



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 14, 2025 – 04:48 PM JST

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](mailto: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>.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

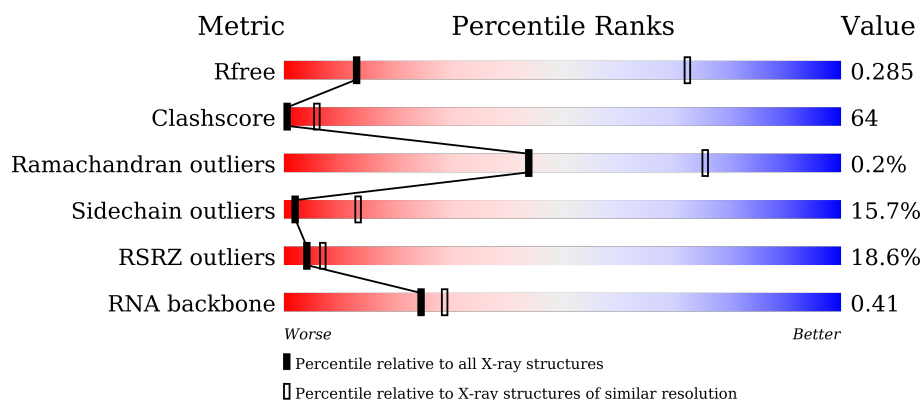
# 1 Overall quality at a glance

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))
$R_{free}$	164625	1175 (4.14-3.70)
Clashscore	180529	1045 (4.12-3.72)
Ramachandran outliers	177936	1006 (4.12-3.72)
Sidechain outliers	177891	1185 (4.14-3.70)
RSRZ outliers	164620	1175 (4.14-3.70)
RNA backbone	3690	1136 (4.84-3.00)

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  $\geq 3$ , 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	<div> <div>34%</div> <div> <div>33%</div> <div>43%</div> <div>20%</div> <div>.</div> </div> </div>
2	B	1368	<div> <div>17%</div> <div> <div>39%</div> <div>46%</div> <div>12%</div> <div>..</div> </div> </div>
3	C	24	<div> <div>12%</div> <div> <div>38%</div> <div>63%</div> </div> </div>
4	D	11	<div> <div>27%</div> <div> <div>64%</div> <div>36%</div> </div> </div>

## 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			

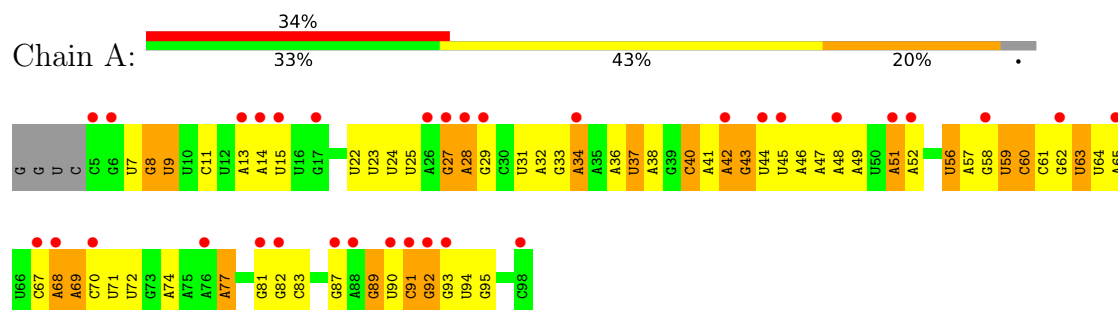
- Molecule 5 is water.

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

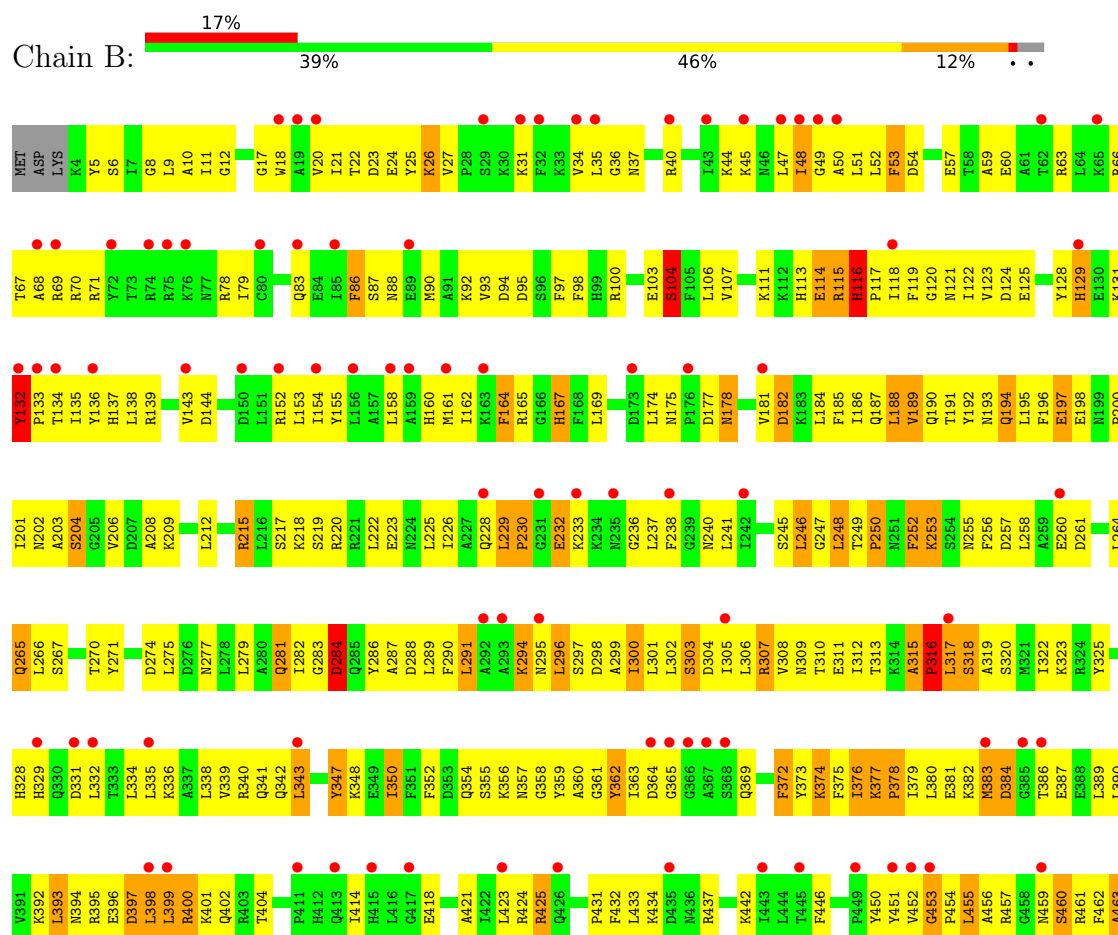
### 3 Residue-property plots [i](#)

