Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:09 PM GMT

PDB ID	:	1S0V
Title	:	Structural basis for substrate selection by T7 RNA polymerase
Authors	:	Temiakov, D.; Patlan, V.; Anikin, M.; McAllister, W.T.; Yokoyama, S.; Vassylyev, D.G.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on	:	2004-01-05
Resolution	:	3.20 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:

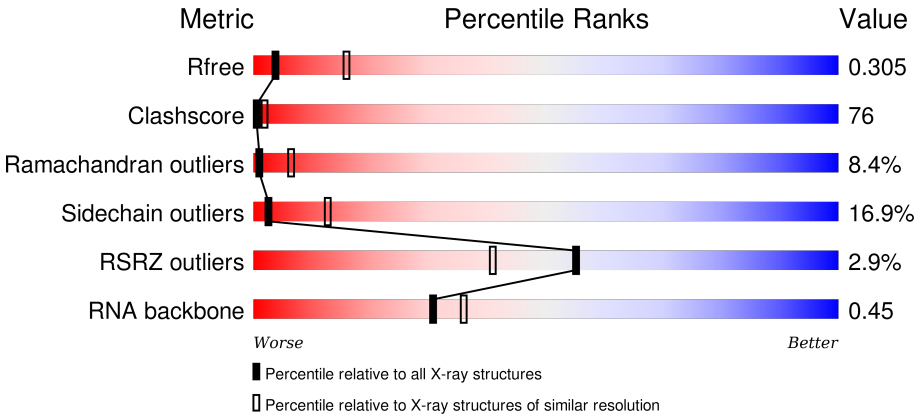
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)
RNA backbone	2183	1079 (3.70-2.70)

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

Mol	Chain	Length	Quality of chain
1	E	18	11% 39% 11% 33% 6%
1	H	18	6% 17% 28% 22% 28% 6%
1	K	18	56% 11% 28% 6%
1	N	18	6% 56% 22% 11% 6%

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Mol	Chain	Length	Quality of chain
2	F	12	8% 33% 25% 33%
2	I	12	42% 17% 8% 33%
2	L	12	50% 17% 33%
2	O	12	17% 33% 17% 33%
3	G	10	20% 90% 10%
3	J	10	10% 90% 10%
3	M	10	90% 10%
3	P	10	10% 80% 10% 10%
4	A	883	4% 21% 54% 18%
4	B	883	2% 19% 55% 21%
4	C	883	2% 24% 57% 15%
4	D	883	3% 26% 57% 13%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	APC	A	2000	-	-	X	-
6	APC	B	2001	-	-	X	-
6	APC	C	2002	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 30899 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 DNA chain called 5'-D(*G*GP*GP*AP*AP*TP*CP*GP*AP*TP*AP*TP*CP*GP*CP*CP*GP*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	17	Total	C	N	O	P	0	0	0
			346	165	66	99	16			
1	H	17	Total	C	N	O	P	0	0	0
			346	165	66	99	16			
1	K	17	Total	C	N	O	P	0	0	0
			346	165	66	99	16			
1	N	17	Total	C	N	O	P	0	0	0
			346	165	66	99	16			

- Molecule 2 is a RNA chain called 5'-R(*AP*AP*CP*U*GP*CP*GP*GP*CP*GP*AP*U)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	8	Total	C	N	O	P	0	0	0
			171	77	33	54	7			
2	I	8	Total	C	N	O	P	0	0	0
			171	77	33	54	7			
2	L	8	Total	C	N	O	P	0	0	0
			171	77	33	54	7			
2	O	8	Total	C	N	O	P	0	0	0
			171	77	33	54	7			

- Molecule 3 is a DNA chain called 5'-D(*GP*TP*CP*GP*AP*TP*TP*CP*CP*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	9	Total	C	N	O	P	0	0	0
			179	87	30	54	8			
3	J	9	Total	C	N	O	P	0	0	0
			179	87	30	54	8			
3	M	9	Total	C	N	O	P	0	0	0
			179	87	30	54	8			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	P	9	Total	C	N	O	P	0	0	0
			179	87	30	54	8			

- Molecule 4 is a protein called DNA-directed RNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	A	857	Total	C	N	O	S	0	0	0
			6746	4296	1173	1242	35			
4	B	857	Total	C	N	O	S	0	0	0
			6746	4296	1173	1242	35			
4	C	857	Total	C	N	O	S	0	0	0
			6746	4296	1173	1242	35			
4	D	857	Total	C	N	O	S	0	0	0
			6746	4296	1173	1242	35			

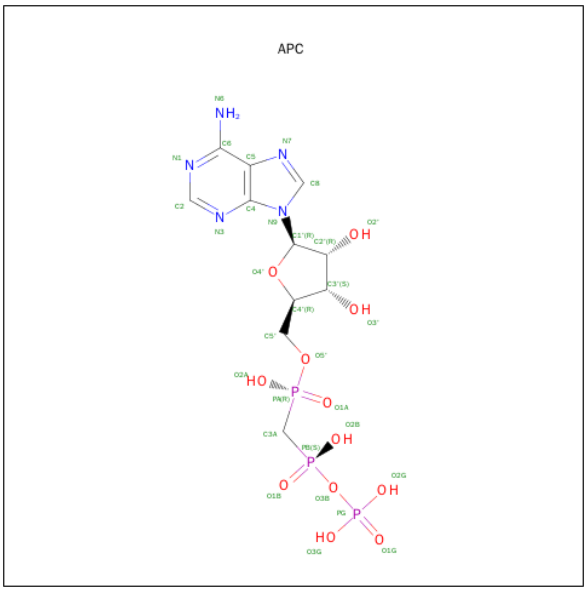
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	497	LEU	-	INSERTION	UNP P00573
B	497	LEU	-	INSERTION	UNP P00573
C	497	LEU	-	INSERTION	UNP P00573
D	497	LEU	-	INSERTION	UNP P00573

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	2	Total	Mg	0	0
			2	2		
5	A	1	Total	Mg	0	0
			1	1		
5	D	2	Total	Mg	0	0
			2	2		
5	C	2	Total	Mg	0	0
			2	2		
5	F	1	Total	Mg	0	0
			1	1		

- Molecule 6 is DIPHOSPHOMETHYLPHOSPHONIC ACID ADENOSYL ESTER (three-letter code: APC) (formula: $C_{11}H_{18}N_5O_{12}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	P	0	0
			31	11	5	12	3		
6	B	1	Total	C	N	O	P	0	0
			31	11	5	12	3		
6	C	1	Total	C	N	O	P	0	0
			31	11	5	12	3		
6	D	1	Total	C	N	O	P	0	0
			31	11	5	12	3		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	237	Total	O	0	0
			237	237		
7	B	212	Total	O	0	0
			212	212		
7	C	201	Total	O	0	0
			201	201		
7	D	173	Total	O	0	0
			173	173		
7	E	39	Total	O	0	0
			39	39		
7	F	9	Total	O	0	0
			9	9		
7	G	9	Total	O	0	0
			9	9		
7	H	19	Total	O	0	0
			19	19		

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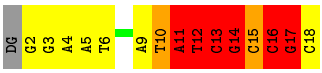
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	I	14	Total O 14 14	0	0
7	J	13	Total O 13 13	0	0
7	K	20	Total O 20 20	0	0
7	L	8	Total O 8 8	0	0
7	M	10	Total O 10 10	0	0
7	N	14	Total O 14 14	0	0
7	O	15	Total O 15 15	0	0
7	P	6	Total O 6 6	0	0

3 Residue-property plots

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 and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

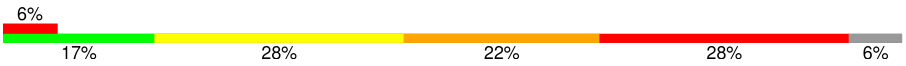
• Molecule 1: 5'-D(*G*GP*GP*AP*AP*TP*CP*GP*AP*TP*AP*TP*CP*GP*CP*CP*GP*C)-3'

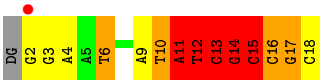
Chain E:



• Molecule 1: 5'-D(*G*GP*GP*AP*AP*TP*CP*GP*AP*TP*AP*TP*CP*GP*CP*CP*GP*C)-3'

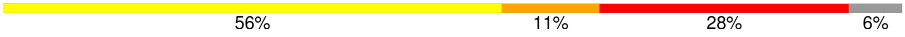
Chain H:





• Molecule 1: 5'-D(*G*GP*GP*AP*AP*TP*CP*GP*AP*TP*AP*TP*CP*GP*CP*CP*GP*C)-3'

Chain K:

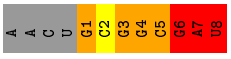


• Molecule 1: 5'-D(*G*GP*GP*AP*AP*TP*CP*GP*AP*TP*AP*TP*CP*GP*CP*CP*GP*C)-3'

Chain N:

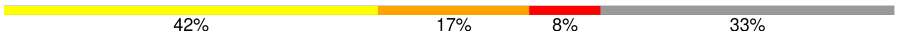
• Molecule 2: 5'-R(*AP*AP*CP*U*GP*CP*GP*GP*CP*GP*AP*U)-3'

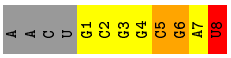
Chain F:



• Molecule 2: 5'-R(*AP*AP*CP*U*GP*CP*GP*GP*CP*GP*AP*U)-3'

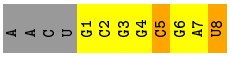
Chain I:





• Molecule 2: 5'-R(*AP*AP*CP*U*GP*CP*GP*GP*CP*GP*AP*U)-3'

Chain L:

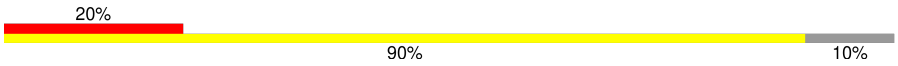


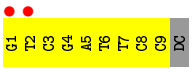
• Molecule 2: 5'-R(*AP*AP*CP*U*GP*CP*GP*GP*CP*GP*AP*U)-3'

Chain O:

• Molecule 3: 5'-D(*GP*TP*CP*GP*AP*TP*TP*CP*CP*C)-3'

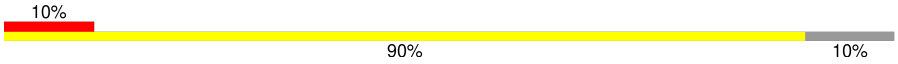
Chain G:

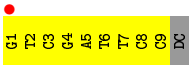




• Molecule 3: 5'-D(*GP*TP*CP*GP*AP*TP*TP*CP*CP*C)-3'

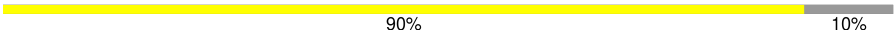
Chain J:

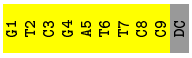




• Molecule 3: 5'-D(*GP*TP*CP*GP*AP*TP*TP*CP*CP*C)-3'

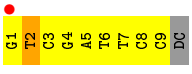
Chain M:





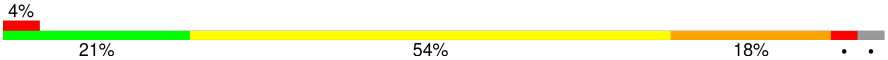
• Molecule 3: 5'-D(*GP*TP*CP*GP*AP*TP*TP*CP*CP*C)-3'

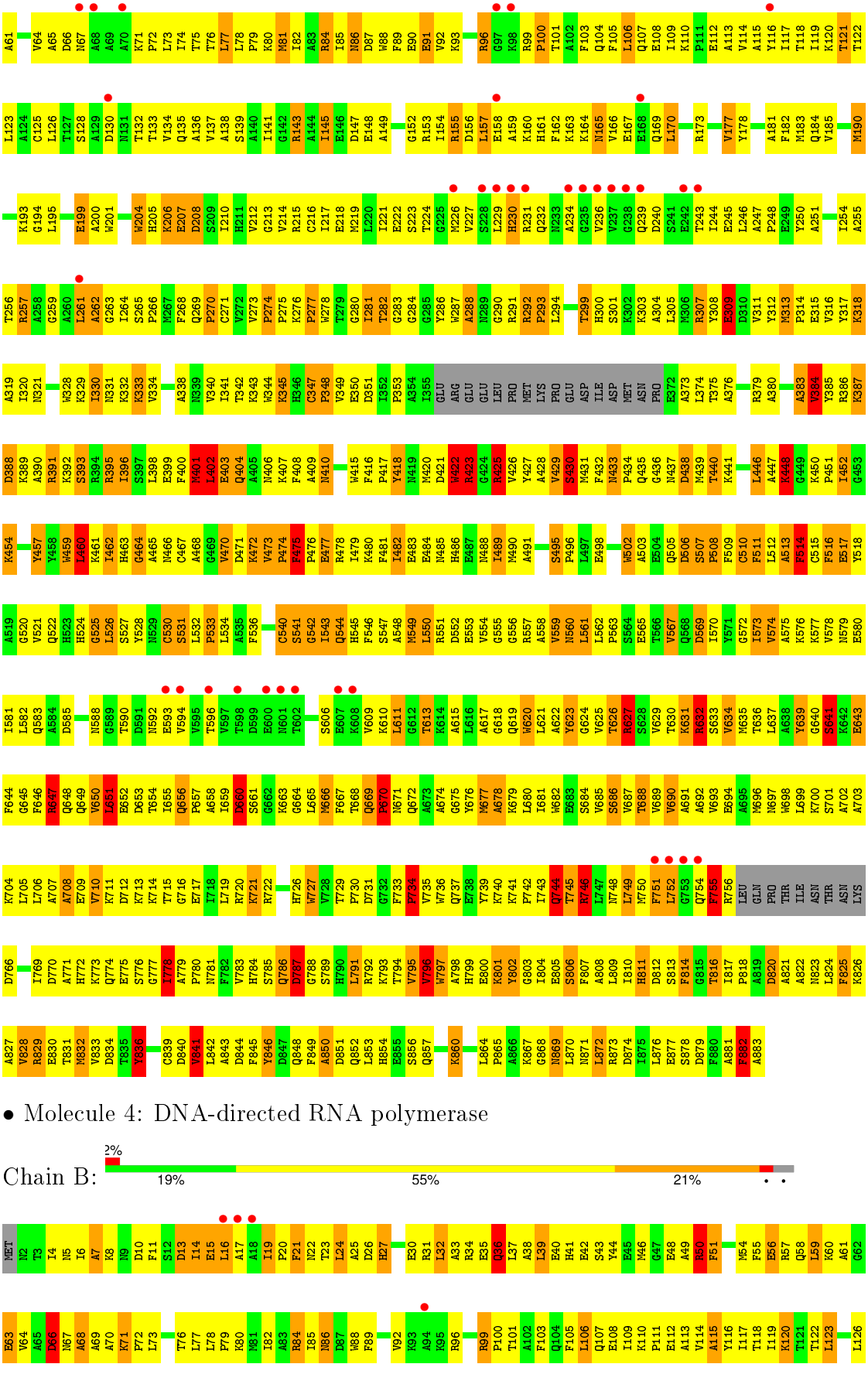
Chain P:



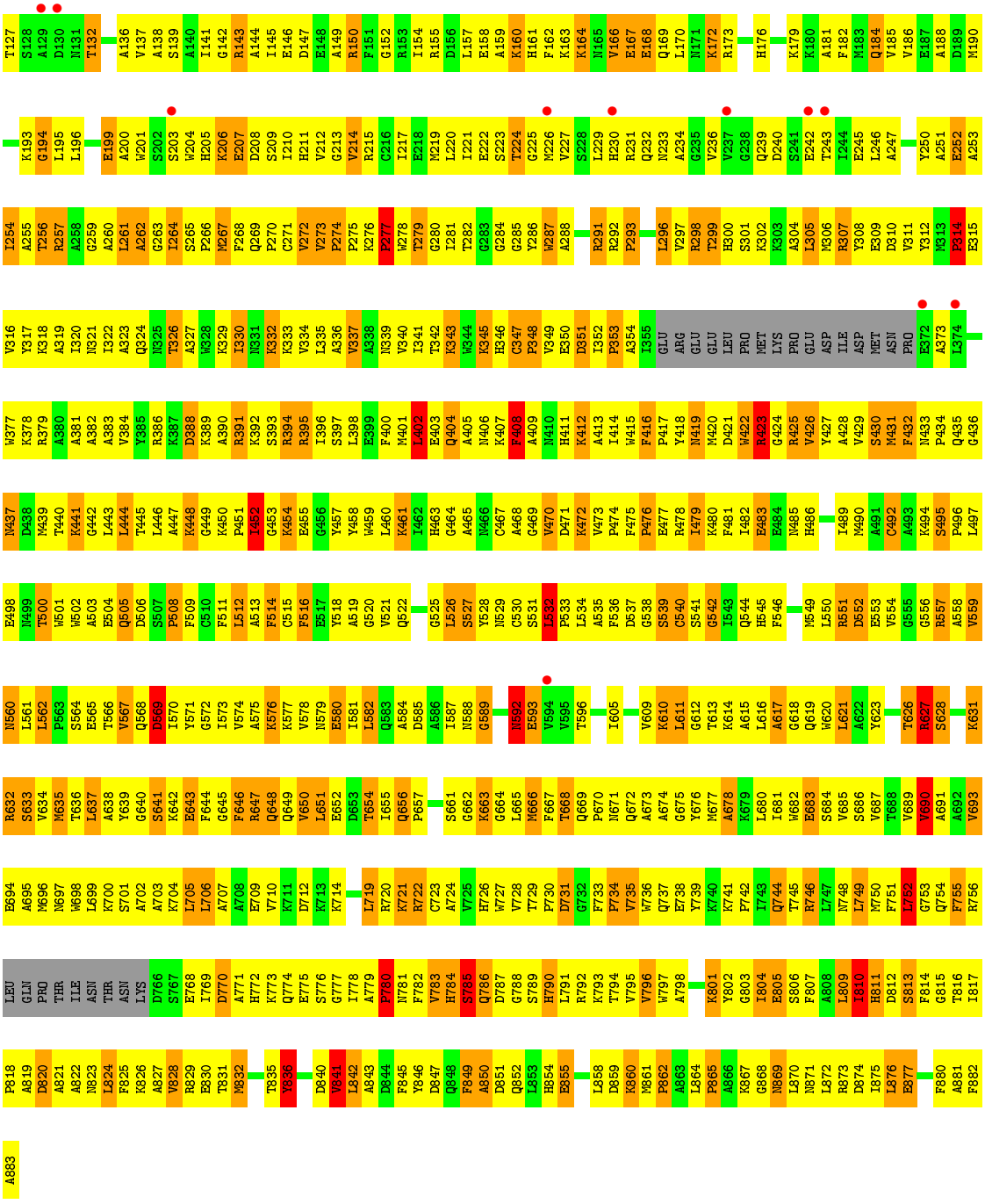
• Molecule 4: DNA-directed RNA polymerase

Chain A:

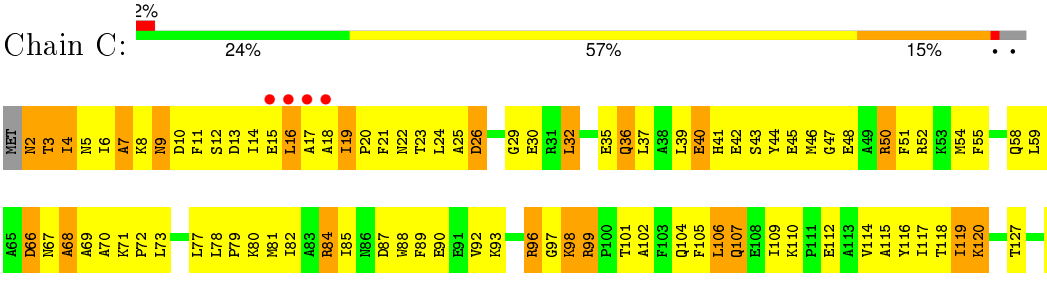


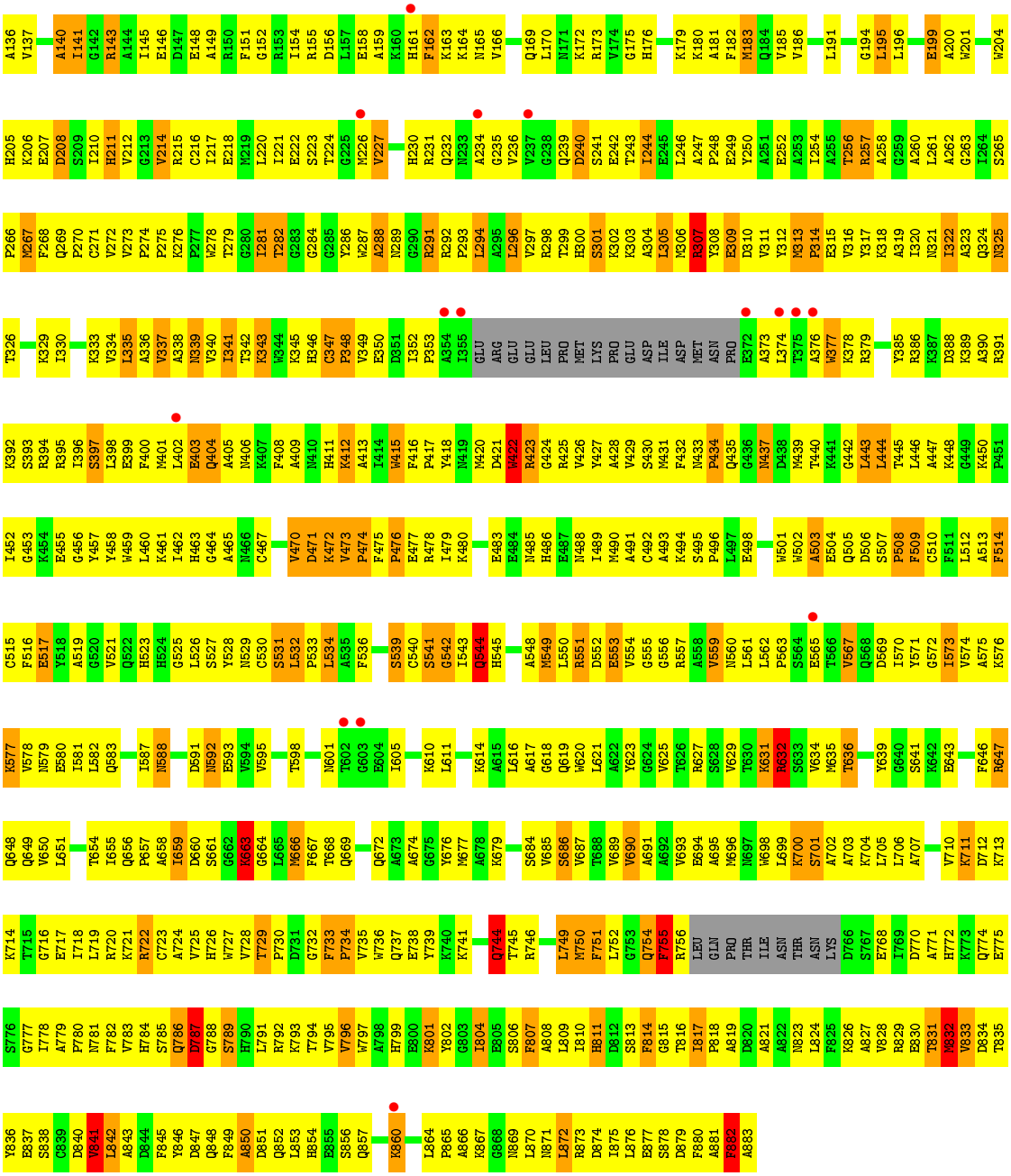


• Molecule 4: DNA-directed RNA polymerase

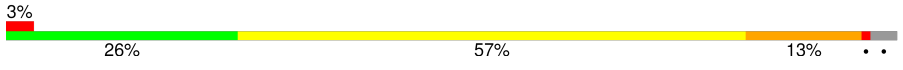


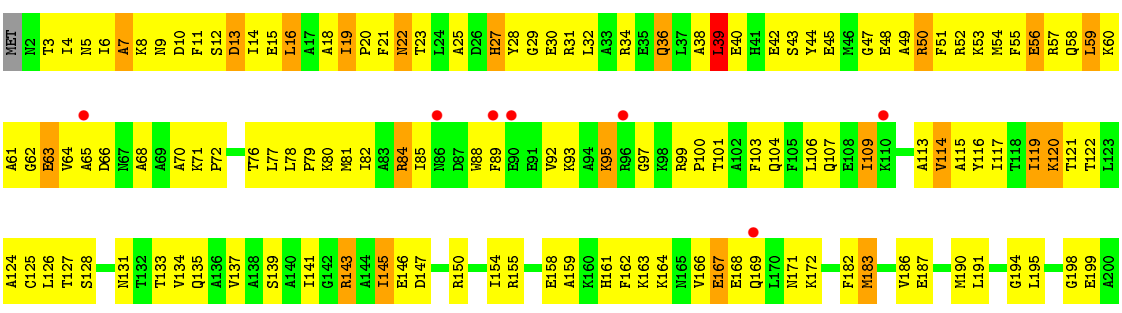
• Molecule 4: DNA-directed RNA polymerase

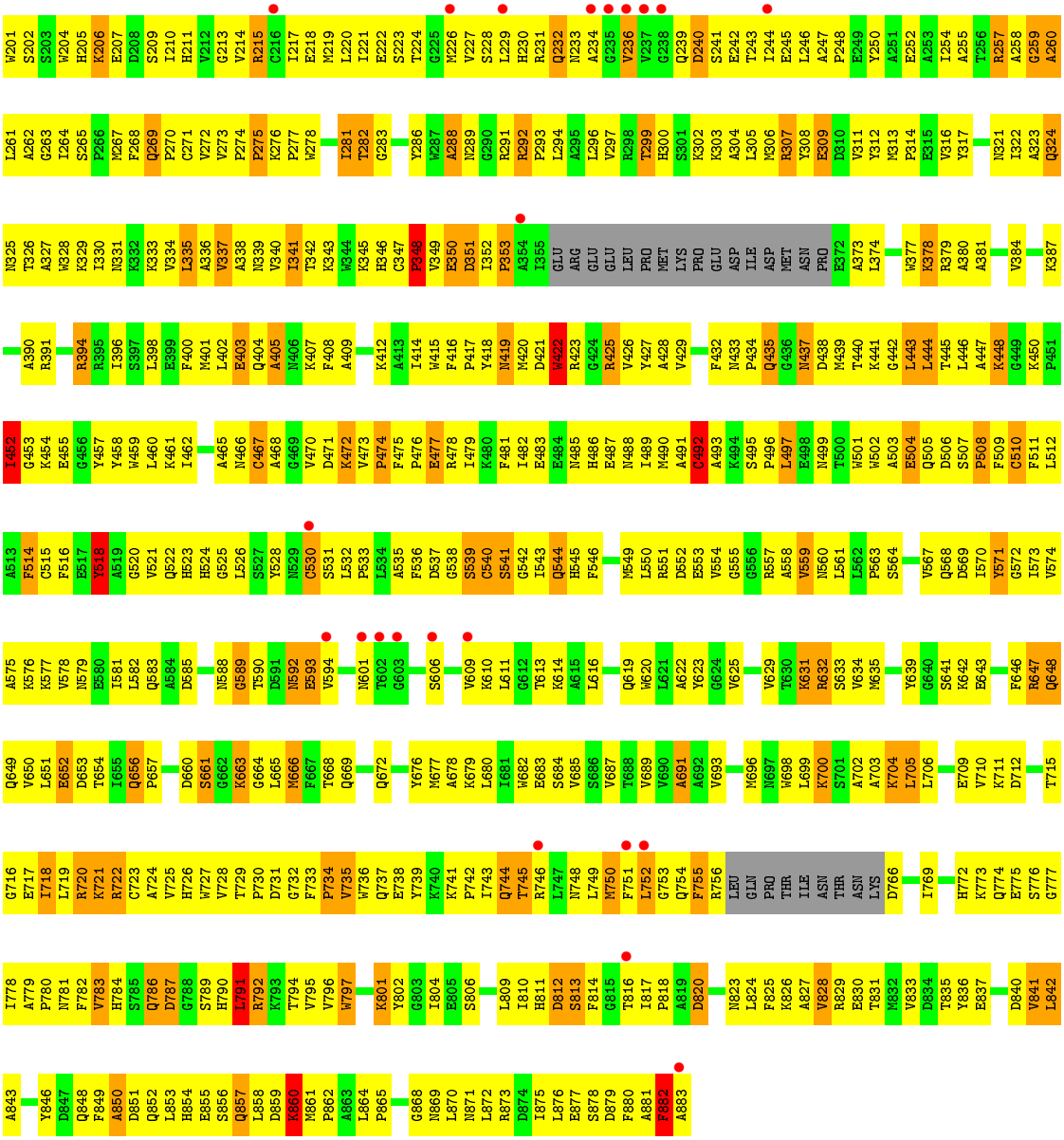




• Molecule 4: DNA-directed RNA polymerase






W201 S202 S203 W204 H205 K206 E207 D208 S209 I210 H211 V212 G213 V214 R215 C216 I217 E218 M219 L220 I221 E222 S223 T224 G225 M226 V227 S228 L229 H230 R231 Q232 N233 A234 G235 V236 V237 G238 Q239 D240 S241 E242 T243 I244 E245 L246 A247 P248 E249 Y250 A251 E252 A253 I254 A255 T256 R257 A258 G259 A260
L261 A262 G263 I264 S265 P266 M267 F268 Q269 P270 C271 V272 V273 P274 P275 K276 P277 W278 I281 T282 G283 Y286 W287 A288 N289 G290 R291 R292 P293 L294 A295 L296 V297 R298 T299 H300 S301 K302 K303 A304 L305 M306 R307 Y308 E309 D310 V311 Y312 M313 P314 E315 V316 Y317 N321 I322 A323 Q324
N325 T326 A327 W328 K329 I330 N331 K332 K333 V334 L335 A336 V337 A338 N339 V340 I341 T342 K343 W344 K345 H346 C347 P348 V349 E350 D351 I352 P353 A354 I355 GLU ARG GLU GLU LEU PRO MET LYS PRO GLU ASP ILE ASP MET ASN PRO E372 A373 L374 W377 K378 R379 A380 A381 V384 K387
A390 R391 R394 R395 I396 S397 L398 E399 F400 M401 L402 E403 Q404 A405 N406 K407 F408 A409 K412 A413 I414 W415 F416 P417 Y418 N419 M420 D421 W422 R423 G424 R425 V426 Y427 A428 V429 F432 M433 P434 Q435 G436 M437 D438 M439 T440 K441 G442 L443 L444 T445 L446 A447 K448 G449 K450 P451
I462 G453 K454 E455 G456 Y457 Y458 W459 L460 K461 I462 A465 N466 C467 A468 G469 V470 D471 K472 V473 P474 F475 P476 E477 R478 I479 K480 F481 I482 E483 E484 N485 H486 E487 N488 I489 M490 A491 C492 A493 K494 S495 P496 L497 E498 N499 T500 W501 W502 A503 E504 Q505 D506 S507 P508 F509 C510 F511 L512
A513 F514 C515 F516 E517 Y518 A519 G520 V521 Q522 H523 H524 G525 L526 S527 Y528 N529 C530 S531 L532 P533 L534 A535 F536 D537 G538 S539 C540 S541 G542 I543 Q544 H545 F546 M549 L550 R551 D552 E553 V554 G555 G556 R557 A558 V559 N560 L561 L562 P563 S564 V567 Q568 D569 I570 Y571 G572 I573 V574
A575 K576 K577 V578 N579 E580 I581 L582 Q583 A584 D585 N588 G589 T590 D591 N592 E593 V594 N601 T602 G603 S606 V609 K610 L611 G612 T613 K614 A615 L616 Q619 W620 L621 A622 Y623 G624 V625 V629 T630 K631 R632 S633 V634 M635 Y639 G640 S641 K642 E643 F646 R647 Q648
Q649 V650 L651 E652 D653 T654 I655 Q656 P657 D660 S661 G662 K663 G664 L665 M666 F667 T668 Q669 Q672 Y676 M677 A678 K679 L680 I681 W682 E683 S684 V685 S686 V687 T688 V689 V690 A691 A692 V693 M696 N697 W698 L699 K700 S701 A702 A703 K704 L705 L706 E709 V710 K711 D712 T715
G716 E717 I718 L719 R720 K721 R722 C723 A724 V725 H726 W727 V728 T729 P730 D731 G732 F733 P734 V735 W736 Q737 E738 Y739 K740 K741 P742 I743 Q744 T745 R746 L747 N748 L749 N750 F751 L752 G753 Q754 F755 R756 LEU GLN PRO THR ILE ASN THR ASN LYS D766 I769 H772 K773 Q774 E775 S776 G777
I778 A779 P780 N781 F782 V783 H784 S785 Q786 D787 G788 S789 H790 L791 R792 K793 T794 V795 V796 W797 K801 Y802 G803 I804 E805 S806 L809 I810 H811 D812 S813 F814 G815 T816 I817 P818 A819 D820 N823 L824 F825 K826 A827 V828 R829 E830 T831 M832 V833 D834 T835 Y836 E837 D840 V841 L842
A843 Y846 D847 Q848 F849 A850 D851 Q852 L853 H854 E855 S856 Q857 L858 D859 K860 M861 P862 A863 L864 P865 G868 N869 L870 N871 L872 R873 D874 I875 L876 E877 S878 D879 F880 A881 F882 A883

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	81.13Å 87.70Å 206.53Å 91.93° 91.02° 110.66°	Depositor
Resolution (Å)	40.00 – 3.20 39.88 – 3.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-3.20) 82.3 (39.88-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.42 (at 3.01Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.255 , 0.307 0.255 , 0.305	Depositor DCC
R_{free} test set	3685 reflections (5.04%)	DCC
Wilson B-factor (Å^2)	59.0	Xtriage
Anisotropy	0.201	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 107.2	EDS
Estimated twinning fraction	0.014 for -h,-k,l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.53$, $< L^2 > = 0.37$	Xtriage
Outliers	0 of 88725 reflections	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	30899	wwPDB-VP
Average B, all atoms (Å^2)	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.34% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	E	1.74	9/388 (2.3%)	1.60	9/597 (1.5%)
1	H	1.62	7/388 (1.8%)	1.47	6/597 (1.0%)
1	K	1.59	7/388 (1.8%)	1.31	1/597 (0.2%)
1	N	1.26	3/388 (0.8%)	1.27	4/597 (0.7%)
2	F	2.39	9/191 (4.7%)	2.00	11/297 (3.7%)
2	I	2.25	7/191 (3.7%)	1.68	2/297 (0.7%)
2	L	1.65	1/191 (0.5%)	1.36	0/297
2	O	1.47	0/191	1.38	0/297
3	G	0.82	0/199	0.92	0/305
3	J	0.78	0/199	0.93	0/305
3	M	0.88	0/199	0.86	0/305
3	P	0.94	0/199	1.07	0/305
4	A	1.20	22/6897 (0.3%)	1.14	24/9329 (0.3%)
4	B	1.21	24/6897 (0.3%)	1.14	24/9329 (0.3%)
4	C	0.97	5/6897 (0.1%)	0.97	7/9329 (0.1%)
4	D	0.92	3/6897 (0.0%)	0.91	4/9329 (0.0%)
All	All	1.14	97/30700 (0.3%)	1.09	92/42112 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	0	6
1	H	0	9
1	K	0	6
1	N	0	4
2	F	0	4
2	I	0	2
2	L	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	O	0	3
3	P	0	1
4	A	0	1
4	B	0	1
4	D	0	1
All	All	0	39

All (97) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	502	TRP	CB-CG	-13.18	1.26	1.50
1	K	14	DG	C5-C6	-11.28	1.31	1.42
4	A	467	CYS	CB-SG	-10.63	1.64	1.82
2	I	8	U	N1-C6	-9.75	1.29	1.38
2	I	7	A	C5-C6	-8.93	1.33	1.41
4	A	271	CYS	CB-SG	-8.70	1.67	1.82
2	F	7	A	C5-C6	-8.57	1.33	1.41
1	E	11	DA	C5-C6	-8.44	1.33	1.41
2	I	8	U	N1-C2	-8.39	1.30	1.38
4	B	310	ASP	CB-CG	8.28	1.69	1.51
1	H	12	DT	C2-O2	8.07	1.28	1.22
4	B	805	GLU	CG-CD	7.74	1.63	1.51
2	I	8	U	C4-C5	-7.73	1.36	1.43
2	F	5	C	N1-C2	-7.63	1.32	1.40
4	A	482	ILE	CA-CB	-7.61	1.37	1.54
1	H	11	DA	N3-C4	-7.16	1.30	1.34
2	F	6	G	C5-C6	7.14	1.49	1.42
1	K	14	DG	C2-N3	-7.13	1.27	1.32
2	F	6	G	C6-N1	-7.09	1.34	1.39
4	B	63	GLU	CG-CD	7.08	1.62	1.51
1	H	14	DG	C5-C6	-7.06	1.35	1.42
4	B	330	ILE	CA-CB	-7.02	1.38	1.54
4	B	416	PHE	CB-CG	-6.93	1.39	1.51
2	L	5	C	C4-C5	-6.88	1.37	1.43
1	K	11	DA	C5-C6	-6.86	1.34	1.41
1	E	11	DA	N9-C4	-6.77	1.33	1.37
1	K	16	DC	N1-C2	-6.72	1.33	1.40
1	E	12	DT	N1-C2	-6.68	1.32	1.38
4	C	807	PHE	CB-CG	-6.60	1.40	1.51
4	B	498	GLU	CG-CD	6.55	1.61	1.51
4	B	683	GLU	CG-CD	6.46	1.61	1.51
1	K	14	DG	C2-N2	-6.40	1.28	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	30	GLU	CG-CD	6.34	1.61	1.51
4	A	384	VAL	CA-CB	-6.24	1.41	1.54
1	N	11	DA	C5-C6	-6.15	1.35	1.41
4	A	448	LYS	CD-CE	6.12	1.66	1.51
4	B	516	PHE	CB-CG	-6.06	1.41	1.51
4	A	727	TRP	CB-CG	6.05	1.61	1.50
2	F	1	G	C5-C6	6.01	1.48	1.42
2	F	7	A	N3-C4	-5.89	1.31	1.34
4	B	635	MET	CG-SD	5.88	1.96	1.81
4	A	35	GLU	CG-CD	5.84	1.60	1.51
4	C	30	GLU	CB-CG	5.82	1.63	1.52
1	K	13	DC	N1-C2	-5.82	1.34	1.40
4	D	797	TRP	CB-CG	-5.79	1.39	1.50
1	E	13	DC	C4-N4	-5.76	1.28	1.33
4	A	347	CYS	CB-SG	-5.76	1.72	1.81
4	A	775	GLU	CG-CD	5.75	1.60	1.51
2	I	7	A	C5'-C4'	-5.74	1.44	1.51
4	D	504	GLU	CG-CD	5.73	1.60	1.51
4	D	504	GLU	CB-CG	5.71	1.63	1.52
1	H	11	DA	C5-C4	-5.68	1.34	1.38
2	F	8	U	C2-O2	-5.66	1.17	1.22
4	B	51	PHE	CB-CG	-5.66	1.41	1.51
4	C	802	TYR	CB-CG	-5.64	1.43	1.51
1	E	10	DT	N1-C2	-5.63	1.33	1.38
1	E	12	DT	C4-C5	-5.62	1.39	1.45
4	B	66	ASP	CB-CG	5.60	1.63	1.51
1	N	14	DG	C5-C6	-5.57	1.36	1.42
2	I	7	A	N1-C2	-5.54	1.29	1.34
4	A	459	TRP	CB-CG	5.50	1.60	1.50
4	A	477	GLU	CG-CD	5.47	1.60	1.51
1	H	12	DT	C3'-O3'	-5.47	1.36	1.44
4	B	271	CYS	CB-SG	-5.45	1.73	1.81
4	B	63	GLU	CB-CG	5.44	1.62	1.52
4	A	514	PHE	CB-CG	-5.43	1.42	1.51
2	F	7	A	C8-N7	5.41	1.35	1.31
4	B	559	VAL	CB-CG2	-5.36	1.41	1.52
4	B	432	PHE	CE2-CZ	-5.34	1.27	1.37
4	C	347	CYS	CB-SG	5.33	1.91	1.82
4	B	416	PHE	CE2-CZ	5.33	1.47	1.37
2	F	8	U	C2-N3	-5.30	1.34	1.37
4	A	805	GLU	CG-CD	5.29	1.59	1.51
4	B	287	TRP	CB-CG	-5.26	1.40	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	820	ASP	CB-CG	5.25	1.62	1.51
4	B	326	THR	CA-CB	5.23	1.67	1.53
4	B	836	TYR	CD1-CE1	5.23	1.47	1.39
4	A	91	GLU	CB-CG	5.22	1.62	1.52
1	E	14	DG	N3-C4	-5.20	1.31	1.35
1	H	14	DG	N9-C4	-5.19	1.33	1.38
4	B	408	PHE	CB-CG	-5.17	1.42	1.51
4	A	639	TYR	CG-CD1	-5.15	1.32	1.39
1	E	12	DT	C3'-O3'	-5.15	1.37	1.44
1	N	13	DC	C3'-O3'	-5.14	1.37	1.44
4	A	808	ALA	CA-CB	-5.11	1.41	1.52
1	H	12	DT	C5-C6	-5.10	1.30	1.34
4	B	408	PHE	CD2-CE2	-5.10	1.29	1.39
4	B	855	GLU	CG-CD	5.10	1.59	1.51
4	A	530	CYS	CB-SG	-5.08	1.73	1.81
4	B	805	GLU	CB-CG	5.03	1.61	1.52
4	A	422	TRP	CZ3-CH2	5.03	1.48	1.40
4	A	795	VAL	CB-CG2	-5.02	1.42	1.52
1	E	11	DA	C3'-O3'	-5.02	1.37	1.44
1	K	15	DC	N1-C2	-5.02	1.35	1.40
4	A	623	TYR	CD2-CE2	5.01	1.46	1.39
4	A	483	GLU	CG-CD	5.01	1.59	1.51
2	I	8	U	C3'-O3'	5.00	1.49	1.42

All (92) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	460	LEU	CB-CG-CD1	-10.01	93.98	111.00
1	E	14	DG	O5'-P-OP1	-9.17	97.45	105.70
4	A	460	LEU	CB-CG-CD2	9.03	126.35	111.00
4	D	791	LEU	CA-CB-CG	8.79	135.52	115.30
4	A	425	ARG	NE-CZ-NH1	-8.45	116.07	120.30
1	E	13	DC	C5'-C4'-O4'	-8.23	93.67	109.30
4	B	425	ARG	NE-CZ-NH2	-8.00	116.30	120.30
4	B	444	LEU	CA-CB-CG	-7.97	96.96	115.30
2	F	4	G	O4'-C4'-C3'	-7.96	96.04	104.00
4	B	635	MET	CA-CB-CG	7.91	126.75	113.30
4	A	627	ARG	NE-CZ-NH1	7.66	124.13	120.30
2	F	8	U	N1-C1'-C2'	-7.58	103.66	112.00
4	A	507	SER	C-N-CD	-7.58	103.93	120.60
1	H	13	DC	OP2-P-O3'	7.03	120.66	105.20
4	A	448	LYS	CD-CE-NZ	6.95	127.68	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	13	DC	N1-C1'-C2'	-6.88	99.52	112.60
4	B	423	ARG	NE-CZ-NH1	6.77	123.69	120.30
4	A	778	ILE	CG1-CB-CG2	-6.74	96.58	111.40
2	I	8	U	C2'-C3'-O3'	6.72	124.46	113.70
1	H	14	DG	O5'-P-OP2	-6.66	99.71	105.70
2	F	8	U	C4'-C3'-O3'	6.65	126.30	113.00
2	F	5	C	N1-C2-O2	-6.63	114.92	118.90
4	D	492	CYS	CA-CB-SG	-6.50	102.29	114.00
1	H	15	DC	N1-C1'-C2'	-6.49	100.26	112.60
1	K	12	DT	OP1-P-O3'	6.48	119.46	105.20
4	A	423	ARG	NE-CZ-NH1	-6.45	117.08	120.30
4	B	569	ASP	CB-CG-OD1	6.42	124.08	118.30
4	C	534	LEU	CA-CB-CG	6.36	129.94	115.30
1	H	14	DG	N9-C1'-C2'	-6.36	100.52	112.60
4	B	330	ILE	CB-CA-C	-6.30	99.01	111.60
2	F	6	G	O4'-C4'-C3'	-6.29	97.71	104.00
4	A	441	LYS	CD-CE-NZ	-6.26	97.30	111.70
4	B	16	LEU	CA-CB-CG	6.24	129.65	115.30
4	A	569	ASP	CB-CG-OD1	-6.23	112.69	118.30
4	B	425	ARG	NE-CZ-NH1	6.21	123.40	120.30
4	D	39	LEU	CA-CB-CG	6.17	129.50	115.30
4	A	387	LYS	CD-CE-NZ	6.06	125.64	111.70
4	B	296	LEU	CA-CB-CG	-6.04	101.40	115.30
2	I	8	U	O4'-C4'-C3'	-6.04	97.96	104.00
4	C	632	ARG	NE-CZ-NH1	6.01	123.30	120.30
4	B	347	CYS	CA-CB-SG	-6.00	103.19	114.00
4	A	660	ASP	CB-CG-OD1	5.99	123.69	118.30
2	F	7	A	C5'-C4'-C3'	-5.96	106.46	116.00
4	B	810	ILE	CG1-CB-CG2	-5.95	98.30	111.40
1	E	17	DG	C5'-C4'-C3'	-5.93	103.43	114.10
4	D	792	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	N	11	DA	N9-C1'-C2'	-5.90	101.39	112.60
4	C	307	ARG	NE-CZ-NH1	5.78	123.19	120.30
4	B	637	LEU	CA-CB-CG	-5.73	102.11	115.30
4	C	296	LEU	CA-CB-CG	-5.71	102.17	115.30
1	E	18	DC	C2'-C3'-O3'	-5.70	93.81	112.60
2	F	6	G	OP1-P-O3'	-5.69	92.69	105.20
4	A	450	LYS	C-N-CA	-5.68	98.14	122.00
1	N	12	DT	O5'-P-OP2	-5.67	100.60	105.70
1	H	15	DC	OP2-P-O3'	5.65	117.64	105.20
4	B	532	LEU	CA-CB-CG	-5.65	102.31	115.30
4	A	651	LEU	CA-CB-CG	5.59	128.17	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	470	VAL	CB-CA-C	-5.54	100.88	111.40
4	B	562	LEU	CA-CB-CG	5.53	128.02	115.30
1	E	16	DC	N1-C1'-C2'	-5.52	102.11	112.60
4	B	345	LYS	CD-CE-NZ	5.52	124.39	111.70
4	C	444	LEU	CB-CG-CD1	-5.44	101.75	111.00
2	F	5	C	N3-C2-O2	5.42	125.69	121.90
2	F	8	U	C1'-C2'-O2'	5.42	126.85	110.60
4	B	332	LYS	CD-CE-NZ	5.42	124.16	111.70
4	A	396	ILE	CG1-CB-CG2	-5.42	99.49	111.40
4	B	632	ARG	NE-CZ-NH1	5.41	123.00	120.30
1	E	11	DA	O5'-P-OP2	-5.41	100.83	105.70
4	A	475	PHE	C-N-CD	5.36	139.66	128.40
2	F	8	U	O5'-P-OP1	5.35	117.12	110.70
1	E	14	DG	O5'-P-OP2	5.31	117.08	110.70
4	B	426	VAL	CB-CA-C	-5.29	101.34	111.40
4	A	836	TYR	CA-CB-CG	-5.24	103.45	113.40
4	B	402	LEU	CA-CB-CG	-5.23	103.27	115.30
4	A	318	LYS	CD-CE-NZ	5.22	123.71	111.70
4	C	471	ASP	CB-CG-OD1	5.20	122.98	118.30
1	N	11	DA	O4'-C1'-N9	5.19	111.63	108.00
4	B	448	LYS	CD-CE-NZ	5.17	123.59	111.70
4	B	59	LEU	CA-CB-CG	-5.17	103.41	115.30
1	N	13	DC	N1-C1'-C2'	-5.16	102.80	112.60
4	C	627	ARG	NE-CZ-NH1	5.14	122.87	120.30
4	A	513	ALA	O-C-N	5.12	130.89	122.70
1	E	12	DT	C6-N1-C1'	5.09	128.03	120.40
4	A	489	ILE	CB-CA-C	-5.09	101.43	111.60
4	A	514	PHE	CB-CG-CD2	-5.08	117.25	120.80
4	B	719	LEU	CA-CB-CG	-5.07	103.64	115.30
2	F	6	G	N1-C2-N3	5.04	126.93	123.90
4	A	787	ASP	CB-CG-OD1	5.04	122.84	118.30
1	E	15	DC	N1-C1'-C2'	-5.03	103.04	112.60
4	A	446	LEU	CB-CG-CD2	-5.03	102.45	111.00
4	B	650	VAL	CB-CA-C	-5.02	101.85	111.40
4	B	576	LYS	CD-CE-NZ	5.02	123.24	111.70

There are no chirality outliers.

All (39) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	A	836	TYR	Sidechain
4	B	836	TYR	Sidechain

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Mol	Chain	Res	Type	Group
4	D	518	TYR	Sidechain
1	E	11	DA	Sidechain
1	E	12	DT	Sidechain
1	E	13	DC	Sidechain
1	E	14	DG	Sidechain
1	E	16	DC	Sidechain
1	E	17	DG	Sidechain
2	F	3	G	Sidechain
2	F	6	G	Sidechain
2	F	7	A	Sidechain
2	F	8	U	Sidechain
1	H	10	DT	Sidechain
1	H	11	DA	Sidechain
1	H	12	DT	Sidechain
1	H	13	DC	Sidechain
1	H	14	DG	Sidechain
1	H	15	DC	Sidechain
1	H	16	DC	Sidechain
1	H	17	DG	Sidechain
1	H	6	DT	Sidechain
2	I	5	C	Sidechain
2	I	6	G	Sidechain
1	K	11	DA	Sidechain
1	K	13	DC	Sidechain
1	K	14	DG	Sidechain
1	K	15	DC	Sidechain
1	K	16	DC	Sidechain
1	K	17	DG	Sidechain
2	L	8	U	Sidechain
1	N	13	DC	Sidechain
1	N	14	DG	Sidechain
1	N	15	DC	Sidechain
1	N	17	DG	Sidechain
2	O	4	G	Sidechain
2	O	6	G	Sidechain
2	O	8	U	Sidechain
3	P	2	DT	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	E	346	0	190	28	0
1	H	346	0	192	66	0
1	K	346	0	190	57	0
1	N	346	0	192	38	0
2	F	171	0	89	10	0
2	I	171	0	89	11	0
2	L	171	0	89	14	0
2	O	171	0	89	5	0
3	G	179	0	104	13	0
3	J	179	0	104	17	0
3	M	179	0	104	13	0
3	P	179	0	104	8	0
4	A	6746	0	6708	1151	0
4	B	6746	0	6708	1190	0
4	C	6746	0	6708	1007	0
4	D	6746	0	6708	899	0
5	A	1	0	0	0	0
5	B	2	0	0	0	0
5	C	2	0	0	0	0
5	D	2	0	0	0	0
5	F	1	0	0	0	0
6	A	31	0	13	16	0
6	B	31	0	13	9	0
6	C	31	0	14	16	0
6	D	31	0	13	7	0
7	A	237	0	0	82	0
7	B	212	0	0	68	0
7	C	201	0	0	70	0
7	D	173	0	0	53	0
7	E	39	0	0	1	0
7	F	9	0	0	1	0
7	G	9	0	0	1	0
7	H	19	0	0	9	0
7	I	14	0	0	4	0
7	J	13	0	0	0	0
7	K	20	0	0	7	0
7	L	8	0	0	0	0
7	M	10	0	0	2	0
7	N	14	0	0	3	0
7	O	15	0	0	2	0
7	P	6	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	30899	0	28421	4458	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 76.

