



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:16 PM UTC

PDB ID : 8KAM / pdb_00008kam
Title : Crystal structure of SpyCas9 in complex with sgRNA and 16nt target DNA
Authors : Chen, Y.; Chen, J.; Liu, L.
Deposited on : 2023-08-03
Resolution : 3.91 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

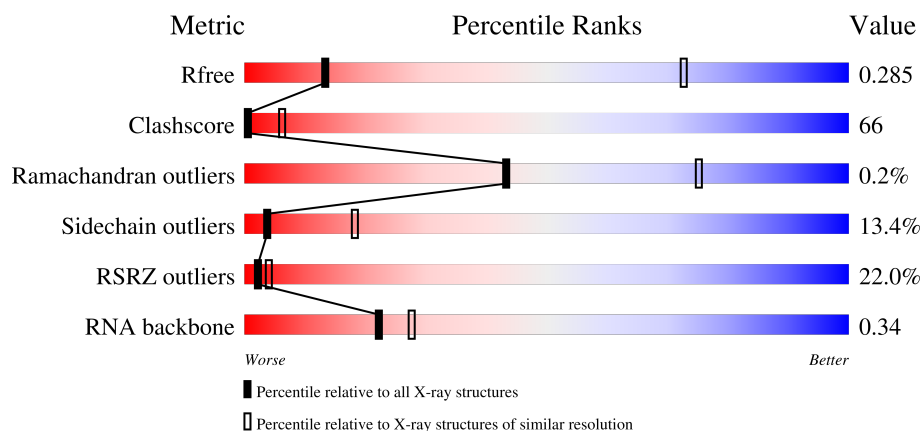
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.91 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1033 (4.10-3.74)
Clashscore	190562	1070 (4.10-3.74)
Ramachandran outliers	187476	1017 (4.10-3.74)
Sidechain outliers	187428	1010 (4.10-3.74)
RSRZ outliers	180081	1033 (4.10-3.74)
RNA backbone	3983	1014 (4.70-3.10)

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

Mol	Chain	Length	Quality of chain
1	A	98	43% 33% 43% 20% .
2	B	1368	20% 39% 45% 11% . .
3	C	24	21% 38% 63%
4	D	11	27% 64% 36%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 13534 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called RNA (98-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	94	Total	C	N	O	P	0	0	0
			2009	899	362	654	94			

- Molecule 2 is a protein called CRISPR-associated endonuclease Cas9/Csn1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1326	Total	C	N	O	S	0	0	0
			10816	6890	1877	2027	22			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	10	ALA	ASP	engineered mutation	UNP Q99ZW2
B	840	ALA	HIS	engineered mutation	UNP Q99ZW2

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	24	Total	C	N	O	P	0	0	0
			483	233	88	139	23			

- Molecule 4 is a DNA chain called DNA (5'-D(*TP*TP*TP*AP*GP*GP*TP*AP*TP*TP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	11	Total	C	N	O	P	0	0	0
			225	110	37	68	10			

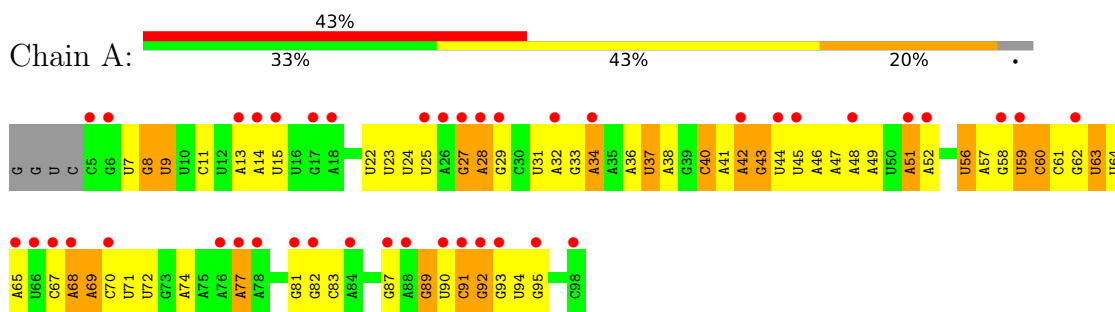
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	O	0	0
			1	1		

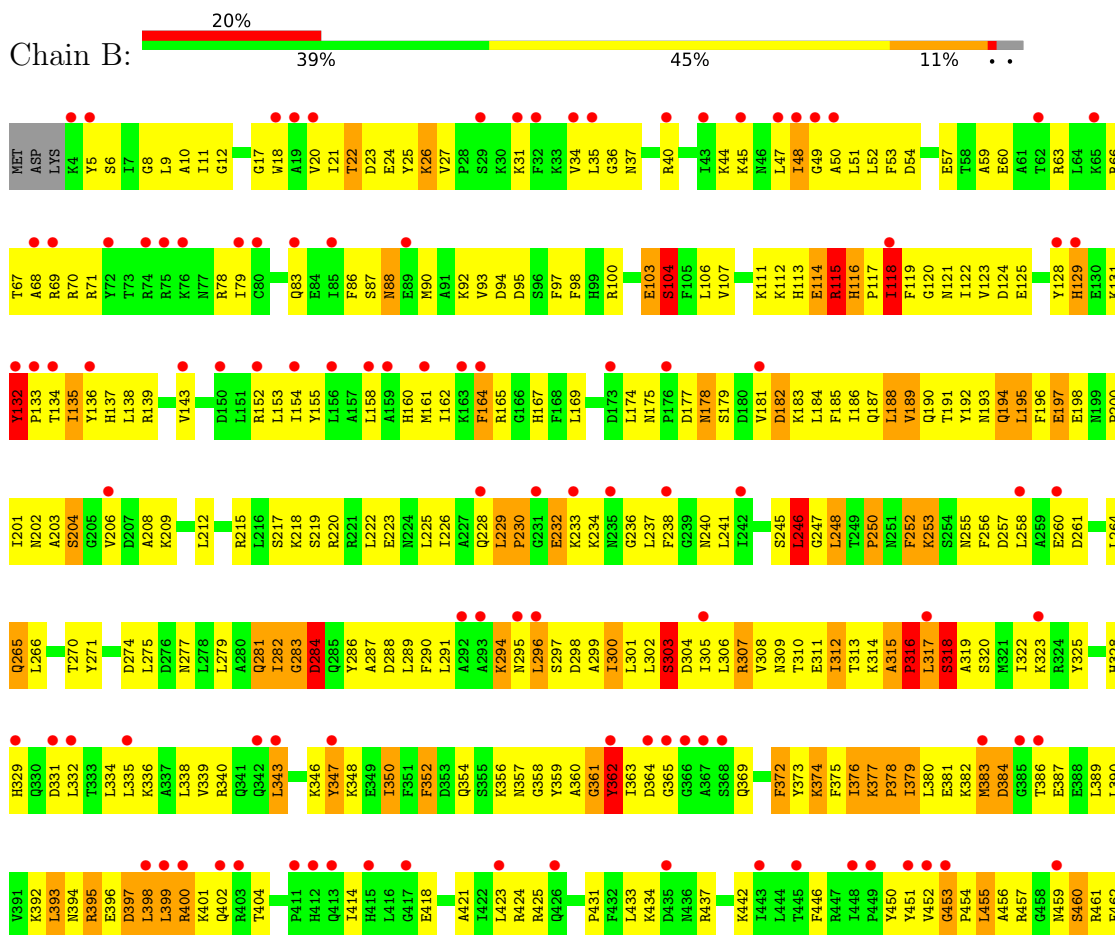
3 Residue-property plots

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

• Molecule 1: RNA (98-MER)



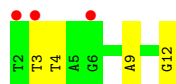
• Molecule 2: CRISPR-associated endonuclease Cas9/Csn1







● Molecule 4: DNA (5'-D(*TP*TP*TP*AP*GP*GP*TP*AP*TP*TP*G)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	199.03Å 70.39Å 186.96Å 90.00° 109.62° 90.00°	Depositor
Resolution (Å)	38.78 – 3.91 38.78 – 3.91	Depositor EDS
% Data completeness (in resolution range)	36.0 (38.78-3.91) 47.6 (38.78-3.91)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.86 (at 3.88Å)	Xtriage
Refinement program	PHENIX 1.17.1 _3660	Depositor
R, R_{free}	0.260 , 0.290 0.260 , 0.285	Depositor DCC
R_{free} test set	1138 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	-2.7	Xtriage
Anisotropy	8.165	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.16 , 0.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.72	EDS
Total number of atoms	13534	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.79% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.15	0/2249	0.35	0/3503
2	B	0.46	14/11008 (0.1%)	0.98	100/14794 (0.7%)
3	C	0.25	0/541	0.48	0/831
4	D	0.23	0/251	0.44	0/387
All	All	0.42	14/14049 (0.1%)	0.87	100/19515 (0.5%)

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

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

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1228	LEU	C-N	5.92	1.40	1.33
2	B	870	VAL	C-N	5.85	1.41	1.33
2	B	453	GLY	C-N	5.75	1.41	1.33
2	B	1136	SER	C-N	5.70	1.41	1.33
2	B	377	LYS	C-N	5.68	1.40	1.34
2	B	1137	PRO	N-CD	5.39	1.55	1.47
2	B	842	VAL	C-N	5.38	1.40	1.33
2	B	378	PRO	N-CD	5.33	1.55	1.47
2	B	132	TYR	C-N	5.32	1.40	1.34
2	B	230	PRO	N-CD	5.22	1.55	1.47
2	B	133	PRO	N-CD	5.14	1.54	1.47
2	B	843	PRO	N-CD	5.14	1.54	1.47
2	B	316	PRO	N-CD	5.12	1.54	1.47
2	B	1229	PRO	N-CD	5.05	1.54	1.47

All (100) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	675	SER	CB-CA-C	-24.02	72.11	111.02
2	B	1222	LYS	CB-CA-C	-16.96	82.39	111.05
2	B	1222	LYS	N-CA-C	16.95	137.38	108.23
2	B	164	PHE	N-CA-C	-14.98	83.39	108.26
2	B	675	SER	N-CA-C	14.84	131.70	112.41
2	B	572	ILE	CB-CA-C	-12.86	99.74	111.06
2	B	284	ASP	CB-CA-C	-11.72	88.67	110.36
2	B	464	TRP	N-CA-C	11.09	123.12	111.14
2	B	178	ASN	N-CA-C	-10.24	90.74	108.56
2	B	572	ILE	N-CA-C	9.86	122.82	112.96
2	B	825	ASP	N-CA-C	9.79	127.78	113.40
2	B	164	PHE	CB-CA-C	9.70	125.08	110.14
2	B	104	SER	N-CA-C	-9.70	98.57	113.02
2	B	1191	LYS	N-CA-C	9.37	124.34	108.23
2	B	831	ASN	N-CA-C	9.14	121.01	111.14
2	B	591	LEU	N-CA-C	-9.04	92.83	108.56
2	B	1280	VAL	CB-CA-C	-8.83	102.82	111.30
2	B	455	LEU	N-CA-C	-8.78	93.13	108.23
2	B	246	LEU	N-CA-C	-8.69	97.15	110.10
2	B	879	MET	CB-CA-C	8.52	123.38	109.07
2	B	675	SER	CA-C-N	8.41	138.21	121.06
2	B	675	SER	C-N-CA	8.41	138.21	121.06
2	B	463	ALA	N-CA-C	8.39	121.68	108.67
2	B	1189	GLU	N-CA-C	8.30	122.94	111.74
2	B	118	ILE	N-CA-C	7.87	117.93	110.53
2	B	95	ASP	CB-CA-C	7.63	125.94	110.38
2	B	567	ASP	CB-CA-C	7.45	125.24	110.42
2	B	1041	ASN	CB-CA-C	7.33	121.87	109.55
2	B	1191	LYS	CB-CA-C	-7.26	98.79	111.05
2	B	265	GLN	CB-CA-C	7.22	122.86	109.86
2	B	1177	ASN	N-CA-C	-7.20	93.89	109.81
2	B	315	ALA	CB-CA-C	-7.14	100.14	110.13
2	B	1228	LEU	CA-C-N	-7.06	113.05	120.03
2	B	1228	LEU	C-N-CA	-7.06	113.05	120.03
2	B	1041	ASN	N-CA-C	6.97	122.78	113.72
2	B	905	ARG	CB-CA-C	6.93	125.70	110.18
2	B	1351	SER	CB-CA-C	-6.91	96.71	113.15
2	B	568	TYR	N-CA-C	6.73	121.63	112.68
2	B	453	GLY	CA-C-N	-6.66	113.12	119.85
2	B	453	GLY	C-N-CA	-6.66	113.12	119.85
2	B	870	VAL	CA-C-N	-6.62	112.95	119.76
2	B	870	VAL	C-N-CA	-6.62	112.95	119.76
2	B	1262	HIS	N-CA-C	-6.61	97.06	108.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	842	VAL	CA-C-N	-6.57	113.01	119.78
2	B	842	VAL	C-N-CA	-6.57	113.01	119.78
2	B	283	GLY	N-CA-C	-6.56	104.14	112.54
2	B	1215	ALA	CB-CA-C	6.51	122.47	110.56
2	B	1215	ALA	N-CA-C	-6.48	102.71	112.04
2	B	303	SER	N-CA-C	6.45	117.97	111.07
2	B	352	PHE	N-CA-C	6.37	118.31	111.36
2	B	1088	SER	N-CA-C	6.36	120.50	112.87
2	B	361	GLY	N-CA-C	-6.29	105.19	112.73
2	B	1136	SER	CA-C-N	-6.29	113.47	119.76
2	B	1136	SER	C-N-CA	-6.29	113.47	119.76
2	B	132	TYR	CA-C-N	-6.23	112.49	118.97
2	B	132	TYR	C-N-CA	-6.23	112.49	118.97
2	B	997	LEU	N-CA-C	6.23	121.01	112.04
2	B	878	LYS	CB-CA-C	6.17	121.17	110.68
2	B	115	ARG	N-CA-C	6.16	117.99	111.28
2	B	1272	GLN	N-CA-C	-6.14	104.58	111.28
2	B	1177	ASN	CB-CA-C	5.97	121.92	110.17
2	B	554	LYS	N-CA-C	-5.96	104.78	111.28
2	B	997	LEU	CB-CA-C	-5.92	99.73	110.56
2	B	88	ASN	N-CA-C	5.89	118.58	111.40
2	B	520	VAL	N-CA-C	5.85	116.03	110.53
2	B	463	ALA	CB-CA-C	-5.84	101.02	110.77
2	B	116	HIS	CA-C-N	-5.77	112.63	119.84
2	B	116	HIS	C-N-CA	-5.77	112.63	119.84
2	B	1222	LYS	CA-C-N	5.75	133.18	122.83
2	B	1222	LYS	C-N-CA	5.75	133.18	122.83
2	B	250	PRO	CA-N-CD	-5.70	104.02	112.00
2	B	318	SER	N-CA-C	-5.68	105.08	111.28
2	B	103	GLU	CB-CA-C	-5.66	103.53	111.85
2	B	661	ARG	N-CA-C	5.61	117.47	111.36
2	B	584	GLU	CB-CA-C	-5.59	99.23	111.71
2	B	593	THR	N-CA-C	-5.55	105.23	111.28
2	B	315	ALA	N-CA-C	5.52	120.87	109.11
2	B	1136	SER	N-CA-C	5.51	121.98	109.81
2	B	552	LEU	N-CA-C	5.48	117.06	111.14
2	B	343	LEU	N-CA-C	5.48	121.93	109.81
2	B	887	LEU	N-CA-C	-5.45	105.34	111.28
2	B	664	ARG	N-CA-C	5.39	117.15	111.28
2	B	377	LYS	CA-C-N	-5.37	113.00	118.85
2	B	377	LYS	C-N-CA	-5.37	113.00	118.85
2	B	1043	MET	N-CA-C	-5.35	100.89	109.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	467	ARG	N-CA-C	5.34	117.50	109.23
2	B	571	LYS	CB-CA-C	5.32	121.00	110.42
2	B	1088	SER	CB-CA-C	5.30	121.82	110.21
2	B	104	SER	N-CA-CB	5.29	120.05	111.27
2	B	831	ASN	CB-CA-C	-5.22	102.66	110.90
2	B	553	PHE	N-CA-C	5.18	117.00	111.36
2	B	103	GLU	N-CA-C	-5.17	99.96	108.49
2	B	1041	ASN	CA-C-N	5.16	127.17	120.56
2	B	1041	ASN	C-N-CA	5.16	127.17	120.56
2	B	362	TYR	N-CA-C	-5.16	105.66	111.28
2	B	229	LEU	CA-C-N	-5.06	113.51	119.84
2	B	229	LEU	C-N-CA	-5.06	113.51	119.84
2	B	265	GLN	N-CA-C	-5.05	100.36	108.55
2	B	175	ASN	CA-C-N	-5.01	112.27	120.88
2	B	175	ASN	C-N-CA	-5.01	112.27	120.88

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	1222	LYS	Peptide
2	B	675	SER	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2009	0	1009	89	0
2	B	10816	0	10957	1659	3
3	C	483	0	272	48	0
4	D	225	0	129	6	0
5	B	1	0	0	0	0
All	All	13534	0	12367	1698	3

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 66.

All (1698) 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)
2:B:1204:PHE:CE1	2:B:1347:LEU:HD12	1.32	1.59
2:B:557:ARG:HG2	2:B:595:HIS:CD2	1.33	1.57
2:B:520:VAL:HG21	2:B:591:LEU:CD2	1.32	1.57
2:B:446:PHE:CZ	2:B:478:PHE:CD1	1.92	1.56
2:B:178:ASN:CB	2:B:299:ALA:HA	1.26	1.56
2:B:520:VAL:CG2	2:B:591:LEU:HD23	1.35	1.56
2:B:451:TYR:HA	2:B:491:PHE:CD1	1.41	1.53
2:B:446:PHE:CE1	2:B:478:PHE:HD1	1.26	1.50
2:B:557:ARG:HA	2:B:595:HIS:CD2	1.43	1.50
2:B:178:ASN:CB	2:B:299:ALA:CA	1.87	1.50
2:B:1204:PHE:HD2	2:B:1342:VAL:CG1	1.22	1.49
2:B:340:ARG:NH2	2:B:347:TYR:CE2	1.79	1.48
2:B:1206:LEU:HB3	2:B:1345:ALA:CB	1.40	1.47
2:B:245:SER:CB	2:B:296:LEU:HD23	1.43	1.45
2:B:1203:LEU:HD11	2:B:1211:LYS:CD	1.48	1.43
2:B:340:ARG:CZ	2:B:347:TYR:CE2	2.02	1.43
2:B:340:ARG:CZ	2:B:347:TYR:HE2	1.31	1.43
2:B:1204:PHE:CD2	2:B:1342:VAL:CG1	1.99	1.43
2:B:1204:PHE:CD2	2:B:1342:VAL:HG11	1.52	1.41
2:B:1204:PHE:HE1	2:B:1347:LEU:CD1	1.32	1.41
2:B:195:LEU:CD1	2:B:289:LEU:HD12	1.53	1.39
2:B:195:LEU:HD13	2:B:289:LEU:CD1	1.52	1.39
2:B:668:ASN:HD21	2:B:680:LEU:CD2	1.34	1.39
2:B:456:ALA:HB2	2:B:463:ALA:CB	1.51	1.39
2:B:553:PHE:CE2	2:B:559:VAL:HG21	1.57	1.39
2:B:545:LYS:HZ1	2:B:690:ASN:CG	1.30	1.38
2:B:556:ASN:C	2:B:595:HIS:NE2	1.81	1.37
2:B:978:ILE:HD11	2:B:1236:LEU:CD1	1.51	1.37
2:B:318:SER:OG	2:B:418:GLU:CD	1.66	1.36
2:B:1348:ILE:HD12	2:B:1359:ARG:NH1	1.37	1.35
2:B:446:PHE:HZ	2:B:478:PHE:CE1	1.44	1.35
2:B:1210:ARG:HG2	2:B:1280:VAL:CG1	1.54	1.35
2:B:379:ILE:O	2:B:383:MET:CG	1.73	1.34
2:B:557:ARG:CA	2:B:595:HIS:CD2	2.07	1.34
2:B:282:ILE:CG2	2:B:286:TYR:CE1	2.12	1.33
2:B:178:ASN:CB	2:B:299:ALA:CB	2.05	1.33
2:B:362:TYR:CD2	2:B:372:PHE:CD2	2.16	1.32
2:B:557:ARG:CG	2:B:595:HIS:HD2	1.42	1.32
2:B:601:ILE:CD1	2:B:607:LEU:HD21	1.59	1.32
2:B:201:ILE:HD13	2:B:232:GLU:OE1	1.20	1.32
2:B:518:PHE:CE2	2:B:683:LEU:HD12	1.64	1.31