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)



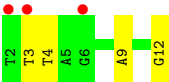
#### • Molecule 2: CRISPR-associated endonuclease Cas9/Csn1







● 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, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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	21237 reflections (9.96%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	-2.7	Xtriage
Anisotropy	8.165	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.16 , 0.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.38$ , $\langle L^2 \rangle = 0.21$	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 <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	0.25	0/2249	0.81	0/3503
2	B	0.39	6/11008 (0.1%)	0.71	48/14794 (0.3%)
3	C	0.64	0/541	1.01	0/831
4	D	0.55	0/251	1.05	0/387
All	All	0.39	6/14049 (0.0%)	0.75	48/19515 (0.2%)

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

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

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1137	PRO	N-CD	5.32	1.55	1.47
2	B	378	PRO	N-CD	5.26	1.55	1.47
2	B	230	PRO	N-CD	5.15	1.55	1.47
2	B	133	PRO	N-CD	5.07	1.54	1.47
2	B	843	PRO	N-CD	5.07	1.54	1.47
2	B	316	PRO	N-CD	5.04	1.54	1.47

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	675	SER	CB-CA-C	-19.99	72.11	110.10
2	B	1222	LYS	CB-CA-C	-14.01	82.39	110.40
2	B	284	ASP	CB-CA-C	-10.87	88.67	110.40
2	B	164	PHE	N-CA-C	-10.23	83.39	111.00
2	B	1222	LYS	N-CA-C	9.77	137.38	111.00
2	B	1215	ALA	CB-CA-C	8.25	122.47	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	95	ASP	CB-CA-C	7.77	125.94	110.40
2	B	675	SER	N-CA-C	7.67	131.70	111.00
2	B	905	ARG	CB-CA-C	7.65	125.70	110.40
2	B	675	SER	C-N-CA	7.58	138.21	122.30
2	B	178	ASN	N-CA-C	-7.50	90.74	111.00
2	B	567	ASP	CB-CA-C	7.42	125.24	110.40
2	B	164	PHE	CB-CA-C	7.34	125.08	110.40
2	B	1351	SER	CB-CA-C	-7.05	96.71	110.10
2	B	591	LEU	N-CA-C	-6.73	92.83	111.00
2	B	315	ALA	CB-CA-C	-6.64	100.14	110.10
2	B	455	LEU	N-CA-C	-6.62	93.13	111.00
2	B	879	MET	CB-CA-C	6.49	123.38	110.40
2	B	104	SER	N-CA-CB	6.37	120.05	110.50
2	B	1177	ASN	N-CA-C	-6.34	93.89	111.00
2	B	265	GLN	CB-CA-C	6.23	122.86	110.40
2	B	825	ASP	N-CA-C	6.22	127.78	111.00
2	B	1088	SER	CB-CA-C	6.17	121.82	110.10
2	B	249	THR	C-N-CD	6.15	141.32	128.40
2	B	175	ASN	C-N-CD	6.12	141.24	128.40
2	B	463	ALA	CB-CA-C	-6.06	101.02	110.10
2	B	453	GLY	C-N-CD	5.98	140.96	128.40
2	B	229	LEU	C-N-CD	5.94	140.87	128.40
2	B	572	ILE	CB-CA-C	-5.93	99.74	111.60
2	B	116	HIS	C-N-CD	5.93	140.84	128.40
2	B	1228	LEU	C-N-CD	5.92	140.83	128.40
2	B	870	VAL	C-N-CD	5.85	140.69	128.40
2	B	1191	LYS	CB-CA-C	-5.81	98.79	110.40
2	B	132	TYR	C-N-CD	5.79	140.55	128.40
2	B	842	VAL	C-N-CD	5.79	140.55	128.40
2	B	1177	ASN	CB-CA-C	5.76	121.92	110.40
2	B	1041	ASN	CB-CA-C	5.74	121.87	110.40
2	B	1032	ALA	CB-CA-C	5.70	118.66	110.10
2	B	377	LYS	C-N-CD	5.60	140.17	128.40
2	B	584	GLU	CB-CA-C	-5.58	99.23	110.40
2	B	997	LEU	CB-CA-C	-5.51	99.73	110.20
2	B	1136	SER	C-N-CD	5.44	139.83	128.40
2	B	878	LYS	CB-CA-C	5.39	121.17	110.40
2	B	250	PRO	CA-N-CD	-5.35	104.02	111.50
2	B	571	LYS	CB-CA-C	5.30	121.00	110.40
2	B	1222	LYS	C-N-CA	5.18	133.18	122.30
2	B	1262	HIS	N-CA-C	-5.16	97.06	111.00
2	B	246	LEU	N-CA-C	-5.13	97.15	111.00

