U:C4	2.39	0.57
5:A:233:ILE:CD1	5:A:254:LEU:CB	2.69	0.57
5:A:390:MET:HG3	6:B:15:ARG:NH1	2.16	0.57
6:B:49:ILE:HG23	6:B:50:ILE:N	2.20	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:26:ARG:HG3	6:B:26:ARG:O	2.04	0.57
5:A:12:PRO:HB3	7:C:28:VAL:HG21	1.87	0.57
5:A:23:PHE:CD1	5:A:431:GLU:HB3	2.40	0.57
7:C:32:HIS:O	7:C:36:VAL:HG23	2.05	0.57
5:A:166:ILE:HG22	5:A:167:GLY:H	1.70	0.57
5:A:141:PHE:CZ	5:A:145:ILE:HD11	2.40	0.57
5:A:233:ILE:HD11	5:A:254:LEU:HD13	1.81	0.57
5:A:98:LEU:O	5:A:99:SER:C	2.43	0.57
5:A:135:LEU:O	5:A:137:PRO:HD3	2.04	0.57
5:A:264:ILE:N	5:A:265:PRO:CD	2.68	0.56
5:A:415:LEU:HD23	5:A:416:LEU:N	2.21	0.56
5:A:286:MET:O	5:A:286:MET:HG2	2.06	0.56
5:A:237:TYR:CD2	5:A:238:ALA:N	2.74	0.56
5:A:241:GLN:HB2	5:A:247:TYR:CA	2.33	0.56
5:A:365:GLY:C	5:A:366:ILE:HG23	2.25	0.56
5:A:189:PRO:C	5:A:191:GLY:H	2.09	0.56
5:A:233:ILE:CD1	5:A:254:LEU:CD1	2.72	0.56
5:A:363:VAL:CG2	5:A:364:PRO:HD3	2.34	0.56
6:B:18:VAL:O	6:B:21:VAL:CG1	2.53	0.56
6:B:47:LEU:O	6:B:50:ILE:CG2	2.53	0.56
5:A:403:ASN:HD21	5:A:412:THR:N	2.03	0.56
5:A:390:MET:HG3	6:B:15:ARG:HH12	1.70	0.56
5:A:361:ALA:O	5:A:362:PHE:CB	2.53	0.56
5:A:80:THR:O	5:A:83:ILE:HB	2.05	0.56
5:A:147:ILE:HG22	5:A:148:ALA:N	2.20	0.56
1:D:82:U:H2'	1:D:83:A:C8	2.41	0.56
1:D:103:A:H2'	1:D:104:A:O4'	2.05	0.56
5:A:182:ILE:HD12	6:B:44:ILE:HD11	1.87	0.56
4:G:1548:A:H2'	4:G:1549:A:H8	1.70	0.56
5:A:246:VAL:CG2	5:A:247:TYR:H	1.92	0.56
5:A:156:TYR:O	5:A:160:ILE:HG13	2.06	0.56
5:A:30:THR:O	5:A:33:VAL:HG23	2.05	0.56
6:B:61:ILE:HA	6:B:64:ILE:CG2	2.35	0.56
2:E:499:U:H2'	2:E:500:G:O4'	2.06	0.56
5:A:254:LEU:HB3	5:A:255:PRO:C	2.25	0.56
5:A:335:VAL:CG2	5:A:392:SER:HB3	2.36	0.56
5:A:34:LEU:HD11	6:B:47:LEU:CD1	2.36	0.56
5:A:116:ILE:HD12	5:A:116:ILE:H	1.71	0.55
3:F:1386:C:H2'	3:F:1387:A:H8	1.68	0.55
1:D:83:A:H61	1:D:101:A:H5'	1.70	0.55
5:A:234:VAL:HG11	5:A:252:THR:O	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:420:ILE:O	5:A:424:MET:HB2	2.05	0.55
6:B:41:ALA:O	6:B:44:ILE:HG22	2.06	0.55
5:A:380:LEU:O	5:A:384:ILE:N	2.37	0.55
5:A:390:MET:C	5:A:394:PHE:HB3	2.24	0.55
5:A:85:MET:HE1	5:A:111:GLN:N	2.21	0.55
5:A:167:GLY:HA2	5:A:427:GLN:NE2	2.20	0.55
5:A:389:VAL:HG13	5:A:391:SER:CB	2.31	0.55
5:A:87:LEU:CD2	5:A:336:MET:CE	2.84	0.55
5:A:241:GLN:HB3	5:A:247:TYR:O	2.05	0.55
5:A:246:VAL:HG13	5:A:247:TYR:N	2.21	0.55
5:A:386:PRO:CB	6:B:15:ARG:CD	2.77	0.55
5:A:253:HIS:C	5:A:254:LEU:HG	2.27	0.55
5:A:233:ILE:CG1	5:A:254:LEU:CG	2.85	0.55
5:A:365:GLY:O	5:A:366:ILE:CG2	2.54	0.55
6:B:32:GLU:O	6:B:35:ALA:N	2.37	0.55
5:A:242:GLN:C	5:A:244:ARG:N	2.44	0.55
5:A:391:SER:C	5:A:393:ALA:N	2.56	0.55
5:A:375:TYR:CD1	5:A:375:TYR:O	2.60	0.55
1:D:91:A:H1'	1:D:92:U:C6	2.41	0.55
5:A:98:LEU:O	5:A:100:ILE:O	2.24	0.55
5:A:146:GLN:HE21	7:C:44:GLU:HG2	1.72	0.54
5:A:228:CYS:SG	6:B:33:TYR:HD2	2.31	0.54
5:A:260:TYR:CE1	5:A:423:ARG:HB3	2.42	0.54
5:A:63:THR:HG23	5:A:76:GLY:CA	2.38	0.54
5:A:13:GLU:CG	5:A:14:VAL:H	2.15	0.54
5:A:355:ARG:CZ	5:A:442:LYS:O	2.55	0.54
6:B:64:ILE:HG12	6:B:64:ILE:O	2.07	0.54
1:D:99:U:O2	1:D:99:U:O4'	2.26	0.54
5:A:236:ASN:O	5:A:251:SER:OG	2.25	0.54
5:A:230:ARG:HB3	6:B:32:GLU:OE2	2.06	0.54
5:A:176:ALA:CB	6:B:47:LEU:HD11	2.36	0.54
5:A:112:LYS:O	5:A:116:ILE:HD12	2.07	0.54
4:G:1547:C:H2'	4:G:1548:A:C8	2.43	0.54
5:A:75:ILE:HD11	5:A:173:PHE:CD1	2.43	0.54
5:A:315:SER:HB3	5:A:404:PHE:O	2.07	0.54