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:G:H4'	2:B:457:ARG:CD	1.59	1.31
2:B:557:ARG:CG	2:B:595:HIS:CD2	2.14	1.31
2:B:1139:VAL:HG12	2:B:1167:THR:CA	1.59	1.31
2:B:557:ARG:N	2:B:595:HIS:NE2	1.78	1.30
2:B:1224:ASN:ND2	2:B:1280:VAL:HG21	1.46	1.30
2:B:1139:VAL:HB	2:B:1166:ILE:O	1.14	1.29
2:B:553:PHE:CD2	2:B:559:VAL:HG21	1.67	1.29
2:B:1210:ARG:HD2	2:B:1280:VAL:O	1.25	1.29
2:B:245:SER:CB	2:B:296:LEU:CD2	2.13	1.27
2:B:18:TRP:CD1	2:B:49:GLY:C	2.08	1.27
2:B:839:ASP:OD1	2:B:864:ARG:NH1	1.64	1.27
2:B:1210:ARG:HD2	2:B:1280:VAL:C	1.59	1.27
2:B:518:PHE:HE2	2:B:683:LEU:CD1	1.46	1.27
1:A:58:G:O2'	2:B:457:ARG:CB	1.82	1.26
2:B:520:VAL:CG2	2:B:591:LEU:CD2	1.98	1.26
2:B:1245:LEU:HD22	2:B:1252:ASN:OD1	1.26	1.26
2:B:446:PHE:HZ	2:B:478:PHE:CD1	1.35	1.26
2:B:511:HIS:O	2:B:593:THR:HG21	1.36	1.25
2:B:507:VAL:HG11	2:B:660:GLY:O	1.14	1.25
2:B:1210:ARG:CD	2:B:1280:VAL:HA	1.67	1.25
2:B:201:ILE:CD1	2:B:232:GLU:OE1	1.85	1.24
1:A:58:G:C4'	2:B:457:ARG:HD3	1.68	1.22
2:B:318:SER:OG	2:B:418:GLU:OE1	1.55	1.22
2:B:668:ASN:OD1	2:B:680:LEU:HB2	1.10	1.22
2:B:668:ASN:OD1	2:B:680:LEU:CB	1.87	1.22
2:B:1210:ARG:CG	2:B:1280:VAL:HA	1.68	1.22
2:B:161:MET:O	2:B:164:PHE:O	1.53	1.21
2:B:668:ASN:ND2	2:B:680:LEU:CD2	2.03	1.21
1:A:58:G:O2'	2:B:457:ARG:HB2	1.03	1.19
2:B:107:VAL:HG13	2:B:1131:TYR:CE1	1.76	1.19
2:B:1312:LEU:HD21	2:B:1326:TYR:HD1	1.02	1.19
2:B:116:HIS:NE2	2:B:122:ILE:HB	1.56	1.19
2:B:282:ILE:HG21	2:B:286:TYR:CD1	1.77	1.19
2:B:1297:HIS:CE1	2:B:1327:PHE:HE2	1.59	1.19
2:B:1210:ARG:CG	2:B:1280:VAL:HG13	1.72	1.19
2:B:116:HIS:HD2	2:B:122:ILE:HA	1.06	1.18
2:B:978:ILE:CD1	2:B:1236:LEU:CD1	2.20	1.18
2:B:107:VAL:HG22	2:B:1131:TYR:OH	1.42	1.18
2:B:518:PHE:CZ	2:B:679:ILE:CG2	2.27	1.18
2:B:1212:ARG:NH1	2:B:1336:TYR:CE2	2.13	1.17
2:B:340:ARG:NH2	2:B:347:TYR:HE2	1.23	1.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:455:LEU:HD23	2:B:473:ILE:CD1	1.74	1.17
2:B:1139:VAL:HG12	2:B:1167:THR:N	1.58	1.17
2:B:107:VAL:N	2:B:1131:TYR:OH	1.76	1.17
2:B:282:ILE:HG21	2:B:286:TYR:CE1	1.73	1.17
2:B:318:SER:OG	2:B:418:GLU:OE2	1.59	1.16
2:B:446:PHE:CE1	2:B:478:PHE:CD1	2.17	1.16
2:B:978:ILE:CD1	2:B:1236:LEU:HD11	1.76	1.16
2:B:1270:ILE:O	2:B:1273:ILE:CG1	1.92	1.16
2:B:1204:PHE:CD2	2:B:1342:VAL:HG12	1.81	1.15
2:B:446:PHE:CZ	2:B:478:PHE:CE1	2.26	1.15
2:B:1270:ILE:HA	2:B:1273:ILE:CD1	1.77	1.15
2:B:282:ILE:CG2	2:B:286:TYR:CD1	2.30	1.14
2:B:1270:ILE:CA	2:B:1273:ILE:HG12	1.78	1.14
2:B:379:ILE:O	2:B:383:MET:HG3	1.37	1.14
2:B:451:TYR:CA	2:B:491:PHE:CD1	2.30	1.14
2:B:507:VAL:CG1	2:B:660:GLY:O	1.95	1.14
2:B:787:GLY:HA3	2:B:891:LEU:HD21	1.18	1.14
2:B:1206:LEU:HB3	2:B:1345:ALA:HB2	1.16	1.14
2:B:557:ARG:HA	2:B:595:HIS:NE2	1.60	1.14
2:B:453:GLY:CA	2:B:464:TRP:HD1	1.60	1.13
2:B:354:GLN:HB2	2:B:361:GLY:HA2	1.14	1.13
2:B:450:TYR:HD2	2:B:491:PHE:CZ	1.66	1.13
2:B:1240:SER:OG	2:B:1307:GLU:HG3	1.45	1.13
2:B:1270:ILE:C	2:B:1273:ILE:HG12	1.73	1.13
2:B:1312:LEU:HD21	2:B:1326:TYR:CD1	1.84	1.12
1:A:58:G:C4'	2:B:457:ARG:CD	2.26	1.12
2:B:446:PHE:CZ	2:B:478:PHE:HD1	1.40	1.11
1:A:58:G:H4'	2:B:457:ARG:HD2	1.12	1.11
2:B:226:ILE:HG22	2:B:229:LEU:HD21	1.25	1.11
2:B:270:THR:O	2:B:274:ASP:HB2	1.51	1.11
2:B:483:ASP:HB3	2:B:486:ALA:HB3	1.32	1.11
2:B:557:ARG:CA	2:B:595:HIS:NE2	2.07	1.11
2:B:456:ALA:CB	2:B:463:ALA:CB	2.29	1.10
2:B:668:ASN:HD21	2:B:680:LEU:HD23	0.99	1.10
2:B:107:VAL:HG13	2:B:1131:TYR:HE1	1.02	1.10
2:B:456:ALA:CB	2:B:463:ALA:HB1	1.82	1.10
2:B:839:ASP:OD2	2:B:864:ARG:HD2	1.51	1.10
2:B:841:ILE:CD1	2:B:900:LEU:HG	1.81	1.10
2:B:18:TRP:NE1	2:B:50:ALA:N	1.87	1.09
2:B:762:GLU:OE1	2:B:990:ASN:CG	1.95	1.09
2:B:1139:VAL:CB	2:B:1166:ILE:O	1.99	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1243:GLU:HB3	2:B:1246:LYS:CE	1.82	1.09
2:B:1270:ILE:O	2:B:1273:ILE:HG13	1.48	1.09
2:B:966:PHE:CE1	2:B:970:PHE:CE2	2.40	1.09
2:B:1226:LEU:CD1	2:B:1276:PHE:HB2	1.82	1.09
2:B:762:GLU:OE1	2:B:990:ASN:OD1	1.68	1.09
2:B:134:THR:HB	2:B:137:HIS:ND1	1.67	1.08
2:B:1203:LEU:HD11	2:B:1211:LYS:HD2	1.16	1.08
2:B:601:ILE:HD12	2:B:607:LEU:CD2	1.82	1.08
2:B:379:ILE:O	2:B:383:MET:HG2	1.48	1.08
2:B:1226:LEU:HD13	2:B:1276:PHE:HB2	1.17	1.08
2:B:6:SER:O	2:B:21:ILE:HG13	1.52	1.08
2:B:1203:LEU:HD21	2:B:1211:LYS:HD3	1.12	1.08
2:B:1210:ARG:CG	2:B:1280:VAL:CA	2.31	1.08
2:B:1297:HIS:CG	2:B:1327:PHE:CZ	2.42	1.08
2:B:116:HIS:CD2	2:B:122:ILE:HB	1.87	1.07
2:B:189:VAL:HG23	2:B:238:PHE:CZ	1.89	1.07
2:B:453:GLY:HA3	2:B:464:TRP:HD1	1.10	1.07
2:B:1210:ARG:HG3	2:B:1280:VAL:HA	1.33	1.07
2:B:1226:LEU:HD13	2:B:1276:PHE:CB	1.84	1.07
2:B:603:ASP:OD1	2:B:606:PHE:HB2	1.55	1.07
2:B:202:ASN:ND2	2:B:204:SER:OG	1.88	1.07
2:B:451:TYR:CA	2:B:491:PHE:HD1	1.65	1.07
2:B:1203:LEU:CD2	2:B:1211:LYS:HD3	1.83	1.07
2:B:362:TYR:CE2	2:B:372:PHE:CD2	2.42	1.07
2:B:479:GLU:OE1	2:B:484:LYS:NZ	1.88	1.06
2:B:1203:LEU:CD1	2:B:1211:LYS:CD	2.32	1.06
2:B:453:GLY:HA3	2:B:464:TRP:CD1	1.89	1.06
2:B:6:SER:CB	2:B:21:ILE:HD11	1.86	1.06
2:B:453:GLY:CA	2:B:464:TRP:CD1	2.38	1.06
2:B:456:ALA:HB2	2:B:463:ALA:HB1	1.12	1.06
2:B:967:ARG:HB3	2:B:972:PHE:O	1.55	1.06
2:B:1139:VAL:HB	2:B:1166:ILE:C	1.80	1.06
2:B:516:GLU:HG3	2:B:593:THR:OG1	1.54	1.06
2:B:1139:VAL:HG12	2:B:1167:THR:HA	1.34	1.06
2:B:189:VAL:HG23	2:B:238:PHE:HZ	1.15	1.05
2:B:489:GLN:NE2	2:B:493:GLU:OE2	1.88	1.05
2:B:839:ASP:OD2	2:B:864:ARG:CD	2.04	1.05
2:B:1270:ILE:HA	2:B:1273:ILE:CG1	1.87	1.05
2:B:1297:HIS:CG	2:B:1327:PHE:HZ	1.74	1.05
2:B:545:LYS:NZ	2:B:690:ASN:CG	2.15	1.05
2:B:853:ASP:O	2:B:896:LYS:HG3	1.55	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:116:HIS:CD2	2:B:122:ILE:CB	2.39	1.05
2:B:320:SER:O	2:B:323:LYS:HB3	1.57	1.05
2:B:360:ALA:O	2:B:364:ASP:N	1.88	1.05
2:B:378:PRO:HG2	2:B:379:ILE:HD12	1.35	1.05
2:B:518:PHE:HZ	2:B:679:ILE:CG2	1.63	1.05
2:B:978:ILE:HD11	2:B:1236:LEU:HD11	1.05	1.05
2:B:1203:LEU:HD11	2:B:1211:LYS:CG	1.85	1.04
2:B:762:GLU:OE1	2:B:990:ASN:ND2	1.89	1.04
2:B:1325:LYS:NZ	2:B:1330:THR:OG1	1.88	1.04
2:B:1203:LEU:CD1	2:B:1211:LYS:HD2	1.87	1.04
2:B:22:THR:N	2:B:26:LYS:O	1.90	1.03
2:B:518:PHE:CE2	2:B:683:LEU:CD1	2.32	1.03
2:B:557:ARG:CB	2:B:595:HIS:HD2	1.71	1.03
2:B:1297:HIS:CE1	2:B:1327:PHE:CE2	2.45	1.03
2:B:50:ALA:HB3	2:B:1093:ASN:O	1.58	1.03
2:B:966:PHE:CE1	2:B:970:PHE:HE2	1.74	1.03
2:B:1206:LEU:CB	2:B:1345:ALA:CB	2.36	1.03
2:B:121:ASN:ND2	2:B:124:ASP:OD2	1.91	1.03
2:B:839:ASP:CG	2:B:864:ARG:HH11	1.65	1.03
2:B:870:VAL:HG12	2:B:871:PRO:HD2	1.08	1.03
2:B:48:ILE:HD11	2:B:984:ALA:HB1	1.39	1.03
2:B:328:HIS:CD2	2:B:399:LEU:HB3	1.93	1.03
2:B:557:ARG:HG2	2:B:595:HIS:CG	1.91	1.03
2:B:178:ASN:CB	2:B:299:ALA:HB2	1.85	1.03
2:B:869:ASN:OD1	2:B:870:VAL:N	1.92	1.03
2:B:1210:ARG:HD2	2:B:1280:VAL:CA	1.89	1.03
2:B:107:VAL:CG1	2:B:1131:TYR:HE1	1.71	1.02
2:B:376:ILE:CA	2:B:379:ILE:HD13	1.89	1.02
2:B:553:PHE:CE2	2:B:559:VAL:CG2	2.41	1.02
2:B:1063:ILE:HG23	2:B:1074:TRP:O	1.57	1.02
2:B:1236:LEU:HB3	2:B:1310:ILE:HD11	1.41	1.02
2:B:456:ALA:HB2	2:B:463:ALA:HB2	1.39	1.02
2:B:1210:ARG:CD	2:B:1280:VAL:O	2.07	1.02
2:B:508:LEU:HD11	2:B:664:ARG:HB2	1.04	1.01
2:B:945:GLU:OE1	2:B:945:GLU:N	1.93	1.01
2:B:1210:ARG:CD	2:B:1280:VAL:CA	2.36	1.01
2:B:1269:ILE:O	2:B:1273:ILE:HG23	1.60	1.01
2:B:116:HIS:HD2	2:B:122:ILE:CA	1.73	1.01
2:B:508:LEU:CD1	2:B:664:ARG:HB2	1.89	1.01
2:B:567:ASP:O	2:B:571:LYS:CG	2.09	1.01
2:B:297:SER:HA	2:B:300:ILE:HG22	1.39	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:478:PHE:HE2	2:B:482:VAL:HG21	1.26	1.01
2:B:1206:LEU:HB3	2:B:1345:ALA:HB1	1.37	1.01
2:B:497:ASN:OD1	3:C:19:DA:OP1	1.79	1.01
2:B:560:THR:N	2:B:563:GLN:OE1	1.94	1.01
2:B:508:LEU:HD11	2:B:664:ARG:CB	1.91	1.00
1:A:58:G:O4'	2:B:457:ARG:HD3	1.60	1.00
2:B:131:LYS:HD3	2:B:132:TYR:HE1	1.23	1.00
2:B:495:MET:HB3	3:C:17:DA:C1'	1.91	1.00
2:B:279:LEU:CD2	2:B:284:ASP:HA	1.91	1.00
1:A:51:A:O2'	2:B:1134:PHE:HE1	1.44	1.00
2:B:1240:SER:OG	2:B:1307:GLU:CG	2.09	1.00
2:B:495:MET:HB2	3:C:17:DA:C4'	1.90	1.00
2:B:719:SER:N	2:B:722:GLU:OE1	1.94	1.00
2:B:520:VAL:HG21	2:B:591:LEU:HD21	1.37	0.99
2:B:668:ASN:ND2	2:B:680:LEU:HD23	1.68	0.99
2:B:245:SER:HB2	2:B:296:LEU:CD2	1.89	0.99
2:B:189:VAL:CG2	2:B:238:PHE:CZ	2.45	0.99
2:B:853:ASP:HA	2:B:896:LYS:HD2	1.41	0.99
1:A:59:U:OP1	2:B:467:ARG:NH2	1.96	0.98
2:B:354:GLN:HB2	2:B:361:GLY:CA	1.94	0.98
2:B:567:ASP:O	2:B:571:LYS:HG3	1.63	0.98
2:B:1297:HIS:ND1	2:B:1327:PHE:CE2	2.31	0.98
2:B:18:TRP:CD1	2:B:49:GLY:O	2.16	0.98
2:B:226:ILE:HA	2:B:229:LEU:CD2	1.94	0.98
2:B:362:TYR:CE2	2:B:372:PHE:HD2	1.77	0.98
2:B:978:ILE:CD1	2:B:1236:LEU:HD12	1.89	0.98
2:B:1270:ILE:HA	2:B:1273:ILE:HG12	1.40	0.98
2:B:455:LEU:CD2	2:B:473:ILE:HD12	1.92	0.98
2:B:116:HIS:CD2	2:B:122:ILE:HA	1.98	0.98
2:B:376:ILE:HA	2:B:379:ILE:HD13	0.99	0.97
2:B:1270:ILE:HD13	2:B:1273:ILE:CD1	1.94	0.97
2:B:870:VAL:HG12	2:B:871:PRO:CD	1.94	0.97
2:B:103:GLU:HG3	2:B:103:GLU:O	1.63	0.97
2:B:354:GLN:CB	2:B:361:GLY:HA2	1.94	0.97
2:B:859:ARG:NE	2:B:860:SER:OG	1.96	0.97
2:B:1312:LEU:HD11	2:B:1326:TYR:CE1	2.00	0.97
2:B:340:ARG:NE	2:B:347:TYR:HE2	1.62	0.96
2:B:18:TRP:O	2:B:48:ILE:CD1	2.13	0.96
2:B:495:MET:CB	3:C:17:DA:C1'	2.44	0.96
2:B:1139:VAL:CG1	2:B:1167:THR:N	2.29	0.96
1:A:60:C:O3'	2:B:460:SER:OG	1.84	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:887:LEU:HB2	2:B:892:ILE:HD11	1.48	0.96
2:B:450:TYR:CD2	2:B:491:PHE:CZ	2.53	0.96
2:B:1203:LEU:HD12	2:B:1212:ARG:O	1.66	0.96
2:B:530:VAL:HG22	2:B:537:PRO:HB3	1.45	0.96
2:B:591:LEU:HD12	2:B:594:TYR:HD1	1.27	0.96
2:B:48:ILE:HD12	2:B:49:GLY:N	1.81	0.95
2:B:328:HIS:CE1	2:B:399:LEU:HB2	2.01	0.95
2:B:1206:LEU:CB	2:B:1345:ALA:HB2	1.96	0.95
2:B:226:ILE:HA	2:B:229:LEU:HG	1.48	0.95
2:B:229:LEU:CD1	2:B:232:GLU:HB2	1.96	0.95
2:B:455:LEU:HD23	2:B:473:ILE:HD12	0.96	0.95
2:B:495:MET:CG	3:C:17:DA:O4'	2.13	0.95
2:B:229:LEU:HD13	2:B:232:GLU:HB2	1.49	0.95
2:B:103:GLU:O	2:B:103:GLU:CG	2.13	0.95
2:B:245:SER:HB3	2:B:296:LEU:HD23	0.97	0.95
2:B:520:VAL:HG22	2:B:591:LEU:HD23	1.44	0.95
2:B:597:LEU:CD1	2:B:607:LEU:HD13	1.97	0.95
2:B:668:ASN:ND2	2:B:680:LEU:HD22	1.78	0.95
2:B:853:ASP:HA	2:B:896:LYS:CD	1.97	0.95
2:B:495:MET:HB3	3:C:17:DA:H1'	1.49	0.95
2:B:450:TYR:HD2	2:B:491:PHE:CE1	1.84	0.94
2:B:518:PHE:HE2	2:B:683:LEU:HD12	0.81	0.94
2:B:495:MET:HB2	3:C:17:DA:H4'	1.45	0.94
2:B:1114:ARG:NH1	4:D:9:DA:OP1	2.00	0.94
2:B:1157:LEU:H	2:B:1157:LEU:HD12	1.29	0.94
2:B:597:LEU:HD12	2:B:607:LEU:HD13	1.47	0.94
2:B:1348:ILE:CD1	2:B:1359:ARG:NH1	2.29	0.94
2:B:376:ILE:HA	2:B:379:ILE:CD1	1.95	0.94
2:B:18:TRP:CG	2:B:49:GLY:O	2.21	0.94
2:B:483:ASP:O	2:B:487:SER:OG	1.85	0.94
2:B:686:ASP:OD2	2:B:691:ARG:NE	2.01	0.93
2:B:206:VAL:HG12	2:B:228:GLN:HG3	1.46	0.93
2:B:591:LEU:HD12	2:B:594:TYR:CD1	2.04	0.93
2:B:1139:VAL:CG1	2:B:1166:ILE:C	2.41	0.93
2:B:1359:ARG:HG2	2:B:1359:ARG:HH11	1.33	0.93
2:B:350:ILE:HD11	2:B:375:PHE:HZ	1.34	0.93
2:B:116:HIS:NE2	2:B:122:ILE:CB	2.32	0.93
2:B:495:MET:HG3	3:C:17:DA:O4'	1.66	0.93
2:B:551:LEU:O	2:B:555:THR:OG1	1.85	0.93
2:B:885:GLN:HA	2:B:888:ASN:HB2	1.50	0.93
2:B:559:VAL:HA	2:B:563:GLN:OE1	1.67	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:949:LEU:HD12	2:B:950:ILE:H	1.31	0.93
2:B:1339:THR:O	2:B:1343:LEU:HD21	1.68	0.93
2:B:202:ASN:OD1	2:B:204:SER:N	2.01	0.93
2:B:1270:ILE:O	2:B:1273:ILE:HG12	1.64	0.93
2:B:1148:LYS:HD2	2:B:1157:LEU:HD22	1.48	0.93
2:B:1210:ARG:HG3	2:B:1280:VAL:CA	1.95	0.92
2:B:186:ILE:O	2:B:190:GLN:HB3	1.69	0.92
2:B:116:HIS:CD2	2:B:122:ILE:CA	2.52	0.92
2:B:226:ILE:HA	2:B:229:LEU:CG	2.00	0.91
2:B:556:ASN:O	2:B:595:HIS:NE2	2.00	0.91
2:B:557:ARG:CB	2:B:595:HIS:CD2	2.50	0.91
2:B:1236:LEU:HD22	2:B:1310:ILE:CG1	2.00	0.91
2:B:131:LYS:HG2	2:B:132:TYR:CD1	2.06	0.91
2:B:1243:GLU:HB3	2:B:1246:LYS:NZ	1.86	0.91
2:B:1130:LYS:O	2:B:1131:TYR:HD1	1.53	0.90
2:B:1236:LEU:HD22	2:B:1310:ILE:HG13	1.52	0.90
2:B:53:PHE:CD1	2:B:54:ASP:O	2.23	0.90
2:B:116:HIS:HB2	2:B:120:GLY:O	1.71	0.90
2:B:226:ILE:CG2	2:B:229:LEU:HD21	2.02	0.90
2:B:307:ARG:HH22	2:B:323:LYS:HE2	1.35	0.90
2:B:197:GLU:N	2:B:197:GLU:OE1	2.02	0.90
2:B:340:ARG:NE	2:B:347:TYR:CE2	2.35	0.90
2:B:297:SER:HA	2:B:300:ILE:CG2	2.01	0.89
2:B:340:ARG:NH2	2:B:347:TYR:CZ	2.40	0.89
2:B:978:ILE:CG1	2:B:1236:LEU:CD1	2.51	0.89
2:B:446:PHE:HE1	2:B:478:PHE:HD1	1.10	0.89
1:A:43:G:O2'	2:B:363:ILE:HD12	1.72	0.89
2:B:195:LEU:HD13	2:B:289:LEU:HD12	0.89	0.89
2:B:375:PHE:CD2	2:B:376:ILE:HG23	2.08	0.89
2:B:193:ASN:ND2	2:B:201:ILE:O	2.06	0.88
2:B:202:ASN:HB3	2:B:230:PRO:HG3	1.52	0.88
2:B:1139:VAL:CB	2:B:1166:ILE:C	2.45	0.88
2:B:1297:HIS:CB	2:B:1327:PHE:HZ	1.84	0.88
2:B:556:ASN:C	2:B:595:HIS:CE1	2.50	0.88
2:B:523:GLU:OE2	2:B:588:ASN:ND2	2.06	0.88
2:B:1210:ARG:CG	2:B:1280:VAL:CG1	2.42	0.88
1:A:58:G:C2'	2:B:457:ARG:HB2	2.02	0.88
2:B:316:PRO:O	2:B:320:SER:N	2.07	0.88
2:B:1228:LEU:CB	2:B:1233:VAL:HG22	2.04	0.88
2:B:450:TYR:CD2	2:B:491:PHE:CE1	2.62	0.88
2:B:362:TYR:CD2	2:B:372:PHE:CE2	2.62	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:841:ILE:CD1	2:B:900:LEU:CD2	2.51	0.88
1:A:14:A:O2'	2:B:464:TRP:CZ2	2.28	0.87
2:B:338:LEU:CD1	2:B:386:THR:HB	2.04	0.87
2:B:1245:LEU:CD2	2:B:1252:ASN:OD1	2.18	0.87
2:B:553:PHE:HE2	2:B:559:VAL:HG11	1.39	0.87
2:B:569:PHE:O	2:B:574:CYS:N	2.07	0.87
2:B:1105:PHE:O	2:B:1137:PRO:HB3	1.74	0.87
2:B:516:GLU:O	2:B:520:VAL:HG23	1.74	0.87
2:B:491:PHE:HE2	3:C:16:DT:H1'	1.39	0.87
2:B:601:ILE:HD12	2:B:607:LEU:HD21	0.88	0.87
2:B:1270:ILE:HD13	2:B:1273:ILE:HD13	1.57	0.87
2:B:520:VAL:CG2	2:B:591:LEU:HD21	1.93	0.87
2:B:603:ASP:OD1	2:B:606:PHE:CB	2.23	0.87
2:B:1148:LYS:HE2	2:B:1189:GLU:CB	2.04	0.87
2:B:841:ILE:CD1	2:B:900:LEU:CG	2.52	0.86
2:B:494:ARG:HG2	2:B:494:ARG:HH11	1.39	0.86
2:B:518:PHE:CZ	2:B:679:ILE:HG21	2.10	0.86
2:B:1348:ILE:HD12	2:B:1359:ARG:HH11	1.10	0.86
2:B:6:SER:OG	2:B:21:ILE:HD11	1.75	0.86
2:B:859:ARG:HE	2:B:860:SER:HG	1.18	0.86
2:B:1237:TYR:HA	2:B:1242:TYR:HE1	1.40	0.86
2:B:107:VAL:HG22	2:B:1131:TYR:CZ	2.11	0.86
2:B:452:VAL:O	2:B:465:MET:HB3	1.75	0.86
2:B:1269:ILE:HG22	2:B:1273:ILE:CG2	2.06	0.86
2:B:1139:VAL:HG11	2:B:1165:GLY:O	1.75	0.86
2:B:668:ASN:CG	2:B:680:LEU:CB	2.47	0.86
2:B:297:SER:CA	2:B:300:ILE:HG22	2.04	0.86
2:B:841:ILE:HD13	2:B:900:LEU:HG	1.55	0.86
2:B:121:ASN:OD1	2:B:124:ASP:N	2.07	0.86
2:B:340:ARG:CZ	2:B:347:TYR:CD2	2.58	0.86
2:B:1224:ASN:ND2	2:B:1280:VAL:CG2	2.38	0.86
2:B:282:ILE:HG22	2:B:286:TYR:CD1	2.08	0.85
2:B:978:ILE:HD11	2:B:1236:LEU:HD12	1.51	0.85
2:B:1204:PHE:HD2	2:B:1342:VAL:HG11	0.69	0.85
2:B:279:LEU:O	2:B:282:ILE:O	1.92	0.85
2:B:453:GLY:HA2	2:B:464:TRP:CD1	2.10	0.85
2:B:761:ILE:HD13	2:B:931:VAL:HG12	1.57	0.85
2:B:1203:LEU:HD11	2:B:1211:LYS:HG2	1.58	0.85
2:B:338:LEU:HD13	2:B:386:THR:HB	1.57	0.85
2:B:511:HIS:O	2:B:593:THR:CG2	2.24	0.85