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	88	0
2	B	10816	0	10957	1624	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	1663	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 64.

All (1663) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:978:ILE:HD11	2:B:1236:LEU:CD1	1.51	1.37
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:545:LYS:HZ1	2:B:690:ASN:CG	1.29	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:556:ASN:C	2:B:595:HIS:NE2	1.81	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
2:B:557:ARG:N	2:B:595:HIS:NE2	1.78	1.31
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:318:SER:OG	2:B:418:GLU:CD	1.66	1.31
2:B:1139:VAL:HG12	2:B:1167:THR:CA	1.59	1.31
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:839:ASP:OD1	2:B:864:ARG:NH1	1.64	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:18:TRP:CD1	2:B:49:GLY:C	2.08	1.22
2:B:1210:ARG:HD2	2:B:1280:VAL:C	1.59	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:1139:VAL:CB	2:B:1166:ILE:O	1.99	1.09
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:1270:ILE:C	2:B:1273:ILE:HG12	1.73	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:853:ASP:O	2:B:896:LYS:HG3	1.55	1.05
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:762:GLU:OE1	2:B:990:ASN:CG	1.95	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:1139:VAL:HB	2:B:1166:ILE:C	1.80	1.01
2:B:297:SER:HA	2:B:300:ILE:HG22	1.39	1.01
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:545:LYS:NZ	2:B:690:ASN:CG	2.15	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:839:ASP:CG	2:B:864:ARG:HH11	1.65	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:O	2:B:103:GLU:HG3	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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
1:A:58:G:HO2'	2:B:457:ARG:HB2	1.26	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:OE1	2:B:197:GLU:N	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:1297:HIS:CB	2:B:1327:PHE:HZ	1.84	0.88
2:B:523:GLU:OE2	2:B:588:ASN:ND2	2.06	0.88
2:B:1139:VAL:CG1	2:B:1166:ILE:C	2.41	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:494:ARG:HH11	2:B:494:ARG:HG2	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: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
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:545:LYS:HZ1	2:B:690:ASN:ND2	1.76	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:1139:VAL:CB	2:B:1166:ILE:C	2.45	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:556:ASN:C	2:B:595:HIS:CE1	2.50	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: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:HG3	2:B:859:ARG:HH11	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:O	2:B:720:LEU:HD12	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
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:668:ASN:CG	2:B:680:LEU:CB	2.47	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: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:N	2:B:194:GLN:OE1	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:A:61:C:P	2:B:460:SER:HG	2.05	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
2:B:307:ARG:NH2	2:B:323:LYS:HE2	1.97	0.79
2:B:1270:ILE:CA	2:B:1273:ILE:CG1	2.53	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:762:GLU:CD	2:B:990:ASN:HD21	1.85	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:493:GLU:O	2:B:496:THR:HG23	1.83	0.78
2:B:545:LYS:HZ1	2:B:690:ASN:CB	1.96	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: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
1:A:51:A:HO2'	2:B:1134:PHE:HE1	0.77	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
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:O	2:B:457:ARG:HG3	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: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:121:ASN:HD21	2:B:124:ASP:CG	1.91	0.74
2:B:1148:LYS:HE2	2:B:1189:GLU:HB2	1.69	0.74
2:B:761:ILE:HG13	2:B:761:ILE:O	1.87	0.74
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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: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:1245:LEU:HD22	2:B:1252:ASN:CG	2.08	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:NH1	2:B:664:ARG:HG3	2.05	0.71
2:B:1269:ILE:O	2:B:1273:ILE:N	2.21	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:380:LEU:HA	2:B:383:MET:HG3	1.72	0.71
2:B:668:ASN:CG	2:B:680:LEU:HB3	2.11	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:489:GLN:HE21	2:B:493:GLU:CD	1.93	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:107:VAL:HG22	2:B:1131:TYR:HH	1.56	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HD12	2:B:1206:LEU:O	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
2:B:1139:VAL:HG21	2:B:1165:GLY:C	2.12	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
1:A:61:C:OP1	2:B:460:SER:OG	2.11	0.69
2:B:556:ASN:O	2:B:595:HIS:CE1	2.46	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:790:GLU:CD	2:B:889:ALA:HA	2.13	0.69
2:B:1245:LEU:HD12	2:B:1245:LEU:C	2.13	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