All (4458) 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)
4:A:313:MET:SD	4:A:313:MET:CE	2.05	1.44
4:C:631:LYS:NZ	6:C:2002:APC:H3A2	1.52	1.22
2:F:1:G:H5"	7:F:3008:HOH:O	1.40	1.19
4:A:631:LYS:NZ	6:A:2000:APC:H3A2	1.58	1.18
4:A:546:PHE:CE1	4:A:783:VAL:HG22	1.78	1.16
4:A:631:LYS:HZ1	6:A:2000:APC:H3A2	0.97	1.13
4:B:452:ILE:HG23	4:B:453:GLY:N	1.57	1.13
4:A:281:ILE:HG22	4:A:282:THR:HG23	1.20	1.13
4:D:720:ARG:HH11	4:D:720:ARG:HG2	0.95	1.12
4:B:59:LEU:HD23	4:B:64:VAL:HG22	1.17	1.12
4:A:109:ILE:HD13	4:A:145:ILE:HG22	1.31	1.11
4:A:471:ASP:OD1	4:A:472:LYS:HD2	1.47	1.11
4:C:281:ILE:HG22	4:C:282:THR:HG22	1.18	1.11
1:K:12:DT:H2"	1:K:13:DC:H5'	1.16	1.11
4:A:722:ARG:HB2	4:A:769:ILE:HD13	1.27	1.11
4:A:804:ILE:HG12	4:A:820:ASP:HB3	1.33	1.10
4:B:452:ILE:CG2	4:B:453:GLY:H	1.64	1.10
4:A:647:ARG:HD2	4:A:675:GLY:HA2	1.34	1.10
1:N:12:DT:H2"	1:N:13:DC:H5'	1.33	1.10
4:B:816:THR:HG22	4:B:817:ILE:H	1.09	1.09
4:A:560:ASN:O	4:A:881:ALA:HB2	1.50	1.09
4:D:36:GLN:OE1	4:D:273:VAL:HG22	1.52	1.09
4:C:158:GLU:HG2	4:C:195:LEU:HD22	1.10	1.08
4:A:871:ASN:HD21	4:A:873:ARG:HB2	1.08	1.08
4:D:718:ILE:H	4:D:718:ILE:HD12	1.11	1.08
4:C:556:GLY:HA2	4:C:561:LEU:HD22	1.35	1.08
4:B:435:GLN:HG2	4:B:810:ILE:HG23	1.36	1.07
4:C:19:ILE:HG12	4:C:20:PRO:HD2	1.30	1.07
1:E:12:DT:H2"	1:E:13:DC:H5'	1.37	1.06
4:B:706:LEU:HD21	4:B:849:PHE:HB2	1.33	1.06
4:B:720:ARG:HH11	4:B:720:ARG:HG2	1.19	1.06
4:B:433:ASN:HB2	4:B:434:PRO:HD3	1.34	1.06
1:H:13:DC:H2"	1:H:14:DG:H5'	1.32	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:433:ASN:HB2	4:B:434:PRO:CD	1.87	1.05
4:D:512:LEU:HA	4:D:515:CYS:SG	1.97	1.05
4:C:333:LYS:HB3	4:C:516:PHE:CE2	1.91	1.05
4:C:536:PHE:HB3	4:C:882:PHE:HB3	1.35	1.05
4:B:473:VAL:HG13	4:B:474:PRO:HD2	1.36	1.04
1:H:9:DA:H5"	7:H:484:HOH:O	1.57	1.04
4:A:281:ILE:HG22	4:A:282:THR:CG2	1.86	1.03
4:B:829:ARG:HH22	4:B:882:PHE:HA	1.16	1.03
4:C:158:GLU:HG2	4:C:195:LEU:CD2	1.89	1.03
4:D:120:LYS:HG3	4:D:752:LEU:HD21	1.38	1.03
4:A:16:LEU:HD13	4:A:38:ALA:HB2	1.41	1.02
4:C:792:ARG:O	4:C:796:VAL:HG23	1.59	1.02
4:B:268:PHE:HB3	4:B:286:TYR:OH	1.59	1.02
4:B:829:ARG:NH2	4:B:882:PHE:HA	1.73	1.02
4:C:54:MET:O	4:C:58:GLN:HG2	1.58	1.01
4:D:737:GLN:HE22	4:D:778:ILE:HA	1.23	1.01
4:A:794:THR:OG1	4:A:831:THR:HG21	1.58	1.01
4:A:829:ARG:HH11	4:A:829:ARG:HG3	1.18	1.01
1:E:12:DT:H2"	1:E:13:DC:C5'	1.90	1.01
4:B:751:PHE:HB3	4:B:752:LEU:HD12	1.36	1.01
4:A:688:THR:HG22	4:A:689:VAL:HG13	1.41	1.01
4:D:794:THR:OG1	4:D:831:THR:HG21	1.58	1.00
4:D:560:ASN:O	4:D:881:ALA:HB2	1.60	1.00
4:C:342:THR:HG22	4:C:348:PRO:HG2	1.40	1.00
4:A:304:ALA:O	4:A:307:ARG:HG3	1.62	1.00
4:C:437:ASN:H	4:C:437:ASN:HD22	1.10	1.00
4:C:457:TYR:CD1	4:C:521:VAL:HG11	1.97	1.00
4:B:418:TYR:HE2	4:B:428:ALA:HB2	1.27	1.00
4:C:651:LEU:O	4:C:651:LEU:HD13	1.61	1.00
4:A:690:VAL:HG23	7:A:3200:HOH:O	1.61	0.99
4:A:687:VAL:HG23	7:A:3114:HOH:O	1.61	0.99
4:A:786:GLN:HA	4:A:786:GLN:HE21	1.27	0.99
4:D:198:GLY:HA3	7:D:3152:HOH:O	1.61	0.99
4:A:841:VAL:HG12	7:A:3070:HOH:O	1.60	0.99
4:C:84:ARG:HH12	4:C:87:ASP:HB2	1.27	0.99
4:B:669:GLN:HG2	4:B:672:GLN:HG3	1.45	0.98
4:D:790:HIS:HE1	4:D:831:THR:HG23	1.28	0.98
4:A:463:HIS:HA	4:A:466:ASN:HD22	1.27	0.98
4:C:281:ILE:HG22	4:C:282:THR:CG2	1.92	0.98
4:D:32:LEU:HD12	4:D:32:LEU:H	1.29	0.97
4:A:280:GLY:HA2	4:A:317:TYR:OH	1.62	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:11:PHE:HB3	4:B:41:HIS:HE1	1.28	0.97
4:B:14:ILE:HD12	4:B:14:ILE:H	1.28	0.97
4:A:169:GLN:O	4:A:173:ARG:HG2	1.65	0.97
4:C:423:ARG:HB2	4:C:423:ARG:HH11	1.26	0.97
4:C:551:ARG:NE	4:C:872:LEU:HD21	1.80	0.96
4:B:84:ARG:HD2	4:B:219:MET:HG2	1.47	0.96
4:B:407:LYS:HG2	4:B:408:PHE:CE2	2.00	0.96
4:A:562:LEU:HD21	4:A:870:LEU:CD1	1.94	0.96
4:A:80:LYS:HE2	4:A:223:SER:O	1.66	0.95
4:B:59:LEU:HD23	4:B:64:VAL:CG2	1.95	0.95
4:C:631:LYS:HZ1	6:C:2002:APC:H3A2	1.29	0.95
4:A:308:TYR:HE2	4:A:734:PRO:HG2	1.29	0.95
4:A:379:ARG:HD3	4:A:660:ASP:OD2	1.66	0.95
1:K:15:DC:H2"	1:K:16:DC:O5'	1.64	0.95
4:C:338:ALA:HB2	4:C:509:PHE:HE1	1.28	0.95
4:C:92:VAL:HG12	4:C:99:ARG:HG3	1.44	0.95
4:A:404:GLN:HA	4:A:404:GLN:HE21	1.30	0.95
4:C:706:LEU:HD22	4:C:725:VAL:HG13	1.49	0.94
4:A:546:PHE:HE1	4:A:783:VAL:HG22	1.28	0.94
4:C:341:ILE:HD12	4:C:348:PRO:HB3	1.49	0.94
1:K:12:DT:H2"	1:K:13:DC:C5'	1.96	0.94
4:B:505:GLN:N	4:B:505:GLN:NE2	2.14	0.94
4:A:544:GLN:HG2	4:A:559:VAL:HG21	1.47	0.94
4:C:133:THR:HA	4:C:243:THR:HG22	1.49	0.94
4:D:16:LEU:HD13	4:D:38:ALA:HB2	1.50	0.94
4:C:629:VAL:HG22	4:C:654:THR:HG21	1.50	0.93
4:B:490:MET:SD	4:B:522:GLN:HG3	2.07	0.93
4:C:236:VAL:HB	4:C:239:GLN:HB2	1.49	0.93
4:A:421:ASP:OD2	4:A:425:ARG:HB2	1.67	0.93
1:H:15:DC:H2"	1:H:16:DC:O5'	1.66	0.93
4:C:632:ARG:HH22	6:C:2002:APC:H5'1	1.31	0.93
4:C:404:GLN:HG2	4:C:432:PHE:CG	2.04	0.93
4:A:105:PHE:HB3	4:A:204:TRP:HZ2	1.34	0.93
4:B:116:TYR:OH	4:B:752:LEU:HD22	1.69	0.93
4:B:492:CYS:O	4:B:496:PRO:HD3	1.68	0.93
2:I:4:G:H2'	2:I:5:C:H6	1.33	0.93
4:A:457:TYR:CE2	4:A:461:LYS:HD3	2.03	0.92
4:A:457:TYR:CZ	4:A:461:LYS:HD3	2.05	0.92
4:C:457:TYR:CE1	4:C:521:VAL:HG11	2.04	0.92
4:A:154:ILE:HG23	4:A:190:MET:CE	1.99	0.92
4:D:380:ALA:O	4:D:384:VAL:HG23	1.69	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:281:ILE:CG2	4:C:282:THR:HG22	2.00	0.92
4:D:264:ILE:HG23	4:D:292:ARG:HB2	1.52	0.92
4:D:718:ILE:HD12	4:D:718:ILE:N	1.85	0.92
1:H:13:DC:H2"	1:H:14:DG:C5'	1.99	0.92
4:B:163:LYS:HZ3	4:B:166:VAL:HB	1.35	0.92
4:C:778:ILE:HG23	4:C:779:ALA:N	1.83	0.92
4:A:85:ILE:HG12	4:A:219:MET:SD	2.10	0.92
4:C:334:VAL:HG21	4:C:513:ALA:HB2	1.49	0.92
4:A:871:ASN:HD21	4:A:873:ARG:CB	1.83	0.91
4:C:333:LYS:HD3	4:C:516:PHE:HD2	1.34	0.91
4:A:5:ASN:HD21	4:A:7:ALA:HB3	1.34	0.91
4:D:810:ILE:HB	4:D:813:SER:OG	1.70	0.91
4:A:828:VAL:HG23	4:A:829:ARG:H	1.33	0.91
4:B:11:PHE:HB3	4:B:41:HIS:CE1	2.05	0.91
4:C:556:GLY:CA	4:C:561:LEU:HD22	2.00	0.91
4:A:280:GLY:O	4:A:282:THR:N	2.04	0.91
4:C:560:ASN:O	4:C:881:ALA:HB2	1.70	0.91
4:B:706:LEU:HD11	4:B:849:PHE:CD2	2.05	0.91
4:A:341:ILE:HD12	4:A:348:PRO:HB3	1.49	0.91
4:C:249:GLU:CD	4:C:249:GLU:H	1.73	0.91
4:A:502:TRP:CD2	4:A:512:LEU:HD13	2.06	0.91
4:D:718:ILE:H	4:D:718:ILE:CD1	1.84	0.91
4:B:646:PHE:O	4:B:650:VAL:HG23	1.69	0.91
4:A:825:PHE:CE1	4:A:829:ARG:NH1	2.39	0.91
4:D:720:ARG:NH1	4:D:720:ARG:HG2	1.74	0.91
4:D:552:ASP:HB2	4:D:691:ALA:HB2	1.53	0.91
4:B:85:ILE:HG12	4:B:219:MET:SD	2.11	0.90
4:B:448:LYS:HD2	7:B:3017:HOH:O	1.70	0.90
6:A:2000:APC:H4'	7:A:3238:HOH:O	1.70	0.90
4:A:103:PHE:O	4:A:107:GLN:HG3	1.71	0.90
4:A:423:ARG:NH2	4:A:784:HIS:ND1	2.18	0.90
4:C:751:PHE:HB3	4:C:752:LEU:HD12	1.51	0.90
4:A:829:ARG:HH11	4:A:829:ARG:CG	1.84	0.90
4:A:294:LEU:HD13	4:A:429:VAL:HG21	1.52	0.90
4:C:460:LEU:HA	4:C:534:LEU:HD21	1.54	0.90
4:B:137:VAL:HG12	4:B:217:ILE:HD11	1.54	0.90
4:A:464:GLY:HA3	4:A:514:PHE:CE2	2.07	0.90
4:C:536:PHE:HB3	4:C:882:PHE:CB	2.01	0.90
4:D:273:VAL:HA	4:D:415:TRP:CZ3	2.06	0.90
4:C:551:ARG:HH21	4:C:872:LEU:HD11	1.37	0.90
4:B:702:ALA:HB1	4:B:849:PHE:CE2	2.07	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:204:TRP:CH2	4:A:212:VAL:HG21	2.06	0.90
4:A:452:ILE:HG22	4:A:528:TYR:O	1.72	0.89
4:B:163:LYS:NZ	4:B:166:VAL:HB	1.87	0.89
3:P:9:DC:H4'	7:P:872:HOH:O	1.72	0.89
4:B:793:LYS:HA	7:B:3141:HOH:O	1.71	0.89
4:D:473:VAL:HG22	4:D:477:GLU:HG3	1.54	0.89
4:B:296:LEU:HG	4:B:296:LEU:O	1.69	0.89
4:C:333:LYS:HB3	4:C:516:PHE:CD2	2.07	0.89
4:B:571:TYR:CE2	4:B:631:LYS:HG3	2.08	0.89
4:C:452:ILE:HD11	4:C:457:TYR:HA	1.52	0.89
4:D:864:LEU:HA	7:D:3079:HOH:O	1.72	0.89
4:C:96:ARG:HB3	7:C:3133:HOH:O	1.72	0.89
4:D:854:HIS:CD2	4:D:856:SER:H	1.90	0.89
4:B:430:SER:O	4:B:431:MET:C	2.09	0.88
4:B:236:VAL:HB	4:B:239:GLN:HB2	1.54	0.88
4:C:109:ILE:HD11	4:C:149:ALA:HB2	1.54	0.88
4:B:77:LEU:HD12	4:B:224:THR:HG21	1.55	0.88
4:A:154:ILE:HG23	4:A:190:MET:HE1	1.54	0.88
4:B:585:ASP:O	4:B:614:LYS:HA	1.73	0.88
4:B:452:ILE:HG23	4:B:453:GLY:H	0.76	0.88
4:C:421:ASP:O	4:C:423:ARG:N	2.07	0.88
4:B:231:ARG:HG2	4:B:234:ALA:HB2	1.55	0.88
4:A:546:PHE:HD2	4:A:692:ALA:HA	1.39	0.88
1:H:12:DT:C4'	4:B:423:ARG:HE	1.86	0.88
4:A:60:LYS:HZ1	4:A:61:ALA:HB2	1.39	0.88
4:A:563:PRO:HB3	4:A:878:SER:HA	1.55	0.88
4:B:695:ALA:O	4:B:699:LEU:HD13	1.72	0.88
4:A:105:PHE:HB3	4:A:204:TRP:CZ2	2.09	0.88
4:B:110:LYS:HD3	4:B:111:PRO:HD2	1.55	0.88
4:D:231:ARG:HG2	4:D:234:ALA:HB2	1.53	0.88
4:A:452:ILE:HD11	4:A:457:TYR:HB2	1.55	0.88
4:C:221:ILE:HG12	4:C:227:VAL:HG23	1.55	0.87
1:N:7:DC:H2"	1:N:8:DG:O5'	1.73	0.87
4:B:264:ILE:HG23	4:B:292:ARG:HB2	1.56	0.87
1:N:2:DG:H2"	1:N:3:DG:H8	1.40	0.87
1:E:12:DT:C2'	1:E:13:DC:H5'	2.04	0.87
4:D:333:LYS:HB3	4:D:516:PHE:CE2	2.10	0.87
4:A:155:ARG:HB2	4:A:163:LYS:HE3	1.55	0.87
4:C:437:ASN:H	4:C:437:ASN:ND2	1.70	0.87
4:A:308:TYR:O	4:A:311:VAL:HG23	1.75	0.87
4:B:829:ARG:HG3	4:B:829:ARG:HH11	1.38	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:420:MET:HA	4:B:425:ARG:O	1.75	0.87
4:A:231:ARG:HG2	4:A:234:ALA:HB2	1.54	0.87
4:A:871:ASN:ND2	4:A:873:ARG:HB2	1.90	0.86
4:B:118:THR:HG23	4:B:141:ILE:HD13	1.55	0.86
4:D:536:PHE:HB3	4:D:882:PHE:HB3	1.57	0.86
4:B:408:PHE:HD1	4:B:414:ILE:HG21	1.40	0.86
1:H:2:DG:H2"	1:H:3:DG:C8	2.10	0.86
4:C:84:ARG:HD3	4:C:84:ARG:O	1.75	0.86
4:D:89:PHE:O	4:D:93:LYS:HG3	1.74	0.86
4:D:437:ASN:ND2	4:D:440:THR:H	1.73	0.86
4:D:724:ALA:HB2	4:D:738:GLU:HG3	1.57	0.86
4:D:39:LEU:HD23	7:D:3105:HOH:O	1.74	0.86
4:D:204:TRP:HE3	7:D:3053:HOH:O	1.56	0.86
4:A:383:ALA:O	4:A:385:TYR:N	2.08	0.86
4:C:828:VAL:HG23	4:C:829:ARG:H	1.40	0.86
4:B:300:HIS:HE2	4:B:422:TRP:HZ3	1.21	0.86
4:D:137:VAL:O	4:D:141:ILE:HG13	1.75	0.86
4:A:791:LEU:HD11	4:A:809:LEU:HD22	1.55	0.86
4:C:317:TYR:O	4:C:321:ASN:ND2	2.07	0.86
4:C:574:VAL:O	4:C:578:VAL:HG23	1.75	0.86
4:B:706:LEU:HD21	4:B:849:PHE:CB	2.05	0.86
4:C:570:ILE:HA	4:C:573:ILE:CG2	2.05	0.86
4:D:308:TYR:HE2	4:D:734:PRO:HG2	1.39	0.86
4:B:122:THR:HG21	4:B:226:MET:HE2	1.56	0.85
4:A:109:ILE:HD11	4:A:145:ILE:O	1.76	0.85
4:C:845:PHE:O	4:C:848:GLN:HB2	1.75	0.85
4:C:84:ARG:NH1	4:C:87:ASP:HB2	1.91	0.85
4:B:463:HIS:CB	4:B:534:LEU:HD22	2.06	0.85
4:C:690:VAL:O	4:C:693:VAL:HB	1.76	0.85
4:B:408:PHE:HD2	4:B:408:PHE:N	1.72	0.85
4:D:804:ILE:HG23	4:D:816:THR:HG21	1.57	0.85
4:A:647:ARG:CD	4:A:675:GLY:HA2	2.05	0.85
1:N:12:DT:H2"	1:N:13:DC:C5'	2.06	0.85
4:B:737:GLN:HE21	4:B:739:TYR:HE2	1.22	0.85
4:C:338:ALA:O	4:C:340:VAL:N	2.10	0.85
3:P:1:DG:H1'	3:P:2:DT:H71	1.56	0.85
4:C:227:VAL:HB	4:C:244:ILE:HD12	1.58	0.85
4:C:276:LYS:HE2	7:C:3084:HOH:O	1.76	0.85
4:B:37:LEU:H	4:B:37:LEU:HD12	1.42	0.85
4:C:404:GLN:HE21	4:C:404:GLN:HA	1.39	0.85
4:D:117:ILE:HG21	4:D:145:ILE:HD13	1.58	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:59:LEU:HA	4:A:64:VAL:CG2	2.06	0.85
4:A:574:VAL:HG11	4:A:685:VAL:HG12	1.56	0.85
4:B:333:LYS:O	4:B:337:VAL:HG23	1.77	0.85
4:A:386:ARG:O	4:A:389:LYS:N	2.09	0.85
4:D:705:LEU:HB3	4:D:857:GLN:NE2	1.92	0.84
4:B:111:PRO:HG2	4:B:112:GLU:OE1	1.77	0.84
4:B:473:VAL:HG13	4:B:474:PRO:CD	2.07	0.84
4:A:505:GLN:O	4:A:507:SER:N	2.10	0.84
4:C:232:GLN:HB2	4:C:241:SER:O	1.77	0.84
4:A:256:THR:HG23	7:A:3067:HOH:O	1.77	0.84
4:B:423:ARG:HG3	4:B:781:ASN:HD22	1.40	0.84
4:C:452:ILE:HD11	4:C:457:TYR:CA	2.07	0.84
4:A:881:ALA:O	4:A:882:PHE:C	2.14	0.84
4:C:158:GLU:CG	4:C:195:LEU:HD22	2.01	0.84
4:C:278:TRP:CE3	4:C:284:GLY:HA3	2.13	0.84
1:H:9:DA:N6	3:J:1:DG:N2	2.26	0.84
4:C:92:VAL:CG1	4:C:99:ARG:HG3	2.06	0.84
4:A:727:TRP:CE2	4:A:735:VAL:HG11	2.12	0.84
4:C:559:VAL:HG23	4:C:561:LEU:HD13	1.58	0.84
4:A:452:ILE:HD11	4:A:457:TYR:CA	2.07	0.84
4:B:168:GLU:O	4:B:172:LYS:HG2	1.77	0.84
4:B:17:ALA:HA	7:B:3012:HOH:O	1.78	0.84
4:A:721:LYS:HD3	4:A:722:ARG:H	1.41	0.84
4:B:816:THR:HG22	4:B:817:ILE:N	1.91	0.84
4:B:632:ARG:HD2	6:B:2001:APC:HN61	1.43	0.84
4:B:728:VAL:HG22	4:B:734:PRO:HA	1.60	0.84
4:C:423:ARG:NH1	4:C:423:ARG:HB2	1.93	0.83
4:B:201:TRP:HB3	7:B:3009:HOH:O	1.78	0.83
4:A:816:THR:HG22	4:A:817:ILE:H	1.43	0.83
4:C:636:THR:HG22	4:C:639:TYR:HD2	1.41	0.83
4:A:646:PHE:O	4:A:650:VAL:HG23	1.78	0.83
4:A:731:ASP:OD1	4:A:792:ARG:NH2	2.11	0.83
4:A:720:ARG:HG2	4:A:720:ARG:HH11	1.42	0.83
4:B:574:VAL:HG21	4:B:685:VAL:HG12	1.57	0.83
4:B:432:PHE:HE2	4:B:444:LEU:HD21	1.40	0.83
4:B:505:GLN:N	4:B:505:GLN:HE21	1.75	0.83
4:B:339:ASN:O	4:B:343:LYS:CD	2.26	0.83
4:C:275:PRO:HG2	4:C:324:GLN:HG2	1.61	0.83
4:A:574:VAL:O	4:A:578:VAL:HG23	1.76	0.83
4:C:437:ASN:N	4:C:437:ASN:HD22	1.72	0.83
4:A:386:ARG:HD2	7:A:3138:HOH:O	1.76	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:744:GLN:HA	4:D:756:ARG:CZ	2.08	0.83
4:A:833:VAL:HG13	4:A:872:LEU:HB3	1.58	0.83
4:C:728:VAL:HG22	4:C:734:PRO:HA	1.59	0.83
4:C:551:ARG:HE	4:C:872:LEU:HD21	1.42	0.83
4:C:404:GLN:HG2	4:C:432:PHE:CB	2.09	0.83
4:A:66:ASP:OD2	4:A:752:LEU:HD23	1.79	0.83
4:B:691:ALA:O	4:B:694:GLU:HB2	1.79	0.83
4:A:280:GLY:HA2	4:A:317:TYR:CZ	2.13	0.82
4:B:437:ASN:HD22	4:B:437:ASN:C	1.81	0.82
4:B:172:LYS:HB3	4:B:172:LYS:NZ	1.93	0.82
4:B:122:THR:HG21	4:B:226:MET:CE	2.09	0.82
4:D:778:ILE:HG23	4:D:779:ALA:N	1.93	0.82
4:B:881:ALA:O	4:B:882:PHE:C	2.14	0.82
4:D:329:LYS:HG2	4:D:445:THR:O	1.78	0.82
4:D:59:LEU:HD23	4:D:64:VAL:HG22	1.59	0.82
4:B:846:TYR:HA	4:B:849:PHE:HE1	1.42	0.82
4:C:582:LEU:HB3	4:C:621:LEU:HD21	1.62	0.82
4:C:663:LYS:HD3	4:C:664:GLY:H	1.45	0.82
4:A:881:ALA:O	4:A:882:PHE:O	1.98	0.82
4:D:668:THR:HG22	4:D:669:GLN:HE21	1.45	0.82
4:C:308:TYR:O	4:C:311:VAL:HG23	1.79	0.82
4:D:828:VAL:HB	4:D:883:ALA:HA	1.61	0.82
4:B:574:VAL:CG1	4:B:574:VAL:O	2.26	0.82
4:B:345:LYS:NZ	4:B:351:ASP:H	1.77	0.82
4:A:278:TRP:CE3	4:A:284:GLY:HA3	2.15	0.82
1:E:14:DG:H2'	1:E:15:DC:C6	2.15	0.82
4:B:298:ARG:HG3	4:B:420:MET:O	1.78	0.82
4:B:574:VAL:HG12	4:B:574:VAL:O	1.76	0.82
4:C:579:ASN:HA	4:C:582:LEU:HD12	1.62	0.82
4:D:275:PRO:HG2	4:D:324:GLN:HG2	1.61	0.82
4:D:470:VAL:HG12	4:D:473:VAL:HG11	1.61	0.82
4:C:169:GLN:O	4:C:173:ARG:HG2	1.80	0.82
4:A:486:HIS:HD2	4:A:518:TYR:CE1	1.98	0.82
1:N:10:DT:H5'	4:D:641:SER:CA	2.09	0.82
4:B:408:PHE:CD2	4:B:408:PHE:N	2.47	0.82
4:A:512:LEU:HG	4:A:516:PHE:HE1	1.43	0.82
4:B:231:ARG:HD2	4:B:240:ASP:OD2	1.80	0.82
4:C:236:VAL:CB	4:C:239:GLN:HB2	2.10	0.81
4:D:486:HIS:HA	4:D:489:ILE:HD12	1.59	0.81
4:A:19:ILE:HG13	7:A:3121:HOH:O	1.78	0.81
4:D:342:THR:HG22	4:D:348:PRO:HG2	1.62	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:229:LEU:HD11	4:B:242:GLU:HG2	1.61	0.81
4:A:421:ASP:OD1	4:A:423:ARG:HD3	1.79	0.81
4:D:870:LEU:HD22	4:D:872:LEU:HD23	1.62	0.81
1:H:13:DC:O4'	4:B:427:TYR:HE2	1.60	0.81
4:D:541:SER:HA	4:D:544:GLN:NE2	1.95	0.81
4:C:271:CYS:SG	4:C:417:PRO:HD3	2.20	0.81
2:I:4:G:H2'	2:I:5:C:C6	2.16	0.81
4:C:231:ARG:HG2	4:C:234:ALA:HB2	1.63	0.81
4:B:51:PHE:O	4:B:51:PHE:CD2	2.34	0.81
4:C:550:LEU:HD21	4:C:865:PRO:HG2	1.62	0.81
4:D:308:TYR:CE2	4:D:734:PRO:HG2	2.14	0.81
4:C:249:GLU:CD	4:C:249:GLU:N	2.31	0.81
4:C:631:LYS:HZ3	6:C:2002:APC:H3A2	1.43	0.81
4:D:699:LEU:O	4:D:778:ILE:HG21	1.80	0.81
4:A:401:MET:O	4:A:403:GLU:N	2.14	0.81
4:D:16:LEU:HD22	4:D:38:ALA:HA	1.61	0.81
4:B:632:ARG:O	4:B:636:THR:HG23	1.79	0.81
4:B:742:PRO:HB3	4:B:744:GLN:OE1	1.81	0.81
4:D:80:LYS:HD3	4:D:224:THR:HB	1.62	0.81
4:A:583:GLN:HB2	7:A:3056:HOH:O	1.79	0.81
4:B:587:ILE:HG22	4:B:588:ASN:ND2	1.96	0.81
4:D:551:ARG:HB2	4:D:868:GLY:H	1.45	0.81
4:A:184:GLN:HG3	7:A:3137:HOH:O	1.81	0.81
4:D:871:ASN:HD21	4:D:873:ARG:HB2	1.46	0.80
4:B:470:VAL:HG12	4:B:470:VAL:O	1.81	0.80
4:C:610:LYS:HE3	7:C:3172:HOH:O	1.80	0.80
4:A:303:LYS:HD2	7:D:3155:HOH:O	1.81	0.80
4:C:291:ARG:HG3	7:C:3104:HOH:O	1.81	0.80
4:A:280:GLY:HA2	4:A:317:TYR:CE1	2.16	0.80
4:D:286:TYR:CE1	4:D:417:PRO:HG3	2.15	0.80
4:B:275:PRO:HD2	7:B:3116:HOH:O	1.81	0.80
4:B:869:ASN:ND2	4:B:869:ASN:N	2.28	0.80
4:B:126:LEU:HD13	4:B:246:LEU:HB2	1.61	0.80
4:A:15:GLU:HB3	4:A:19:ILE:HG12	1.63	0.80
4:D:840:ASP:O	4:D:842:LEU:N	2.14	0.80
4:A:801:LYS:HD3	4:A:801:LYS:C	2.01	0.80
4:A:669:GLN:HG2	4:A:672:GLN:HE21	1.47	0.80
4:A:278:TRP:CZ3	4:A:284:GLY:HA3	2.17	0.80
4:D:582:LEU:HD11	4:D:625:VAL:HG21	1.62	0.80
4:A:624:GLY:HA3	7:A:3045:HOH:O	1.79	0.80
4:C:631:LYS:CE	6:C:2002:APC:H3A2	2.11	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:502:TRP:CG	4:A:512:LEU:HD13	2.16	0.80
4:B:158:GLU:HA	4:B:195:LEU:HD13	1.63	0.80
4:D:448:LYS:NZ	4:D:806:SER:HB3	1.96	0.80
4:A:802:TYR:O	4:A:804:ILE:N	2.13	0.80
4:B:537:ASP:H	4:B:882:PHE:HD2	1.28	0.80
4:B:669:GLN:CG	4:B:672:GLN:HG3	2.11	0.80
4:D:552:ASP:OD1	4:D:555:GLY:N	2.11	0.80
4:C:211:HIS:O	4:C:214:VAL:HG23	1.81	0.80
1:H:6:DT:H5'	1:H:6:DT:C6	2.16	0.80
7:I:777:HOH:O	4:B:386:ARG:HD3	1.82	0.79
1:N:2:DG:H2"	1:N:3:DG:C8	2.16	0.79
4:D:281:ILE:HG22	4:D:282:THR:HG22	1.62	0.79
4:D:489:ILE:O	4:D:492:CYS:SG	2.40	0.79
4:D:14:ILE:H	4:D:14:ILE:HD12	1.45	0.79
4:A:478:ARG:HH12	4:A:882:PHE:HZ	1.29	0.79
4:D:125:CYS:O	4:D:128:SER:HB3	1.81	0.79
4:D:490:MET:O	4:D:493:ALA:HB3	1.81	0.79
4:A:15:GLU:HG3	4:A:18:ALA:H	1.45	0.79
4:A:610:LYS:HG2	4:A:610:LYS:O	1.79	0.79
4:C:214:VAL:HA	4:C:217:ILE:HD12	1.65	0.79
4:A:462:ILE:HG12	4:A:479:ILE:HD11	1.64	0.79
4:B:881:ALA:O	4:B:883:ALA:OXT	1.99	0.79
4:A:452:ILE:HD11	4:A:457:TYR:CB	2.13	0.79
4:A:526:LEU:N	4:A:526:LEU:HD12	1.97	0.79
4:D:804:ILE:HG12	4:D:820:ASP:HB3	1.63	0.79
4:A:157:LEU:HB3	7:A:3133:HOH:O	1.80	0.79
4:C:78:LEU:N	4:C:79:PRO:HD2	1.97	0.79
1:H:14:DG:H2"	1:H:15:DC:C5'	2.13	0.79
4:A:119:ILE:O	4:A:123:LEU:HD12	1.81	0.79
4:B:770:ASP:OD1	4:B:770:ASP:C	2.21	0.79
4:D:860:LYS:O	4:D:860:LYS:HD2	1.83	0.79
4:A:342:THR:HG21	4:A:398:LEU:HD21	1.61	0.79
4:A:806:SER:O	4:A:816:THR:HG23	1.82	0.79
4:C:158:GLU:HA	4:C:195:LEU:HD13	1.63	0.79
4:C:19:ILE:HD13	7:C:3117:HOH:O	1.83	0.79
4:C:59:LEU:HD22	4:C:64:VAL:HG13	1.65	0.79
4:B:748:ASN:ND2	4:B:751:PHE:HB2	1.98	0.79
4:D:139:SER:HB2	4:D:210:ILE:CD1	2.13	0.79
4:C:396:ILE:HG22	7:C:3188:HOH:O	1.82	0.79
4:C:299:THR:HG22	4:C:300:HIS:N	1.98	0.79
4:A:291:ARG:HB2	7:A:3193:HOH:O	1.83	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:452:ILE:HD11	4:A:457:TYR:HA	1.65	0.78
4:C:47:GLY:HA3	4:C:265:SER:O	1.83	0.78
4:C:563:PRO:HB3	4:C:877:GLU:O	1.82	0.78
4:B:814:PHE:HB3	4:B:824:LEU:HD21	1.65	0.78
4:B:24:LEU:HD13	4:B:37:LEU:HD11	1.62	0.78
4:A:16:LEU:HD13	4:A:38:ALA:CB	2.13	0.78
4:D:475:PHE:HE2	4:D:879:ASP:HB3	1.48	0.78
4:B:712:ASP:HB3	7:B:3078:HOH:O	1.84	0.78
4:A:871:ASN:HB3	4:A:874:ASP:OD2	1.83	0.78
4:B:816:THR:CG2	4:B:817:ILE:H	1.89	0.78
4:B:449:GLY:HA3	4:B:529:ASN:ND2	1.99	0.78
4:A:133:THR:HA	4:A:243:THR:HG22	1.65	0.78
4:C:778:ILE:CG2	4:C:779:ALA:N	2.46	0.78
4:C:404:GLN:HG2	4:C:432:PHE:HB2	1.65	0.78
4:D:806:SER:O	4:D:816:THR:HG23	1.81	0.78
4:C:505:GLN:O	4:C:508:PRO:HD3	1.82	0.78
4:A:748:ASN:ND2	4:A:751:PHE:H	1.82	0.78
4:A:546:PHE:CE1	4:A:783:VAL:CG2	2.63	0.78
4:A:791:LEU:CD1	4:A:809:LEU:HD22	2.14	0.78
1:K:11:DA:C8	4:C:639:TYR:HB3	2.18	0.78
4:B:446:LEU:HD12	4:B:817:ILE:HG23	1.64	0.78
4:C:84:ARG:HH11	4:C:84:ARG:HA	1.47	0.78
4:A:475:PHE:O	4:A:479:ILE:HG12	1.84	0.78
4:A:44:TYR:OH	4:A:292:ARG:HB3	1.83	0.78
4:D:427:TYR:HA	4:D:435:GLN:HE22	1.48	0.78
4:D:323:ALA:O	4:D:325:ASN:N	2.16	0.78
4:B:869:ASN:HD22	4:B:869:ASN:N	1.81	0.78
4:C:448:LYS:HE3	4:C:806:SER:OG	1.84	0.78
4:A:546:PHE:CZ	4:A:783:VAL:HG22	2.19	0.78
4:C:545:HIS:O	4:C:549:MET:HG2	1.84	0.78
4:A:562:LEU:HD21	4:A:870:LEU:HD12	1.65	0.78
4:D:454:LYS:HG3	4:D:455:GLU:H	1.48	0.78
4:A:860:LYS:HD2	4:A:860:LYS:O	1.84	0.78
4:D:475:PHE:CE2	4:D:879:ASP:HB3	2.19	0.77
1:N:15:DC:C2	1:N:16:DC:C5	2.72	0.77
4:B:423:ARG:HH12	4:B:784:HIS:HB3	1.48	0.77
4:B:398:LEU:HD21	4:B:439:MET:HE1	1.65	0.77
4:B:274:PRO:HD3	4:B:415:TRP:CZ3	2.19	0.77
4:C:706:LEU:HD22	4:C:725:VAL:HG22	1.67	0.77
4:A:727:TRP:HA	4:A:848:GLN:HE21	1.46	0.77
4:B:80:LYS:O	4:B:223:SER:HB2	1.83	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:159:ALA:O	4:D:163:LYS:HB2	1.84	0.77
4:B:631:LYS:HE2	6:B:2001:APC:H3A2	1.67	0.77
4:C:460:LEU:HG	4:C:460:LEU:O	1.84	0.77
1:H:2:DG:H2"	1:H:3:DG:H8	1.48	0.77
4:C:155:ARG:HB2	4:C:163:LYS:NZ	2.00	0.77
2:O:4:G:O2'	2:O:5:C:H5'	1.85	0.77
4:B:264:ILE:C	4:B:266:PRO:HD3	2.05	0.77
4:B:233:ASN:HD22	4:B:239:GLN:NE2	1.82	0.77
4:C:181:ALA:O	4:C:185:VAL:HG22	1.85	0.77
4:B:273:VAL:O	4:B:274:PRO:O	2.02	0.77
4:D:563:PRO:HB2	7:D:3032:HOH:O	1.85	0.77
4:D:57:ARG:O	4:D:60:LYS:HB3	1.85	0.77
4:A:468:ALA:HB2	4:A:511:PHE:CE1	2.20	0.77
4:D:720:ARG:HH11	4:D:720:ARG:CG	1.86	0.77
4:A:141:ILE:HG22	4:A:145:ILE:HD11	1.66	0.77
4:C:275:PRO:HB2	4:C:324:GLN:OE1	1.85	0.77
4:B:663:LYS:HG2	4:B:664:GLY:H	1.49	0.77
4:B:407:LYS:HG2	4:B:408:PHE:CD2	2.19	0.77
4:B:489:ILE:HG22	4:B:515:CYS:HB3	1.67	0.77
4:D:51:PHE:CE2	4:D:55:PHE:HB2	2.20	0.77
4:D:55:PHE:CZ	4:D:59:LEU:HD21	2.20	0.77
4:C:81:MET:O	4:C:85:ILE:HG13	1.85	0.77
4:A:664:GLY:HA2	4:A:667:PHE:HD2	1.50	0.77
4:C:433:ASN:CA	7:C:3164:HOH:O	2.33	0.77
1:H:14:DG:H2"	1:H:15:DC:H5'	1.67	0.77
4:C:337:VAL:HG21	4:C:512:LEU:HD21	1.66	0.77
4:B:5:ASN:HD22	4:B:8:LYS:HG3	1.49	0.77
4:A:825:PHE:CZ	4:A:829:ARG:NH2	2.52	0.76
1:K:11:DA:H2'	1:K:12:DT:C7	2.14	0.76
4:A:60:LYS:O	4:A:60:LYS:NZ	2.18	0.76
4:D:744:GLN:HA	4:D:756:ARG:NE	2.00	0.76
4:C:516:PHE:O	4:C:519:ALA:HB3	1.84	0.76
4:C:401:MET:O	4:C:404:GLN:HB3	1.85	0.76
4:D:95:LYS:HD3	7:D:3062:HOH:O	1.85	0.76
4:A:210:ILE:O	4:A:214:VAL:HG23	1.85	0.76
4:B:582:LEU:HB3	4:B:621:LEU:HD11	1.65	0.76
4:C:55:PHE:O	4:C:58:GLN:HB2	1.85	0.76
4:D:473:VAL:N	4:D:567:VAL:HG21	2.00	0.76
4:A:390:ALA:O	4:A:392:LYS:N	2.18	0.76
4:A:495:SER:HA	7:A:3203:HOH:O	1.85	0.76
4:A:281:ILE:CG1	4:A:309:GLU:HA	2.15	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:423:ARG:CG	4:B:781:ASN:HD22	1.98	0.76
4:A:87:ASP:O	4:A:91:GLU:HG3	1.85	0.76
4:D:651:LEU:O	4:D:651:LEU:HD13	1.85	0.76
4:B:690:VAL:O	4:B:693:VAL:HG23	1.84	0.76
4:B:784:HIS:O	4:B:786:GLN:N	2.18	0.76
4:B:790:HIS:HE1	4:B:831:THR:HG23	1.50	0.76
4:A:512:LEU:HG	4:A:516:PHE:CE1	2.21	0.76
4:B:418:TYR:CD2	4:B:428:ALA:HA	2.21	0.76
4:A:92:VAL:HG11	4:A:100:PRO:HD2	1.66	0.76
4:B:390:ALA:C	4:B:392:LYS:H	1.87	0.76
4:A:454:LYS:N	4:A:526:LEU:HD23	2.00	0.76
4:C:15:GLU:HG3	4:C:18:ALA:H	1.49	0.76
4:C:744:GLN:CB	7:C:3076:HOH:O	2.34	0.76
4:C:778:ILE:CG2	4:C:779:ALA:H	1.99	0.76
4:D:790:HIS:CE1	4:D:831:THR:HG23	2.16	0.76
4:A:548:ALA:O	4:A:550:LEU:N	2.18	0.76
4:A:464:GLY:HA3	4:A:514:PHE:CZ	2.21	0.75
4:C:308:TYR:OH	4:C:734:PRO:O	2.05	0.75
4:D:540:CYS:O	4:D:542:GLY:N	2.18	0.75
4:A:825:PHE:CE1	4:A:829:ARG:CZ	2.68	0.75
4:A:84:ARG:HD3	4:A:84:ARG:O	1.87	0.75
4:A:668:THR:HG22	4:A:669:GLN:OE1	1.86	0.75
4:A:290:GLY:O	4:A:293:PRO:HD3	1.86	0.75
4:C:308:TYR:OH	4:C:733:PHE:HE2	1.69	0.75
4:D:228:SER:HB3	7:D:3168:HOH:O	1.86	0.75
4:A:457:TYR:HD1	4:A:521:VAL:HG21	1.52	0.75
4:A:816:THR:OG1	4:A:824:LEU:HD22	1.87	0.75
4:D:829:ARG:HG3	4:D:829:ARG:HH11	1.51	0.75
4:C:299:THR:HG22	4:C:300:HIS:H	1.51	0.75
4:D:141:ILE:O	4:D:145:ILE:HG12	1.87	0.75
4:D:871:ASN:ND2	4:D:873:ARG:HB2	2.00	0.75
4:D:465:ALA:CB	4:D:478:ARG:HB3	2.16	0.75
4:B:719:LEU:HD23	4:B:854:HIS:NE2	2.01	0.75
4:C:5:ASN:HD21	4:C:7:ALA:HB3	1.50	0.75
4:A:280:GLY:CA	4:A:317:TYR:OH	2.35	0.75
4:B:463:HIS:HB2	4:B:534:LEU:HD22	1.68	0.75
4:D:297:VAL:HG12	4:D:299:THR:HG22	1.68	0.75
4:C:539:SER:HA	7:C:3124:HOH:O	1.86	0.75
4:B:391:ARG:HG3	7:B:3101:HOH:O	1.86	0.75
4:A:463:HIS:HA	4:A:466:ASN:ND2	2.01	0.75
4:A:273:VAL:O	4:A:273:VAL:CG2	2.35	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:10:DT:H5'	4:D:641:SER:N	2.02	0.75
4:D:435:GLN:HB3	4:D:810:ILE:HG12	1.69	0.75
4:A:544:GLN:CG	4:A:559:VAL:HG21	2.16	0.74
4:B:55:PHE:CD2	4:B:55:PHE:O	2.40	0.74
4:C:810:ILE:HG22	4:C:810:ILE:O	1.86	0.74
1:H:15:DC:H2"	1:H:16:DC:C5'	2.18	0.74
7:I:777:HOH:O	4:B:386:ARG:CD	2.33	0.74
4:A:486:HIS:CD2	4:A:518:TYR:HE1	2.06	0.74
4:A:514:PHE:HD1	4:A:515:CYS:N	1.85	0.74
4:A:793:LYS:O	4:A:796:VAL:HG23	1.86	0.74
4:C:324:GLN:HE21	4:C:418:TYR:H	1.36	0.74
4:B:56:GLU:OE1	4:B:57:ARG:HA	1.87	0.74
4:D:454:LYS:HG3	4:D:455:GLU:N	2.03	0.74
4:C:4:ILE:HD12	4:C:256:THR:HG23	1.69	0.74
4:A:825:PHE:CE1	4:A:829:ARG:NH2	2.55	0.74
4:B:92:VAL:HA	7:B:3193:HOH:O	1.88	0.74
4:B:871:ASN:HB3	4:B:874:ASP:OD2	1.88	0.74
4:D:351:ASP:HA	7:D:3124:HOH:O	1.86	0.74
4:B:475:PHE:O	4:B:476:PRO:C	2.23	0.74
4:C:141:ILE:O	4:C:145:ILE:HG12	1.86	0.74
4:C:109:ILE:CD1	4:C:149:ALA:HB2	2.17	0.74
4:B:143:ARG:O	4:B:146:GLU:HB3	1.86	0.74
4:A:60:LYS:O	4:A:60:LYS:HG2	1.86	0.74
4:A:77:LEU:HD23	4:A:119:ILE:HD12	1.70	0.74
4:A:418:TYR:HD2	4:A:426:VAL:CG1	2.01	0.74
4:B:651:LEU:O	4:B:651:LEU:HD22	1.86	0.74
4:C:749:LEU:HD12	4:C:750:MET:HG2	1.69	0.74
4:A:275:PRO:HD2	7:A:3206:HOH:O	1.88	0.74
4:B:846:TYR:HA	4:B:849:PHE:CE1	2.23	0.74
4:C:84:ARG:HH12	4:C:87:ASP:CB	2.00	0.74
4:B:855:GLU:O	4:B:858:LEU:HD12	1.87	0.74
4:B:71:LYS:N	4:B:72:PRO:HD2	2.03	0.74
4:C:706:LEU:CD2	4:C:725:VAL:HG13	2.18	0.74
4:A:116:TYR:OH	4:A:752:LEU:HD22	1.88	0.74
4:C:738:GLU:HA	4:C:774:GLN:HE22	1.53	0.74
4:B:663:LYS:CG	4:B:664:GLY:H	2.00	0.74
4:B:537:ASP:O	4:B:882:PHE:HB2	1.87	0.74
4:C:744:GLN:HB3	4:C:756:ARG:HB3	1.70	0.74
4:A:395:ARG:HG3	4:A:395:ARG:O	1.88	0.74
4:D:250:TYR:O	4:D:254:ILE:HG13	1.88	0.74
4:B:636:THR:HG21	4:B:649:GLN:HE22	1.53	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:172:LYS:HB3	4:B:172:LYS:HZ2	1.52	0.73
4:D:663:LYS:HG2	4:D:664:GLY:H	1.52	0.73
4:C:656:GLN:N	4:C:657:PRO:HD2	2.02	0.73
1:H:12:DT:H4'	4:B:423:ARG:HE	1.52	0.73
4:B:780:PRO:HA	4:B:783:VAL:HG23	1.70	0.73
4:C:866:ALA:HB2	7:C:3189:HOH:O	1.86	0.73
4:C:850:ALA:O	4:C:853:LEU:HG	1.89	0.73
4:B:226:MET:O	4:B:247:ALA:HB2	1.88	0.73
4:B:662:GLY:O	4:B:663:LYS:O	2.06	0.73
4:C:655:ILE:HD12	4:C:674:ALA:HB2	1.69	0.73
4:B:557:ARG:O	4:B:557:ARG:HG2	1.86	0.73
4:B:278:TRP:CE3	4:B:284:GLY:HA3	2.23	0.73
4:D:881:ALA:O	4:D:882:PHE:C	2.27	0.73
4:C:744:GLN:HB2	7:C:3076:HOH:O	1.89	0.73
4:C:492:CYS:HA	7:C:3071:HOH:O	1.89	0.73
4:D:457:TYR:CE1	4:D:521:VAL:HG11	2.23	0.73
4:C:636:THR:HG22	4:C:639:TYR:CD2	2.22	0.73
4:C:778:ILE:HG23	4:C:779:ALA:H	1.51	0.73
1:K:13:DC:H2"	1:K:14:DG:C5'	2.18	0.73
4:D:417:PRO:O	4:D:429:VAL:HG23	1.87	0.73
4:A:100:PRO:HG2	4:A:103:PHE:HB2	1.69	0.73
4:A:380:ALA:O	4:A:384:VAL:HG23	1.87	0.73
4:C:210:ILE:O	4:C:214:VAL:HG22	1.89	0.73
4:D:457:TYR:CD1	4:D:521:VAL:HG11	2.24	0.73
4:C:337:VAL:HG12	4:C:338:ALA:N	2.03	0.73
4:A:562:LEU:HD21	4:A:870:LEU:HD11	1.69	0.73
4:C:281:ILE:HG12	4:C:309:GLU:HA	1.70	0.73
4:D:14:ILE:CG2	4:D:288:ALA:HB1	2.19	0.73
4:C:70:ALA:C	4:C:72:PRO:HD2	2.09	0.73
4:A:54:MET:O	4:A:58:GLN:HG2	1.89	0.73
1:K:13:DC:H2"	1:K:14:DG:O5'	1.89	0.73
4:B:748:ASN:ND2	4:B:751:PHE:H	1.86	0.73
4:D:330:ILE:HG13	4:D:408:PHE:O	1.88	0.73
4:A:281:ILE:CG2	4:A:282:THR:HG23	2.11	0.73
4:A:138:ALA:O	4:A:213:GLY:HA3	1.89	0.73
4:C:739:TYR:HB2	4:C:774:GLN:OE1	1.89	0.73
1:K:11:DA:H2'	1:K:12:DT:H72	1.69	0.73
4:D:623:TYR:HA	4:D:666:MET:HE1	1.70	0.73
4:B:291:ARG:HB2	7:B:3037:HOH:O	1.89	0.73
4:C:269:GLN:O	4:C:430:SER:HB3	1.88	0.72
4:D:278:TRP:HB2	4:D:321:ASN:HD21	1.53	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1:G:H5"	7:I:873:HOH:O	1.89	0.72
4:A:514:PHE:CD1	4:A:515:CYS:N	2.57	0.72
4:A:736:TRP:HB2	7:A:3116:HOH:O	1.88	0.72
4:C:728:VAL:HG22	4:C:734:PRO:CA	2.19	0.72
4:D:833:VAL:CG2	4:D:875:ILE:HB	2.19	0.72
4:A:829:ARG:NH1	4:A:829:ARG:HG3	1.98	0.72
4:B:418:TYR:HE2	4:B:428:ALA:CB	2.01	0.72
4:B:345:LYS:HZ3	4:B:351:ASP:H	1.37	0.72
4:A:428:ALA:H	4:A:435:GLN:HE22	1.34	0.72
4:B:119:ILE:O	4:B:122:THR:HB	1.88	0.72
4:C:423:ARG:NH2	4:C:784:HIS:ND1	2.37	0.72
4:D:39:LEU:HD22	4:D:272:VAL:CG2	2.19	0.72
4:B:395:ARG:O	4:B:398:LEU:N	2.22	0.72
4:A:59:LEU:HA	4:A:64:VAL:HG22	1.70	0.72
4:B:454:LYS:HE2	7:B:3020:HOH:O	1.88	0.72
2:F:1:G:H2'	2:F:2:C:C6	2.24	0.72
4:D:272:VAL:O	4:D:415:TRP:HZ3	1.72	0.72
4:D:505:GLN:N	4:D:505:GLN:NE2	2.37	0.72
4:D:472:LYS:HA	4:D:567:VAL:HG11	1.71	0.72
4:B:339:ASN:O	4:B:343:LYS:HD2	1.88	0.72
4:A:113:ALA:O	4:A:117:ILE:HG13	1.89	0.72
4:C:423:ARG:HD2	4:C:781:ASN:ND2	2.03	0.72
4:D:328:TRP:O	4:D:414:ILE:N	2.20	0.72
4:B:268:PHE:CB	4:B:286:TYR:OH	2.35	0.72
4:B:567:VAL:HG13	4:B:880:PHE:CG	2.25	0.72
4:B:314:PRO:O	4:B:316:VAL:N	2.23	0.72
4:D:327:ALA:HB2	4:D:415:TRP:NE1	2.05	0.72
4:B:578:VAL:HG22	4:B:680:LEU:HB3	1.72	0.72
4:B:432:PHE:CE2	4:B:444:LEU:HD21	2.23	0.72
4:C:459:TRP:HB3	4:C:534:LEU:HD13	1.70	0.72
1:H:3:DG:N3	7:H:1116:HOH:O	2.22	0.72
4:D:448:LYS:CE	4:D:806:SER:HB3	2.19	0.72
4:D:593:GLU:O	4:D:610:LYS:N	2.19	0.72
4:A:423:ARG:NH2	4:A:784:HIS:HB3	2.05	0.72
4:C:420:MET:HA	4:C:425:ARG:O	1.89	0.72
4:B:281:ILE:CD1	4:B:309:GLU:HA	2.20	0.72
4:B:505:GLN:H	4:B:505:GLN:HE21	1.36	0.72
4:D:766:ASP:HB3	7:D:3085:HOH:O	1.88	0.72
4:B:741:LYS:HB2	4:B:770:ASP:HB2	1.70	0.72
4:A:182:PHE:O	4:A:185:VAL:HG22	1.90	0.72
4:C:335:LEU:HD21	4:C:339:ASN:HD22	1.55	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:471:ASP:O	4:B:472:LYS:HD2	1.90	0.71
4:A:502:TRP:CE2	4:A:512:LEU:HD13	2.25	0.71
4:A:84:ARG:HD3	4:A:84:ARG:C	2.10	0.71
4:A:421:ASP:O	4:A:423:ARG:N	2.22	0.71
4:B:300:HIS:NE2	4:B:422:TRP:CZ3	2.56	0.71
4:D:443:LEU:N	4:D:443:LEU:HD23	2.04	0.71
4:C:247:ALA:HB1	4:C:249:GLU:OE1	1.90	0.71
4:C:78:LEU:HG	4:C:78:LEU:O	1.88	0.71
4:D:352:ILE:N	4:D:352:ILE:HD12	2.05	0.71
4:C:433:ASN:OD1	4:C:435:GLN:N	2.21	0.71
4:B:281:ILE:HD13	4:B:309:GLU:HA	1.72	0.71
4:C:663:LYS:CD	4:C:664:GLY:H	2.03	0.71
1:E:15:DC:H2"	1:E:16:DC:H5'	1.71	0.71
4:C:291:ARG:HB2	7:C:3192:HOH:O	1.89	0.71
4:C:797:TRP:CZ2	4:C:801:LYS:HG3	2.26	0.71
4:C:551:ARG:HD2	7:C:3087:HOH:O	1.91	0.71
4:B:423:ARG:CG	4:B:781:ASN:ND2	2.53	0.71
4:B:609:VAL:O	4:B:611:LEU:N	2.23	0.71
4:A:666:MET:N	4:A:666:MET:SD	2.64	0.71
4:C:557:ARG:HB2	4:C:562:LEU:HD12	1.70	0.71
4:B:623:TYR:HA	4:B:666:MET:HE1	1.71	0.71
4:B:236:VAL:HG21	4:B:239:GLN:NE2	2.06	0.71
4:B:274:PRO:HD3	4:B:415:TRP:CH2	2.25	0.71
4:B:454:LYS:HB2	7:B:3020:HOH:O	1.90	0.71
4:A:457:TYR:CE1	4:A:521:VAL:HG11	2.25	0.71
4:B:308:TYR:CE2	4:B:734:PRO:HG2	2.25	0.71
4:B:617:ALA:HB2	4:B:676:TYR:OH	1.91	0.71
4:A:5:ASN:ND2	4:A:7:ALA:HB3	2.06	0.71
4:D:541:SER:HA	4:D:544:GLN:HE21	1.53	0.71
4:C:40:GLU:CD	4:C:286:TYR:HB3	2.10	0.71
4:B:100:PRO:HG2	4:B:103:PHE:HB2	1.71	0.71
4:A:351:ASP:HA	7:A:3222:HOH:O	1.89	0.71
4:D:231:ARG:CG	4:D:234:ALA:HB2	2.21	0.71
4:A:423:ARG:NH2	4:A:784:HIS:CG	2.59	0.71
4:C:828:VAL:O	4:C:831:THR:HG22	1.89	0.71
4:D:324:GLN:HG3	4:D:417:PRO:HA	1.73	0.71
1:H:14:DG:H2"	1:H:15:DC:O5'	1.90	0.71
4:B:11:PHE:CZ	4:B:44:TYR:HB3	2.24	0.71
4:D:257:ARG:O	4:D:261:LEU:HB2	1.91	0.71
4:C:201:TRP:O	4:C:204:TRP:HB2	1.90	0.71
4:B:564:SER:OG	4:B:566:THR:N	2.20	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:720:ARG:NH1	4:A:720:ARG:HG2	2.03	0.71
4:B:816:THR:HG21	4:B:820:ASP:HB3	1.73	0.71
4:D:269:GLN:HE22	4:D:407:LYS:HE2	1.56	0.71
4:A:643:GLU:HB2	7:A:3076:HOH:O	1.90	0.71
4:A:786:GLN:HA	4:A:786:GLN:NE2	2.03	0.71
4:A:828:VAL:HB	4:A:883:ALA:HA	1.73	0.71
4:A:109:ILE:CD1	4:A:145:ILE:O	2.39	0.71
4:D:435:GLN:HA	4:D:810:ILE:HD11	1.72	0.71
4:B:390:ALA:O	4:B:393:SER:N	2.24	0.71
4:D:772:HIS:O	4:D:773:LYS:C	2.28	0.71
4:A:786:GLN:OE1	4:A:841:VAL:HG11	1.91	0.70
4:C:553:GLU:HA	4:C:870:LEU:HD12	1.73	0.70
4:D:428:ALA:H	4:D:435:GLN:NE2	1.89	0.70
4:D:116:TYR:OH	4:D:752:LEU:HD22	1.90	0.70
4:B:213:GLY:O	4:B:217:ILE:HG13	1.91	0.70
4:A:161:HIS:O	4:A:164:LYS:HG2	1.90	0.70
4:A:633:SER:HB2	7:A:3199:HOH:O	1.91	0.70
4:A:810:ILE:HB	4:A:813:SER:HB3	1.72	0.70
4:B:849:PHE:O	4:B:852:GLN:N	2.22	0.70
4:C:120:LYS:HG3	4:C:752:LEU:HD11	1.74	0.70
4:A:827:ALA:O	4:A:830:GLU:HB2	1.91	0.70
4:D:810:ILE:O	4:D:810:ILE:HG22	1.89	0.70
4:B:645:GLY:O	4:B:647:ARG:N	2.24	0.70
4:C:338:ALA:HB2	4:C:509:PHE:CE1	2.20	0.70
4:D:264:ILE:CG2	4:D:292:ARG:HB2	2.21	0.70
4:B:312:TYR:HA	7:B:3069:HOH:O	1.89	0.70
4:A:281:ILE:HG12	4:A:309:GLU:HA	1.73	0.70
4:A:720:ARG:O	4:A:721:LYS:O	2.09	0.70
4:B:777:GLY:O	4:B:780:PRO:HD2	1.92	0.70
4:B:475:PHE:O	4:B:477:GLU:N	2.25	0.70
4:A:89:PHE:HA	4:A:103:PHE:CE1	2.26	0.70
4:D:29:GLY:HA2	7:D:3080:HOH:O	1.91	0.70
4:A:158:GLU:HG2	4:A:195:LEU:HD23	1.74	0.70
4:A:480:LYS:O	4:A:484:GLU:HG3	1.91	0.70
4:C:40:GLU:OE2	4:C:286:TYR:HD1	1.74	0.70
4:D:221:ILE:HG12	4:D:227:VAL:HG23	1.73	0.70
4:C:572:GLY:O	4:C:575:ALA:HB3	1.91	0.70
4:C:67:ASN:O	4:C:69:ALA:N	2.25	0.70
1:E:12:DT:H2"	1:E:13:DC:H5"	1.71	0.70
4:D:739:TYR:OH	4:D:781:ASN:OD1	2.10	0.70
4:D:432:PHE:CE1	4:D:444:LEU:HD11	2.26	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:306:MET:O	4:D:308:TYR:N	2.25	0.70
4:C:330:ILE:HG13	4:C:408:PHE:O	1.91	0.70
4:A:525:GLY:O	4:A:527:SER:N	2.24	0.70
4:C:703:ALA:HB2	4:C:778:ILE:HG12	1.73	0.70
4:D:36:GLN:CD	4:D:273:VAL:HG22	2.12	0.70
4:D:268:PHE:CD2	4:D:429:VAL:HG12	2.26	0.70
4:C:333:LYS:HD3	4:C:516:PHE:CD2	2.22	0.70
4:A:78:LEU:N	4:A:79:PRO:HD2	2.06	0.70
4:B:326:THR:HA	7:B:3162:HOH:O	1.90	0.70
4:B:632:ARG:HD3	6:B:2001:APC:N7	2.07	0.70
4:A:16:LEU:HA	4:A:37:LEU:HD22	1.73	0.70
4:A:4:ILE:HD12	7:A:3067:HOH:O	1.92	0.70
4:B:868:GLY:C	4:B:869:ASN:HD22	1.95	0.70
4:D:14:ILE:HG23	4:D:288:ALA:HB1	1.74	0.70
4:C:105:PHE:HE1	4:C:208:ASP:HB3	1.56	0.70
4:A:647:ARG:HG3	4:A:674:ALA:O	1.92	0.70
4:D:402:LEU:HD23	4:D:443:LEU:CD1	2.22	0.70
4:A:611:LEU:HD12	4:A:669:GLN:HB2	1.74	0.70
4:C:270:PRO:HG3	4:C:430:SER:OG	1.92	0.70
4:C:551:ARG:HH11	4:C:551:ARG:CG	2.05	0.70
4:D:882:PHE:O	4:D:883:ALA:HB3	1.92	0.70
4:B:544:GLN:HG3	4:B:561:LEU:HD11	1.74	0.70
4:B:734:PRO:HG2	4:B:734:PRO:O	1.91	0.70
4:B:416:PHE:CE1	4:B:433:ASN:HA	2.26	0.70
4:B:557:ARG:HD3	7:B:3119:HOH:O	1.91	0.70
2:I:1:G:H2'	2:I:2:C:C6	2.27	0.70
1:K:11:DA:C2	1:K:12:DT:C4	2.80	0.69
4:D:779:ALA:O	4:D:783:VAL:HG22	1.90	0.69
4:B:264:ILE:O	4:B:266:PRO:HD3	1.92	0.69
4:B:298:ARG:HE	4:B:419:ASN:HB3	1.57	0.69
4:B:647:ARG:O	4:B:648:GLN:C	2.31	0.69
4:B:788:GLY:O	4:B:792:ARG:HG3	1.92	0.69
4:D:71:LYS:HD3	7:D:3030:HOH:O	1.92	0.69
4:A:746:ARG:HH12	4:A:754:GLN:H	1.37	0.69
4:A:273:VAL:O	4:A:273:VAL:HG23	1.91	0.69
4:B:308:TYR:HA	4:B:311:VAL:CG2	2.21	0.69
4:C:322:ILE:HG13	7:C:3131:HOH:O	1.91	0.69
4:A:721:LYS:HD3	4:A:722:ARG:N	2.07	0.69
4:D:324:GLN:O	4:D:324:GLN:HG2	1.91	0.69
4:D:471:ASP:O	4:D:472:LYS:HD2	1.92	0.69
4:C:570:ILE:O	4:C:574:VAL:HG23	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:278:TRP:HA	7:B:3014:HOH:O	1.92	0.69
4:A:14:ILE:HD12	4:A:14:ILE:N	2.07	0.69
4:A:275:PRO:HD3	4:A:415:TRP:HB3	1.74	0.69
4:D:573:ILE:HA	4:D:576:LYS:HD2	1.73	0.69
4:B:307:ARG:HD3	4:B:736:TRP:CE3	2.28	0.69
4:B:824:LEU:O	4:B:828:VAL:HG23	1.92	0.69
4:B:390:ALA:C	4:B:392:LYS:N	2.46	0.69
4:A:19:ILE:HG23	4:A:20:PRO:HD2	1.73	0.69
4:A:452:ILE:CD1	4:A:457:TYR:HB2	2.22	0.69
4:B:473:VAL:CG1	4:B:477:GLU:HB2	2.23	0.69
4:B:801:LYS:C	4:B:801:LYS:HD3	2.13	0.69
4:C:29:GLY:HA3	7:C:3129:HOH:O	1.93	0.69
4:B:829:ARG:NH2	4:B:882:PHE:CA	2.54	0.69
4:B:512:LEU:O	4:B:515:CYS:N	2.25	0.69
4:D:158:GLU:HA	4:D:195:LEU:HD22	1.75	0.69
4:A:474:PRO:HG2	4:A:477:GLU:HG3	1.75	0.69
4:C:308:TYR:HE2	4:C:734:PRO:HG2	1.57	0.69
4:D:274:PRO:HD3	4:D:415:TRP:CH2	2.27	0.69
1:H:12:DT:H4'	4:B:423:ARG:NE	2.08	0.69
4:B:418:TYR:CE2	4:B:428:ALA:HB2	2.18	0.69
4:B:549:MET:CE	4:B:841:VAL:HG21	2.22	0.69
4:D:120:LYS:HD2	4:D:752:LEU:HD11	1.73	0.69
4:D:210:ILE:O	4:D:214:VAL:HG23	1.93	0.69
4:D:657:PRO:O	4:D:661:SER:HB2	1.92	0.69
4:C:25:ALA:HA	4:C:29:GLY:O	1.92	0.69
4:A:236:VAL:HG11	4:A:239:GLN:CD	2.13	0.69
4:A:6:ILE:O	4:A:8:LYS:N	2.22	0.69
1:K:7:DC:H2"	1:K:8:DG:O5'	1.91	0.69
4:D:206:LYS:HD3	4:D:206:LYS:H	1.57	0.69
4:B:423:ARG:HH12	4:B:784:HIS:CB	2.06	0.69
4:D:337:VAL:HG21	4:D:512:LEU:HD21	1.74	0.69
4:B:390:ALA:O	4:B:392:LYS:N	2.25	0.69
4:B:132:THR:HG21	7:B:3161:HOH:O	1.92	0.69
4:A:311:VAL:HG12	4:A:312:TYR:N	2.08	0.69
4:A:526:LEU:CD1	4:A:526:LEU:H	2.06	0.69
4:B:452:ILE:CG2	4:B:453:GLY:N	2.33	0.69
4:B:247:ALA:HB3	4:B:250:TYR:HB2	1.76	0.69
4:D:333:LYS:NZ	4:D:516:PHE:HB3	2.08	0.69
1:H:3:DG:N2	7:H:948:HOH:O	2.25	0.69
4:A:665:LEU:HD12	4:A:665:LEU:H	1.58	0.69
4:A:308:TYR:CE2	4:A:734:PRO:HG2	2.21	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:428:ALA:H	4:C:435:GLN:NE2	1.90	0.68
4:B:308:TYR:HA	4:B:311:VAL:HG23	1.75	0.68
4:D:470:VAL:HG12	4:D:473:VAL:CG1	2.23	0.68
4:B:109:ILE:N	4:B:109:ILE:HD12	2.08	0.68
4:D:390:ALA:HB1	4:D:394:ARG:HH21	1.58	0.68
4:A:275:PRO:HD3	4:A:415:TRP:CB	2.22	0.68
4:C:840:ASP:O	4:C:842:LEU:N	2.27	0.68
4:A:404:GLN:NE2	4:A:404:GLN:HA	2.08	0.68
4:A:59:LEU:HD23	4:A:64:VAL:CG2	2.23	0.68
4:A:4:ILE:HD11	4:A:256:THR:OG1	1.92	0.68
4:A:668:THR:HG22	4:A:669:GLN:CD	2.14	0.68
4:A:236:VAL:HG11	4:A:239:GLN:CG	2.24	0.68
4:D:433:ASN:HB2	4:D:434:PRO:CD	2.23	0.68
4:B:571:TYR:HE1	7:B:3067:HOH:O	1.75	0.68
4:B:301:SER:O	4:B:304:ALA:N	2.27	0.68
4:C:335:LEU:HD11	4:C:406:ASN:OD1	1.94	0.68
4:B:261:LEU:O	4:B:263:GLY:N	2.27	0.68
4:A:11:PHE:CE1	4:A:44:TYR:HB3	2.29	0.68
4:B:840:ASP:O	4:B:842:LEU:N	2.27	0.68
4:A:551:ARG:HB2	4:A:868:GLY:H	1.58	0.68
4:D:326:THR:O	4:D:415:TRP:HD1	1.76	0.68
4:B:730:PRO:CD	4:B:786:GLN:HE21	2.06	0.68
4:B:720:ARG:NH1	4:B:720:ARG:HG2	1.92	0.68
4:D:437:ASN:HD21	4:D:440:THR:H	1.41	0.68
4:D:55:PHE:HA	4:D:58:GLN:HG3	1.75	0.68
4:B:801:LYS:HD3	4:B:801:LYS:O	1.94	0.68
4:B:31:ARG:HB3	4:B:31:ARG:HH11	1.59	0.68
4:A:655:ILE:HD12	4:A:674:ALA:HB2	1.76	0.68
1:E:12:DT:H5"	4:A:422:TRP:CH2	2.29	0.68
4:C:40:GLU:OE1	4:C:286:TYR:HB3	1.92	0.68
4:B:301:SER:O	4:B:304:ALA:HB3	1.94	0.68
4:C:432:PHE:CZ	4:C:444:LEU:HD21	2.28	0.68
4:C:465:ALA:O	4:C:470:VAL:HG23	1.94	0.68
4:A:486:HIS:CD2	4:A:518:TYR:CE1	2.80	0.68
4:D:433:ASN:HB2	4:D:434:PRO:HD2	1.74	0.68
4:B:354:ALA:HA	7:B:3118:HOH:O	1.94	0.68
4:C:17:ALA:HB2	7:C:3201:HOH:O	1.92	0.68
4:B:706:LEU:HD11	4:B:849:PHE:HD2	1.58	0.68
4:D:233:ASN:HD22	4:D:239:GLN:NE2	1.92	0.68
4:B:564:SER:OG	4:B:565:GLU:N	2.25	0.68
4:C:173:ARG:CZ	4:C:182:PHE:HB2	2.23	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:159:ALA:O	4:C:163:LYS:HB2	1.93	0.68
4:C:134:VAL:HG12	4:C:242:GLU:O	1.94	0.68
4:A:552:ASP:OD2	7:A:3223:HOH:O	2.10	0.68
4:C:785:SER:HA	7:C:3159:HOH:O	1.93	0.67
4:B:299:THR:HG21	4:B:305:LEU:HA	1.76	0.67
4:C:338:ALA:C	4:C:340:VAL:N	2.46	0.67
4:C:340:VAL:O	4:C:342:THR:N	2.27	0.67
4:A:404:GLN:HE21	4:A:404:GLN:CA	2.02	0.67
4:C:514:PHE:CG	4:C:514:PHE:O	2.47	0.67
4:C:475:PHE:CE2	4:C:879:ASP:HB3	2.29	0.67
4:D:100:PRO:HG2	4:D:103:PHE:CB	2.23	0.67
4:D:55:PHE:CE1	4:D:59:LEU:HD21	2.30	0.67
4:D:161:HIS:O	4:D:164:LYS:HG2	1.94	0.67
4:C:146:GLU:OE2	4:C:201:TRP:HB3	1.94	0.67
4:A:631:LYS:NZ	6:A:2000:APC:C3A	2.49	0.67
4:D:829:ARG:NH1	4:D:829:ARG:HG3	2.07	0.67
4:D:718:ILE:HD12	7:D:3025:HOH:O	1.94	0.67
4:B:418:TYR:HD2	4:B:428:ALA:HA	1.59	0.67
4:B:571:TYR:OH	4:B:635:MET:HE3	1.94	0.67
4:D:333:LYS:HB3	4:D:516:PHE:CD2	2.28	0.67
4:A:748:ASN:HD22	4:A:751:PHE:H	1.40	0.67
4:A:526:LEU:N	4:A:526:LEU:CD1	2.57	0.67
4:B:623:TYR:HA	4:B:666:MET:CE	2.23	0.67
4:B:552:ASP:C	4:B:552:ASP:OD1	2.32	0.67
4:C:866:ALA:HB1	7:C:3057:HOH:O	1.94	0.67
4:A:744:GLN:HA	4:A:756:ARG:NH2	2.09	0.67
4:C:50:ARG:HG2	4:C:50:ARG:NH1	2.07	0.67
4:A:464:GLY:CA	4:A:514:PHE:CE2	2.78	0.67
4:A:551:ARG:NH2	4:A:872:LEU:HD11	2.10	0.67
4:A:423:ARG:NH2	4:A:784:HIS:CB	2.58	0.67
4:B:418:TYR:HD2	4:B:427:TYR:O	1.78	0.67
1:H:12:DT:O4'	4:B:423:ARG:NH2	2.27	0.67
4:B:269:GLN:NE2	4:B:407:LYS:NZ	2.42	0.67
4:C:475:PHE:HE2	4:C:879:ASP:HB3	1.58	0.67
4:D:855:GLU:O	4:D:858:LEU:HD12	1.94	0.67
4:A:78:LEU:HD21	4:A:116:TYR:HB2	1.74	0.67
1:N:14:DG:N7	7:N:81:HOH:O	2.27	0.67
4:D:330:ILE:HD11	4:D:405:ALA:HA	1.75	0.67
4:C:32:LEU:HB2	7:C:3157:HOH:O	1.94	0.67
4:A:630:THR:O	7:A:3199:HOH:O	2.12	0.67
4:C:59:LEU:CD2	4:C:64:VAL:HG13	2.24	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:510:CYS:O	4:A:513:ALA:N	2.26	0.67
4:A:495:SER:HB3	4:A:498:GLU:HG3	1.77	0.67
4:C:2:ASN:O	7:C:3169:HOH:O	2.11	0.67
4:C:631:LYS:HZ1	6:C:2002:APC:C3A	2.07	0.67
4:B:449:GLY:HA3	4:B:529:ASN:HD21	1.58	0.67
4:A:109:ILE:HG13	4:A:149:ALA:HB2	1.75	0.67
4:C:24:LEU:HD21	4:C:287:TRP:CE2	2.29	0.67
4:B:829:ARG:HG3	4:B:829:ARG:NH1	2.05	0.67
4:A:428:ALA:HB3	4:A:433:ASN:HD22	1.57	0.67
4:C:330:ILE:CG1	4:C:408:PHE:O	2.43	0.67
4:D:303:LYS:HG3	4:D:304:ALA:N	2.10	0.67
4:C:632:ARG:NH2	6:C:2002:APC:H5'1	2.08	0.67
4:A:802:TYR:CD2	4:A:802:TYR:N	2.61	0.67
4:D:778:ILE:CG2	4:D:779:ALA:N	2.57	0.67
4:D:797:TRP:HE1	4:D:802:TYR:HE2	1.41	0.67
4:B:794:THR:OG1	4:B:831:THR:HG21	1.92	0.67
4:A:716:GLY:HA3	7:A:3184:HOH:O	1.93	0.67
4:A:849:PHE:HD2	4:A:853:LEU:HD21	1.60	0.67
4:C:338:ALA:C	4:C:340:VAL:H	1.96	0.67
4:C:534:LEU:HD12	4:C:821:ALA:CB	2.25	0.67
4:A:518:TYR:O	4:A:518:TYR:CD1	2.48	0.67
4:D:656:GLN:N	4:D:657:PRO:HD2	2.10	0.67
4:C:279:THR:HG22	7:C:3038:HOH:O	1.95	0.67
4:D:769:ILE:H	4:D:769:ILE:HD12	1.60	0.67
4:D:19:ILE:HD12	4:D:20:PRO:HD2	1.77	0.67
4:B:449:GLY:CA	4:B:529:ASN:HD21	2.08	0.67
4:B:64:VAL:HG21	4:B:127:THR:HG21	1.76	0.67
4:C:308:TYR:CZ	4:C:733:PHE:HE2	2.12	0.67
4:B:423:ARG:HH11	4:B:423:ARG:CB	2.08	0.67
4:C:349:VAL:HG11	4:C:508:PRO:HG3	1.77	0.67
4:B:77:LEU:CD1	4:B:224:THR:HG21	2.25	0.67
4:A:746:ARG:HG3	4:A:756:ARG:HB2	1.77	0.67
4:C:9:ASN:HA	4:C:12:SER:HB3	1.76	0.67
4:B:549:MET:HE2	4:B:841:VAL:HG21	1.76	0.67
4:B:720:ARG:HH11	4:B:720:ARG:CG	2.03	0.67
4:C:77:LEU:C	4:C:79:PRO:HD2	2.15	0.67
4:A:428:ALA:HB3	4:A:433:ASN:ND2	2.09	0.67
4:A:843:ALA:O	4:A:846:TYR:N	2.27	0.67
4:B:254:ILE:HG22	4:B:255:ALA:N	2.10	0.67
4:C:707:ALA:O	4:C:722:ARG:HB3	1.95	0.67
4:A:786:GLN:CA	4:A:786:GLN:HE21	2.03	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:635:MET:HE1	6:D:2003:APC:H3'	1.77	0.66
4:D:272:VAL:O	4:D:415:TRP:CZ3	2.47	0.66
4:D:39:LEU:HD22	4:D:272:VAL:HG23	1.76	0.66
4:C:443:LEU:O	4:C:444:LEU:HD23	1.95	0.66
4:C:460:LEU:HA	4:C:534:LEU:CD2	2.24	0.66
4:C:105:PHE:CE1	4:C:208:ASP:HB3	2.30	0.66
4:C:706:LEU:HD22	4:C:725:VAL:CG1	2.24	0.66
4:B:671:ASN:O	4:B:674:ALA:HB3	1.96	0.66
4:B:850:ALA:O	4:B:852:GLN:N	2.28	0.66
4:A:46:MET:HG2	7:A:3162:HOH:O	1.94	0.66
4:B:731:ASP:HB3	4:B:789:SER:OG	1.96	0.66
4:D:89:PHE:HZ	4:D:106:LEU:HB3	1.60	0.66
4:A:669:GLN:O	4:A:670:PRO:C	2.33	0.66
4:A:548:ALA:C	4:A:550:LEU:H	1.97	0.66
4:D:269:GLN:HG2	4:D:408:PHE:HZ	1.59	0.66
4:B:35:GLU:O	4:B:38:ALA:HB3	1.96	0.66
4:A:881:ALA:O	4:A:883:ALA:OXT	2.14	0.66
4:C:551:ARG:CD	4:C:872:LEU:HD21	2.24	0.66
4:D:829:ARG:HH22	4:D:882:PHE:HA	1.61	0.66
4:D:109:ILE:HD13	4:D:114:VAL:HG22	1.76	0.66
4:D:744:GLN:HG2	4:D:756:ARG:HB3	1.75	0.66
4:A:308:TYR:OH	4:A:734:PRO:O	2.14	0.66
4:A:540:CYS:O	4:A:541:SER:C	2.33	0.66
4:A:828:VAL:HG23	4:A:829:ARG:N	2.06	0.66
4:D:275:PRO:HD2	7:D:3108:HOH:O	1.94	0.66
4:D:560:ASN:OD1	4:D:568:GLN:HB2	1.95	0.66
4:B:424:GLY:O	4:B:792:ARG:NH1	2.29	0.66
4:B:233:ASN:HD22	4:B:239:GLN:CD	1.97	0.66
4:C:105:PHE:O	4:C:107:GLN:N	2.29	0.66
4:C:50:ARG:HG2	4:C:50:ARG:HH11	1.60	0.66
4:C:50:ARG:CG	4:C:50:ARG:HH11	2.08	0.66
4:D:84:ARG:HD3	4:D:84:ARG:O	1.94	0.66
4:A:574:VAL:HG11	4:A:685:VAL:CG1	2.25	0.66
4:A:769:ILE:HD12	4:A:769:ILE:H	1.60	0.66
4:B:437:ASN:HB2	7:B:3149:HOH:O	1.95	0.66
4:A:418:TYR:HD2	4:A:426:VAL:HG12	1.60	0.66
4:A:44:TYR:CE2	4:A:266:PRO:HB3	2.31	0.66
4:C:36:GLN:HG3	4:C:273:VAL:HG22	1.78	0.66
4:C:286:TYR:CZ	4:C:417:PRO:HG3	2.31	0.66
4:C:553:GLU:HG2	4:C:554:VAL:H	1.60	0.66
4:C:562:LEU:HD21	4:C:870:LEU:HG	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:402:LEU:HD23	4:D:443:LEU:HD11	1.77	0.66
4:A:157:LEU:HD23	7:A:3133:HOH:O	1.95	0.66
4:B:525:GLY:O	4:B:527:SER:N	2.28	0.66
4:A:30:GLU:HB3	4:A:34:ARG:NH2	2.10	0.66
4:C:605:ILE:HG23	7:C:3098:HOH:O	1.96	0.66
4:A:463:HIS:HD2	7:A:3167:HOH:O	1.77	0.66
4:A:459:TRP:HE1	4:A:822:ALA:HA	1.61	0.66
4:A:869:ASN:ND2	4:A:869:ASN:N	2.44	0.66
4:C:553:GLU:CD	4:C:553:GLU:H	1.99	0.66
4:B:616:LEU:O	4:B:619:GLN:N	2.29	0.66
4:D:337:VAL:O	4:D:341:ILE:HG12	1.96	0.66
4:B:336:ALA:O	4:B:340:VAL:HG23	1.95	0.66
4:A:119:ILE:O	4:A:122:THR:HB	1.95	0.66
4:D:574:VAL:O	4:D:578:VAL:HG23	1.95	0.66
4:D:23:THR:O	4:D:27:HIS:HB2	1.96	0.66
4:A:485:ASN:HB3	4:A:488:ASN:HD22	1.61	0.66
4:A:563:PRO:HB3	4:A:877:GLU:O	1.96	0.66
4:A:281:ILE:HD11	4:A:309:GLU:N	2.11	0.66
4:D:425:ARG:HB3	4:D:427:TYR:HE1	1.61	0.66
4:B:825:PHE:O	4:B:829:ARG:NH1	2.29	0.66
1:K:12:DT:C2	1:K:13:DC:C5	2.83	0.66
4:B:730:PRO:CD	4:B:786:GLN:NE2	2.59	0.66
4:B:475:PHE:HA	4:B:478:ARG:HD2	1.78	0.66
4:B:291:ARG:CG	7:B:3037:HOH:O	2.44	0.66
4:B:536:PHE:HB3	4:B:882:PHE:HB3	1.76	0.65
4:A:80:LYS:HD3	4:A:224:THR:HG22	1.76	0.65
4:B:273:VAL:O	4:B:274:PRO:C	2.32	0.65
4:B:173:ARG:HH11	4:B:182:PHE:HD1	1.44	0.65
4:A:475:PHE:HD2	7:A:3202:HOH:O	1.79	0.65
4:C:551:ARG:HH11	4:C:551:ARG:HG3	1.61	0.65
4:D:718:ILE:CD1	7:D:3025:HOH:O	2.43	0.65
4:B:639:TYR:HE1	7:B:3084:HOH:O	1.79	0.65
4:B:726:HIS:CD2	4:B:735:VAL:O	2.49	0.65
4:B:37:LEU:N	4:B:37:LEU:HD12	2.09	0.65
4:C:340:VAL:O	4:C:341:ILE:C	2.33	0.65
4:C:182:PHE:O	4:C:186:VAL:HG23	1.97	0.65
4:A:737:GLN:O	4:A:774:GLN:NE2	2.29	0.65
4:C:551:ARG:NH2	4:C:872:LEU:HD11	2.11	0.65
4:B:428:ALA:H	4:B:435:GLN:HE22	1.43	0.65
4:B:330:ILE:HD12	4:B:405:ALA:HB1	1.78	0.65
4:D:508:PRO:O	4:D:511:PHE:N	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:159:ALA:O	4:B:160:LYS:C	2.32	0.65
4:D:106:LEU:HA	4:D:109:ILE:HD11	1.78	0.65
4:A:433:ASN:C	4:A:433:ASN:OD1	2.34	0.65
4:D:629:VAL:HG13	4:D:654:THR:HG21	1.77	0.65
4:D:252:GLU:O	4:D:255:ALA:HB3	1.97	0.65
4:D:553:GLU:OE1	4:D:869:ASN:HB2	1.97	0.65
4:A:24:LEU:HD21	4:A:287:TRP:CE2	2.31	0.65
4:C:298:ARG:HB2	4:C:421:ASP:HA	1.79	0.65
4:D:796:VAL:HA	7:D:3013:HOH:O	1.96	0.65
4:B:780:PRO:HD2	4:B:781:ASN:H	1.61	0.65
4:C:64:VAL:HG21	4:C:127:THR:HG21	1.77	0.65
4:A:668:THR:HG22	4:A:669:GLN:NE2	2.11	0.65
4:B:266:PRO:HG2	4:B:268:PHE:CZ	2.31	0.65
4:B:663:LYS:HE2	4:B:666:MET:HE1	1.77	0.65
4:B:790:HIS:CE1	4:B:831:THR:HG23	2.30	0.65
4:B:236:VAL:HG21	4:B:239:GLN:HE21	1.60	0.65
4:D:236:VAL:HG21	4:D:239:GLN:NE2	2.11	0.65
4:B:552:ASP:O	4:B:552:ASP:OD1	2.14	0.65
4:B:705:LEU:O	4:B:707:ALA:N	2.29	0.65
1:E:5:DA:C2	3:G:7:DT:O2	2.50	0.65
4:A:3:THR:HB	4:A:52:ARG:NH1	2.12	0.65
4:C:631:LYS:HE2	4:C:635:MET:SD	2.36	0.65
4:A:632:ARG:O	4:A:633:SER:C	2.34	0.65
4:A:292:ARG:H	4:A:293:PRO:HD3	1.62	0.65
4:A:141:ILE:O	4:A:145:ILE:HG12	1.96	0.65
4:B:728:VAL:O	7:B:3081:HOH:O	2.15	0.65
1:N:16:DC:H2"	1:N:17:DG:O5'	1.97	0.65
4:B:257:ARG:HG2	4:B:257:ARG:HH11	1.60	0.65
4:D:9:ASN:HA	4:D:12:SER:HB2	1.79	0.65
4:C:551:ARG:NH2	4:C:836:TYR:O	2.30	0.65
1:K:13:DC:H2"	1:K:14:DG:H5'	1.78	0.65
4:B:446:LEU:HD12	4:B:817:ILE:CG2	2.27	0.65
4:B:540:CYS:O	4:B:541:SER:C	2.35	0.65
4:D:475:PHE:N	4:D:476:PRO:HD2	2.11	0.65
4:D:109:ILE:HG12	4:D:145:ILE:HG22	1.79	0.65
4:C:801:LYS:C	4:C:801:LYS:HD3	2.17	0.65
3:G:7:DT:H2"	3:G:8:DC:C6	2.31	0.65
4:A:590:THR:HG1	4:A:613:THR:HG1	1.41	0.65
4:B:119:ILE:N	4:B:119:ILE:HD13	2.11	0.65
4:D:428:ALA:H	4:D:435:GLN:HE21	1.43	0.65
4:A:154:ILE:HG23	4:A:190:MET:HE2	1.76	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:218:GLU:O	4:D:222:GLU:HB2	1.95	0.65
4:A:793:LYS:HA	4:A:796:VAL:CG2	2.27	0.65
4:B:631:LYS:CE	6:B:2001:APC:H3A2	2.26	0.65
4:B:807:PHE:HA	4:B:815:GLY:O	1.96	0.65
4:B:14:ILE:HD12	4:B:14:ILE:N	2.08	0.65
4:D:340:VAL:O	4:D:341:ILE:C	2.35	0.65
4:C:474:PRO:HB2	4:C:476:PRO:HD2	1.78	0.65
4:A:19:ILE:CG2	7:A:3120:HOH:O	2.45	0.65
4:A:744:GLN:HA	4:A:756:ARG:CZ	2.27	0.65
4:A:221:ILE:HG23	4:A:227:VAL:O	1.97	0.65
1:K:17:DG:H2"	1:K:18:DC:C5	2.32	0.65
4:D:737:GLN:NE2	4:D:778:ILE:HA	2.06	0.65
4:B:296:LEU:O	4:B:296:LEU:CG	2.44	0.65
4:A:16:LEU:HD22	4:A:38:ALA:HA	1.77	0.65
4:C:595:VAL:HG21	7:C:3085:HOH:O	1.97	0.65
4:C:346:HIS:HA	4:C:395:ARG:HH11	1.61	0.65
4:B:122:THR:CG2	4:B:226:MET:CE	2.74	0.64
4:C:727:TRP:CE3	4:C:735:VAL:HG13	2.32	0.64
4:B:559:VAL:HG23	4:B:559:VAL:O	1.98	0.64
4:B:435:GLN:CG	4:B:810:ILE:HG23	2.20	0.64
4:B:138:ALA:HB2	4:B:214:VAL:HG13	1.79	0.64
4:D:564:SER:O	7:D:3040:HOH:O	2.14	0.64
4:A:26:ASP:HB2	7:A:3183:HOH:O	1.97	0.64
4:A:421:ASP:O	4:A:422:TRP:C	2.31	0.64
4:B:281:ILE:CG2	4:B:282:THR:HG23	2.27	0.64
4:B:828:VAL:CG1	4:B:883:ALA:HA	2.28	0.64
4:B:33:ALA:O	4:B:37:LEU:HD13	1.97	0.64
4:D:134:VAL:H	4:D:243:THR:HA	1.62	0.64
4:A:40:GLU:HG2	4:A:286:TYR:HD1	1.62	0.64
4:D:426:VAL:HG21	4:D:791:LEU:HD21	1.78	0.64
4:A:817:ILE:HB	4:A:818:PRO:HD2	1.79	0.64
4:B:449:GLY:C	4:B:529:ASN:HD21	2.01	0.64
4:C:837:GLU:CG	4:C:872:LEU:HD12	2.27	0.64
4:D:471:ASP:C	4:D:472:LYS:HD2	2.17	0.64
4:A:78:LEU:N	4:A:79:PRO:CD	2.60	0.64
4:A:50:ARG:NH1	4:A:50:ARG:HG2	2.11	0.64
4:C:746:ARG:HD3	4:C:755:PHE:O	1.97	0.64
4:D:326:THR:O	4:D:415:TRP:CD1	2.50	0.64
4:B:702:ALA:O	4:B:706:LEU:HD12	1.96	0.64
4:B:37:LEU:CD1	4:B:37:LEU:H	2.10	0.64
4:D:438:ASP:OD2	4:D:508:PRO:HG2	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:402:LEU:CD2	4:D:443:LEU:HD11	2.28	0.64
4:C:342:THR:HG22	4:C:348:PRO:CG	2.24	0.64