2:B:1148:LYS:HE2	2:B:1189:GLU:HG3	1.58	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:135:ILE:HD11	2:B:138:LEU:HD23	1.59	0.85
2:B:206:VAL:HG12	2:B:228:GLN:CG	2.06	0.85
2:B:520:VAL:HG21	2:B:591:LEU:HD23	0.88	0.85
2:B:1312:LEU:HD11	2:B:1326:TYR:HE1	1.41	0.85
1:A:61:C:P	2:B:460:SER:OG	2.34	0.84
2:B:107:VAL:CG2	2:B:1131:TYR:OH	2.25	0.84
2:B:518:PHE:HZ	2:B:679:ILE:HG23	1.41	0.84
2:B:495:MET:HB3	3:C:17:DA:C2'	2.06	0.84
2:B:516:GLU:CG	2:B:593:THR:OG1	2.26	0.84
2:B:885:GLN:O	2:B:889:ALA:N	2.10	0.84
2:B:186:ILE:O	2:B:190:GLN:CB	2.25	0.84
2:B:1203:LEU:HD21	2:B:1211:LYS:CD	2.03	0.84
2:B:518:PHE:CZ	2:B:679:ILE:HG22	2.11	0.84
2:B:720:LEU:CD1	2:B:724:ILE:HG13	2.07	0.84
2:B:564:LEU:HD23	2:B:569:PHE:HE2	1.41	0.83
2:B:841:ILE:HD11	2:B:900:LEU:CD2	2.08	0.83
2:B:6:SER:N	2:B:21:ILE:HD11	1.93	0.83
2:B:762:GLU:CD	2:B:990:ASN:HD21	1.85	0.83
2:B:495:MET:CB	3:C:17:DA:H2''	2.08	0.83
2:B:787:GLY:HA3	2:B:891:LEU:CD2	2.07	0.83
2:B:6:SER:O	2:B:21:ILE:CG1	2.25	0.83
2:B:859:ARG:HH11	2:B:859:ARG:HG3	1.41	0.83
2:B:282:ILE:HG22	2:B:286:TYR:CE1	2.14	0.83
2:B:245:SER:HB3	2:B:296:LEU:CD2	1.93	0.83
2:B:495:MET:CB	3:C:17:DA:C2'	2.56	0.83
2:B:1120:ILE:HD11	2:B:1137:PRO:CD	2.09	0.82
2:B:1148:LYS:HE2	2:B:1189:GLU:CG	2.09	0.82
1:A:43:G:O2'	2:B:363:ILE:CD1	2.27	0.82
2:B:1204:PHE:CE1	2:B:1347:LEU:CD1	2.22	0.82
2:B:1224:ASN:HD22	2:B:1280:VAL:HG21	1.40	0.82
2:B:1361:ASP:OD1	2:B:1363:SER:OG	1.96	0.82
2:B:720:LEU:HD12	2:B:720:LEU:O	1.78	0.82
2:B:841:ILE:HD11	2:B:900:LEU:HG	1.59	0.82
2:B:859:ARG:HD2	2:B:859:ARG:O	1.79	0.82
2:B:1287:LEU:HD12	2:B:1287:LEU:O	1.78	0.82
2:B:317:LEU:CD2	2:B:414:ILE:HD12	2.10	0.82
2:B:1297:HIS:HB3	2:B:1327:PHE:HZ	1.44	0.82
2:B:521:TYR:CE1	2:B:684:LYS:HG2	2.15	0.82
2:B:839:ASP:OD2	2:B:864:ARG:HD3	1.80	0.81
2:B:386:THR:OG1	2:B:389:LEU:HB2	1.80	0.81
2:B:978:ILE:CG1	2:B:1236:LEU:HD11	2.08	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:53:PHE:CE1	2:B:54:ASP:O	2.33	0.81
2:B:491:PHE:CE2	3:C:16:DT:H1'	2.15	0.81
2:B:597:LEU:HD12	2:B:607:LEU:CD1	2.10	0.81
2:B:1243:GLU:HB3	2:B:1246:LYS:HE2	1.60	0.81
2:B:379:ILE:HD12	2:B:379:ILE:H	1.45	0.81
2:B:545:LYS:HZ1	2:B:690:ASN:ND2	1.79	0.81
2:B:841:ILE:HD11	2:B:900:LEU:CG	2.11	0.81
2:B:1210:ARG:CG	2:B:1280:VAL:CB	2.58	0.80
2:B:1348:ILE:HD12	2:B:1359:ARG:HH12	1.41	0.80
1:A:60:C:H5''	2:B:455:LEU:O	1.81	0.80
2:B:194:GLN:OE1	2:B:194:GLN:N	2.15	0.80
2:B:478:PHE:CE2	2:B:482:VAL:HG21	2.16	0.80
2:B:1139:VAL:CG1	2:B:1167:THR:HA	2.11	0.80
2:B:208:ALA:O	2:B:212:LEU:HB2	1.81	0.80
2:B:362:TYR:CD2	2:B:372:PHE:HD2	1.77	0.80
2:B:545:LYS:NZ	2:B:690:ASN:ND2	2.29	0.80
2:B:131:LYS:HG2	2:B:132:TYR:HD1	1.44	0.80
2:B:294:LYS:NZ	2:B:295:ASN:OD1	2.14	0.80
2:B:545:LYS:HZ1	2:B:690:ASN:CB	1.94	0.80
2:B:839:ASP:OD1	2:B:840:ALA:N	2.15	0.80
2:B:18:TRP:HE1	2:B:50:ALA:N	1.76	0.80
2:B:354:GLN:CB	2:B:361:GLY:CA	2.57	0.80
2:B:362:TYR:CE2	2:B:372:PHE:CE2	2.70	0.79
2:B:465:MET:HE2	2:B:482:VAL:HG22	1.63	0.79
2:B:334:LEU:CD1	2:B:338:LEU:HD11	2.12	0.79
2:B:369:GLN:O	2:B:373:TYR:HD2	1.64	0.79
2:B:554:LYS:CB	2:B:604:LYS:NZ	2.44	0.79
2:B:591:LEU:HB3	2:B:594:TYR:HB3	1.64	0.79
2:B:520:VAL:CG1	2:B:553:PHE:CD1	2.65	0.79
2:B:265:GLN:O	2:B:271:TYR:CD1	2.35	0.79
2:B:379:ILE:HG22	2:B:383:MET:SD	2.22	0.79
2:B:1108:GLU:O	2:B:1134:PHE:HE2	1.64	0.79
2:B:282:ILE:CG2	2:B:286:TYR:HE1	1.92	0.79
2:B:1148:LYS:CD	2:B:1157:LEU:HD22	2.11	0.79
2:B:189:VAL:O	2:B:193:ASN:N	2.16	0.79
2:B:317:LEU:HD23	2:B:414:ILE:HD12	1.62	0.79
2:B:356:LYS:O	2:B:357:ASN:HB2	1.81	0.79
2:B:392:LYS:HB3	2:B:397:ASP:O	1.82	0.79
2:B:1139:VAL:CG1	2:B:1167:THR:CA	2.54	0.79
2:B:317:LEU:O	2:B:320:SER:OG	2.00	0.79
2:B:967:ARG:CB	2:B:972:PHE:O	2.30	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:121:ASN:HD21	2:B:124:ASP:CG	1.91	0.79
2:B:307:ARG:NH2	2:B:323:LYS:HE2	1.97	0.79
2:B:195:LEU:HD12	2:B:289:LEU:HD12	1.63	0.79
2:B:282:ILE:HG23	2:B:286:TYR:CE1	2.18	0.79
2:B:131:LYS:HD3	2:B:132:TYR:CE1	2.15	0.78
2:B:720:LEU:HD12	2:B:724:ILE:HG13	1.63	0.78
2:B:1229:PRO:O	2:B:1233:VAL:HG23	1.81	0.78
1:A:61:C:P	2:B:460:SER:HG	2.06	0.78
2:B:591:LEU:CD1	2:B:594:TYR:HB2	2.13	0.78
2:B:1139:VAL:HG21	2:B:1165:GLY:CA	2.13	0.78
2:B:182:ASP:OD1	2:B:209:LYS:HB2	1.84	0.78
2:B:887:LEU:CB	2:B:892:ILE:HD11	2.14	0.78
2:B:362:TYR:HD2	2:B:372:PHE:CD2	1.98	0.78
2:B:195:LEU:HD13	2:B:289:LEU:HD13	1.59	0.78
2:B:316:PRO:HA	2:B:319:ALA:HB3	1.66	0.78
2:B:493:GLU:O	2:B:496:THR:HG23	1.83	0.78
2:B:686:ASP:CB	2:B:690:ASN:HA	2.13	0.78
2:B:840:ALA:O	2:B:864:ARG:NH1	2.17	0.78
2:B:1245:LEU:HD22	2:B:1252:ASN:CG	2.08	0.77
1:A:51:A:HO2'	2:B:1134:PHE:HE1	0.78	0.77
2:B:226:ILE:HA	2:B:229:LEU:HD21	1.66	0.77
2:B:668:ASN:ND2	2:B:680:LEU:HB3	1.99	0.77
2:B:378:PRO:HG2	2:B:379:ILE:CD1	2.12	0.77
2:B:842:VAL:HG12	2:B:854:ASN:OD1	1.83	0.77
2:B:520:VAL:HG11	2:B:553:PHE:HD1	1.50	0.77
2:B:18:TRP:O	2:B:48:ILE:HD12	1.83	0.77
2:B:375:PHE:HD2	2:B:376:ILE:HG23	1.47	0.77
2:B:553:PHE:CD2	2:B:559:VAL:CG2	2.61	0.77
2:B:1270:ILE:HD13	2:B:1273:ILE:HD11	1.64	0.77
2:B:1297:HIS:CG	2:B:1327:PHE:CE2	2.72	0.77
2:B:1245:LEU:HD13	2:B:1252:ASN:HD21	1.50	0.77
2:B:270:THR:O	2:B:274:ASP:CB	2.31	0.77
2:B:315:ALA:HB1	2:B:418:GLU:OE2	1.84	0.76
2:B:350:ILE:HD11	2:B:375:PHE:CZ	2.20	0.76
2:B:359:TYR:CE1	2:B:363:ILE:HG13	2.20	0.76
2:B:564:LEU:HD23	2:B:569:PHE:CE2	2.20	0.76
2:B:567:ASP:O	2:B:571:LYS:HB2	1.84	0.76
2:B:1210:ARG:HG2	2:B:1280:VAL:HG13	0.79	0.76
2:B:686:ASP:HB2	2:B:690:ASN:HD22	1.48	0.76
2:B:1069:THR:OG1	2:B:1071:GLU:HG3	1.85	0.76
2:B:1325:LYS:NZ	2:B:1330:THR:HG1	1.83	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1327:PHE:HD2	2:B:1328:ASP:H	1.34	0.76
1:A:14:A:O2'	2:B:464:TRP:HZ2	1.68	0.76
2:B:495:MET:HB3	3:C:17:DA:H2''	1.62	0.76
2:B:1130:LYS:O	2:B:1131:TYR:CD1	2.38	0.76
2:B:398:LEU:HG	2:B:399:LEU:HG	1.67	0.76
2:B:520:VAL:HG23	2:B:591:LEU:CD2	2.09	0.76
2:B:567:ASP:O	2:B:571:LYS:CB	2.34	0.76
2:B:668:ASN:CG	2:B:680:LEU:HB3	2.11	0.76
2:B:1325:LYS:CB	2:B:1330:THR:HA	2.16	0.76
2:B:966:PHE:CE1	2:B:970:PHE:CD2	2.74	0.76
2:B:193:ASN:OD1	2:B:201:ILE:N	2.17	0.76
2:B:489:GLN:HE21	2:B:493:GLU:CD	1.93	0.76
2:B:350:ILE:CD1	2:B:375:PHE:HZ	1.98	0.75
2:B:1218:GLY:O	2:B:1337:THR:O	2.03	0.75
2:B:1270:ILE:HA	2:B:1273:ILE:HD11	1.65	0.75
2:B:48:ILE:HD12	2:B:49:GLY:H	1.47	0.75
2:B:841:ILE:HD13	2:B:900:LEU:CG	2.15	0.75
2:B:135:ILE:CD1	2:B:138:LEU:HD23	2.16	0.75
2:B:226:ILE:CA	2:B:229:LEU:HG	2.17	0.75
2:B:842:VAL:HG21	2:B:847:LEU:CD2	2.16	0.75
2:B:966:PHE:CD1	2:B:970:PHE:CE2	2.75	0.75
2:B:457:ARG:HG3	2:B:457:ARG:O	1.87	0.75
2:B:245:SER:HB2	2:B:296:LEU:HD21	1.67	0.75
2:B:724:ILE:HD13	2:B:737:ILE:HG22	1.67	0.75
2:B:873:GLU:O	2:B:877:LYS:HG2	1.87	0.75
2:B:566:GLU:O	2:B:571:LYS:HG2	1.85	0.75
2:B:1284:ASP:OD1	2:B:1285:ALA:N	2.20	0.75
2:B:516:GLU:O	2:B:519:THR:HG22	1.86	0.75
2:B:1210:ARG:HG3	2:B:1280:VAL:HG22	1.67	0.75
2:B:495:MET:CB	3:C:17:DA:C4'	2.64	0.74
2:B:279:LEU:HD21	2:B:284:ASP:HA	1.68	0.74
2:B:354:GLN:HA	2:B:361:GLY:HA3	1.69	0.74
2:B:1308:ASN:OD1	2:B:1327:PHE:HB3	1.88	0.74
2:B:520:VAL:CG1	2:B:553:PHE:HD1	1.98	0.74
2:B:328:HIS:CE1	2:B:399:LEU:CB	2.71	0.74
2:B:1139:VAL:HG21	2:B:1165:GLY:C	2.12	0.74
2:B:1119:LEU:HD13	2:B:1119:LEU:N	2.00	0.74
2:B:131:LYS:CD	2:B:132:TYR:HE1	1.98	0.74
2:B:1210:ARG:HG2	2:B:1280:VAL:CB	2.17	0.74
2:B:1148:LYS:HE2	2:B:1189:GLU:HB2	1.69	0.74
2:B:761:ILE:O	2:B:761:ILE:HG13	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:G:N1	2:B:1272:GLN:OE1	2.21	0.74
2:B:393:LEU:HD23	2:B:394:ASN:N	2.03	0.74
2:B:668:ASN:HD21	2:B:680:LEU:CG	2.01	0.74
2:B:485:GLY:HA2	2:B:488:ALA:HB3	1.70	0.74
2:B:978:ILE:HG13	2:B:1236:LEU:CD1	2.17	0.74
2:B:275:LEU:O	2:B:279:LEU:N	2.14	0.73
2:B:853:ASP:CA	2:B:896:LYS:HD2	2.16	0.73
2:B:1359:ARG:NH1	2:B:1359:ARG:HG2	1.95	0.73
2:B:790:GLU:CD	2:B:889:ALA:HA	2.13	0.73
2:B:178:ASN:HA	2:B:299:ALA:HB2	1.68	0.73
2:B:823:TYR:CE2	2:B:858:THR:HG21	2.23	0.73
2:B:1120:ILE:HD11	2:B:1137:PRO:CG	2.18	0.73
2:B:178:ASN:CA	2:B:299:ALA:HB2	2.17	0.73
2:B:446:PHE:HE1	2:B:478:PHE:CD1	1.88	0.73
2:B:1245:LEU:C	2:B:1245:LEU:HD12	2.13	0.73
2:B:1343:LEU:N	2:B:1343:LEU:HD23	2.03	0.73
2:B:21:ILE:O	2:B:21:ILE:HD12	1.88	0.73
2:B:302:LEU:O	2:B:305:ILE:HG12	1.89	0.73
2:B:312:ILE:HD12	2:B:312:ILE:N	2.03	0.73
2:B:686:ASP:HB2	2:B:690:ASN:ND2	2.03	0.73
2:B:1207:GLU:OE2	2:B:1210:ARG:NH1	2.22	0.73
2:B:1232:TYR:OH	2:B:1268:GLU:HB3	1.88	0.73
2:B:18:TRP:CG	2:B:49:GLY:C	2.38	0.73
2:B:724:ILE:O	2:B:727:LEU:HG	1.89	0.73
2:B:852:ILE:O	2:B:896:LYS:HD2	1.88	0.73
2:B:1204:PHE:CZ	2:B:1347:LEU:HD12	2.16	0.73
2:B:841:ILE:O	2:B:870:VAL:HG13	1.89	0.73
2:B:1065:THR:OG1	2:B:1071:GLU:O	2.06	0.73
2:B:1203:LEU:CG	2:B:1211:LYS:HD3	2.18	0.73
2:B:359:TYR:HA	2:B:362:TYR:HB3	1.69	0.72
2:B:495:MET:CB	3:C:17:DA:O4'	2.36	0.72
2:B:569:PHE:CE1	2:B:578:VAL:HG11	2.23	0.72
2:B:949:LEU:HD12	2:B:950:ILE:N	2.03	0.72
2:B:1271:GLU:HA	2:B:1274:SER:HB2	1.71	0.72
2:B:307:ARG:HH22	2:B:323:LYS:CE	2.02	0.72
2:B:312:ILE:HD12	2:B:312:ILE:H	1.51	0.72
2:B:1236:LEU:CB	2:B:1310:ILE:HD11	2.19	0.72
2:B:559:VAL:CA	2:B:563:GLN:OE1	2.36	0.72
2:B:1148:LYS:CE	2:B:1189:GLU:HG3	2.19	0.72
2:B:116:HIS:NE2	2:B:122:ILE:HD12	2.04	0.72
2:B:1232:TYR:OH	2:B:1268:GLU:OE1	2.05	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1290:VAL:HG22	2:B:1331:ILE:CD1	2.19	0.72
2:B:1229:PRO:HD2	2:B:1232:TYR:HD2	1.54	0.72
2:B:1237:TYR:HA	2:B:1242:TYR:CE1	2.24	0.72
2:B:78:ARG:NH1	2:B:162:ILE:O	2.23	0.72
2:B:307:ARG:NH2	2:B:323:LYS:NZ	2.37	0.72
2:B:551:LEU:C	2:B:551:LEU:HD12	2.15	0.72
2:B:1120:ILE:CD1	2:B:1137:PRO:CD	2.67	0.72
2:B:379:ILE:HD12	2:B:379:ILE:N	2.04	0.72
2:B:966:PHE:HE1	2:B:970:PHE:HE2	1.35	0.72
2:B:1269:ILE:HG22	2:B:1273:ILE:HG23	1.71	0.72
2:B:265:GLN:O	2:B:271:TYR:HB2	1.90	0.72
2:B:1297:HIS:CB	2:B:1327:PHE:CZ	2.72	0.72
2:B:332:LEU:HD11	2:B:359:TYR:HE2	1.54	0.72
2:B:1229:PRO:CG	2:B:1232:TYR:HD2	2.02	0.72
2:B:6:SER:CB	2:B:21:ILE:CD1	2.67	0.71
2:B:116:HIS:NE2	2:B:122:ILE:CG1	2.52	0.71
2:B:664:ARG:HG3	2:B:664:ARG:NH1	2.05	0.71
2:B:1269:ILE:O	2:B:1273:ILE:N	2.21	0.71
2:B:188:LEU:HD13	2:B:188:LEU:C	2.15	0.71
2:B:455:LEU:CD2	2:B:473:ILE:CD1	2.61	0.71
2:B:1270:ILE:O	2:B:1274:SER:N	2.21	0.71
2:B:380:LEU:HA	2:B:383:MET:HG3	1.72	0.71
2:B:857:LEU:C	2:B:857:LEU:HD23	2.15	0.71
2:B:895:ARG:HD2	2:B:895:ARG:C	2.15	0.71
2:B:1277:SER:OG	2:B:1287:LEU:HD22	1.91	0.71
1:A:83:C:H42	1:A:95:G:H1	1.36	0.71
2:B:861:ASP:OD2	2:B:861:ASP:N	2.23	0.71
2:B:1139:VAL:HA	2:B:1167:THR:HA	1.73	0.71
2:B:307:ARG:HH21	2:B:323:LYS:NZ	1.88	0.71
2:B:348:LYS:HA	2:B:352:PHE:HD1	1.56	0.71
2:B:393:LEU:HD23	2:B:393:LEU:C	2.16	0.71
2:B:70:ARG:HH22	2:B:462:PHE:HE2	1.38	0.71
2:B:203:ALA:O	2:B:206:VAL:HG13	1.89	0.71
2:B:1325:LYS:HB2	2:B:1329:THR:O	1.91	0.71
2:B:315:ALA:O	2:B:319:ALA:HB2	1.91	0.71
2:B:465:MET:CE	2:B:482:VAL:HG22	2.21	0.71
2:B:1210:ARG:HG3	2:B:1280:VAL:CB	2.21	0.71
2:B:229:LEU:C	2:B:229:LEU:HD12	2.15	0.71
2:B:307:ARG:NH2	2:B:323:LYS:CE	2.54	0.71
2:B:1139:VAL:CG1	2:B:1167:THR:HG22	2.21	0.71
2:B:45:LYS:HB3	2:B:1091:GLN:HE22	1.56	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:174:LEU:HD23	2:B:302:LEU:HD21	1.73	0.70
2:B:870:VAL:CG1	2:B:871:PRO:HD2	2.03	0.70
2:B:961:LYS:NZ	2:B:965:ASP:OD2	2.21	0.70
2:B:1312:LEU:HA	2:B:1324:PHE:CE2	2.26	0.70
1:A:44:U:H5'	2:B:363:ILE:HD13	1.73	0.70
2:B:201:ILE:HD11	2:B:232:GLU:OE1	1.88	0.70
2:B:1114:ARG:NH1	4:D:9:DA:H5'	2.06	0.70
2:B:495:MET:HB2	3:C:17:DA:C2'	2.21	0.70
2:B:963:VAL:HG21	2:B:990:ASN:OD1	1.91	0.70
2:B:992:VAL:O	2:B:996:ALA:N	2.21	0.70
2:B:1105:PHE:O	2:B:1137:PRO:CB	2.39	0.70
2:B:1347:LEU:C	2:B:1347:LEU:HD23	2.16	0.70
2:B:137:HIS:HA	2:B:322:ILE:HD11	1.74	0.70
2:B:1205:GLU:OE1	2:B:1359:ARG:NH2	2.24	0.70
2:B:1270:ILE:CD1	2:B:1273:ILE:HD11	2.22	0.70
2:B:317:LEU:HD23	2:B:414:ILE:CD1	2.21	0.70
2:B:225:LEU:HD13	2:B:229:LEU:HD23	1.72	0.70
2:B:495:MET:SD	3:C:17:DA:H1'	2.30	0.70
2:B:668:ASN:ND2	2:B:680:LEU:CB	2.54	0.70
2:B:851:SER:O	2:B:855:LYS:HG3	1.91	0.70
2:B:1269:ILE:HG22	2:B:1273:ILE:HG21	1.72	0.70
2:B:1290:VAL:HG22	2:B:1331:ILE:HD13	1.73	0.70
2:B:478:PHE:HE2	2:B:482:VAL:CG2	2.02	0.70
2:B:492:ILE:HD12	2:B:625:LEU:O	1.91	0.70
2:B:279:LEU:HD23	2:B:284:ASP:HA	1.73	0.70
2:B:1297:HIS:ND1	2:B:1327:PHE:CZ	2.56	0.70
2:B:664:ARG:HG3	2:B:664:ARG:HH11	1.55	0.69
2:B:1348:ILE:CD1	2:B:1359:ARG:HH11	1.99	0.69
2:B:518:PHE:CE2	2:B:683:LEU:HD11	2.26	0.69
2:B:841:ILE:HD11	2:B:900:LEU:HD21	1.74	0.69
2:B:1206:LEU:O	2:B:1206:LEU:HD12	1.91	0.69
2:B:442:LYS:HE2	2:B:476:TRP:HA	1.74	0.69
2:B:522:ASN:HA	2:B:525:THR:OG1	1.93	0.69
2:B:686:ASP:HB3	2:B:689:ALA:O	1.92	0.69
1:A:58:G:C5'	2:B:457:ARG:HH11	2.05	0.69
2:B:956:ILE:HD11	2:B:998:ILE:HD13	1.75	0.69
2:B:245:SER:OG	2:B:296:LEU:CD2	2.39	0.69
2:B:359:TYR:O	2:B:362:TYR:HB3	1.91	0.69
2:B:187:GLN:O	2:B:191:THR:HG23	1.92	0.69
2:B:328:HIS:CD2	2:B:399:LEU:CB	2.74	0.69
2:B:1270:ILE:C	2:B:1273:ILE:CG1	2.47	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:C:OP1	2:B:460:SER:OG	2.11	0.69
2:B:466:THR:C	2:B:467:ARG:HG3	2.18	0.69
2:B:1204:PHE:CE1	2:B:1347:LEU:CG	2.76	0.69
2:B:188:LEU:HD11	2:B:238:PHE:CE1	2.28	0.69
2:B:489:GLN:HG2	2:B:493:GLU:OE1	1.92	0.69
2:B:1281:ILE:HG22	2:B:1283:ALA:HB2	1.74	0.69
2:B:369:GLN:OE1	2:B:400:ARG:NH1	2.24	0.68
2:B:5:TYR:OH	2:B:754:HIS:O	2.10	0.68
2:B:1239:ALA:HB1	2:B:1306:ALA:HB2	1.76	0.68
2:B:328:HIS:CG	2:B:399:LEU:HB3	2.29	0.68
2:B:563:GLN:O	2:B:567:ASP:HB2	1.93	0.68
2:B:1135:ASP:OD1	2:B:1136:SER:N	2.26	0.68
2:B:1297:HIS:HB3	2:B:1327:PHE:CZ	2.28	0.68
2:B:118:ILE:HG22	2:B:119:PHE:CE1	2.27	0.68
2:B:317:LEU:CD2	2:B:414:ILE:CD1	2.71	0.68
2:B:1204:PHE:HE1	2:B:1347:LEU:CG	2.06	0.68
1:A:77:A:OP1	2:B:721:HIS:CD2	2.46	0.68
2:B:6:SER:CA	2:B:21:ILE:HD11	2.23	0.68
2:B:885:GLN:CA	2:B:888:ASN:HB2	2.24	0.68
2:B:53:PHE:HD1	2:B:54:ASP:O	1.72	0.68
2:B:841:ILE:HD13	2:B:900:LEU:CD2	2.24	0.68
2:B:1065:THR:HB	2:B:1072:ILE:HA	1.75	0.68
2:B:1269:ILE:CG2	2:B:1273:ILE:CG2	2.71	0.67
2:B:1312:LEU:HA	2:B:1324:PHE:CD2	2.29	0.67
2:B:666:LEU:O	2:B:666:LEU:HD23	1.94	0.67
2:B:1271:GLU:O	2:B:1275:GLU:N	2.26	0.67
2:B:309:ASN:ND2	2:B:312:ILE:HD13	2.09	0.67
2:B:1215:ALA:HB2	2:B:1221:GLN:HG3	1.74	0.67
2:B:18:TRP:N	2:B:49:GLY:O	2.27	0.67
2:B:143:VAL:O	2:B:425:ARG:NE	2.27	0.67
2:B:188:LEU:O	2:B:191:THR:OG1	2.13	0.67
2:B:296:LEU:O	2:B:300:ILE:N	2.22	0.67
2:B:524:LEU:O	2:B:524:LEU:HD23	1.94	0.67
2:B:565:LYS:HG2	2:B:578:VAL:HG12	1.77	0.67
2:B:1032:ALA:HA	2:B:1035:LYS:HB3	1.75	0.67
2:B:1324:PHE:O	2:B:1331:ILE:N	2.24	0.67
2:B:188:LEU:CD1	2:B:238:PHE:HE1	2.08	0.67
2:B:283:GLY:O	2:B:286:TYR:HD1	1.78	0.67
2:B:300:ILE:HD12	2:B:300:ILE:O	1.94	0.67
2:B:1229:PRO:CD	2:B:1232:TYR:HD2	2.06	0.67
2:B:1308:ASN:OD1	2:B:1327:PHE:CA	2.43	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:317:LEU:HB3	2:B:414:ILE:HD12	1.77	0.67