1:A:43:G:HO2'	2:B:363:ILE:HD12	1.59	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:551:LEU:HD12	2:B:551:LEU:C	2.15	0.67
2:B:465:MET:HE1	2:B:482:VAL:HG22	1.76	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
2:B:317:LEU:HB3	2:B:414:ILE:HD12	1.77	0.67
2:B:661:ARG:NH1	2:B:661:ARG:HG3	2.10	0.67
2:B:188:LEU:C	2:B:188:LEU:HD13	2.15	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:1269:ILE:CG2	2:B:1273:ILE:HG23	2.25	0.67
2:B:895:ARG:HD2	2:B:895:ARG:C	2.15	0.66
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:229:LEU:HD12	2:B:229:LEU:C	2.15	0.66
2:B:393:LEU:HD23	2:B:393:LEU:C	2.16	0.66
2:B:591:LEU:HD13	2:B:594:TYR:HB2	1.76	0.66
2:B:857:LEU:C	2:B:857:LEU:HD23	2.15	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
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:1347:LEU:C	2:B:1347:LEU:HD23	2.16	0.65
2:B:553:PHE:HE2	2:B:559:VAL:CG1	2.08	0.65
2:B:602:LYS:O	2:B:602:LYS:HG3	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:297:SER:OG	2:B:301:LEU:HD11	1.96	0.64
2:B:1270:ILE:C	2:B:1273:ILE:CG1	2.47	0.64
2:B:362:TYR:HD2	2:B:372:PHE:CE2	2.11	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:466:THR:C	2:B:467:ARG:HG3	2.18	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: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: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
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:334:LEU:HD13	2:B:338:LEU:CD1	2.28	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:HD2	2:B:594:TYR:O	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:859:ARG:HD2	2:B:859:ARG:C	2.20	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:545:LYS:NZ	2:B:690:ASN:CB	2.59	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:1270:ILE:HA	2:B:1273:ILE:HD13	1.81	0.61
2:B:165:ARG:NH2	2:B:446:PHE:O	2.34	0.61
2:B:297:SER:C	2:B:300:ILE:HG22	2.21	0.61
2:B:720:LEU:HD11	2:B:724:ILE:HD11	1.82	0.61
2:B:1348:ILE:HD11	2:B:1357:GLU:CD	2.21	0.61
2:B:247:GLY:O	2:B:248:LEU:HD23	2.00	0.61
2:B:886:LEU:N	2:B:886:LEU:HD23	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: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:HD11	2:B:238:PHE:HE1	1.64	0.60
2:B:188:LEU:HD13	2:B:189:VAL:N	2.16	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:395:ARG:C	2:B:396:GLU:HG3	2.21	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:197:GLU:H	2:B:197:GLU:CD	1.98	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: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:842:VAL:HG12	2:B:854:ASN:CG	2.22	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
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:N	2:B:942:LYS:HD3	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:720:LEU:HD12	2:B:720:LEU:C	2.23	0.59
2:B:763:MET:HG3	2:B:928:THR:HB	1.84	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: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:857:LEU:HD23	2:B:857:LEU:O	2.03	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:HH11	2:B:661:ARG:CG	2.15	0.58
2:B:723:HIS:CE1	2:B:727:LEU:CD2	2.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:979:ASN:OD1	2:B:980:ASN:N	2.36	0.58
2:B:1207:GLU:CD	2:B:1208:ASN:H	2.07	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:1130:LYS:C	2:B:1131:TYR:CD1	2.76	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: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
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:307:ARG:NH2	2:B:323:LYS:HZ1	2.01	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:N	2:B:973:TYR:CD2	2.73	0.57
2:B:1224:ASN:HB2	2:B:1280:VAL:HG11	1.85	0.57
2:B:307:ARG:HH21	2:B:323:LYS:HZ1	1.51	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:384:ASP:N	2:B:384:ASP:OD1	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:1225:GLU:HA	2:B:1225:GLU:OE1	2.05	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:944:ASP:OD1	2:B:944:ASP:N	2.37	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:516:GLU:CD	2:B:593:THR:OG1	2.44	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1146:VAL:HG13	2:B:1191:LYS:HG3	1.86	0.56
2:B:161:MET:C	2:B:164:PHE:O	2.39	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: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
2:B:1243:GLU:CB	2:B:1246:LYS:NZ	2.66	0.55
2:B:484:LYS:O	2:B:488:ALA:HB2	2.06	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:O	2:B:343:LEU:HG	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:1114:ARG:HH12	4:D:9:DA:P	2.30	0.55
2:B:1287:LEU:HD12	2:B:1287:LEU:C	2.26	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1349:HIS:HB2	2:B:1358:THR:OG1	2.06	0.54
2:B:222:LEU:O	2:B:226:ILE:HG12	2.06	0.54
2:B:853:ASP:C	2:B:896:LYS:HG3	2.25	0.54
2:B:967:ARG:NH1	2:B:986:ASP:OD1	2.40	0.54
2:B:47:LEU:O	2:B:48:ILE:C	2.45	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:941:THR:C	2:B:942:LYS:HD3	2.28	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
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
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:482:VAL:HG12	2:B:483:ASP:N	2.22	0.54
2:B:1243:GLU:O	2:B:1246:LYS:HD2	2.07	0.54