4:D:471:ASP:OD1	4:D:472:LYS:HD3	1.97	0.64
1:E:14:DG:H2'	1:E:15:DC:C5	2.31	0.64
4:B:275:PRO:O	4:B:277:PRO:HD3	1.97	0.64
4:B:58:GLN:HG3	4:B:67:ASN:HD22	1.63	0.64
4:D:269:GLN:HG2	4:D:408:PHE:CZ	2.33	0.64
4:C:400:PHE:CE1	4:C:431:MET:HE2	2.32	0.64
4:A:476:PRO:O	4:A:479:ILE:N	2.28	0.64
4:A:274:PRO:HG3	4:A:415:TRP:CE2	2.32	0.64
4:C:433:ASN:HA	7:C:3164:HOH:O	1.93	0.64
4:B:473:VAL:CG1	4:B:474:PRO:N	2.59	0.64
4:B:486:HIS:CE1	4:B:490:MET:HG3	2.32	0.64
4:B:231:ARG:CG	4:B:234:ALA:HB2	2.27	0.64
4:A:257:ARG:HG2	4:A:257:ARG:HH11	1.62	0.64
4:B:446:LEU:HB2	4:B:531:SER:O	1.98	0.64
4:B:779:ALA:N	4:B:780:PRO:CD	2.60	0.64
4:B:423:ARG:NH1	4:B:784:HIS:HB3	2.13	0.64
4:B:720:ARG:CG	4:B:720:ARG:NH1	2.59	0.64
4:B:46:MET:HE1	4:B:269:GLN:HE22	1.61	0.64
4:B:401:MET:HE3	4:B:440:THR:HG21	1.80	0.64
4:C:475:PHE:N	4:C:476:PRO:HD2	2.13	0.64
4:D:135:GLN:HG3	7:D:3160:HOH:O	1.97	0.64
4:D:572:GLY:O	4:D:575:ALA:N	2.30	0.64
2:F:7:A:H2'	2:F:8:U:H6	1.62	0.64
4:A:545:HIS:CE1	4:A:787:ASP:HA	2.33	0.64
4:B:492:CYS:SG	4:B:502:TRP:CD1	2.90	0.64
4:D:281:ILE:HD12	4:D:317:TYR:OH	1.96	0.64
4:B:5:ASN:ND2	4:B:7:ALA:N	2.46	0.64
4:A:10:ASP:O	4:A:13:ASP:HB2	1.98	0.64
4:D:421:ASP:O	4:D:423:ARG:N	2.31	0.64
4:B:469:GLY:O	4:B:471:ASP:N	2.31	0.64
4:A:502:TRP:CD1	4:A:512:LEU:CD1	2.81	0.64
4:D:161:HIS:HE1	7:D:3114:HOH:O	1.80	0.64
4:C:163:LYS:HB3	4:C:164:LYS:HZ3	1.63	0.64
4:C:423:ARG:HE	4:C:781:ASN:HD22	1.45	0.64
4:D:734:PRO:O	4:D:734:PRO:HG2	1.97	0.64
4:C:744:GLN:HB3	7:C:3076:HOH:O	1.96	0.64
4:D:311:VAL:HG12	4:D:312:TYR:N	2.13	0.64
4:A:582:LEU:HD11	4:A:625:VAL:HG21	1.78	0.63
4:C:423:ARG:HD2	4:C:781:ASN:CB	2.27	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:17:DG:H2"	1:K:18:DC:C6	2.33	0.63
4:B:433:ASN:CB	4:B:434:PRO:CD	2.63	0.63
4:B:751:PHE:HB3	4:B:752:LEU:CD1	2.19	0.63
4:C:292:ARG:N	4:C:293:PRO:HD3	2.13	0.63
4:B:5:ASN:HD21	4:B:7:ALA:N	1.95	0.63
4:C:424:GLY:HA3	7:C:3159:HOH:O	1.98	0.63
4:B:217:ILE:O	4:B:221:ILE:HG13	1.98	0.63
4:A:634:VAL:HG23	4:A:685:VAL:HG11	1.80	0.63
4:D:273:VAL:CA	4:D:415:TRP:CZ3	2.82	0.63
4:C:335:LEU:HD21	4:C:339:ASN:ND2	2.13	0.63
4:D:804:ILE:CG2	4:D:816:THR:HG21	2.29	0.63
4:C:881:ALA:O	4:C:883:ALA:N	2.31	0.63
4:C:882:PHE:HD1	4:C:882:PHE:H	1.44	0.63
4:B:463:HIS:HB3	4:B:534:LEU:HD22	1.79	0.63
4:B:537:ASP:N	4:B:882:PHE:HD2	1.96	0.63
4:D:649:GLN:HA	4:D:652:GLU:OE2	1.98	0.63
4:D:10:ASP:O	4:D:13:ASP:HB3	1.98	0.63
4:B:113:ALA:O	4:B:117:ILE:HG13	1.98	0.63
4:D:550:LEU:HD21	4:D:865:PRO:HG2	1.81	0.63
4:C:423:ARG:NE	4:C:781:ASN:HD22	1.96	0.63
4:B:777:GLY:O	4:B:781:ASN:HB2	1.98	0.63
4:B:51:PHE:CE2	4:B:55:PHE:HD1	2.16	0.63
4:A:92:VAL:HG12	4:A:99:ARG:HG3	1.80	0.63
4:D:552:ASP:CB	4:D:691:ALA:HB2	2.28	0.63
4:D:432:PHE:HE1	4:D:440:THR:HG23	1.64	0.63
4:D:278:TRP:HB2	4:D:321:ASN:ND2	2.13	0.63
4:B:860:LYS:O	4:B:860:LYS:HD2	1.99	0.63
4:A:871:ASN:ND2	4:A:871:ASN:O	2.32	0.63
4:D:274:PRO:HD3	4:D:415:TRP:CZ3	2.33	0.63
4:C:552:ASP:OD1	4:C:555:GLY:N	2.27	0.63
4:C:881:ALA:O	4:C:882:PHE:C	2.37	0.63
4:C:530:CYS:SG	4:C:818:PRO:HG2	2.39	0.63
4:D:446:LEU:O	4:D:531:SER:HB2	1.99	0.63
4:D:141:ILE:HG22	4:D:145:ILE:HD11	1.80	0.63
4:A:65:ALA:HB3	4:A:120:LYS:HE3	1.79	0.63
4:A:446:LEU:O	4:A:531:SER:HB2	1.99	0.63
4:A:472:LYS:HA	4:A:567:VAL:HG11	1.81	0.63
4:B:281:ILE:HG22	4:B:282:THR:HG23	1.80	0.63
1:H:12:DT:C4'	4:B:423:ARG:NE	2.59	0.63
4:B:549:MET:HG2	4:B:836:TYR:HE1	1.63	0.63
4:B:830:GLU:HA	4:B:876:LEU:HD21	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:14:ILE:H	4:B:14:ILE:CD1	2.03	0.63
4:B:329:LYS:HD3	4:B:447:ALA:HA	1.78	0.63
4:A:383:ALA:C	4:A:385:TYR:N	2.52	0.63
4:D:95:LYS:HB2	4:D:95:LYS:NZ	2.13	0.63
4:A:716:GLY:CA	7:A:3184:HOH:O	2.47	0.63
4:C:296:LEU:O	4:C:296:LEU:HG	1.99	0.63
4:A:478:ARG:O	4:A:482:ILE:HG12	1.98	0.63
4:A:729:THR:N	4:A:733:PHE:O	2.31	0.63
4:B:297:VAL:O	4:B:297:VAL:HG12	1.95	0.63
4:B:730:PRO:HD2	4:B:786:GLN:NE2	2.13	0.63
4:A:304:ALA:O	4:A:307:ARG:CG	2.44	0.63
4:D:28:TYR:O	4:D:32:LEU:HD13	1.99	0.63
4:A:437:ASN:ND2	4:A:440:THR:OG1	2.32	0.63
4:D:221:ILE:HG12	4:D:227:VAL:O	1.99	0.63
1:E:16:DC:H2"	1:E:17:DG:H5'	1.81	0.63
4:C:110:LYS:HE2	4:C:112:GLU:OE1	1.98	0.63
4:B:278:TRP:CZ3	4:B:284:GLY:HA3	2.33	0.63
4:D:452:ILE:HG23	4:D:453:GLY:H	1.63	0.63
4:B:626:THR:O	4:B:628:SER:N	2.31	0.63
4:B:27:HIS:HA	7:B:3169:HOH:O	1.98	0.63
4:A:570:ILE:O	4:A:573:ILE:HG23	1.99	0.62
4:A:459:TRP:O	4:A:460:LEU:O	2.16	0.62
4:A:280:GLY:O	4:A:281:ILE:C	2.35	0.62
4:C:313:MET:HA	7:C:3099:HOH:O	1.99	0.62
4:C:317:TYR:C	4:C:321:ASN:ND2	2.52	0.62
4:D:139:SER:HB2	4:D:210:ILE:HD13	1.81	0.62
4:C:163:LYS:HB3	4:C:164:LYS:NZ	2.13	0.62
4:A:270:PRO:HD2	4:A:408:PHE:CE2	2.34	0.62
4:B:539:SER:OG	4:B:560:ASN:ND2	2.32	0.62
4:A:423:ARG:O	4:A:785:SER:HA	1.99	0.62
4:C:824:LEU:O	4:C:824:LEU:HD12	1.99	0.62
4:B:163:LYS:O	4:B:166:VAL:HG23	1.98	0.62
4:D:133:THR:HA	4:D:243:THR:HG22	1.79	0.62
4:A:118:THR:O	4:A:122:THR:OG1	2.03	0.62
4:C:563:PRO:HD2	4:C:874:ASP:HB3	1.80	0.62
2:L:1:G:H2'	2:L:2:C:C6	2.34	0.62
4:D:590:THR:O	4:D:614:LYS:HB2	1.99	0.62
4:A:630:THR:HA	7:A:3199:HOH:O	1.98	0.62
4:D:725:VAL:HB	4:D:737:GLN:HB3	1.81	0.62
4:B:728:VAL:HG22	4:B:734:PRO:CA	2.29	0.62
4:B:828:VAL:HG11	4:B:883:ALA:HA	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:4:ILE:CD1	4:A:256:THR:HA	2.29	0.62
4:A:457:TYR:CE2	4:A:461:LYS:CD	2.82	0.62
4:A:540:CYS:O	4:A:542:GLY:N	2.33	0.62
4:C:423:ARG:HD2	4:C:781:ASN:HB3	1.81	0.62
4:D:698:TRP:CE3	4:D:699:LEU:HD23	2.34	0.62
4:D:725:VAL:HG23	4:D:774:GLN:NE2	2.14	0.62
4:C:474:PRO:HB2	4:C:476:PRO:CG	2.29	0.62
4:C:346:HIS:HA	4:C:395:ARG:NH1	2.14	0.62
4:A:544:GLN:OE1	4:A:559:VAL:HG23	1.99	0.62
4:B:571:TYR:CD2	4:B:631:LYS:HA	2.35	0.62
4:B:668:THR:O	4:B:670:PRO:HD3	1.99	0.62
1:H:10:DT:OP2	4:B:641:SER:CB	2.48	0.62
4:B:403:GLU:OE1	4:B:404:GLN:N	2.32	0.62
4:A:106:LEU:HD21	4:A:212:VAL:HG13	1.81	0.62
4:B:158:GLU:HG2	4:B:195:LEU:HD22	1.81	0.62
4:A:632:ARG:HB3	4:A:649:GLN:HE21	1.63	0.62
4:B:508:PRO:O	4:B:511:PHE:N	2.32	0.62
4:C:137:VAL:O	4:C:140:ALA:HB3	1.99	0.62
4:D:540:CYS:O	4:D:541:SER:C	2.37	0.62
4:B:610:LYS:O	4:B:611:LEU:O	2.17	0.62
4:B:569:ASP:CG	4:B:627:ARG:HH21	2.02	0.62
4:B:553:GLU:HG3	7:B:3114:HOH:O	2.00	0.62
4:D:169:GLN:HB3	4:D:182:PHE:CE2	2.34	0.62
4:A:823:ASN:O	4:A:824:LEU:C	2.36	0.62
4:A:11:PHE:HB3	4:A:41:HIS:CE1	2.34	0.62
4:D:327:ALA:HB2	4:D:415:TRP:HE1	1.61	0.62
4:B:578:VAL:HG13	4:B:680:LEU:HD23	1.80	0.62
4:D:582:LEU:CD1	4:D:625:VAL:HG21	2.28	0.62
2:L:6:G:OP1	4:C:394:ARG:NH1	2.32	0.62
4:A:540:CYS:HB3	4:A:543:ILE:HG13	1.82	0.62
4:A:793:LYS:HA	4:A:796:VAL:HG23	1.82	0.62
4:A:425:ARG:HD3	4:A:811:HIS:CD2	2.35	0.62
4:B:122:THR:CG2	4:B:226:MET:HE1	2.28	0.62
4:A:512:LEU:O	4:A:516:PHE:CE1	2.53	0.62
4:A:392:LYS:O	4:A:396:ILE:HG12	1.99	0.62
4:C:303:LYS:NZ	4:C:303:LYS:CB	2.63	0.62
4:C:875:ILE:CG2	4:C:875:ILE:O	2.48	0.62
4:B:748:ASN:HD22	4:B:751:PHE:H	1.46	0.62
4:A:132:THR:O	4:A:132:THR:HG22	1.99	0.62
4:B:689:VAL:HG23	4:B:689:VAL:O	1.99	0.62
4:B:391:ARG:CG	7:B:3101:HOH:O	2.46	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:488:ASN:O	4:D:491:ALA:HB3	2.00	0.62
4:A:588:ASN:HB3	7:A:3224:HOH:O	1.99	0.62
4:A:632:ARG:HH21	6:A:2000:APC:C8	2.12	0.62
4:A:578:VAL:HG13	4:A:680:LEU:HB3	1.82	0.62
4:A:818:PRO:O	4:A:821:ALA:HB3	1.98	0.62
4:A:24:LEU:HD11	4:A:287:TRP:CG	2.35	0.62
4:D:705:LEU:HD12	4:D:853:LEU:HD22	1.81	0.62
4:D:324:GLN:HA	4:D:418:TYR:CD1	2.35	0.62
4:B:792:ARG:O	4:B:796:VAL:HG23	2.00	0.62
4:B:475:PHE:O	4:B:478:ARG:N	2.32	0.62
4:B:26:ASP:HB3	7:B:3098:HOH:O	2.00	0.62
4:C:557:ARG:HB3	4:C:557:ARG:HH11	1.64	0.61
4:B:24:LEU:HD22	4:B:33:ALA:HA	1.80	0.61
4:B:464:GLY:HA3	4:B:514:PHE:CE2	2.35	0.61
4:A:226:MET:HA	4:A:250:TYR:CD1	2.35	0.61
4:C:635:MET:CE	6:C:2002:APC:H8	2.30	0.61
4:A:798:ALA:HB2	4:A:827:ALA:CB	2.30	0.61
4:A:825:PHE:CD1	4:A:829:ARG:NH1	2.63	0.61
4:C:549:MET:HE1	4:C:786:GLN:HG2	1.83	0.61
4:C:882:PHE:N	4:C:882:PHE:CD1	2.68	0.61
1:H:6:DT:H5'	1:H:6:DT:H6	1.65	0.61
4:A:704:LYS:HE3	4:A:860:LYS:NZ	2.15	0.61
4:C:398:LEU:O	4:C:398:LEU:HD23	1.99	0.61
4:C:730:PRO:HD3	4:C:786:GLN:HE22	1.66	0.61
4:B:726:HIS:HD2	4:B:735:VAL:O	1.82	0.61
4:B:470:VAL:HG21	4:B:481:PHE:CD2	2.35	0.61
4:A:112:GLU:O	4:A:115:ALA:HB3	2.00	0.61
4:D:304:ALA:HA	4:D:307:ARG:HD2	1.81	0.61
4:A:786:GLN:OE1	4:A:841:VAL:HG21	2.00	0.61
4:C:14:ILE:CG2	4:C:288:ALA:HB1	2.31	0.61
4:C:728:VAL:HG22	4:C:734:PRO:CB	2.30	0.61
4:D:273:VAL:HA	4:D:415:TRP:HZ3	1.61	0.61
4:B:823:ASN:N	4:B:823:ASN:HD22	1.98	0.61
4:C:19:ILE:HG12	4:C:20:PRO:CD	2.20	0.61
4:B:88:TRP:CZ2	4:B:215:ARG:HD3	2.35	0.61
4:A:347:CYS:O	4:A:349:VAL:N	2.33	0.61
4:A:231:ARG:CG	4:A:234:ALA:HB2	2.30	0.61
4:D:11:PHE:CE1	4:D:44:TYR:HB3	2.35	0.61
4:A:459:TRP:CZ3	4:A:475:PHE:HE1	2.18	0.61
4:A:563:PRO:HB3	4:A:878:SER:CA	2.29	0.61
4:B:538:GLY:HA2	4:B:882:PHE:O	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:783:VAL:O	4:B:786:GLN:N	2.31	0.61
4:A:386:ARG:O	4:A:388:ASP:N	2.34	0.61
4:B:574:VAL:CG2	4:B:685:VAL:HG12	2.30	0.61
4:D:139:SER:HB2	4:D:210:ILE:HD11	1.83	0.61
4:D:592:ASN:O	4:D:593:GLU:HB2	2.00	0.61
4:C:727:TRP:HB3	4:C:845:PHE:CD1	2.36	0.61
4:B:292:ARG:O	4:B:293:PRO:O	2.19	0.61
4:B:485:ASN:O	4:B:486:HIS:C	2.39	0.61
4:C:455:GLU:O	4:C:458:TYR:HB3	2.00	0.61
4:D:221:ILE:CG1	4:D:227:VAL:HG23	2.30	0.61
4:C:291:ARG:HG2	7:C:3066:HOH:O	2.00	0.61
4:C:643:GLU:OE2	4:C:679:LYS:HD2	2.00	0.61
4:D:422:TRP:C	4:D:422:TRP:CD1	2.74	0.61
4:A:459:TRP:O	4:A:460:LEU:C	2.36	0.61
4:A:778:ILE:HG23	4:A:779:ALA:N	2.16	0.61
4:A:817:ILE:HB	4:A:818:PRO:CD	2.30	0.61
4:B:460:LEU:N	4:B:534:LEU:HD11	2.15	0.61
4:B:631:LYS:NZ	6:B:2001:APC:H3A2	2.16	0.61
4:B:676:TYR:CE1	4:B:680:LEU:HD11	2.36	0.61
4:D:329:LYS:HD2	4:D:447:ALA:HA	1.82	0.61
4:D:187:GLU:O	4:D:191:LEU:HG	2.00	0.61
4:C:495:SER:HB2	4:C:498:GLU:HB2	1.82	0.61
4:D:573:ILE:O	4:D:577:LYS:HG3	2.01	0.61
4:B:571:TYR:CD2	4:B:631:LYS:HG3	2.34	0.61
4:B:682:TRP:O	4:B:686:SER:OG	2.16	0.61
4:B:706:LEU:O	4:B:723:CYS:O	2.19	0.61
4:C:405:ALA:HB2	4:C:443:LEU:HD13	1.81	0.61
4:D:448:LYS:HZ2	4:D:806:SER:HB3	1.64	0.61
4:D:643:GLU:OE1	4:D:679:LYS:HD3	2.01	0.61
4:A:727:TRP:CD2	4:A:735:VAL:CG1	2.84	0.61
4:B:55:PHE:CE2	4:B:59:LEU:HD11	2.36	0.61
4:C:849:PHE:CD2	4:C:853:LEU:HD21	2.35	0.61
4:D:631:LYS:CE	6:D:2003:APC:H3A2	2.31	0.61
4:D:327:ALA:HA	4:D:415:TRP:CD1	2.35	0.61
4:B:206:LYS:O	4:B:210:ILE:HG12	2.01	0.61
4:C:292:ARG:HG3	4:C:292:ARG:O	2.00	0.61
4:D:859:ASP:HA	7:D:3136:HOH:O	2.00	0.61
4:C:828:VAL:HG23	4:C:829:ARG:N	2.12	0.61
4:B:281:ILE:HG22	4:B:282:THR:N	2.15	0.61
4:B:582:LEU:HD13	4:B:621:LEU:HD12	1.82	0.61
4:C:461:LYS:O	4:C:464:GLY:N	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:432:PHE:CE1	4:D:440:THR:HG23	2.36	0.61
4:C:570:ILE:HA	4:C:573:ILE:HG22	1.81	0.61
4:A:77:LEU:CD2	4:A:119:ILE:HD12	2.31	0.61
4:B:326:THR:O	4:B:415:TRP:CD1	2.54	0.61
4:C:155:ARG:HB2	4:C:163:LYS:HZ2	1.65	0.61
4:A:390:ALA:O	4:A:393:SER:N	2.33	0.61
4:D:330:ILE:HG21	4:D:409:ALA:HA	1.81	0.61
4:C:303:LYS:HB2	4:C:303:LYS:HZ2	1.65	0.61
1:N:11:DA:C6	4:D:639:TYR:CE2	2.89	0.60
1:H:10:DT:H5'	4:B:641:SER:N	2.15	0.60
4:C:84:ARG:NH1	4:C:84:ARG:HA	2.15	0.60
4:C:754:GLN:O	4:C:755:PHE:O	2.19	0.60
4:A:373:ALA:HB2	7:A:3006:HOH:O	2.01	0.60
4:B:551:ARG:HG3	7:B:3047:HOH:O	2.01	0.60
4:C:386:ARG:HB3	7:C:3082:HOH:O	2.01	0.60
4:A:457:TYR:OH	4:A:461:LYS:HD3	2.00	0.60
4:A:14:ILE:HA	7:A:3082:HOH:O	2.00	0.60
4:B:329:LYS:CG	4:B:329:LYS:O	2.49	0.60
4:A:402:LEU:HG	4:A:439:MET:CE	2.31	0.60
4:A:516:PHE:N	4:A:516:PHE:HD1	1.99	0.60
4:A:682:TRP:CG	4:A:682:TRP:O	2.54	0.60
4:A:316:VAL:HG13	4:A:792:ARG:HE	1.66	0.60
4:C:788:GLY:C	4:C:792:ARG:NH1	2.54	0.60
4:C:823:ASN:O	4:C:826:LYS:N	2.32	0.60
4:B:427:TYR:CE1	4:B:811:HIS:NE2	2.69	0.60
4:B:423:ARG:CD	4:B:781:ASN:ND2	2.64	0.60
4:B:536:PHE:HE2	4:B:825:PHE:HB2	1.65	0.60
4:B:269:GLN:HG2	4:B:404:GLN:OE1	2.00	0.60
4:B:439:MET:O	4:B:442:GLY:N	2.33	0.60
4:C:236:VAL:O	4:C:240:ASP:HB2	2.01	0.60
4:C:329:LYS:CD	4:C:447:ALA:HA	2.31	0.60
4:B:345:LYS:NZ	4:B:351:ASP:N	2.48	0.60
4:C:208:ASP:O	4:C:212:VAL:HG23	2.01	0.60
4:A:488:ASN:O	4:A:491:ALA:HB3	2.01	0.60
4:C:631:LYS:O	4:C:632:ARG:C	2.37	0.60
4:A:802:TYR:OH	4:A:830:GLU:OE2	2.20	0.60
4:A:25:ALA:O	4:A:29:GLY:N	2.32	0.60
4:B:677:MET:HG3	4:B:681:ILE:HD13	1.82	0.60
7:N:1048:HOH:O	4:D:772:HIS:HD2	1.83	0.60
4:D:486:HIS:NE2	4:D:490:MET:HG3	2.16	0.60
1:N:15:DC:C2'	1:N:16:DC:OP2	2.48	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:496:PRO:HD2	7:A:3203:HOH:O	2.00	0.60
4:C:35:GLU:HG2	4:C:272:VAL:HG21	1.84	0.60
4:D:373:ALA:HB1	4:D:377:TRP:HE1	1.67	0.60
4:A:791:LEU:O	4:A:795:VAL:HG23	2.02	0.60
4:C:551:ARG:HE	4:C:872:LEU:CD2	2.14	0.60
4:B:875:ILE:HG22	4:B:876:LEU:N	2.15	0.60
4:B:433:ASN:CB	4:B:434:PRO:HD3	2.11	0.60
4:D:292:ARG:H	4:D:293:PRO:HD3	1.65	0.60
1:N:8:DG:H4'	7:N:1048:HOH:O	2.02	0.60
1:H:3:DG:H2"	1:H:4:DA:C8	2.36	0.60
4:D:207:GLU:HB3	4:D:211:HIS:NE2	2.15	0.60
4:B:347:CYS:HB3	4:B:350:GLU:CG	2.32	0.60
4:A:459:TRP:HZ3	4:A:475:PHE:HE1	1.50	0.60
4:A:882:PHE:H	4:A:882:PHE:HD1	1.47	0.60
4:B:320:ILE:O	4:B:324:GLN:HB2	2.01	0.60
4:C:651:LEU:C	4:C:651:LEU:HD13	2.22	0.60
4:B:84:ARG:CD	4:B:219:MET:HG2	2.25	0.60
4:B:398:LEU:O	4:B:398:LEU:HD23	2.01	0.60
4:A:390:ALA:C	4:A:392:LYS:N	2.52	0.60
4:C:266:PRO:HG2	4:C:268:PHE:CZ	2.37	0.60
4:A:574:VAL:HG12	4:A:684:SER:HB3	1.82	0.60
4:A:546:PHE:CD2	4:A:692:ALA:HA	2.30	0.60
4:B:59:LEU:HA	4:B:64:VAL:HG22	1.82	0.60
4:B:460:LEU:HA	4:B:534:LEU:HD21	1.82	0.60
4:B:680:LEU:N	4:B:680:LEU:HD12	2.15	0.60
1:H:9:DA:N6	3:J:1:DG:H21	2.00	0.60
4:B:120:LYS:NZ	4:B:752:LEU:HD11	2.17	0.60
4:A:342:THR:HG22	4:A:348:PRO:HG3	1.83	0.60
4:A:159:ALA:O	4:A:163:LYS:HB2	2.02	0.60
4:D:729:THR:HB	4:D:789:SER:HB2	1.83	0.60
4:A:610:LYS:O	4:A:611:LEU:C	2.38	0.60
4:B:454:LYS:HG3	4:B:455:GLU:N	2.15	0.60
4:A:47:GLY:O	4:A:50:ARG:HB3	2.01	0.60
4:C:175:GLY:O	4:C:176:HIS:C	2.37	0.60
4:D:833:VAL:HG22	4:D:875:ILE:HB	1.83	0.60
4:C:333:LYS:CB	4:C:516:PHE:CD2	2.84	0.60
4:A:89:PHE:HA	4:A:103:PHE:HE1	1.64	0.60
4:B:73:LEU:HD21	4:B:77:LEU:HD22	1.83	0.60
4:B:437:ASN:C	4:B:437:ASN:ND2	2.54	0.60
1:N:15:DC:H2"	1:N:16:DC:O5'	2.01	0.60
4:B:291:ARG:HG3	7:B:3037:HOH:O	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:181:ALA:O	4:B:185:VAL:HG13	2.00	0.60
4:A:329:LYS:HG2	4:A:447:ALA:HA	1.84	0.60
4:A:633:SER:OG	4:A:646:PHE:CG	2.44	0.60
4:D:571:TYR:CD1	4:D:631:LYS:HA	2.37	0.60
4:B:398:LEU:C	4:B:398:LEU:HD23	2.21	0.60
4:D:113:ALA:O	4:D:117:ILE:HG13	2.01	0.60
4:A:116:TYR:CE2	4:A:752:LEU:HD13	2.37	0.60
4:C:492:CYS:SG	4:C:501:TRP:HE3	2.25	0.60
4:A:536:PHE:HB3	4:A:882:PHE:HB3	1.84	0.60
4:C:14:ILE:HG21	4:C:288:ALA:HB1	1.83	0.60
4:B:292:ARG:N	4:B:293:PRO:HD3	2.16	0.60
4:B:300:HIS:NE2	4:B:422:TRP:HZ3	1.97	0.60
4:A:82:ILE:HG21	4:A:112:GLU:OE2	2.01	0.60
4:D:54:MET:O	4:D:58:GLN:HG2	2.02	0.60
4:D:213:GLY:O	4:D:217:ILE:HG13	2.02	0.60
4:A:842:LEU:O	4:A:845:PHE:HB3	2.02	0.60
4:A:778:ILE:CG2	4:A:779:ALA:N	2.65	0.59
4:C:324:GLN:HG3	4:C:417:PRO:HA	1.84	0.59
4:B:571:TYR:CE1	7:B:3067:HOH:O	2.51	0.59
4:B:780:PRO:O	4:B:781:ASN:C	2.35	0.59
4:A:689:VAL:O	4:A:690:VAL:C	2.39	0.59
4:A:342:THR:CG2	4:A:398:LEU:HD21	2.33	0.59
4:A:159:ALA:HB1	4:A:163:LYS:N	2.17	0.59
4:D:646:PHE:O	4:D:647:ARG:O	2.19	0.59
4:D:846:TYR:HA	4:D:849:PHE:CE1	2.36	0.59
4:B:698:TRP:O	4:B:701:SER:N	2.35	0.59
4:B:66:ASP:OD1	4:B:120:LYS:HE3	2.01	0.59
4:A:380:ALA:O	4:A:383:ALA:HB3	2.02	0.59
2:F:3:G:O2'	4:A:389:LYS:NZ	2.35	0.59
4:A:669:GLN:CG	4:A:672:GLN:HE21	2.15	0.59
4:D:95:LYS:HD2	7:D:3092:HOH:O	2.02	0.59
4:A:428:ALA:N	4:A:435:GLN:HE22	2.00	0.59
4:C:496:PRO:HA	7:C:3071:HOH:O	2.02	0.59
4:A:712:ASP:HA	7:A:3088:HOH:O	2.00	0.59
4:C:525:GLY:O	4:C:527:SER:N	2.35	0.59
4:B:418:TYR:CE2	4:B:428:ALA:CB	2.82	0.59
4:C:333:LYS:NZ	7:C:3010:HOH:O	2.34	0.59
4:B:473:VAL:CG1	4:B:474:PRO:CD	2.79	0.59
4:B:163:LYS:HB3	4:B:164:LYS:NZ	2.17	0.59
4:B:21:PHE:C	4:B:23:THR:H	2.05	0.59
4:C:299:THR:CG2	4:C:300:HIS:H	2.13	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:4:G:H2'	2:O:5:C:H6	1.67	0.59
4:A:741:LYS:HB2	4:A:770:ASP:HB2	1.84	0.59
4:D:3:THR:HG23	7:D:3098:HOH:O	2.00	0.59
4:C:695:ALA:O	4:C:699:LEU:HD12	2.03	0.59
4:D:322:ILE:HG22	4:D:323:ALA:N	2.17	0.59
4:B:561:LEU:HD23	4:B:875:ILE:HD11	1.84	0.59
4:B:398:LEU:HD21	4:B:439:MET:CE	2.33	0.59
4:D:623:TYR:HA	4:D:666:MET:CE	2.32	0.59
4:C:78:LEU:HD11	4:C:115:ALA:HB3	1.84	0.59
4:C:330:ILE:HG12	7:C:3016:HOH:O	2.02	0.59
4:B:861:MET:O	4:B:862:PRO:C	2.40	0.59
4:C:875:ILE:HG22	4:C:875:ILE:O	2.01	0.59
4:A:585:ASP:O	4:A:588:ASN:O	2.19	0.59
4:C:14:ILE:HG21	4:C:288:ALA:CB	2.33	0.59
4:C:318:LYS:HE2	4:C:796:VAL:HG13	1.84	0.59
4:D:229:LEU:HA	4:D:244:ILE:HD13	1.84	0.59
4:A:849:PHE:CD2	4:A:853:LEU:HD21	2.37	0.59
4:D:19:ILE:HG23	4:D:20:PRO:HD2	1.84	0.59
4:D:53:LYS:O	4:D:56:GLU:HB3	2.02	0.59
4:A:205:HIS:HB3	4:A:207:GLU:HG2	1.84	0.59
4:C:24:LEU:HD22	4:C:273:VAL:HG21	1.85	0.59
4:C:306:MET:O	4:C:308:TYR:N	2.35	0.59
4:C:706:LEU:O	4:C:723:CYS:O	2.20	0.59
4:C:726:HIS:HB2	4:C:736:TRP:CD1	2.37	0.59
4:C:850:ALA:C	4:C:852:GLN:H	2.06	0.59
4:D:725:VAL:HG23	4:D:774:GLN:HE21	1.66	0.59
4:B:663:LYS:CG	4:B:664:GLY:N	2.66	0.59
4:B:751:PHE:C	4:B:752:LEU:HD12	2.23	0.59
4:A:92:VAL:HG22	7:A:3011:HOH:O	2.01	0.59
4:A:294:LEU:CD1	4:A:429:VAL:HG21	2.29	0.59
4:D:100:PRO:HG2	4:D:103:PHE:HB2	1.83	0.59
4:C:78:LEU:N	4:C:79:PRO:CD	2.65	0.59
3:M:5:DA:H2"	3:M:6:DT:H72	1.84	0.59
4:D:710:VAL:CG1	4:D:720:ARG:HB3	2.33	0.59
4:C:837:GLU:HG3	4:C:872:LEU:HD12	1.85	0.59
4:A:15:GLU:HG2	4:A:18:ALA:O	2.03	0.59
4:A:143:ARG:HD3	7:A:3118:HOH:O	2.01	0.59
4:A:178:TYR:H	4:A:178:TYR:HD1	1.47	0.59
4:A:96:ARG:NE	7:A:3009:HOH:O	2.33	0.59
4:A:629:VAL:HG12	4:A:629:VAL:O	2.02	0.59
4:A:727:TRP:CH2	4:A:735:VAL:HG21	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:281:ILE:CG1	4:C:309:GLU:HA	2.33	0.59
1:N:10:DT:H5'	4:D:641:SER:HA	1.83	0.59
4:D:273:VAL:C	4:D:415:TRP:CE3	2.76	0.59
4:B:36:GLN:HA	4:B:36:GLN:OE1	2.03	0.59
4:C:452:ILE:HD11	4:C:457:TYR:N	2.18	0.59
4:A:80:LYS:CD	4:A:224:THR:HG22	2.32	0.59
2:I:5:C:N3	2:I:6:G:N7	2.50	0.59
4:B:770:ASP:OD1	4:B:772:HIS:N	2.36	0.59
4:A:660:ASP:HB3	7:A:3072:HOH:O	2.02	0.59
4:A:727:TRP:CE3	4:A:735:VAL:HG13	2.37	0.59
4:A:802:TYR:HD2	4:A:802:TYR:N	1.99	0.59
4:C:308:TYR:HH	4:C:733:PHE:HE2	1.49	0.59
4:B:40:GLU:OE1	4:B:288:ALA:HB3	2.02	0.59
4:C:21:PHE:C	4:C:23:THR:N	2.54	0.59
4:C:724:ALA:HB2	4:C:738:GLU:HG3	1.85	0.59
4:A:720:ARG:HH21	4:A:857:GLN:HE22	1.51	0.59
4:B:576:LYS:O	4:B:579:ASN:N	2.36	0.59
3:J:1:DG:H1'	3:J:2:DT:H71	1.83	0.59
4:B:473:VAL:HG12	4:B:474:PRO:N	2.17	0.59
4:B:514:PHE:CG	4:B:514:PHE:O	2.56	0.59
4:D:479:ILE:HG22	4:D:483:GLU:CD	2.23	0.59
4:D:726:HIS:CD2	4:D:736:TRP:CE2	2.90	0.59
4:A:425:ARG:NH2	4:A:784:HIS:CE1	2.71	0.58
1:H:13:DC:C4'	4:B:427:TYR:HE2	2.15	0.58
4:D:619:GLN:NE2	4:D:668:THR:H	2.01	0.58
4:D:668:THR:HG22	4:D:669:GLN:NE2	2.17	0.58
4:D:465:ALA:HB1	4:D:478:ARG:HB3	1.84	0.58
4:C:268:PHE:HB3	4:C:430:SER:HA	1.85	0.58
4:D:616:LEU:HD13	4:D:676:TYR:HB2	1.85	0.58
1:K:9:DA:H5'	7:K:731:HOH:O	2.01	0.58
4:C:632:ARG:HA	4:C:635:MET:HG2	1.85	0.58
4:A:810:ILE:O	4:A:812:ASP:N	2.36	0.58
4:C:728:VAL:HG13	4:C:733:PHE:C	2.24	0.58
4:C:727:TRP:CZ2	4:C:735:VAL:HG11	2.38	0.58
4:D:472:LYS:HG3	4:D:567:VAL:HG11	1.84	0.58
4:A:40:GLU:O	4:A:43:SER:HB2	2.04	0.58
4:C:252:GLU:HG2	7:C:3072:HOH:O	2.02	0.58
4:A:570:ILE:O	4:A:574:VAL:HG23	2.02	0.58
4:A:619:GLN:O	4:A:622:ALA:HB3	2.03	0.58
4:A:549:MET:HB3	4:A:836:TYR:HE1	1.67	0.58
4:D:560:ASN:O	4:D:878:SER:OG	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:748:ASN:HD21	4:B:751:PHE:HB2	1.67	0.58
4:A:404:GLN:HG2	4:A:432:PHE:CB	2.33	0.58
4:D:458:TYR:O	4:D:462:ILE:HG12	2.03	0.58
4:D:473:VAL:CG2	4:D:477:GLU:HG3	2.32	0.58
4:B:236:VAL:CB	4:B:239:GLN:HB2	2.31	0.58
4:C:501:TRP:HB2	7:C:3116:HOH:O	2.03	0.58
4:C:50:ARG:CZ	4:C:267:MET:HE3	2.33	0.58
4:A:108:GLU:HG3	7:A:3115:HOH:O	2.02	0.58
4:B:814:PHE:CE2	4:B:828:VAL:HG13	2.39	0.58
4:C:92:VAL:HG12	4:C:99:ARG:CG	2.27	0.58
4:C:329:LYS:HG3	4:C:445:THR:CG2	2.32	0.58
4:C:816:THR:HG22	4:C:817:ILE:HG13	1.86	0.58
4:D:475:PHE:O	4:D:476:PRO:C	2.37	0.58
4:B:585:ASP:OD2	4:B:613:THR:HB	2.03	0.58
4:C:161:HIS:O	4:C:163:LYS:N	2.36	0.58
4:D:496:PRO:HD2	7:D:3035:HOH:O	2.02	0.58
4:A:48:GLU:O	4:A:49:ALA:C	2.42	0.58
3:G:4:DG:H1'	3:G:5:DA:C8	2.38	0.58
4:C:588:ASN:N	4:C:588:ASN:HD22	2.02	0.58
4:A:551:ARG:HH21	4:A:872:LEU:HD11	1.67	0.58
4:A:727:TRP:CD2	4:A:735:VAL:HG13	2.39	0.58
4:B:55:PHE:HD2	4:B:55:PHE:O	1.87	0.58
4:C:319:ALA:CB	4:C:792:ARG:HB3	2.34	0.58
4:C:322:ILE:HG21	4:C:795:VAL:HG12	1.85	0.58
4:C:882:PHE:O	4:C:883:ALA:HB3	2.02	0.58
4:B:850:ALA:C	4:B:852:GLN:H	2.06	0.58
4:B:46:MET:O	4:B:49:ALA:HB3	2.03	0.58
4:A:516:PHE:CD1	4:A:516:PHE:N	2.70	0.58
4:C:477:GLU:HA	4:C:480:LYS:HB3	1.86	0.58
4:D:619:GLN:O	4:D:622:ALA:HB3	2.03	0.58
4:C:299:THR:HG21	4:C:304:ALA:HB3	1.85	0.58
4:B:182:PHE:O	4:B:185:VAL:HG22	2.02	0.58
4:C:423:ARG:NH1	4:C:423:ARG:CB	2.67	0.58
4:D:830:GLU:HG2	4:D:876:LEU:CD2	2.34	0.58
4:C:432:PHE:HZ	4:C:444:LEU:HD21	1.67	0.58
4:A:502:TRP:CD1	4:A:512:LEU:HD13	2.39	0.58
4:B:389:LYS:O	4:B:392:LYS:HB3	2.03	0.58
4:B:206:LYS:HB2	7:B:3155:HOH:O	2.02	0.58
4:C:579:ASN:HA	4:C:582:LEU:HB2	1.86	0.58
4:D:40:GLU:OE1	4:D:288:ALA:N	2.34	0.58
4:A:582:LEU:HB2	4:A:621:LEU:HD21	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:461:LYS:O	4:A:462:ILE:C	2.40	0.58
4:A:792:ARG:HH11	4:A:792:ARG:HG3	1.68	0.58
4:B:423:ARG:HD2	4:B:781:ASN:HD21	1.68	0.58
4:B:702:ALA:CB	4:B:849:PHE:CE2	2.84	0.58
4:B:751:PHE:CB	4:B:752:LEU:HD12	2.23	0.58
4:B:162:PHE:CD1	4:B:190:MET:SD	2.97	0.58
4:D:77:LEU:HD11	4:D:224:THR:OG1	2.03	0.58
4:D:308:TYR:CE2	4:D:734:PRO:O	2.56	0.58
4:D:619:GLN:NE2	4:D:666:MET:O	2.36	0.58
4:A:392:LYS:O	4:A:392:LYS:HG2	2.03	0.58
4:D:230:HIS:NE2	4:D:245:GLU:HB2	2.19	0.58
4:D:680:LEU:O	4:D:683:GLU:N	2.37	0.58
4:B:99:ARG:HG2	4:B:99:ARG:NH1	2.19	0.58
4:C:553:GLU:HG2	4:C:554:VAL:N	2.19	0.58
4:C:849:PHE:HD2	4:C:853:LEU:HD21	1.68	0.58
4:B:423:ARG:HD2	4:B:781:ASN:ND2	2.18	0.58
4:C:19:ILE:CG1	4:C:20:PRO:HD2	2.20	0.58
4:C:452:ILE:HG22	4:C:528:TYR:O	2.04	0.58
4:B:5:ASN:HD21	4:B:7:ALA:CA	2.17	0.58
4:B:54:MET:O	4:B:58:GLN:HG2	2.03	0.58
4:A:3:THR:HB	4:A:52:ARG:HH12	1.69	0.58
4:D:720:ARG:NH1	4:D:720:ARG:CG	2.52	0.58
4:C:433:ASN:HB2	4:C:434:PRO:HD2	1.85	0.58
4:C:701:SER:O	4:C:704:LYS:HB3	2.04	0.58
4:C:727:TRP:NE1	4:C:782:PHE:CD1	2.72	0.58
4:B:843:ALA:HA	4:B:864:LEU:HD21	1.85	0.58
4:B:753:GLY:O	4:B:754:GLN:HG2	2.04	0.58
4:A:400:PHE:O	4:A:401:MET:C	2.42	0.58
4:D:292:ARG:N	4:D:293:PRO:HD3	2.18	0.58
4:A:511:PHE:CD2	4:A:511:PHE:O	2.57	0.58
4:A:270:PRO:HB3	4:A:416:PHE:CE1	2.39	0.58
4:A:50:ARG:HH11	4:A:50:ARG:HG2	1.68	0.58
4:B:861:MET:O	4:B:862:PRO:O	2.21	0.58
4:A:463:HIS:O	4:A:466:ASN:N	2.36	0.58
4:C:737:GLN:OE1	4:C:778:ILE:HD13	2.04	0.58
4:D:794:THR:OG1	4:D:831:THR:CG2	2.45	0.58
4:D:748:ASN:HB2	4:D:753:GLY:CA	2.33	0.58
4:C:401:MET:O	4:C:404:GLN:CB	2.52	0.58
4:B:439:MET:HG3	4:B:509:PHE:CG	2.38	0.58
4:A:105:PHE:C	4:A:107:GLN:H	2.07	0.58
4:C:476:PRO:HG2	4:C:477:GLU:H	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:623:TYR:HD1	4:A:663:LYS:HE3	1.69	0.57
4:A:727:TRP:CZ2	4:A:735:VAL:HG11	2.39	0.57
4:A:788:GLY:C	4:A:792:ARG:HH12	2.08	0.57
4:C:308:TYR:O	4:C:310:ASP:N	2.37	0.57
4:D:870:LEU:C	4:D:870:LEU:HD23	2.25	0.57
4:B:582:LEU:HD13	4:B:621:LEU:CD1	2.33	0.57
4:B:41:HIS:O	4:B:42:GLU:C	2.43	0.57
4:A:448:LYS:HG2	7:A:3094:HOH:O	2.04	0.57
4:B:450:LYS:HB3	4:B:819:ALA:HB3	1.86	0.57
4:B:123:LEU:O	4:B:127:THR:HG23	2.04	0.57
4:A:471:ASP:OD1	4:A:472:LYS:CD	2.38	0.57
4:B:823:ASN:O	4:B:826:LYS:N	2.36	0.57
4:B:436:GLY:HA3	7:B:3166:HOH:O	2.03	0.57
1:E:14:DG:C2'	1:E:15:DC:C6	2.85	0.57
4:A:669:GLN:HB3	4:A:672:GLN:HG3	1.86	0.57
4:A:416:PHE:CE2	4:A:434:PRO:HD3	2.40	0.57
4:C:67:ASN:C	4:C:69:ALA:H	2.06	0.57
4:D:84:ARG:HB2	4:D:223:SER:HB3	1.87	0.57
4:B:99:ARG:HG2	4:B:99:ARG:HH11	1.68	0.57
4:A:135:GLN:HB2	7:A:3052:HOH:O	2.02	0.57
4:C:275:PRO:CG	4:C:324:GLN:HG2	2.34	0.57
4:C:326:THR:O	4:C:415:TRP:CD1	2.57	0.57
4:C:308:TYR:CE2	4:C:734:PRO:HG2	2.38	0.57
4:C:700:LYS:HA	4:C:778:ILE:HG21	1.86	0.57
4:C:787:ASP:C	4:C:787:ASP:OD1	2.42	0.57
4:D:323:ALA:C	4:D:325:ASN:H	2.07	0.57
4:D:814:PHE:CE1	4:D:883:ALA:CB	2.87	0.57
4:B:737:GLN:HG2	4:B:774:GLN:NE2	2.18	0.57
4:D:100:PRO:O	4:D:104:GLN:HG2	2.04	0.57
4:D:155:ARG:HA	4:D:163:LYS:HE3	1.86	0.57
4:A:657:PRO:O	4:A:661:SER:OG	2.13	0.57
4:A:462:ILE:CD1	4:A:478:ARG:HD2	2.34	0.57
4:A:828:VAL:O	4:A:831:THR:HG22	2.04	0.57
4:B:642:LYS:HG2	4:B:682:TRP:CZ3	2.38	0.57
4:B:492:CYS:SG	4:B:502:TRP:HD1	2.25	0.57
4:B:164:LYS:NZ	4:B:164:LYS:N	2.52	0.57
4:D:471:ASP:CG	4:D:472:LYS:HD3	2.24	0.57
4:B:21:PHE:C	4:B:23:THR:N	2.58	0.57
4:D:270:PRO:HD2	4:D:408:PHE:CE2	2.39	0.57
4:D:61:ALA:HB3	4:D:63:GLU:HG3	1.84	0.57
3:M:2:DT:H2"	3:M:3:DC:O5'	2.02	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:651:LEU:HD11	4:A:656:GLN:HE22	1.70	0.57
4:C:281:ILE:CD1	4:C:309:GLU:HA	2.34	0.57
4:C:281:ILE:HG12	4:C:309:GLU:CA	2.34	0.57
4:C:704:LYS:NZ	4:C:775:GLU:OE2	2.32	0.57
4:B:281:ILE:HD11	4:B:308:TYR:C	2.24	0.57
2:I:4:G:H5"	4:B:386:ARG:HD3	1.86	0.57
4:C:531:SER:OG	7:C:3088:HOH:O	2.17	0.57
4:D:486:HIS:NE2	4:D:490:MET:CG	2.67	0.57
4:B:261:LEU:C	4:B:263:GLY:H	2.07	0.57
4:A:712:ASP:O	4:A:716:GLY:N	2.36	0.57
3:P:3:DC:H5'	7:D:3034:HOH:O	2.04	0.57
4:C:583:GLN:O	4:C:587:ILE:HG12	2.05	0.57
4:A:882:PHE:N	4:A:882:PHE:CD1	2.71	0.57
4:C:727:TRP:CE2	4:C:735:VAL:HG11	2.39	0.57
4:D:870:LEU:CD2	4:D:872:LEU:HD23	2.34	0.57
4:B:823:ASN:O	4:B:824:LEU:C	2.40	0.57
4:A:438:ASP:O	4:A:439:MET:C	2.42	0.57
4:A:849:PHE:O	4:A:852:GLN:N	2.38	0.57
4:A:461:LYS:HE3	4:A:479:ILE:HG23	1.84	0.57
4:A:514:PHE:CD1	4:A:514:PHE:C	2.76	0.57
4:D:632:ARG:HH22	6:D:2003:APC:C5'	2.18	0.57
4:B:298:ARG:HE	4:B:419:ASN:CB	2.18	0.57
4:B:828:VAL:O	4:B:831:THR:HG22	2.05	0.57
4:D:297:VAL:HG21	4:D:733:PHE:HZ	1.69	0.57
4:C:10:ASP:OD1	7:C:3066:HOH:O	2.18	0.57
4:A:468:ALA:HB2	4:A:511:PHE:CD1	2.38	0.57
4:D:543:ILE:HG22	4:D:543:ILE:O	2.05	0.57
4:A:643:GLU:HG3	4:A:682:TRP:CG	2.39	0.57
4:D:720:ARG:NH1	4:D:721:LYS:O	2.38	0.57
4:C:322:ILE:HG22	4:C:323:ALA:N	2.19	0.57
4:B:571:TYR:HD2	4:B:631:LYS:HA	1.69	0.57
4:A:562:LEU:CD2	4:A:870:LEU:HD11	2.35	0.57
4:D:19:ILE:CG2	7:D:3014:HOH:O	2.51	0.57
4:B:677:MET:SD	4:B:681:ILE:CD1	2.93	0.57
4:B:780:PRO:HA	4:B:783:VAL:CG2	2.35	0.57
4:D:439:MET:HG3	4:D:509:PHE:CD2	2.40	0.57
4:A:404:GLN:HG2	4:A:432:PHE:HB2	1.86	0.57
4:D:236:VAL:HB	4:D:239:GLN:HB2	1.87	0.57
4:D:88:TRP:O	4:D:92:VAL:HG23	2.04	0.57
4:C:579:ASN:HA	4:C:582:LEU:CD1	2.33	0.57
4:B:557:ARG:HB2	4:B:562:LEU:HD12	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:374:LEU:H	4:A:374:LEU:HD12	1.68	0.57
4:A:779:ALA:O	4:A:783:VAL:HG23	2.05	0.57
4:A:137:VAL:HG12	4:A:217:ILE:HD11	1.86	0.57
4:B:264:ILE:HG22	4:B:264:ILE:O	2.05	0.57
4:B:702:ALA:HB1	4:B:849:PHE:HE2	1.67	0.57
4:D:338:ALA:HB2	4:D:509:PHE:CE1	2.40	0.57
4:B:162:PHE:HD1	4:B:190:MET:SD	2.27	0.57
4:A:429:VAL:HG12	4:A:430:SER:N	2.18	0.57
4:D:551:ARG:HB2	4:D:868:GLY:N	2.16	0.57
4:D:42:GLU:O	4:D:43:SER:C	2.43	0.57
4:C:711:LYS:HG2	4:C:718:ILE:HA	1.87	0.57
4:A:685:VAL:O	4:A:687:VAL:N	2.37	0.56
4:A:312:TYR:CZ	4:A:314:PRO:HG3	2.40	0.56
4:A:777:GLY:O	4:A:781:ASN:OD1	2.23	0.56
4:A:828:VAL:CG2	4:A:829:ARG:H	2.14	0.56
1:E:12:DT:C2'	1:E:13:DC:C5'	2.69	0.56
4:A:109:ILE:CD1	4:A:149:ALA:HB2	2.35	0.56
4:B:536:PHE:CE2	4:B:825:PHE:HD2	2.23	0.56
4:B:571:TYR:OH	4:B:635:MET:CE	2.52	0.56
4:B:734:PRO:O	4:B:734:PRO:CG	2.52	0.56
4:A:502:TRP:CG	4:A:512:LEU:CD1	2.88	0.56
4:A:88:TRP:HE3	4:A:91:GLU:OE1	1.88	0.56
4:D:401:MET:HE3	4:D:440:THR:HG21	1.87	0.56
4:D:201:TRP:HA	4:D:204:TRP:HD1	1.69	0.56
4:C:676:TYR:O	4:C:677:MET:C	2.43	0.56
4:A:583:GLN:CB	7:A:3056:HOH:O	2.46	0.56
4:C:721:LYS:HG2	4:C:722:ARG:N	2.19	0.56
4:B:457:TYR:CE1	4:B:521:VAL:HG11	2.40	0.56
4:C:632:ARG:HH22	6:C:2002:APC:C5'	2.13	0.56
4:A:423:ARG:HG2	4:A:781:ASN:HD22	1.70	0.56
4:B:532:LEU:O	4:B:818:PRO:HD3	2.04	0.56
4:B:42:GLU:O	4:B:43:SER:C	2.44	0.56
4:D:505:GLN:NE2	4:D:505:GLN:CA	2.66	0.56
4:B:163:LYS:NZ	4:B:167:GLU:N	2.54	0.56
4:D:745:THR:HB	4:D:756:ARG:NH1	2.21	0.56
4:C:5:ASN:ND2	4:C:7:ALA:HB3	2.19	0.56
4:A:807:PHE:N	4:A:807:PHE:CD1	2.73	0.56
4:A:579:ASN:HA	4:A:582:LEU:CD1	2.35	0.56
4:A:379:ARG:HE	4:A:656:GLN:HG2	1.70	0.56
4:A:308:TYR:CE2	4:A:736:TRP:HZ3	2.23	0.56
4:A:820:ASP:O	4:A:823:ASN:HB2	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:831:THR:CG2	4:C:832:MET:N	2.69	0.56
7:K:1088:HOH:O	4:C:641:SER:HA	2.06	0.56
4:D:420:MET:HA	4:D:425:ARG:O	2.04	0.56
4:B:541:SER:O	4:B:542:GLY:C	2.43	0.56
4:B:841:VAL:HG12	7:B:3081:HOH:O	2.05	0.56
4:B:632:ARG:CD	6:B:2001:APC:HN61	2.16	0.56
1:H:17:DG:H3'	4:B:57:ARG:NH2	2.20	0.56
4:B:616:LEU:O	4:B:618:GLY:N	2.38	0.56
4:D:512:LEU:O	4:D:515:CYS:HB2	2.05	0.56
4:C:334:VAL:HG21	4:C:513:ALA:CB	2.29	0.56
4:B:66:ASP:OD1	4:B:752:LEU:HD21	2.05	0.56
4:A:268:PHE:HB3	4:A:430:SER:HA	1.86	0.56
4:C:534:LEU:HD12	4:C:821:ALA:HB2	1.86	0.56
4:A:155:ARG:CB	4:A:163:LYS:HE3	2.31	0.56
4:A:383:ALA:O	4:A:384:VAL:C	2.41	0.56
4:B:173:ARG:NH1	4:B:182:PHE:CD1	2.74	0.56
4:C:472:LYS:HE3	7:C:3049:HOH:O	2.05	0.56
4:A:734:PRO:O	4:A:734:PRO:HG2	2.05	0.56
4:A:816:THR:HG22	4:A:817:ILE:N	2.18	0.56
4:B:51:PHE:CD2	4:B:51:PHE:C	2.78	0.56
4:C:551:ARG:NH1	4:C:551:ARG:CG	2.68	0.56
4:B:541:SER:O	4:B:544:GLN:HB3	2.04	0.56
4:B:56:GLU:OE1	4:B:57:ARG:CA	2.53	0.56
4:B:634:VAL:O	4:B:634:VAL:HG22	2.05	0.56
4:B:695:ALA:O	4:B:699:LEU:CD1	2.50	0.56
4:B:846:TYR:CD2	4:B:864:LEU:HD11	2.40	0.56
4:B:465:ALA:O	4:B:468:ALA:HB3	2.05	0.56
4:A:436:GLY:HA3	4:A:440:THR:HB	1.87	0.56
4:A:508:PRO:HG2	4:A:509:PHE:H	1.69	0.56
4:C:474:PRO:HB2	4:C:476:PRO:CD	2.36	0.56
4:B:233:ASN:CB	4:B:239:GLN:HB3	2.35	0.56
4:B:335:LEU:HD21	4:B:406:ASN:OD1	2.06	0.56
4:D:390:ALA:HB1	4:D:394:ARG:NH2	2.19	0.56
4:D:303:LYS:HG3	4:D:304:ALA:H	1.68	0.56
4:C:741:LYS:HB2	4:C:770:ASP:HB2	1.86	0.56
4:C:152:GLY:O	4:C:156:ASP:OD2	2.22	0.56
4:A:792:ARG:O	4:A:796:VAL:HG22	2.06	0.56
4:A:798:ALA:HB2	4:A:827:ALA:HB1	1.86	0.56
4:A:14:ILE:HG13	7:A:3082:HOH:O	2.05	0.56
4:A:109:ILE:HD13	4:A:145:ILE:CG2	2.20	0.56
4:B:446:LEU:HD13	4:B:806:SER:HB3	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:620:TRP:CD2	4:B:677:MET:HE2	2.41	0.56
4:B:210:ILE:O	4:B:214:VAL:HG22	2.06	0.56
4:B:587:ILE:O	4:B:614:LYS:HE3	2.05	0.56
4:D:437:ASN:HD22	4:D:437:ASN:C	2.07	0.56
4:B:19:ILE:CD1	4:B:20:PRO:HD2	2.35	0.56
4:A:620:TRP:HA	4:A:620:TRP:CE3	2.40	0.56
4:A:314:PRO:HD2	4:A:315:GLU:H	1.70	0.56
4:D:828:VAL:HA	4:D:831:THR:CG2	2.35	0.56
4:D:712:ASP:HB2	4:D:719:LEU:HD11	1.88	0.56
4:B:783:VAL:O	4:B:784:HIS:O	2.24	0.56
4:B:827:ALA:O	4:B:828:VAL:C	2.44	0.56
4:C:335:LEU:HD21	4:C:406:ASN:OD1	2.06	0.56
4:A:81:MET:SD	4:A:85:ILE:HD11	2.45	0.56
4:D:669:GLN:HG3	4:D:672:GLN:NE2	2.21	0.56
4:B:5:ASN:HB3	4:B:8:LYS:HE3	1.88	0.56
4:A:143:ARG:HG2	7:A:3010:HOH:O	2.05	0.56
4:B:89:PHE:HZ	4:B:106:LEU:O	1.89	0.56
4:C:275:PRO:HB2	4:C:324:GLN:CD	2.25	0.56
4:C:421:ASP:O	4:C:422:TRP:C	2.44	0.56
4:A:854:HIS:HD2	4:A:856:SER:OG	1.89	0.56
4:D:824:LEU:O	4:D:828:VAL:HG22	2.06	0.56
4:B:550:LEU:HD11	4:B:695:ALA:HB2	1.88	0.56
4:B:795:VAL:O	4:B:796:VAL:C	2.39	0.56
4:B:804:ILE:HA	7:B:3072:HOH:O	2.04	0.56
4:C:452:ILE:HG13	4:C:456:GLY:HA3	1.86	0.56
4:A:347:CYS:SG	4:A:350:GLU:HG2	2.46	0.56
4:B:109:ILE:HG13	4:B:149:ALA:HB2	1.88	0.56
4:B:199:GLU:HG2	4:B:201:TRP:HD1	1.70	0.56
4:A:486:HIS:HE1	7:A:3212:HOH:O	1.89	0.56
4:C:485:ASN:O	4:C:489:ILE:HG13	2.06	0.56
4:C:711:LYS:HG2	4:C:717:GLU:O	2.06	0.56
4:D:199:GLU:OE2	4:D:202:SER:HB2	2.04	0.56
4:C:42:GLU:O	4:C:46:MET:HE2	2.06	0.56
4:A:316:VAL:HG13	4:A:792:ARG:NE	2.20	0.56
4:C:278:TRP:CZ3	4:C:284:GLY:HA3	2.41	0.56
4:C:423:ARG:CD	4:C:781:ASN:ND2	2.68	0.56
1:K:11:DA:H2'	1:K:12:DT:H73	1.88	0.56
4:D:421:ASP:OD1	4:D:421:ASP:O	2.24	0.56
4:C:882:PHE:N	4:C:882:PHE:HD1	2.02	0.56
4:B:478:ARG:O	4:B:481:PHE:HB3	2.06	0.56
4:A:390:ALA:C	4:A:392:LYS:H	2.10	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:173:ARG:NH1	4:B:182:PHE:HD1	2.03	0.56
4:B:626:THR:O	4:B:627:ARG:C	2.43	0.56
4:B:86:ASN:HB3	7:B:3090:HOH:O	2.04	0.56
4:A:700:LYS:NZ	7:A:3017:HOH:O	2.25	0.56
4:A:534:LEU:N	4:A:534:LEU:HD23	2.19	0.56
4:A:656:GLN:N	4:A:657:PRO:HD2	2.21	0.56
4:C:273:VAL:O	4:C:274:PRO:C	2.42	0.56
4:C:281:ILE:HG22	4:C:282:THR:N	2.21	0.56
4:C:322:ILE:HG21	4:C:795:VAL:CG1	2.36	0.56
4:B:620:TRP:O	4:B:623:TYR:HB3	2.05	0.56
4:B:779:ALA:O	4:B:783:VAL:HG22	2.06	0.56
4:B:730:PRO:HD2	4:B:786:GLN:HE21	1.69	0.56
4:B:846:TYR:CD1	4:B:850:ALA:HB2	2.41	0.56
4:B:746:ARG:NH2	4:B:753:GLY:HA2	2.21	0.56
4:A:80:LYS:CE	4:A:224:THR:HG22	2.36	0.56
4:A:348:PRO:C	4:A:349:VAL:CG2	2.74	0.56
4:D:432:PHE:CZ	4:D:444:LEU:HD11	2.40	0.56
4:D:313:MET:O	4:D:317:TYR:HD2	1.89	0.56
4:B:89:PHE:CZ	4:B:106:LEU:O	2.58	0.56
4:D:812:ASP:N	4:D:812:ASP:OD1	2.38	0.56
4:A:281:ILE:HG13	4:A:309:GLU:HA	1.88	0.56
4:C:416:PHE:HB2	4:C:418:TYR:HE1	1.70	0.56
4:B:639:TYR:HA	7:B:3018:HOH:O	2.04	0.56
4:B:737:GLN:HE22	4:B:777:GLY:C	2.09	0.56
4:B:849:PHE:O	4:B:852:GLN:HB2	2.06	0.56
4:B:329:LYS:HG2	4:B:445:THR:O	2.05	0.56
4:C:341:ILE:CD1	4:C:348:PRO:HB3	2.29	0.56
4:C:512:LEU:O	4:C:512:LEU:HD12	2.06	0.56
4:A:333:LYS:CB	4:A:516:PHE:CD2	2.89	0.56
4:C:532:LEU:HD23	4:C:532:LEU:O	2.06	0.56
1:E:9:DA:N6	3:G:1:DG:N2	2.54	0.56
4:D:30:GLU:HB3	4:D:34:ARG:HH21	1.70	0.56
4:C:571:TYR:CE2	4:C:631:LYS:HE3	2.42	0.55
4:A:545:HIS:HE1	4:A:787:ASP:HA	1.71	0.55
4:C:814:PHE:N	4:C:814:PHE:CD1	2.75	0.55
3:J:1:DG:H1'	3:J:2:DT:C7	2.36	0.55
4:C:116:TYR:OH	4:C:752:LEU:HD22	2.06	0.55
4:C:543:ILE:HD13	4:C:689:VAL:HG11	1.88	0.55
4:A:433:ASN:HB2	4:A:434:PRO:HD2	1.88	0.55
4:C:205:HIS:O	4:C:207:GLU:N	2.39	0.55
4:A:824:LEU:O	4:A:827:ALA:N	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:563:PRO:CB	4:A:878:SER:HA	2.33	0.55
4:A:14:ILE:HD11	4:A:290:GLY:HA2	1.86	0.55
4:C:423:ARG:HD2	4:C:781:ASN:CG	2.26	0.55
4:C:421:ASP:C	4:C:423:ARG:N	2.57	0.55
1:N:12:DT:H5'	4:D:781:ASN:HD21	1.71	0.55
4:B:576:LYS:NZ	7:B:3102:HOH:O	2.39	0.55
4:B:407:LYS:CG	4:B:408:PHE:CE2	2.85	0.55
4:A:342:THR:HG22	4:A:348:PRO:CG	2.35	0.55
4:D:744:GLN:HB3	4:D:756:ARG:HB2	1.88	0.55
4:C:155:ARG:HG2	4:C:155:ARG:O	2.06	0.55
4:C:105:PHE:C	4:C:107:GLN:H	2.10	0.55
4:A:236:VAL:HB	4:A:239:GLN:HB2	1.88	0.55
4:C:50:ARG:CG	4:C:50:ARG:NH1	2.69	0.55
4:A:706:LEU:HD11	4:A:849:PHE:CD2	2.41	0.55
4:A:715:THR:CG2	4:A:717:GLU:HB2	2.36	0.55
4:C:16:LEU:HD21	4:C:41:HIS:ND1	2.20	0.55
4:A:526:LEU:H	4:A:526:LEU:HD12	1.66	0.55
4:A:292:ARG:N	4:A:293:PRO:HD3	2.21	0.55
4:D:717:GLU:O	4:D:719:LEU:HD12	2.07	0.55
4:B:423:ARG:HH11	4:B:423:ARG:CG	2.19	0.55
4:B:698:TRP:CZ2	4:B:864:LEU:HG	2.41	0.55
4:D:505:GLN:N	4:D:505:GLN:HE21	2.04	0.55
4:B:473:VAL:HG11	4:B:477:GLU:CB	2.36	0.55
4:D:772:HIS:O	4:D:775:GLU:N	2.38	0.55
4:B:71:LYS:N	4:B:72:PRO:CD	2.69	0.55
4:B:525:GLY:C	4:B:527:SER:H	2.10	0.55
4:B:182:PHE:O	4:B:186:VAL:HG23	2.06	0.55
4:C:711:LYS:CG	4:C:718:ILE:HA	2.36	0.55
4:A:578:VAL:CG1	4:A:680:LEU:HB3	2.36	0.55
4:A:650:VAL:O	4:A:654:THR:HG22	2.07	0.55
1:N:9:DA:H2"	1:N:10:DT:OP1	2.05	0.55
4:B:492:CYS:O	4:B:496:PRO:CD	2.50	0.55
4:B:489:ILE:CG2	4:B:515:CYS:HB3	2.37	0.55
4:A:59:LEU:HD23	4:A:64:VAL:HG22	1.88	0.55
4:B:291:ARG:CB	7:B:3037:HOH:O	2.51	0.55
4:B:411:HIS:O	4:B:413:ALA:N	2.40	0.55
1:E:10:DT:OP2	4:A:645:GLY:HA3	2.05	0.55
4:A:778:ILE:CG2	4:A:779:ALA:H	2.19	0.55
4:B:308:TYR:HE2	4:B:734:PRO:HG2	1.72	0.55
4:B:780:PRO:CD	4:B:781:ASN:H	2.19	0.55
4:D:817:ILE:HG12	4:D:820:ASP:OD2	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:9:DA:N6	3:M:1:DG:N2	2.54	0.55
4:A:632:ARG:HG2	7:A:3022:HOH:O	2.06	0.55
4:A:474:PRO:HB2	4:A:476:PRO:HD2	1.88	0.55
3:J:1:DG:H4'	3:J:2:DT:H5'	1.87	0.55
4:B:588:ASN:O	4:B:614:LYS:HD2	2.06	0.55
4:C:395:ARG:HE	4:C:399:GLU:CG	2.20	0.55
4:D:826:LYS:HD2	7:D:3041:HOH:O	2.05	0.55
4:A:308:TYR:O	4:A:311:VAL:N	2.35	0.55
4:A:797:TRP:CZ2	4:A:801:LYS:HG3	2.40	0.55
4:D:286:TYR:CZ	4:D:417:PRO:HG3	2.41	0.55
4:B:285:GLY:HA2	4:B:324:GLN:HE22	1.71	0.55
4:A:401:MET:N	4:A:401:MET:SD	2.79	0.55
4:A:350:GLU:O	7:A:3222:HOH:O	2.18	0.55
4:B:137:VAL:HG12	4:B:217:ILE:CD1	2.34	0.55
4:C:582:LEU:HD11	4:C:625:VAL:HG21	1.88	0.55
4:C:623:TYR:HA	4:C:666:MET:HE1	1.89	0.55
4:C:173:ARG:NH2	4:C:182:PHE:HB2	2.22	0.55
4:B:275:PRO:CD	7:B:3116:HOH:O	2.48	0.55
4:A:669:GLN:HG2	4:A:672:GLN:NE2	2.20	0.55
4:B:854:HIS:HD1	4:B:855:GLU:H	1.55	0.55
4:D:277:PRO:HA	7:D:3029:HOH:O	2.06	0.55
4:C:807:PHE:N	4:C:807:PHE:CD1	2.74	0.55
4:D:743:ILE:O	4:D:756:ARG:NH2	2.40	0.55
4:B:689:VAL:O	4:B:690:VAL:C	2.45	0.55
4:B:345:LYS:HZ1	4:B:351:ASP:H	1.55	0.55
4:C:183:MET:HE3	4:C:186:VAL:HG21	1.89	0.55
4:A:707:ALA:O	4:A:708:ALA:O	2.25	0.55
4:C:744:GLN:HA	4:C:756:ARG:HD3	1.89	0.55
4:B:569:ASP:OD1	4:B:569:ASP:O	2.24	0.55
4:A:619:GLN:O	4:A:623:TYR:N	2.37	0.55
4:A:630:THR:O	4:A:631:LYS:O	2.25	0.55
4:A:779:ALA:HB3	4:A:780:PRO:CD	2.37	0.55
4:A:829:ARG:O	4:A:833:VAL:HG23	2.06	0.55
4:A:317:TYR:O	4:A:321:ASN:ND2	2.33	0.55
4:C:40:GLU:OE2	4:C:286:TYR:CD1	2.58	0.55
4:D:448:LYS:CD	4:D:806:SER:HB3	2.36	0.55
4:B:345:LYS:O	4:B:346:HIS:C	2.45	0.55
4:D:652:GLU:O	4:D:657:PRO:HD3	2.06	0.55
4:C:770:ASP:O	4:C:770:ASP:OD1	2.25	0.55
4:C:684:SER:O	4:C:687:VAL:HG22	2.07	0.55
4:B:76:THR:CG2	7:B:3212:HOH:O	2.54	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:14:ILE:CD1	4:A:14:ILE:N	2.69	0.55
4:A:287:TRP:O	4:A:288:ALA:O	2.25	0.55
4:B:803:GLY:O	4:B:804:ILE:O	2.25	0.55
4:B:813:SER:C	4:B:814:PHE:CD1	2.81	0.55
4:B:388:ASP:C	4:B:388:ASP:OD1	2.45	0.55
4:D:816:THR:HG22	4:D:817:ILE:H	1.71	0.55
4:C:579:ASN:OD1	4:C:582:LEU:HD12	2.07	0.55
4:C:106:LEU:HG	4:C:212:VAL:HG13	1.89	0.55
4:D:311:VAL:CG1	4:D:312:TYR:N	2.70	0.55
4:C:710:VAL:HG13	4:C:710:VAL:O	2.07	0.55
4:C:278:TRP:CD2	4:C:284:GLY:HA3	2.42	0.54
4:B:419:ASN:O	4:B:426:VAL:HA	2.07	0.54
4:B:398:LEU:HG	4:B:439:MET:HE2	1.89	0.54
4:B:587:ILE:HG22	4:B:588:ASN:HD22	1.71	0.54
4:D:241:SER:O	4:D:243:THR:HG23	2.06	0.54
4:C:448:LYS:CE	4:C:806:SER:OG	2.54	0.54
1:E:5:DA:H2	3:G:7:DT:O2	1.89	0.54
4:C:21:PHE:C	4:C:23:THR:H	2.11	0.54
1:E:9:DA:C2	4:A:644:PHE:CD1	2.95	0.54
4:A:177:VAL:HB	7:A:3038:HOH:O	2.06	0.54
4:A:13:ASP:HB3	4:A:14:ILE:HD12	1.88	0.54
4:C:433:ASN:C	4:C:433:ASN:OD1	2.46	0.54
4:C:728:VAL:HG22	4:C:734:PRO:HB3	1.89	0.54
4:C:777:GLY:O	4:C:781:ASN:OD1	2.25	0.54
4:D:558:ALA:HB1	4:D:570:ILE:HD13	1.88	0.54
4:B:532:LEU:HG	4:B:533:PRO:HD2	1.90	0.54
4:C:814:PHE:CE1	4:C:883:ALA:CB	2.91	0.54
4:B:266:PRO:HG2	4:B:268:PHE:CE1	2.41	0.54
4:B:545:HIS:O	4:B:546:PHE:C	2.42	0.54
4:B:662:GLY:C	4:B:663:LYS:O	2.45	0.54
4:B:849:PHE:O	4:B:850:ALA:C	2.46	0.54
4:C:340:VAL:C	4:C:342:THR:N	2.60	0.54
4:B:398:LEU:C	4:B:398:LEU:CD2	2.75	0.54
4:D:155:ARG:CA	4:D:163:LYS:HE3	2.37	0.54
4:C:45:GLU:O	4:C:48:GLU:HB3	2.07	0.54
4:A:641:SER:HB2	4:A:646:PHE:HE1	1.73	0.54
4:C:278:TRP:CD1	4:C:320:ILE:HG22	2.43	0.54
1:K:12:DT:H5"	4:C:422:TRP:CH2	2.42	0.54
4:C:334:VAL:CG2	4:C:513:ALA:HB2	2.29	0.54
4:C:84:ARG:HB2	4:C:223:SER:HB3	1.89	0.54
4:B:109:ILE:O	4:B:110:LYS:C	2.46	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:564:SER:HG	4:B:566:THR:H	1.53	0.54
4:B:27:HIS:HD2	7:B:3169:HOH:O	1.88	0.54
4:B:318:LYS:O	4:B:319:ALA:C	2.45	0.54
4:A:640:GLY:O	4:A:641:SER:C	2.46	0.54
4:A:35:GLU:O	4:A:36:GLN:C	2.46	0.54
4:D:577:LYS:O	4:D:581:ILE:HG13	2.07	0.54
4:D:632:ARG:HH22	6:D:2003:APC:H5'2	1.72	0.54
4:B:639:TYR:CA	7:B:3018:HOH:O	2.55	0.54
4:B:423:ARG:NH2	4:B:784:HIS:ND1	2.53	0.54
4:B:784:HIS:O	4:B:785:SER:C	2.44	0.54
1:H:12:DT:C2'	1:H:13:DC:H6	2.19	0.54
4:C:508:PRO:HB2	4:C:509:PHE:HD2	1.71	0.54
4:C:509:PHE:H	4:C:509:PHE:HD2	1.54	0.54
3:P:9:DC:H2"	7:P:1110:HOH:O	2.06	0.54
4:B:454:LYS:HG3	4:B:455:GLU:H	1.72	0.54
4:C:576:LYS:O	4:C:580:GLU:HG3	2.07	0.54
4:C:403:GLU:N	7:C:3123:HOH:O	2.39	0.54
4:B:334:VAL:HG12	4:B:443:LEU:HD23	1.88	0.54
4:A:649:GLN:O	4:A:650:VAL:C	2.46	0.54
4:A:316:VAL:HG13	4:A:792:ARG:HD2	1.89	0.54
4:A:793:LYS:O	4:A:794:THR:C	2.45	0.54
4:A:11:PHE:HB3	4:A:41:HIS:HE1	1.72	0.54
4:C:793:LYS:NZ	4:C:835:THR:OG1	2.32	0.54
4:C:833:VAL:HG22	4:C:872:LEU:O	2.08	0.54
4:B:573:ILE:HD13	7:B:3102:HOH:O	2.07	0.54
4:B:677:MET:O	4:B:678:ALA:C	2.44	0.54
4:B:810:ILE:O	4:B:813:SER:HB2	2.07	0.54
4:D:446:LEU:HG	4:D:533:PRO:HD3	1.90	0.54
4:B:181:ALA:HA	4:B:184:GLN:NE2	2.22	0.54
2:I:8:U:O3'	4:B:812:ASP:OD2	2.24	0.54
4:D:47:GLY:O	4:D:50:ARG:HB3	2.08	0.54
4:A:620:TRP:CE2	4:A:677:MET:HB2	2.43	0.54
4:A:13:ASP:CG	4:A:291:ARG:HH21	2.10	0.54
4:A:720:ARG:HH21	4:A:857:GLN:NE2	2.06	0.54
4:B:803:GLY:O	4:B:804:ILE:C	2.46	0.54
4:D:512:LEU:CA	4:D:515:CYS:SG	2.86	0.54
4:B:473:VAL:HG11	4:B:477:GLU:HB2	1.88	0.54
4:A:204:TRP:HH2	4:A:212:VAL:HG21	1.67	0.54
4:D:817:ILE:HB	4:D:818:PRO:CD	2.38	0.54
4:A:76:THR:C	4:A:79:PRO:HD2	2.27	0.54
4:B:742:PRO:HB3	4:B:744:GLN:CD	2.27	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:669:GLN:O	4:A:672:GLN:N	2.41	0.54
4:C:656:GLN:HE21	4:C:656:GLN:HA	1.72	0.54
4:D:50:ARG:NH1	4:D:267:MET:HG2	2.23	0.54
4:A:555:GLY:O	4:A:558:ALA:HB3	2.08	0.54
4:D:258:ALA:O	4:D:259:GLY:O	2.26	0.54
4:A:474:PRO:O	4:A:477:GLU:HB2	2.07	0.54
4:A:275:PRO:O	4:A:277:PRO:HD3	2.07	0.54
4:A:471:ASP:O	4:A:472:LYS:HG3	2.08	0.54
4:C:273:VAL:HG23	4:C:274:PRO:O	2.08	0.54
4:C:726:HIS:CD2	4:C:736:TRP:CE2	2.96	0.54
4:B:297:VAL:HG12	4:B:299:THR:HG22	1.88	0.54
4:B:790:HIS:HE1	4:B:831:THR:CG2	2.20	0.54
4:B:814:PHE:N	4:B:814:PHE:CD1	2.76	0.54
4:A:88:TRP:CE3	4:A:91:GLU:OE1	2.61	0.54
4:B:211:HIS:O	4:B:214:VAL:HG23	2.08	0.54
4:D:744:GLN:HE21	4:D:756:ARG:H	1.56	0.54
4:A:120:LYS:HG3	4:A:752:LEU:HD21	1.90	0.54
4:D:19:ILE:CD1	4:D:20:PRO:HD2	2.36	0.54
4:D:21:PHE:C	4:D:23:THR:N	2.61	0.54
4:C:6:ILE:HD13	7:C:3031:HOH:O	2.06	0.54
6:A:2000:APC:C4'	7:A:3238:HOH:O	2.41	0.54
4:A:636:THR:HG21	6:A:2000:APC:N6	2.23	0.54
4:D:882:PHE:O	4:D:883:ALA:CB	2.56	0.54
4:B:728:VAL:HG13	4:B:733:PHE:C	2.28	0.54
4:B:823:ASN:O	4:B:825:PHE:N	2.40	0.54
4:B:882:PHE:HE2	7:B:3089:HOH:O	1.90	0.54
4:A:216:CYS:O	4:A:219:MET:N	2.40	0.54
4:C:474:PRO:CB	4:C:476:PRO:HD2	2.37	0.54
4:C:161:HIS:C	4:C:163:LYS:N	2.62	0.54
4:A:428:ALA:H	4:A:435:GLN:NE2	2.04	0.54
4:A:395:ARG:O	4:A:399:GLU:HG3	2.08	0.54
4:A:654:THR:O	4:A:658:ALA:HB2	2.07	0.54
4:A:810:ILE:HG22	4:A:810:ILE:O	2.07	0.54
4:A:44:TYR:CD2	4:A:266:PRO:HB3	2.43	0.54
4:C:312:TYR:CE1	4:C:314:PRO:HG3	2.42	0.54
1:H:15:DC:H2"	1:H:16:DC:H5'	1.89	0.54
4:D:507:SER:O	4:D:511:PHE:N	2.41	0.54
4:B:754:GLN:O	4:B:755:PHE:O	2.25	0.54
4:C:457:TYR:CE1	4:C:521:VAL:CG1	2.87	0.54
4:C:120:LYS:HD2	4:C:751:PHE:HE2	1.72	0.54
4:D:201:TRP:O	4:D:204:TRP:HB2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:201:TRP:CD2	7:B:3009:HOH:O	2.61	0.54
4:C:199:GLU:HB2	7:C:3075:HOH:O	2.08	0.54
4:A:485:ASN:HD22	4:A:488:ASN:ND2	2.06	0.54
4:A:573:ILE:O	4:A:576:LYS:HB2	2.07	0.54
4:A:656:GLN:O	4:A:658:ALA:N	2.41	0.54
4:C:306:MET:C	4:C:308:TYR:N	2.61	0.54
4:C:830:GLU:O	4:C:831:THR:C	2.46	0.54
4:C:846:TYR:HA	4:C:849:PHE:CE1	2.42	0.54
4:D:829:ARG:O	4:D:833:VAL:HG23	2.08	0.54
1:H:12:DT:H2"	1:H:13:DC:H5'	1.89	0.54
4:B:42:GLU:HG2	4:B:46:MET:HE1	1.89	0.54
4:B:439:MET:O	4:B:440:THR:C	2.43	0.54
4:B:163:LYS:C	4:B:166:VAL:HG23	2.28	0.54
4:B:144:ALA:O	4:B:145:ILE:C	2.46	0.54
4:D:530:CYS:HB3	4:D:818:PRO:HG2	1.90	0.54
4:B:333:LYS:O	4:B:337:VAL:CG2	2.54	0.54
4:B:229:LEU:HD21	4:B:242:GLU:CD	2.29	0.54
4:D:551:ARG:HG3	4:D:551:ARG:HH11	1.73	0.54
4:B:610:LYS:O	4:B:611:LEU:C	2.46	0.54
4:C:89:PHE:HZ	4:C:106:LEU:O	1.91	0.54
4:D:21:PHE:C	4:D:23:THR:H	2.10	0.54
3:M:8:DC:H2"	3:M:9:DC:OP2	2.07	0.54
4:D:594:VAL:HA	4:D:609:VAL:HA	1.90	0.54
4:A:648:GLN:O	4:A:652:GLU:HG2	2.08	0.53
4:A:459:TRP:HZ3	4:A:475:PHE:CE1	2.25	0.53
4:A:544:GLN:OE1	4:A:559:VAL:CG2	2.56	0.53
4:A:882:PHE:N	4:A:882:PHE:HD1	2.05	0.53
4:A:36:GLN:HG3	4:A:273:VAL:HG22	1.91	0.53
4:A:134:VAL:O	4:A:134:VAL:HG22	2.08	0.53
4:C:706:LEU:HD22	4:C:725:VAL:CG2	2.36	0.53
4:D:508:PRO:O	4:D:510:CYS:N	2.41	0.53
4:D:264:ILE:HG22	4:D:292:ARG:HG2	1.89	0.53
4:C:539:SER:HB2	4:C:544:GLN:OE1	2.08	0.53
4:C:291:ARG:CG	7:C:3066:HOH:O	2.56	0.53
4:A:755:PHE:CD1	4:A:755:PHE:N	2.77	0.53
4:C:398:LEU:HD23	4:C:398:LEU:C	2.29	0.53
2:F:6:G:O2'	2:F:7:A:H5'	2.07	0.53
4:A:316:VAL:HG13	4:A:792:ARG:CD	2.38	0.53
4:A:825:PHE:C	4:A:825:PHE:CD1	2.81	0.53
4:A:563:PRO:HB3	4:A:877:GLU:C	2.28	0.53
4:A:292:ARG:O	4:A:292:ARG:HG3	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:11:DA:C5	4:D:639:TYR:CE2	2.96	0.53
4:B:816:THR:HG21	4:B:820:ASP:CB	2.38	0.53
4:D:274:PRO:HB3	4:D:325:ASN:OD1	2.07	0.53
4:B:645:GLY:C	4:B:647:ARG:N	2.60	0.53
4:B:730:PRO:HD3	4:B:786:GLN:NE2	2.24	0.53
4:B:843:ALA:HA	4:B:864:LEU:CD2	2.38	0.53
4:C:514:PHE:CD1	4:C:514:PHE:C	2.81	0.53
4:A:78:LEU:O	4:A:82:ILE:HG13	2.08	0.53
4:D:19:ILE:HG21	7:D:3014:HOH:O	2.08	0.53
4:B:76:THR:HG22	7:B:3212:HOH:O	2.07	0.53
4:C:705:LEU:HD21	4:C:860:LYS:HE3	1.90	0.53
4:A:594:VAL:HA	4:A:609:VAL:HA	1.89	0.53
4:D:523:HIS:O	4:D:524:HIS:ND1	2.41	0.53
4:C:421:ASP:C	4:C:423:ARG:H	2.10	0.53
4:C:739:TYR:HD2	4:C:774:GLN:HA	1.73	0.53
4:B:840:ASP:O	4:B:841:VAL:C	2.46	0.53
4:A:105:PHE:O	4:A:107:GLN:N	2.41	0.53
4:D:302:LYS:HE3	4:D:306:MET:CE	2.38	0.53
4:B:201:TRP:CG	7:B:3009:HOH:O	2.60	0.53
4:A:19:ILE:HG22	7:A:3120:HOH:O	2.04	0.53
4:D:14:ILE:HG21	4:D:288:ALA:HB1	1.89	0.53
4:A:236:VAL:HG11	4:A:239:GLN:HG3	1.89	0.53
4:C:791:LEU:C	4:C:791:LEU:HD23	2.29	0.53
4:B:710:VAL:O	4:B:710:VAL:HG13	2.08	0.53
4:A:651:LEU:CD1	4:A:656:GLN:NE2	2.72	0.53
4:A:328:TRP:HA	4:A:446:LEU:HA	1.91	0.53
4:A:546:PHE:CZ	4:A:783:VAL:CG2	2.88	0.53
4:C:826:LYS:O	4:C:830:GLU:HG3	2.08	0.53
4:C:840:ASP:O	4:C:843:ALA:N	2.41	0.53
4:D:419:ASN:HD22	4:D:419:ASN:N	2.06	0.53
4:B:633:SER:HB3	4:B:646:PHE:CD1	2.43	0.53
4:B:465:ALA:HB1	4:B:470:VAL:HB	1.89	0.53
4:A:333:LYS:HB2	4:A:516:PHE:CD2	2.43	0.53
4:B:112:GLU:H	4:B:112:GLU:CD	2.11	0.53
4:B:69:ALA:O	4:B:72:PRO:HD2	2.08	0.53
4:A:643:GLU:HG3	4:A:682:TRP:CB	2.39	0.53
4:A:423:ARG:HH21	4:A:784:HIS:CB	2.22	0.53
4:A:809:LEU:C	4:A:810:ILE:HG13	2.28	0.53
4:A:11:PHE:CZ	4:A:44:TYR:HB3	2.43	0.53
4:C:830:GLU:HG2	4:C:876:LEU:CD2	2.38	0.53
4:D:810:ILE:HB	4:D:813:SER:CB	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:427:TYR:HE1	4:B:811:HIS:NE2	2.06	0.53
4:C:452:ILE:HG23	4:C:453:GLY:H	1.74	0.53
4:C:88:TRP:O	4:C:92:VAL:HG23	2.07	0.53
2:I:5:C:C2	2:I:6:G:C8	2.96	0.53
4:D:677:MET:O	4:D:680:LEU:HB2	2.08	0.53
4:A:374:LEU:C	4:A:376:ALA:H	2.12	0.53
4:A:229:LEU:HD13	4:A:244:ILE:HD13	1.90	0.53
4:C:719:LEU:N	4:C:719:LEU:HD12	2.24	0.53
4:A:796:VAL:O	4:A:797:TRP:C	2.45	0.53
4:A:881:ALA:C	4:A:882:PHE:O	2.45	0.53
4:D:537:ASP:O	4:D:882:PHE:HB2	2.08	0.53
4:B:696:MET:O	4:B:700:LYS:HB2	2.08	0.53
4:B:795:VAL:O	4:B:796:VAL:O	2.27	0.53
4:B:430:SER:O	4:B:430:SER:OG	2.21	0.53
4:B:50:ARG:CG	4:B:50:ARG:HH11	2.22	0.53
7:I:777:HOH:O	4:B:386:ARG:HD2	2.02	0.53
4:D:619:GLN:HG2	4:D:666:MET:O	2.09	0.53
4:B:99:ARG:NH2	7:B:3046:HOH:O	2.40	0.53
4:A:457:TYR:HE1	4:A:521:VAL:HG11	1.70	0.53
4:A:729:THR:OG1	4:A:733:PHE:HB3	2.08	0.53
4:C:14:ILE:HA	7:C:3014:HOH:O	2.09	0.53
4:C:553:GLU:O	4:C:554:VAL:C	2.47	0.53
4:B:631:LYS:O	4:B:632:ARG:C	2.47	0.53
4:C:118:THR:HG23	4:C:141:ILE:HD13	1.90	0.53
4:B:278:TRP:N	4:B:321:ASN:OD1	2.27	0.53
4:D:754:GLN:O	4:D:755:PHE:O	2.27	0.53
4:A:165:ASN:N	4:A:165:ASN:OD1	2.35	0.53
4:A:828:VAL:C	4:A:830:GLU:N	2.61	0.53
4:A:136:ALA:O	4:A:139:SER:HB3	2.08	0.53
4:C:849:PHE:O	4:C:852:GLN:N	2.42	0.53
1:N:10:DT:H3	6:D:2003:APC:HN62	1.56	0.53
1:H:10:DT:H4'	4:B:639:TYR:O	2.08	0.53
4:C:90:GLU:OE2	4:C:93:LYS:HD2	2.08	0.53
4:D:281:ILE:HD12	4:D:317:TYR:HH	1.73	0.53
4:B:21:PHE:HD1	4:B:21:PHE:O	1.91	0.53
4:D:230:HIS:O	4:D:230:HIS:ND1	2.41	0.53
4:B:68:ALA:HB3	4:B:261:LEU:HD21	1.91	0.53
4:A:30:GLU:HB2	7:A:3035:HOH:O	2.09	0.53
4:C:472:LYS:HA	4:C:567:VAL:HG11	1.89	0.53
4:C:592:ASN:O	4:C:593:GLU:HB2	2.09	0.53
4:C:80:LYS:HD2	4:C:224:THR:CG2	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:4:G:H1'	4:C:389:LYS:NZ	2.23	0.53
4:A:446:LEU:HB2	4:A:531:SER:O	2.09	0.53
4:C:737:GLN:OE1	4:C:778:ILE:HA	2.08	0.53
4:D:428:ALA:N	4:D:435:GLN:NE2	2.55	0.53
4:B:737:GLN:NE2	4:B:739:TYR:HE2	1.99	0.53
1:H:13:DC:H4'	4:B:427:TYR:CE2	2.44	0.53
4:B:407:LYS:HE2	4:B:408:PHE:CE2	2.44	0.53
4:D:402:LEU:O	4:D:403:GLU:C	2.47	0.53
4:C:96:ARG:HG2	4:C:96:ARG:HH11	1.74	0.53
4:D:854:HIS:CG	4:D:855:GLU:N	2.76	0.53