6:B:23:TRP:NE1	6:B:27:LYS:HB3	2.20	0.54
6:B:25:THR:HG22	6:B:28:PRO:O	2.08	0.54
5:A:4:LEU:C	5:A:6:PRO:HD2	2.28	0.54
5:A:142:LEU:O	5:A:145:ILE:HB	2.08	0.54
5:A:342:VAL:O	5:A:344:THR:N	2.41	0.54
5:A:389:VAL:HG12	5:A:391:SER:OG	2.03	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:26:ARG:C	6:B:28:PRO:C	2.67	0.54
6:B:56:VAL:HG12	6:B:57:PRO:CD	2.15	0.54
5:A:149:PHE:HB3	7:C:40:PHE:CZ	2.43	0.54
6:B:46:LEU:C	6:B:49:ILE:HG22	2.28	0.54
5:A:206:ASN:OD1	5:A:208:GLU:HB2	2.07	0.54
5:A:232:ARG:HB3	5:A:255:PRO:HD3	1.90	0.53
1:D:100:U:H1'	1:D:101:A:N1	2.23	0.53
5:A:391:SER:O	5:A:392:SER:C	2.46	0.53
5:A:39:ILE:N	6:B:54:ILE:CD1	2.72	0.53
1:D:84:A:H4'	1:D:85:G:O5'	2.08	0.53
5:A:280:GLY:HA3	5:A:294:TYR:OH	2.07	0.53
5:A:311:TYR:HD1	5:A:312:GLY:N	2.05	0.53
5:A:18:VAL:HG12	5:A:18:VAL:O	2.08	0.53
5:A:300:VAL:O	5:A:300:VAL:HG12	2.07	0.53
5:A:415:LEU:HD23	5:A:415:LEU:C	2.29	0.53
5:A:149:PHE:HB3	7:C:40:PHE:CE2	2.43	0.53
5:A:390:MET:O	5:A:394:PHE:HB2	2.09	0.53
6:B:41:ALA:HA	6:B:44:ILE:HG22	1.90	0.53
6:B:55:HIS:O	6:B:59:THR:HG23	2.09	0.53
5:A:152:ILE:HD13	5:A:155:ILE:CD1	2.38	0.53
5:A:238:ALA:C	5:A:249:ALA:HB3	2.27	0.53
5:A:155:ILE:O	5:A:159:GLU:HG2	2.09	0.53
2:E:493:G:H2'	2:E:494:G:O4'	2.09	0.52
3:F:1400:U:H2'	3:F:1401:G:C8	2.43	0.52
4:G:1547:C:H2'	4:G:1548:A:H8	1.74	0.52
5:A:386:PRO:HB2	6:B:15:ARG:HD2	1.89	0.52
5:A:92:GLY:O	5:A:94:ILE:N	2.42	0.52
5:A:342:VAL:C	5:A:344:THR:N	2.63	0.52
5:A:39:ILE:CG1	6:B:54:ILE:HD11	2.38	0.52
5:A:113:LEU:O	5:A:116:ILE:N	2.43	0.52
5:A:23:PHE:HD1	5:A:431:GLU:HB3	1.72	0.52
6:B:46:LEU:HA	6:B:49:ILE:HG22	1.92	0.52
3:F:1400:U:H2'	3:F:1401:G:H8	1.73	0.52
4:G:1545:A:H2'	4:G:1546:G:O4'	2.09	0.52
5:A:87:LEU:HD21	5:A:336:MET:CE	2.39	0.52
5:A:228:CYS:HB3	6:B:33:TYR:CE2	2.41	0.52
6:B:18:VAL:HG13	6:B:19:ARG:N	2.24	0.52
5:A:294:TYR:CE2	5:A:299:ALA:HB2	2.44	0.52
5:A:72:THR:HB	5:A:147:ILE:HD12	1.92	0.52
5:A:172:LEU:HD23	5:A:172:LEU:C	2.30	0.52
3:F:1386:C:H5"	3:F:1396:U:O2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:227:GLU:O	6:B:36:VAL:HG11	2.10	0.52
5:A:357:LYS:HD2	5:A:374:LYS:CA	2.38	0.52
5:A:108:GLN:O	5:A:109:GLY:C	2.47	0.52
5:A:5:ILE:HG22	5:A:9:GLU:OE1	2.10	0.51
5:A:164:TYR:CZ	7:C:30:PRO:HG2	2.46	0.51
5:A:231:ARG:CG	6:B:22:ILE:HD12	2.32	0.51
5:A:166:ILE:HG22	5:A:167:GLY:N	2.25	0.51
5:A:399:ALA:O	5:A:402:ALA:HB3	2.09	0.51
5:A:238:ALA:HB1	5:A:369:GLY:N	2.18	0.51
5:A:294:TYR:HB3	5:A:298:ARG:O	2.09	0.51
3:F:1399:C:O2'	3:F:1400:U:H5'	2.10	0.51
5:A:231:ARG:HG2	6:B:22:ILE:CD1	2.31	0.51
6:B:36:VAL:HG13	6:B:37:ALA:H	1.74	0.51
4:G:1535:A:H3'	4:G:1536:C:C6	2.45	0.51
5:A:427:GLN:O	5:A:431:GLU:HG2	2.11	0.51
5:A:83:ILE:HG23	5:A:337:PHE:CE2	2.46	0.51
5:A:331:ILE:HG23	5:A:393:ALA:HB2	1.91	0.51
6:B:29:THR:OG1	6:B:32:GLU:HB3	2.09	0.51
6:B:52:TYR:O	6:B:53:ILE:O	2.29	0.51
2:E:480:A:H3'	2:E:481:G:C5'	2.40	0.51
5:A:317:ILE:O	5:A:319:ASP:N	2.38	0.51
5:A:24:LYS:O	5:A:28:LYS:HG3	2.11	0.51
5:A:238:ALA:O	5:A:249:ALA:O	2.29	0.51
5:A:389:VAL:CG1	5:A:391:SER:OG	2.58	0.51
6:B:32:GLU:O	6:B:35:ALA:HB3	2.10	0.51
5:A:206:ASN:HB3	5:A:209:TYR:HD1	1.74	0.51
5:A:321:ILE:O	5:A:325:VAL:HG23	2.11	0.51
2:E:480:A:H2'	2:E:480:A:N3	2.25	0.51
5:A:389:VAL:CB	5:A:391:SER:HB3	2.34	0.51
5:A:246:VAL:HG22	5:A:248:ALA:H	1.76	0.51
5:A:360:GLY:CA	5:A:370:GLU:CD	2.54	0.51
4:G:1537:G:C6	4:G:1538:G:H1'	2.45	0.51
5:A:88:LEU:C	5:A:90:GLY:N	2.63	0.51