2:B:666:LEU:HD23	2:B:666:LEU:C	2.29	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
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:465:MET:HE2	2:B:482:VAL:HG22	1.91	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:553:PHE:HE2	2:B:559:VAL:HG21	1.52	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:362:TYR:HD1	2:B:362:TYR:O	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:241:LEU:HD21	2:B:290:PHE:HE2	1.74	0.53
2:B:379:ILE:C	2:B:383:MET:HG3	2.22	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
2:B:609:ASN:ND2	2:B:612:ASN:OD1	2.34	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: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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:303:SER:O	2:B:306:LEU:C	2.48	0.52
2:B:359:TYR:O	2:B:363:ILE:N	2.38	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:78:ARG:CZ	2:B:165:ARG:HD2	2.40	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:851:SER:C	2:B:855:LYS:HG3	2.31	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: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: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:OE1	2:B:1243:GLU:HA	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:1207:GLU:CG	2:B:1208:ASN:N	2.73	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:226:ILE:C	2:B:229:LEU:HG	2.31	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:282:ILE:N	2:B:282:ILE:CD1	2.73	0.51
2:B:347:TYR:C	2:B:347:TYR:CD1	2.84	0.51
2:B:433:LEU:O	2:B:437:ARG:N	2.44	0.51
2:B:879:MET:O	2:B:880:LYS:C	2.49	0.51
2:B:936:ASP:CG	2:B:951:ARG:HE	2.14	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
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: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:1348:ILE:HG23	2:B:1348:ILE:O	2.11	0.50
2:B:135:ILE:O	2:B:138:LEU:HB3	2.11	0.50
2:B:661:ARG:N	2:B:661:ARG:CD	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: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:559:VAL:C	2:B:563:GLN:OE1	2.49	0.50
2:B:760:VAL:HG11	2:B:990:ASN:O	2.11	0.50
2:B:118:ILE:C	2:B:119:PHE:CD1	2.85	0.50
2:B:509:PRO:HA	2:B:659:TRP:HA	1.93	0.50
2:B:192:TYR:C	2:B:192:TYR:CD2	2.85	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1270:ILE:CA	2:B:1273:ILE:HD11	2.40	0.50
2:B:53:PHE:CD1	2:B:53:PHE:C	2.85	0.49
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:491:PHE:C	2:B:491:PHE:CD2	2.85	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
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: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: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:1309:ILE:HG12	2:B:1326:TYR:OH	2.12	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
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: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:545:LYS:HZ2	2:B:690:ASN:ND2	2.08	0.49
2:B:279:LEU:HD11	2:B:287:ALA:HB2	1.95	0.49
2:B:359:TYR:CD1	2:B:359:TYR:C	2.85	0.49
2:B:401:LYS:HB2	2:B:404:THR:CG2	2.43	0.49
2:B:733:ILE:HD11	2:B:763:MET:HE3	1.94	0.49
2:B:128:TYR:CD1	2:B:153:LEU:HD21	2.48	0.49
2:B:362:TYR:CD1	2:B:362:TYR:C	2.85	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:1204:PHE:CE1	2:B:1347:LEU:HB2	2.48	0.48
1:A:8:G:HO2'	1:A:9:U:P	2.37	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:524:LEU:HD23	2:B:524:LEU:C	2.34	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:869:ASN:CG	2:B:870:VAL:N	2.65	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: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
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:347:TYR:C	2:B:347:TYR:HD1	2.17	0.47
2:B:489:GLN:O	2:B:493:GLU:HB2	2.14	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: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:372:PHE:CD1	2:B:372:PHE:C	2.85	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: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: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:825:ASP:CG	2:B:825:ASP:O	2.53	0.47
2:B:887:LEU:HA	2:B:892:ILE:HG12	1.97	0.47
2:B:1045:PHE:HB2	2:B:1064:GLU:CD	2.35	0.47
2:B:1075:ASP:OD1	2:B:1078:ARG:N	2.33	0.47
2:B:1139:VAL:HG11	2:B:1165:GLY:C	2.32	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: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:572:ILE:O	2:B:572:ILE:CG2	2.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:2:DA:H2''	3:C:3:DA:C8	2.50	0.47
2:B:421:ALA:O	2:B:425:ARG:N	2.48	0.47
2:B:478:PHE:C	2:B:478:PHE:CD2	2.85	0.47
2:B:516:GLU:HA	2:B:519:THR:HG22	1.97	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:121:ASN:CG	2:B:124:ASP:HB2	2.35	0.46
2:B:949:LEU:CG	2:B:950:ILE:N	2.78	0.46
2:B:969:ASP:OD1	2:B:969:ASP:N	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:197:GLU:O	2:B:198:GLU:C	2.51	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: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: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: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:914:ALA:HB3	2:B:1032:ALA:HB1	1.95	0.46
2:B:515:TYR:HD2	2:B:515:TYR:O	1.98	0.46
2:B:967:ARG:C	2:B:972:PHE:O	2.53	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:348:LYS:HG2	2:B:352:PHE:HB2	1.96	0.46