4:D:849:PHE:O	4:D:852:GLN:N	2.34	0.53
4:C:698:TRP:CZ2	4:C:864:LEU:HG	2.44	0.53
4:D:570:ILE:HA	4:D:573:ILE:HG22	1.91	0.53
4:D:571:TYR:HD1	4:D:631:LYS:HA	1.72	0.53
4:D:711:LYS:C	4:D:719:LEU:HD13	2.29	0.53
4:B:423:ARG:NH1	4:B:784:HIS:CB	2.71	0.53
4:B:793:LYS:HG3	7:B:3181:HOH:O	2.08	0.53
4:B:416:PHE:HE1	4:B:432:PHE:O	1.92	0.53
4:D:349:VAL:HG12	4:D:349:VAL:O	2.09	0.53
4:C:509:PHE:N	4:C:509:PHE:CD2	2.76	0.53
4:C:512:LEU:O	4:C:516:PHE:HD1	1.92	0.53
4:D:32:LEU:CD1	4:D:32:LEU:H	2.08	0.53
4:A:502:TRP:O	4:A:505:GLN:HB2	2.09	0.53
4:D:100:PRO:HG2	4:D:103:PHE:HB3	1.90	0.53
4:D:817:ILE:HB	4:D:818:PRO:HD2	1.90	0.53
4:C:82:ILE:CD1	4:C:112:GLU:HA	2.39	0.53
3:M:5:DA:H2"	3:M:6:DT:C7	2.39	0.53
4:A:109:ILE:CG1	4:A:149:ALA:HB2	2.39	0.52
4:C:871:ASN:ND2	4:C:873:ARG:HB2	2.24	0.52
4:C:158:GLU:OE1	4:C:195:LEU:HB3	2.08	0.52
4:B:663:LYS:HG2	4:B:664:GLY:N	2.21	0.52
4:B:11:PHE:CE1	4:B:44:TYR:HB3	2.43	0.52
4:B:669:GLN:CB	4:B:672:GLN:HE21	2.22	0.52
4:D:233:ASN:HD22	4:D:239:GLN:HE21	1.56	0.52
4:D:744:GLN:CA	4:D:756:ARG:CZ	2.85	0.52
4:D:543:ILE:HG21	4:D:689:VAL:HG11	1.91	0.52
3:J:4:DG:H1'	3:J:5:DA:C8	2.44	0.52
4:A:569:ASP:O	4:A:573:ILE:HG22	2.08	0.52
4:A:727:TRP:CE2	4:A:735:VAL:CG1	2.88	0.52
4:C:320:ILE:O	4:C:324:GLN:HB2	2.09	0.52
4:C:36:GLN:HG3	4:C:273:VAL:CG2	2.38	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:845:PHE:O	4:C:848:GLN:N	2.41	0.52
4:D:739:TYR:HD2	4:D:774:GLN:HA	1.74	0.52
4:B:307:ARG:HB3	4:B:736:TRP:CZ3	2.44	0.52
4:C:19:ILE:HG23	4:C:20:PRO:N	2.23	0.52
4:B:486:HIS:HE1	4:B:490:MET:HG3	1.73	0.52
4:D:114:VAL:HA	4:D:117:ILE:HD12	1.91	0.52
4:A:664:GLY:HA2	4:A:667:PHE:CD2	2.39	0.52
4:D:545:HIS:O	4:D:546:PHE:C	2.47	0.52
2:O:2:C:H5	7:O:443:HOH:O	1.92	0.52
4:D:557:ARG:NH2	7:D:3021:HOH:O	2.43	0.52
4:A:626:THR:O	4:A:627:ARG:C	2.48	0.52
4:A:646:PHE:O	4:A:647:ARG:C	2.48	0.52
1:E:11:DA:H2'	1:E:12:DT:C7	2.39	0.52
4:B:122:THR:HG22	4:B:123:LEU:N	2.24	0.52
4:C:322:ILE:CG2	4:C:795:VAL:CG1	2.88	0.52
4:C:788:GLY:O	4:C:792:ARG:NH1	2.42	0.52
4:C:551:ARG:HD3	4:C:872:LEU:HD21	1.91	0.52
4:C:830:GLU:HG2	4:C:876:LEU:HD21	1.91	0.52
4:D:751:PHE:HB3	4:D:752:LEU:HD12	1.90	0.52
4:C:474:PRO:O	4:C:478:ARG:HG3	2.09	0.52
4:B:146:GLU:O	4:B:147:ASP:C	2.46	0.52
4:D:731:ASP:OD1	4:D:792:ARG:NH2	2.42	0.52
4:B:21:PHE:C	4:B:21:PHE:CD1	2.82	0.52
4:D:154:ILE:O	4:D:159:ALA:HB3	2.09	0.52
4:C:205:HIS:C	4:C:207:GLU:H	2.12	0.52
4:A:755:PHE:N	4:A:755:PHE:HD1	2.07	0.52
4:B:272:VAL:HG11	4:B:411:HIS:HD2	1.73	0.52
3:J:5:DA:H2"	3:J:6:DT:H72	1.91	0.52
1:N:6:DT:C6	1:N:6:DT:H5'	2.44	0.52
4:A:544:GLN:HG2	4:A:559:VAL:CG2	2.30	0.52
4:A:551:ARG:O	4:A:868:GLY:HA3	2.08	0.52
4:C:278:TRP:CD1	4:C:320:ILE:CG2	2.92	0.52
4:C:315:GLU:OE1	4:C:796:VAL:HG11	2.08	0.52
4:C:794:THR:OG1	4:C:831:THR:HG21	2.09	0.52
4:C:843:ALA:HA	4:C:864:LEU:HD21	1.92	0.52
4:D:323:ALA:C	4:D:325:ASN:N	2.61	0.52
4:D:833:VAL:O	4:D:837:GLU:HG3	2.09	0.52
1:H:12:DT:C5'	4:B:423:ARG:HE	2.22	0.52
4:D:384:VAL:HA	7:D:3158:HOH:O	2.10	0.52
4:A:269:GLN:O	4:A:430:SER:HB2	2.10	0.52
4:D:458:TYR:CD2	4:D:458:TYR:C	2.82	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:383:ALA:C	4:A:385:TYR:H	2.11	0.52
4:B:19:ILE:HG23	4:B:20:PRO:CD	2.39	0.52
4:D:207:GLU:O	4:D:211:HIS:CE1	2.63	0.52
4:C:770:ASP:O	4:C:772:HIS:N	2.42	0.52
4:A:476:PRO:HG2	4:A:477:GLU:H	1.74	0.52
4:A:546:PHE:HE2	4:A:696:MET:CG	2.22	0.52
4:C:325:ASN:O	4:C:415:TRP:CD1	2.62	0.52
4:C:433:ASN:N	7:C:3164:HOH:O	2.41	0.52
1:H:18:DC:H2"	4:B:63:GLU:OE1	2.10	0.52
4:B:810:ILE:N	4:B:813:SER:HB3	2.25	0.52
4:B:407:LYS:HG2	4:B:408:PHE:HE2	1.66	0.52
4:B:430:SER:O	4:B:432:PHE:N	2.43	0.52
4:B:327:ALA:HB1	4:B:447:ALA:HB3	1.91	0.52
4:D:116:TYR:CE2	4:D:752:LEU:HD22	2.44	0.52
4:C:116:TYR:O	4:C:119:ILE:HG12	2.10	0.52
4:B:231:ARG:HG2	4:B:234:ALA:CB	2.35	0.52
4:A:694:GLU:OE1	4:A:865:PRO:HB3	2.10	0.52
4:B:569:ASP:O	4:B:572:GLY:N	2.41	0.52
2:O:6:G:O2'	2:O:7:A:H5'	2.09	0.52
4:A:422:TRP:CD1	4:A:423:ARG:HG3	2.45	0.52
1:K:14:DG:H3'	7:K:520:HOH:O	2.08	0.52
4:D:777:GLY:O	4:D:778:ILE:C	2.46	0.52
4:D:322:ILE:HG21	4:D:795:VAL:HG12	1.92	0.52
4:B:422:TRP:CD1	4:B:422:TRP:C	2.83	0.52
4:B:720:ARG:NH1	4:B:721:LYS:O	2.43	0.52
4:D:506:ASP:O	4:D:508:PRO:HD2	2.09	0.52
4:B:473:VAL:HG12	4:B:477:GLU:HB2	1.91	0.52
4:D:232:GLN:HB2	4:D:241:SER:O	2.09	0.52
4:A:42:GLU:O	4:A:45:GLU:N	2.42	0.52
4:A:433:ASN:OD1	4:A:435:GLN:N	2.41	0.52
4:B:58:GLN:NE2	7:B:3136:HOH:O	2.41	0.52
4:B:278:TRP:CD2	4:B:284:GLY:HA3	2.44	0.52
4:A:34:ARG:NH2	7:A:3166:HOH:O	2.43	0.52
3:G:5:DA:N6	7:G:73:HOH:O	2.43	0.52
4:C:591:ASP:OD1	7:C:3122:HOH:O	2.19	0.52
4:A:134:VAL:HA	4:A:137:VAL:HB	1.92	0.52
4:B:699:LEU:HD11	4:B:842:LEU:HD11	1.90	0.52
4:B:882:PHE:O	4:B:883:ALA:HB3	2.09	0.52
4:B:330:ILE:HD11	4:B:405:ALA:HA	1.90	0.52
4:B:267:MET:HE3	4:B:431:MET:SD	2.50	0.52
4:A:16:LEU:HB3	4:A:37:LEU:HB3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:95:LYS:HB2	4:D:95:LYS:HZ2	1.75	0.52
4:B:872:LEU:O	4:B:874:ASP:N	2.43	0.52
4:A:299:THR:HG22	4:A:300:HIS:H	1.75	0.52
4:A:627:ARG:NH2	6:A:2000:APC:O2G	2.43	0.52
4:A:830:GLU:O	4:A:831:THR:C	2.47	0.52
4:A:141:ILE:CG2	4:A:145:ILE:HD11	2.39	0.52
4:C:846:TYR:HD2	4:C:864:LEU:HD11	1.74	0.52
1:N:11:DA:H2"	1:N:12:DT:O5'	2.10	0.52
4:D:809:LEU:O	4:D:810:ILE:HG13	2.10	0.52
4:B:422:TRP:NE1	4:B:781:ASN:ND2	2.57	0.52
4:B:403:GLU:O	4:B:404:GLN:C	2.48	0.52
4:D:337:VAL:HG12	4:D:341:ILE:HD11	1.92	0.52
3:G:4:DG:H2"	3:G:5:DA:C8	2.45	0.52
4:C:685:VAL:C	4:C:687:VAL:H	2.13	0.52
4:A:596:THR:HG23	4:A:606:SER:O	2.09	0.52
4:B:276:LYS:HB2	4:B:287:TRP:CD2	2.45	0.52
4:D:848:GLN:OE1	4:D:848:GLN:HA	2.09	0.52
4:A:620:TRP:CZ2	4:A:677:MET:HB2	2.45	0.52
4:A:871:ASN:O	4:A:874:ASP:OD2	2.28	0.52
4:A:206:LYS:O	4:A:210:ILE:HG12	2.10	0.52
4:B:779:ALA:N	4:B:780:PRO:HD3	2.25	0.52
4:B:780:PRO:HB3	7:B:3018:HOH:O	2.10	0.52
4:B:849:PHE:H	4:B:849:PHE:HD1	1.56	0.52
4:C:333:LYS:CD	4:C:516:PHE:HD2	2.15	0.52
4:A:437:ASN:O	4:A:438:ASP:C	2.46	0.52
4:B:157:LEU:O	4:B:160:LYS:N	2.32	0.52
4:C:455:GLU:OE1	4:C:455:GLU:HA	2.09	0.52
4:D:404:GLN:HG2	4:D:432:PHE:CB	2.40	0.52
4:C:4:ILE:CD1	4:C:256:THR:HG23	2.37	0.52
4:A:166:VAL:O	4:A:167:GLU:C	2.47	0.52
4:B:48:GLU:HG3	4:B:262:ALA:HB1	1.92	0.52
4:A:459:TRP:CH2	4:A:825:PHE:CE2	2.98	0.52
4:B:450:LYS:N	4:B:529:ASN:HD21	2.07	0.52
4:A:281:ILE:HG13	4:A:309:GLU:CG	2.40	0.52
4:A:281:ILE:HG22	4:A:282:THR:N	2.23	0.52
4:B:471:ASP:C	4:B:472:LYS:HD2	2.31	0.52
4:D:66:ASP:OD2	4:D:752:LEU:HD23	2.10	0.52
2:I:5:C:N3	2:I:6:G:C8	2.78	0.52
4:D:236:VAL:O	4:D:240:ASP:HB2	2.09	0.52
4:D:582:LEU:HD22	4:D:620:TRP:HB2	1.92	0.52
4:D:613:THR:HG22	4:D:676:TYR:HE1	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:501:TRP:HA	4:D:504:GLU:CD	2.30	0.52
4:B:722:ARG:NH1	4:B:768:GLU:OE2	2.42	0.52
4:A:521:VAL:HG12	4:A:522:GLN:N	2.24	0.51
4:A:457:TYR:CD1	4:A:521:VAL:HG21	2.40	0.51
4:A:810:ILE:CD1	7:A:3145:HOH:O	2.58	0.51
1:H:9:DA:N6	3:J:1:DG:H22	2.05	0.51
4:C:404:GLN:NE2	4:C:404:GLN:HA	2.19	0.51
4:C:649:GLN:O	4:C:650:VAL:C	2.48	0.51
4:C:93:LYS:HA	4:C:99:ARG:NH2	2.25	0.51
4:B:194:GLY:O	4:B:196:LEU:HD23	2.11	0.51
4:C:569:ASP:O	4:C:572:GLY:N	2.43	0.51
4:D:466:ASN:OD1	4:D:478:ARG:NH1	2.44	0.51
4:A:270:PRO:HB3	4:A:416:PHE:CD1	2.45	0.51
4:C:42:GLU:OE1	4:C:46:MET:HE1	2.09	0.51
4:B:105:PHE:C	4:B:107:GLN:H	2.13	0.51
4:A:459:TRP:CZ3	4:A:475:PHE:CE1	2.99	0.51
4:C:729:THR:OG1	4:C:733:PHE:N	2.40	0.51
4:C:405:ALA:CB	4:C:443:LEU:HD13	2.41	0.51
4:D:745:THR:CG2	7:D:3056:HOH:O	2.59	0.51
4:C:579:ASN:O	4:C:582:LEU:HB2	2.09	0.51
4:C:155:ARG:HB2	4:C:163:LYS:HZ3	1.74	0.51
4:C:215:ARG:O	4:C:218:GLU:HB2	2.10	0.51
4:B:516:PHE:O	4:B:519:ALA:HB3	2.10	0.51
4:A:379:ARG:HE	4:A:656:GLN:CG	2.23	0.51
4:A:812:ASP:OD1	4:A:812:ASP:N	2.38	0.51
4:D:814:PHE:CE1	4:D:883:ALA:HB1	2.45	0.51
4:B:704:LYS:HG3	4:B:775:GLU:OE1	2.10	0.51
4:B:875:ILE:O	4:B:877:GLU:N	2.43	0.51
4:B:194:GLY:O	4:B:196:LEU:CD2	2.59	0.51
4:C:668:THR:HB	4:C:669:GLN:NE2	2.25	0.51
4:C:15:GLU:CG	4:C:18:ALA:H	2.22	0.51
4:D:84:ARG:CB	4:D:223:SER:HB3	2.41	0.51
1:E:3:DG:H2"	1:E:4:DA:C8	2.45	0.51
4:A:50:ARG:CG	4:A:50:ARG:HH11	2.23	0.51
4:A:729:THR:HB	4:A:789:SER:HB2	1.92	0.51
4:A:551:ARG:HB2	4:A:868:GLY:N	2.24	0.51
4:C:36:GLN:HA	4:C:36:GLN:OE1	2.10	0.51
4:B:639:TYR:C	7:B:3018:HOH:O	2.48	0.51
1:H:17:DG:H2"	1:H:18:DC:C5	2.46	0.51
4:D:338:ALA:O	4:D:342:THR:HG23	2.10	0.51
4:D:472:LYS:CA	4:D:567:VAL:HG11	2.38	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:339:ASN:O	4:B:343:LYS:CG	2.59	0.51
4:C:32:LEU:N	7:C:3157:HOH:O	2.29	0.51
4:C:400:PHE:CZ	4:C:431:MET:HE2	2.44	0.51
4:C:51:PHE:CZ	4:C:261:LEU:HD23	2.45	0.51
4:B:381:ALA:C	4:B:383:ALA:H	2.14	0.51
4:A:292:ARG:N	4:A:293:PRO:CD	2.73	0.51
4:D:849:PHE:O	4:D:850:ALA:C	2.48	0.51
1:K:11:DA:C8	4:C:639:TYR:CG	2.98	0.51
4:D:724:ALA:HB1	4:D:737:GLN:O	2.10	0.51
1:N:12:DT:H4'	4:D:423:ARG:HD2	1.93	0.51
4:B:580:GLU:O	4:B:581:ILE:C	2.47	0.51
1:H:12:DT:H2"	1:H:13:DC:H6	1.76	0.51
1:H:15:DC:C2	1:H:16:DC:C5	2.99	0.51
4:B:432:PHE:CE2	4:B:444:LEU:HD11	2.44	0.51
4:A:689:VAL:O	4:A:691:ALA:N	2.44	0.51
4:A:513:ALA:O	7:A:3098:HOH:O	2.19	0.51
4:C:239:GLN:O	4:C:241:SER:N	2.43	0.51
4:D:475:PHE:HE2	4:D:879:ASP:CB	2.21	0.51
4:B:112:GLU:CD	4:B:112:GLU:N	2.63	0.51
4:D:486:HIS:O	4:D:487:GLU:C	2.47	0.51
4:D:578:VAL:HG13	4:D:680:LEU:HB3	1.93	0.51
4:A:754:GLN:O	4:A:755:PHE:O	2.28	0.51
4:D:6:ILE:C	4:D:8:LYS:H	2.13	0.51
4:C:643:GLU:OE2	4:C:679:LYS:HA	2.11	0.51
4:B:136:ALA:O	4:B:139:SER:HB3	2.10	0.51
4:B:322:ILE:HG22	4:B:323:ALA:N	2.24	0.51
4:D:859:ASP:C	4:D:861:MET:H	2.14	0.51
4:B:55:PHE:CD2	4:B:59:LEU:HD11	2.45	0.51
4:A:213:GLY:O	4:A:217:ILE:HG13	2.11	0.51
4:B:417:PRO:O	4:B:429:VAL:HG23	2.10	0.51
4:A:439:MET:HG3	4:A:509:PHE:CD2	2.45	0.51
4:A:430:SER:OG	4:A:431:MET:N	2.41	0.51
4:C:462:ILE:O	4:C:465:ALA:HB3	2.11	0.51
4:C:109:ILE:H	4:C:109:ILE:HD12	1.74	0.51
4:D:308:TYR:HE2	4:D:734:PRO:O	1.94	0.51
4:B:854:HIS:ND1	4:B:855:GLU:N	2.58	0.51
4:D:726:HIS:CD2	4:D:736:TRP:NE1	2.78	0.51
2:L:4:G:O2'	2:L:5:C:H5'	2.10	0.51
4:D:538:GLY:O	4:D:539:SER:C	2.49	0.51
4:D:15:GLU:OE2	4:D:18:ALA:HB3	2.11	0.51
4:C:294:LEU:HD23	4:C:294:LEU:N	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:324:GLN:HA	4:D:418:TYR:CE1	2.45	0.51
4:B:576:LYS:O	4:B:577:LYS:C	2.49	0.51
4:C:59:LEU:HD22	4:C:64:VAL:CG1	2.39	0.51
4:B:157:LEU:O	4:B:158:GLU:C	2.48	0.51
4:B:172:LYS:HB3	4:B:172:LYS:HZ3	1.76	0.51
4:D:306:MET:O	4:D:309:GLU:N	2.42	0.51
4:B:19:ILE:HG23	4:B:20:PRO:HD2	1.92	0.51
4:A:40:GLU:OE1	4:A:286:TYR:HB3	2.10	0.51
4:D:277:PRO:CA	7:D:3029:HOH:O	2.59	0.51
4:D:259:GLY:O	4:D:262:ALA:N	2.43	0.51
4:D:835:THR:HG22	4:D:836:TYR:CD2	2.46	0.51
4:A:726:HIS:HB2	4:A:736:TRP:CD1	2.45	0.51
4:C:308:TYR:CZ	4:C:733:PHE:CE2	2.97	0.51
4:C:840:ASP:O	4:C:841:VAL:C	2.50	0.51
1:N:11:DA:C4'	4:D:780:PRO:HG3	2.40	0.51
4:D:797:TRP:NE1	4:D:802:TYR:HE2	2.08	0.51
4:B:308:TYR:HA	4:B:311:VAL:HG21	1.91	0.51
4:C:437:ASN:ND2	4:C:440:THR:OG1	2.44	0.51
4:B:505:GLN:N	4:B:505:GLN:CD	2.58	0.51
4:A:268:PHE:CB	4:A:430:SER:HA	2.40	0.51
4:B:585:ASP:OD2	4:B:613:THR:CB	2.58	0.51
4:B:82:ILE:CD1	4:B:112:GLU:HG3	2.41	0.51
4:D:221:ILE:HA	4:D:224:THR:O	2.11	0.51
4:B:744:GLN:HB3	4:B:756:ARG:HB3	1.92	0.51
4:A:303:LYS:NZ	7:A:3108:HOH:O	2.42	0.51
4:A:746:ARG:HH12	4:A:754:GLN:N	2.06	0.51
4:A:843:ALA:O	4:A:844:ASP:C	2.48	0.51
4:D:207:GLU:O	4:D:211:HIS:CG	2.64	0.51
6:A:2000:APC:H5'2	7:A:3048:HOH:O	2.11	0.51
4:D:843:ALA:O	4:D:846:TYR:N	2.42	0.51
4:C:824:LEU:O	4:C:828:VAL:HG22	2.10	0.51
4:D:327:ALA:CB	4:D:415:TRP:NE1	2.73	0.51
4:B:61:ALA:C	4:B:63:GLU:H	2.14	0.51
4:B:571:TYR:HE2	4:B:631:LYS:HG3	1.68	0.51
4:B:729:THR:HG23	4:B:733:PHE:O	2.10	0.51
4:B:783:VAL:O	4:B:784:HIS:C	2.48	0.51
4:B:158:GLU:HG2	4:B:195:LEU:CB	2.41	0.51
4:D:455:GLU:O	4:D:458:TYR:HB3	2.11	0.51
4:A:548:ALA:C	4:A:550:LEU:N	2.63	0.51
4:A:418:TYR:HD2	4:A:426:VAL:HG11	1.75	0.51
4:C:345:LYS:NZ	4:C:352:ILE:HG12	2.24	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:480:LYS:HE3	4:A:484:GLU:CD	2.31	0.51
4:A:514:PHE:O	4:A:515:CYS:C	2.45	0.51
4:C:313:MET:O	4:C:317:TYR:HD2	1.94	0.51
4:A:721:LYS:CD	4:A:722:ARG:H	2.17	0.51
4:B:535:ALA:HA	4:B:815:GLY:HA2	1.94	0.51
4:A:115:ALA:O	4:A:119:ILE:HG12	2.11	0.51
1:N:15:DC:H2"	1:N:16:DC:OP2	2.09	0.51
4:B:871:ASN:O	4:B:872:LEU:C	2.49	0.51
4:D:7:ALA:HA	4:D:11:PHE:HD2	1.76	0.51
4:B:4:ILE:HD12	4:B:256:THR:HG23	1.92	0.51
4:C:307:ARG:HD3	4:C:736:TRP:CD2	2.45	0.50
4:C:852:GLN:NE2	7:C:3094:HOH:O	2.21	0.50
1:K:15:DC:H5'	1:K:15:DC:H6	1.75	0.50
1:H:14:DG:C4	1:H:15:DC:C5	2.99	0.50
4:B:40:GLU:O	4:B:41:HIS:C	2.48	0.50
4:B:42:GLU:HG2	4:B:46:MET:CE	2.41	0.50
4:C:333:LYS:CD	4:C:516:PHE:CD2	2.93	0.50
4:C:442:GLY:O	4:C:444:LEU:N	2.44	0.50
4:C:329:LYS:HG3	4:C:445:THR:HG23	1.93	0.50
4:D:452:ILE:HD11	4:D:457:TYR:HA	1.94	0.50
4:D:71:LYS:N	4:D:72:PRO:HD2	2.25	0.50
4:D:377:TRP:HA	7:D:3074:HOH:O	2.10	0.50
4:A:651:LEU:HD11	4:A:656:GLN:NE2	2.25	0.50
4:A:685:VAL:C	4:A:687:VAL:H	2.13	0.50
4:A:308:TYR:HE2	4:A:734:PRO:CG	2.12	0.50
1:K:10:DT:H4'	4:C:639:TYR:O	2.12	0.50
4:C:737:GLN:HE22	4:C:777:GLY:C	2.14	0.50
4:C:779:ALA:N	4:C:780:PRO:HD2	2.26	0.50
4:C:837:GLU:HG2	4:C:872:LEU:HD12	1.93	0.50
1:H:9:DA:C2	4:B:644:PHE:CD1	2.98	0.50
4:B:777:GLY:C	4:B:780:PRO:HD2	2.31	0.50
4:B:780:PRO:CD	4:B:781:ASN:N	2.73	0.50
1:H:9:DA:C5'	7:H:484:HOH:O	2.32	0.50
4:B:478:ARG:O	4:B:479:ILE:C	2.48	0.50
4:C:120:LYS:HD2	4:C:751:PHE:CE2	2.46	0.50
4:C:291:ARG:CB	7:C:3192:HOH:O	2.54	0.50
4:D:676:TYR:CZ	4:D:680:LEU:HD11	2.46	0.50
4:C:205:HIS:C	4:C:207:GLU:N	2.64	0.50
4:C:60:LYS:O	4:C:60:LYS:HG2	2.12	0.50
4:A:421:ASP:OD2	4:A:427:TYR:HE1	1.93	0.50
4:D:275:PRO:HG2	4:D:324:GLN:CG	2.38	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:426:VAL:C	4:B:427:TYR:HD1	2.14	0.50
4:B:422:TRP:CE2	4:B:781:ASN:ND2	2.79	0.50
4:B:791:LEU:O	4:B:794:THR:N	2.42	0.50
4:B:824:LEU:O	4:B:824:LEU:HG	2.11	0.50
4:A:223:SER:OG	4:A:224:THR:HG23	2.11	0.50
4:B:505:GLN:H	4:B:505:GLN:NE2	1.94	0.50
4:D:215:ARG:HA	4:D:218:GLU:OE1	2.10	0.50
4:D:158:GLU:HA	4:D:195:LEU:HD13	1.94	0.50
4:C:569:ASP:O	4:C:573:ILE:HG22	2.11	0.50
4:D:789:SER:HA	4:D:792:ARG:CZ	2.41	0.50
4:D:448:LYS:NZ	4:D:806:SER:CB	2.73	0.50
4:A:611:LEU:HD11	4:A:669:GLN:NE2	2.27	0.50
4:B:70:ALA:C	4:B:72:PRO:HD2	2.31	0.50
4:B:821:ALA:O	4:B:822:ALA:C	2.49	0.50
4:A:281:ILE:HD11	4:A:309:GLU:H	1.75	0.50
4:B:632:ARG:HH11	6:B:2001:APC:C8	2.24	0.50
4:B:120:LYS:HG3	4:B:752:LEU:HD11	1.94	0.50
4:B:508:PRO:O	4:B:509:PHE:C	2.49	0.50
4:D:236:VAL:HG11	4:D:239:GLN:CD	2.31	0.50
4:A:82:ILE:CG2	4:A:112:GLU:OE2	2.59	0.50
4:C:291:ARG:C	4:C:293:PRO:HD3	2.31	0.50
4:D:205:HIS:C	4:D:207:GLU:H	2.14	0.50
4:A:463:HIS:O	4:A:464:GLY:C	2.48	0.50
4:D:702:ALA:HB2	4:D:861:MET:CE	2.41	0.50
4:D:706:LEU:HD11	4:D:849:PHE:CG	2.46	0.50
1:K:11:DA:C8	4:C:639:TYR:CB	2.93	0.50
1:K:11:DA:C2'	1:K:12:DT:C7	2.89	0.50
1:N:12:DT:O4'	4:D:423:ARG:CZ	2.58	0.50
4:D:828:VAL:HA	4:D:831:THR:HG22	1.93	0.50
4:B:422:TRP:CD1	4:B:423:ARG:N	2.80	0.50
4:B:470:VAL:HG11	4:B:478:ARG:HA	1.93	0.50
4:B:159:ALA:HA	4:B:162:PHE:HB3	1.94	0.50
4:A:610:LYS:CG	4:A:610:LYS:O	2.51	0.50
4:B:770:ASP:OD1	4:B:770:ASP:O	2.29	0.50
4:C:43:SER:OG	4:C:269:GLN:HG3	2.12	0.50
4:D:70:ALA:C	4:D:72:PRO:HD2	2.32	0.50
4:D:19:ILE:HG23	4:D:20:PRO:CD	2.41	0.50
4:B:272:VAL:CG1	4:B:411:HIS:HD2	2.25	0.50
4:C:672:GLN:HG3	7:C:3033:HOH:O	2.10	0.50
4:D:665:LEU:HB2	7:D:3125:HOH:O	2.12	0.50
4:A:572:GLY:O	4:A:576:LYS:HG3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:706:LEU:HD23	4:D:853:LEU:HD23	1.94	0.50
4:B:51:PHE:O	4:B:55:PHE:HB2	2.11	0.50
4:B:631:LYS:HZ1	6:B:2001:APC:H3A2	1.76	0.50
4:B:638:ALA:O	4:B:780:PRO:HB3	2.11	0.50
4:B:14:ILE:HG23	4:B:288:ALA:HB1	1.93	0.50
4:D:335:LEU:O	4:D:339:ASN:HB2	2.12	0.50
4:B:84:ARG:C	4:B:84:ARG:HD3	2.31	0.50
4:C:474:PRO:C	4:C:476:PRO:HD2	2.32	0.50
4:D:150:ARG:HG3	4:D:201:TRP:CD1	2.46	0.50
4:D:209:SER:HB2	7:D:3053:HOH:O	2.11	0.50
4:A:386:ARG:CD	7:A:3138:HOH:O	2.45	0.50
4:C:9:ASN:CA	4:C:12:SER:HB3	2.41	0.50
4:D:685:VAL:C	4:D:687:VAL:H	2.15	0.50
4:A:579:ASN:HA	4:A:582:LEU:HG	1.93	0.50
4:D:706:LEU:HD21	4:D:849:PHE:HD2	1.76	0.50
4:B:405:ALA:O	4:B:409:ALA:N	2.45	0.50
4:B:475:PHE:HB2	4:B:476:PRO:CD	2.42	0.50
4:B:479:ILE:O	4:B:480:LYS:C	2.49	0.50
4:A:333:LYS:CB	4:A:516:PHE:HD2	2.23	0.50
4:C:446:LEU:H	4:C:533:PRO:HD3	1.76	0.50
4:C:446:LEU:HD12	4:C:817:ILE:HG23	1.93	0.50
4:D:92:VAL:CG1	4:D:99:ARG:HG3	2.41	0.50
4:D:485:ASN:O	4:D:489:ILE:HG13	2.12	0.50
4:A:42:GLU:O	4:A:43:SER:C	2.50	0.50
4:D:304:ALA:HB1	7:D:3038:HOH:O	2.10	0.50
4:D:585:ASP:O	4:D:614:LYS:HA	2.12	0.50
4:B:412:LYS:O	4:B:413:ALA:HB2	2.12	0.50
4:B:450:LYS:N	4:B:529:ASN:ND2	2.60	0.50
4:D:857:GLN:C	4:D:859:ASP:H	2.15	0.50
4:C:306:MET:O	4:C:307:ARG:C	2.51	0.50
1:K:11:DA:H8	4:C:639:TYR:HB3	1.74	0.50
1:K:16:DC:H2"	1:K:17:DG:H5'	1.93	0.50
4:D:794:THR:O	4:D:795:VAL:C	2.49	0.50
4:D:402:LEU:CD2	4:D:443:LEU:CD1	2.88	0.50
4:B:162:PHE:HE1	4:B:190:MET:HG2	1.76	0.50
4:B:159:ALA:HB1	4:B:163:LYS:N	2.27	0.50
4:C:248:PRO:HB2	4:C:249:GLU:OE2	2.12	0.50
4:A:19:ILE:HG23	4:A:20:PRO:CD	2.39	0.50
4:A:21:PHE:C	4:A:23:THR:N	2.64	0.50
4:C:656:GLN:N	4:C:657:PRO:CD	2.75	0.50
3:J:5:DA:C2	3:J:6:DT:C2	2.99	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:490:MET:HE3	4:C:490:MET:HA	1.94	0.50
4:B:500:THR:O	4:B:503:ALA:HB3	2.11	0.50
4:C:22:ASN:O	4:C:26:ASP:HB3	2.11	0.50
4:A:422:TRP:HD1	7:A:3029:HOH:O	1.95	0.50
4:A:829:ARG:NE	4:A:878:SER:O	2.42	0.50
1:K:10:DT:H5'	4:C:641:SER:CA	2.42	0.50
4:A:719:LEU:HD22	4:A:854:HIS:CE1	2.47	0.50
4:B:268:PHE:HD2	4:B:429:VAL:HG12	1.77	0.50
1:H:10:DT:OP2	4:B:641:SER:HB3	2.12	0.50
4:D:508:PRO:O	4:D:509:PHE:C	2.48	0.50
4:A:42:GLU:HG2	4:A:46:MET:CE	2.42	0.50
4:D:433:ASN:CB	4:D:434:PRO:CD	2.88	0.50
4:A:846:TYR:CD1	4:A:850:ALA:HB2	2.47	0.50
3:P:4:DG:H2"	3:P:5:DA:C8	2.47	0.50
4:D:115:ALA:O	4:D:119:ILE:HG12	2.11	0.50
4:C:632:ARG:CZ	6:C:2002:APC:C8	2.90	0.49
4:A:786:GLN:C	4:A:788:GLY:N	2.63	0.49
4:A:273:VAL:O	4:A:274:PRO:C	2.50	0.49
4:C:14:ILE:HG12	4:C:288:ALA:HB1	1.94	0.49
4:C:417:PRO:O	4:C:429:VAL:HG23	2.12	0.49
1:K:16:DC:H2"	1:K:17:DG:C5'	2.42	0.49
1:N:10:DT:C5'	4:D:641:SER:N	2.75	0.49
4:D:797:TRP:CH2	4:D:801:LYS:HG3	2.47	0.49
4:D:560:ASN:C	4:D:881:ALA:HB2	2.30	0.49
1:H:15:DC:OP2	7:H:411:HOH:O	2.19	0.49
4:B:92:VAL:HG11	4:B:100:PRO:HD2	1.94	0.49
4:C:232:GLN:NE2	7:C:3040:HOH:O	2.45	0.49
4:A:338:ALA:C	4:A:340:VAL:N	2.66	0.49
4:C:221:ILE:HG23	4:C:227:VAL:O	2.12	0.49
4:D:404:GLN:HG2	4:D:432:PHE:HB2	1.94	0.49
4:C:668:THR:HB	4:C:669:GLN:HE22	1.75	0.49
4:D:489:ILE:HA	4:D:492:CYS:SG	2.52	0.49
4:D:72:PRO:HG3	4:D:257:ARG:HG3	1.94	0.49
4:C:272:VAL:HG13	4:C:411:HIS:HD2	1.76	0.49
4:B:51:PHE:HE2	4:B:55:PHE:HD1	1.57	0.49
1:H:13:DC:C4'	4:B:427:TYR:CE2	2.95	0.49
1:H:18:DC:C2'	4:B:63:GLU:OE1	2.60	0.49
4:B:578:VAL:HG13	4:B:680:LEU:CD2	2.40	0.49
1:H:14:DG:H2"	1:H:15:DC:H6	1.77	0.49
4:A:401:MET:C	4:A:403:GLU:H	2.14	0.49
4:D:745:THR:H	4:D:756:ARG:HD3	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:544:GLN:HG2	4:D:561:LEU:HD11	1.93	0.49
4:A:704:LYS:O	4:A:707:ALA:HB3	2.12	0.49
4:B:261:LEU:C	4:B:263:GLY:N	2.63	0.49
1:K:5:DA:N6	3:M:5:DA:N6	2.60	0.49
4:B:860:LYS:O	4:B:862:PRO:HD2	2.12	0.49
3:J:6:DT:H2"	3:J:7:DT:H71	1.94	0.49
4:A:71:LYS:N	4:A:72:PRO:HD2	2.27	0.49
4:A:473:VAL:CG1	4:A:473:VAL:O	2.60	0.49
4:A:543:ILE:O	4:A:544:GLN:C	2.50	0.49
4:B:55:PHE:CD2	4:B:55:PHE:C	2.84	0.49
4:C:316:VAL:O	4:C:317:TYR:C	2.50	0.49
4:C:870:LEU:HA	7:C:3053:HOH:O	2.11	0.49
4:B:647:ARG:HD3	7:B:3138:HOH:O	2.11	0.49
4:B:829:ARG:CG	4:B:829:ARG:NH1	2.68	0.49
4:A:84:ARG:HG3	4:A:222:GLU:HG2	1.93	0.49
4:C:458:TYR:CE1	4:C:479:ILE:HD11	2.47	0.49
4:C:474:PRO:HB2	4:C:476:PRO:HG2	1.94	0.49
1:N:15:DC:N3	1:N:16:DC:C4	2.80	0.49
4:A:182:PHE:O	4:A:185:VAL:CG2	2.59	0.49
3:G:6:DT:H2"	3:G:7:DT:OP2	2.12	0.49
4:C:711:LYS:HE2	4:C:716:GLY:O	2.12	0.49
4:A:715:THR:HB	4:A:717:GLU:HB2	1.94	0.49
4:A:344:TRP:O	4:A:345:LYS:HG3	2.12	0.49
4:B:155:ARG:HH21	4:B:749:LEU:HB2	1.77	0.49
4:A:425:ARG:HD3	4:A:811:HIS:HD2	1.76	0.49
4:A:136:ALA:HA	7:A:3053:HOH:O	2.11	0.49
4:A:720:ARG:HE	4:A:854:HIS:H	1.60	0.49
4:B:826:LYS:HG2	4:B:830:GLU:HG3	1.94	0.49
4:B:193:LYS:HG3	4:B:194:GLY:H	1.77	0.49
4:C:461:LYS:O	4:C:462:ILE:C	2.49	0.49
4:C:669:GLN:N	4:C:669:GLN:NE2	2.60	0.49
4:D:551:ARG:O	4:D:868:GLY:HA3	2.12	0.49
4:A:488:ASN:O	4:A:491:ALA:N	2.45	0.49
4:C:854:HIS:O	4:C:857:GLN:HG2	2.13	0.49
4:B:232:GLN:HG3	4:B:243:THR:CG2	2.43	0.49
4:C:250:TYR:O	4:C:254:ILE:HG13	2.12	0.49
4:B:203:SER:O	4:B:205:HIS:N	2.38	0.49
4:D:379:ARG:HD2	7:D:3122:HOH:O	2.12	0.49
4:A:460:LEU:O	4:A:461:LYS:C	2.50	0.49
4:C:324:GLN:CG	4:C:417:PRO:HA	2.42	0.49
4:D:830:GLU:HG2	4:D:876:LEU:HD21	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:421:ASP:O	4:B:424:GLY:N	2.45	0.49
4:B:459:TRP:CZ3	4:B:536:PHE:CZ	3.01	0.49
4:A:402:LEU:HG	4:A:439:MET:HE1	1.94	0.49
4:B:485:ASN:ND2	4:B:501:TRP:CZ2	2.80	0.49
4:A:60:LYS:O	4:A:60:LYS:CG	2.56	0.49
4:D:139:SER:CA	4:D:210:ILE:HD13	2.42	0.49
3:M:5:DA:C2'	3:M:6:DT:H72	2.42	0.49
4:A:772:HIS:O	4:A:773:LYS:C	2.50	0.49
4:D:10:ASP:O	4:D:13:ASP:CB	2.61	0.49
4:B:272:VAL:HG11	4:B:411:HIS:CD2	2.48	0.49
4:C:345:LYS:HZ3	4:C:352:ILE:HG12	1.77	0.49
2:F:1:G:C2	2:F:2:C:C2	3.01	0.49
4:A:629:VAL:HG11	4:A:677:MET:CE	2.43	0.49
4:A:643:GLU:OE2	4:A:679:LYS:HA	2.13	0.49
4:A:465:ALA:CB	4:A:478:ARG:HB3	2.43	0.49
4:A:480:LYS:HG2	7:A:3046:HOH:O	2.13	0.49
4:A:524:HIS:O	4:A:525:GLY:O	2.30	0.49
4:A:264:ILE:HG22	4:A:292:ARG:HD3	1.95	0.49
4:C:423:ARG:CD	4:C:781:ASN:HD22	2.25	0.49
4:D:810:ILE:CB	4:D:813:SER:OG	2.53	0.49
4:D:814:PHE:CE1	4:D:883:ALA:HB2	2.47	0.49
4:B:544:GLN:HA	4:B:559:VAL:HG21	1.94	0.49
4:B:60:LYS:HE2	4:B:61:ALA:HB2	1.95	0.49
4:C:84:ARG:CA	4:C:84:ARG:HH11	2.22	0.49
4:B:512:LEU:C	4:B:514:PHE:N	2.64	0.49
1:E:15:DC:H2"	1:E:16:DC:C5'	2.41	0.49
4:D:330:ILE:CG1	4:D:408:PHE:O	2.60	0.49
4:B:454:LYS:N	4:B:526:LEU:HD22	2.27	0.49
4:D:646:PHE:O	4:D:647:ARG:C	2.51	0.49
4:B:560:ASN:OD1	4:B:568:GLN:HB2	2.12	0.49
4:B:334:VAL:HG12	4:B:443:LEU:CD2	2.42	0.49
4:A:462:ILE:O	4:A:465:ALA:N	2.45	0.49
4:C:24:LEU:CD2	4:C:273:VAL:HG21	2.42	0.49
4:D:810:ILE:N	4:D:813:SER:OG	2.46	0.49
4:B:292:ARG:CG	4:B:292:ARG:O	2.61	0.49
4:B:726:HIS:CD2	4:B:736:TRP:CE2	3.01	0.49
4:B:546:PHE:CE1	4:B:783:VAL:HG13	2.47	0.49
4:A:169:GLN:O	4:A:173:ARG:CG	2.50	0.49
4:A:401:MET:C	4:A:403:GLU:N	2.63	0.49
4:D:518:TYR:O	4:D:522:GLN:HG2	2.13	0.49
4:A:485:ASN:HA	7:A:3028:HOH:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:259:GLY:O	4:D:260:ALA:C	2.50	0.49
4:C:734:PRO:HG2	4:C:734:PRO:O	2.13	0.49
4:C:786:GLN:O	4:C:789:SER:HB3	2.12	0.49
4:C:549:MET:HB3	4:C:836:TYR:CE1	2.48	0.49
4:B:281:ILE:HD11	4:B:309:GLU:N	2.28	0.49
4:B:703:ALA:O	4:B:704:LYS:C	2.50	0.49
4:B:804:ILE:CG2	4:B:807:PHE:CE2	2.96	0.49
4:B:826:LYS:O	4:B:830:GLU:HG3	2.13	0.49
4:B:404:GLN:HB3	4:B:432:PHE:CD1	2.48	0.49
4:C:340:VAL:HA	4:C:343:LYS:HD3	1.95	0.49
4:B:388:ASP:O	4:B:389:LYS:C	2.51	0.49
4:D:381:ALA:O	4:D:384:VAL:HB	2.12	0.49
4:B:111:PRO:HG2	4:B:112:GLU:CD	2.33	0.49
4:D:840:ASP:C	4:D:842:LEU:N	2.65	0.49
1:K:7:DC:C6	1:K:8:DG:N7	2.80	0.49
4:D:78:LEU:N	4:D:79:PRO:HD2	2.27	0.49
4:A:617:ALA:O	4:A:620:TRP:N	2.46	0.49
4:C:846:TYR:CD1	4:C:850:ALA:HB2	2.48	0.49
4:C:552:ASP:HB2	4:C:691:ALA:HB2	1.94	0.49
4:B:810:ILE:O	4:B:811:HIS:HB2	2.11	0.49
4:B:846:TYR:O	4:B:847:ASP:C	2.50	0.49
1:H:15:DC:N3	1:H:16:DC:C4	2.80	0.49
1:H:3:DG:H1'	7:H:1116:HOH:O	2.12	0.49
4:D:452:ILE:HG23	4:D:526:LEU:O	2.13	0.49
4:B:105:PHE:HB3	4:B:204:TRP:CZ2	2.48	0.49
4:C:151:PHE:O	4:C:154:ILE:HG13	2.13	0.49
4:A:631:LYS:HG2	4:A:632:ARG:N	2.28	0.49
4:C:36:GLN:CG	4:C:273:VAL:HG22	2.41	0.49
4:C:553:GLU:CG	4:C:554:VAL:H	2.25	0.49
4:C:730:PRO:HD3	4:C:786:GLN:NE2	2.27	0.49
4:A:721:LYS:HE2	7:A:3021:HOH:O	2.12	0.49
4:D:275:PRO:HB2	4:D:324:GLN:CD	2.33	0.49
4:B:292:ARG:HG3	4:B:292:ARG:O	2.13	0.49
4:B:463:HIS:O	4:B:467:CYS:SG	2.71	0.49
1:H:17:DG:H2"	1:H:18:DC:C6	2.47	0.49
4:D:116:TYR:HE2	4:D:752:LEU:HD13	1.77	0.49
4:C:475:PHE:O	4:C:479:ILE:HG12	2.13	0.49
4:A:159:ALA:HA	4:A:162:PHE:HB3	1.94	0.49
4:B:263:GLY:C	7:B:3137:HOH:O	2.51	0.49
4:D:84:ARG:CG	4:D:223:SER:HB3	2.43	0.49
4:A:51:PHE:CZ	4:A:261:LEU:HB3	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:178:TYR:CD1	4:A:178:TYR:N	2.77	0.49
4:A:619:GLN:NE2	4:A:666:MET:O	2.46	0.48
4:C:786:GLN:NE2	4:C:841:VAL:HG11	2.28	0.48
4:C:871:ASN:HD21	4:C:873:ARG:HB2	1.78	0.48
4:B:301:SER:O	4:B:304:ALA:CB	2.59	0.48
4:B:698:TRP:O	4:B:701:SER:HB2	2.12	0.48
1:H:9:DA:C5	4:B:644:PHE:CZ	3.01	0.48
4:B:13:ASP:O	4:B:15:GLU:N	2.43	0.48
4:D:347:CYS:O	4:D:349:VAL:N	2.46	0.48
4:A:89:PHE:HA	4:A:103:PHE:CZ	2.47	0.48
1:E:16:DC:H2"	1:E:17:DG:C5'	2.42	0.48
4:C:82:ILE:HD13	4:C:112:GLU:HA	1.95	0.48
4:D:646:PHE:O	4:D:650:VAL:HG23	2.13	0.48
1:K:9:DA:N6	3:M:1:DG:H22	2.11	0.48
4:A:532:LEU:HA	4:A:533:PRO:HD2	1.64	0.48
4:A:634:VAL:O	4:A:637:LEU:HB3	2.13	0.48
4:A:559:VAL:HG23	4:A:559:VAL:O	2.12	0.48
4:A:797:TRP:CZ2	4:A:830:GLU:OE1	2.67	0.48
1:K:13:DC:C2	1:K:14:DG:C8	3.00	0.48
4:A:720:ARG:HG2	4:A:720:ARG:O	2.13	0.48
4:B:418:TYR:HB3	4:B:426:VAL:CG1	2.44	0.48
4:B:549:MET:HG2	4:B:836:TYR:CE1	2.46	0.48
4:B:680:LEU:H	4:B:680:LEU:HD12	1.75	0.48
1:H:16:DC:H2"	1:H:17:DG:OP2	2.13	0.48
4:D:338:ALA:C	4:D:340:VAL:H	2.16	0.48
4:A:340:VAL:O	4:A:341:ILE:C	2.49	0.48
4:D:231:ARG:HG2	4:D:234:ALA:CB	2.36	0.48
4:D:92:VAL:HG11	4:D:103:PHE:CG	2.48	0.48
4:D:158:GLU:CA	4:D:195:LEU:HD22	2.43	0.48
1:N:14:DG:C4	1:N:15:DC:C5	3.02	0.48
4:C:330:ILE:HG12	4:C:408:PHE:O	2.13	0.48
4:B:32:LEU:HA	4:B:32:LEU:HD12	1.67	0.48
4:A:637:LEU:O	4:A:637:LEU:HG	2.11	0.48
4:A:633:SER:HB3	4:A:646:PHE:CE2	2.48	0.48
4:A:463:HIS:O	4:A:465:ALA:N	2.46	0.48
4:A:777:GLY:O	4:A:781:ASN:HB2	2.12	0.48
4:C:297:VAL:HG21	4:C:733:PHE:HZ	1.78	0.48
4:C:846:TYR:CD2	4:C:864:LEU:HD11	2.48	0.48
1:K:11:DA:H2"	1:K:12:DT:O5'	2.12	0.48
4:B:428:ALA:N	4:B:435:GLN:HE22	2.08	0.48
4:B:556:GLY:C	4:B:558:ALA:H	2.17	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:670:PRO:O	4:B:671:ASN:C	2.48	0.48
4:B:546:PHE:CE2	4:B:696:MET:HG3	2.48	0.48
4:B:794:THR:CG2	4:B:828:VAL:HA	2.43	0.48
4:A:333:LYS:HB3	4:A:516:PHE:CD2	2.48	0.48
4:A:512:LEU:O	4:A:516:PHE:CD1	2.66	0.48
4:A:89:PHE:CZ	4:A:106:LEU:O	2.65	0.48
4:A:85:ILE:O	4:A:85:ILE:HG22	2.13	0.48
4:B:109:ILE:CD1	4:B:109:ILE:N	2.75	0.48
4:B:109:ILE:HG22	4:B:110:LYS:O	2.13	0.48
4:D:745:THR:HG21	7:D:3056:HOH:O	2.13	0.48
4:D:62:GLY:C	4:D:64:VAL:H	2.17	0.48
4:D:485:ASN:OD1	4:D:485:ASN:N	2.46	0.48
4:A:668:THR:HG22	4:A:669:GLN:HE22	1.79	0.48
4:A:670:PRO:O	4:A:671:ASN:C	2.52	0.48
4:D:230:HIS:HB3	7:D:3168:HOH:O	2.13	0.48
4:A:39:LEU:O	4:A:42:GLU:N	2.46	0.48
4:D:269:GLN:NE2	4:D:407:LYS:HE2	2.25	0.48
4:A:744:GLN:H	4:A:744:GLN:HG3	1.36	0.48
4:A:745:THR:HG22	4:A:746:ARG:N	2.28	0.48
4:A:6:ILE:HD11	4:A:259:GLY:C	2.33	0.48
4:B:860:LYS:O	4:B:862:PRO:CD	2.61	0.48
4:B:347:CYS:HA	4:B:348:PRO:HD3	1.68	0.48
4:C:252:GLU:HA	7:C:3072:HOH:O	2.13	0.48
4:A:619:GLN:O	4:A:622:ALA:N	2.47	0.48
4:A:477:GLU:O	4:A:480:LYS:N	2.46	0.48
4:C:706:LEU:CD2	4:C:725:VAL:HG22	2.42	0.48
4:C:850:ALA:O	4:C:852:GLN:N	2.42	0.48
4:D:779:ALA:O	4:D:783:VAL:CG2	2.61	0.48
4:D:273:VAL:CA	4:D:415:TRP:CE3	2.96	0.48
4:B:264:ILE:O	4:B:292:ARG:NH1	2.45	0.48
4:B:850:ALA:C	4:B:852:GLN:N	2.64	0.48
4:D:468:ALA:HA	4:D:505:GLN:HB3	1.96	0.48
4:C:502:TRP:CZ3	4:C:503:ALA:HB2	2.48	0.48
4:C:512:LEU:HG	4:C:516:PHE:HE1	1.77	0.48
4:B:84:ARG:HD3	4:B:84:ARG:O	2.13	0.48
4:A:401:MET:HG3	4:A:440:THR:HG23	1.96	0.48
4:C:78:LEU:HD21	4:C:82:ILE:HD11	1.96	0.48
4:D:84:ARG:HG3	4:D:223:SER:HB3	1.95	0.48
4:C:303:LYS:HB2	4:C:303:LYS:NZ	2.28	0.48
4:C:490:MET:O	4:C:493:ALA:HB3	2.14	0.48
2:L:8:U:O4	6:C:2002:APC:H1'	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:639:TYR:HA	4:A:780:PRO:HB3	1.95	0.48
4:A:817:ILE:CB	4:A:818:PRO:CD	2.89	0.48
4:B:450:LYS:HG2	4:B:451:PRO:HD2	1.94	0.48
4:A:274:PRO:HD3	4:A:415:TRP:CZ3	2.48	0.48
4:B:787:ASP:OD1	4:B:788:GLY:N	2.46	0.48
3:J:2:DT:H2"	3:J:3:DC:O5'	2.14	0.48
4:B:116:TYR:CE2	4:B:120:LYS:HB2	2.48	0.48
4:A:304:ALA:HA	4:A:307:ARG:HD2	1.96	0.48
4:C:464:GLY:HA3	4:C:514:PHE:CE2	2.48	0.48
4:D:490:MET:C	4:D:493:ALA:HB3	2.33	0.48
4:D:544:GLN:HG2	4:D:561:LEU:CD1	2.43	0.48
4:B:126:LEU:CD1	4:B:246:LEU:HB2	2.39	0.48
4:D:161:HIS:C	4:D:163:LYS:H	2.17	0.48
4:C:489:ILE:O	4:C:492:CYS:HB2	2.13	0.48
4:A:770:ASP:O	4:A:772:HIS:N	2.47	0.48
4:C:755:PHE:N	4:C:755:PHE:CD1	2.80	0.48
4:A:193:LYS:HA	7:A:3220:HOH:O	2.12	0.48
4:A:546:PHE:HE2	4:A:696:MET:HG3	1.78	0.48
4:C:36:GLN:HE21	4:C:273:VAL:HG22	1.78	0.48
4:D:631:LYS:O	4:D:632:ARG:C	2.51	0.48
4:D:502:TRP:CD1	4:D:512:LEU:HD13	2.49	0.48
4:A:105:PHE:CB	4:A:204:TRP:CZ2	2.89	0.48
4:D:88:TRP:CZ2	4:D:215:ARG:NH2	2.81	0.48
2:F:4:G:H2'	2:F:5:C:O4'	2.13	0.48
4:A:65:ALA:HB3	4:A:120:LYS:CE	2.42	0.48
4:A:278:TRP:CZ3	4:A:284:GLY:CA	2.93	0.48
4:C:173:ARG:NH1	4:C:182:PHE:HB2	2.28	0.48
4:C:299:THR:HG21	4:C:304:ALA:CB	2.44	0.48
4:D:452:ILE:HG23	4:D:453:GLY:N	2.28	0.48
4:B:34:ARG:O	4:B:38:ALA:HB2	2.14	0.48
4:B:705:LEU:C	4:B:707:ALA:H	2.17	0.48
4:A:617:ALA:O	4:A:618:GLY:C	2.52	0.48
4:A:649:GLN:O	4:A:653:ASP:HB2	2.14	0.48
4:A:680:LEU:O	4:A:681:ILE:C	2.50	0.48
4:A:794:THR:O	4:A:795:VAL:C	2.51	0.48
1:K:11:DA:C4	1:K:12:DT:H72	2.48	0.48
4:A:709:GLU:HB2	4:A:722:ARG:HE	1.79	0.48
4:D:828:VAL:CA	4:D:831:THR:HG22	2.43	0.48
4:B:304:ALA:O	4:B:307:ARG:HB2	2.13	0.48
4:B:422:TRP:CZ2	4:B:781:ASN:ND2	2.82	0.48
4:B:616:LEU:C	4:B:618:GLY:N	2.66	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:787:ASP:O	4:B:790:HIS:HB3	2.14	0.48
4:D:752:LEU:N	4:D:752:LEU:HD12	2.29	0.48
4:C:404:GLN:CG	4:C:432:PHE:HB2	2.41	0.48
4:D:387:LYS:HD3	7:D:3157:HOH:O	2.12	0.48
4:A:81:MET:O	4:A:85:ILE:HG13	2.14	0.48
4:C:473:VAL:O	4:C:474:PRO:O	2.32	0.48
4:C:689:VAL:O	4:C:690:VAL:C	2.52	0.48
2:F:5:C:O2	2:F:5:C:H2'	2.14	0.48
4:C:183:MET:HA	4:C:186:VAL:HB	1.96	0.48
4:D:261:LEU:C	4:D:263:GLY:N	2.66	0.48
1:K:5:DA:H2"	1:K:6:DT:OP2	2.13	0.48
4:C:400:PHE:CZ	4:C:431:MET:CE	2.96	0.48
4:C:711:LYS:HG2	4:C:717:GLU:C	2.34	0.48
4:D:121:THR:O	4:D:124:ALA:HB3	2.14	0.48
2:L:8:U:O4	6:C:2002:APC:N3	2.47	0.48
4:A:540:CYS:HB3	4:A:543:ILE:CG1	2.44	0.48
4:C:298:ARG:HA	7:C:3165:HOH:O	2.14	0.48
4:C:307:ARG:HD3	4:C:736:TRP:CE3	2.49	0.48
4:C:324:GLN:HE21	4:C:418:TYR:N	2.09	0.48
4:D:783:VAL:O	4:D:786:GLN:HB2	2.14	0.48
4:B:467:CYS:O	4:B:506:ASP:HB2	2.14	0.48
4:B:535:ALA:O	4:B:536:PHE:HD1	1.96	0.48
4:B:823:ASN:ND2	4:B:823:ASN:N	2.60	0.48
4:D:477:GLU:HG2	4:D:477:GLU:H	1.37	0.48
4:D:442:GLY:C	4:D:444:LEU:H	2.17	0.48
4:C:744:GLN:HB2	4:C:744:GLN:HE21	1.46	0.48
4:A:418:TYR:CD2	4:A:426:VAL:HG12	2.47	0.48
4:B:457:TYR:CD1	4:B:521:VAL:HG11	2.49	0.48
4:C:97:GLY:O	4:C:98:LYS:C	2.52	0.48
4:A:864:LEU:HD12	4:A:864:LEU:N	2.29	0.48
4:A:786:GLN:CA	4:A:786:GLN:NE2	2.70	0.48
4:A:138:ALA:HB1	4:A:214:VAL:HG23	1.96	0.48
6:B:2001:APC:O2B	6:B:2001:APC:O1A	2.32	0.48
4:D:343:LYS:HA	7:D:3020:HOH:O	2.13	0.48
4:C:646:PHE:O	4:C:649:GLN:HB2	2.14	0.48
4:C:629:VAL:O	4:C:629:VAL:HG12	2.14	0.48
4:A:82:ILE:HG12	4:A:115:ALA:CB	2.44	0.48
4:B:552:ASP:OD1	4:B:554:VAL:N	2.46	0.48
4:C:392:LYS:O	4:C:396:ILE:HG12	2.14	0.48
4:D:646:PHE:HE2	4:D:682:TRP:HE3	1.60	0.48
4:C:199:GLU:HG2	4:C:201:TRP:HD1	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:647:ARG:O	4:A:648:GLN:C	2.53	0.48
4:C:435:GLN:HA	4:C:810:ILE:HD11	1.96	0.48
4:D:322:ILE:HG13	7:D:3013:HOH:O	2.13	0.48
4:B:642:LYS:HG2	4:B:682:TRP:HZ3	1.77	0.48
4:B:790:HIS:ND1	4:B:790:HIS:C	2.67	0.48
4:B:810:ILE:H	4:B:813:SER:HB3	1.79	0.48
1:H:12:DT:H2'	1:H:13:DC:C6	2.49	0.48
4:C:349:VAL:HG12	4:C:349:VAL:O	2.13	0.48
4:C:515:CYS:O	4:C:516:PHE:C	2.51	0.48
4:D:752:LEU:HB2	4:D:753:GLY:H	1.54	0.48
4:C:54:MET:SD	4:C:54:MET:C	2.93	0.48
4:D:134:VAL:HG12	4:D:242:GLU:O	2.13	0.48
4:A:19:ILE:HG21	7:A:3120:HOH:O	2.08	0.48
4:D:579:ASN:HD21	4:D:625:VAL:HG12	1.79	0.48
4:A:393:SER:O	4:A:396:ILE:N	2.45	0.48
4:B:525:GLY:C	4:B:527:SER:N	2.66	0.48
4:C:101:THR:HA	4:C:104:GLN:NE2	2.28	0.48
4:A:379:ARG:HD3	4:A:660:ASP:CG	2.34	0.47
4:A:530:CYS:HB3	4:A:818:PRO:HG2	1.96	0.47
4:C:36:GLN:HG2	4:C:273:VAL:HG13	1.96	0.47
4:C:421:ASP:OD2	4:C:423:ARG:NH1	2.44	0.47
4:D:833:VAL:HG22	4:D:875:ILE:HD12	1.95	0.47
4:B:840:ASP:O	4:B:843:ALA:N	2.47	0.47
4:A:502:TRP:CG	4:A:503:ALA:N	2.81	0.47
4:A:438:ASP:OD1	4:A:507:SER:HB3	2.14	0.47
4:C:816:THR:HG22	4:C:817:ILE:N	2.29	0.47
4:B:21:PHE:O	4:B:21:PHE:CD1	2.67	0.47
4:B:687:VAL:HG23	4:B:687:VAL:O	2.14	0.47
4:A:77:LEU:HD11	4:A:226:MET:SD	2.54	0.47
4:C:292:ARG:O	4:C:292:ARG:CG	2.62	0.47
4:B:5:ASN:HD21	4:B:7:ALA:C	2.17	0.47
4:A:286:TYR:CE2	4:A:417:PRO:HG3	2.49	0.47
4:C:657:PRO:HG2	4:C:658:ALA:H	1.79	0.47
4:D:647:ARG:O	4:D:649:GLN:N	2.47	0.47
4:D:564:SER:C	7:D:3040:HOH:O	2.51	0.47
4:C:397:SER:OG	4:C:398:LEU:N	2.42	0.47
4:A:580:GLU:HG3	7:A:3111:HOH:O	2.13	0.47
4:C:391:ARG:O	4:C:391:ARG:HG2	2.14	0.47
4:A:632:ARG:HA	4:A:635:MET:HG2	1.96	0.47
4:A:277:PRO:HA	4:A:321:ASN:OD1	2.14	0.47
4:C:416:PHE:CZ	4:C:434:PRO:HD3	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:831:THR:HG22	4:C:832:MET:N	2.29	0.47
4:B:423:ARG:HG3	4:B:781:ASN:ND2	2.14	0.47
4:B:470:VAL:CG1	4:B:470:VAL:O	2.52	0.47
4:D:120:LYS:HG3	4:D:752:LEU:CD2	2.27	0.47
4:B:501:TRP:O	4:B:505:GLN:NE2	2.47	0.47
4:B:439:MET:HG3	4:B:509:PHE:CD2	2.49	0.47
4:A:216:CYS:HA	4:A:219:MET:CE	2.44	0.47
4:D:445:THR:OG1	4:D:533:PRO:HD2	2.15	0.47
4:B:199:GLU:O	4:B:201:TRP:N	2.41	0.47
4:B:201:TRP:CB	7:B:3009:HOH:O	2.50	0.47
4:A:518:TYR:C	4:A:518:TYR:CD1	2.87	0.47
4:B:67:ASN:O	4:B:69:ALA:N	2.47	0.47
4:D:569:ASP:OD2	4:D:572:GLY:N	2.45	0.47
4:B:592:ASN:N	4:B:592:ASN:OD1	2.47	0.47
4:A:829:ARG:NH2	4:A:878:SER:O	2.47	0.47
4:A:274:PRO:HD3	4:A:415:TRP:CH2	2.48	0.47
4:C:557:ARG:HD3	7:C:3150:HOH:O	2.15	0.47
4:A:403:GLU:O	4:A:404:GLN:C	2.52	0.47
4:B:461:LYS:HG2	4:B:482:ILE:HG21	1.96	0.47
4:B:504:GLU:HB3	7:B:3140:HOH:O	2.13	0.47
4:C:575:ALA:O	4:C:578:VAL:HB	2.13	0.47
4:A:751:PHE:HB3	4:A:752:LEU:HD12	1.96	0.47
4:D:345:LYS:NZ	4:D:351:ASP:O	2.43	0.47
4:A:416:PHE:CE2	4:A:434:PRO:CD	2.98	0.47
4:D:592:ASN:OD1	4:D:611:LEU:HA	2.15	0.47
1:K:8:DG:H2"	1:K:9:DA:C8	2.49	0.47
4:A:30:GLU:OE1	4:A:30:GLU:HA	2.13	0.47
4:B:106:LEU:HD11	4:B:212:VAL:HG13	1.95	0.47
4:B:155:ARG:NE	4:B:749:LEU:HD23	2.28	0.47
4:C:811:HIS:N	4:C:811:HIS:CD2	2.82	0.47
4:A:318:LYS:HE3	4:A:800:GLU:OE2	2.14	0.47
4:A:629:VAL:HG11	4:A:677:MET:HE2	1.96	0.47
4:A:545:HIS:O	4:A:546:PHE:C	2.52	0.47
4:C:777:GLY:C	4:C:780:PRO:HD2	2.35	0.47
4:C:794:THR:O	4:C:795:VAL:C	2.50	0.47
4:D:830:GLU:HA	4:D:876:LEU:HD21	1.95	0.47
4:B:329:LYS:O	4:B:330:ILE:C	2.52	0.47
4:A:60:LYS:HG3	7:A:3125:HOH:O	2.14	0.47
4:C:686:SER:HA	4:C:693:VAL:HG21	1.96	0.47
4:A:418:TYR:CD2	4:A:426:VAL:CG1	2.90	0.47
4:B:272:VAL:CG1	4:B:411:HIS:CD2	2.98	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:559:VAL:O	4:A:560:ASN:HB2	2.14	0.47
4:D:720:ARG:HD2	4:D:852:GLN:O	2.14	0.47
4:B:51:PHE:HE2	4:B:55:PHE:CD1	2.33	0.47
4:C:727:TRP:NE1	4:C:782:PHE:HD1	2.11	0.47
4:B:696:MET:HG2	4:B:779:ALA:HB1	1.95	0.47
4:B:669:GLN:HB3	4:B:672:GLN:HB2	1.97	0.47
4:B:512:LEU:O	4:B:513:ALA:C	2.49	0.47
4:A:105:PHE:C	4:A:107:GLN:N	2.67	0.47
4:A:59:LEU:CA	4:A:64:VAL:HG22	2.41	0.47
4:C:161:HIS:O	4:C:164:LYS:HG2	2.14	0.47
4:A:739:TYR:HB2	4:A:774:GLN:OE1	2.14	0.47
4:A:152:GLY:O	4:A:156:ASP:OD2	2.32	0.47
4:D:168:GLU:O	4:D:172:LYS:HG2	2.15	0.47
4:A:313:MET:HG3	4:A:313:MET:O	2.15	0.47
2:L:6:G:C2	2:L:7:A:C8	3.03	0.47
4:A:473:VAL:HG13	4:A:477:GLU:HB2	1.96	0.47
4:A:477:GLU:O	4:A:480:LYS:HB3	2.13	0.47
1:K:11:DA:C2	1:K:12:DT:N3	2.83	0.47
4:D:631:LYS:HE2	4:D:635:MET:SD	2.55	0.47
4:C:559:VAL:CG2	4:C:561:LEU:HD13	2.37	0.47
4:B:308:TYR:CA	4:B:311:VAL:HG23	2.44	0.47
4:B:634:VAL:O	4:B:637:LEU:HB2	2.14	0.47
4:B:726:HIS:CD2	4:B:736:TRP:CD2	3.03	0.47
4:B:794:THR:HG21	4:B:828:VAL:HA	1.97	0.47
4:D:333:LYS:HZ2	4:D:516:PHE:HB3	1.78	0.47
4:D:387:LYS:HE2	7:D:3158:HOH:O	2.14	0.47
4:A:85:ILE:HG23	4:A:219:MET:SD	2.54	0.47
4:C:180:LYS:O	4:C:183:MET:N	2.41	0.47
4:C:183:MET:O	4:C:186:VAL:HB	2.15	0.47
3:M:4:DG:H4'	3:M:5:DA:OP1	2.15	0.47
4:C:39:LEU:HD22	4:C:272:VAL:HG23	1.95	0.47
1:K:2:DG:H1'	7:K:268:HOH:O	2.14	0.47
1:N:4:DA:C6	1:N:5:DA:C6	3.02	0.47
4:A:632:ARG:HH22	6:A:2000:APC:H5'2	1.79	0.47
4:A:676:TYR:O	4:A:677:MET:C	2.51	0.47
4:A:791:LEU:HA	4:A:814:PHE:HE2	1.80	0.47
4:A:869:ASN:HD22	4:A:869:ASN:N	2.13	0.47
4:A:828:VAL:CB	4:A:883:ALA:HA	2.44	0.47
4:A:141:ILE:HB	4:A:213:GLY:HA2	1.97	0.47
4:D:558:ALA:CB	4:D:570:ILE:HD13	2.45	0.47
4:D:435:GLN:HA	4:D:810:ILE:CD1	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:797:TRP:CZ2	4:D:801:LYS:HG3	2.50	0.47
4:B:44:TYR:HD1	4:B:44:TYR:H	1.63	0.47
4:D:515:CYS:O	4:D:516:PHE:C	2.51	0.47
4:B:469:GLY:C	4:B:471:ASP:H	2.15	0.47
4:A:80:LYS:HE2	4:A:224:THR:HG22	1.96	0.47
4:A:99:ARG:N	4:A:99:ARG:HD2	2.29	0.47
4:A:103:PHE:O	4:A:107:GLN:NE2	2.44	0.47
4:A:190:MET:HB3	7:A:3103:HOH:O	2.14	0.47
4:B:159:ALA:O	4:B:161:HIS:N	2.47	0.47
4:C:109:ILE:HD12	4:C:109:ILE:N	2.29	0.47
4:D:236:VAL:CG2	4:D:239:GLN:HB2	2.45	0.47
1:N:2:DG:C2'	1:N:3:DG:C8	2.95	0.47
4:D:316:VAL:O	4:D:317:TYR:C	2.52	0.47
4:C:616:LEU:HD13	4:C:676:TYR:HB2	1.95	0.47
4:D:14:ILE:N	4:D:14:ILE:HD12	2.23	0.47
4:A:42:GLU:O	4:A:46:MET:N	2.44	0.47
4:D:521:VAL:O	4:D:525:GLY:N	2.46	0.47
4:C:71:LYS:N	4:C:72:PRO:HD2	2.30	0.47
2:I:2:C:H2'	2:I:3:G:H8	1.80	0.47
4:D:629:VAL:HG22	4:D:654:THR:HG21	1.95	0.47
2:L:2:C:O5'	2:L:2:C:H6	1.98	0.47
3:J:7:DT:H2"	3:J:8:DC:C6	2.49	0.47
4:D:836:TYR:N	4:D:836:TYR:CD2	2.81	0.47
4:C:101:THR:HA	4:C:104:GLN:CD	2.35	0.47
4:B:652:GLU:O	4:B:657:PRO:HD3	2.13	0.47
4:D:143:ARG:O	4:D:147:ASP:OD2	2.32	0.47
4:B:279:THR:HG22	7:B:3148:HOH:O	2.14	0.47
4:A:801:LYS:C	4:A:801:LYS:CD	2.80	0.47
4:A:280:GLY:HA2	4:A:317:TYR:HE1	1.74	0.47
4:C:417:PRO:O	4:C:418:TYR:HD1	1.98	0.47
4:C:830:GLU:HA	4:C:876:LEU:HD21	1.96	0.47
4:D:631:LYS:HD3	4:D:635:MET:SD	2.54	0.47
4:B:806:SER:O	4:B:816:THR:HG23	2.14	0.47
4:B:428:ALA:H	4:B:435:GLN:NE2	2.11	0.47
4:B:647:ARG:O	4:B:650:VAL:N	2.48	0.47
4:B:24:LEU:O	4:B:25:ALA:C	2.52	0.47
4:C:337:VAL:HG12	4:C:338:ALA:H	1.79	0.47
4:C:651:LEU:HB2	4:C:674:ALA:CB	2.45	0.47
4:D:472:LYS:C	4:D:567:VAL:HG21	2.35	0.47
4:C:117:ILE:HG21	4:C:145:ILE:HD13	1.97	0.47
4:D:308:TYR:OH	4:D:734:PRO:O	2.26	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:579:ASN:HA	4:C:582:LEU:CG	2.45	0.47
4:D:159:ALA:HB3	4:D:163:LYS:HD3	1.96	0.47
4:B:314:PRO:C	4:B:316:VAL:N	2.65	0.47
3:P:5:DA:H2"	3:P:6:DT:H72	1.97	0.47
4:B:656:GLN:N	4:B:657:PRO:HD2	2.29	0.47
4:A:86:ASN:O	4:A:90:GLU:HG2	2.15	0.47
4:A:631:LYS:O	4:A:632:ARG:C	2.53	0.47
4:A:635:MET:HE1	6:A:2000:APC:H3'	1.97	0.47
4:A:311:VAL:HG12	4:A:312:TYR:H	1.77	0.47
4:A:797:TRP:CH2	4:A:801:LYS:HG3	2.50	0.47
4:D:416:PHE:O	4:D:418:TYR:CE1	2.68	0.47
4:B:56:GLU:CD	4:B:57:ARG:N	2.68	0.47
4:B:49:ALA:O	4:B:50:ARG:C	2.52	0.47
4:C:452:ILE:HG23	4:C:453:GLY:N	2.29	0.47
4:D:31:ARG:O	4:D:32:LEU:C	2.53	0.47
4:B:485:ASN:N	4:B:485:ASN:OD1	2.44	0.47
4:B:166:VAL:O	4:B:167:GLU:C	2.53	0.47
4:A:77:LEU:CD1	4:A:226:MET:SD	3.03	0.47
4:D:647:ARG:O	4:D:648:GLN:C	2.53	0.47
4:A:706:LEU:HD11	4:A:849:PHE:CG	2.50	0.47
4:D:166:VAL:O	4:D:167:GLU:C	2.53	0.47
4:B:778:ILE:HG13	4:B:778:ILE:O	2.14	0.47
4:C:517:GLU:OE1	4:C:517:GLU:HA	2.14	0.47
4:D:374:LEU:O	4:D:378:LYS:HB2	2.14	0.47
4:A:679:LYS:O	4:A:680:LEU:C	2.51	0.47
4:A:794:THR:HG1	4:A:831:THR:HG21	1.76	0.47
4:C:274:PRO:HA	4:C:275:PRO:HD3	1.77	0.47
4:C:314:PRO:HD3	7:C:3099:HOH:O	2.13	0.47
4:C:727:TRP:HB3	4:C:845:PHE:CE1	2.50	0.47
4:C:870:LEU:HD23	4:C:871:ASN:C	2.35	0.47
4:D:419:ASN:ND2	4:D:429:VAL:HG22	2.30	0.47
4:B:648:GLN:O	4:B:649:GLN:C	2.53	0.47
4:B:567:VAL:HG13	4:B:880:PHE:CD2	2.50	0.47
4:B:492:CYS:SG	4:B:502:TRP:HB3	2.55	0.47
4:D:448:LYS:HZ1	4:D:806:SER:HA	1.79	0.47
4:C:746:ARG:NH1	4:C:754:GLN:O	2.47	0.47
4:B:411:HIS:C	4:B:413:ALA:N	2.67	0.47
4:A:647:ARG:CG	4:A:675:GLY:HA2	2.45	0.46
4:A:420:MET:HA	4:A:425:ARG:O	2.15	0.46
4:D:706:LEU:CD2	4:D:853:LEU:HD23	2.44	0.46
4:D:631:LYS:HE2	6:D:2003:APC:H3A2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:782:PHE:CE2	4:D:786:GLN:OE1	2.68	0.46
4:B:570:ILE:HG13	4:B:570:ILE:O	2.14	0.46
4:B:675:GLY:O	4:B:678:ALA:HB3	2.15	0.46
4:B:729:THR:HB	4:B:789:SER:HB2	1.96	0.46
4:B:36:GLN:OE1	4:B:36:GLN:CA	2.63	0.46
4:B:403:GLU:O	4:B:405:ALA:N	2.48	0.46
4:C:404:GLN:CA	4:C:404:GLN:HE21	2.15	0.46
4:A:439:MET:HG3	4:A:509:PHE:CE2	2.49	0.46
4:C:616:LEU:O	4:C:617:ALA:C	2.53	0.46
1:E:14:DG:C2'	1:E:15:DC:H6	2.28	0.46
4:A:390:ALA:O	4:A:391:ARG:C	2.52	0.46
4:C:4:ILE:CD1	7:C:3146:HOH:O	2.62	0.46
4:B:254:ILE:O	4:B:255:ALA:C	2.52	0.46
3:G:4:DG:C1'	3:G:5:DA:C8	2.98	0.46
4:D:823:ASN:O	4:D:826:LYS:N	2.48	0.46
4:A:711:LYS:CB	4:A:711:LYS:NZ	2.78	0.46
4:A:311:VAL:CG1	4:A:312:TYR:N	2.77	0.46
4:A:308:TYR:CE2	4:A:736:TRP:CZ3	3.03	0.46
4:B:247:ALA:CB	4:B:250:TYR:CD1	2.99	0.46
4:D:828:VAL:O	4:D:831:THR:HG22	2.16	0.46
4:C:540:CYS:O	4:C:541:SER:C	2.54	0.46
4:B:268:PHE:CD2	4:B:429:VAL:HG12	2.51	0.46
4:B:787:ASP:O	4:B:790:HIS:N	2.48	0.46
1:H:12:DT:C2'	1:H:13:DC:C6	2.98	0.46
4:B:116:TYR:CD2	4:B:116:TYR:C	2.89	0.46
4:C:84:ARG:HD2	4:C:222:GLU:OE1	2.14	0.46
4:C:246:LEU:HG	4:C:247:ALA:N	2.29	0.46
4:C:140:ALA:O	4:C:143:ARG:N	2.48	0.46
4:C:623:TYR:HD1	4:C:663:LYS:HE2	1.80	0.46
4:A:303:LYS:HE2	4:A:740:LYS:HZ1	1.81	0.46
4:C:598:THR:OG1	4:C:605:ILE:HD13	2.16	0.46
4:A:410:ASN:N	4:A:410:ASN:HD22	2.12	0.46
4:A:473:VAL:HA	4:A:474:PRO:HD2	1.62	0.46
4:A:871:ASN:O	4:A:872:LEU:C	2.54	0.46
4:C:416:PHE:HB2	4:C:418:TYR:CE1	2.51	0.46
4:D:739:TYR:CD2	4:D:774:GLN:HA	2.50	0.46
4:D:784:HIS:O	4:D:787:ASP:N	2.49	0.46
4:B:643:GLU:C	4:B:645:GLY:N	2.66	0.46
4:A:403:GLU:O	4:A:406:ASN:N	2.48	0.46
4:A:347:CYS:HB3	4:A:350:GLU:CG	2.45	0.46
4:A:347:CYS:HB3	4:A:350:GLU:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:450:LYS:HD2	4:C:817:ILE:CD1	2.46	0.46
4:A:386:ARG:C	4:A:388:ASP:N	2.68	0.46
4:D:21:PHE:CD1	4:D:21:PHE:O	2.68	0.46
2:F:7:A:H2'	2:F:8:U:C6	2.46	0.46
4:D:373:ALA:O	4:D:377:TRP:CD1	2.68	0.46
4:A:711:LYS:HB2	4:A:711:LYS:NZ	2.30	0.46
4:C:659:ILE:HG22	4:C:660:ASP:N	2.29	0.46
4:A:796:VAL:O	4:A:799:HIS:N	2.40	0.46
4:B:450:LYS:HB3	4:B:819:ALA:CB	2.45	0.46
4:A:281:ILE:HG22	4:A:282:THR:HG22	1.86	0.46
4:C:729:THR:O	4:C:732:GLY:N	2.29	0.46
4:B:324:GLN:HG3	4:B:418:TYR:H	1.80	0.46
4:B:549:MET:HE1	4:B:782:PHE:HE2	1.81	0.46
4:C:92:VAL:HG12	4:C:92:VAL:O	2.15	0.46
4:A:59:LEU:HD23	4:A:64:VAL:CG1	2.46	0.46
4:D:390:ALA:CB	4:D:394:ARG:HH21	2.28	0.46
4:A:261:LEU:C	4:A:263:GLY:H	2.19	0.46
4:D:684:SER:O	4:D:687:VAL:HG22	2.16	0.46
4:B:520:GLY:HA3	4:B:528:TYR:CE1	2.50	0.46
4:A:646:PHE:O	4:A:647:ARG:O	2.33	0.46
4:A:726:HIS:CD2	4:A:736:TRP:CE2	3.03	0.46
4:A:274:PRO:HA	4:A:415:TRP:CG	2.50	0.46
4:C:698:TRP:O	4:C:701:SER:HB2	2.16	0.46
4:C:777:GLY:O	4:C:781:ASN:CG	2.54	0.46
4:C:727:TRP:CD1	4:C:782:PHE:HE1	2.33	0.46
4:C:549:MET:CE	4:C:786:GLN:HG2	2.46	0.46
4:D:632:ARG:HG2	4:D:653:ASP:OD2	2.15	0.46
1:N:12:DT:C2'	1:N:13:DC:H5'	2.22	0.46
4:D:328:TRP:CG	4:D:416:PHE:HE2	2.33	0.46
4:D:797:TRP:HD1	4:D:827:ALA:HB1	1.81	0.46
4:B:644:PHE:CD2	4:B:644:PHE:C	2.89	0.46
4:B:469:GLY:C	4:B:471:ASP:N	2.68	0.46
4:A:89:PHE:HZ	4:A:106:LEU:O	1.99	0.46
4:B:158:GLU:HA	4:B:195:LEU:CD1	2.42	0.46
4:C:475:PHE:N	4:C:476:PRO:CD	2.78	0.46
4:D:541:SER:O	4:D:542:GLY:C	2.53	0.46
4:C:165:ASN:ND2	7:C:3138:HOH:O	2.48	0.46
4:D:593:GLU:O	4:D:610:LYS:HB3	2.16	0.46
4:D:21:PHE:CD1	4:D:21:PHE:C	2.89	0.46
4:D:588:ASN:O	4:D:614:LYS:HG3	2.15	0.46
3:M:9:DC:H2"	7:M:350:HOH:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:76:THR:C	4:D:79:PRO:HD2	2.36	0.46
4:A:520:GLY:HA3	4:A:528:TYR:CE2	2.50	0.46
4:A:727:TRP:CH2	4:A:735:VAL:CG2	2.99	0.46
4:A:109:ILE:HG12	4:A:148:GLU:HB3	1.97	0.46
4:C:829:ARG:NH2	4:C:878:SER:O	2.47	0.46
4:B:60:LYS:O	4:B:60:LYS:HG2	2.15	0.46
4:B:459:TRP:CH2	4:B:825:PHE:CD2	3.04	0.46
4:B:432:PHE:CD2	4:B:432:PHE:C	2.89	0.46
4:C:338:ALA:O	4:C:339:ASN:C	2.43	0.46
4:C:655:ILE:O	4:C:655:ILE:HG22	2.15	0.46
4:C:329:LYS:HD3	4:C:447:ALA:HA	1.98	0.46
4:D:476:PRO:HG2	4:D:477:GLU:OE2	2.15	0.46
1:H:3:DG:N2	3:J:9:DC:O2	2.48	0.46
4:D:89:PHE:CZ	4:D:106:LEU:HB3	2.46	0.46
4:C:82:ILE:HA	4:C:85:ILE:HD12	1.96	0.46
4:C:268:PHE:O	4:C:430:SER:HB2	2.15	0.46
4:D:613:THR:HG22	4:D:676:TYR:CE1	2.51	0.46
4:C:754:GLN:HB3	4:C:755:PHE:HD1	1.80	0.46
3:G:1:DG:H1'	3:G:2:DT:H72	1.98	0.46
4:D:81:MET:O	4:D:85:ILE:HG13	2.15	0.46
4:A:577:LYS:HB3	4:A:684:SER:OG	2.15	0.46
4:A:446:LEU:HD12	4:A:531:SER:O	2.15	0.46
4:A:541:SER:O	4:A:542:GLY:C	2.52	0.46
4:A:829:ARG:NH1	4:A:829:ARG:CG	2.57	0.46
4:A:139:SER:HB2	4:A:210:ILE:CD1	2.46	0.46
4:C:551:ARG:HH12	4:C:867:LYS:HZ3	1.63	0.46
4:C:840:ASP:OD2	4:C:867:LYS:NZ	2.49	0.46
4:C:849:PHE:O	4:C:850:ALA:C	2.54	0.46
4:B:680:LEU:H	4:B:680:LEU:CD1	2.29	0.46
4:C:349:VAL:HG13	4:C:503:ALA:O	2.16	0.46
4:B:748:ASN:ND2	4:B:751:PHE:N	2.60	0.46
4:B:482:ILE:O	4:B:485:ASN:N	2.48	0.46
4:B:172:LYS:NZ	4:B:172:LYS:CB	2.70	0.46
4:D:122:THR:O	4:D:125:CYS:N	2.48	0.46
4:D:422:TRP:O	4:D:422:TRP:CD1	2.69	0.46
4:D:205:HIS:C	4:D:207:GLU:N	2.69	0.46
4:C:577:LYS:O	4:C:581:ILE:HG13	2.15	0.46
4:A:517:GLU:OE1	4:A:517:GLU:HA	2.16	0.46
4:B:55:PHE:HE2	4:B:59:LEU:HD11	1.79	0.46
4:C:550:LEU:C	4:C:867:LYS:HG3	2.36	0.46
4:D:825:PHE:O	4:D:828:VAL:HG23	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:460:LEU:HD12	4:B:460:LEU:O	2.15	0.46
4:B:556:GLY:HA2	4:B:561:LEU:HD13	1.98	0.46
4:B:727:TRP:CZ2	4:B:782:PHE:HA	2.51	0.46
4:D:502:TRP:CG	4:D:512:LEU:HD13	2.50	0.46
4:B:475:PHE:HB2	4:B:476:PRO:HD2	1.98	0.46
4:A:404:GLN:NE2	4:A:404:GLN:CA	2.73	0.46
4:A:429:VAL:O	4:A:430:SER:O	2.33	0.46
4:D:221:ILE:HG23	4:D:227:VAL:O	2.16	0.46
4:D:55:PHE:CZ	4:D:59:LEU:HD11	2.51	0.46
4:B:229:LEU:CD1	4:B:242:GLU:HG2	2.41	0.46
4:C:42:GLU:HG2	4:C:46:MET:HE2	1.96	0.46
4:A:644:PHE:C	4:A:644:PHE:CD2	2.88	0.46
4:B:105:PHE:O	4:B:107:GLN:N	2.49	0.46
4:A:230:HIS:CE1	4:A:232:GLN:HE21	2.34	0.46
4:A:475:PHE:O	4:A:476:PRO:C	2.50	0.46
4:C:319:ALA:HB2	4:C:792:ARG:HB3	1.97	0.46
4:C:418:TYR:HD2	4:C:426:VAL:HG11	1.80	0.46
4:C:786:GLN:O	4:C:788:GLY:N	2.49	0.46
4:C:435:GLN:HG2	4:C:810:ILE:HG12	1.97	0.46
4:C:848:GLN:OE1	4:C:848:GLN:HA	2.15	0.46
4:B:408:PHE:CD1	4:B:414:ILE:HG21	2.31	0.46
4:C:506:ASP:O	4:C:508:PRO:HD2	2.15	0.46
4:B:164:LYS:HZ2	4:B:164:LYS:N	2.13	0.46
4:C:534:LEU:CD1	4:C:818:PRO:HA	2.46	0.46
4:D:470:VAL:CG1	4:D:473:VAL:HG11	2.40	0.46
4:D:281:ILE:HG12	4:D:309:GLU:HA	1.97	0.46
4:D:744:GLN:HB3	4:D:756:ARG:CB	2.45	0.46
4:B:67:ASN:O	4:B:68:ALA:C	2.54	0.46
4:C:257:ARG:HH11	4:C:257:ARG:HG2	1.81	0.46
4:B:30:GLU:O	4:B:31:ARG:C	2.53	0.46
4:D:543:ILE:HG21	4:D:689:VAL:CG1	2.45	0.46
4:A:656:GLN:C	4:A:658:ALA:N	2.68	0.46
4:A:831:THR:CG2	4:A:832:MET:N	2.78	0.46
4:C:14:ILE:CG2	4:C:288:ALA:CB	2.91	0.46
4:C:700:LYS:O	4:C:701:SER:C	2.54	0.46
4:D:699:LEU:HD11	4:D:782:PHE:CD2	2.50	0.46
4:B:433:ASN:HB2	4:B:434:PRO:HD2	1.88	0.46
4:D:468:ALA:HB2	4:D:511:PHE:CE1	2.51	0.46
4:C:646:PHE:HD1	4:C:649:GLN:OE1	1.99	0.46
4:A:404:GLN:O	4:A:407:LYS:HB3	2.16	0.46
4:B:163:LYS:HA	4:B:163:LYS:HD2	1.71	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:462:ILE:CD1	4:C:479:ILE:HD11	2.45	0.46
4:D:135:GLN:HB3	7:D:3160:HOH:O	2.15	0.46
4:C:180:LYS:O	4:C:181:ALA:C	2.54	0.46
4:D:139:SER:CB	4:D:210:ILE:HD13	2.45	0.46
4:B:72:PRO:HG3	4:B:257:ARG:HG3	1.97	0.46
4:A:746:ARG:HB3	4:A:746:ARG:CZ	2.45	0.46
4:D:182:PHE:O	4:D:186:VAL:HG23	2.16	0.46
4:B:322:ILE:O	4:B:323:ALA:C	2.52	0.46
4:A:147:ASP:HB3	4:A:750:MET:CE	2.46	0.46
4:C:809:LEU:HA	4:C:813:SER:O	2.17	0.46
4:A:480:LYS:HG3	4:A:484:GLU:OE1	2.16	0.45
4:C:551:ARG:HE	4:C:872:LEU:HD11	1.80	0.45
1:K:15:DC:C5'	1:K:15:DC:H6	2.28	0.45
4:B:620:TRP:CD2	4:B:677:MET:CE	2.99	0.45
4:B:676:TYR:O	4:B:677:MET:C	2.53	0.45
4:D:116:TYR:HH	4:D:752:LEU:HD22	1.82	0.45
4:B:163:LYS:HB3	4:B:164:LYS:HZ2	1.79	0.45
4:B:164:LYS:HA	4:B:164:LYS:HD3	1.78	0.45
4:D:460:LEU:HD13	4:D:532:LEU:HD23	1.97	0.45
4:D:236:VAL:O	4:D:240:ASP:CB	2.64	0.45
4:B:199:GLU:C	4:B:201:TRP:H	2.20	0.45
4:C:164:LYS:N	4:C:164:LYS:HZ3	2.14	0.45
4:C:148:GLU:OE1	4:C:749:LEU:HB2	2.15	0.45
4:A:158:GLU:CD	4:A:195:LEU:HB3	2.37	0.45
4:C:89:PHE:CZ	4:C:106:LEU:O	2.68	0.45
4:B:797:TRP:CZ2	4:B:801:LYS:HG3	2.51	0.45
4:A:798:ALA:HB1	4:A:804:ILE:HD12	1.98	0.45
4:A:801:LYS:HD3	4:A:801:LYS:O	2.13	0.45
4:A:828:VAL:C	4:A:830:GLU:H	2.19	0.45