2:B:661:ARG:HG3	2:B:661:ARG:NH1	2.10	0.67
2:B:348:LYS:CG	2:B:352:PHE:HB2	2.25	0.67
2:B:1139:VAL:HG21	2:B:1165:GLY:HA3	1.75	0.67
2:B:597:LEU:O	2:B:601:ILE:HG12	1.95	0.67
2:B:859:ARG:HD2	2:B:859:ARG:C	2.20	0.67
2:B:1269:ILE:CG2	2:B:1273:ILE:HG23	2.25	0.67
2:B:1120:ILE:HD11	2:B:1137:PRO:HG3	1.76	0.66
2:B:1240:SER:HB3	2:B:1242:TYR:CE1	2.31	0.66
2:B:1308:ASN:OD1	2:B:1327:PHE:CB	2.43	0.66
2:B:591:LEU:HD13	2:B:594:TYR:HB2	1.76	0.66
2:B:1231:LYS:HD2	2:B:1265:TYR:OH	1.95	0.66
2:B:284:ASP:OD2	2:B:284:ASP:N	2.29	0.66
2:B:477:ASN:O	2:B:481:VAL:HG23	1.96	0.66
2:B:564:LEU:CD2	2:B:569:PHE:HE2	2.09	0.66
2:B:1210:ARG:HG3	2:B:1280:VAL:CG2	2.25	0.66
2:B:1276:PHE:CZ	2:B:1281:ILE:HD11	2.31	0.66
2:B:229:LEU:HD11	2:B:232:GLU:HB2	1.75	0.66
2:B:282:ILE:N	2:B:282:ILE:HD12	2.10	0.66
2:B:455:LEU:HD21	2:B:473:ILE:HG21	1.77	0.66
2:B:297:SER:C	2:B:300:ILE:HG22	2.21	0.66
2:B:446:PHE:CZ	2:B:478:PHE:HE1	2.08	0.66
2:B:1229:PRO:HD2	2:B:1232:TYR:CD2	2.30	0.66
2:B:1348:ILE:HD11	2:B:1357:GLU:CD	2.21	0.66
2:B:303:SER:O	2:B:306:LEU:O	2.14	0.66
2:B:554:LYS:CB	2:B:604:LYS:HZ3	2.06	0.66
2:B:115:ARG:HG3	2:B:116:HIS:HD1	1.60	0.65
2:B:495:MET:CG	3:C:17:DA:C1'	2.74	0.65
2:B:1204:PHE:CE2	2:B:1342:VAL:HG11	2.26	0.65
2:B:1207:GLU:OE1	2:B:1208:ASN:N	2.27	0.65
2:B:1226:LEU:HD13	2:B:1276:PHE:CG	2.30	0.65
2:B:1206:LEU:CB	2:B:1345:ALA:HB1	2.16	0.65
2:B:1229:PRO:HG2	2:B:1232:TYR:CD2	2.31	0.65
2:B:696:LEU:HD13	2:B:702:LEU:HD13	1.78	0.65
2:B:1120:ILE:CD1	2:B:1137:PRO:HG3	2.26	0.65
1:A:14:A:O2'	2:B:464:TRP:CH2	2.49	0.65
1:A:58:G:H5'	2:B:457:ARG:NH1	2.12	0.65
2:B:887:LEU:CA	2:B:892:ILE:HD11	2.27	0.65
2:B:1204:PHE:CD1	2:B:1347:LEU:HB2	2.31	0.65
2:B:6:SER:N	2:B:21:ILE:CD1	2.59	0.65
2:B:115:ARG:HG3	2:B:116:HIS:ND1	2.12	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:350:ILE:CD1	2:B:375:PHE:CZ	2.79	0.65
2:B:516:GLU:HG3	2:B:593:THR:CB	2.27	0.65
2:B:691:ARG:HB2	2:B:696:LEU:CD2	2.27	0.65
2:B:720:LEU:HD11	2:B:724:ILE:CD1	2.27	0.65
2:B:354:GLN:CA	2:B:361:GLY:HA3	2.26	0.65
2:B:1203:LEU:CD1	2:B:1211:LYS:HD3	2.21	0.65
2:B:395:ARG:C	2:B:396:GLU:HG3	2.21	0.65
2:B:553:PHE:HE2	2:B:559:VAL:CG1	2.08	0.65
2:B:602:LYS:HG3	2:B:602:LYS:O	1.97	0.65
2:B:6:SER:HB2	2:B:21:ILE:HD11	1.78	0.65
2:B:189:VAL:HG22	2:B:238:PHE:CZ	2.31	0.65
2:B:975:VAL:HG11	2:B:978:ILE:HG13	1.77	0.65
2:B:1308:ASN:OD1	2:B:1327:PHE:N	2.30	0.65
2:B:597:LEU:HD13	2:B:607:LEU:HD13	1.79	0.64
2:B:601:ILE:CD1	2:B:607:LEU:CD2	2.56	0.64
2:B:195:LEU:CD1	2:B:289:LEU:CD1	2.37	0.64
2:B:843:PRO:HD2	2:B:846:PHE:CD2	2.31	0.64
2:B:35:LEU:HB2	2:B:1358:THR:HG22	1.78	0.64
2:B:188:LEU:CD1	2:B:238:PHE:CE1	2.80	0.64
2:B:197:GLU:H	2:B:197:GLU:CD	1.98	0.64
2:B:297:SER:OG	2:B:301:LEU:HD11	1.96	0.64
2:B:362:TYR:HD2	2:B:372:PHE:CE2	2.11	0.64
2:B:556:ASN:O	2:B:595:HIS:CE1	2.46	0.64
2:B:902:LYS:HG3	2:B:907:GLY:HA2	1.80	0.64
2:B:6:SER:HB2	2:B:21:ILE:CD1	2.27	0.64
2:B:553:PHE:CE2	2:B:559:VAL:CB	2.79	0.64
2:B:1120:ILE:CD1	2:B:1137:PRO:HD3	2.28	0.64
2:B:6:SER:HB2	2:B:21:ILE:HG12	1.79	0.64
2:B:229:LEU:HD12	2:B:229:LEU:O	1.97	0.64
2:B:842:VAL:HG12	2:B:854:ASN:CG	2.22	0.64
2:B:1269:ILE:O	2:B:1273:ILE:CG2	2.41	0.64
2:B:136:TYR:HE2	2:B:402:GLN:HB3	1.60	0.64
2:B:18:TRP:CD1	2:B:50:ALA:N	2.49	0.64
2:B:354:GLN:HA	2:B:361:GLY:CA	2.26	0.64
2:B:557:ARG:CA	2:B:595:HIS:HD2	1.72	0.64
1:A:56:U:O2	1:A:58:G:N2	2.31	0.64
2:B:720:LEU:HD12	2:B:720:LEU:C	2.23	0.64
2:B:861:ASP:O	2:B:864:ARG:HG2	1.98	0.64
2:B:513:LEU:O	2:B:517:TYR:N	2.28	0.64
2:B:851:SER:O	2:B:855:LYS:CG	2.46	0.64
1:A:41:A:H2'	1:A:42:A:H5''	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:131:LYS:HG2	2:B:132:TYR:CE1	2.33	0.63
2:B:167:HIS:HD2	2:B:169:LEU:HD12	1.63	0.63
2:B:184:LEU:O	2:B:187:GLN:N	2.30	0.63
2:B:334:LEU:HD13	2:B:338:LEU:HD11	1.80	0.63
2:B:1327:PHE:HD2	2:B:1328:ASP:N	1.95	0.63
2:B:521:TYR:HE1	2:B:684:LYS:HG2	1.60	0.63
2:B:665:LYS:O	2:B:669:GLY:N	2.32	0.63
2:B:1207:GLU:CD	2:B:1208:ASN:H	2.07	0.63
2:B:334:LEU:HD13	2:B:338:LEU:CD1	2.28	0.63
2:B:1130:LYS:C	2:B:1131:TYR:CD1	2.76	0.63
2:B:1203:LEU:CD2	2:B:1211:LYS:CD	2.71	0.63
2:B:277:ASN:HB3	2:B:653:ARG:HE	1.62	0.63
2:B:379:ILE:CD1	2:B:379:ILE:H	2.10	0.63
2:B:594:TYR:O	2:B:594:TYR:HD2	1.80	0.63
2:B:668:ASN:HD21	2:B:680:LEU:CB	2.10	0.63
3:C:13:DA:H2'	3:C:14:DA:H8	1.62	0.63
2:B:188:LEU:O	2:B:188:LEU:HD22	1.97	0.63
2:B:379:ILE:C	2:B:383:MET:HG3	2.22	0.63
2:B:495:MET:HG3	3:C:17:DA:C4'	2.29	0.63
2:B:859:ARG:HG3	2:B:859:ARG:NH1	2.11	0.63
2:B:1245:LEU:HD12	2:B:1245:LEU:O	1.99	0.63
1:A:48:A:H2'	1:A:49:A:C8	2.34	0.63
2:B:378:PRO:O	2:B:382:LYS:N	2.32	0.63
2:B:483:ASP:CB	2:B:486:ALA:HB3	2.18	0.63
2:B:591:LEU:HD12	2:B:594:TYR:HB2	1.79	0.63
2:B:1240:SER:OG	2:B:1307:GLU:HG2	1.98	0.63
1:A:63:U:OP2	2:B:69:ARG:NH2	2.32	0.63
2:B:524:LEU:HD11	2:B:548:ILE:HD12	1.80	0.63
2:B:36:GLY:HA3	2:B:1359:ARG:O	1.99	0.63
2:B:348:LYS:O	2:B:352:PHE:N	2.32	0.63
1:A:52:A:OP2	1:A:62:G:N2	2.32	0.62
2:B:491:PHE:HE2	3:C:16:DT:C1'	2.10	0.62
2:B:761:ILE:HD13	2:B:931:VAL:CG1	2.28	0.62
2:B:116:HIS:CD2	2:B:122:ILE:CG1	2.82	0.62
2:B:869:ASN:OD1	2:B:870:VAL:HG23	1.99	0.62
2:B:6:SER:HB2	2:B:21:ILE:CG1	2.29	0.62
2:B:423:LEU:HD13	2:B:437:ARG:HG3	1.81	0.62
2:B:93:VAL:O	2:B:152:ARG:NH1	2.33	0.62
2:B:94:ASP:HB2	2:B:152:ARG:HH11	1.63	0.62
2:B:282:ILE:HG22	2:B:283:GLY:N	2.15	0.62
2:B:495:MET:SD	3:C:17:DA:C1'	2.88	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:720:LEU:HD11	2:B:724:ILE:HG13	1.80	0.62
2:B:975:VAL:HG11	2:B:1236:LEU:CD1	2.29	0.62
2:B:1139:VAL:HG12	2:B:1167:THR:CG2	2.29	0.62
2:B:1243:GLU:HB3	2:B:1246:LYS:CD	2.29	0.62
2:B:316:PRO:O	2:B:319:ALA:HB3	2.00	0.62
2:B:520:VAL:HG13	2:B:553:PHE:CE1	2.33	0.62
2:B:572:ILE:O	2:B:572:ILE:HG22	1.99	0.62
2:B:591:LEU:HB3	2:B:594:TYR:CB	2.30	0.62
2:B:328:HIS:NE2	2:B:399:LEU:CB	2.63	0.62
2:B:1120:ILE:HD12	2:B:1137:PRO:HD3	1.82	0.62
2:B:83:GLN:O	2:B:87:SER:N	2.33	0.61
2:B:664:ARG:HH11	2:B:664:ARG:CG	2.13	0.61
2:B:1203:LEU:CD1	2:B:1211:LYS:HG2	2.28	0.61
1:A:67:C:OP1	2:B:739:GLN:NE2	2.32	0.61
2:B:181:VAL:HG21	2:B:209:LYS:HA	1.83	0.61
2:B:187:GLN:O	2:B:191:THR:CG2	2.48	0.61
2:B:1106:SER:HB2	2:B:1135:ASP:O	2.00	0.61
2:B:1243:GLU:CB	2:B:1246:LYS:HE2	2.28	0.61
2:B:1273:ILE:HG13	2:B:1274:SER:N	2.14	0.61
2:B:189:VAL:CG2	2:B:238:PHE:HZ	1.92	0.61
2:B:723:HIS:NE2	2:B:934:ILE:HD11	2.15	0.61
2:B:1270:ILE:CA	2:B:1273:ILE:CG1	2.53	0.61
2:B:348:LYS:HG3	2:B:352:PHE:CB	2.30	0.61
2:B:358:GLY:O	2:B:362:TYR:N	2.32	0.61
2:B:850:ASP:O	2:B:855:LYS:CD	2.48	0.61
2:B:1139:VAL:HG12	2:B:1166:ILE:C	2.14	0.61
2:B:1270:ILE:HA	2:B:1273:ILE:HD13	1.81	0.61
2:B:18:TRP:NE1	2:B:50:ALA:H	1.95	0.61
2:B:165:ARG:NH2	2:B:446:PHE:O	2.34	0.61
2:B:720:LEU:HD11	2:B:724:ILE:HD11	1.82	0.61
2:B:247:GLY:O	2:B:248:LEU:HD23	2.00	0.61
2:B:886:LEU:HD23	2:B:886:LEU:N	2.15	0.61
2:B:1239:ALA:HB1	2:B:1306:ALA:CB	2.30	0.61
2:B:282:ILE:HG22	2:B:283:GLY:O	2.01	0.61
2:B:557:ARG:N	2:B:595:HIS:CD2	2.47	0.61
2:B:748:VAL:HG12	2:B:753:ARG:HA	1.82	0.61
2:B:1139:VAL:HG12	2:B:1167:THR:CB	2.29	0.61
2:B:182:ASP:OD1	2:B:209:LYS:CB	2.48	0.61
2:B:518:PHE:CE1	2:B:679:ILE:HG21	2.36	0.61
2:B:1257:LEU:O	2:B:1261:GLN:N	2.31	0.61
2:B:161:MET:C	2:B:164:PHE:O	2.39	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:359:TYR:CE1	2:B:363:ILE:HD11	2.37	0.60
2:B:502:LEU:HD23	2:B:505:GLU:HG3	1.84	0.60
2:B:354:GLN:CA	2:B:361:GLY:CA	2.78	0.60
2:B:647:VAL:O	2:B:651:LEU:N	2.34	0.60
2:B:841:ILE:CD1	2:B:900:LEU:HD23	2.30	0.60
2:B:188:LEU:HD13	2:B:189:VAL:N	2.16	0.60
2:B:188:LEU:HD11	2:B:238:PHE:HE1	1.64	0.60
2:B:842:VAL:HG21	2:B:847:LEU:HD21	1.83	0.60
2:B:1109:SER:OG	3:C:9:DC:OP2	2.16	0.60
2:B:51:LEU:O	2:B:52:LEU:HD22	2.01	0.60
2:B:253:LYS:O	2:B:257:ASP:N	2.33	0.60
2:B:369:GLN:O	2:B:373:TYR:CD2	2.51	0.60
2:B:877:LYS:HG3	2:B:878:LYS:H	1.66	0.60
1:A:27:G:H1'	2:B:129:HIS:CD2	2.36	0.60
2:B:553:PHE:CE2	2:B:559:VAL:HG11	2.28	0.60
2:B:809:GLU:HA	2:B:812:TYR:HB3	1.82	0.60
1:A:43:G:N2	2:B:360:ALA:HB2	2.17	0.60
2:B:90:MET:HG2	2:B:98:PHE:CE1	2.36	0.60
2:B:516:GLU:CD	2:B:593:THR:OG1	2.44	0.60
2:B:520:VAL:HG13	2:B:553:PHE:CD1	2.36	0.60
2:B:889:ALA:O	2:B:890:LYS:HB2	2.01	0.60
2:B:901:THR:O	2:B:905:ARG:NH2	2.34	0.60
2:B:1224:ASN:HD22	2:B:1280:VAL:CG2	2.10	0.60
2:B:178:ASN:CA	2:B:299:ALA:CB	2.75	0.60
2:B:841:ILE:HD13	2:B:900:LEU:HD23	1.83	0.60
2:B:1063:ILE:CG2	2:B:1074:TRP:O	2.43	0.60
1:A:42:A:O2'	1:A:43:G:OP1	2.18	0.59
2:B:545:LYS:NZ	2:B:690:ASN:CB	2.59	0.59
2:B:850:ASP:O	2:B:855:LYS:HG3	2.01	0.59
2:B:279:LEU:CD2	2:B:284:ASP:CA	2.76	0.59
2:B:721:HIS:CE1	2:B:738:LEU:HD21	2.37	0.59
2:B:1287:LEU:HD12	2:B:1287:LEU:C	2.26	0.59
2:B:68:ALA:HA	2:B:71:ARG:HB3	1.84	0.59
2:B:118:ILE:CG2	2:B:119:PHE:CE1	2.86	0.59
2:B:601:ILE:HD11	2:B:607:LEU:HD11	1.83	0.59
2:B:845:SER:O	2:B:920:GLN:NE2	2.35	0.59
2:B:174:LEU:CD2	2:B:302:LEU:HD21	2.32	0.59
2:B:208:ALA:O	2:B:212:LEU:CB	2.50	0.59
2:B:593:THR:O	2:B:597:LEU:HG	2.02	0.59
2:B:1229:PRO:CG	2:B:1232:TYR:CD2	2.85	0.59
2:B:11:ILE:HD13	2:B:740:THR:HG21	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:116:HIS:NE2	2:B:122:ILE:CD1	2.65	0.59
2:B:569:PHE:CD1	2:B:578:VAL:HG11	2.37	0.59
2:B:942:LYS:HD3	2:B:942:LYS:N	2.18	0.59
2:B:967:ARG:CA	2:B:972:PHE:O	2.50	0.59
2:B:495:MET:HB2	3:C:17:DA:H2"	1.81	0.59
2:B:763:MET:HG3	2:B:928:THR:HB	1.84	0.59
2:B:853:ASP:C	2:B:896:LYS:HG3	2.25	0.59
2:B:47:LEU:O	2:B:48:ILE:C	2.45	0.59
2:B:121:ASN:OD1	2:B:123:VAL:HG13	2.03	0.59
2:B:893:THR:HG23	2:B:896:LYS:HB2	1.85	0.59
2:B:941:THR:C	2:B:942:LYS:HD3	2.28	0.59
2:B:1148:LYS:HA	2:B:1159:SER:HA	1.84	0.59
2:B:1240:SER:CB	2:B:1242:TYR:CE1	2.85	0.59
2:B:139:ARG:HH11	2:B:161:MET:HG2	1.66	0.59
2:B:131:LYS:CG	2:B:132:TYR:CE1	2.86	0.59
2:B:186:ILE:O	2:B:190:GLN:HB2	2.03	0.59
2:B:359:TYR:CE1	2:B:363:ILE:CD1	2.85	0.59
2:B:1228:LEU:CB	2:B:1233:VAL:CG2	2.79	0.59
2:B:312:ILE:H	2:B:312:ILE:CD1	2.16	0.58
2:B:386:THR:HG1	2:B:389:LEU:HB2	1.66	0.58
2:B:661:ARG:CG	2:B:661:ARG:HH11	2.15	0.58
2:B:723:HIS:CE1	2:B:727:LEU:CD2	2.86	0.58
2:B:979:ASN:OD1	2:B:980:ASN:N	2.36	0.58
2:B:18:TRP:CZ3	2:B:49:GLY:CA	2.70	0.58
2:B:317:LEU:CB	2:B:414:ILE:HD12	2.33	0.58
2:B:552:LEU:HD21	2:B:563:GLN:NE2	2.17	0.58
2:B:592:GLY:O	2:B:596:ASP:N	2.32	0.58
2:B:661:ARG:HG3	2:B:661:ARG:HH11	1.66	0.58
2:B:823:TYR:HE2	2:B:858:THR:HG21	1.68	0.58
2:B:381:GLU:O	2:B:382:LYS:HD3	2.03	0.58
2:B:749:LYS:HG3	2:B:753:ARG:HH12	1.67	0.58
2:B:821:ASP:OD2	2:B:859:ARG:HB2	2.02	0.58
2:B:1045:PHE:O	2:B:1076:LYS:NZ	2.25	0.58
2:B:1157:LEU:HD12	2:B:1157:LEU:N	2.03	0.58
3:C:1:DC:H42	4:D:12:DG:H1	1.51	0.58
1:A:33:G:N2	1:A:36:A:OP2	2.36	0.58
2:B:666:LEU:HD23	2:B:666:LEU:C	2.29	0.58
2:B:378:PRO:CG	2:B:379:ILE:HD12	2.23	0.58
2:B:359:TYR:CE1	2:B:363:ILE:CG1	2.86	0.58
2:B:297:SER:O	2:B:300:ILE:HG22	2.02	0.58
2:B:328:HIS:NE2	2:B:399:LEU:HB3	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:522:ASN:O	2:B:525:THR:OG1	2.22	0.58
2:B:544:GLN:O	2:B:548:ILE:HG13	2.04	0.58
2:B:718:ASP:HB3	2:B:722:GLU:HB2	1.86	0.58
2:B:288:ASP:HA	2:B:291:LEU:HD22	1.84	0.58
2:B:1222:LYS:NZ	2:B:1314:THR:O	2.37	0.58
3:C:17:DA:H2'	3:C:18:DG:H8	1.69	0.58
2:B:850:ASP:O	2:B:855:LYS:CG	2.52	0.57
2:B:348:LYS:HG3	2:B:352:PHE:HB2	1.85	0.57
2:B:494:ARG:HH11	2:B:494:ARG:CG	2.12	0.57
2:B:202:ASN:HD21	2:B:204:SER:HA	1.69	0.57
2:B:328:HIS:CG	2:B:399:LEU:CB	2.87	0.57
2:B:634:GLU:HA	2:B:637:LYS:HE2	1.85	0.57
2:B:973:TYR:CD2	2:B:973:TYR:N	2.73	0.57
2:B:1224:ASN:HB2	2:B:1280:VAL:HG11	1.85	0.57
2:B:564:LEU:CD2	2:B:569:PHE:CE2	2.86	0.57
2:B:1269:ILE:O	2:B:1273:ILE:HG12	2.05	0.57
2:B:857:LEU:HD23	2:B:857:LEU:O	2.03	0.57
2:B:1142:SER:HA	2:B:1165:GLY:HA2	1.86	0.57
2:B:334:LEU:O	2:B:338:LEU:HG	2.05	0.57
2:B:340:ARG:HH21	2:B:347:TYR:HE2	1.24	0.57
2:B:384:ASP:OD1	2:B:384:ASP:N	2.35	0.57
2:B:594:TYR:OH	2:B:608:ASP:OD1	2.22	0.57
2:B:6:SER:H	2:B:21:ILE:CD1	2.18	0.57
2:B:494:ARG:HG2	2:B:494:ARG:NH1	2.16	0.57
2:B:720:LEU:HD11	2:B:724:ILE:CG1	2.34	0.57
2:B:755:LYS:NZ	2:B:942:LYS:HE2	2.19	0.57
2:B:1127:ASP:HB3	2:B:1130:LYS:HG3	1.87	0.57
2:B:237:LEU:HD13	2:B:256:PHE:CE1	2.40	0.57
2:B:265:GLN:O	2:B:271:TYR:HD1	1.86	0.57
2:B:540:LEU:O	2:B:545:LYS:HE3	2.04	0.57
2:B:1315:LEU:HD13	2:B:1324:PHE:HE1	1.70	0.57
2:B:8:GLY:HA3	2:B:991:ALA:HB2	1.86	0.57
2:B:178:ASN:CB	2:B:299:ALA:HB1	2.22	0.57
2:B:348:LYS:O	2:B:352:PHE:HB2	2.05	0.57
2:B:1062:LEU:HD23	2:B:1062:LEU:H	1.70	0.57
2:B:1108:GLU:HB2	3:C:9:DC:H5''	1.87	0.57
2:B:1281:ILE:CG2	2:B:1283:ALA:HB2	2.35	0.57
2:B:484:LYS:O	2:B:488:ALA:N	2.37	0.56
2:B:842:VAL:CG2	2:B:847:LEU:CD2	2.82	0.56
2:B:483:ASP:HB3	2:B:486:ALA:CB	2.20	0.56
2:B:945:GLU:H	2:B:945:GLU:CD	1.97	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:303:SER:O	2:B:306:LEU:C	2.48	0.56
2:B:315:ALA:CB	2:B:418:GLU:HG2	2.35	0.56
2:B:499:ASP:CB	2:B:502:LEU:O	2.53	0.56
2:B:522:ASN:HD22	2:B:523:GLU:N	2.02	0.56
2:B:895:ARG:HH11	2:B:899:ASN:ND2	2.04	0.56
2:B:1139:VAL:CG1	2:B:1167:THR:CG2	2.83	0.56
2:B:1198:LEU:HD13	2:B:1204:PHE:HZ	1.69	0.56
2:B:1270:ILE:CA	2:B:1273:ILE:CD1	2.70	0.56
2:B:100:ARG:NE	2:B:117:PRO:O	2.37	0.56
2:B:325:TYR:O	2:B:329:HIS:N	2.34	0.56
2:B:851:SER:C	2:B:855:LYS:HG3	2.31	0.56
2:B:1206:LEU:O	2:B:1207:GLU:HG3	2.06	0.56
2:B:1236:LEU:HD22	2:B:1310:ILE:CD1	2.35	0.56
1:A:13:A:H5"	2:B:59:ALA:HB3	1.86	0.56
2:B:18:TRP:CE3	2:B:49:GLY:N	2.69	0.56
2:B:169:LEU:HD21	3:C:13:DA:H2"	1.88	0.56
2:B:217:SER:OG	2:B:220:ARG:NH1	2.39	0.56
2:B:686:ASP:OD2	2:B:690:ASN:HA	2.05	0.56
2:B:897:PHE:CZ	2:B:901:THR:HG21	2.40	0.56
2:B:1041:ASN:O	2:B:1044:ASN:HB2	2.06	0.56
2:B:1146:VAL:HG13	2:B:1191:LYS:HG3	1.86	0.56
2:B:761:ILE:CD1	2:B:931:VAL:HG12	2.35	0.56
2:B:856:VAL:HG22	2:B:857:LEU:N	2.20	0.56
2:B:975:VAL:HG11	2:B:1236:LEU:HD13	1.87	0.56
2:B:1119:LEU:HD13	2:B:1119:LEU:H	1.69	0.56
2:B:1123:LYS:HB2	2:B:1126:TRP:CE3	2.41	0.56
2:B:1240:SER:CB	2:B:1242:TYR:CZ	2.88	0.56
2:B:245:SER:OG	2:B:296:LEU:HD22	2.04	0.56
2:B:252:PHE:CZ	2:B:264:LEU:HD13	2.41	0.56
2:B:594:TYR:HA	2:B:597:LEU:HD11	1.88	0.56
2:B:1210:ARG:HD3	2:B:1280:VAL:HA	1.76	0.56
2:B:18:TRP:CZ3	2:B:47:LEU:O	2.59	0.56
2:B:107:VAL:CG1	2:B:1131:TYR:CE1	2.60	0.56
2:B:135:ILE:HG23	2:B:136:TYR:N	2.20	0.56
2:B:887:LEU:N	2:B:892:ILE:HD11	2.21	0.56
2:B:749:LYS:HG3	2:B:753:ARG:NH1	2.21	0.56
2:B:1297:HIS:NE2	2:B:1327:PHE:HE2	2.01	0.56
2:B:226:ILE:C	2:B:229:LEU:HG	2.31	0.55
2:B:451:TYR:CB	2:B:491:PHE:CD1	2.89	0.55
2:B:520:VAL:HG11	2:B:553:PHE:CD1	2.34	0.55
2:B:721:HIS:ND1	2:B:738:LEU:HD11	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1243:GLU:CB	2:B:1246:LYS:NZ	2.66	0.55
2:B:347:TYR:C	2:B:347:TYR:CD1	2.84	0.55
2:B:484:LYS:O	2:B:488:ALA:HB2	2.06	0.55
2:B:879:MET:O	2:B:880:LYS:C	2.49	0.55
2:B:936:ASP:CG	2:B:951:ARG:HE	2.14	0.55
2:B:31:LYS:HG3	2:B:44:LYS:HB2	1.87	0.55