2:B:794:GLN:CD	2:B:794:GLN:H	2.19	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: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:188:LEU:C	2:B:188:LEU:HD22	2.33	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:895:ARG:HD2	2:B:895:ARG:O	2.16	0.45
2:B:966:PHE:CD1	2:B:970:PHE:CD2	3.04	0.45
2:B:971:GLN:C	2:B:972:PHE:HD1	2.19	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
2:B:193:ASN:CG	2:B:201:ILE:H	2.14	0.45
1:A:49:A:H1'	2:B:1122:ARG:HH11	1.81	0.45
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: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:1308:ASN:CG	2:B:1327:PHE:HB3	2.36	0.45
2:B:350:ILE:O	2:B:359:TYR:N	2.47	0.45
2:B:362:TYR:O	2:B:362:TYR:CD1	2.70	0.45
2:B:723:HIS:CE1	2:B:727:LEU:HD21	2.51	0.45
2:B:762:GLU:CD	2:B:990:ASN:ND2	2.57	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:933:GLN:OE1	2:B:934:ILE:HG13	2.16	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: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:664:ARG:CD	2:B:664:ARG:C	2.86	0.45
2:B:686:ASP:CG	2:B:691:ARG:CZ	2.85	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:376:ILE:CD1	2:B:376:ILE:C	2.86	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:265:GLN:O	2:B:271:TYR:CB	2.63	0.44
2:B:265:GLN:C	2:B:271:TYR:CD1	2.90	0.44
2:B:1276:PHE:CD1	2:B:1276:PHE:O	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:270:THR:O	2:B:270:THR:OG1	2.34	0.44
2:B:277:ASN:ND2	2:B:649:LYS:O	2.50	0.44
2:B:359:TYR:CZ	2:B:363:ILE:HD11	2.52	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:887:LEU:HD23	2:B:887:LEU:O	2.16	0.44
2:B:450:TYR:C	2:B:491:PHE:HE1	2.20	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:HD13	2:B:811:LEU:O	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:666:LEU:C	2:B:666:LEU:CD2	2.85	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:859:ARG:C	2:B:859:ARG:CD	2.86	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:1272:GLN:HE21	2:B:1272:GLN:C	2.19	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
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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:882:TYR:HD2	2:B:883:TRP:HD1	1.66	0.43
2:B:895:ARG:C	2:B:895:ARG:CD	2.85	0.43
2:B:1211:LYS:HZ3	2:B:1211:LYS:HB2	1.84	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:450:TYR:C	2:B:491:PHE:CE1	2.92	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: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: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: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:672:ASP:HB2	2:B:704:PHE:HE2	1.84	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
2:B:1324:PHE:N	2:B:1324:PHE:CD1	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: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:723:HIS:ND1	2:B:723:HIS:C	2.73	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:229:LEU:CD1	2:B:229:LEU:C	2.85	0.42
2:B:513:LEU:O	2:B:516:GLU:N	2.53	0.42
2:B:573:GLU:HA	2:B:573:GLU:OE1	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:594:TYR:C	2:B:594:TYR:CD2	2.93	0.42
2:B:672:ASP:HB2	2:B:704:PHE:CE2	2.54	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:191:THR:HG1	2:B:192:TYR:N	2.18	0.42
2:B:201:ILE:HG22	2:B:202:ASN:H	1.85	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:522:ASN:ND2	2:B:522:ASN:C	2.73	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:555:THR:C	2:B:556:ASN:ND2	2.73	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:594:TYR:HD2	2:B:594:TYR:C	2.23	0.42
2:B:818:ASN:O	2:B:818:ASN:ND2	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
2:B:465:MET:HE1	2:B:467:ARG:HG2	2.02	0.42
2:B:465:MET:SD	2:B:465:MET:C	2.98	0.42
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:O	2:B:1364:GLN:HG2	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:27:VAL:HG12	2:B:1086:VAL:HG22	2.02	0.41
2:B:202:ASN:CG	2:B:204:SER:N	2.73	0.41
2:B:256:PHE:N	2:B:256:PHE:HD1	2.18	0.41
2:B:492:ILE:HG23	3:C:17:DA:H5'	2.02	0.41
2:B:555:THR:C	2:B:556:ASN:HD22	2.23	0.41
2:B:591:LEU:HD12	2:B:594:TYR:CG	2.54	0.41
2:B:359:TYR:C	2:B:362:TYR:HB3	2.39	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:668:ASN:OD1	2:B:680:LEU:HB3	1.96	0.41
2:B:905:ARG:NH1	3:C:24:DG:OP1	2.54	0.41
2:B:1149:VAL:HG23	2:B:1149:VAL:O	2.20	0.41
2:B:1207:GLU:CD	2:B:1210:ARG:NH1	2.73	0.41
2:B:313:THR:HG23	2:B:313:THR:O	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:686:ASP:CG	2:B:691:ARG:NH2	2.73	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:398:LEU:C	2:B:398:LEU:HD12	2.41	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:857:LEU:C	2:B:857:LEU:CD2	2.86	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: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: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:969:ASP:C	2:B:970:PHE:HD1	2.25	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
2:B:681:ASP:HA	2:B:684:LYS:HE2	2.03	0.40
2:B:686:ASP:CG	2:B:690:ASN:HA	2.42	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:489:GLN:CG	2:B:493:GLU:CD	2.89	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 ⓘ