5:A:300:VAL:O	5:A:301:ASP:HB2	2.11	0.51
4:G:1541:C:H2'	4:G:1542:U:O4'	2.11	0.51
5:A:21:ILE:HD12	5:A:21:ILE:H	1.76	0.51
5:A:227:GLU:CG	5:A:257:LYS:HZ1	2.16	0.51
5:A:412:THR:O	5:A:415:LEU:HB3	2.11	0.51
6:B:29:THR:C	6:B:31:ASP:H	2.13	0.51
5:A:98:LEU:O	5:A:100:ILE:N	2.43	0.51
5:A:439:ALA:O	5:A:441:ALA:N	2.39	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:1540:G:H2'	4:G:1541:C:C6	2.46	0.50
5:A:365:GLY:O	5:A:366:ILE:CD1	2.60	0.50
6:B:23:TRP:HE1	6:B:27:LYS:HB2	1.76	0.50
5:A:39:ILE:CA	6:B:54:ILE:HD11	2.41	0.50
5:A:398:LEU:O	5:A:402:ALA:HB2	2.11	0.50
3:F:1394:U:O2'	3:F:1395:A:H5'	2.10	0.50
5:A:172:LEU:CD2	5:A:172:LEU:C	2.80	0.50
5:A:231:ARG:O	5:A:232:ARG:HB3	2.11	0.50
5:A:281:LEU:HD13	5:A:281:LEU:C	2.32	0.50
5:A:435:GLU:HG3	5:A:435:GLU:O	2.12	0.50
5:A:377:GLU:O	5:A:379:ARG:N	2.44	0.50
7:C:22:THR:HG22	7:C:24:SER:H	1.76	0.50
5:A:255:PRO:HB2	5:A:256:LEU:HD23	1.93	0.50
6:B:46:LEU:CA	6:B:49:ILE:HG22	2.42	0.50
5:A:136:THR:HG22	5:A:139:LEU:H	1.76	0.50
6:B:25:THR:CG2	6:B:29:THR:HG22	2.39	0.50
5:A:189:PRO:HG3	6:B:56:VAL:CG2	2.41	0.50
5:A:227:GLU:HB3	5:A:257:LYS:NZ	2.27	0.50
5:A:373:ALA:O	5:A:374:LYS:HB2	2.11	0.50
5:A:75:ILE:HG21	5:A:170:ILE:HG23	1.93	0.49
5:A:370:GLU:O	5:A:372:THR:N	2.45	0.49
5:A:80:THR:HG23	5:A:275:ASN:HD21	1.76	0.49
5:A:336:MET:HG3	5:A:340:PHE:CE1	2.47	0.49
5:A:116:ILE:HD12	5:A:116:ILE:N	2.26	0.49
5:A:355:ARG:NE	5:A:442:LYS:O	2.45	0.49
6:B:5:LYS:HA	6:B:8:VAL:CG1	2.42	0.49
5:A:306:TYR:O	5:A:307:LEU:HD23	2.12	0.49
1:D:104:A:H2'	1:D:105:C:C6	2.47	0.49
5:A:238:ALA:O	5:A:249:ALA:C	2.51	0.49
5:A:189:PRO:HG3	6:B:56:VAL:HG23	1.94	0.49
5:A:82:GLY:O	5:A:86:GLN:HG2	2.11	0.49
5:A:89:VAL:O	5:A:89:VAL:HG12	2.12	0.49
5:A:261:VAL:C	5:A:263:ASN:N	2.62	0.49
5:A:102:GLU:C	5:A:106:LEU:HG	2.31	0.49
5:A:29:TRP:CE2	5:A:164:TYR:HD2	2.31	0.49
5:A:89:VAL:HG21	5:A:107:PHE:CD1	2.47	0.49
5:A:241:GLN:CB	5:A:247:TYR:N	2.74	0.49
7:C:30:PRO:HA	7:C:33:VAL:CG2	2.42	0.49
5:A:160:ILE:HD11	7:C:33:VAL:CG2	2.43	0.49
7:C:34:ILE:O	7:C:38:VAL:HG23	2.13	0.49
6:B:58:ALA:O	6:B:61:ILE:CG2	2.57	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:381:LYS:O	5:A:385:PRO:CG	2.60	0.49
6:B:32:GLU:O	6:B:33:TYR:C	2.50	0.49
4:G:1533:C:H2'	4:G:1534:U:O4'	2.12	0.49
6:B:5:LYS:HA	6:B:8:VAL:HG12	1.94	0.49
5:A:376:ILE:HG22	5:A:376:ILE:O	2.11	0.49
5:A:260:TYR:O	5:A:261:VAL:C	2.51	0.49
7:C:35:GLY:HA2	7:C:38:VAL:HG23	1.94	0.49
5:A:43:ILE:HG22	5:A:70:LEU:HD11	1.93	0.49
5:A:358:LYS:O	5:A:360:GLY:N	2.45	0.49
5:A:384:ILE:N	5:A:385:PRO:CD	2.75	0.49
5:A:228:CYS:SG	5:A:229:MET:N	2.84	0.49
5:A:233:ILE:O	5:A:234:VAL:HG23	2.13	0.49
5:A:239:LYS:CD	5:A:240:ARG:NH2	2.75	0.49
5:A:34:LEU:HD21	6:B:50:ILE:HG21	1.94	0.49
6:B:26:ARG:CA	6:B:27:LYS:HD3	2.35	0.49
5:A:228:CYS:O	5:A:229:MET:O	2.30	0.49
5:A:118:MET:O	5:A:122:GLU:HG2	2.13	0.49
5:A:321:ILE:HD12	5:A:322:HIS:N	2.19	0.49
5:A:15:GLU:O	5:A:17:PRO:HD3	2.12	0.49
5:A:250:GLN:O	5:A:251:SER:OG	2.30	0.48
5:A:429:LEU:C	5:A:431:GLU:N	2.65	0.48
5:A:179:SER:HB3	6:B:48:GLY:N	2.28	0.48
2:E:490:C:H42	5:A:358:LYS:HZ2	1.55	0.48
5:A:350:LYS:O	5:A:351:SER:HB2	2.13	0.48
5:A:75:ILE:HD11	5:A:173:PHE:HD1	1.78	0.48
5:A:34:LEU:HD23	6:B:50:ILE:HD12	1.94	0.48
5:A:360:GLY:HA3	5:A:370:GLU:OE1	2.10	0.48
5:A:367:ARG:N	5:A:368:PRO:HD3	2.26	0.48
5:A:261:VAL:HG21	5:A:388:THR:HG22	0.54	0.48
5:A:257:LYS:HD2	5:A:422:TYR:HE2	1.73	0.48