1:A:58:G:H5'	2:B:457:ARG:HH11	1.71	0.55
2:B:107:VAL:HG22	2:B:1131:TYR:CE1	2.42	0.55
2:B:132:TYR:CD1	2:B:132:TYR:N	2.73	0.55
2:B:279:LEU:HD21	2:B:284:ASP:CA	2.37	0.55
2:B:886:LEU:HB2	2:B:892:ILE:HD13	1.87	0.55
2:B:343:LEU:HG	2:B:343:LEU:O	2.07	0.55
2:B:379:ILE:CG2	2:B:383:MET:SD	2.95	0.55
2:B:749:LYS:HD2	2:B:753:ARG:HH22	1.71	0.55
2:B:1204:PHE:CD1	2:B:1347:LEU:CB	2.89	0.55
2:B:393:LEU:HD23	2:B:394:ASN:CA	2.37	0.55
2:B:559:VAL:C	2:B:563:GLN:OE1	2.49	0.55
2:B:1114:ARG:HH12	4:D:9:DA:P	2.30	0.55
2:B:118:ILE:C	2:B:119:PHE:CD1	2.85	0.55
2:B:288:ASP:HA	2:B:291:LEU:CD2	2.36	0.55
2:B:300:ILE:HG23	2:B:301:LEU:N	2.21	0.55
2:B:456:ALA:CB	2:B:463:ALA:HB2	2.19	0.55
2:B:1139:VAL:HG11	2:B:1165:GLY:C	2.32	0.55
2:B:192:TYR:C	2:B:192:TYR:CD2	2.85	0.54
2:B:328:HIS:NE2	2:B:399:LEU:HB2	2.21	0.54
2:B:497:ASN:OD1	3:C:19:DA:P	2.65	0.54
2:B:1349:HIS:HB2	2:B:1358:THR:OG1	2.06	0.54
2:B:53:PHE:CD1	2:B:53:PHE:C	2.85	0.54
2:B:222:LEU:O	2:B:226:ILE:HG12	2.06	0.54
2:B:491:PHE:CD2	2:B:491:PHE:C	2.85	0.54
2:B:967:ARG:NH1	2:B:986:ASP:OD1	2.40	0.54
2:B:513:LEU:O	2:B:516:GLU:HB2	2.08	0.54
2:B:531:THR:HG22	2:B:534:MET:SD	2.47	0.54
2:B:972:PHE:N	2:B:972:PHE:CD1	2.73	0.54
1:A:15:U:OP2	2:B:66:ARG:NH2	2.40	0.54
2:B:520:VAL:CG1	2:B:553:PHE:CE1	2.90	0.54
2:B:978:ILE:HD12	2:B:1236:LEU:HD12	1.86	0.54
2:B:1207:GLU:CG	2:B:1208:ASN:H	2.20	0.54
2:B:1225:GLU:OE1	2:B:1225:GLU:HA	2.05	0.54
1:A:92:G:OP1	2:B:40:ARG:NH2	2.41	0.54
2:B:316:PRO:HD2	2:B:317:LEU:H	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:473:ILE:HG12	2:B:481:VAL:HG11	1.89	0.54
2:B:22:THR:OG1	2:B:26:LYS:O	2.26	0.54
2:B:107:VAL:N	2:B:1131:TYR:CZ	2.64	0.54
2:B:338:LEU:HD13	2:B:386:THR:CB	2.35	0.54
2:B:843:PRO:HD2	2:B:846:PHE:HD2	1.71	0.54
2:B:1325:LYS:HA	2:B:1330:THR:HA	1.89	0.54
2:B:318:SER:CB	2:B:418:GLU:OE2	2.53	0.54
2:B:680:LEU:O	2:B:684:LYS:HG3	2.07	0.54
2:B:879:MET:O	2:B:882:TYR:N	2.40	0.54
2:B:131:LYS:CD	2:B:132:TYR:CE1	2.86	0.54
2:B:359:TYR:C	2:B:359:TYR:CD1	2.85	0.54
2:B:1243:GLU:O	2:B:1246:LYS:HD2	2.07	0.54
2:B:482:VAL:HG12	2:B:483:ASP:N	2.22	0.54
2:B:727:LEU:O	2:B:734:LYS:HD3	2.08	0.54
2:B:895:ARG:NH1	2:B:899:ASN:ND2	2.54	0.54
2:B:682:PHE:CG	2:B:696:LEU:HD11	2.43	0.53
2:B:686:ASP:HB2	2:B:690:ASN:HA	1.88	0.53
2:B:944:ASP:OD1	2:B:944:ASP:N	2.37	0.53
1:A:68:A:H2'	1:A:69:A:C8	2.43	0.53
2:B:115:ARG:CG	2:B:116:HIS:HD1	2.21	0.53
2:B:359:TYR:CA	2:B:362:TYR:HB3	2.38	0.53
2:B:361:GLY:HA2	2:B:365:GLY:H	1.74	0.53
2:B:362:TYR:CD1	2:B:362:TYR:C	2.85	0.53
2:B:554:LYS:CB	2:B:604:LYS:HZ1	2.19	0.53
2:B:316:PRO:CD	2:B:317:LEU:H	2.21	0.53
2:B:455:LEU:CD2	2:B:473:ILE:HG21	2.38	0.53
2:B:545:LYS:HZ2	2:B:690:ASN:ND2	2.04	0.53
2:B:553:PHE:HE2	2:B:559:VAL:HG21	1.52	0.53
2:B:362:TYR:O	2:B:362:TYR:HD1	1.92	0.53
2:B:395:ARG:O	2:B:396:GLU:HG3	2.07	0.53
2:B:1229:PRO:HD2	2:B:1232:TYR:HB2	1.91	0.53
3:C:17:DA:H2'	3:C:18:DG:C8	2.43	0.53
2:B:374:LYS:HA	2:B:374:LYS:CE	2.37	0.53
2:B:686:ASP:H	2:B:690:ASN:ND2	2.06	0.53
2:B:1207:GLU:HG2	2:B:1210:ARG:HH12	1.71	0.53
2:B:188:LEU:C	2:B:188:LEU:HD22	2.33	0.53
2:B:241:LEU:HD21	2:B:290:PHE:HE2	1.74	0.53
2:B:524:LEU:HD23	2:B:524:LEU:C	2.34	0.53
2:B:1351:SER:OG	2:B:1356:TYR:HB2	2.08	0.53
3:C:1:DC:N4	4:D:12:DG:H1	2.06	0.53
2:B:116:HIS:CD2	2:B:122:ILE:HG13	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:609:ASN:ND2	2:B:612:ASN:OD1	2.34	0.53
2:B:1130:LYS:C	2:B:1131:TYR:HD1	2.11	0.53
2:B:307:ARG:NH2	2:B:323:LYS:HZ1	2.06	0.53
2:B:850:ASP:O	2:B:855:LYS:HD2	2.09	0.53
2:B:884:ARG:O	2:B:888:ASN:N	2.32	0.53
2:B:1276:PHE:HE2	2:B:1316:THR:HA	1.74	0.53
1:A:51:A:O2'	2:B:1134:PHE:CE1	2.37	0.53
2:B:359:TYR:OH	2:B:363:ILE:HD11	2.09	0.53
2:B:131:LYS:CG	2:B:132:TYR:CD1	2.88	0.53
2:B:226:ILE:O	2:B:229:LEU:HG	2.09	0.53
2:B:266:LEU:HD21	2:B:294:LYS:HA	1.90	0.53
2:B:334:LEU:CD1	2:B:338:LEU:CD1	2.85	0.53
2:B:869:ASN:CG	2:B:870:VAL:N	2.65	0.53
2:B:63:ARG:O	2:B:67:THR:OG1	2.20	0.52
2:B:335:LEU:O	2:B:339:VAL:HG23	2.10	0.52
2:B:478:PHE:CE2	2:B:482:VAL:CG2	2.86	0.52
2:B:1202:SER:O	2:B:1214:LEU:N	2.28	0.52
2:B:48:ILE:HD12	2:B:48:ILE:C	2.35	0.52
2:B:297:SER:O	2:B:301:LEU:HD12	2.10	0.52
2:B:315:ALA:HB2	2:B:418:GLU:HG2	1.90	0.52
2:B:398:LEU:HG	2:B:399:LEU:H	1.75	0.52
2:B:600:ILE:N	2:B:600:ILE:CD1	2.73	0.52
2:B:942:LYS:O	2:B:950:ILE:HB	2.09	0.52
2:B:347:TYR:C	2:B:347:TYR:HD1	2.17	0.52
2:B:356:LYS:O	2:B:357:ASN:CB	2.53	0.52
2:B:1207:GLU:OE1	2:B:1208:ASN:HB3	2.10	0.52
3:C:11:DT:H2'	3:C:12:DC:O4'	2.09	0.52
3:C:13:DA:H2'	3:C:14:DA:C8	2.41	0.52
2:B:312:ILE:N	2:B:312:ILE:CD1	2.73	0.52
2:B:372:PHE:C	2:B:372:PHE:CD1	2.85	0.52
2:B:454:PRO:O	2:B:456:ALA:N	2.42	0.52
2:B:1315:LEU:HD13	2:B:1324:PHE:CE1	2.44	0.52
2:B:282:ILE:HG22	2:B:286:TYR:HD1	1.68	0.52
2:B:966:PHE:CZ	2:B:970:PHE:HD2	2.28	0.52
2:B:1107:LYS:HD3	3:C:8:DT:H4'	1.92	0.52
2:B:1325:LYS:CA	2:B:1330:THR:HA	2.40	0.52
2:B:1347:LEU:HD23	2:B:1347:LEU:O	2.10	0.52
2:B:189:VAL:HA	2:B:192:TYR:HB3	1.92	0.52
2:B:1325:LYS:HB3	2:B:1330:THR:OG1	2.10	0.52
2:B:1348:ILE:HD11	2:B:1357:GLU:CG	2.40	0.52
3:C:18:DG:H2'	3:C:19:DA:C8	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:134:THR:CB	2:B:137:HIS:ND1	2.58	0.52
2:B:236:GLY:O	2:B:240:ASN:ND2	2.42	0.52
2:B:359:TYR:O	2:B:363:ILE:N	2.38	0.52
2:B:825:ASP:CG	2:B:825:ASP:O	2.53	0.52
2:B:1045:PHE:HB2	2:B:1064:GLU:CD	2.35	0.52
2:B:1339:THR:O	2:B:1343:LEU:CD2	2.50	0.52
2:B:374:LYS:CE	2:B:374:LYS:CA	2.86	0.51
2:B:1119:LEU:H	2:B:1119:LEU:HD22	1.75	0.51
2:B:1269:ILE:C	2:B:1273:ILE:HG23	2.34	0.51
2:B:78:ARG:CZ	2:B:165:ARG:HD2	2.40	0.51
2:B:307:ARG:HH21	2:B:323:LYS:HZ1	1.57	0.51
2:B:308:VAL:HG12	2:B:309:ASN:N	2.25	0.51
2:B:509:PRO:HB3	2:B:624:THR:HG21	1.91	0.51
2:B:70:ARG:NH2	2:B:462:PHE:CD2	2.78	0.51
2:B:115:ARG:CG	2:B:116:HIS:ND1	2.73	0.51
2:B:245:SER:OG	2:B:296:LEU:HD23	2.02	0.51
2:B:478:PHE:C	2:B:478:PHE:CD2	2.85	0.51
2:B:523:GLU:OE1	2:B:589:ALA:HB2	2.10	0.51
2:B:1236:LEU:O	2:B:1240:SER:HB2	2.11	0.51
1:A:81:G:N1	2:B:1356:TYR:HB3	2.26	0.51
2:B:686:ASP:CB	2:B:690:ASN:ND2	2.73	0.51
2:B:713:VAL:O	2:B:716:GLN:N	2.32	0.51
2:B:853:ASP:HA	2:B:896:LYS:CG	2.40	0.51
2:B:1127:ASP:O	2:B:1131:TYR:N	2.37	0.51
2:B:115:ARG:HG3	2:B:116:HIS:CE1	2.45	0.51
2:B:121:ASN:CG	2:B:124:ASP:HB2	2.35	0.51
2:B:134:THR:HG22	2:B:136:TYR:H	1.75	0.51
2:B:887:LEU:N	2:B:892:ILE:CD1	2.73	0.51
2:B:1243:GLU:HA	2:B:1243:GLU:OE1	2.11	0.51
2:B:1245:LEU:HD13	2:B:1252:ASN:ND2	2.23	0.51
2:B:114:GLU:HG2	2:B:120:GLY:HA2	1.92	0.51
2:B:520:VAL:HG21	2:B:591:LEU:CG	2.27	0.51
2:B:591:LEU:HD12	2:B:594:TYR:CB	2.40	0.51
2:B:966:PHE:CZ	2:B:970:PHE:CD2	2.99	0.51
2:B:999:LYS:HB3	2:B:1073:VAL:HG11	1.92	0.51
2:B:197:GLU:O	2:B:198:GLU:C	2.51	0.51
2:B:336:LYS:O	2:B:340:ARG:HG2	2.11	0.51
2:B:569:PHE:HA	2:B:573:GLU:HB2	1.92	0.51
2:B:790:GLU:OE2	2:B:888:ASN:O	2.28	0.51
2:B:1224:ASN:HD21	2:B:1280:VAL:HG21	1.60	0.51
2:B:45:LYS:CB	2:B:1091:GLN:HE22	2.22	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:282:ILE:N	2:B:282:ILE:CD1	2.73	0.51
2:B:433:LEU:O	2:B:437:ARG:N	2.44	0.51
2:B:1062:LEU:O	2:B:1076:LYS:HG3	2.11	0.51
2:B:1100:VAL:HG13	2:B:1140:ALA:HB1	1.92	0.51
2:B:1272:GLN:HE21	2:B:1272:GLN:C	2.19	0.51
1:A:22:U:H2'	1:A:23:U:C6	2.46	0.51
2:B:465:MET:SD	2:B:467:ARG:HG3	2.51	0.51
2:B:679:ILE:HG12	2:B:704:PHE:CE1	2.46	0.51
2:B:967:ARG:C	2:B:972:PHE:O	2.53	0.51
2:B:1120:ILE:HD11	2:B:1137:PRO:HD2	1.91	0.51
2:B:1343:LEU:HD23	2:B:1343:LEU:H	1.72	0.51
1:A:8:G:O2'	1:A:9:U:OP1	2.27	0.50
2:B:334:LEU:HD12	2:B:389:LEU:HD11	1.93	0.50
2:B:780:ARG:HD3	2:B:812:TYR:CE2	2.46	0.50
2:B:691:ARG:HB2	2:B:696:LEU:HD22	1.94	0.50
2:B:135:ILE:O	2:B:138:LEU:HB3	2.11	0.50
2:B:661:ARG:CD	2:B:661:ARG:N	2.73	0.50
2:B:1220:LEU:CD2	2:B:1342:VAL:HG21	2.42	0.50
2:B:1363:SER:O	2:B:1364:GLN:HB3	2.12	0.50
2:B:620:VAL:HG13	2:B:656:TYR:CE2	2.46	0.50
2:B:971:GLN:C	2:B:972:PHE:HD1	2.19	0.50
2:B:970:PHE:O	2:B:971:GLN:HB2	2.11	0.50
2:B:48:ILE:HG21	2:B:1092:VAL:HG22	1.92	0.50
2:B:60:GLU:HG3	2:B:63:ARG:HH22	1.76	0.50
2:B:202:ASN:OD1	2:B:203:ALA:N	2.45	0.50
2:B:457:ARG:HG2	2:B:459:ASN:ND2	2.26	0.50
2:B:552:LEU:O	2:B:555:THR:OG1	2.29	0.50
2:B:760:VAL:HG11	2:B:990:ASN:O	2.11	0.50
2:B:794:GLN:H	2:B:794:GLN:CD	2.19	0.50
2:B:509:PRO:HA	2:B:659:TRP:HA	1.93	0.50
2:B:277:ASN:O	2:B:281:GLN:OE1	2.30	0.50
2:B:291:LEU:O	2:B:294:LYS:HD3	2.11	0.50
2:B:359:TYR:HE1	2:B:363:ILE:CG1	2.25	0.50
2:B:666:LEU:HA	2:B:670:ILE:HG12	1.94	0.50
2:B:940:ASN:HB3	2:B:950:ILE:O	2.11	0.50
2:B:1270:ILE:CA	2:B:1273:ILE:HD11	2.40	0.50
2:B:193:ASN:CG	2:B:201:ILE:H	2.14	0.50
2:B:121:ASN:OD1	2:B:124:ASP:HB2	2.11	0.49
2:B:202:ASN:ND2	2:B:204:SER:CB	2.74	0.49
2:B:495:MET:CB	3:C:17:DA:H1'	2.22	0.49
2:B:522:ASN:ND2	2:B:523:GLU:N	2.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1308:ASN:CG	2:B:1327:PHE:HB3	2.36	0.49
1:A:70:C:H2'	1:A:71:U:C6	2.47	0.49
2:B:648:MET:HA	2:B:651:LEU:HB2	1.94	0.49
2:B:668:ASN:CG	2:B:680:LEU:HB2	2.06	0.49
2:B:1204:PHE:CE2	2:B:1342:VAL:CG1	2.85	0.49
2:B:1235:PHE:CD1	2:B:1258:PHE:CE2	3.00	0.49
2:B:1348:ILE:CD1	2:B:1359:ARG:HH12	2.10	0.49
2:B:376:ILE:CD1	2:B:376:ILE:C	2.86	0.49
2:B:491:PHE:HD2	2:B:492:ILE:HG12	1.77	0.49
2:B:495:MET:HB2	3:C:17:DA:C3'	2.42	0.49
2:B:762:GLU:CD	2:B:990:ASN:ND2	2.57	0.49
2:B:1309:ILE:HG12	2:B:1326:TYR:OH	2.12	0.49
2:B:1348:ILE:HG23	2:B:1348:ILE:O	2.11	0.49
1:A:58:G:C5'	2:B:457:ARG:NH1	2.71	0.49
2:B:373:TYR:O	2:B:376:ILE:HD12	2.13	0.49
2:B:664:ARG:C	2:B:664:ARG:CD	2.86	0.49
2:B:686:ASP:CG	2:B:691:ARG:CZ	2.85	0.49
1:A:15:U:H4'	2:B:464:TRP:HE1	1.77	0.49
2:B:282:ILE:CG2	2:B:283:GLY:N	2.75	0.49
2:B:331:ASP:HB3	2:B:398:LEU:HD11	1.94	0.49
2:B:334:LEU:HD12	2:B:389:LEU:CD1	2.42	0.49
2:B:787:GLY:O	2:B:791:LEU:N	2.32	0.49
2:B:1120:ILE:CD1	2:B:1137:PRO:CG	2.84	0.49
1:A:8:G:O4'	2:B:894:GLN:OE1	2.30	0.49
2:B:11:ILE:HG22	2:B:12:GLY:H	1.77	0.49
2:B:201:ILE:HG22	2:B:202:ASN:N	2.27	0.49
2:B:1279:ARG:HG2	2:B:1280:VAL:HG23	1.94	0.49
2:B:1325:LYS:HB3	2:B:1330:THR:HA	1.90	0.49
1:A:32:A:H61	1:A:37:U:H3	1.60	0.49
2:B:218:LYS:H	2:B:218:LYS:HD2	1.78	0.49
2:B:265:GLN:C	2:B:271:TYR:CD1	2.90	0.49
2:B:450:TYR:HD2	2:B:491:PHE:HZ	1.45	0.49
2:B:513:LEU:HB2	2:B:617:GLU:OE2	2.12	0.49
2:B:859:ARG:C	2:B:859:ARG:CD	2.86	0.49
2:B:279:LEU:HD11	2:B:287:ALA:HB2	1.95	0.49
2:B:401:LYS:HB2	2:B:404:THR:CG2	2.43	0.49
2:B:666:LEU:C	2:B:666:LEU:CD2	2.85	0.49
2:B:128:TYR:CD1	2:B:153:LEU:HD21	2.48	0.49
2:B:1207:GLU:CG	2:B:1208:ASN:N	2.73	0.49
1:A:27:G:N2	1:A:44:U:OP2	2.46	0.48
2:B:1239:ALA:CB	2:B:1306:ALA:HB1	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:U:H2'	1:A:46:A:C8	2.47	0.48
1:A:59:U:P	2:B:467:ARG:HH22	2.36	0.48
2:B:377:LYS:O	2:B:381:GLU:HB2	2.13	0.48
2:B:450:TYR:C	2:B:491:PHE:HE1	2.20	0.48
2:B:1204:PHE:CE1	2:B:1347:LEU:HB2	2.48	0.48
2:B:186:ILE:HD12	2:B:203:ALA:HB2	1.95	0.48
2:B:1276:PHE:CE2	2:B:1316:THR:HB	2.49	0.48
2:B:512:SER:O	2:B:516:GLU:HG2	2.12	0.48
2:B:316:PRO:CA	2:B:319:ALA:HB3	2.39	0.48
2:B:746:GLU:HA	2:B:749:LYS:HB3	1.95	0.48
2:B:1262:HIS:HD2	2:B:1265:TYR:CZ	2.30	0.48
1:A:33:G:H2'	1:A:34:A:H5''	1.95	0.48
1:A:49:A:H1'	2:B:1122:ARG:NH1	2.29	0.48
2:B:720:LEU:CD1	2:B:724:ILE:CG1	2.86	0.48
2:B:949:LEU:CD1	2:B:950:ILE:N	2.73	0.48
2:B:169:LEU:HD22	3:C:14:DA:H5'	1.95	0.48
2:B:275:LEU:HD11	2:B:290:PHE:CD1	2.49	0.48
2:B:362:TYR:HE2	2:B:372:PHE:CE2	2.29	0.48
1:A:45:U:H2'	1:A:46:A:H8	1.78	0.48
1:A:65:A:OP1	2:B:57:GLU:N	2.46	0.48
2:B:206:VAL:HG12	2:B:228:GLN:HG2	1.94	0.48
2:B:975:VAL:HG21	2:B:1236:LEU:HB2	1.96	0.48
2:B:1229:PRO:HG2	2:B:1232:TYR:CE2	2.48	0.48
2:B:332:LEU:HD11	2:B:359:TYR:CE2	2.42	0.48
2:B:93:VAL:HG12	2:B:152:ARG:NH1	2.28	0.48
2:B:343:LEU:O	2:B:343:LEU:CG	2.62	0.48
2:B:393:LEU:HD23	2:B:394:ASN:HA	1.94	0.48
2:B:450:TYR:C	2:B:491:PHE:CE1	2.92	0.48
2:B:1240:SER:HB3	2:B:1242:TYR:CZ	2.49	0.48
3:C:3:DA:H2'	3:C:4:DT:H71	1.95	0.48
1:A:67:C:OP2	2:B:1097:LYS:NZ	2.46	0.47
2:B:270:THR:OG1	2:B:629:ARG:NH1	2.47	0.47
2:B:668:ASN:HD21	2:B:680:LEU:HB3	1.67	0.47
2:B:975:VAL:HG11	2:B:1236:LEU:HD12	1.94	0.47
2:B:1206:LEU:HB3	2:B:1345:ALA:HB3	1.71	0.47
2:B:1334:LYS:NZ	3:C:2:DA:O3'	2.46	0.47
1:A:43:G:H22	2:B:360:ALA:HB2	1.79	0.47
2:B:121:ASN:ND2	2:B:124:ASP:HB2	2.29	0.47
2:B:489:GLN:O	2:B:493:GLU:HB2	2.14	0.47
2:B:668:ASN:CG	2:B:680:LEU:HD22	2.39	0.47
2:B:897:PHE:HA	2:B:900:LEU:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:594:TYR:C	2:B:594:TYR:CD2	2.93	0.47
2:B:877:LYS:HG3	2:B:878:LYS:N	2.29	0.47
1:A:47:A:O2'	2:B:104:SER:OG	2.23	0.47
2:B:484:LYS:HA	2:B:487:SER:OG	2.14	0.47
2:B:495:MET:CG	3:C:17:DA:C4'	2.88	0.47
2:B:601:ILE:HD11	2:B:607:LEU:HD21	1.80	0.47
2:B:1065:THR:CB	2:B:1072:ILE:HA	2.42	0.47
2:B:727:LEU:O	2:B:734:LYS:NZ	2.38	0.47
2:B:1276:PHE:HE2	2:B:1316:THR:CA	2.27	0.47
2:B:485:GLY:HA2	2:B:488:ALA:CB	2.41	0.47
2:B:723:HIS:C	2:B:723:HIS:ND1	2.73	0.47
2:B:755:LYS:HZ2	2:B:942:LYS:HE2	1.80	0.47
2:B:1118:LYS:HA	2:B:1118:LYS:HD3	1.73	0.47
2:B:1139:VAL:CA	2:B:1167:THR:HA	2.43	0.47
2:B:1297:HIS:CD2	2:B:1327:PHE:CE2	3.03	0.47
2:B:119:PHE:HD2	2:B:124:ASP:O	1.98	0.47
2:B:317:LEU:HD22	2:B:414:ILE:CD1	2.43	0.47
2:B:340:ARG:NE	2:B:347:TYR:CD2	2.77	0.47
2:B:375:PHE:CE2	2:B:376:ILE:HG23	2.48	0.47
2:B:380:LEU:CA	2:B:383:MET:HG3	2.44	0.47
2:B:431:PRO:O	2:B:434:LYS:HG2	2.14	0.47
2:B:494:ARG:CG	2:B:494:ARG:NH1	2.73	0.47
2:B:679:ILE:HG12	2:B:704:PHE:HE1	1.80	0.47
2:B:778:ARG:NH1	3:C:11:DT:OP1	2.48	0.47
2:B:887:LEU:HA	2:B:892:ILE:HG12	1.97	0.47
2:B:1075:ASP:OD1	2:B:1078:ARG:N	2.33	0.47
2:B:1144:LEU:HB3	2:B:1196:ILE:HB	1.95	0.47
2:B:1148:LYS:HB2	2:B:1157:LEU:HB2	1.96	0.47
2:B:1203:LEU:CD1	2:B:1212:ARG:O	2.53	0.47
2:B:1236:LEU:CG	2:B:1310:ILE:HD11	2.45	0.47
2:B:1239:ALA:CB	2:B:1306:ALA:CB	2.92	0.47
2:B:1270:ILE:HG13	2:B:1294:TYR:CE2	2.50	0.47
2:B:1281:ILE:O	2:B:1336:TYR:OH	2.26	0.47
2:B:328:HIS:CG	2:B:399:LEU:HA	2.49	0.47
2:B:465:MET:SD	2:B:467:ARG:CG	3.02	0.47
2:B:491:PHE:CD2	2:B:492:ILE:HG12	2.49	0.47
2:B:518:PHE:CZ	2:B:679:ILE:HG23	2.25	0.47
2:B:522:ASN:ND2	2:B:522:ASN:C	2.73	0.47
2:B:942:LYS:N	2:B:942:LYS:CD	2.73	0.47
2:B:86:PHE:HE2	2:B:155:TYR:HB2	1.79	0.47
2:B:555:THR:C	2:B:556:ASN:ND2	2.73	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:594:TYR:HD2	2:B:594:TYR:C	2.23	0.47
3:C:2:DA:H2''	3:C:3:DA:C8	2.50	0.47
1:A:43:G:HO2'	2:B:363:ILE:HD12	1.78	0.47
2:B:421:ALA:O	2:B:425:ARG:N	2.48	0.47
2:B:465:MET:SD	2:B:465:MET:C	2.98	0.47
2:B:516:GLU:HA	2:B:519:THR:HG22	1.97	0.47
2:B:686:ASP:CG	2:B:691:ARG:NE	2.73	0.47
2:B:721:HIS:HE1	2:B:738:LEU:HD21	1.79	0.47
2:B:784:ILE:HG22	2:B:796:LEU:HD11	1.96	0.47
2:B:954:LYS:HD2	2:B:998:ILE:HD12	1.97	0.47
2:B:949:LEU:CG	2:B:950:ILE:N	2.78	0.46
2:B:969:ASP:N	2:B:969:ASP:OD1	2.47	0.46
2:B:686:ASP:HB3	2:B:690:ASN:HA	1.95	0.46