4:D:705:LEU:HB3	4:D:857:GLN:HE22	1.78	0.45
4:C:548:ALA:C	4:C:550:LEU:H	2.19	0.45
4:C:882:PHE:O	4:C:883:ALA:CB	2.64	0.45
1:H:9:DA:H62	3:J:1:DG:H22	1.64	0.45
4:C:334:VAL:O	4:C:337:VAL:HB	2.16	0.45
4:C:437:ASN:ND2	4:C:440:THR:H	2.13	0.45
4:C:432:PHE:HE1	4:C:440:THR:HG23	1.81	0.45
4:A:92:VAL:CG1	4:A:99:ARG:HG3	2.45	0.45
4:C:110:LYS:O	4:C:114:VAL:HG23	2.16	0.45
4:A:704:LYS:HE3	4:A:860:LYS:CE	2.46	0.45
4:B:257:ARG:HG2	4:B:257:ARG:NH1	2.30	0.45
1:E:4:DA:H2"	1:E:5:DA:OP2	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:1:G:C2	2:L:2:C:C2	3.04	0.45
4:D:501:TRP:HA	4:D:504:GLU:OE2	2.16	0.45
1:K:2:DG:H2"	1:K:3:DG:C8	2.52	0.45
4:B:279:THR:O	4:B:279:THR:HG23	2.15	0.45
4:B:373:ALA:O	4:B:377:TRP:CD1	2.70	0.45
4:B:384:VAL:O	4:B:384:VAL:HG12	2.16	0.45
4:D:704:LYS:HE3	4:D:860:LYS:NZ	2.32	0.45
4:A:113:ALA:O	4:A:114:VAL:C	2.54	0.45
4:D:709:GLU:O	4:D:711:LYS:HG3	2.16	0.45
4:C:556:GLY:HA3	4:C:561:LEU:HD22	1.91	0.45
1:H:14:DG:H8	1:H:14:DG:H5'	1.82	0.45
4:D:342:THR:CG2	4:D:348:PRO:HG2	2.41	0.45
4:D:126:LEU:HD11	4:D:227:VAL:HG12	1.97	0.45
4:D:440:THR:O	4:D:444:LEU:HD12	2.16	0.45
4:B:552:ASP:HB3	4:B:691:ALA:HB2	1.99	0.45
4:A:416:PHE:HA	4:A:417:PRO:HD2	1.75	0.45
4:C:656:GLN:H	4:C:657:PRO:HD2	1.78	0.45
4:D:656:GLN:N	4:D:657:PRO:CD	2.77	0.45
4:A:261:LEU:O	4:A:263:GLY:N	2.50	0.45
4:C:567:VAL:HG12	4:C:567:VAL:O	2.15	0.45
4:D:47:GLY:HA3	4:D:265:SER:O	2.16	0.45
4:A:153:ARG:HD2	7:A:3089:HOH:O	2.17	0.45
4:D:696:MET:O	4:D:700:LYS:HB2	2.16	0.45
4:A:281:ILE:HG13	4:A:309:GLU:HG2	1.98	0.45
4:A:145:ILE:H	4:A:145:ILE:HG12	1.55	0.45
4:C:433:ASN:C	7:C:3164:HOH:O	2.52	0.45
4:C:425:ARG:NH2	4:C:787:ASP:OD2	2.49	0.45
4:B:577:LYS:O	4:B:580:GLU:HB2	2.16	0.45
4:B:698:TRP:O	4:B:699:LEU:C	2.54	0.45
4:B:690:VAL:C	4:B:693:VAL:HG23	2.36	0.45
4:D:669:GLN:HG3	4:D:672:GLN:HE21	1.80	0.45
4:B:770:ASP:OD2	4:B:773:LYS:HD2	2.17	0.45
4:B:314:PRO:C	4:B:316:VAL:H	2.20	0.45
4:B:232:GLN:HG3	4:B:243:THR:HG23	1.98	0.45
1:E:2:DG:C2	7:E:42:HOH:O	2.56	0.45
4:A:462:ILE:HG22	4:A:463:HIS:N	2.31	0.45
4:D:322:ILE:HG21	7:D:3013:HOH:O	2.16	0.45
4:C:814:PHE:CE1	4:C:883:ALA:HB1	2.52	0.45
4:B:167:GLU:O	4:B:168:GLU:C	2.54	0.45
4:B:685:VAL:O	4:B:687:VAL:N	2.49	0.45
4:A:112:GLU:H	4:A:112:GLU:CD	2.19	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:278:TRP:CD2	4:A:284:GLY:HA3	2.49	0.45
4:C:164:LYS:N	4:C:164:LYS:NZ	2.64	0.45
4:A:664:GLY:O	4:A:667:PHE:HB2	2.17	0.45
4:D:42:GLU:O	4:D:45:GLU:N	2.50	0.45
2:L:4:G:H1'	4:C:389:LYS:HZ1	1.80	0.45
3:J:5:DA:C2'	3:J:6:DT:H72	2.47	0.45
4:B:225:GLY:HA2	7:B:3035:HOH:O	2.16	0.45
4:A:423:ARG:O	4:A:785:SER:HB2	2.16	0.45
4:A:109:ILE:HG13	4:A:149:ALA:CB	2.46	0.45
4:A:148:GLU:OE2	4:A:749:LEU:HB2	2.15	0.45
1:K:12:DT:N3	1:K:13:DC:C5	2.85	0.45
1:K:16:DC:H2"	1:K:17:DG:O5'	2.15	0.45
4:D:322:ILE:HD13	4:D:322:ILE:HA	1.79	0.45
4:B:404:GLN:HB2	4:B:404:GLN:HE21	1.35	0.45
4:C:140:ALA:O	4:C:141:ILE:C	2.55	0.45
4:D:316:VAL:HG22	4:D:731:ASP:OD2	2.15	0.45
4:D:448:LYS:HZ2	4:D:806:SER:CB	2.29	0.45
4:B:552:ASP:CB	4:B:691:ALA:HB2	2.46	0.45
4:B:436:GLY:O	4:B:441:LYS:HE2	2.15	0.45
4:A:518:TYR:HD1	4:A:518:TYR:O	1.98	0.45
7:M:542:HOH:O	4:C:164:LYS:HB3	2.16	0.45
4:B:6:ILE:C	4:B:8:LYS:H	2.19	0.45
4:A:416:PHE:CZ	4:A:434:PRO:HD3	2.51	0.45
4:A:746:ARG:NH1	4:A:754:GLN:H	2.11	0.45
4:D:6:ILE:O	4:D:8:LYS:N	2.39	0.45
4:A:208:ASP:OD2	4:A:208:ASP:N	2.50	0.45
4:A:330:ILE:HD13	4:A:330:ILE:HA	1.39	0.45
4:A:778:ILE:O	4:A:779:ALA:C	2.54	0.45
4:D:859:ASP:OD2	4:D:860:LYS:N	2.50	0.45
4:B:418:TYR:HE1	7:B:3028:HOH:O	1.99	0.45
4:B:459:TRP:HH2	4:B:825:PHE:CE2	2.34	0.45
1:H:9:DA:C6	4:B:644:PHE:CE1	3.04	0.45
4:B:726:HIS:HB2	4:B:736:TRP:CD1	2.52	0.45
4:B:804:ILE:HG22	4:B:807:PHE:CE2	2.52	0.45
4:B:36:GLN:HB3	4:B:37:LEU:HD12	1.97	0.45
4:D:220:LEU:HD21	4:D:226:MET:HE2	1.99	0.45
4:A:385:TYR:CD2	4:A:385:TYR:C	2.90	0.45
4:B:455:GLU:O	4:B:458:TYR:HB3	2.16	0.45
4:D:633:SER:HA	4:D:649:GLN:HE22	1.82	0.45
4:A:849:PHE:O	4:A:850:ALA:C	2.55	0.45
4:C:279:THR:CG2	7:C:3038:HOH:O	2.59	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:84:ARG:HA	4:D:84:ARG:HH11	1.80	0.45
4:B:334:VAL:CG1	4:B:443:LEU:HD23	2.46	0.45
4:B:402:LEU:HA	4:B:402:LEU:HD23	1.45	0.45
4:A:421:ASP:C	4:A:423:ARG:N	2.70	0.45
4:A:473:VAL:HG13	4:A:473:VAL:O	2.17	0.45
4:D:702:ALA:O	4:D:703:ALA:C	2.55	0.45
4:B:620:TRP:CH2	4:B:677:MET:HE3	2.52	0.45
1:H:15:DC:H3'	7:H:334:HOH:O	2.16	0.45
4:B:486:HIS:C	4:B:486:HIS:ND1	2.71	0.45
4:D:462:ILE:HD12	4:D:475:PHE:HD1	1.82	0.45
4:D:246:LEU:HD23	4:D:247:ALA:O	2.17	0.45
4:B:19:ILE:O	4:B:21:PHE:N	2.42	0.45
4:C:161:HIS:C	4:C:163:LYS:H	2.20	0.45
4:C:269:GLN:HB3	4:C:269:GLN:HE21	1.56	0.45
4:A:318:LYS:O	4:A:319:ALA:C	2.55	0.45
4:A:786:GLN:O	4:A:787:ASP:C	2.54	0.45
4:C:287:TRP:O	4:C:288:ALA:O	2.35	0.45
4:C:849:PHE:O	4:C:852:GLN:HB2	2.17	0.45
1:N:10:DT:H5'	4:D:641:SER:CB	2.46	0.45
4:D:829:ARG:HH12	4:D:883:ALA:H	1.64	0.45
4:B:419:ASN:O	4:B:420:MET:CG	2.65	0.45
1:H:10:DT:H5'	4:B:641:SER:H	1.79	0.45
4:C:507:SER:HA	4:C:508:PRO:HD2	1.62	0.45
4:B:400:PHE:O	4:B:401:MET:C	2.50	0.45
3:G:4:DG:H2"	3:G:5:DA:H8	1.81	0.45
4:B:205:HIS:O	4:B:207:GLU:N	2.50	0.45
4:D:5:ASN:HA	4:D:52:ARG:NH1	2.32	0.45
4:A:802:TYR:C	4:A:804:ILE:H	2.17	0.45
4:C:323:ALA:O	4:C:324:GLN:C	2.55	0.45
4:C:553:GLU:CG	4:C:554:VAL:N	2.80	0.45
4:B:549:MET:HE1	4:B:841:VAL:HG21	1.96	0.45
1:H:15:DC:N3	1:H:16:DC:C5	2.85	0.45
4:B:267:MET:HB3	4:B:267:MET:HE3	1.83	0.45
4:B:50:ARG:HH11	4:B:50:ARG:HG2	1.82	0.45
4:D:331:ASN:ND2	4:D:334:VAL:HG23	2.32	0.45
4:D:439:MET:CE	4:D:443:LEU:HD11	2.47	0.45
4:D:402:LEU:HD21	4:D:439:MET:HE3	1.99	0.45
4:D:502:TRP:CE3	4:D:503:ALA:N	2.85	0.45
4:A:688:THR:CG2	4:A:689:VAL:HG13	2.30	0.45
4:C:432:PHE:CE1	4:C:440:THR:HG23	2.51	0.45
4:C:329:LYS:HG3	4:C:445:THR:HG22	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:60:LYS:HG3	7:A:3023:HOH:O	2.16	0.45
4:D:816:THR:HG22	4:D:817:ILE:N	2.32	0.45
4:B:345:LYS:HZ1	4:B:351:ASP:N	2.13	0.45
4:A:8:LYS:O	4:A:12:SER:HB2	2.16	0.45
1:E:6:DT:H2'	1:E:6:DT:H6	1.55	0.45
4:C:3:THR:HB	4:C:52:ARG:CZ	2.46	0.45
4:A:474:PRO:C	4:A:476:PRO:HD2	2.37	0.44
4:C:845:PHE:O	4:C:848:GLN:CB	2.57	0.44
4:B:532:LEU:HG	4:B:533:PRO:CD	2.47	0.44
4:B:571:TYR:H	4:B:571:TYR:HD1	1.65	0.44
4:B:579:ASN:HA	4:B:582:LEU:HB2	1.98	0.44
4:B:643:GLU:HG3	4:B:682:TRP:HB3	1.99	0.44
4:C:651:LEU:C	4:C:651:LEU:CD1	2.86	0.44
4:B:164:LYS:N	4:B:164:LYS:HZ3	2.15	0.44
4:B:138:ALA:O	4:B:213:GLY:HA3	2.17	0.44
4:D:729:THR:HG23	4:D:733:PHE:O	2.17	0.44
4:A:47:GLY:HA3	4:A:265:SER:O	2.18	0.44
4:B:347:CYS:HB3	4:B:350:GLU:HG3	1.99	0.44
4:C:488:ASN:O	4:C:491:ALA:HB3	2.16	0.44
4:A:554:VAL:O	4:A:557:ARG:HB3	2.17	0.44
4:A:572:GLY:O	4:A:575:ALA:HB3	2.18	0.44
4:C:313:MET:O	4:C:317:TYR:CD2	2.70	0.44
4:C:323:ALA:O	4:C:325:ASN:N	2.49	0.44
4:D:631:LYS:HD2	4:D:632:ARG:NH1	2.32	0.44
4:B:570:ILE:HA	4:B:573:ILE:HG22	1.98	0.44
4:B:640:GLY:O	4:B:641:SER:O	2.36	0.44
4:B:643:GLU:HG3	4:B:682:TRP:CB	2.47	0.44
4:B:784:HIS:C	4:B:786:GLN:N	2.69	0.44
4:B:404:GLN:HG3	4:B:404:GLN:O	2.17	0.44
4:B:416:PHE:HD1	4:B:430:SER:OG	2.01	0.44
4:D:340:VAL:O	4:D:343:LYS:HG2	2.17	0.44
4:D:511:PHE:O	4:D:514:PHE:HB3	2.16	0.44
4:B:194:GLY:O	4:B:195:LEU:C	2.56	0.44
4:C:460:LEU:O	4:C:514:PHE:CE2	2.70	0.44
4:D:133:THR:C	4:D:135:GLN:N	2.71	0.44
4:A:19:ILE:HA	4:A:19:ILE:HD13	1.89	0.44
4:C:210:ILE:O	4:C:214:VAL:CG2	2.63	0.44
4:D:345:LYS:O	4:D:346:HIS:C	2.51	0.44
4:C:71:LYS:N	4:C:72:PRO:CD	2.81	0.44
4:A:205:HIS:C	4:A:207:GLU:N	2.70	0.44
4:D:706:LEU:HD21	4:D:849:PHE:CD2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:14:ILE:HG22	4:C:14:ILE:O	2.18	0.44
4:D:327:ALA:CA	4:D:415:TRP:NE1	2.81	0.44
4:B:701:SER:O	4:B:702:ALA:C	2.55	0.44
4:D:443:LEU:HD23	4:D:443:LEU:H	1.81	0.44
4:B:473:VAL:HG12	4:B:474:PRO:O	2.18	0.44
4:A:505:GLN:O	4:A:506:ASP:C	2.51	0.44
4:A:333:LYS:HB3	4:A:516:PHE:CE2	2.52	0.44
4:D:306:MET:C	4:D:308:TYR:N	2.70	0.44
4:B:685:VAL:C	4:B:687:VAL:N	2.70	0.44
4:C:617:ALA:O	4:C:621:LEU:HG	2.18	0.44
4:C:620:TRP:CZ3	4:C:667:PHE:HZ	2.35	0.44
4:C:155:ARG:CG	4:C:155:ARG:O	2.65	0.44
4:A:417:PRO:C	4:A:418:TYR:HD1	2.21	0.44
4:A:746:ARG:NH1	4:A:746:ARG:HB3	2.32	0.44
4:A:739:TYR:CD2	4:A:773:LYS:HB3	2.52	0.44
4:A:56:GLU:HB2	7:A:3057:HOH:O	2.17	0.44
4:A:308:TYR:OH	4:A:733:PHE:CE2	2.70	0.44
4:A:788:GLY:O	4:A:789:SER:C	2.56	0.44
4:D:857:GLN:C	4:D:859:ASP:N	2.70	0.44
4:C:728:VAL:CG2	4:C:734:PRO:HB3	2.47	0.44
1:K:15:DC:H2"	1:K:16:DC:C5'	2.46	0.44
4:D:326:THR:C	4:D:415:TRP:CD1	2.91	0.44
4:D:795:VAL:HG12	7:D:3013:HOH:O	2.18	0.44
4:C:536:PHE:HB3	4:C:882:PHE:HB2	1.94	0.44
4:B:460:LEU:CA	4:B:534:LEU:HD11	2.48	0.44
4:B:570:ILE:CG1	4:B:570:ILE:O	2.59	0.44
4:B:430:SER:OG	4:B:432:PHE:O	2.34	0.44
4:D:502:TRP:CZ3	4:D:503:ALA:HB2	2.52	0.44
2:F:4:G:H4'	4:A:389:LYS:HD3	1.99	0.44
4:B:19:ILE:HD13	4:B:20:PRO:HD2	1.98	0.44
4:A:42:GLU:C	4:A:46:MET:HE2	2.38	0.44
4:B:609:VAL:O	4:B:609:VAL:HG22	2.17	0.44
1:K:6:DT:H5'	1:K:6:DT:C6	2.52	0.44
4:A:846:TYR:HD1	4:A:850:ALA:HB2	1.82	0.44
4:B:626:THR:C	4:B:628:SER:N	2.70	0.44
4:D:49:ALA:O	4:D:52:ARG:HB2	2.17	0.44
4:D:300:HIS:HA	7:D:3088:HOH:O	2.17	0.44
4:B:169:GLN:HB3	4:B:169:GLN:HE21	1.51	0.44
4:A:631:LYS:NZ	6:A:2000:APC:O2A	2.39	0.44
4:B:421:ASP:OD2	4:B:425:ARG:HB2	2.17	0.44
4:B:823:ASN:C	4:B:825:PHE:N	2.70	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:15:DC:OP1	7:H:313:HOH:O	2.21	0.44
4:D:482:ILE:HD12	4:D:514:PHE:HZ	1.83	0.44
4:A:400:PHE:O	4:A:401:MET:O	2.36	0.44
4:A:60:LYS:NZ	4:A:61:ALA:HB2	2.22	0.44
4:B:340:VAL:O	4:B:343:LYS:HG3	2.17	0.44
4:B:273:VAL:C	4:B:274:PRO:O	2.56	0.44
4:A:286:TYR:CD2	4:A:286:TYR:N	2.86	0.44
4:D:646:PHE:HA	4:D:649:GLN:OE1	2.17	0.44
4:A:86:ASN:HD22	4:A:86:ASN:N	2.15	0.44
4:B:665:LEU:HD23	4:B:665:LEU:HA	1.82	0.44
4:C:305:LEU:C	4:C:305:LEU:CD2	2.86	0.44
4:A:697:ASN:O	4:A:698:TRP:C	2.55	0.44
4:C:571:TYR:HD1	4:C:634:VAL:HG11	1.83	0.44
4:A:794:THR:OG1	4:A:831:THR:CG2	2.48	0.44
4:A:797:TRP:CZ3	4:A:801:LYS:HB2	2.52	0.44
4:A:264:ILE:O	4:A:264:ILE:HG22	2.18	0.44
4:C:307:ARG:HG3	4:C:307:ARG:HH11	1.82	0.44
4:C:308:TYR:CE2	4:C:734:PRO:O	2.71	0.44
4:C:824:LEU:C	4:C:824:LEU:HD12	2.37	0.44
1:K:13:DC:C2'	1:K:14:DG:H5'	2.45	0.44
4:D:870:LEU:HD23	4:D:871:ASN:N	2.33	0.44
4:B:460:LEU:HA	4:B:534:LEU:HD11	1.99	0.44
4:B:556:GLY:O	4:B:558:ALA:N	2.51	0.44
4:B:737:GLN:C	4:B:774:GLN:HE22	2.21	0.44
4:B:780:PRO:HD2	4:B:781:ASN:N	2.31	0.44
4:B:796:VAL:HG21	7:B:3141:HOH:O	2.18	0.44
4:B:329:LYS:O	4:B:445:THR:HG23	2.17	0.44
4:D:338:ALA:C	4:D:340:VAL:N	2.70	0.44
4:D:333:LYS:HZ1	4:D:516:PHE:HB3	1.83	0.44
4:A:16:LEU:HA	4:A:37:LEU:CD2	2.46	0.44
4:B:512:LEU:O	4:B:514:PHE:N	2.51	0.44
4:D:486:HIS:NE2	4:D:490:MET:HG2	2.33	0.44
4:C:291:ARG:HD2	7:C:3077:HOH:O	2.17	0.44
4:D:14:ILE:HG21	4:D:288:ALA:CB	2.48	0.44
4:B:278:TRP:CZ3	4:B:284:GLY:CA	2.99	0.44
4:C:270:PRO:HD2	4:C:408:PHE:CE2	2.53	0.44
4:D:611:LEU:HB2	4:D:616:LEU:HD21	2.00	0.44
4:C:69:ALA:HA	4:C:257:ARG:HD2	1.99	0.44
4:A:699:LEU:O	4:A:702:ALA:HB3	2.18	0.44
4:A:710:VAL:HG13	4:A:710:VAL:O	2.18	0.44
4:A:133:THR:O	4:A:137:VAL:HG23	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:296:LEU:O	4:B:420:MET:HE2	2.18	0.44
4:B:699:LEU:HD12	4:B:699:LEU:H	1.82	0.44
4:B:269:GLN:NE2	4:B:407:LYS:HZ3	2.15	0.44
4:B:40:GLU:O	4:B:43:SER:HB2	2.17	0.44
4:B:50:ARG:NH1	4:B:50:ARG:HG2	2.33	0.44
4:B:220:LEU:O	4:B:223:SER:N	2.46	0.44
4:D:804:ILE:H	4:D:804:ILE:HG13	1.47	0.44
4:B:199:GLU:HG2	4:B:201:TRP:CD1	2.51	0.44
4:D:743:ILE:HD12	4:D:766:ASP:HB3	2.00	0.44
4:D:840:ASP:O	4:D:841:VAL:C	2.54	0.44
4:D:14:ILE:CG2	4:D:288:ALA:CB	2.91	0.44
4:A:320:ILE:HG23	4:A:418:TYR:O	2.18	0.44
4:B:651:LEU:HA	4:B:655:ILE:HD12	1.99	0.44
4:C:685:VAL:O	4:C:687:VAL:N	2.51	0.44
4:B:170:LEU:C	4:B:170:LEU:HD13	2.38	0.44
4:A:578:VAL:O	4:A:581:ILE:N	2.50	0.44
4:A:462:ILE:O	4:A:463:HIS:C	2.55	0.44
4:A:802:TYR:H	4:A:802:TYR:HD2	1.63	0.44
4:A:446:LEU:HD13	4:A:817:ILE:HG23	1.99	0.44
4:C:550:LEU:O	4:C:867:LYS:HG3	2.18	0.44
4:A:436:GLY:HA3	4:A:440:THR:CB	2.48	0.44
4:B:505:GLN:HG3	4:B:511:PHE:CD2	2.53	0.44
4:C:236:VAL:CG1	4:C:239:GLN:HB2	2.48	0.44
4:B:164:LYS:HZ3	4:B:164:LYS:H	1.65	0.44
4:A:347:CYS:C	4:A:349:VAL:N	2.68	0.44
4:C:450:LYS:O	4:C:529:ASN:HA	2.18	0.44
4:D:233:ASN:O	4:D:236:VAL:HG23	2.17	0.44
4:D:161:HIS:C	4:D:163:LYS:N	2.71	0.44
4:D:523:HIS:C	4:D:524:HIS:HD1	2.21	0.44
4:A:676:TYR:O	4:A:678:ALA:N	2.50	0.44
1:E:12:DT:C2	1:E:13:DC:C6	3.06	0.44
4:A:282:THR:OG1	4:A:283:GLY:N	2.45	0.44
1:K:10:DT:H5'	4:C:641:SER:HA	1.99	0.44
4:C:832:MET:O	4:C:833:VAL:C	2.56	0.44
4:D:778:ILE:O	4:D:782:PHE:HB2	2.18	0.44
1:N:10:DT:H4'	4:D:639:TYR:O	2.17	0.44
4:B:570:ILE:HG23	4:B:571:TYR:N	2.32	0.44
4:B:752:LEU:HB2	4:B:753:GLY:H	1.69	0.44
4:B:495:SER:N	4:B:496:PRO:CD	2.80	0.44
4:D:459:TRP:O	4:D:462:ILE:N	2.51	0.44
4:C:269:GLN:C	4:C:430:SER:HB3	2.38	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:296:LEU:HD12	4:C:296:LEU:HA	1.85	0.44
4:B:322:ILE:HD13	4:B:322:ILE:HA	1.73	0.44
1:K:3:DG:H5'	7:K:268:HOH:O	2.17	0.44
4:A:73:LEU:C	4:A:75:THR:H	2.20	0.44
4:B:227:VAL:HB	4:B:245:GLU:O	2.17	0.44
4:A:620:TRP:NE1	4:A:677:MET:HB2	2.33	0.43
1:E:13:DC:H6	1:E:13:DC:H5'	1.82	0.43
4:D:268:PHE:CD2	4:D:429:VAL:CG1	3.00	0.43
4:B:421:ASP:O	4:B:422:TRP:C	2.55	0.43
4:B:556:GLY:O	4:B:559:VAL:N	2.51	0.43
4:B:616:LEU:O	4:B:617:ALA:C	2.56	0.43
4:B:84:ARG:NH1	4:B:84:ARG:O	2.51	0.43
4:B:398:LEU:CD2	4:B:439:MET:CE	2.96	0.43
4:A:215:ARG:NH1	4:A:218:GLU:OE2	2.47	0.43
4:A:226:MET:O	4:A:247:ALA:CB	2.66	0.43
4:A:78:LEU:CD1	4:A:119:ILE:HG13	2.48	0.43
1:E:15:DC:H2'	1:E:16:DC:C6	2.53	0.43
4:A:286:TYR:HD2	4:A:286:TYR:H	1.66	0.43
4:C:402:LEU:HD23	4:C:402:LEU:HA	1.79	0.43
4:A:713:LYS:O	4:A:714:LYS:HD3	2.18	0.43
4:A:804:ILE:HG23	4:A:816:THR:HG21	2.00	0.43
4:A:826:LYS:O	4:A:827:ALA:C	2.56	0.43
4:A:276:LYS:O	4:A:277:PRO:C	2.57	0.43
4:A:110:LYS:O	4:A:113:ALA:HB3	2.18	0.43
4:C:317:TYR:C	4:C:321:ASN:HD21	2.21	0.43
4:C:706:LEU:HD11	4:C:849:PHE:CG	2.54	0.43
4:C:698:TRP:NE1	4:C:864:LEU:HA	2.33	0.43
4:C:462:ILE:CD1	4:C:479:ILE:CD1	2.96	0.43
4:C:462:ILE:HG23	4:C:478:ARG:HD2	2.00	0.43
4:C:818:PRO:O	4:C:821:ALA:HB3	2.18	0.43
4:D:532:LEU:HA	4:D:533:PRO:HD2	1.58	0.43
4:B:233:ASN:HB3	4:B:239:GLN:HB3	2.00	0.43
4:A:388:ASP:O	4:A:388:ASP:CG	2.56	0.43
4:A:320:ILE:CG2	4:A:418:TYR:O	2.67	0.43
1:K:7:DC:H6	1:K:7:DC:H2'	1.47	0.43
4:C:721:LYS:HG2	4:C:722:ARG:H	1.81	0.43
4:D:422:TRP:O	4:D:422:TRP:HD1	2.00	0.43
1:K:2:DG:N2	7:K:239:HOH:O	2.50	0.43
4:C:66:ASP:OD2	4:C:66:ASP:N	2.51	0.43
4:C:220:LEU:HD21	4:C:226:MET:CE	2.49	0.43
4:C:136:ALA:HA	7:C:3021:HOH:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:647:ARG:HD2	4:A:675:GLY:CA	2.25	0.43
4:A:521:VAL:O	4:A:525:GLY:N	2.51	0.43
4:A:780:PRO:O	4:A:784:HIS:HB2	2.18	0.43
4:C:727:TRP:CD2	4:C:735:VAL:CG1	3.01	0.43
4:C:737:GLN:O	4:C:774:GLN:NE2	2.51	0.43
4:D:794:THR:HA	4:D:797:TRP:HB3	1.99	0.43
4:C:541:SER:O	4:C:542:GLY:C	2.56	0.43
4:B:459:TRP:O	4:B:460:LEU:C	2.56	0.43
4:B:556:GLY:C	4:B:558:ALA:N	2.72	0.43
4:B:582:LEU:HD23	4:B:582:LEU:HA	1.86	0.43
4:B:46:MET:CE	4:B:269:GLN:HE22	2.30	0.43
4:D:402:LEU:CD2	4:D:439:MET:HE3	2.48	0.43
4:C:532:LEU:HA	4:C:533:PRO:HD2	1.77	0.43
4:D:232:GLN:O	4:D:233:ASN:C	2.56	0.43
4:D:122:THR:HG21	4:D:226:MET:CE	2.48	0.43
4:C:570:ILE:O	4:C:573:ILE:HG23	2.18	0.43
4:C:231:ARG:CG	4:C:234:ALA:HB2	2.42	0.43
4:A:320:ILE:HG23	4:A:320:ILE:HD12	1.74	0.43
4:C:592:ASN:ND2	4:C:611:LEU:CD2	2.81	0.43
4:D:379:ARG:HD3	4:D:660:ASP:OD2	2.18	0.43
4:A:125:CYS:O	4:A:128:SER:HB3	2.18	0.43
4:C:808:ALA:HB3	4:C:815:GLY:HA3	2.00	0.43
4:A:651:LEU:HA	4:A:655:ILE:HB	1.99	0.43
4:A:422:TRP:C	4:A:422:TRP:CD1	2.91	0.43
4:A:820:ASP:OD1	4:A:820:ASP:N	2.51	0.43
4:A:276:LYS:O	4:A:277:PRO:O	2.36	0.43
4:C:298:ARG:HG3	4:C:420:MET:O	2.17	0.43
4:C:308:TYR:HA	4:C:311:VAL:CG2	2.48	0.43
4:C:306:MET:C	4:C:308:TYR:H	2.20	0.43
1:K:11:DA:N1	1:K:12:DT:C4	2.86	0.43
4:D:825:PHE:O	4:D:828:VAL:CG2	2.67	0.43
4:D:829:ARG:HB3	4:D:876:LEU:HD23	2.00	0.43
4:B:577:LYS:CB	4:B:684:SER:HB3	2.47	0.43
4:C:646:PHE:O	4:C:647:ARG:C	2.56	0.43
4:A:234:ALA:HA	4:A:240:ASP:OD2	2.18	0.43
4:D:744:GLN:HA	4:D:756:ARG:NH2	2.33	0.43
4:A:65:ALA:CB	4:A:120:LYS:HG2	2.48	0.43
4:C:68:ALA:O	4:C:257:ARG:HD2	2.17	0.43
4:D:169:GLN:HB3	4:D:182:PHE:CZ	2.53	0.43
4:B:86:ASN:ND2	7:B:3033:HOH:O	2.37	0.43
4:D:545:HIS:O	4:D:549:MET:HG2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:643:GLU:OE2	4:A:679:LYS:CA	2.67	0.43
4:C:696:MET:O	4:C:700:LYS:HB2	2.18	0.43
4:C:778:ILE:HD12	4:C:778:ILE:HA	1.65	0.43
4:D:830:GLU:HG2	4:D:876:LEU:HD22	2.00	0.43
4:B:324:GLN:HE21	4:B:417:PRO:HA	1.84	0.43
4:B:307:ARG:HD3	4:B:736:TRP:CD2	2.52	0.43
4:C:452:ILE:CG1	4:C:457:TYR:N	2.81	0.43
4:A:204:TRP:CZ3	4:A:212:VAL:HG21	2.50	0.43
4:D:401:MET:HG3	4:D:440:THR:OG1	2.19	0.43
4:D:743:ILE:HG22	4:D:743:ILE:O	2.19	0.43
4:C:47:GLY:CA	4:C:265:SER:O	2.59	0.43
4:C:269:GLN:C	4:C:430:SER:CB	2.87	0.43
4:C:755:PHE:N	4:C:755:PHE:HD1	2.16	0.43
4:A:51:PHE:HZ	4:A:261:LEU:HD23	1.83	0.43
4:D:461:LYS:HE3	4:D:479:ILE:HG23	2.00	0.43
4:D:554:VAL:O	4:D:557:ARG:HB3	2.19	0.43
4:C:374:LEU:C	4:C:376:ALA:H	2.22	0.43
4:B:394:ARG:HB2	4:B:394:ARG:HE	1.49	0.43
4:D:837:GLU:HG2	4:D:872:LEU:HD12	2.01	0.43
4:B:306:MET:O	4:B:308:TYR:N	2.52	0.43
4:B:831:THR:HG23	4:B:832:MET:N	2.33	0.43
1:H:9:DA:H2"	1:H:10:DT:OP1	2.18	0.43
4:C:248:PRO:HD2	4:C:249:GLU:OE2	2.19	0.43
4:D:472:LYS:CG	4:D:567:VAL:HG11	2.49	0.43
4:B:341:ILE:O	4:B:343:LYS:N	2.51	0.43
4:A:77:LEU:C	4:A:79:PRO:HD2	2.39	0.43
4:D:489:ILE:H	4:D:489:ILE:HG13	1.40	0.43
4:C:563:PRO:HD3	4:C:874:ASP:O	2.19	0.43
4:C:485:ASN:OD1	4:C:485:ASN:N	2.51	0.43
4:C:50:ARG:NH1	4:C:267:MET:HE3	2.33	0.43
4:C:397:SER:O	4:C:398:LEU:C	2.56	0.43
4:D:276:LYS:O	4:D:277:PRO:C	2.56	0.43
4:A:147:ASP:HB3	4:A:750:MET:HE1	2.01	0.43
4:A:73:LEU:HD11	4:A:254:ILE:HG13	2.00	0.43
4:A:635:MET:HE1	6:A:2000:APC:C3'	2.49	0.43
4:A:308:TYR:HA	4:A:311:VAL:HG23	1.99	0.43
4:A:461:LYS:HE3	4:A:479:ILE:CG2	2.48	0.43
4:A:465:ALA:HB2	4:A:482:ILE:HD11	2.00	0.43
4:A:545:HIS:H	4:A:545:HIS:CD2	2.36	0.43
4:A:549:MET:HB3	4:A:836:TYR:CE1	2.51	0.43
4:A:459:TRP:NE1	4:A:822:ALA:HA	2.29	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:274:PRO:HA	4:A:275:PRO:HD3	1.89	0.43
4:A:109:ILE:O	4:A:110:LYS:C	2.55	0.43
4:C:555:GLY:O	4:C:556:GLY:C	2.57	0.43
4:B:435:GLN:HG2	4:B:810:ILE:HG12	2.00	0.43
4:B:407:LYS:CG	4:B:408:PHE:HE2	2.27	0.43
4:B:416:PHE:CD1	4:B:430:SER:OG	2.71	0.43
4:C:502:TRP:O	4:C:504:GLU:N	2.51	0.43
4:A:502:TRP:CE2	4:A:512:LEU:CD1	2.97	0.43
4:B:400:PHE:C	4:B:400:PHE:CD1	2.91	0.43
4:B:504:GLU:C	4:B:505:GLN:O	2.56	0.43
4:A:122:THR:O	4:A:126:LEU:HG	2.19	0.43
4:D:485:ASN:O	4:D:486:HIS:C	2.57	0.43
4:D:95:LYS:HE3	7:D:3065:HOH:O	2.17	0.43
4:D:452:ILE:HG22	4:D:528:TYR:O	2.18	0.43
4:A:8:LYS:HB3	4:A:9:ASN:H	1.49	0.43
4:D:21:PHE:CE1	4:D:25:ALA:HB2	2.54	0.43
4:A:178:TYR:O	4:A:181:ALA:HB3	2.18	0.43
2:L:5:C:H5"	4:C:390:ALA:HB1	2.01	0.43
3:J:5:DA:H2"	3:J:6:DT:C7	2.48	0.43
4:A:344:TRP:O	4:A:345:LYS:CB	2.66	0.43
4:D:78:LEU:O	4:D:82:ILE:HG13	2.18	0.43
4:D:583:GLN:HB3	7:D:3135:HOH:O	2.19	0.43
4:B:78:LEU:N	4:B:79:PRO:HD2	2.34	0.43
4:A:793:LYS:CA	4:A:796:VAL:HG23	2.48	0.43
4:C:846:TYR:O	4:C:847:ASP:C	2.57	0.43
4:D:419:ASN:HB3	4:D:420:MET:H	1.53	0.43
4:C:881:ALA:O	4:C:883:ALA:OXT	2.37	0.43
4:B:865:PRO:HA	7:B:3135:HOH:O	2.19	0.43
4:B:13:ASP:OD1	4:B:14:ILE:N	2.51	0.43
4:A:402:LEU:HG	4:A:439:MET:HE3	2.01	0.43
4:B:163:LYS:HA	4:B:166:VAL:HG23	2.00	0.43
4:C:246:LEU:HD12	4:C:247:ALA:H	1.83	0.43
4:B:233:ASN:ND2	4:B:239:GLN:CD	2.70	0.43
4:B:220:LEU:C	4:B:222:GLU:N	2.70	0.43
4:D:744:GLN:NE2	4:D:756:ARG:H	2.16	0.43
4:D:159:ALA:CB	4:D:163:LYS:HD3	2.49	0.43
4:A:396:ILE:HG23	4:A:396:ILE:HD12	1.65	0.43
4:C:70:ALA:O	4:C:73:LEU:HB2	2.18	0.43
4:C:105:PHE:C	4:C:107:GLN:N	2.70	0.43
4:D:741:LYS:HA	4:D:742:PRO:HD3	1.79	0.43
4:C:412:LYS:O	4:C:413:ALA:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:615:ALA:O	4:A:618:GLY:N	2.51	0.43
4:A:630:THR:O	4:A:631:LYS:C	2.55	0.43
4:A:525:GLY:O	4:A:526:LEU:C	2.57	0.43
4:B:122:THR:HG22	4:B:226:MET:HE1	2.01	0.43
4:C:289:ASN:HB2	7:C:3014:HOH:O	2.17	0.43
4:C:308:TYR:O	4:C:309:GLU:C	2.56	0.43
4:C:548:ALA:O	4:C:550:LEU:N	2.52	0.43
4:B:421:ASP:OD1	4:B:424:GLY:N	2.50	0.43
4:B:61:ALA:C	4:B:63:GLU:N	2.71	0.43
4:A:201:TRP:O	4:A:204:TRP:HB2	2.19	0.43
4:A:219:MET:O	4:A:222:GLU:HB3	2.19	0.43
4:C:120:LYS:HG3	4:C:752:LEU:CD1	2.46	0.43
4:C:531:SER:O	4:C:817:ILE:HG22	2.18	0.43
4:A:57:ARG:HA	4:A:60:LYS:HB3	2.01	0.43
4:B:109:ILE:H	4:B:109:ILE:HD12	1.78	0.43
4:D:126:LEU:HD13	4:D:246:LEU:HB2	2.00	0.43
4:A:78:LEU:HD13	4:A:119:ILE:HG13	2.00	0.43
4:B:437:ASN:O	4:B:441:LYS:HG2	2.19	0.43
4:B:261:LEU:HD12	4:B:261:LEU:HA	1.81	0.43
4:B:455:GLU:HG2	4:B:822:ALA:HB2	2.00	0.43
4:C:67:ASN:C	4:C:69:ALA:N	2.69	0.43
3:G:8:DC:H2"	3:G:9:DC:OP2	2.19	0.43
4:C:373:ALA:O	4:C:377:TRP:CD1	2.71	0.43
4:B:724:ALA:HB2	4:B:738:GLU:HG3	2.00	0.43
4:A:619:GLN:HA	4:A:622:ALA:HB3	2.01	0.43
4:A:517:GLU:O	4:A:520:GLY:N	2.42	0.43
4:A:546:PHE:HA	4:A:549:MET:HG2	2.01	0.43
4:A:14:ILE:CD1	4:A:14:ILE:H	2.32	0.43
4:C:727:TRP:CD1	4:C:782:PHE:CE1	3.06	0.43
4:B:56:GLU:OE1	4:B:57:ARG:N	2.52	0.43
4:B:643:GLU:HB2	7:B:3053:HOH:O	2.19	0.43
4:B:726:HIS:CD2	4:B:736:TRP:CD1	3.06	0.43
4:B:14:ILE:O	4:B:14:ILE:HG22	2.19	0.43
4:A:223:SER:HA	7:A:3147:HOH:O	2.19	0.43
4:B:158:GLU:HG2	4:B:195:LEU:CD2	2.47	0.43
4:A:159:ALA:HB3	4:A:163:LYS:HD3	2.01	0.43
4:B:141:ILE:O	4:B:145:ILE:HG12	2.19	0.43
4:D:306:MET:O	4:D:309:GLU:HB2	2.19	0.43
4:D:164:LYS:NZ	7:D:3179:HOH:O	2.50	0.43
4:C:164:LYS:C	4:C:166:VAL:H	2.22	0.43
4:D:303:LYS:HE2	4:D:307:ARG:HH12	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:9:ASN:HA	4:C:12:SER:CB	2.47	0.43
4:C:710:VAL:HG21	4:C:856:SER:OG	2.18	0.43
4:B:520:GLY:HA3	4:B:528:TYR:CZ	2.54	0.43
4:B:596:THR:CG2	4:B:605:ILE:HG23	2.49	0.43
4:A:617:ALA:C	4:A:621:LEU:HD12	2.40	0.42
4:A:631:LYS:HZ2	6:A:2000:APC:PA	2.41	0.42
4:A:840:ASP:O	4:A:841:VAL:C	2.56	0.42
4:C:786:GLN:O	4:C:789:SER:N	2.51	0.42
4:D:535:ALA:HA	4:D:814:PHE:O	2.19	0.42
4:B:620:TRP:CE2	4:B:677:MET:HE2	2.54	0.42
4:B:623:TYR:HA	4:B:666:MET:HE2	2.00	0.42
4:D:340:VAL:HG11	4:D:497:LEU:HD11	2.01	0.42
4:B:80:LYS:HD3	4:B:224:THR:HG23	1.99	0.42
4:B:110:LYS:CD	4:B:111:PRO:HD2	2.39	0.42
4:D:134:VAL:HB	4:D:244:ILE:HG12	2.01	0.42
4:B:17:ALA:O	4:B:21:PHE:HE2	2.02	0.42
4:B:744:GLN:HA	4:B:756:ARG:HD3	2.01	0.42
4:B:6:ILE:HG23	4:B:10:ASP:CG	2.39	0.42
4:D:478:ARG:O	4:D:481:PHE:HB3	2.19	0.42
4:D:352:ILE:HA	4:D:353:PRO:HD2	1.54	0.42
4:A:742:PRO:HB3	4:A:744:GLN:OE1	2.19	0.42
4:D:520:GLY:O	4:D:524:HIS:HB2	2.18	0.42
4:C:8:LYS:HB2	7:C:3187:HOH:O	2.18	0.42
4:C:632:ARG:NH1	6:C:2002:APC:C8	2.83	0.42
4:A:640:GLY:O	4:A:641:SER:O	2.37	0.42
4:A:24:LEU:O	4:A:25:ALA:C	2.56	0.42
4:A:266:PRO:HD2	4:A:292:ARG:NH1	2.34	0.42
4:D:861:MET:HA	4:D:862:PRO:HD2	1.84	0.42
4:B:864:LEU:O	4:B:865:PRO:O	2.36	0.42
4:D:337:VAL:HG12	4:D:341:ILE:CD1	2.48	0.42
4:B:504:GLU:O	4:B:505:GLN:O	2.37	0.42
4:A:89:PHE:O	4:A:93:LYS:HG3	2.19	0.42
4:D:231:ARG:NH1	4:D:242:GLU:HB2	2.34	0.42
4:B:142:GLY:O	4:B:143:ARG:C	2.57	0.42
4:D:106:LEU:HD11	4:D:215:ARG:HG2	2.01	0.42
4:D:442:GLY:O	4:D:444:LEU:N	2.52	0.42
4:A:610:LYS:O	4:A:611:LEU:O	2.37	0.42
4:D:677:MET:O	4:D:678:ALA:C	2.55	0.42
4:B:31:ARG:HB3	4:B:31:ARG:NH1	2.32	0.42
4:B:259:GLY:O	4:B:262:ALA:N	2.52	0.42
4:A:246:LEU:HD23	4:A:251:ALA:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:798:ALA:O	4:B:802:TYR:O	2.38	0.42
4:B:714:LYS:HD3	4:B:714:LYS:HA	1.77	0.42
4:A:810:ILE:N	4:A:813:SER:O	2.46	0.42
4:C:318:LYS:HE2	4:C:796:VAL:CG1	2.48	0.42
4:C:326:THR:O	4:C:415:TRP:HD1	1.99	0.42
4:C:428:ALA:H	4:C:435:GLN:HE22	1.66	0.42
4:C:699:LEU:O	4:C:778:ILE:HG12	2.19	0.42
4:A:720:ARG:O	4:A:721:LYS:C	2.57	0.42
4:B:533:PRO:HA	4:B:816:THR:O	2.18	0.42
4:B:301:SER:O	4:B:302:LYS:C	2.56	0.42
4:B:305:LEU:O	4:B:307:ARG:N	2.53	0.42
4:B:682:TRP:C	4:B:682:TRP:CD1	2.90	0.42
4:D:334:VAL:HG12	4:D:443:LEU:HD22	2.01	0.42
4:A:331:ASN:O	4:A:333:LYS:N	2.53	0.42
4:A:84:ARG:NH1	4:A:91:GLU:OE2	2.52	0.42
4:A:347:CYS:C	4:A:349:VAL:H	2.22	0.42
4:B:613:THR:HG21	7:B:3104:HOH:O	2.19	0.42
4:D:125:CYS:O	4:D:128:SER:CB	2.62	0.42
4:A:703:ALA:O	4:A:704:LYS:C	2.57	0.42
4:D:68:ALA:HB3	4:D:261:LEU:HD21	2.01	0.42
3:M:4:DG:C2	3:M:5:DA:C2	3.07	0.42
4:A:205:HIS:O	4:A:208:ASP:N	2.52	0.42
4:C:305:LEU:HD23	4:C:305:LEU:O	2.19	0.42
4:D:474:PRO:HA	4:D:880:PHE:CE1	2.54	0.42
4:B:150:ARG:C	4:B:152:GLY:N	2.70	0.42
4:B:152:GLY:C	4:B:154:ILE:N	2.72	0.42
4:A:675:GLY:O	4:A:678:ALA:HB3	2.18	0.42
4:A:308:TYR:OH	4:A:733:PHE:HE2	2.02	0.42
4:A:801:LYS:HD3	4:A:802:TYR:CD2	2.54	0.42
4:A:793:LYS:HB3	4:A:831:THR:OG1	2.19	0.42
4:B:51:PHE:CE2	4:B:55:PHE:CD1	3.03	0.42
4:C:36:GLN:NE2	4:C:273:VAL:HG22	2.34	0.42
4:B:36:GLN:O	4:B:39:LEU:N	2.45	0.42
4:C:512:LEU:O	4:C:516:PHE:CD1	2.71	0.42
4:B:511:PHE:O	4:B:514:PHE:HB3	2.19	0.42
4:C:462:ILE:HG12	4:C:479:ILE:HD11	2.02	0.42
4:B:144:ALA:O	4:B:147:ASP:N	2.53	0.42
4:D:89:PHE:CD2	4:D:107:GLN:OE1	2.73	0.42
4:D:247:ALA:HA	4:D:248:PRO:HD3	1.80	0.42
4:C:693:VAL:HG12	4:C:694:GLU:N	2.34	0.42
4:B:19:ILE:HG23	4:B:20:PRO:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:486:HIS:HA	4:D:489:ILE:CD1	2.40	0.42
4:D:579:ASN:ND2	4:D:625:VAL:HG12	2.35	0.42
4:C:162:PHE:CE2	4:C:165:ASN:HB2	2.54	0.42
4:D:207:GLU:O	4:D:211:HIS:CD2	2.73	0.42
4:B:749:LEU:HD12	4:B:750:MET:HG3	2.01	0.42
4:D:147:ASP:HB3	4:D:750:MET:HE2	2.01	0.42
4:A:830:GLU:O	4:A:832:MET:N	2.51	0.42
4:A:276:LYS:HB2	4:A:287:TRP:CD2	2.54	0.42
4:C:698:TRP:O	4:C:701:SER:N	2.53	0.42
4:D:326:THR:C	4:D:415:TRP:HD1	2.22	0.42
1:H:14:DG:H2'	1:H:15:DC:C5	2.55	0.42
4:D:116:TYR:CZ	4:D:752:LEU:HD22	2.54	0.42
4:C:650:VAL:HG11	4:C:674:ALA:HA	2.00	0.42
4:D:122:THR:O	4:D:125:CYS:HB2	2.19	0.42
4:A:226:MET:HG3	4:A:250:TYR:HD1	1.83	0.42
4:D:64:VAL:HG21	4:D:127:THR:HG21	2.01	0.42
4:A:704:LYS:O	4:A:707:ALA:N	2.47	0.42
4:A:395:ARG:O	4:A:399:GLU:CG	2.68	0.42
4:C:205:HIS:HB3	4:C:208:ASP:OD2	2.18	0.42
4:A:236:VAL:HG11	4:A:239:GLN:OE1	2.19	0.42
4:D:303:LYS:HE2	4:D:307:ARG:NH1	2.34	0.42
4:D:727:TRP:CE2	4:D:735:VAL:CG1	3.03	0.42
3:G:3:DC:C4	3:G:4:DG:N7	2.88	0.42
4:C:41:HIS:CD2	4:C:41:HIS:C	2.92	0.42
4:C:799:HIS:HA	4:C:804:ILE:O	2.20	0.42
4:C:714:LYS:HA	4:C:714:LYS:HD3	1.74	0.42
4:A:832:MET:O	4:A:834:ASP:N	2.53	0.42
4:C:322:ILE:HA	4:C:322:ILE:HD13	1.74	0.42
4:C:286:TYR:CE2	4:C:417:PRO:HG3	2.54	0.42
4:C:834:ASP:O	4:C:837:GLU:N	2.44	0.42
4:C:833:VAL:HG11	4:C:873:ARG:HD3	2.01	0.42
4:A:722:ARG:CB	4:A:769:ILE:HD13	2.19	0.42
4:D:631:LYS:CD	4:D:635:MET:SD	3.08	0.42
4:D:425:ARG:HB3	4:D:427:TYR:CE1	2.49	0.42
4:D:794:THR:CB	4:D:831:THR:HG21	2.47	0.42
4:C:556:GLY:C	4:C:561:LEU:HB2	2.40	0.42
4:B:264:ILE:CG2	4:B:292:ARG:HB2	2.39	0.42
4:B:305:LEU:O	4:B:306:MET:C	2.57	0.42
4:B:39:LEU:O	4:B:40:GLU:C	2.57	0.42
4:A:333:LYS:HE3	4:A:516:PHE:HB3	2.01	0.42
4:A:333:LYS:CB	4:A:516:PHE:CE2	3.03	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:518:TYR:CE1	4:B:522:GLN:NE2	2.88	0.42
4:D:384:VAL:O	4:D:384:VAL:HG12	2.19	0.42
4:A:88:TRP:HA	4:A:91:GLU:CD	2.40	0.42
4:C:329:LYS:HD2	4:C:447:ALA:HA	2.02	0.42
4:A:163:LYS:HA	4:A:163:LYS:HD2	1.93	0.42
4:D:113:ALA:O	4:D:114:VAL:C	2.57	0.42
4:B:690:VAL:O	4:B:691:ALA:C	2.58	0.42
4:D:579:ASN:OD1	4:D:625:VAL:HB	2.18	0.42
4:D:257:ARG:NH1	4:D:261:LEU:HD13	2.34	0.42
4:D:836:TYR:N	4:D:836:TYR:HD2	2.16	0.42
4:A:166:VAL:HG12	4:A:170:LEU:HD12	2.01	0.42
4:B:381:ALA:C	4:B:383:ALA:N	2.71	0.42
4:A:556:GLY:CA	4:A:561:LEU:HB2	2.49	0.42
4:C:631:LYS:NZ	6:C:2002:APC:C3A	2.47	0.42
4:A:656:GLN:C	4:A:658:ALA:H	2.22	0.42
4:A:457:TYR:C	4:A:457:TYR:CD2	2.93	0.42
4:A:543:ILE:O	4:A:544:GLN:O	2.37	0.42
4:A:779:ALA:HB3	4:A:780:PRO:HD3	2.02	0.42
4:A:471:ASP:OD1	4:A:471:ASP:C	2.55	0.42
4:D:631:LYS:HE2	4:D:635:MET:CE	2.50	0.42
4:D:712:ASP:O	4:D:716:GLY:N	2.46	0.42
4:B:581:ILE:O	4:B:584:ALA:HB3	2.20	0.42
4:B:643:GLU:O	4:B:644:PHE:C	2.56	0.42
4:B:545:HIS:HE1	4:B:787:ASP:HA	1.84	0.42
4:B:793:LYS:CG	7:B:3181:HOH:O	2.66	0.42
4:B:804:ILE:HG21	4:B:807:PHE:CE2	2.54	0.42
4:B:840:ASP:HB3	4:B:843:ALA:HB3	2.02	0.42
4:B:432:PHE:HD2	4:B:432:PHE:O	2.01	0.42
4:B:567:VAL:CG1	4:B:880:PHE:CG	3.01	0.42
4:A:407:LYS:HE3	4:A:407:LYS:HB2	1.85	0.42
4:A:510:CYS:O	4:A:512:LEU:N	2.53	0.42
4:A:215:ARG:O	4:A:219:MET:HG3	2.20	0.42
4:A:348:PRO:C	4:A:349:VAL:HG23	2.37	0.42
4:C:247:ALA:HA	4:C:248:PRO:HD3	1.89	0.42
4:D:473:VAL:N	4:D:567:VAL:CG2	2.79	0.42
4:D:239:GLN:O	4:D:241:SER:N	2.52	0.42
4:C:132:THR:HG21	4:C:244:ILE:O	2.20	0.42
4:D:728:VAL:HG22	4:D:734:PRO:HA	2.01	0.42
4:D:745:THR:O	4:D:746:ARG:HG3	2.20	0.42
4:A:121:THR:OG1	4:A:751:PHE:HE1	2.02	0.42
4:C:161:HIS:O	4:C:162:PHE:C	2.58	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:756:ARG:HG3	7:C:3143:HOH:O	2.20	0.42
4:D:643:GLU:HB2	4:D:682:TRP:CD1	2.54	0.42
4:C:257:ARG:HG2	4:C:257:ARG:NH1	2.34	0.42
4:A:488:ASN:O	4:A:491:ALA:CB	2.67	0.42
4:B:208:ASP:OD2	4:B:208:ASP:N	2.53	0.42
4:D:166:VAL:HG11	4:D:183:MET:CE	2.50	0.42
4:D:396:ILE:HA	4:D:396:ILE:HD13	1.84	0.42
4:A:308:TYR:C	4:A:311:VAL:HG23	2.37	0.42
4:A:13:ASP:OD2	4:A:291:ARG:NH2	2.50	0.42
4:A:281:ILE:HG23	4:A:305:LEU:HD11	2.01	0.42
4:C:322:ILE:CG1	7:C:3131:HOH:O	2.59	0.42
4:D:632:ARG:HH22	6:D:2003:APC:H5'1	1.85	0.42
1:N:12:DT:H5'	4:D:781:ASN:ND2	2.34	0.42
4:B:530:CYS:SG	4:B:818:PRO:HG2	2.60	0.42
4:D:36:GLN:HE21	4:D:36:GLN:CA	2.28	0.42
4:B:726:HIS:CD2	4:B:736:TRP:CG	3.08	0.42
4:D:339:ASN:O	4:D:343:LYS:HD3	2.20	0.42
4:C:109:ILE:HD13	4:C:145:ILE:HG22	2.01	0.42
4:D:133:THR:HA	4:D:243:THR:CG2	2.48	0.42
4:B:19:ILE:CG2	4:B:20:PRO:N	2.83	0.42
4:A:65:ALA:HB3	4:A:120:LYS:CD	2.49	0.42
4:A:19:ILE:O	4:A:21:PHE:N	2.49	0.42
4:A:668:THR:CG2	4:A:669:GLN:HE22	2.32	0.42
4:D:161:HIS:CE1	7:D:3114:HOH:O	2.64	0.42
4:A:686:SER:HA	4:A:693:VAL:HG21	2.01	0.42
4:C:330:ILE:HA	4:C:330:ILE:HD13	1.74	0.42
4:C:42:GLU:HG2	4:C:46:MET:CE	2.49	0.42
4:B:205:HIS:C	4:B:207:GLU:N	2.72	0.42
4:B:661:SER:CB	7:B:3192:HOH:O	2.68	0.42
4:C:191:LEU:O	4:C:196:LEU:HD22	2.20	0.42
2:L:3:G:H5"	4:C:172:LYS:CD	2.50	0.42
4:B:709:GLU:HG2	4:B:709:GLU:O	2.20	0.42
4:C:571:TYR:HD1	4:C:634:VAL:CG1	2.33	0.42
4:C:789:SER:O	4:C:793:LYS:HG3	2.19	0.42
4:C:845:PHE:O	4:C:846:TYR:C	2.58	0.42
4:D:423:ARG:NH2	4:D:784:HIS:ND1	2.67	0.42
4:D:809:LEU:HA	4:D:813:SER:O	2.19	0.42
4:B:308:TYR:CE2	4:B:734:PRO:O	2.73	0.42
1:H:11:DA:N3	4:B:784:HIS:HE1	2.17	0.42
4:B:11:PHE:C	4:B:13:ASP:N	2.73	0.42
4:A:333:LYS:O	4:A:334:VAL:C	2.58	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:505:GLN:O	4:A:508:PRO:HD3	2.19	0.42
4:D:854:HIS:HD2	4:D:856:SER:H	1.55	0.42
4:B:19:ILE:HD12	4:B:20:PRO:HD2	2.00	0.42
4:B:19:ILE:HG22	4:B:21:PHE:HB3	2.01	0.42
4:C:216:CYS:O	4:C:217:ILE:C	2.57	0.42
4:C:303:LYS:NZ	4:C:303:LYS:HB3	2.35	0.42
4:B:347:CYS:HB3	4:B:350:GLU:HG2	2.00	0.42
4:C:101:THR:HG23	4:C:104:GLN:HE22	1.84	0.42
4:A:254:ILE:HG22	4:A:255:ALA:N	2.34	0.42
4:C:63:GLU:O	4:C:66:ASP:HB2	2.20	0.42
4:B:280:GLY:HA2	4:B:317:TYR:OH	2.20	0.42
4:C:713:LYS:HD2	4:C:713:LYS:HA	1.83	0.42
4:A:481:PHE:O	4:A:482:ILE:C	2.54	0.42
4:A:801:LYS:CD	4:A:802:TYR:CD2	3.02	0.42
4:A:292:ARG:O	4:A:292:ARG:CG	2.63	0.42
4:B:247:ALA:HB3	4:B:250:TYR:CD1	2.55	0.42
4:C:553:GLU:CD	4:C:553:GLU:N	2.71	0.42
4:B:561:LEU:HD12	4:B:561:LEU:N	2.35	0.42
4:A:100:PRO:HG2	4:A:103:PHE:CB	2.46	0.42
4:B:158:GLU:HA	4:B:195:LEU:HD22	2.01	0.42
4:C:329:LYS:HD3	4:C:446:LEU:O	2.20	0.42
4:D:281:ILE:HG22	4:D:282:THR:CG2	2.42	0.42
4:B:339:ASN:O	4:B:343:LYS:HD3	2.15	0.42
4:B:6:ILE:O	4:B:8:LYS:N	2.44	0.42
4:C:260:ALA:O	4:C:261:LEU:C	2.59	0.42
4:A:71:LYS:N	4:A:72:PRO:CD	2.82	0.42
4:B:170:LEU:HD22	4:B:179:LYS:HG2	2.01	0.42
4:A:254:ILE:O	4:A:255:ALA:C	2.58	0.42
4:B:352:ILE:HA	4:B:353:PRO:HD2	1.69	0.42
4:A:489:ILE:O	4:A:490:MET:C	2.56	0.42
4:A:553:GLU:OE1	4:A:553:GLU:N	2.53	0.42
4:A:659:ILE:HG22	4:A:660:ASP:N	2.35	0.41
4:A:291:ARG:CB	7:A:3193:HOH:O	2.56	0.41
4:A:291:ARG:CG	7:A:3193:HOH:O	2.67	0.41
4:B:247:ALA:CB	4:B:250:TYR:HD1	2.33	0.41
4:C:870:LEU:HD23	4:C:871:ASN:N	2.35	0.41
1:N:11:DA:H4'	4:D:780:PRO:HG3	2.00	0.41
4:B:578:VAL:HG21	4:B:681:ILE:HD12	2.01	0.41
4:B:416:PHE:CD2	4:B:416:PHE:N	2.88	0.41
4:D:32:LEU:HD12	4:D:32:LEU:N	2.12	0.41
4:D:264:ILE:O	4:D:264:ILE:HG22	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:473:VAL:HA	4:C:474:PRO:HD2	1.90	0.41
4:D:459:TRP:O	4:D:460:LEU:C	2.56	0.41
4:C:619:GLN:O	4:C:666:MET:HG3	2.20	0.41
4:A:21:PHE:C	4:A:23:THR:H	2.23	0.41
4:C:610:LYS:HD2	7:C:3085:HOH:O	2.19	0.41
4:C:292:ARG:N	4:C:293:PRO:CD	2.82	0.41
4:D:161:HIS:O	4:D:163:LYS:N	2.53	0.41
4:C:9:ASN:C	4:C:12:SER:HB3	2.40	0.41
4:C:385:TYR:O	4:C:386:ARG:C	2.56	0.41
4:A:108:GLU:CG	7:A:3115:HOH:O	2.63	0.41
4:B:179:LYS:O	4:B:750:MET:SD	2.78	0.41
4:A:864:LEU:H	4:A:864:LEU:HD12	1.84	0.41
4:A:330:ILE:HG21	4:A:409:ALA:HA	2.02	0.41
4:C:402:LEU:HG	4:C:439:MET:CE	2.50	0.41
3:P:7:DT:H2"	3:P:8:DC:OP2	2.21	0.41
4:C:635:MET:HG3	6:C:2002:APC:N7	2.36	0.41
4:A:421:ASP:OD2	4:A:427:TYR:CE1	2.71	0.41
4:C:420:MET:SD	4:C:733:PHE:CE1	3.13	0.41
4:C:850:ALA:C	4:C:852:GLN:N	2.72	0.41
1:K:14:DG:C4	1:K:15:DC:C5	3.08	0.41
4:B:541:SER:O	4:B:542:GLY:O	2.38	0.41
4:B:650:VAL:O	4:B:654:THR:HG23	2.20	0.41
4:B:864:LEU:HA	4:B:865:PRO:HD2	1.72	0.41
4:B:537:ASP:N	4:B:882:PHE:CD2	2.73	0.41
4:B:472:LYS:C	4:B:567:VAL:HG21	2.40	0.41
4:C:437:ASN:ND2	4:C:440:THR:CB	2.83	0.41
4:A:401:MET:O	4:A:404:GLN:N	2.53	0.41
4:D:291:ARG:O	4:D:292:ARG:HB2	2.20	0.41
4:A:348:PRO:HB2	4:A:349:VAL:HG23	2.03	0.41
4:B:773:LYS:HE3	7:B:3124:HOH:O	2.19	0.41
4:B:6:ILE:O	4:B:10:ASP:HB3	2.19	0.41
4:A:693:VAL:HG12	4:A:694:GLU:N	2.35	0.41
4:A:244:ILE:HG22	4:A:245:GLU:N	2.34	0.41
4:C:261:LEU:O	4:C:263:GLY:N	2.52	0.41
4:B:155:ARG:NH2	4:B:749:LEU:HB2	2.34	0.41
4:A:482:ILE:O	4:A:482:ILE:HG22	2.20	0.41
4:A:454:LYS:H	4:A:526:LEU:HD23	1.81	0.41
4:B:115:ALA:O	4:B:119:ILE:HG12	2.21	0.41
4:C:423:ARG:HD2	4:C:781:ASN:HD22	1.81	0.41
4:C:727:TRP:CD2	4:C:735:VAL:HG13	2.55	0.41
4:C:738:GLU:CA	4:C:774:GLN:HE22	2.28	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:570:ILE:HG23	4:D:571:TYR:N	2.35	0.41
4:B:537:ASP:O	4:B:882:PHE:CD2	2.72	0.41
1:H:13:DC:O4'	4:B:427:TYR:CE2	2.53	0.41
4:D:116:TYR:HE2	4:D:752:LEU:HD22	1.86	0.41
4:C:58:GLN:NE2	4:C:58:GLN:HA	2.35	0.41
4:C:55:PHE:CE2	4:C:59:LEU:HD21	2.55	0.41
4:C:461:LYS:O	4:C:463:HIS:N	2.53	0.41
4:B:587:ILE:HA	4:B:587:ILE:HD13	1.83	0.41
4:D:733:PHE:HA	4:D:734:PRO:HD2	1.93	0.41
4:B:345:LYS:HB3	4:B:345:LYS:HE2	1.68	0.41
4:C:448:LYS:CG	4:C:806:SER:OG	2.69	0.41
4:A:40:GLU:HG2	4:A:286:TYR:CD1	2.49	0.41
4:B:655:ILE:HG12	4:B:667:PHE:CE1	2.55	0.41
4:A:706:LEU:HD11	4:A:849:PHE:HB2	2.02	0.41
4:B:381:ALA:O	4:B:383:ALA:N	2.53	0.41
1:K:3:DG:C2	1:K:4:DA:C2	3.08	0.41
4:B:738:GLU:HG2	4:B:738:GLU:O	2.20	0.41
2:L:7:A:H2'	2:L:8:U:H6	1.85	0.41
4:A:314:PRO:CD	4:A:315:GLU:H	2.33	0.41
4:A:462:ILE:CD1	4:A:475:PHE:CD1	3.03	0.41
4:A:475:PHE:HD2	4:A:475:PHE:H	1.68	0.41
4:B:250:TYR:O	4:B:251:ALA:C	2.59	0.41
4:C:278:TRP:HB2	4:C:321:ASN:OD1	2.20	0.41
4:C:788:GLY:C	4:C:792:ARG:HH12	2.24	0.41
1:K:14:DG:H2"	1:K:15:DC:C6	2.56	0.41
4:D:717:GLU:HA	7:D:3025:HOH:O	2.20	0.41
4:B:617:ALA:O	4:B:621:LEU:HD12	2.19	0.41
4:B:793:LYS:HE2	4:B:835:THR:OG1	2.20	0.41
4:B:881:ALA:O	4:B:883:ALA:N	2.52	0.41
4:B:745:THR:O	4:B:746:ARG:HB2	2.20	0.41
4:B:464:GLY:HA3	4:B:514:PHE:CZ	2.55	0.41
4:D:191:LEU:HD23	4:D:195:LEU:O	2.21	0.41
4:D:146:GLU:HG3	4:D:204:TRP:CE2	2.55	0.41
4:D:734:PRO:CG	4:D:734:PRO:O	2.65	0.41
4:A:668:THR:O	4:A:670:PRO:HD3	2.20	0.41
4:C:330:ILE:HG13	4:C:409:ALA:HA	2.00	0.41
4:D:261:LEU:C	4:D:263:GLY:H	2.23	0.41
4:D:19:ILE:HD13	4:D:19:ILE:HA	1.95	0.41
4:D:19:ILE:CG2	4:D:20:PRO:N	2.84	0.41
4:A:261:LEU:C	4:A:263:GLY:N	2.72	0.41
4:D:735:VAL:HG23	4:D:736:TRP:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:592:ASN:O	4:B:593:GLU:HB2	2.20	0.41
4:A:873:ARG:O	4:A:876:LEU:HD12	2.20	0.41
4:B:451:PRO:O	4:B:452:ILE:C	2.58	0.41
4:C:827:ALA:O	4:C:828:VAL:C	2.54	0.41
4:D:724:ALA:HA	4:D:774:GLN:NE2	2.35	0.41
4:D:778:ILE:CG2	4:D:779:ALA:H	2.30	0.41
4:A:689:VAL:C	4:A:691:ALA:N	2.72	0.41
4:C:452:ILE:HG13	4:C:456:GLY:CA	2.50	0.41
4:C:329:LYS:CG	4:C:445:THR:HG23	2.50	0.41
4:D:455:GLU:HA	4:D:455:GLU:OE1	2.19	0.41
4:B:589:GLY:O	4:B:614:LYS:HD2	2.20	0.41
4:B:111:PRO:HG2	4:B:112:GLU:H	1.86	0.41
4:A:59:LEU:HD23	4:A:64:VAL:HG21	1.99	0.41
4:C:620:TRP:NE1	4:C:677:MET:HB2	2.36	0.41
4:D:642:LYS:HB3	4:D:682:TRP:CH2	2.56	0.41
4:B:569:ASP:CG	4:B:569:ASP:O	2.58	0.41
4:A:31:ARG:NH2	4:A:32:LEU:HD11	2.34	0.41
4:A:743:ILE:HA	7:A:3130:HOH:O	2.19	0.41
4:A:632:ARG:O	4:A:636:THR:HG23	2.20	0.41
4:A:454:LYS:HA	4:A:526:LEU:HD21	2.01	0.41
4:C:416:PHE:HA	4:C:417:PRO:HD2	1.99	0.41
4:C:557:ARG:HB3	4:C:557:ARG:NH1	2.33	0.41
4:D:420:MET:HG2	4:D:425:ARG:O	2.20	0.41
4:D:829:ARG:CG	4:D:829:ARG:HH11	2.25	0.41
4:C:158:GLU:HA	4:C:195:LEU:CD1	2.43	0.41
4:C:559:VAL:O	4:C:560:ASN:HB2	2.21	0.41
4:B:615:ALA:O	4:B:616:LEU:C	2.58	0.41
4:B:329:LYS:O	4:B:329:LYS:HG3	2.20	0.41
4:C:337:VAL:HG21	4:C:512:LEU:CD2	2.45	0.41
4:C:336:ALA:O	4:C:337:VAL:O	2.38	0.41
4:C:534:LEU:HD12	4:C:818:PRO:HA	2.03	0.41
4:C:137:VAL:O	4:C:141:ILE:HG13	2.20	0.41
4:B:612:GLY:O	4:B:613:THR:C	2.58	0.41
4:D:133:THR:C	4:D:135:GLN:H	2.22	0.41
4:D:125:CYS:HB3	4:D:137:VAL:HG22	2.02	0.41
4:C:543:ILE:O	4:C:544:GLN:O	2.39	0.41
4:A:112:GLU:N	4:A:112:GLU:CD	2.74	0.41
4:C:135:GLN:OE1	4:C:210:ILE:HG21	2.21	0.41
4:B:771:ALA:O	4:B:772:HIS:C	2.57	0.41
4:C:486:HIS:O	4:C:489:ILE:HB	2.20	0.41
4:D:646:PHE:HD1	4:D:649:GLN:OE1	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:588:ASN:HD22	4:A:588:ASN:N	2.19	0.41
4:C:176:HIS:O	4:C:179:LYS:HB2	2.20	0.41
4:B:845:PHE:O	4:B:845:PHE:CD1	2.73	0.41
4:A:544:GLN:O	4:A:547:SER:N	2.54	0.41
4:A:825:PHE:HE1	4:A:829:ARG:CZ	2.26	0.41
4:A:14:ILE:HG23	4:A:288:ALA:HB1	2.02	0.41
4:C:557:ARG:O	4:C:557:ARG:HG2	2.19	0.41
1:N:9:DA:N6	3:P:1:DG:N2	2.68	0.41
4:B:817:ILE:HG13	4:B:820:ASP:HB2	2.02	0.41
4:D:416:PHE:HA	4:D:417:PRO:HD2	1.80	0.41
4:D:828:VAL:CB	4:D:883:ALA:HA	2.40	0.41
4:C:556:GLY:O	4:C:561:LEU:HB2	2.21	0.41
4:B:474:PRO:HA	4:B:880:PHE:CE1	2.56	0.41
4:B:475:PHE:C	4:B:477:GLU:N	2.74	0.41
4:B:477:GLU:O	4:B:480:LYS:HB3	2.20	0.41
4:B:505:GLN:NE2	4:B:505:GLN:CA	2.79	0.41
4:C:446:LEU:CD1	4:C:817:ILE:HG23	2.50	0.41
4:B:233:ASN:HB2	4:B:239:GLN:O	2.21	0.41
4:B:114:VAL:HG13	4:B:145:ILE:HD12	2.03	0.41
4:D:92:VAL:HG11	4:D:103:PHE:CD1	2.54	0.41
4:D:440:THR:C	4:D:442:GLY:N	2.74	0.41
4:A:384:VAL:HG12	4:A:384:VAL:O	2.20	0.41
4:D:732:GLY:O	4:D:734:PRO:HD3	2.19	0.41
4:D:744:GLN:CG	4:D:756:ARG:HB3	2.46	0.41
4:A:78:LEU:HA	4:A:78:LEU:HD12	1.83	0.41
4:D:254:ILE:HG13	4:D:254:ILE:H	1.70	0.41
1:K:6:DT:H2"	1:K:7:DC:OP2	2.20	0.41
4:D:304:ALA:HA	4:D:307:ARG:HG3	2.03	0.41
4:D:21:PHE:O	4:D:21:PHE:HD1	2.03	0.41
4:A:635:MET:CE	6:A:2000:APC:H2'	2.51	0.41
4:A:457:TYR:CD1	4:A:521:VAL:HG11	2.55	0.41
4:A:792:ARG:CG	4:A:792:ARG:HH11	2.30	0.41
4:A:290:GLY:C	4:A:292:ARG:H	2.24	0.41
4:D:702:ALA:O	4:D:704:LYS:N	2.54	0.41
4:C:297:VAL:CG2	4:C:733:PHE:HZ	2.34	0.41
4:C:322:ILE:O	4:C:323:ALA:C	2.59	0.41
4:A:709:GLU:HB2	4:A:722:ARG:NE	2.35	0.41
4:B:268:PHE:CD1	4:B:286:TYR:CE2	3.09	0.41
4:B:57:ARG:O	4:B:60:LYS:HB3	2.21	0.41
4:B:633:SER:O	4:B:634:VAL:C	2.54	0.41
4:B:676:TYR:CD1	4:B:680:LEU:HD11	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:730:PRO:HD3	7:B:3081:HOH:O	2.21	0.41
4:D:439:MET:HE3	4:D:443:LEU:HD11	2.02	0.41
4:B:461:LYS:HD3	4:B:483:GLU:OE2	2.21	0.41
4:D:282:THR:OG1	4:D:283:GLY:N	2.52	0.41
4:C:619:GLN:NE2	4:C:668:THR:H	2.19	0.41
4:C:393:SER:C	4:C:395:ARG:H	2.24	0.41
1:N:17:DG:P	4:D:57:ARG:HH12	2.44	0.41
4:A:511:PHE:CD2	4:A:511:PHE:C	2.93	0.41
4:D:678:ALA:O	4:D:679:LYS:C	2.59	0.41
4:A:257:ARG:CD	4:A:261:LEU:HD13	2.49	0.41
4:C:272:VAL:HG13	4:C:411:HIS:CD2	2.55	0.41
4:C:711:LYS:HG3	4:C:718:ILE:HA	2.03	0.41
4:B:323:ALA:HB1	4:B:809:LEU:HD11	2.02	0.41
4:C:632:ARG:CZ	6:C:2002:APC:N7	2.84	0.41
4:A:678:ALA:O	4:A:679:LYS:C	2.59	0.41
4:A:630:THR:CA	7:A:3199:HOH:O	2.62	0.41
4:A:308:TYR:HH	4:A:733:PHE:HE2	1.68	0.41
4:A:559:VAL:CG1	7:A:3104:HOH:O	2.68	0.41
4:A:794:THR:HG21	4:A:828:VAL:HG13	2.02	0.41
4:A:514:PHE:O	4:A:517:GLU:N	2.45	0.41
4:D:843:ALA:HB2	4:D:864:LEU:HD21	2.03	0.41
4:A:110:LYS:O	4:A:114:VAL:HG23	2.21	0.41
4:C:36:GLN:NE2	4:C:271:CYS:HB3	2.35	0.41
4:C:698:TRP:HE3	4:C:699:LEU:HG	1.85	0.41
4:C:699:LEU:HD22	4:C:782:PHE:CG	2.56	0.41
4:C:702:ALA:O	4:C:703:ALA:C	2.56	0.41
4:C:308:TYR:CE2	4:C:736:TRP:HZ3	2.38	0.41
1:K:12:DT:O4'	4:C:423:ARG:NH2	2.54	0.41
4:C:729:THR:OG1	4:C:733:PHE:HB3	2.21	0.41
4:C:696:MET:HG2	4:C:779:ALA:HB1	2.02	0.41
4:D:570:ILE:O	4:D:573:ILE:HG22	2.20	0.41
4:D:323:ALA:O	4:D:324:GLN:C	2.55	0.41
4:B:619:GLN:HE22	4:B:668:THR:H	1.68	0.41
4:B:673:ALA:O	4:B:676:TYR:HB3	2.20	0.41
4:B:581:ILE:O	4:B:584:ALA:N	2.50	0.41
4:B:636:THR:O	4:B:637:LEU:C	2.59	0.41
4:B:700:LYS:HE3	4:B:775:GLU:HG2	2.03	0.41
4:A:437:ASN:O	4:A:438:ASP:O	2.39	0.41
4:C:445:THR:OG1	4:C:532:LEU:HA	2.21	0.41
4:D:400:PHE:O	4:D:404:GLN:HB2	2.21	0.41
4:D:150:ARG:HH21	4:D:187:GLU:CD	2.22	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:335:LEU:HG	4:B:339:ASN:ND2	2.36	0.41
4:C:617:ALA:O	4:C:618:GLY:C	2.58	0.41
4:D:840:ASP:C	4:D:842:LEU:H	2.23	0.41
4:D:582:LEU:CD2	4:D:620:TRP:HB2	2.49	0.41
4:C:78:LEU:HD11	4:C:115:ALA:CB	2.51	0.41
4:C:395:ARG:O	4:C:396:ILE:C	2.58	0.41
4:D:457:TYR:HH	4:D:518:TYR:HE2	1.67	0.41
4:C:269:GLN:O	4:C:430:SER:CB	2.65	0.41
4:C:199:GLU:HG2	4:C:201:TRP:CD1	2.55	0.41
4:B:705:LEU:C	4:B:707:ALA:N	2.75	0.41
4:D:12:SER:O	4:D:13:ASP:C	2.59	0.41
4:B:569:ASP:OD1	4:B:572:GLY:N	2.50	0.41
4:D:6:ILE:HB	4:D:11:PHE:CE2	2.55	0.41
4:C:385:TYR:O	4:C:388:ASP:N	2.54	0.41
4:A:374:LEU:C	4:A:376:ALA:N	2.74	0.41
4:A:715:THR:HG21	4:A:717:GLU:OE2	2.21	0.41
4:C:576:LYS:HB3	7:C:3018:HOH:O	2.19	0.41
4:B:105:PHE:CE1	4:B:208:ASP:HB3	2.55	0.41
4:A:701:SER:O	4:A:702:ALA:C	2.59	0.41
4:B:805:GLU:HB2	7:B:3030:HOH:O	2.21	0.41
4:C:301:SER:O	4:C:302:LYS:C	2.59	0.41
4:A:727:TRP:O	4:A:734:PRO:HA	2.21	0.41
4:A:734:PRO:O	4:A:734:PRO:CG	2.68	0.41
4:A:825:PHE:C	4:A:825:PHE:HD1	2.22	0.41
1:E:12:DT:C2'	1:E:13:DC:H6	2.33	0.41
4:C:421:ASP:O	4:C:424:GLY:N	2.48	0.41
4:C:733:PHE:HB2	4:C:792:ARG:HH21	1.86	0.41
4:D:698:TRP:CZ3	4:D:699:LEU:HD23	2.56	0.41
4:D:36:GLN:HG2	4:D:272:VAL:HB	2.02	0.41
4:D:827:ALA:O	4:D:828:VAL:C	2.59	0.41
4:B:634:VAL:O	4:B:634:VAL:CG2	2.69	0.41
4:B:678:ALA:O	4:B:681:ILE:N	2.54	0.41
4:D:402:LEU:HD23	4:D:402:LEU:HA	1.59	0.41
4:D:482:ILE:HD12	4:D:514:PHE:CZ	2.55	0.41
4:C:452:ILE:HG13	4:C:456:GLY:C	2.41	0.41
4:A:505:GLN:C	4:A:507:SER:N	2.71	0.41
4:A:103:PHE:CE2	7:A:3227:HOH:O	2.57	0.41
4:A:199:GLU:O	4:A:201:TRP:N	2.44	0.41
4:A:341:ILE:O	4:A:342:THR:C	2.58	0.41
4:D:133:THR:HG22	4:D:243:THR:HG22	2.03	0.41
4:D:77:LEU:HD21	4:D:226:MET:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:201:TRP:HA	4:D:204:TRP:CD1	2.51	0.41
4:D:448:LYS:HD2	4:D:806:SER:HB3	2.03	0.41
4:D:619:GLN:CG	4:D:666:MET:O	2.68	0.41
4:A:705:LEU:O	4:A:708:ALA:HB3	2.21	0.41
4:D:563:PRO:HB3	4:D:877:GLU:C	2.42	0.41
4:C:106:LEU:HG	4:C:212:VAL:CG1	2.51	0.41
4:C:397:SER:O	4:C:400:PHE:N	2.44	0.41
4:C:3:THR:HG23	4:C:258:ALA:HB3	2.02	0.41
4:C:11:PHE:CE1	4:C:44:TYR:HB3	2.56	0.41
4:A:646:PHE:N	4:A:646:PHE:CD1	2.88	0.40
4:A:658:ALA:O	4:A:661:SER:HB2	2.21	0.40
4:C:834:ASP:O	4:C:837:GLU:HB2	2.21	0.40
1:K:12:DT:H4'	4:C:423:ARG:NH1	2.36	0.40
4:D:417:PRO:C	4:D:429:VAL:HG23	2.40	0.40
4:B:645:GLY:O	4:B:646:PHE:C	2.59	0.40
4:B:646:PHE:O	4:B:647:ARG:O	2.39	0.40
4:D:349:VAL:HG13	4:D:503:ALA:HB1	2.03	0.40
4:D:347:CYS:HB3	4:D:350:GLU:CG	2.50	0.40
4:B:502:TRP:CE3	4:B:512:LEU:HD22	2.56	0.40
2:I:4:G:H4'	4:B:389:LYS:HE3	2.03	0.40
4:D:437:ASN:ND2	4:D:437:ASN:C	2.75	0.40
4:B:341:ILE:N	4:B:341:ILE:HD12	2.36	0.40
4:A:19:ILE:CG2	4:A:20:PRO:N	2.84	0.40
1:N:15:DC:N3	1:N:16:DC:C5	2.89	0.40
4:D:642:LYS:O	4:D:646:PHE:CD2	2.74	0.40
4:B:797:TRP:CH2	4:B:801:LYS:HG3	2.56	0.40
4:A:741:LYS:HB3	4:A:741:LYS:HE2	1.82	0.40
4:D:588:ASN:HB3	4:D:589:GLY:H	1.65	0.40
4:B:150:ARG:C	4:B:152:GLY:H	2.23	0.40
4:A:620:TRP:HZ3	4:A:623:TYR:HD2	1.69	0.40
4:A:816:THR:HG21	4:A:820:ASP:HB2	2.03	0.40
4:C:281:ILE:HD12	4:C:281:ILE:HA	1.83	0.40
4:C:425:ARG:HB2	4:C:427:TYR:HE1	1.86	0.40
4:D:327:ALA:HB2	4:D:415:TRP:CE2	2.56	0.40
4:D:827:ALA:O	4:D:831:THR:HG22	2.21	0.40
4:B:418:TYR:CD2	4:B:427:TYR:O	2.67	0.40
4:B:680:LEU:N	4:B:680:LEU:CD1	2.80	0.40
1:H:15:DC:C5'	7:H:642:HOH:O	2.69	0.40
4:B:329:LYS:CD	4:B:447:ALA:HA	2.45	0.40
4:D:439:MET:HG3	4:D:509:PHE:CE2	2.56	0.40
4:A:304:ALA:C	4:A:307:ARG:HG3	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:103:PHE:CD2	4:A:107:GLN:NE2	2.89	0.40
4:D:733:PHE:HB2	4:D:792:ARG:NH2	2.37	0.40
4:A:126:LEU:HD23	4:A:132:THR:HG23	2.03	0.40
4:C:13:ASP:CB	7:C:3077:HOH:O	2.69	0.40
4:C:563:PRO:CD	4:C:874:ASP:HB3	2.48	0.40
4:A:433:ASN:CB	4:A:434:PRO:HD2	2.50	0.40
4:D:735:VAL:CG2	4:D:736:TRP:N	2.85	0.40
4:D:539:SER:HB3	4:D:559:VAL:HG12	2.02	0.40
4:B:230:HIS:CE1	4:B:232:GLN:HE21	2.39	0.40
4:C:402:LEU:CD1	4:C:439:MET:HE3	2.51	0.40
4:A:74:ILE:HG22	4:A:74:ILE:O	2.21	0.40
4:A:867:LYS:N	4:A:867:LYS:HD2	2.36	0.40
4:D:296:LEU:HG	4:D:296:LEU:O	2.21	0.40
4:C:720:ARG:HG2	4:C:720:ARG:HH11	1.85	0.40
2:L:6:G:C6	2:L:7:A:N7	2.89	0.40
4:C:730:PRO:CD	4:C:786:GLN:NE2	2.84	0.40
4:C:729:THR:HA	4:C:730:PRO:HD3	1.88	0.40
4:D:571:TYR:CD1	4:D:634:VAL:CG1	3.04	0.40
4:D:737:GLN:HG2	4:D:774:GLN:OE1	2.20	0.40
4:D:274:PRO:HA	4:D:275:PRO:HD3	1.93	0.40
4:B:779:ALA:O	4:B:783:VAL:CG2	2.69	0.40
4:D:236:VAL:CB	4:D:239:GLN:HB2	2.51	0.40
4:A:386:ARG:HE	4:A:386:ARG:HB2	1.20	0.40
4:D:744:GLN:HE21	4:D:756:ARG:N	2.18	0.40
4:A:58:GLN:HG3	4:A:67:ASN:ND2	2.36	0.40
1:K:5:DA:H1'	7:K:712:HOH:O	2.20	0.40
4:A:51:PHE:CD2	4:A:262:ALA:HB2	2.56	0.40
4:C:712:ASP:O	4:C:716:GLY:N	2.55	0.40
4:C:576:LYS:HD3	7:C:3018:HOH:O	2.21	0.40
3:M:7:DT:H2"	3:M:8:DC:C6	2.56	0.40
4:B:105:PHE:C	4:B:107:GLN:N	2.75	0.40
4:C:491:ALA:O	4:C:494:LYS:N	2.55	0.40
4:A:635:MET:HE1	6:A:2000:APC:H2'	2.03	0.40
4:D:294:LEU:HD13	4:D:419:ASN:HD21	1.86	0.40
4:C:540:CYS:HB2	4:C:559:VAL:HG12	2.04	0.40
4:B:643:GLU:O	4:B:645:GLY:N	2.54	0.40
4:B:577:LYS:HB3	4:B:684:SER:HB3	2.03	0.40
4:B:790:HIS:HD1	4:B:790:HIS:C	2.24	0.40
4:B:810:ILE:HB	4:B:813:SER:HB2	2.03	0.40
4:D:508:PRO:C	4:D:510:CYS:N	2.73	0.40
4:C:59:LEU:HA	4:C:64:VAL:HG22	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:116:TYR:CE2	4:B:752:LEU:HD13	2.56	0.40
4:C:84:ARG:CB	4:C:223:SER:HB3	2.49	0.40
4:B:88:TRP:O	4:B:92:VAL:HG23	2.22	0.40
4:A:404:GLN:HG2	4:A:432:PHE:CD2	2.55	0.40
4:C:463:HIS:HE1	4:C:532:LEU:HD11	1.86	0.40
4:B:220:LEU:O	4:B:222:GLU:N	2.54	0.40
4:B:109:ILE:H	4:B:109:ILE:CD1	2.33	0.40
4:D:141:ILE:O	4:D:145:ILE:CG1	2.66	0.40
4:A:704:LYS:HE3	4:A:860:LYS:HZ1	1.83	0.40
4:A:550:LEU:HD21	4:A:865:PRO:HG2	2.04	0.40
4:A:39:LEU:O	4:A:40:GLU:C	2.60	0.40
3:M:4:DG:H2"	3:M:5:DA:C8	2.57	0.40
4:B:572:GLY:O	4:B:575:ALA:HB3	2.21	0.40
4:D:726:HIS:CD2	4:D:735:VAL:O	2.74	0.40
3:J:6:DT:C2'	3:J:7:DT:H71	2.50	0.40
2:O:6:G:H3'	7:O:144:HOH:O	2.20	0.40
4:A:56:GLU:HG3	7:A:3057:HOH:O	2.20	0.40
4:B:252:GLU:O	4:B:253:ALA:C	2.58	0.40
4:B:108:GLU:HA	4:B:108:GLU:OE2	2.21	0.40
4:A:868:GLY:N	7:A:3164:HOH:O	2.54	0.40
4:A:868:GLY:C	4:A:869:ASN:HD22	2.25	0.40
4:A:24:LEU:HD21	4:A:287:TRP:CD2	2.56	0.40
4:D:702:ALA:HB2	4:D:861:MET:HE1	2.03	0.40
4:C:551:ARG:HE	4:C:872:LEU:CG	2.34	0.40
4:C:786:GLN:C	4:C:788:GLY:N	2.75	0.40
4:B:306:MET:O	4:B:309:GLU:N	2.51	0.40
4:B:215:ARG:O	4:B:219:MET:HE3	2.21	0.40
4:C:817:ILE:HD12	4:C:819:ALA:HB3	2.04	0.40
4:B:229:LEU:HD11	4:B:242:GLU:CG	2.42	0.40
4:C:756:ARG:CG	7:C:3143:HOH:O	2.70	0.40
4:C:749:LEU:CD1	4:C:750:MET:HG2	2.46	0.40
4:C:483:GLU:O	4:C:486:HIS:N	2.52	0.40
4:D:22:ASN:HA	4:D:25:ALA:HB3	2.03	0.40
4:B:185:VAL:O	4:B:188:ALA:HB3	2.22	0.40
4:C:525:GLY:C	4:C:527:SER:H	2.24	0.40
4:D:549:MET:HE3	4:D:836:TYR:HE1	1.86	0.40
4:C:261:LEU:HA	4:C:261:LEU:HD12	1.82	0.40
4:C:523:HIS:N	4:C:523:HIS:CD2	2.90	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
4	A	851/883 (96%)	570 (67%)	198 (23%)	83 (10%)	1 4
4	B	851/883 (96%)	578 (68%)	188 (22%)	85 (10%)	1 4
4	C	851/883 (96%)	608 (71%)	178 (21%)	65 (8%)	1 9
4	D	851/883 (96%)	623 (73%)	174 (20%)	54 (6%)	2 13
All	All	3404/3532 (96%)	2379 (70%)	738 (22%)	287 (8%)	1 6