6:B:25:THR:HG22	6:B:26:ARG:N	2.28	0.48
5:A:46:TYR:CB	5:A:146:GLN:HE22	2.19	0.48
5:A:256:LEU:CD2	5:A:256:LEU:N	2.76	0.48
5:A:381:LYS:C	5:A:385:PRO:HD3	2.28	0.48
5:A:75:ILE:O	5:A:79:VAL:HG23	2.13	0.48
1:D:100:U:H1'	1:D:101:A:C2	2.49	0.48
5:A:92:GLY:O	5:A:95:GLN:HG3	2.14	0.48
6:B:50:ILE:O	6:B:54:ILE:HG22	2.13	0.48
5:A:67:ILE:HG23	5:A:72:THR:HG23	1.94	0.48
5:A:38:PHE:CB	6:B:54:ILE:CD1	2.66	0.48
1:D:104:A:H2'	1:D:105:C:H6	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:179:SER:HB3	6:B:48:GLY:CA	2.44	0.48
5:A:181:THR:HG21	5:A:409:GLY:HA2	1.96	0.48
5:A:239:LYS:HB3	5:A:240:ARG:NH2	2.27	0.48
5:A:167:GLY:HA2	5:A:427:GLN:CD	2.34	0.48
5:A:350:LYS:O	5:A:351:SER:OG	2.30	0.48
6:B:65:LEU:O	6:B:65:LEU:HG	2.14	0.48
5:A:237:TYR:CG	5:A:238:ALA:N	2.82	0.48
5:A:239:LYS:CG	5:A:248:ALA:O	2.61	0.48
5:A:233:ILE:HG12	5:A:254:LEU:HB2	0.50	0.48
6:B:54:ILE:CG2	6:B:55:HIS:N	2.72	0.48
5:A:313:LEU:N	5:A:313:LEU:HD12	2.29	0.48
5:A:34:LEU:HD13	5:A:172:LEU:HD21	1.96	0.47
5:A:136:THR:O	5:A:138:LEU:N	2.47	0.47
6:B:26:ARG:CB	6:B:28:PRO:O	2.60	0.47
5:A:375:TYR:CG	5:A:375:TYR:O	2.66	0.47
5:A:124:VAL:HA	5:A:144:ILE:CD1	2.44	0.47
5:A:354:LYS:C	5:A:355:ARG:HG3	2.35	0.47
5:A:194:TRP:O	5:A:195:LYS:C	2.52	0.47
5:A:94:ILE:O	5:A:94:ILE:HG22	2.14	0.47
5:A:344:THR:O	5:A:345:THR:OG1	2.31	0.47
5:A:309:THR:HG21	5:A:403:ASN:OD1	2.14	0.47
5:A:179:SER:OG	6:B:44:ILE:HG13	2.15	0.47
5:A:235:VAL:CG2	5:A:236:ASN:N	2.51	0.47
5:A:330:MET:O	5:A:331:ILE:C	2.52	0.47
5:A:386:PRO:HB3	6:B:15:ARG:CZ	2.40	0.47
6:B:26:ARG:CG	6:B:30:LYS:H	1.91	0.47
5:A:153:ILE:HG21	7:C:37:THR:HG23	1.96	0.47
5:A:118:MET:O	5:A:122:GLU:CG	2.63	0.47
5:A:227:GLU:CB	6:B:36:VAL:CG2	2.80	0.47
6:B:26:ARG:CD	6:B:27:LYS:HZ1	2.26	0.47
5:A:14:VAL:HG21	5:A:159:GLU:HB3	1.95	0.47
5:A:301:ASP:N	5:A:305:TYR:HB2	2.29	0.47
5:A:227:GLU:O	6:B:36:VAL:CB	2.62	0.47
5:A:239:LYS:CB	5:A:240:ARG:NH1	2.59	0.47
5:A:245:ARG:N	5:A:247:TYR:CE1	2.76	0.47
5:A:341:TRP:O	5:A:344:THR:HG23	2.15	0.47
6:B:52:TYR:O	6:B:56:VAL:HG12	2.15	0.47
5:A:86:GLN:O	5:A:90:GLY:HA3	2.13	0.47
5:A:294:TYR:CD2	5:A:299:ALA:HB2	2.50	0.47
5:A:67:ILE:CA	5:A:72:THR:HG23	2.34	0.47
6:B:5:LYS:O	6:B:8:VAL:HG13	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:74:GLY:O	5:A:77:PRO:HD2	2.14	0.47
3:F:1402:U:H5'	4:G:1521:G:HO2'	1.76	0.47
2:E:479:A:O2'	2:E:481:G:H5'	2.15	0.47
5:A:166:ILE:CD1	5:A:428:LEU:HD21	2.45	0.47
5:A:214:ILE:O	5:A:215:GLY:C	2.52	0.47
5:A:318:SER:O	5:A:319:ASP:CG	2.53	0.47
5:A:172:LEU:CD2	5:A:176:ALA:HB2	2.45	0.47
5:A:171:GLY:HA3	5:A:423:ARG:HH21	1.80	0.47
6:B:5:LYS:CA	6:B:8:VAL:HG12	2.45	0.47
5:A:135:LEU:N	5:A:135:LEU:HD12	2.30	0.47
5:A:232:ARG:HA	5:A:233:ILE:CG2	2.37	0.47
5:A:84:ILE:O	5:A:87:LEU:N	2.47	0.47
1:D:102:U:H4'	1:D:103:A:OP1	2.15	0.47
5:A:123:ALA:HB2	5:A:148:ALA:HB2	1.96	0.46
3:F:1401:G:H2'	3:F:1402:U:C6	2.49	0.46
6:B:26:ARG:CA	6:B:28:PRO:O	2.64	0.46
5:A:98:LEU:HD23	5:A:103:ASN:HB3	1.96	0.46
6:B:61:ILE:CA	6:B:64:ILE:HG22	2.43	0.46
5:A:427:GLN:HB2	5:A:427:GLN:HE21	1.53	0.46
5:A:410:GLY:O	5:A:411:GLY:C	2.53	0.46
5:A:239:LYS:HA	5:A:249:ALA:HB3	1.97	0.46
5:A:233:ILE:CG1	5:A:254:LEU:HD12	2.45	0.46
5:A:366:ILE:CG1	5:A:368:PRO:HG3	2.45	0.46
5:A:12:PRO:HB3	7:C:28:VAL:CG2	2.45	0.46
5:A:227:GLU:HB3	5:A:257:LYS:HZ1	1.81	0.46
5:A:233:ILE:HD11	5:A:254:LEU:CB	2.46	0.46
2:E:488:G:H1'	2:E:492:A:N6	2.30	0.46