2:B:959:LYS:HD2	2:B:960:SER:H	1.79	0.46
2:B:1236:LEU:HD22	2:B:1310:ILE:HD11	1.96	0.46
2:B:453:GLY:HA2	2:B:464:TRP:NE1	2.30	0.46
2:B:822:MET:HG2	2:B:856:VAL:HG21	1.97	0.46
2:B:887:LEU:HA	2:B:892:ILE:CG1	2.45	0.46
1:A:58:G:C4'	2:B:457:ARG:HD2	2.04	0.46
1:A:61:C:H5'	2:B:460:SER:OG	2.16	0.46
1:A:70:C:H2'	1:A:71:U:H6	1.79	0.46
2:B:9:LEU:HD12	2:B:761:ILE:HG22	1.98	0.46
2:B:135:ILE:CG2	2:B:136:TYR:N	2.78	0.46
2:B:202:ASN:CG	2:B:204:SER:N	2.73	0.46
2:B:315:ALA:O	2:B:319:ALA:CB	2.62	0.46
2:B:518:PHE:CD2	2:B:683:LEU:HD12	2.38	0.46
2:B:555:THR:C	2:B:556:ASN:HD22	2.23	0.46
2:B:668:ASN:O	2:B:678:THR:HG21	2.15	0.46
2:B:1231:LYS:CD	2:B:1265:TYR:OH	2.62	0.46
2:B:1243:GLU:O	2:B:1246:LYS:NZ	2.27	0.46
2:B:94:ASP:OD1	2:B:97:PHE:N	2.48	0.46
2:B:359:TYR:C	2:B:362:TYR:HB3	2.39	0.46
2:B:616:LEU:HA	2:B:619:ILE:HG22	1.98	0.46
2:B:677:LYS:HB2	2:B:682:PHE:CE2	2.51	0.46
2:B:1207:GLU:CD	2:B:1210:ARG:NH1	2.73	0.46
2:B:308:VAL:CG1	2:B:309:ASN:N	2.79	0.46
2:B:374:LYS:HA	2:B:374:LYS:HE3	1.96	0.46
2:B:530:VAL:O	2:B:578:VAL:HG22	2.15	0.46
2:B:597:LEU:HG	2:B:597:LEU:H	1.52	0.46
2:B:686:ASP:CG	2:B:691:ARG:NH2	2.73	0.46
2:B:914:ALA:HB3	2:B:1032:ALA:HB1	1.95	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:G:HO2'	2:B:363:ILE:CD1	2.25	0.46
2:B:47:LEU:HG	2:B:751:MET:HE1	1.97	0.46
2:B:515:TYR:O	2:B:515:TYR:HD2	1.98	0.46
2:B:986:ASP:O	2:B:990:ASN:ND2	2.48	0.46
2:B:1139:VAL:HG13	2:B:1167:THR:HG22	1.94	0.46
2:B:297:SER:O	2:B:301:LEU:HG	2.15	0.46
2:B:518:PHE:HZ	2:B:679:ILE:HG21	1.54	0.46
2:B:520:VAL:HG23	2:B:591:LEU:HD21	1.80	0.46
2:B:949:LEU:HD11	2:B:950:ILE:O	2.15	0.46
2:B:1043:MET:HE3	2:B:1046:PHE:HE2	1.81	0.46
2:B:348:LYS:HG2	2:B:352:PHE:HB2	1.96	0.46
2:B:483:ASP:C	2:B:487:SER:HG	2.03	0.46
2:B:859:ARG:NE	2:B:860:SER:HG	1.98	0.46
2:B:1274:SER:O	2:B:1277:SER:HB3	2.16	0.46
2:B:1348:ILE:HD11	2:B:1357:GLU:OE1	2.15	0.46
2:B:245:SER:HA	2:B:297:SER:HB2	1.97	0.46
2:B:1224:ASN:CB	2:B:1280:VAL:HG11	2.46	0.46
2:B:746:GLU:OE1	2:B:1352:ILE:HG22	2.15	0.45
2:B:1045:PHE:O	2:B:1064:GLU:OE2	2.33	0.45
2:B:1065:THR:HB	2:B:1072:ILE:HG12	1.98	0.45
2:B:1211:LYS:NZ	2:B:1211:LYS:CB	2.78	0.45
1:A:8:G:C4'	2:B:894:GLN:OE1	2.64	0.45
1:A:67:C:OP1	2:B:742:LYS:NZ	2.47	0.45
2:B:128:TYR:OH	2:B:135:ILE:HD13	2.16	0.45
2:B:465:MET:HE1	2:B:467:ARG:HG2	1.97	0.45
2:B:572:ILE:O	2:B:572:ILE:CG2	2.63	0.45
2:B:859:ARG:NH1	2:B:859:ARG:CG	2.75	0.45
2:B:557:ARG:HG2	2:B:595:HIS:CB	2.46	0.45
2:B:1212:ARG:NH1	2:B:1336:TYR:CD2	2.77	0.45
2:B:111:LYS:HD3	2:B:115:ARG:HA	1.99	0.45
2:B:201:ILE:HG23	2:B:230:PRO:HD2	1.98	0.45
2:B:348:LYS:HG3	2:B:352:PHE:CG	2.52	0.45
2:B:686:ASP:CG	2:B:690:ASN:HA	2.42	0.45
2:B:857:LEU:C	2:B:857:LEU:CD2	2.86	0.45
2:B:895:ARG:HD2	2:B:895:ARG:O	2.16	0.45
2:B:969:ASP:C	2:B:970:PHE:HD1	2.25	0.45
2:B:398:LEU:C	2:B:398:LEU:HD12	2.41	0.45
2:B:966:PHE:CD1	2:B:970:PHE:CD2	3.04	0.45
2:B:20:VAL:O	2:B:27:VAL:HB	2.16	0.45
2:B:37:ASN:OD1	2:B:1360:ILE:HG23	2.17	0.45
1:A:49:A:H1'	2:B:1122:ARG:HH11	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:C:H2'	2:B:44:LYS:O	2.16	0.45
2:B:372:PHE:CD1	2:B:372:PHE:O	2.70	0.45
2:B:687:GLY:O	2:B:689:ALA:N	2.48	0.45
2:B:478:PHE:CD2	2:B:478:PHE:O	2.70	0.45
2:B:489:GLN:CG	2:B:493:GLU:CD	2.89	0.45
2:B:823:TYR:CD1	2:B:875:VAL:HG11	2.52	0.45
2:B:1270:ILE:HG23	2:B:1273:ILE:HD11	1.97	0.45
2:B:350:ILE:O	2:B:359:TYR:N	2.47	0.45
2:B:362:TYR:CD1	2:B:362:TYR:O	2.70	0.45
2:B:723:HIS:CE1	2:B:727:LEU:HD21	2.51	0.45
2:B:933:GLN:OE1	2:B:934:ILE:HG13	2.16	0.45
2:B:979:ASN:C	2:B:980:ASN:HD22	2.23	0.45
2:B:1078:ARG:O	2:B:1082:THR:HG23	2.16	0.45
2:B:1105:PHE:CE2	2:B:1169:MET:HG3	2.52	0.45
2:B:1218:GLY:O	2:B:1337:THR:C	2.58	0.45
2:B:226:ILE:CA	2:B:229:LEU:HD21	2.44	0.45
2:B:304:ASP:OD1	2:B:304:ASP:N	2.45	0.45
2:B:597:LEU:HB2	2:B:601:ILE:CD1	2.47	0.45
2:B:746:GLU:O	2:B:750:VAL:N	2.48	0.45
2:B:874:GLU:O	2:B:877:LYS:HG3	2.17	0.45
2:B:53:PHE:HE1	2:B:54:ASP:O	1.94	0.44
2:B:225:LEU:CD1	2:B:229:LEU:HD23	2.46	0.44
2:B:686:ASP:N	2:B:690:ASN:ND2	2.64	0.44
2:B:817:GLN:OE1	2:B:857:LEU:O	2.35	0.44
2:B:1139:VAL:CA	2:B:1166:ILE:O	2.63	0.44
2:B:1243:GLU:CG	2:B:1246:LYS:HE2	2.47	0.44
2:B:1325:LYS:HB3	2:B:1330:THR:CB	2.47	0.44
1:A:24:U:H2'	1:A:25:U:O4'	2.17	0.44
1:A:48:A:H2'	1:A:49:A:H8	1.81	0.44
2:B:139:ARG:NH1	2:B:161:MET:HG2	2.32	0.44
2:B:1232:TYR:CZ	2:B:1268:GLU:HB3	2.52	0.44
2:B:1276:PHE:CE2	2:B:1316:THR:HA	2.51	0.44
1:A:42:A:HO2'	1:A:43:G:P	2.39	0.44
2:B:114:GLU:OE2	2:B:120:GLY:C	2.61	0.44
2:B:245:SER:O	2:B:246:LEU:C	2.59	0.44
2:B:265:GLN:O	2:B:271:TYR:CB	2.63	0.44
2:B:763:MET:HE3	2:B:763:MET:HB3	1.75	0.44
2:B:1276:PHE:O	2:B:1276:PHE:CD1	2.70	0.44
2:B:103:GLU:OE2	2:B:113:HIS:HB2	2.18	0.44
2:B:158:LEU:O	2:B:162:ILE:HG13	2.17	0.44
2:B:277:ASN:ND2	2:B:649:LYS:O	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:359:TYR:CZ	2:B:363:ILE:HD11	2.52	0.44
2:B:842:VAL:CG1	2:B:854:ASN:CG	2.89	0.44
2:B:975:VAL:CG1	2:B:978:ILE:HG13	2.47	0.44
2:B:1116:SER:O	2:B:1119:LEU:HD22	2.18	0.44
2:B:316:PRO:CG	2:B:317:LEU:N	2.81	0.44
2:B:359:TYR:O	2:B:359:TYR:CD1	2.70	0.44
2:B:466:THR:O	2:B:467:ARG:HG3	2.17	0.44
2:B:612:ASN:O	2:B:616:LEU:HG	2.17	0.44
2:B:51:LEU:HD13	2:B:1352:ILE:O	2.18	0.44
2:B:181:VAL:HG23	2:B:182:ASP:OD1	2.18	0.44
2:B:730:SER:O	2:B:733:ILE:HG22	2.18	0.44
2:B:887:LEU:O	2:B:887:LEU:HD23	2.16	0.44
2:B:478:PHE:O	2:B:478:PHE:HD2	2.01	0.44
2:B:552:LEU:HD22	2:B:559:VAL:HG22	1.99	0.44
2:B:811:LEU:O	2:B:811:LEU:HD13	2.18	0.44
2:B:1206:LEU:CA	2:B:1345:ALA:HB1	2.46	0.44
2:B:1217:ALA:O	2:B:1339:THR:HG21	2.18	0.44
2:B:790:GLU:OE1	2:B:889:ALA:HA	2.17	0.44
2:B:1039:TYR:O	2:B:1042:ILE:HG22	2.18	0.44
2:B:255:ASN:OD1	2:B:256:PHE:CD1	2.70	0.44
2:B:761:ILE:CD1	2:B:931:VAL:CG1	2.95	0.44
2:B:6:SER:OG	2:B:21:ILE:CD1	2.59	0.43
2:B:134:THR:CG2	2:B:136:TYR:CD2	3.01	0.43
2:B:386:THR:HG23	2:B:386:THR:O	2.18	0.43
2:B:518:PHE:CD1	2:B:667:ILE:HG12	2.52	0.43
2:B:553:PHE:CE2	2:B:559:VAL:CG1	2.93	0.43
2:B:1207:GLU:HG2	2:B:1210:ARG:NH1	2.33	0.43
2:B:780:ARG:HD3	2:B:812:TYR:CZ	2.52	0.43
2:B:966:PHE:O	2:B:970:PHE:HB2	2.19	0.43
2:B:1240:SER:HB2	2:B:1242:TYR:CE1	2.53	0.43
2:B:1245:LEU:C	2:B:1245:LEU:CD1	2.86	0.43
2:B:188:LEU:C	2:B:191:THR:HG1	2.21	0.43
2:B:265:GLN:O	2:B:271:TYR:CG	2.70	0.43
2:B:552:LEU:CD2	2:B:563:GLN:NE2	2.80	0.43
2:B:569:PHE:N	2:B:569:PHE:CD2	2.86	0.43
2:B:602:LYS:HE3	2:B:602:LYS:HB2	1.64	0.43
2:B:1204:PHE:CD1	2:B:1347:LEU:CG	3.01	0.43
2:B:1235:PHE:HD1	2:B:1258:PHE:CE2	2.37	0.43
2:B:1363:SER:C	2:B:1364:GLN:CD	2.85	0.43
1:A:15:U:O2'	2:B:450:TYR:O	2.30	0.43
1:A:58:G:C1'	2:B:457:ARG:HB2	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:18:TRP:O	2:B:48:ILE:HD13	2.07	0.43
2:B:135:ILE:HG21	2:B:160:HIS:CD2	2.53	0.43
2:B:181:VAL:CG2	2:B:209:LYS:HB2	2.48	0.43
2:B:266:LEU:H	2:B:266:LEU:HD12	1.84	0.43
2:B:270:THR:O	2:B:270:THR:OG1	2.34	0.43
2:B:971:GLN:C	2:B:972:PHE:CD1	2.96	0.43
2:B:202:ASN:ND2	2:B:204:SER:HA	2.33	0.43
2:B:1123:LYS:HD2	2:B:1123:LYS:HA	1.85	0.43
1:A:27:G:H4'	1:A:28:A:OP2	2.18	0.43
1:A:94:U:H2'	1:A:95:G:C8	2.52	0.43
2:B:320:SER:O	2:B:323:LYS:CB	2.47	0.43
2:B:334:LEU:HD11	2:B:338:LEU:HD11	1.97	0.43
2:B:882:TYR:HD2	2:B:883:TRP:HD1	1.66	0.43
2:B:1220:LEU:HD21	2:B:1342:VAL:HG21	2.00	0.43
2:B:1310:ILE:HA	2:B:1313:PHE:CD2	2.53	0.43
2:B:1359:ARG:HH11	2:B:1359:ARG:CG	2.11	0.43
2:B:34:VAL:HG11	2:B:1359:ARG:HD3	1.99	0.43
2:B:86:PHE:CE2	2:B:155:TYR:HB2	2.54	0.43
2:B:256:PHE:CD1	2:B:256:PHE:N	2.85	0.43
2:B:520:VAL:HG13	2:B:553:PHE:HE1	1.81	0.43
2:B:1119:LEU:N	2:B:1119:LEU:CD1	2.73	0.43
1:A:71:U:H2'	1:A:72:U:H6	1.83	0.43
2:B:118:ILE:C	2:B:119:PHE:HD1	2.26	0.43
2:B:298:ASP:O	2:B:302:LEU:HG	2.19	0.43
2:B:361:GLY:O	2:B:365:GLY:N	2.52	0.43
2:B:823:TYR:CE2	2:B:864:ARG:HB3	2.54	0.43
2:B:887:LEU:C	2:B:887:LEU:CD2	2.91	0.43
2:B:1203:LEU:HA	2:B:1212:ARG:O	2.18	0.43
2:B:1325:LYS:HB2	2:B:1330:THR:HA	2.00	0.43
1:A:8:G:HO2'	1:A:9:U:P	2.42	0.43
1:A:58:G:O2'	2:B:457:ARG:CA	2.58	0.43
2:B:118:ILE:HG22	2:B:119:PHE:HE1	1.77	0.43
2:B:234:LYS:C	2:B:234:LYS:HD3	2.43	0.43
2:B:482:VAL:HG12	2:B:483:ASP:C	2.44	0.43
2:B:672:ASP:HB2	2:B:704:PHE:HE2	1.84	0.43
2:B:1243:GLU:C	2:B:1246:LYS:HZ3	2.19	0.43
1:A:58:G:O4'	2:B:457:ARG:CD	2.46	0.43
2:B:18:TRP:HE1	2:B:50:ALA:H	1.61	0.43
2:B:256:PHE:CE2	2:B:282:ILE:HG12	2.54	0.43
2:B:307:ARG:HE	2:B:307:ARG:HB2	1.69	0.43
2:B:1143:VAL:HG12	2:B:1164:LEU:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1324:PHE:CD1	2:B:1324:PHE:N	2.86	0.43
2:B:24:GLU:O	2:B:25:TYR:HB2	2.19	0.42
2:B:106:LEU:HA	2:B:1131:TYR:CE2	2.54	0.42
2:B:177:ASP:C	2:B:179:SER:N	2.75	0.42
2:B:229:LEU:HD11	2:B:232:GLU:CB	2.45	0.42
2:B:282:ILE:HG23	2:B:286:TYR:HE1	1.72	0.42
2:B:317:LEU:HA	2:B:320:SER:OG	2.19	0.42
2:B:541:SER:N	2:B:544:GLN:OE1	2.48	0.42
2:B:594:TYR:CE2	2:B:607:LEU:HD12	2.54	0.42
2:B:1308:ASN:O	2:B:1311:HIS:HB2	2.18	0.42
1:A:93:G:H2'	1:A:94:U:C6	2.54	0.42
2:B:193:ASN:OD1	2:B:200:PRO:HA	2.19	0.42
2:B:202:ASN:ND2	2:B:204:SER:CA	2.82	0.42
2:B:1000:LYS:HB2	2:B:1073:VAL:HG21	2.01	0.42
2:B:22:THR:HG22	2:B:23:ASP:H	1.84	0.42
2:B:1222:LYS:O	2:B:1318:LEU:HA	2.19	0.42
2:B:1235:PHE:CE1	2:B:1258:PHE:CE2	3.07	0.42
2:B:513:LEU:O	2:B:516:GLU:N	2.53	0.42
2:B:573:GLU:OE1	2:B:573:GLU:HA	2.18	0.42
2:B:817:GLN:HB3	2:B:820:ARG:O	2.20	0.42
2:B:1157:LEU:N	2:B:1157:LEU:CD1	2.73	0.42
2:B:1163:LEU:HD12	2:B:1339:THR:HB	2.02	0.42
2:B:1211:LYS:NZ	2:B:1211:LYS:HB2	2.35	0.42
2:B:672:ASP:HB2	2:B:704:PHE:CE2	2.54	0.42
2:B:686:ASP:HB3	2:B:689:ALA:C	2.44	0.42
2:B:1154:SER:HB2	2:B:1156:LYS:HG3	2.01	0.42
2:B:1333:ARG:HD2	2:B:1335:ARG:HG3	2.02	0.42
2:B:201:ILE:HG22	2:B:202:ASN:H	1.85	0.42
2:B:229:LEU:CD1	2:B:229:LEU:C	2.85	0.42
2:B:482:VAL:CG1	2:B:483:ASP:N	2.83	0.42
2:B:495:MET:SD	3:C:17:DA:O4'	2.77	0.42
2:B:603:ASP:OD1	2:B:606:PHE:N	2.53	0.42
2:B:1239:ALA:HB3	2:B:1306:ALA:HB1	2.01	0.42
2:B:560:THR:OG1	2:B:563:GLN:HG3	2.19	0.42
2:B:569:PHE:N	2:B:569:PHE:HD2	2.17	0.42
2:B:818:ASN:ND2	2:B:818:ASN:O	2.52	0.42
2:B:843:PRO:HG2	2:B:846:PHE:CE2	2.55	0.42
2:B:1036:TYR:O	2:B:1040:SER:HB3	2.20	0.42
2:B:1210:ARG:CG	2:B:1280:VAL:HG22	2.44	0.42
2:B:60:GLU:HA	2:B:63:ARG:NH1	2.35	0.42
2:B:178:ASN:HA	2:B:299:ALA:CB	2.41	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:495:MET:H	2:B:495:MET:HG2	1.52	0.42
2:B:672:ASP:HA	2:B:703:THR:HG22	2.02	0.42
2:B:733:ILE:O	2:B:737:ILE:HG13	2.18	0.42
2:B:920:GLN:OE1	2:B:961:LYS:HE3	2.20	0.42
1:A:40:C:H2'	1:A:41:A:C8	2.55	0.42
2:B:10:ALA:O	2:B:17:GLY:N	2.52	0.42
2:B:219:SER:O	2:B:223:GLU:HG3	2.20	0.42
2:B:316:PRO:CD	2:B:317:LEU:N	2.83	0.42
2:B:518:PHE:HD1	2:B:667:ILE:CD1	2.32	0.42
2:B:652:LYS:HE2	2:B:652:LYS:HB2	1.82	0.42
2:B:389:LEU:O	2:B:392:LYS:N	2.53	0.42
2:B:704:PHE:O	2:B:708:ILE:HG12	2.20	0.42
2:B:810:LYS:HE2	2:B:838:VAL:HG23	2.02	0.42
2:B:883:TRP:CZ3	2:B:900:LEU:HD22	2.54	0.42
2:B:1364:GLN:HG2	2:B:1364:GLN:O	2.19	0.42
2:B:135:ILE:HG21	2:B:160:HIS:NE2	2.34	0.41
2:B:197:GLU:O	2:B:200:PRO:HD3	2.19	0.41
2:B:374:LYS:HE3	2:B:374:LYS:O	2.20	0.41
2:B:398:LEU:CG	2:B:399:LEU:H	2.30	0.41
2:B:516:GLU:C	2:B:519:THR:HG22	2.45	0.41
2:B:733:ILE:HG12	2:B:763:MET:HE1	2.01	0.41
2:B:27:VAL:HG12	2:B:1086:VAL:HG22	2.02	0.41
2:B:256:PHE:N	2:B:256:PHE:HD1	2.18	0.41
2:B:316:PRO:C	2:B:319:ALA:HB3	2.45	0.41
2:B:492:ILE:HG23	3:C:17:DA:H5'	2.02	0.41
2:B:591:LEU:HD12	2:B:594:TYR:CG	2.54	0.41
2:B:733:ILE:CG1	2:B:763:MET:HE1	2.49	0.41
2:B:361:GLY:CA	2:B:365:GLY:H	2.32	0.41
2:B:625:LEU:HD13	2:B:659:TRP:HZ2	1.86	0.41
2:B:760:VAL:HG13	2:B:956:ILE:CG2	2.50	0.41
2:B:882:TYR:O	2:B:886:LEU:HG	2.21	0.41
2:B:266:LEU:HG	2:B:271:TYR:CZ	2.55	0.41
2:B:905:ARG:NH1	3:C:24:DG:OP1	2.54	0.41
2:B:313:THR:O	2:B:313:THR:HG23	2.20	0.41
2:B:331:ASP:HB3	2:B:398:LEU:CD1	2.49	0.41
2:B:451:TYR:HA	2:B:491:PHE:CE1	2.30	0.41
2:B:519:THR:HG23	2:B:520:VAL:N	2.36	0.41
2:B:551:LEU:HD12	2:B:552:LEU:N	2.36	0.41
2:B:48:ILE:HG13	2:B:1092:VAL:HG13	2.01	0.41
2:B:376:ILE:HD12	2:B:376:ILE:N	2.36	0.41
2:B:512:SER:OG	2:B:617:GLU:OE1	2.24	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:895:ARG:C	2:B:895:ARG:CD	2.85	0.41
1:A:64:U:O3'	2:B:57:GLU:HB2	2.21	0.41
2:B:181:VAL:HG23	2:B:182:ASP:N	2.36	0.41
2:B:492:ILE:CG2	3:C:17:DA:H5'	2.51	0.41
2:B:846:PHE:HB3	2:B:916:PHE:HD2	1.85	0.41
2:B:855:LYS:HB3	2:B:855:LYS:HE2	1.76	0.41
2:B:1105:PHE:CZ	2:B:1169:MET:HG3	2.56	0.41
1:A:67:C:P	2:B:739:GLN:HE22	2.43	0.41
2:B:315:ALA:HB1	2:B:418:GLU:HG2	2.01	0.41
2:B:376:ILE:HD12	2:B:376:ILE:H	1.85	0.41
2:B:563:GLN:O	2:B:567:ASP:N	2.48	0.41
2:B:846:PHE:O	2:B:920:GLN:NE2	2.44	0.41
2:B:1229:PRO:CD	2:B:1232:TYR:CD2	2.94	0.41
1:A:23:U:H3	1:A:48:A:H2	1.66	0.41
2:B:18:TRP:CA	2:B:49:GLY:O	2.69	0.41
2:B:27:VAL:HG12	2:B:1086:VAL:CG2	2.51	0.41
2:B:37:ASN:OD1	2:B:1360:ILE:HA	2.21	0.41
2:B:48:ILE:CG1	2:B:1092:VAL:HG13	2.51	0.41
2:B:188:LEU:O	2:B:192:TYR:N	2.46	0.41
2:B:328:HIS:ND1	2:B:399:LEU:CB	2.84	0.41
2:B:530:VAL:O	2:B:578:VAL:CG2	2.69	0.41
2:B:624:THR:HA	2:B:656:TYR:HB2	2.02	0.41
2:B:686:ASP:H	2:B:690:ASN:HD21	1.68	0.41
2:B:724:ILE:HD12	2:B:738:LEU:HG	2.03	0.41
2:B:1149:VAL:O	2:B:1149:VAL:HG23	2.20	0.41
2:B:1276:PHE:CD2	2:B:1316:THR:HB	2.56	0.41
1:A:7:U:O2'	2:B:894:GLN:OE1	2.28	0.41
1:A:31:U:H2'	1:A:32:A:O4'	2.20	0.41
2:B:21:ILE:HD12	2:B:21:ILE:C	2.44	0.41
2:B:79:ILE:H	2:B:79:ILE:HG12	1.68	0.41
2:B:300:ILE:CG2	2:B:301:LEU:N	2.83	0.41
2:B:421:ALA:HA	2:B:424:ARG:HB2	2.03	0.41
2:B:465:MET:SD	2:B:465:MET:O	2.79	0.41
2:B:1050:ILE:HG13	2:B:1059:LYS:N	2.36	0.41
2:B:1139:VAL:HG11	2:B:1166:ILE:C	2.38	0.41
2:B:100:ARG:HD2	2:B:117:PRO:HA	2.03	0.40
2:B:451:TYR:HA	2:B:491:PHE:HD1	0.68	0.40
2:B:510:LYS:HG2	2:B:659:TRP:C	2.47	0.40
2:B:1205:GLU:O	2:B:1346:THR:OG1	2.35	0.40
4:D:3:DT:H2''	4:D:4:DT:H71	2.03	0.40
2:B:154:ILE:O	2:B:158:LEU:HG	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:681:ASP:HA	2:B:684:LYS:HE2	2.03	0.40
2:B:1276:PHE:CD1	2:B:1276:PHE:C	2.98	0.40
1:A:58:G:O2'	2:B:457:ARG:HB3	2.03	0.40
2:B:27:VAL:HG11	2:B:1086:VAL:HG13	2.02	0.40
2:B:301:LEU:O	2:B:304:ASP:OD1	2.39	0.40
2:B:518:PHE:CE1	2:B:679:ILE:CG2	2.91	0.40
2:B:1235:PHE:CE1	2:B:1259:VAL:HA	2.56	0.40
2:B:215:ARG:O	2:B:215:ARG:NE	2.44	0.40
2:B:557:ARG:HA	2:B:595:HIS:HD2	1.32	0.40
2:B:755:LYS:HZ1	2:B:942:LYS:HE2	1.87	0.40
2:B:939:MET:HG3	2:B:953:VAL:HG11	2.04	0.40
2:B:963:VAL:CG2	2:B:990:ASN:OD1	2.66	0.40
2:B:1183:GLU:HG2	2:B:1187:TYR:O	2.21	0.40
2:B:88:ASN:O	2:B:92:LYS:HE3	2.21	0.40
2:B:188:LEU:HA	2:B:191:THR:OG1	2.22	0.40
2:B:350:ILE:CD1	2:B:350:ILE:N	2.84	0.40
2:B:823:TYR:CD2	2:B:858:THR:HG21	2.56	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:232:GLU:O	2:B:573:GLU:OE2[4_445]	1.99	0.21
2:B:226:ILE:CD1	2:B:574:CYS:SG[4_445]	2.08	0.12
2:B:611:GLU:O	2:B:859:ARG:NH2[1_565]	2.12	0.08