### 5.3.1 Protein backbone ⓘ

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%)	44 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%)	997 (84%)	186 (16%)	<b>2</b> <b>13</b>

All (186) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	26	LYS
2	B	48	ILE
2	B	53	PHE
2	B	86	PHE
2	B	104	SER
2	B	114	GLU
2	B	115	ARG
2	B	116	HIS
2	B	125	GLU
2	B	129	HIS
2	B	132	TYR
2	B	144	ASP
2	B	167	HIS
2	B	177	ASP
2	B	182	ASP
2	B	185	PHE
2	B	188	LEU
2	B	189	VAL
2	B	194	GLN
2	B	196	PHE
2	B	197	GLU
2	B	204	SER
2	B	215	ARG
2	B	232	GLU
2	B	233	LYS
2	B	246	LEU
2	B	248	LEU
2	B	252	PHE
2	B	253	LYS
2	B	258	LEU

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Mol	Chain	Res	Type
2	B	260	GLU
2	B	261	ASP
2	B	267	SER
2	B	281	GLN
2	B	284	ASP
2	B	291	LEU
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	317	LEU
2	B	318	SER
2	B	341	GLN
2	B	342	GLN
2	B	343	LEU
2	B	347	TYR
2	B	350	ILE
2	B	355	SER
2	B	362	TYR
2	B	372	PHE
2	B	374	LYS
2	B	376	ILE
2	B	383	MET
2	B	384	ASP
2	B	387	GLU
2	B	390	LEU
2	B	393	LEU
2	B	397	ASP
2	B	398	LEU
2	B	399	LEU
2	B	400	ARG
2	B	425	ARG
2	B	432	PHE
2	B	460	SER
2	B	461	ARG
2	B	464	TRP
2	B	465	MET
2	B	478	PHE
2	B	480	GLU

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Mol	Chain	Res	Type
2	B	491	PHE
2	B	492	ILE
2	B	494	ARG
2	B	495	MET
2	B	506	LYS
2	B	518	PHE
2	B	521	TYR
2	B	522	ASN
2	B	529	TYR
2	B	535	ARG
2	B	546	LYS
2	B	550	ASP
2	B	551	LEU
2	B	552	LEU
2	B	555	THR
2	B	557	ARG
2	B	564	LEU
2	B	576	ASP
2	B	577	SER
2	B	591	LEU
2	B	593	THR
2	B	594	TYR
2	B	597	LEU
2	B	598	LEU
2	B	600	ILE
2	B	602	LYS
2	B	621	LEU
2	B	631	MET
2	B	661	ARG
2	B	662	LEU
2	B	664	ARG
2	B	665	LYS
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	751	MET
2	B	763	MET
2	B	820	ARG
2	B	821	ASP

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Mol	Chain	Res	Type
2	B	826	GLN
2	B	829	ASP
2	B	855	LYS
2	B	858	THR
2	B	859	ARG
2	B	860	SER
2	B	861	ASP
2	B	868	ASP
2	B	873	GLU
2	B	885	GLN
2	B	887	LEU
2	B	893	THR
2	B	895	ARG
2	B	905	ARG
2	B	926	GLN
2	B	933	GLN
2	B	936	ASP
2	B	937	SER
2	B	944	ASP
2	B	948	LYS
2	B	949	LEU
2	B	964	SER
2	B	968	LYS
2	B	969	ASP
2	B	971	GLN
2	B	973	TYR
2	B	974	LYS
2	B	980	ASN
2	B	1031	LYS
2	B	1037	PHE
2	B	1045	PHE
2	B	1065	THR
2	B	1080	PHE
2	B	1091	GLN
2	B	1116	SER
2	B	1119	LEU
2	B	1123	LYS
2	B	1134	PHE
2	B	1138	THR
2	B	1148	LYS
2	B	1154	SER
2	B	1157	LEU

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Mol	Chain	Res	Type
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	1212	ARG
2	B	1231	LYS
2	B	1235	PHE
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	1255	LYS
2	B	1272	GLN
2	B	1274	SER
2	B	1287	LEU
2	B	1325	LYS
2	B	1326	TYR
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	1364	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	190	GLN
2	B	202	ASN
2	B	342	GLN
2	B	459	ASN
2	B	522	ASN
2	B	668	ASN
2	B	690	ASN
2	B	980	ASN

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Mol	Chain	Res	Type
2	B	990	ASN
2	B	1091	GLN
2	B	1224	ASN
2	B	1262	HIS

### 5.3.3 RNA [i](#)

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 [i](#)

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

#### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

#### 5.6 Ligand geometry [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	94/98 (95%)	1.73	33 (35%) ⓘ ⓘ	12, 36, 69, 103	0
2	B	1326/1368 (96%)	1.16	231 (17%) ⓘ ⓘ	5, 29, 53, 90	0
3	C	24/24 (100%)	1.21	3 (12%) ⓘ ⓘ	22, 36, 57, 65	0
4	D	11/11 (100%)	1.37	3 (27%) ⓘ ⓘ	22, 41, 84, 95	0
All	All	1455/1501 (96%)	1.20	270 (18%) ⓘ ⓘ	5, 29, 56, 103	0

All (270) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	813	LEU	6.9
2	B	1043	MET	6.6
2	B	19	ALA	6.5
2	B	158	LEU	6.5
2	B	1263	LYS	6.4
2	B	1223	GLY	6.3
2	B	994	GLY	6.0
2	B	1007	GLU	5.9
2	B	65	LYS	5.7
2	B	551	LEU	5.7
2	B	1352	ILE	5.7
2	B	399	LEU	5.6
2	B	398	LEU	5.4
2	B	1134	PHE	5.4
2	B	1224	ASN	5.3
2	B	1354	GLY	5.3
2	B	1225	GLU	5.2
2	B	917	ILE	5.2
2	B	136	TYR	5.2
2	B	993	VAL	5.1
2	B	413	GLN	5.0