1:D:100:U:H1'	1:D:101:A:C6	2.50	0.46
5:A:311:TYR:CD1	5:A:312:GLY:N	2.84	0.46
5:A:344:THR:CG2	5:A:345:THR:N	2.51	0.46
5:A:112:LYS:HD3	5:A:116:ILE:HD11	1.98	0.46
5:A:79:VAL:HG11	5:A:271:ALA:CB	2.45	0.46
5:A:120:PHE:O	5:A:123:ALA:HB3	2.15	0.46
7:C:49:TYR:CD1	7:C:49:TYR:N	2.83	0.46
5:A:260:TYR:HE1	5:A:423:ARG:CB	2.28	0.46
5:A:389:VAL:CG2	5:A:390:MET:HB3	2.40	0.46
6:B:27:LYS:CD	6:B:27:LYS:N	2.70	0.46
4:G:1536:C:H1'	4:G:1537:G:H22	1.81	0.46
5:A:321:ILE:CD1	5:A:322:HIS:H	2.21	0.46
5:A:23:PHE:CE1	5:A:431:GLU:HB2	2.48	0.46
5:A:273:PHE:H	5:A:273:PHE:HD1	1.62	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:129:ALA:O	5:A:285:ARG:HD3	2.15	0.46
5:A:263:ASN:HD22	5:A:423:ARG:NH1	2.13	0.46
5:A:124:VAL:CG2	5:A:144:ILE:HD13	2.36	0.46
5:A:230:ARG:HE	5:A:255:PRO:N	2.14	0.46
5:A:357:LYS:CD	5:A:374:LYS:HA	2.42	0.46
5:A:153:ILE:CD1	7:C:37:THR:HG23	2.40	0.46
5:A:153:ILE:HD11	7:C:40:PHE:CD1	2.50	0.46
5:A:386:PRO:CA	6:B:15:ARG:NH1	2.78	0.45
5:A:386:PRO:O	5:A:389:VAL:CG2	2.47	0.45
5:A:38:PHE:CE1	6:B:51:GLY:N	2.84	0.45
5:A:8:LEU:HD23	5:A:8:LEU:C	2.36	0.45
5:A:230:ARG:HE	5:A:255:PRO:CA	2.29	0.45
5:A:239:LYS:CB	5:A:248:ALA:O	2.64	0.45
5:A:227:GLU:CB	5:A:257:LYS:NZ	2.77	0.45
5:A:380:LEU:C	5:A:384:ILE:CG1	2.84	0.45
5:A:195:LYS:HB3	5:A:209:TYR:CE2	2.50	0.45
5:A:245:ARG:C	5:A:246:VAL:CG1	2.83	0.45
5:A:349:PRO:O	5:A:352:MET:N	2.49	0.45
5:A:176:ALA:HA	6:B:47:LEU:HG	1.94	0.45
5:A:245:ARG:O	5:A:246:VAL:HG13	2.14	0.45
5:A:230:ARG:HE	5:A:256:LEU:N	2.14	0.45
5:A:3:LYS:O	5:A:5:ILE:N	2.47	0.45
5:A:39:ILE:HG12	6:B:54:ILE:CD1	2.42	0.45
6:B:45:SER:O	6:B:49:ILE:HG22	2.15	0.45
5:A:340:PHE:CD1	5:A:340:PHE:N	2.85	0.45
5:A:45:VAL:HG11	5:A:147:ILE:HD11	1.98	0.45
5:A:14:VAL:HG13	7:C:30:PRO:HG3	1.98	0.45
5:A:227:GLU:OE2	5:A:419:SER:HA	2.17	0.45
7:C:30:PRO:O	7:C:33:VAL:HG23	2.17	0.45
5:A:237:TYR:CE2	5:A:238:ALA:HB2	2.52	0.45
5:A:260:TYR:HE1	5:A:423:ARG:CG	2.24	0.45
6:B:36:VAL:O	6:B:40:THR:CG2	2.58	0.45
5:A:319:ASP:N	5:A:320:PRO:HD3	2.32	0.45
5:A:346:GLY:O	5:A:348:ASP:N	2.49	0.45
5:A:246:VAL:O	5:A:247:TYR:CG	2.69	0.45
5:A:261:VAL:HG21	5:A:388:THR:CB	2.35	0.45
5:A:42:CYS:SG	6:B:55:HIS:HA	2.57	0.45
5:A:170:ILE:O	5:A:171:GLY:C	2.56	0.45
5:A:262:SER:C	5:A:265:PRO:HD2	2.37	0.45
5:A:369:GLY:O	5:A:370:GLU:HB2	2.17	0.45
5:A:129:ALA:C	5:A:285:ARG:HD3	2.37	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:402:ALA:O	5:A:405:ILE:CG2	2.65	0.45
5:A:117:ILE:O	5:A:121:VAL:HG23	2.17	0.45
5:A:11:ILE:CD1	5:A:113:LEU:HD23	2.32	0.45
5:A:227:GLU:HB3	6:B:36:VAL:CG2	2.42	0.44
5:A:157:LEU:HD23	5:A:160:ILE:CD1	2.35	0.44
6:B:61:ILE:O	6:B:64:ILE:HG22	2.17	0.44
5:A:377:GLU:C	5:A:379:ARG:N	2.70	0.44
5:A:77:PRO:O	5:A:80:THR:N	2.50	0.44
1:D:92:U:H3'	1:D:93:G:H8	1.82	0.44
5:A:169:GLY:O	5:A:170:ILE:C	2.56	0.44
5:A:136:THR:O	5:A:137:PRO:C	2.54	0.44
5:A:248:ALA:O	5:A:249:ALA:HB3	2.17	0.44
5:A:230:ARG:HG3	5:A:255:PRO:CG	2.34	0.44
5:A:388:THR:OG1	5:A:389:VAL:N	2.49	0.44
5:A:87:LEU:HD23	5:A:336:MET:CE	2.47	0.44
5:A:194:TRP:O	5:A:197:LEU:N	2.50	0.44
5:A:414:VAL:O	5:A:418:VAL:HG23	2.17	0.44
5:A:227:GLU:HB2	6:B:36:VAL:CG2	2.29	0.44
5:A:391:SER:O	5:A:395:VAL:N	2.50	0.44
6:B:46:LEU:HA	6:B:49:ILE:CG2	2.47	0.44
6:B:47:LEU:C	6:B:50:ILE:HG22	2.38	0.44
5:A:91:SER:C	5:A:93:ILE:H	2.20	0.44
5:A:263:ASN:HD21	5:A:423:ARG:NH1	2.10	0.44
5:A:63:THR:O	5:A:63:THR:HG22	2.16	0.44