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	B	1318/1368 (96%)	1254 (95%)	62 (5%)	2 (0%)	43 75

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	250	PRO
2	B	316	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	B	1183/1225 (97%)	1024 (87%)	159 (13%)	4 18

All (159) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	22	THR
2	B	26	LYS
2	B	48	ILE
2	B	104	SER
2	B	112	LYS
2	B	114	GLU
2	B	115	ARG
2	B	118	ILE
2	B	125	GLU
2	B	129	HIS
2	B	132	TYR
2	B	135	ILE
2	B	182	ASP
2	B	183	LYS
2	B	185	PHE
2	B	188	LEU
2	B	189	VAL
2	B	194	GLN
2	B	195	LEU
2	B	196	PHE
2	B	197	GLU
2	B	204	SER
2	B	232	GLU

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Mol	Chain	Res	Type
2	B	233	LYS
2	B	246	LEU
2	B	248	LEU
2	B	252	PHE
2	B	253	LYS
2	B	258	LEU
2	B	260	GLU
2	B	261	ASP
2	B	281	GLN
2	B	282	ILE
2	B	284	ASP
2	B	294	LYS
2	B	296	LEU
2	B	300	ILE
2	B	303	SER
2	B	307	ARG
2	B	310	THR
2	B	311	GLU
2	B	312	ILE
2	B	314	LYS
2	B	317	LEU
2	B	318	SER
2	B	346	LYS
2	B	347	TYR
2	B	350	ILE
2	B	362	TYR
2	B	372	PHE
2	B	374	LYS
2	B	376	ILE
2	B	379	ILE
2	B	383	MET
2	B	384	ASP
2	B	387	GLU
2	B	390	LEU
2	B	393	LEU
2	B	395	ARG
2	B	397	ASP
2	B	398	LEU
2	B	399	LEU
2	B	400	ARG
2	B	460	SER
2	B	461	ARG