All (287) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	7	ALA
4	A	194	GLY
4	A	199	GLU
4	A	281	ILE
4	A	288	ALA
4	A	309	GLU
4	A	353	PRO
4	A	387	LYS
4	A	391	ARG
4	A	402	LEU
4	A	430	SER
4	A	506	ASP
4	A	508	PRO
4	A	526	LEU
4	A	549	MET
4	A	592	ASN
4	A	631	LYS
4	A	686	SER
4	A	708	ALA
4	A	721	LYS
4	A	744	GLN
4	A	745	THR

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Mol	Chain	Res	Type
4	A	746	ARG
4	A	755	PHE
4	A	803	GLY
4	A	850	ALA
4	B	262	ALA
4	B	274	PRO
4	B	293	PRO
4	B	391	ARG
4	B	452	ILE
4	B	539	SER
4	B	610	LYS
4	B	611	LEU
4	B	646	PHE
4	B	647	ARG
4	B	663	LYS
4	B	690	VAL
4	B	706	LEU
4	B	755	PHE
4	B	784	HIS
4	B	785	SER
4	B	796	VAL
4	B	804	ILE
4	B	841	VAL
4	B	851	ASP
4	C	68	ALA
4	C	106	LEU
4	C	240	ASP
4	C	288	ALA
4	C	309	GLU
4	C	337	VAL
4	C	422	TRP
4	C	503	ALA
4	C	508	PRO
4	C	526	LEU
4	C	539	SER
4	C	631	LYS
4	C	744	GLN
4	C	745	THR
4	C	755	PHE
4	C	771	ALA
4	C	841	VAL
4	D	307	ARG