7:C:30:PRO:HA	7:C:33:VAL:HG22	2.00	0.44
5:A:149:PHE:CD2	7:C:40:PHE:HZ	2.31	0.44
6:B:51:GLY:O	6:B:55:HIS:CB	2.65	0.44
5:A:13:GLU:O	7:C:28:VAL:HB	2.18	0.44
5:A:319:ASP:O	5:A:320:PRO:C	2.56	0.44
5:A:246:VAL:HG13	5:A:247:TYR:H	1.83	0.44
6:B:23:TRP:CZ2	6:B:27:LYS:CB	2.98	0.44
5:A:130:GLY:HA3	5:A:285:ARG:NH1	2.33	0.44
6:B:13:GLU:O	6:B:16:THR:OG1	2.30	0.44
6:B:41:ALA:O	6:B:44:ILE:CG2	2.66	0.44
5:A:311:TYR:C	5:A:311:TYR:CD1	2.91	0.44
5:A:216:THR:OG1	5:A:408:LEU:HB3	2.18	0.44
5:A:172:LEU:O	5:A:175:ALA:N	2.50	0.43
5:A:238:ALA:CB	5:A:368:PRO:C	2.83	0.43
5:A:38:PHE:CZ	6:B:50:ILE:HG23	2.40	0.43
1:D:83:A:H2'	1:D:84:A:N7	2.33	0.43
5:A:227:GLU:O	6:B:36:VAL:HB	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:33:TYR:O	6:B:36:VAL:CG1	2.51	0.43
5:A:194:TRP:O	5:A:196:PHE:N	2.51	0.43
5:A:358:LYS:O	5:A:359:SER:C	2.57	0.43
5:A:415:LEU:CD2	5:A:416:LEU:N	2.81	0.43
6:B:8:VAL:HG13	6:B:9:ALA:N	2.33	0.43
2:E:492:A:OP1	5:A:244:ARG:HB2	2.18	0.43
5:A:331:ILE:CD1	5:A:392:SER:O	2.65	0.43
6:B:50:ILE:HG23	6:B:51:GLY:N	2.33	0.43
5:A:361:ALA:O	5:A:362:PHE:HB3	2.19	0.43
5:A:284:TYR:C	5:A:286:MET:H	2.22	0.43
5:A:240:ARG:N	5:A:240:ARG:HE	2.13	0.43
6:B:39:VAL:HG13	6:B:40:THR:N	2.34	0.43
5:A:379:ARG:HD2	5:A:383:TYR:CE2	2.54	0.43
5:A:171:GLY:HA2	5:A:420:ILE:HD13	2.00	0.43
5:A:230:ARG:NE	5:A:256:LEU:N	2.66	0.43
5:A:227:GLU:HA	5:A:257:LYS:HE3	1.98	0.43
5:A:385:PRO:CB	5:A:386:PRO:CD	2.59	0.43
6:B:25:THR:CG2	6:B:29:THR:CG2	2.96	0.43
5:A:163:LYS:O	5:A:164:TYR:CD1	2.72	0.43
2:E:483:A:H5"	5:A:245:ARG:NH2	2.34	0.43
5:A:38:PHE:CD1	6:B:51:GLY:HA2	2.54	0.43
5:A:239:LYS:HD2	5:A:240:ARG:NH2	2.26	0.43
5:A:239:LYS:N	5:A:368:PRO:CB	2.78	0.43
5:A:389:VAL:CA	5:A:391:SER:HB3	2.48	0.43
5:A:170:ILE:HG13	5:A:170:ILE:H	1.48	0.43
5:A:266:VAL:CG1	5:A:416:LEU:HD21	2.48	0.43
5:A:386:PRO:CB	6:B:15:ARG:HH11	2.05	0.43
5:A:14:VAL:CG1	7:C:30:PRO:HG3	2.48	0.43
5:A:46:TYR:HB3	5:A:146:GLN:NE2	2.20	0.43
5:A:23:PHE:CE1	5:A:431:GLU:CB	3.02	0.43
5:A:346:GLY:O	5:A:347:LEU:C	2.57	0.43
5:A:240:ARG:CD	5:A:240:ARG:N	2.82	0.42
5:A:79:VAL:HG11	5:A:271:ALA:HB2	2.01	0.42
4:G:1533:C:H2'	4:G:1534:U:C6	2.54	0.42
5:A:98:LEU:CA	5:A:103:ASN:HB2	2.34	0.42
5:A:224:VAL:O	5:A:227:GLU:N	2.52	0.42
5:A:171:GLY:O	5:A:420:ILE:HG21	2.19	0.42
6:B:22:ILE:O	6:B:22:ILE:CG2	2.67	0.42
5:A:29:TRP:O	5:A:30:THR:C	2.57	0.42
3:F:1400:U:O2'	3:F:1401:G:H5'	2.18	0.42
5:A:194:TRP:C	5:A:196:PHE:N	2.71	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:97:C:H2'	1:D:98:G:O4'	2.18	0.42
5:A:143:VAL:O	5:A:144:ILE:C	2.56	0.42
5:A:166:ILE:HD13	5:A:428:LEU:HD23	1.97	0.42
2:E:497:A:H2'	2:E:498:G:C8	2.54	0.42
5:A:224:VAL:HG11	6:B:37:ALA:HB2	1.99	0.42
5:A:342:VAL:O	5:A:343:GLU:C	2.57	0.42
5:A:76:GLY:O	5:A:80:THR:OG1	2.35	0.42
5:A:257:LYS:HZ2	5:A:422:TYR:HD2	1.55	0.42
5:A:124:VAL:HA	5:A:144:ILE:HD11	2.02	0.42
5:A:188:GLY:HA2	6:B:52:TYR:CE1	2.41	0.42
5:A:240:ARG:NE	5:A:240:ARG:CA	2.83	0.42
5:A:241:GLN:OE1	5:A:241:GLN:O	2.38	0.42
5:A:256:LEU:HD23	5:A:256:LEU:H	1.83	0.42
6:B:31:ASP:OD1	6:B:31:ASP:O	2.37	0.42
5:A:87:LEU:CD2	5:A:336:MET:HE1	2.46	0.42
5:A:98:LEU:HD22	5:A:104:ARG:HA	2.02	0.42
3:F:1401:G:H2'	3:F:1402:U:O4'	2.19	0.42
3:F:1397:U:H5"	3:F:1398:C:H5	1.84	0.42
5:A:329:ALA:O	5:A:332:ILE:HG12	2.20	0.42
5:A:228:CYS:SG	6:B:33:TYR:CD2	3.10	0.42
5:A:33:VAL:HG11	5:A:161:VAL:CG2	2.50	0.42
6:B:61:ILE:CG2	6:B:62:LYS:N	2.83	0.42