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Mol	Chain	Res	Type
2	B	464	TRP
2	B	465	MET
2	B	480	GLU
2	B	491	PHE
2	B	492	ILE
2	B	494	ARG
2	B	495	MET
2	B	518	PHE
2	B	521	TYR
2	B	522	ASN
2	B	548	ILE
2	B	551	LEU
2	B	552	LEU
2	B	555	THR
2	B	557	ARG
2	B	564	LEU
2	B	570	LYS
2	B	574	CYS
2	B	576	ASP
2	B	577	SER
2	B	591	LEU
2	B	593	THR
2	B	597	LEU
2	B	598	LEU
2	B	600	ILE
2	B	601	ILE
2	B	602	LYS
2	B	661	ARG
2	B	662	LEU
2	B	664	ARG
2	B	665	LYS
2	B	666	LEU
2	B	686	ASP
2	B	691	ARG
2	B	719	SER
2	B	720	LEU
2	B	723	HIS
2	B	727	LEU
2	B	761	ILE
2	B	763	MET
2	B	844	GLN
2	B	855	LYS

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Mol	Chain	Res	Type
2	B	858	THR
2	B	860	SER
2	B	861	ASP
2	B	870	VAL
2	B	873	GLU
2	B	885	GLN
2	B	886	LEU
2	B	887	LEU
2	B	893	THR
2	B	895	ARG
2	B	944	ASP
2	B	945	GLU
2	B	948	LYS
2	B	949	LEU
2	B	969	ASP
2	B	971	GLN
2	B	973	TYR
2	B	1064	GLU
2	B	1065	THR
2	B	1116	SER
2	B	1119	LEU
2	B	1138	THR
2	B	1148	LYS
2	B	1154	SER
2	B	1157	LEU
2	B	1158	LYS
2	B	1159	SER
2	B	1206	LEU
2	B	1207	GLU
2	B	1210	ARG
2	B	1211	LYS
2	B	1231	LYS
2	B	1240	SER
2	B	1243	GLU
2	B	1244	LYS
2	B	1245	LEU
2	B	1246	LYS
2	B	1248	SER
2	B	1274	SER
2	B	1275	GLU
2	B	1287	LEU
2	B	1325	LYS

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Mol	Chain	Res	Type
2	B	1327	PHE
2	B	1328	ASP
2	B	1329	THR
2	B	1340	LYS
2	B	1341	GLU
2	B	1343	LEU
2	B	1347	LEU
2	B	1359	ARG
2	B	1362	LEU
2	B	1364	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	190	GLN
2	B	199	ASN
2	B	202	ASN
2	B	265	GLN
2	B	330	GLN
2	B	342	GLN
2	B	459	ASN
2	B	522	ASN
2	B	690	ASN
2	B	754	HIS
2	B	799	HIS
2	B	817	GLN
2	B	946	ASN
2	B	980	ASN
2	B	990	ASN
2	B	1091	GLN
2	B	1224	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	93/98 (94%)	27 (29%)	4 (4%)

All (27) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	9	U
1	A	11	C
1	A	27	G
1	A	28	A
1	A	29	G
1	A	34	A
1	A	37	U
1	A	38	A
1	A	40	C
1	A	42	A
1	A	43	G
1	A	51	A
1	A	56	U
1	A	57	A
1	A	59	U
1	A	60	C
1	A	63	U
1	A	68	A
1	A	69	A
1	A	74	A
1	A	77	A
1	A	82	G
1	A	87	G
1	A	89	G
1	A	90	U
1	A	91	C
1	A	92	G

All (4) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	8	G
1	A	27	G
1	A	42	A
1	A	68	A

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	94/98 (95%)	2.06	42 (44%) 0 1	12, 36, 69, 103	0
2	B	1326/1368 (96%)	1.31	270 (20%) 3 5	5, 29, 53, 90	0
3	C	24/24 (100%)	1.36	5 (20%) 2 4	22, 36, 57, 65	0
4	D	11/11 (100%)	1.48	3 (27%) 1 3	22, 41, 84, 95	0
All	All	1455/1501 (96%)	1.36	320 (21%) 2 4	5, 29, 56, 103	0

All (320) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	813	LEU	6.8
2	B	19	ALA	6.8
2	B	1043	MET	6.6
2	B	1223	GLY	6.5
2	B	1263	LYS	6.5
2	B	158	LEU	6.4
2	B	994	GLY	6.2
2	B	1007	GLU	6.2
2	B	65	LYS	5.8
2	B	1352	ILE	5.6
2	B	136	TYR	5.6
2	B	551	LEU	5.6
2	B	1134	PHE	5.6
2	B	399	LEU	5.5
2	B	1354	GLY	5.5
2	B	1225	GLU	5.4
2	B	993	VAL	5.4
2	B	398	LEU	5.4
2	B	1224	ASN	5.3
2	B	917	ILE	5.2
2	B	413	GLN	5.0

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Mol	Chain	Res	Type	RSRZ
2	B	1355	LEU	4.9
1	A	44	U	4.8
2	B	49	GLY	4.8
2	B	1356	TYR	4.7
2	B	48	ILE	4.6
2	B	72	TYR	4.6
2	B	40	ARG	4.6
2	B	728	ALA	4.5
2	B	938	ARG	4.5
2	B	80	CYS	4.5
1	A	93	G	4.5
2	B	76	LYS	4.4
2	B	520	VAL	4.4
1	A	28	A	4.4
2	B	1095	VAL	4.4
2	B	1126	TRP	4.3
1	A	17	G	4.3
2	B	997	LEU	4.3
2	B	50	ALA	4.3
2	B	1204	PHE	4.3
2	B	154	ILE	4.3
2	B	739	GLN	4.2
1	A	92	G	4.2
2	B	1295	ASN	4.2
2	B	978	ILE	4.2
2	B	1342	VAL	4.1
2	B	675	SER	4.1
2	B	74	ARG	4.1
2	B	927	ILE	4.1
2	B	560	THR	4.0
1	A	27	G	3.9
1	A	67	C	3.9
2	B	1220	LEU	3.8
2	B	1236	LEU	3.8
2	B	317	LEU	3.8
2	B	888	ASN	3.7
2	B	852	ILE	3.7
1	A	34	A	3.7
2	B	1085	LYS	3.7
1	A	91	C	3.7
2	B	659	TRP	3.6
2	B	62	THR	3.6

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Mol	Chain	Res	Type	RSRZ
2	B	68	ALA	3.5
2	B	443	ILE	3.5
2	B	688	PHE	3.5
2	B	1098	THR	3.5
2	B	152	ARG	3.5
2	B	587	PHE	3.4
2	B	501	ASN	3.4
2	B	559	VAL	3.4
2	B	1349	HIS	3.4
2	B	18	TRP	3.4
2	B	934	ILE	3.4
1	A	88	A	3.4
2	B	47	LEU	3.3
2	B	946	ASN	3.3
2	B	834	SER	3.3
1	A	90	U	3.3
2	B	385	GLY	3.3
2	B	518	PHE	3.3
2	B	1359	ARG	3.3
2	B	924	THR	3.3
2	B	134	THR	3.3
2	B	742	LYS	3.2
2	B	1138	THR	3.2
1	A	14	A	3.2
2	B	295	ASN	3.2
2	B	979	ASN	3.2
2	B	1216	SER	3.2
2	B	1226	LEU	3.2
2	B	242	ILE	3.2
1	A	70	C	3.1
2	B	133	PRO	3.1
2	B	449	PRO	3.1
2	B	824	VAL	3.1
2	B	614	ASP	3.1
2	B	1137	PRO	3.1
2	B	823	TYR	3.1
2	B	383	MET	3.1
2	B	452	VAL	3.1
2	B	132	TYR	3.1
2	B	476	TRP	3.1
1	A	42	A	3.1
2	B	150	ASP	3.1

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Mol	Chain	Res	Type	RSRZ
2	B	524	LEU	3.0
1	A	29	G	3.0
1	A	82	G	3.0
2	B	841	ILE	3.0
2	B	975	VAL	3.0
2	B	1009	VAL	3.0
2	B	616	LEU	3.0
2	B	1209	GLY	3.0
2	B	31	LYS	3.0
2	B	45	LYS	3.0
2	B	515	TYR	3.0
2	B	617	GLU	3.0
2	B	305	ILE	3.0
2	B	156	LEU	3.0
2	B	621	LEU	3.0
2	B	740	THR	3.0
2	B	935	LEU	3.0
2	B	957	THR	3.0
2	B	231	GLY	2.9
2	B	639	TYR	2.9
2	B	367	ALA	2.9
2	B	69	ARG	2.9
2	B	473	ILE	2.9
2	B	335	LEU	2.9
2	B	364	ASP	2.9
2	B	435	ASP	2.9
2	B	933	GLN	2.9
2	B	1350	GLN	2.9
2	B	445	THR	2.9
2	B	1140	ALA	2.9
2	B	1111	LEU	2.9
2	B	1234	ASN	2.9
2	B	292	ALA	2.9
2	B	1124	LYS	2.8
2	B	931	VAL	2.8
2	B	1075	ASP	2.8
2	B	746	GLU	2.8
2	B	415	HIS	2.8
2	B	544	GLN	2.8
1	A	52	A	2.8
2	B	1211	LYS	2.8
1	A	58	G	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	81	G	2.8
2	B	947	ASP	2.8
1	A	51	A	2.8
2	B	228	GLN	2.8
2	B	1008	PHE	2.8
2	B	818	ASN	2.8
2	B	995	THR	2.7
2	B	29	SER	2.7
2	B	85	ILE	2.7
2	B	368	SER	2.7
2	B	453	GLY	2.7
2	B	747	LEU	2.7
2	B	75	ARG	2.7
2	B	181	VAL	2.7
1	A	68	A	2.7
2	B	564	LEU	2.7
2	B	366	GLY	2.7
2	B	343	LEU	2.7
2	B	423	LEU	2.7
2	B	1336	TYR	2.6
2	B	143	VAL	2.6
2	B	783	ARG	2.6
2	B	332	LEU	2.6
1	A	15	U	2.6
2	B	918	LYS	2.6
2	B	1213	MET	2.6
1	A	62	G	2.6
2	B	43	ILE	2.6
2	B	792	GLY	2.6
2	B	1353	THR	2.6
1	A	48	A	2.6
1	A	45	U	2.6
2	B	235	ASN	2.6
2	B	118	ILE	2.6
1	A	98	C	2.6
2	B	939	MET	2.6
2	B	1110	ILE	2.5
2	B	163	LYS	2.5
2	B	329	HIS	2.5
2	B	654	ARG	2.5
2	B	1335	ARG	2.5
2	B	129	HIS	2.5

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Mol	Chain	Res	Type	RSRZ
2	B	836	TYR	2.5
2	B	785	GLU	2.5
2	B	161	MET	2.5
1	A	87	G	2.5
2	B	862	LYS	2.5
1	A	26	A	2.5
2	B	713	VAL	2.5
2	B	238	PHE	2.5
2	B	83	GLN	2.5
2	B	737	ILE	2.5
2	B	1042	ILE	2.5
2	B	1267	ASP	2.5
2	B	1351	SER	2.5
2	B	743	VAL	2.5
2	B	744	VAL	2.5
1	A	6	G	2.5
1	A	13	A	2.5
2	B	475	PRO	2.5
2	B	1006	SER	2.5
2	B	1119	LEU	2.4
2	B	1164	LEU	2.4
2	B	822	MET	2.4
1	A	65	A	2.4
2	B	20	VAL	2.4
2	B	159	ALA	2.4
2	B	426	GLN	2.4
4	D	2	DT	2.4
2	B	365	GLY	2.4
2	B	451	TYR	2.4
2	B	724	ILE	2.4
1	A	5	C	2.4
1	A	76	A	2.4
2	B	386	THR	2.4
2	B	1202	SER	2.4
2	B	331	ASP	2.4
2	B	260	GLU	2.4
2	B	1092	VAL	2.4
2	B	749	LYS	2.4
1	A	78	A	2.3
2	B	173	ASP	2.3
2	B	698	HIS	2.3
2	B	729	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	828	LEU	2.3
2	B	1266	LEU	2.3
1	A	25	U	2.3
2	B	1153	LYS	2.3
2	B	32	PHE	2.3
2	B	89	GLU	2.3
2	B	417	GLY	2.3
2	B	34	VAL	2.3
2	B	683	LEU	2.3
2	B	850	ASP	2.3
4	D	3	DT	2.3
2	B	1203	LEU	2.3
2	B	1347	LEU	2.3
1	A	59	U	2.3
2	B	543	GLU	2.3
2	B	977	GLU	2.3
2	B	176	PRO	2.3
2	B	233	LYS	2.3
2	B	899	ASN	2.2
2	B	1201	TYR	2.2
2	B	1357	GLU	2.2
1	A	95	G	2.2
2	B	411	PRO	2.2
2	B	412	HIS	2.2
2	B	930	HIS	2.2
2	B	759	ILE	2.2
2	B	293	ALA	2.2
4	D	6	DG	2.2
2	B	362	TYR	2.2
2	B	1109	SER	2.2
2	B	655	ARG	2.2
2	B	1171	ARG	2.2
2	B	697	ILE	2.2
2	B	553	PHE	2.2
2	B	970	PHE	2.2
2	B	5	TYR	2.2
2	B	35	LEU	2.2
2	B	403	ARG	2.2
2	B	990	ASN	2.2
2	B	914	ALA	2.2
3	C	19	DA	2.2
2	B	795	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	509	PRO	2.2
2	B	1128	PRO	2.2
2	B	761	ILE	2.1
3	C	15	DT	2.1
2	B	347	TYR	2.1
3	C	2	DA	2.1
2	B	779	GLU	2.1
2	B	625	LEU	2.1
2	B	459	ASN	2.1
2	B	839	ASP	2.1
2	B	206	VAL	2.1
3	C	9	DC	2.1
1	A	18	A	2.1
1	A	84	A	2.1
2	B	128	TYR	2.1
2	B	4	LYS	2.1
2	B	959	LYS	2.1
2	B	853	ASP	2.1
2	B	1039	TYR	2.1
2	B	466	THR	2.1
2	B	622	THR	2.1
2	B	400	ARG	2.1
2	B	79	ILE	2.1
2	B	734	LYS	2.1
2	B	164	PHE	2.1
2	B	1214	LEU	2.1
2	B	874	GLU	2.1
2	B	448	ILE	2.1
2	B	342	GLN	2.1
2	B	817	GLN	2.1
2	B	1101	GLN	2.1
2	B	549	VAL	2.1
2	B	1010	TYR	2.0
2	B	1334	LYS	2.0
2	B	296	LEU	2.0
2	B	1093	ASN	2.0
2	B	858	THR	2.0
2	B	258	LEU	2.0
3	C	20	DA	2.0
1	A	32	A	2.0
1	A	77	A	2.0
2	B	402	GLN	2.0

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Mol	Chain	Res	Type	RSRZ
2	B	323	LYS	2.0
2	B	915	GLY	2.0
2	B	667	ILE	2.0
1	A	66	U	2.0
2	B	1100	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.