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Mol	Chain	Res	Type
4	D	324	GLN
4	D	353	PRO
4	D	508	PRO
4	D	539	SER
4	D	541	SER
4	D	592	ASN
4	D	647	ARG
4	D	663	LYS
4	D	755	PHE
4	D	841	VAL
4	A	60	LYS
4	A	106	LEU
4	A	177	VAL
4	A	200	ALA
4	A	332	LYS
4	A	375	THR
4	A	384	VAL
4	A	401	MET
4	A	422	TRP
4	A	438	ASP
4	A	474	PRO
4	A	544	GLN
4	A	632	ARG
4	A	641	SER
4	A	678	ALA
4	A	771	ALA
4	A	811	HIS
4	A	882	PHE
4	B	14	ILE
4	B	36	GLN
4	B	106	LEU
4	B	167	GLU
4	B	176	HIS
4	B	194	GLY
4	B	298	ARG
4	B	307	ARG
4	B	314	PRO
4	B	315	GLU
4	B	412	LYS
4	B	430	SER
4	B	431	MET
4	B	470	VAL

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Mol	Chain	Res	Type
4	B	526	LEU
4	B	542	GLY
4	B	589	GLY
4	B	592	ASN
4	B	641	SER
4	B	721	LYS
4	B	746	ARG
4	B	865	PRO
4	B	873	ARG
4	B	876	LEU
4	C	7	ALA
4	C	162	PHE
4	C	307	ARG
4	C	314	PRO
4	C	339	ASN
4	C	443	LEU
4	C	474	PRO
4	C	544	GLN
4	C	686	SER
4	C	690	VAL
4	C	796	VAL
4	C	811	HIS
4	C	882	PHE
4	D	7	ALA
4	D	119	ILE
4	D	167	GLU
4	D	259	GLY
4	D	292	ARG
4	D	422	TRP
4	D	443	LEU
4	D	452	ILE
4	D	593	GLU
4	D	648	GLN
4	D	745	THR
4	D	882	PHE
4	A	100	PRO
4	A	262	ALA
4	A	277	PRO
4	A	460	LEU
4	A	511	PHE
4	A	525	GLY
4	A	541	SER