5:A:173:PHE:O	5:A:176:ALA:HB3	2.20	0.42
5:A:189:PRO:CG	6:B:56:VAL:CG2	2.96	0.42
5:A:149:PHE:O	5:A:152:ILE:HB	2.20	0.42
5:A:220:PHE:CE2	5:A:224:VAL:HG21	2.54	0.42
5:A:63:THR:CG2	5:A:76:GLY:H	2.25	0.42
5:A:79:VAL:O	5:A:80:THR:C	2.58	0.42
5:A:277:GLN:HE21	5:A:308:SER:HB3	1.83	0.42
5:A:211:ALA:HB3	5:A:212:PRO:HD3	2.02	0.42
5:A:216:THR:HA	5:A:407:ALA:HB1	2.02	0.42
5:A:341:TRP:O	5:A:345:THR:O	2.38	0.41
6:B:29:THR:C	6:B:31:ASP:N	2.74	0.41
6:B:32:GLU:O	6:B:35:ALA:CB	2.68	0.41
4:G:1535:A:H3'	4:G:1536:C:C5	2.55	0.41
5:A:230:ARG:NE	5:A:255:PRO:CD	2.83	0.41
5:A:380:LEU:O	5:A:382:ARG:N	2.53	0.41
6:B:19:ARG:HA	6:B:22:ILE:CG2	2.51	0.41
2:E:490:C:H4'	2:E:490:C:OP2	2.20	0.41
5:A:84:ILE:CD1	5:A:114:LEU:HD21	2.24	0.41
5:A:67:ILE:HG23	5:A:72:THR:CG2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:31:GLY:O	5:A:35:VAL:HG23	2.20	0.41
5:A:49:GLY:C	5:A:51:GLN:H	2.22	0.41
5:A:239:LYS:O	5:A:368:PRO:CB	2.65	0.41
5:A:263:ASN:ND2	5:A:423:ARG:HH11	2.14	0.41
5:A:272:LEU:HA	5:A:272:LEU:HD22	1.84	0.41
5:A:34:LEU:HD21	6:B:50:ILE:CD1	2.33	0.41
5:A:370:GLU:O	5:A:371:GLN:C	2.57	0.41
5:A:391:SER:H	5:A:394:PHE:N	2.08	0.41
5:A:239:LYS:H	5:A:368:PRO:HA	1.85	0.41
6:B:26:ARG:NE	6:B:27:LYS:HZ1	2.19	0.41
5:A:85:MET:HG3	5:A:111:GLN:HG3	2.01	0.41
5:A:166:ILE:CG2	5:A:427:GLN:HG2	2.50	0.41
5:A:433:VAL:C	5:A:435:GLU:N	2.74	0.41
5:A:100:ILE:C	5:A:102:GLU:N	2.73	0.41
5:A:156:TYR:HB3	7:C:33:VAL:HG11	2.02	0.41
5:A:157:LEU:HD23	5:A:157:LEU:HA	1.95	0.41
5:A:5:ILE:N	5:A:6:PRO:CD	2.83	0.41
4:G:1542:U:O2'	4:G:1543:G:H5'	2.21	0.41
5:A:370:GLU:C	5:A:372:THR:N	2.74	0.41
5:A:193:LEU:HG	5:A:197:LEU:HD22	2.02	0.41
5:A:69:THR:C	5:A:71:ILE:H	2.22	0.41
7:C:31:GLU:OE2	7:C:31:GLU:N	2.37	0.41
5:A:224:VAL:O	5:A:226:ALA:N	2.54	0.41
5:A:386:PRO:C	6:B:15:ARG:NH1	2.74	0.41
6:B:53:ILE:HG23	6:B:54:ILE:N	2.27	0.41
5:A:85:MET:CE	5:A:111:GLN:HB2	2.49	0.41
7:C:43:ILE:O	7:C:47:LEU:N	2.44	0.41
3:F:1394:U:C2'	3:F:1395:A:H5'	2.50	0.41
6:B:66:LYS:O	6:B:66:LYS:HG2	2.20	0.41
5:A:342:VAL:C	5:A:344:THR:H	2.24	0.41
5:A:240:ARG:CG	5:A:367:ARG:N	2.47	0.41
5:A:116:ILE:HA	5:A:119:CYS:HB2	2.02	0.41
5:A:324:ILE:HG23	5:A:328:ILE:HD11	2.03	0.41
5:A:26:LYS:HA	5:A:165:GLY:HA2	2.03	0.41
5:A:227:GLU:CB	5:A:257:LYS:HZ1	2.33	0.40
5:A:92:GLY:O	5:A:93:ILE:C	2.58	0.40
2:E:497:A:H2'	2:E:498:G:H8	1.87	0.40
5:A:357:LYS:CD	5:A:374:LYS:N	2.84	0.40
5:A:360:GLY:O	5:A:361:ALA:HB2	2.21	0.40
5:A:380:LEU:O	5:A:381:LYS:C	2.59	0.40
6:B:49:ILE:CG2	6:B:50:ILE:N	2.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:43:ILE:C	5:A:70:LEU:HD13	2.41	0.40
5:A:166:ILE:HG22	5:A:427:GLN:HG2	2.02	0.40
5:A:35:VAL:O	5:A:36:LEU:C	2.58	0.40
5:A:36:LEU:HD23	5:A:36:LEU:HA	1.92	0.40
5:A:241:GLN:O	5:A:242:GLN:CB	2.69	0.40
5:A:245:ARG:C	5:A:247:TYR:CE1	2.95	0.40
5:A:236:ASN:N	5:A:251:SER:HB2	2.37	0.40
5:A:357:LYS:HD3	5:A:374:LYS:H	1.86	0.40
5:A:200:LEU:HD23	5:A:200:LEU:HA	1.89	0.40
5:A:89:VAL:HG21	5:A:107:PHE:HD1	1.85	0.40
5:A:263:ASN:HD22	5:A:423:ARG:HH11	1.68	0.40
5:A:335:VAL:HG23	5:A:392:SER:HB2	1.89	0.40
5:A:382:ARG:C	5:A:384:ILE:N	2.75	0.40
5:A:386:PRO:CB	6:B:15:ARG:CZ	2.97	0.40
6:B:41:ALA:CA	6:B:44:ILE:HG22	2.52	0.40
6:B:36:VAL:CG1	6:B:37:ALA:N	2.83	0.40
5:A:325:VAL:O	5:A:326:TYR:C	2.60	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 PDB entries followed by that with respect to all EM entries.

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
5	A	440/442 (100%)	241 (55%)	116 (26%)	83 (19%)	0 3
6	B	63/65 (97%)	45 (71%)	9 (14%)	9 (14%)	0 6
7	C	30/32 (94%)	19 (63%)	11 (37%)	0	100 100
All	All	533/539 (99%)	305 (57%)	136 (26%)	92 (17%)	0 4

All (92) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	A	66	ARG
5	A	99	SER
5	A	229	MET
5	A	230	ARG
5	A	232	ARG
5	A	233	ILE
5	A	238	ALA
5	A	242	GLN
5	A	243	GLY
5	A	244	ARG
5	A	247	TYR
5	A	251	SER
5	A	254	LEU
5	A	255	PRO
5	A	257	LYS
5	A	259	VAL
5	A	260	TYR
5	A	262	SER
5	A	318	SER
5	A	361	ALA
5	A	363	VAL
5	A	364	PRO
5	A	366	ILE
5	A	370	GLU
5	A	373	ALA
5	A	374	LYS
5	A	385	PRO
5	A	387	LEU
5	A	389	VAL
5	A	391	SER
6	B	24	PRO
6	B	25	THR
6	B	53	ILE
6	B	54	ILE
5	A	58	PHE
5	A	89	VAL
5	A	93	ILE
5	A	147	ILE
5	A	170	ILE
5	A	172	LEU
5	A	188	GLY
5	A	189	PRO
5	A	231	ARG

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Mol	Chain	Res	Type
5	A	234	VAL
5	A	261	VAL
5	A	311	TYR
5	A	336	MET
5	A	343	GLU
5	A	347	LEU
5	A	351	SER
5	A	355	ARG
5	A	359	SER
5	A	362	PHE
5	A	375	TYR
5	A	378	HIS
5	A	388	THR
5	A	415	LEU
5	A	440	ILE
6	B	23	TRP
6	B	30	LYS
6	B	31	ASP
6	B	32	GLU
5	A	4	LEU
5	A	108	GLN
5	A	145	ILE
5	A	205	PRO
5	A	252	THR
5	A	295	GLU
5	A	331	ILE
5	A	371	GLN
5	A	392	SER
5	A	439	ALA
5	A	173	PHE
5	A	245	ARG
5	A	246	VAL
5	A	294	TYR
5	A	319	ASP
6	B	55	HIS
5	A	102	GLU
5	A	109	GLY
5	A	249	ALA
5	A	320	PRO
5	A	6	PRO
5	A	136	THR
5	A	137	PRO

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Mol	Chain	Res	Type
5	A	211	ALA
5	A	353	ALA
5	A	367	ARG
5	A	77	PRO
5	A	386	PRO
5	A	406	GLY
5	A	12	PRO

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	
5	A	362/362 (100%)	333 (92%)	29 (8%)	15	50
6	B	52/52 (100%)	51 (98%)	1 (2%)	65	86
7	C	28/28 (100%)	26 (93%)	2 (7%)	18	55
All	All	442/442 (100%)	410 (93%)	32 (7%)	23	55

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	A	3	LYS
5	A	16	LEU
5	A	21	ILE
5	A	27	LEU
5	A	29	TRP
5	A	33	VAL
5	A	62	ILE
5	A	80	THR
5	A	112	LYS
5	A	126	PHE
5	A	135	LEU
5	A	172	LEU
5	A	197	LEU
5	A	202	GLN
5	A	210	ILE

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Mol	Chain	Res	Type
5	A	232	ARG
5	A	234	VAL
5	A	240	ARG
5	A	264	ILE
5	A	266	VAL
5	A	272	LEU
5	A	311	TYR
5	A	313	LEU
5	A	321	ILE
5	A	343	GLU
5	A	367	ARG
5	A	389	VAL
5	A	412	THR
5	A	427	GLN
6	B	27	LYS
7	C	33	VAL
7	C	51	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
5	A	111	GLN
5	A	146	GLN
5	A	180	GLN
5	A	236	ASN
5	A	275	ASN
5	A	403	ASN
5	A	427	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	D	26/27 (96%)	7 (26%)	0
2	E	26/27 (96%)	5 (19%)	0
3	F	18/19 (94%)	2 (11%)	0
4	G	31/32 (96%)	4 (12%)	0
All	All	101/105 (96%)	18 (17%)	0

All (18) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	D	84	A
1	D	91	A
1	D	95	A
1	D	98	G
1	D	100	U
1	D	101	A
1	D	102	U
2	E	479	A
2	E	481	G
2	E	490	C
2	E	491	G
2	E	504	A
3	F	1396	U
3	F	1397	U
4	G	1524	G
4	G	1532	A
4	G	1535	A
4	G	1538	G

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.