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Mol	Chain	Res	Type
4	A	542	GLY
4	A	647	ARG
4	A	660	ASP
4	A	734	PRO
4	A	797	TRP
4	A	825	PHE
4	A	872	LEU
4	B	7	ALA
4	B	68	ALA
4	B	150	ARG
4	B	199	GLU
4	B	200	ALA
4	B	260	ALA
4	B	348	PRO
4	B	382	ALA
4	B	505	GLN
4	B	508	PRO
4	B	551	ARG
4	B	593	GLU
4	B	617	ALA
4	B	627	ARG
4	B	628	SER
4	B	678	ALA
4	B	810	ILE
4	B	862	PRO
4	C	98	LYS
4	C	140	ALA
4	C	199	GLU
4	C	206	LYS
4	C	262	ALA
4	C	549	MET
4	C	647	ARG
4	C	850	ALA
4	C	851	ASP
4	D	240	ASP
4	D	288	ALA
4	D	309	GLU
4	D	314	PRO
4	D	348	PRO
4	D	405	ALA
4	D	544	GLN
4	D	589	GLY

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Mol	Chain	Res	Type
4	A	160	LYS
4	A	204	TRP
4	A	274	PRO
4	A	345	LYS
4	A	425	ARG
4	A	464	GLY
4	A	611	LEU
4	A	670	PRO
4	A	677	MET
4	A	796	VAL
4	B	50	ARG
4	B	160	LYS
4	B	277	PRO
4	B	395	ARG
4	B	396	ILE
4	B	476	PRO
4	B	580	GLU
4	B	631	LYS
4	B	648	GLN
4	B	705	LEU
4	B	752	LEU
4	B	811	HIS
4	B	824	LEU
4	B	850	ALA
4	C	200	ALA
4	C	353	PRO
4	C	476	PRO
4	C	592	ASN
4	C	787	ASP
4	D	65	ALA
4	D	260	ALA
4	D	631	LYS
4	D	722	ARG
4	A	4	ILE
4	A	313	MET
4	A	348	PRO
4	A	383	ALA
4	A	560	ASN
4	A	690	VAL
4	B	115	ALA
4	B	265	SER
4	B	342	THR

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Mol	Chain	Res	Type
4	B	557	ARG
4	B	780	PRO
4	C	102	ALA
4	C	348	PRO
4	C	541	SER
4	C	542	GLY
4	C	632	ARG
4	C	663	LYS
4	C	701	SER
4	C	832	MET
4	D	63	GLU
4	D	162	PHE
4	D	467	CYS
4	D	474	PRO
4	D	691	ALA
4	D	704	LYS
4	D	744	GLN
4	A	292	ARG
4	A	593	GLU
4	B	254	ILE
4	C	4	ILE
4	C	211	HIS
4	C	235	GLY
4	C	341	ILE
4	C	648	GLN
4	C	872	LEU
4	D	275	PRO
4	D	336	ALA
4	D	715	THR
4	D	811	HIS
4	D	850	ALA
4	D	860	LYS
4	A	710	VAL
4	B	270	PRO
4	B	479	ILE
4	C	804	ILE
4	D	114	VAL
4	D	194	GLY
4	D	693	VAL
4	A	533	PRO
4	A	650	VAL
4	C	19	ILE

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Mol	Chain	Res	Type
4	C	141	ILE
4	C	322	ILE
4	C	567	VAL
4	A	841	VAL
4	B	353	PRO
4	C	194	GLY
4	C	833	VAL
4	D	337	VAL
4	A	270	PRO
4	A	567	VAL
4	A	669	GLN
4	D	97	GLY
4	D	4	ILE

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
4	A	703/729 (96%)	573 (82%)	130 (18%)	2 10
4	B	703/729 (96%)	573 (82%)	130 (18%)	2 10
4	C	703/729 (96%)	594 (84%)	109 (16%)	3 15
4	D	703/729 (96%)	598 (85%)	105 (15%)	4 17
All	All	2812/2916 (96%)	2338 (83%)	474 (17%)	2 13

All (474) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	8	LYS
4	A	16	LEU
4	A	19	ILE
4	A	23	THR
4	A	27	HIS
4	A	36	GLN
4	A	50	ARG
4	A	53	LYS

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Mol	Chain	Res	Type
4	A	56	GLU
4	A	57	ARG
4	A	60	LYS
4	A	77	LEU
4	A	81	MET
4	A	84	ARG
4	A	86	ASN
4	A	96	ARG
4	A	101	THR
4	A	104	GLN
4	A	121	THR
4	A	130	ASP
4	A	143	ARG
4	A	145	ILE
4	A	155	ARG
4	A	157	LEU
4	A	165	ASN
4	A	170	LEU
4	A	183	MET
4	A	190	MET
4	A	206	LYS
4	A	207	GLU
4	A	208	ASP
4	A	230	HIS
4	A	248	PRO
4	A	257	ARG
4	A	261	LEU
4	A	282	THR
4	A	293	PRO
4	A	299	THR
4	A	301	SER
4	A	307	ARG
4	A	309	GLU
4	A	330	ILE
4	A	333	LYS
4	A	343	LYS
4	A	388	ASP
4	A	393	SER
4	A	395	ARG
4	A	401	MET
4	A	402	LEU
4	A	403	GLU

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Mol	Chain	Res	Type
4	A	404	GLN
4	A	410	ASN
4	A	418	TYR
4	A	422	TRP
4	A	423	ARG
4	A	429	VAL
4	A	430	SER
4	A	433	ASN
4	A	440	THR
4	A	448	LYS
4	A	451	PRO
4	A	452	ILE
4	A	454	LYS
4	A	457	TYR
4	A	462	ILE
4	A	470	VAL
4	A	472	LYS
4	A	473	VAL
4	A	475	PHE
4	A	495	SER
4	A	510	CYS
4	A	514	PHE
4	A	516	PHE
4	A	517	GLU
4	A	531	SER
4	A	540	CYS
4	A	543	ILE
4	A	550	LEU
4	A	559	VAL
4	A	561	LEU
4	A	565	GLU
4	A	573	ILE
4	A	574	VAL
4	A	613	THR
4	A	620	TRP
4	A	626	THR
4	A	627	ARG
4	A	632	ARG
4	A	634	VAL
4	A	641	SER
4	A	643	GLU
4	A	647	ARG

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Mol	Chain	Res	Type
4	A	651	LEU
4	A	656	GLN
4	A	660	ASP
4	A	666	MET
4	A	670	PRO
4	A	688	THR
4	A	730	PRO
4	A	734	PRO
4	A	744	GLN
4	A	746	ARG
4	A	749	LEU
4	A	751	PHE
4	A	752	LEU
4	A	755	PHE
4	A	766	ASP
4	A	776	SER
4	A	778	ILE
4	A	786	GLN
4	A	787	ASP
4	A	791	LEU
4	A	796	VAL
4	A	801	LYS
4	A	802	TYR
4	A	806	SER
4	A	814	PHE
4	A	816	THR
4	A	820	ASP
4	A	828	VAL
4	A	829	ARG
4	A	832	MET
4	A	839	CYS
4	A	841	VAL
4	A	846	TYR
4	A	851	ASP
4	A	860	LYS
4	A	869	ASN
4	A	879	ASP
4	A	882	PHE
4	B	13	ASP
4	B	15	GLU
4	B	16	LEU
4	B	19	ILE

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Mol	Chain	Res	Type
4	B	21	PHE
4	B	22	ASN
4	B	24	LEU
4	B	27	HIS
4	B	32	LEU
4	B	36	GLN
4	B	39	LEU
4	B	50	ARG
4	B	56	GLU
4	B	66	ASP
4	B	71	LYS
4	B	84	ARG
4	B	86	ASN
4	B	96	ARG
4	B	99	ARG
4	B	101	THR
4	B	120	LYS
4	B	123	LEU
4	B	132	THR
4	B	143	ARG
4	B	164	LYS
4	B	166	VAL
4	B	168	GLU
4	B	172	LYS
4	B	184	GLN
4	B	206	LYS
4	B	207	GLU
4	B	209	SER
4	B	214	VAL
4	B	224	THR
4	B	252	GLU
4	B	256	THR
4	B	257	ARG
4	B	261	LEU
4	B	264	ILE
4	B	267	MET
4	B	272	VAL
4	B	273	VAL
4	B	277	PRO
4	B	279	THR
4	B	291	ARG
4	B	299	THR

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Mol	Chain	Res	Type
4	B	305	LEU
4	B	314	PRO
4	B	332	LYS
4	B	337	VAL
4	B	343	LYS
4	B	349	VAL
4	B	351	ASP
4	B	378	LYS
4	B	379	ARG
4	B	388	ASP
4	B	394	ARG
4	B	397	SER
4	B	402	LEU
4	B	404	GLN
4	B	408	PHE
4	B	419	ASN
4	B	422	TRP
4	B	423	ARG
4	B	437	ASN
4	B	441	LYS
4	B	452	ILE
4	B	454	LYS
4	B	461	LYS
4	B	472	LYS
4	B	483	GLU
4	B	492	CYS
4	B	494	LYS
4	B	495	SER
4	B	497	LEU
4	B	500	THR
4	B	512	LEU
4	B	514	PHE
4	B	527	SER
4	B	532	LEU
4	B	540	CYS
4	B	552	ASP
4	B	560	ASN
4	B	567	VAL
4	B	569	ASP
4	B	582	LEU
4	B	592	ASN
4	B	621	LEU

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Mol	Chain	Res	Type
4	B	626	THR
4	B	627	ARG
4	B	633	SER
4	B	643	GLU
4	B	651	LEU
4	B	654	THR
4	B	656	GLN
4	B	666	MET
4	B	668	THR
4	B	683	GLU
4	B	690	VAL
4	B	693	VAL
4	B	697	ASN
4	B	722	ARG
4	B	731	ASP
4	B	734	PRO
4	B	735	VAL
4	B	744	GLN
4	B	749	LEU
4	B	752	LEU
4	B	769	ILE
4	B	770	ASP
4	B	776	SER
4	B	780	PRO
4	B	783	VAL
4	B	785	SER
4	B	786	GLN
4	B	790	HIS
4	B	801	LYS
4	B	809	LEU
4	B	813	SER
4	B	828	VAL
4	B	832	MET
4	B	841	VAL
4	B	842	LEU
4	B	849	PHE
4	B	859	ASP
4	B	860	LYS
4	B	867	LYS
4	B	869	ASN
4	B	870	LEU
4	B	877	GLU

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Mol	Chain	Res	Type
4	C	2	ASN
4	C	3	THR
4	C	9	ASN
4	C	16	LEU
4	C	26	ASP
4	C	32	LEU
4	C	36	GLN
4	C	37	LEU
4	C	40	GLU
4	C	50	ARG
4	C	64	VAL
4	C	66	ASP
4	C	84	ARG
4	C	96	ARG
4	C	99	ARG
4	C	107	GLN
4	C	119	ILE
4	C	120	LYS
4	C	143	ARG
4	C	170	LEU
4	C	183	MET
4	C	195	LEU
4	C	208	ASP
4	C	214	VAL
4	C	227	VAL
4	C	230	HIS
4	C	244	ILE
4	C	256	THR
4	C	257	ARG
4	C	267	MET
4	C	281	ILE
4	C	282	THR
4	C	291	ARG
4	C	294	LEU
4	C	301	SER
4	C	305	LEU
4	C	313	MET
4	C	325	ASN
4	C	335	LEU
4	C	343	LYS
4	C	347	CYS
4	C	350	GLU

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Mol	Chain	Res	Type
4	C	377	TRP
4	C	378	LYS
4	C	379	ARG
4	C	397	SER
4	C	403	GLU
4	C	404	GLN
4	C	412	LYS
4	C	415	TRP
4	C	422	TRP
4	C	423	ARG
4	C	434	PRO
4	C	437	ASN
4	C	467	CYS
4	C	470	VAL
4	C	471	ASP
4	C	472	LYS
4	C	473	VAL
4	C	509	PHE
4	C	510	CYS
4	C	514	PHE
4	C	517	GLU
4	C	531	SER
4	C	532	LEU
4	C	544	GLN
4	C	551	ARG
4	C	553	GLU
4	C	559	VAL
4	C	565	GLU
4	C	573	ILE
4	C	577	LYS
4	C	588	ASN
4	C	601	ASN
4	C	614	LYS
4	C	636	THR
4	C	659	ILE
4	C	661	SER
4	C	663	LYS
4	C	666	MET
4	C	700	LYS
4	C	711	LYS
4	C	722	ARG
4	C	729	THR

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Mol	Chain	Res	Type
4	C	733	PHE
4	C	734	PRO
4	C	744	GLN
4	C	749	LEU
4	C	750	MET
4	C	751	PHE
4	C	754	GLN
4	C	755	PHE
4	C	768	GLU
4	C	783	VAL
4	C	786	GLN
4	C	787	ASP
4	C	789	SER
4	C	801	LYS
4	C	814	PHE
4	C	817	ILE
4	C	831	THR
4	C	832	MET
4	C	838	SER
4	C	841	VAL
4	C	842	LEU
4	C	860	LYS
4	C	869	ASN
4	C	880	PHE
4	C	882	PHE
4	D	13	ASP
4	D	16	LEU
4	D	19	ILE
4	D	22	ASN
4	D	27	HIS
4	D	36	GLN
4	D	39	LEU
4	D	48	GLU
4	D	50	ARG
4	D	56	GLU
4	D	59	LEU
4	D	84	ARG
4	D	95	LYS
4	D	101	THR
4	D	109	ILE
4	D	120	LYS
4	D	131	ASN

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Mol	Chain	Res	Type
4	D	143	ARG
4	D	145	ILE
4	D	171	ASN
4	D	183	MET
4	D	190	MET
4	D	206	LYS
4	D	215	ARG
4	D	219	MET
4	D	232	GLN
4	D	236	VAL
4	D	257	ARG
4	D	269	GLN
4	D	271	CYS
4	D	281	ILE
4	D	282	THR
4	D	289	ASN
4	D	299	THR
4	D	305	LEU
4	D	335	LEU
4	D	341	ILE
4	D	348	PRO
4	D	350	GLU
4	D	351	ASP
4	D	378	LYS
4	D	391	ARG
4	D	394	ARG
4	D	398	LEU
4	D	403	GLU
4	D	412	LYS
4	D	419	ASN
4	D	422	TRP
4	D	425	ARG
4	D	435	GLN
4	D	437	ASN
4	D	441	LYS
4	D	444	LEU
4	D	448	LYS
4	D	450	LYS
4	D	452	ILE
4	D	467	CYS
4	D	472	LYS
4	D	477	GLU

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Mol	Chain	Res	Type
4	D	492	CYS
4	D	495	SER
4	D	497	LEU
4	D	499	ASN
4	D	510	CYS
4	D	514	PHE
4	D	518	TYR
4	D	530	CYS
4	D	540	CYS
4	D	559	VAL
4	D	571	TYR
4	D	601	ASN
4	D	606	SER
4	D	632	ARG
4	D	652	GLU
4	D	656	GLN
4	D	661	SER
4	D	666	MET
4	D	700	LYS
4	D	705	LEU
4	D	718	ILE
4	D	720	ARG
4	D	721	LYS
4	D	722	ARG
4	D	723	CYS
4	D	730	PRO
4	D	734	PRO
4	D	735	VAL
4	D	749	LEU
4	D	750	MET
4	D	752	LEU
4	D	776	SER
4	D	783	VAL
4	D	786	GLN
4	D	787	ASP
4	D	791	LEU
4	D	801	LYS
4	D	812	ASP
4	D	813	SER
4	D	820	ASP
4	D	828	VAL
4	D	842	LEU

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Mol	Chain	Res	Type
4	D	851	ASP
4	D	857	GLN
4	D	860	LYS
4	D	882	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (125) such sidechains are listed below:

Mol	Chain	Res	Type
4	A	5	ASN
4	A	41	HIS
4	A	86	ASN
4	A	171	ASN
4	A	184	GLN
4	A	205	HIS
4	A	211	HIS
4	A	230	HIS
4	A	232	GLN
4	A	239	GLN
4	A	269	GLN
4	A	289	ASN
4	A	404	GLN
4	A	410	ASN
4	A	419	ASN
4	A	435	GLN
4	A	437	ASN
4	A	466	ASN
4	A	486	HIS
4	A	488	ASN
4	A	545	HIS
4	A	588	ASN
4	A	649	GLN
4	A	656	GLN
4	A	669	GLN
4	A	672	GLN
4	A	748	ASN
4	A	754	GLN
4	A	781	ASN
4	A	823	ASN
4	A	848	GLN
4	A	854	HIS
4	A	857	GLN
4	A	869	ASN

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Mol	Chain	Res	Type
4	A	871	ASN
4	B	5	ASN
4	B	22	ASN
4	B	86	ASN
4	B	107	GLN
4	B	161	HIS
4	B	169	GLN
4	B	171	ASN
4	B	205	HIS
4	B	232	GLN
4	B	233	ASN
4	B	239	GLN
4	B	269	GLN
4	B	324	GLN
4	B	404	GLN
4	B	419	ASN
4	B	435	GLN
4	B	437	ASN
4	B	499	ASN
4	B	505	GLN
4	B	529	ASN
4	B	544	GLN
4	B	545	HIS
4	B	560	ASN
4	B	588	ASN
4	B	619	GLN
4	B	656	GLN
4	B	672	GLN
4	B	726	HIS
4	B	748	ASN
4	B	772	HIS
4	B	774	GLN
4	B	781	ASN
4	B	786	GLN
4	B	823	ASN
4	B	848	GLN
4	B	869	ASN
4	C	5	ASN
4	C	58	GLN
4	C	86	ASN
4	C	104	GLN
4	C	107	GLN

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Mol	Chain	Res	Type
4	C	169	GLN
4	C	171	ASN
4	C	230	HIS
4	C	232	GLN
4	C	269	GLN
4	C	289	ASN
4	C	324	GLN
4	C	339	ASN
4	C	410	ASN
4	C	435	GLN
4	C	437	ASN
4	C	523	HIS
4	C	560	ASN
4	C	588	ASN
4	C	656	GLN
4	C	669	GLN
4	C	726	HIS
4	C	737	GLN
4	C	744	GLN
4	C	754	GLN
4	C	781	ASN
4	C	786	GLN
4	C	799	HIS
4	D	22	ASN
4	D	41	HIS
4	D	86	ASN
4	D	107	GLN
4	D	161	HIS
4	D	239	GLN
4	D	289	ASN
4	D	331	ASN
4	D	410	ASN
4	D	419	ASN
4	D	435	GLN
4	D	437	ASN
4	D	499	ASN
4	D	544	GLN
4	D	619	GLN
4	D	669	GLN
4	D	726	HIS
4	D	737	GLN
4	D	744	GLN

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Mol	Chain	Res	Type
4	D	748	ASN
4	D	754	GLN
4	D	790	HIS
4	D	823	ASN
4	D	854	HIS
4	D	857	GLN
4	D	871	ASN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	F	7/12 (58%)	0	0
2	I	7/12 (58%)	1 (14%)	0
2	L	7/12 (58%)	0	0
2	O	7/12 (58%)	0	0
All	All	28/48 (58%)	1 (3%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	I	8	U

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

Of 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link

column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	APC	A	2000	5	25,33,33	1.95	5 (20%)	30,52,52	1.85	9 (30%)
6	APC	B	2001	5	25,33,33	2.13	7 (28%)	30,52,52	2.14	6 (20%)
6	APC	C	2002	5	25,33,33	2.23	7 (28%)	30,52,52	1.35	5 (16%)
6	APC	D	2003	5	25,33,33	2.00	4 (16%)	30,52,52	1.85	6 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	APC	A	2000	5	-	0/15/38/38	0/3/3/3
6	APC	B	2001	5	-	0/15/38/38	0/3/3/3
6	APC	C	2002	5	-	0/15/38/38	0/3/3/3
6	APC	D	2003	5	-	0/15/38/38	0/3/3/3

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	2001	APC	PB-O2B	-2.76	1.49	1.56
6	B	2001	APC	PA-O2A	-2.50	1.50	1.56
6	C	2002	APC	PA-O2A	-2.47	1.50	1.56
6	A	2000	APC	C8-N7	-2.24	1.30	1.34
6	A	2000	APC	PB-O2B	-2.24	1.50	1.56
6	C	2002	APC	PB-O2B	-2.09	1.51	1.56
6	D	2003	APC	PA-O2A	-2.05	1.51	1.56
6	C	2002	APC	O4'-C1'	2.06	1.43	1.41
6	C	2002	APC	C2-N1	2.24	1.38	1.33
6	B	2001	APC	C5'-C4'	2.25	1.58	1.51
6	A	2000	APC	C2-N3	2.84	1.37	1.32
6	C	2002	APC	C2-N3	3.11	1.37	1.32
6	B	2001	APC	C2-N3	3.28	1.38	1.32
6	D	2003	APC	C2-N3	3.32	1.38	1.32
6	D	2003	APC	PA-O5'	3.40	1.61	1.57
6	B	2001	APC	O4'-C1'	3.65	1.45	1.41
6	A	2000	APC	PA-O5'	3.95	1.61	1.57
6	B	2001	APC	PB-O3B	4.50	1.63	1.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	2002	APC	PB-O3B	5.50	1.64	1.58
6	B	2001	APC	PA-O5'	6.15	1.64	1.57
6	A	2000	APC	PB-O3B	6.55	1.65	1.58
6	D	2003	APC	PB-O3B	7.14	1.66	1.58
6	C	2002	APC	PA-O5'	7.32	1.65	1.57

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	B	2001	APC	O1A-PA-C3A	-4.68	97.24	109.02
6	A	2000	APC	O5'-PA-O1A	-4.59	101.79	113.98
6	B	2001	APC	PG-O3B-PB	-3.67	120.37	132.67
6	A	2000	APC	PG-O3B-PB	-2.88	123.02	132.67
6	C	2002	APC	PG-O3B-PB	-2.43	124.51	132.67
6	C	2002	APC	O5'-PA-O1A	-2.25	107.99	113.98
6	D	2003	APC	PG-O3B-PB	-2.11	125.58	132.67
6	A	2000	APC	C2'-C3'-C4'	2.03	106.78	102.61
6	A	2000	APC	O3G-PG-O3B	2.07	114.49	105.09
6	D	2003	APC	C2'-C3'-C4'	2.12	106.97	102.61
6	A	2000	APC	O4'-C4'-C3'	2.17	109.53	105.15
6	D	2003	APC	O2'-C2'-C3'	2.51	119.99	111.83
6	B	2001	APC	O2A-PA-O1A	2.67	118.51	110.12
6	A	2000	APC	C1'-N9-C4	2.70	131.02	126.94
6	C	2002	APC	C2'-C3'-C4'	2.81	108.40	102.61
6	A	2000	APC	O2B-PB-O1B	2.98	119.50	110.12
6	B	2001	APC	O2B-PB-O1B	3.07	119.77	110.12
6	C	2002	APC	O2A-PA-O1A	3.08	119.80	110.12
6	A	2000	APC	O2A-PA-O1A	3.08	119.80	110.12
6	B	2001	APC	C2'-C3'-C4'	3.22	109.23	102.61
6	D	2003	APC	O2A-PA-O1A	3.22	120.24	110.12
6	C	2002	APC	O2B-PB-O1B	3.24	120.31	110.12
6	D	2003	APC	O2B-PB-O1B	3.41	120.85	110.12
6	A	2000	APC	O1A-PA-C3A	3.72	118.37	109.02
6	D	2003	APC	C2'-C1'-N9	6.68	124.50	114.29
6	B	2001	APC	C2'-C1'-N9	7.03	125.03	114.29

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 48 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	2000	APC	16	0
6	B	2001	APC	9	0
6	C	2002	APC	16	0
6	D	2003	APC	7	0

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

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	E	17/18 (94%)	-0.20	0 100 100	19, 58, 179, 181	0
1	H	17/18 (94%)	0.20	1 (5%) 26 14	21, 75, 158, 171	0
1	K	17/18 (94%)	0.14	0 100 100	48, 94, 157, 159	0
1	N	17/18 (94%)	0.15	0 100 100	51, 102, 172, 173	0
2	F	8/12 (66%)	-0.46	0 100 100	17, 23, 83, 93	0
2	I	8/12 (66%)	-0.01	0 100 100	17, 38, 82, 93	0
2	L	8/12 (66%)	0.21	0 100 100	47, 53, 113, 118	0
2	O	8/12 (66%)	0.16	0 100 100	51, 80, 132, 144	0
3	G	9/10 (90%)	1.06	2 (22%) 1 1	146, 153, 176, 183	0
3	J	9/10 (90%)	0.07	1 (11%) 7 4	130, 138, 162, 163	0
3	M	9/10 (90%)	-0.13	0 100 100	134, 146, 155, 158	0
3	P	9/10 (90%)	1.39	1 (11%) 7 4	157, 167, 172, 172	0
4	A	857/883 (97%)	-0.28	37 (4%) 39 25	15, 76, 141, 153	0
4	B	857/883 (97%)	-0.41	15 (1%) 71 58	10, 69, 131, 150	0
4	C	857/883 (97%)	-0.30	19 (2%) 65 50	47, 93, 134, 160	0
4	D	857/883 (97%)	-0.04	29 (3%) 49 34	41, 102, 144, 156	0
All	All	3564/3692 (96%)	-0.24	105 (2%) 55 41	10, 89, 142, 183	0

All (105) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	P	1	DG	8.5
4	D	235	GLY	7.1
3	G	1	DG	6.9
4	A	235	GLY	6.2
4	A	601	ASN	5.5

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Mol	Chain	Res	Type	RSRZ
4	D	238	GLY	5.1
4	C	372	GLU	4.8
4	B	17	ALA	4.7
4	B	129	ALA	4.6
4	D	237	VAL	4.4
4	A	236	VAL	4.4
4	B	16	LEU	4.3
4	D	226	MET	4.3
4	A	752	LEU	3.9
4	B	94	ALA	3.9
4	C	375	THR	3.8
4	A	753	GLY	3.8
4	A	116	TYR	3.7
4	A	98	LYS	3.7
4	B	243	THR	3.6
4	D	169	GLN	3.6
4	A	168	GLU	3.5
4	D	603	GLY	3.5
4	D	816	THR	3.4
4	A	226	MET	3.4
4	C	16	LEU	3.4
4	D	601	ASN	3.4
4	D	110	LYS	3.4
4	A	608	LYS	3.4
4	B	18	ALA	3.4
4	A	239	GLN	3.4
4	B	372	GLU	3.3
4	A	242	GLU	3.3
4	C	237	VAL	3.3
4	A	234	ALA	3.2
4	A	598	THR	3.2
4	B	374	LEU	3.2
4	B	237	VAL	3.2
4	C	376	ALA	3.2
4	A	596	THR	3.1
4	B	130	ASP	3.1
4	A	231	ARG	3.1
4	D	606	SER	3.1
4	A	67	ASN	3.1
4	C	354	ALA	3.1
4	C	226	MET	3.0
4	A	70	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
4	D	752	LEU	2.9
4	C	374	LEU	2.9
4	C	860	LYS	2.9
4	D	354	ALA	2.9
4	A	243	THR	2.8
4	C	355	ILE	2.8
4	A	600	GLU	2.8
4	B	594	VAL	2.8
4	B	230	HIS	2.8
4	A	237	VAL	2.7
4	A	602	THR	2.7
4	A	607	GLU	2.7
4	C	18	ALA	2.7
4	C	234	ALA	2.7
4	A	158	GLU	2.6
4	A	228	SER	2.6
4	D	746	ARG	2.6
4	A	229	LEU	2.5
4	A	751	PHE	2.5
4	D	602	THR	2.5
4	B	242	GLU	2.5
3	J	1	DG	2.5
4	A	130	ASP	2.4
4	A	593	GLU	2.4
4	D	609	VAL	2.4
4	A	261	LEU	2.4
1	H	2	DG	2.4
4	D	530	CYS	2.4
4	C	17	ALA	2.4
4	A	754	GLN	2.4
4	D	65	ALA	2.3
4	A	238	GLY	2.3
4	C	603	GLY	2.3
4	D	234	ALA	2.3
4	D	229	LEU	2.3
4	B	203	SER	2.3
4	C	15	GLU	2.2
3	G	2	DT	2.2
4	A	9	ASN	2.2
4	D	594	VAL	2.2
4	C	161	HIS	2.2
4	C	565	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
4	D	883	ALA	2.2
4	B	226	MET	2.2
4	A	594	VAL	2.2
4	C	602	THR	2.2
4	D	86	ASN	2.2
4	A	68	ALA	2.1
4	D	244	ILE	2.1
4	D	89	PHE	2.1
4	D	90	GLU	2.1
4	D	216	CYS	2.1
4	D	96	ARG	2.1
4	C	402	LEU	2.0
4	A	230	HIS	2.0
4	A	97	GLY	2.0
4	D	236	VAL	2.0
4	D	751	PHE	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
6	APC	B	2001	31/31	0.94	0.22	1.24	28,47,63,68	0
6	APC	A	2000	31/31	0.95	0.20	1.19	34,58,80,82	0
6	APC	C	2002	31/31	0.93	0.24	0.47	65,70,77,78	0
6	APC	D	2003	31/31	0.94	0.17	-0.82	48,57,61,63	0
5	MG	D	3004	1/1	0.70	0.31	-	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
5	MG	B	3002	1/1	0.95	0.55	-	65,65,65,65	0
5	MG	C	3007	1/1	0.99	0.18	-	46,46,46,46	0
5	MG	F	3005	1/1	0.96	0.16	-	18,18,18,18	0
5	MG	C	3003	1/1	0.99	0.27	-	41,41,41,41	0
5	MG	D	3008	1/1	0.97	0.18	-	16,16,16,16	0
5	MG	B	3006	1/1	0.98	0.17	-	34,34,34,34	0
5	MG	A	3001	1/1	0.94	0.13	-	22,22,22,22	0

6.5 Other polymers

There are no such residues in this entry.