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Mol	Chain	Res	Type	RSRZ
2	B	1355	LEU	5.0
2	B	48	ILE	4.6
2	B	49	GLY	4.6
2	B	675	SER	4.5
2	B	997	LEU	4.3
2	B	728	ALA	4.3
2	B	76	LYS	4.3
2	B	1356	TYR	4.3
2	B	40	ARG	4.2
2	B	154	ILE	4.2
2	B	739	GLN	4.2
2	B	938	ARG	4.2
1	A	44	U	4.2
2	B	72	TYR	4.2
2	B	1295	ASN	4.2
2	B	520	VAL	4.2
2	B	978	ILE	4.1
2	B	1204	PHE	4.1
2	B	1095	VAL	4.1
2	B	80	CYS	4.1
2	B	927	ILE	4.1
2	B	50	ALA	4.1
2	B	560	THR	4.0
1	A	93	G	4.0
2	B	1126	TRP	3.9
1	A	28	A	3.9
1	A	17	G	3.9
2	B	1220	LEU	3.9
2	B	1236	LEU	3.9
2	B	1342	VAL	3.8
2	B	317	LEU	3.8
2	B	74	ARG	3.8
1	A	92	G	3.8
2	B	888	ASN	3.7
2	B	852	ILE	3.6
2	B	834	SER	3.6
2	B	62	THR	3.6
2	B	1085	LYS	3.5
1	A	27	G	3.5
2	B	1098	THR	3.5
2	B	443	ILE	3.5
2	B	1216	SER	3.4

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Mol	Chain	Res	Type	RSRZ
2	B	501	ASN	3.4
1	A	67	C	3.4
2	B	688	PHE	3.4
2	B	47	LEU	3.3
2	B	68	ALA	3.3
2	B	934	ILE	3.3
2	B	946	ASN	3.3
2	B	587	PHE	3.3
2	B	924	THR	3.3
2	B	134	THR	3.3
2	B	659	TRP	3.3
2	B	1138	THR	3.2
1	A	34	A	3.2
1	A	91	C	3.2
2	B	295	ASN	3.2
2	B	559	VAL	3.2
2	B	152	ARG	3.2
2	B	1226	LEU	3.2
2	B	979	ASN	3.2
2	B	518	PHE	3.1
2	B	242	ILE	3.1
2	B	385	GLY	3.1
2	B	1349	HIS	3.1
2	B	742	LYS	3.1
2	B	18	TRP	3.0
2	B	524	LEU	3.0
2	B	1359	ARG	3.0
2	B	133	PRO	3.0
2	B	449	PRO	3.0
2	B	616	LEU	3.0
2	B	841	ILE	3.0
2	B	383	MET	3.0
2	B	740	THR	3.0
2	B	957	THR	3.0
2	B	156	LEU	2.9
2	B	1137	PRO	2.9
2	B	621	LEU	2.9
2	B	935	LEU	2.9
2	B	29	SER	2.9
1	A	88	A	2.9
2	B	305	ILE	2.9
2	B	368	SER	2.9

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Mol	Chain	Res	Type	RSRZ
2	B	614	ASP	2.9
2	B	445	THR	2.9
2	B	824	VAL	2.9
2	B	335	LEU	2.9
2	B	31	LYS	2.9
2	B	45	LYS	2.9
2	B	1111	LEU	2.8
2	B	150	ASP	2.8
2	B	933	GLN	2.8
2	B	1350	GLN	2.8
1	A	90	U	2.8
2	B	473	ILE	2.8
2	B	1209	GLY	2.8
2	B	452	VAL	2.8
2	B	1234	ASN	2.8
1	A	14	A	2.8
2	B	617	GLU	2.8
2	B	231	GLY	2.8
2	B	975	VAL	2.8
2	B	1009	VAL	2.8
2	B	544	GLN	2.8
2	B	823	TYR	2.7
2	B	132	TYR	2.7
2	B	476	TRP	2.7
2	B	995	THR	2.7
2	B	367	ALA	2.7
1	A	70	C	2.7
2	B	228	GLN	2.7
2	B	818	ASN	2.7
2	B	1124	LYS	2.7
2	B	1140	ALA	2.7
2	B	364	ASP	2.7
2	B	435	ASP	2.7
1	A	29	G	2.7
1	A	82	G	2.7
2	B	292	ALA	2.7
2	B	747	LEU	2.7
2	B	515	TYR	2.7
1	A	42	A	2.6
2	B	85	ILE	2.6
2	B	69	ARG	2.6
2	B	1211	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
2	B	1351	SER	2.6
2	B	564	LEU	2.6
2	B	1075	ASP	2.6
2	B	1006	SER	2.6
2	B	343	LEU	2.6
2	B	423	LEU	2.6
2	B	746	GLU	2.6
2	B	1008	PHE	2.6
2	B	639	TYR	2.6
2	B	931	VAL	2.6
2	B	332	LEU	2.6
2	B	1353	THR	2.6
2	B	947	ASP	2.6
2	B	1202	SER	2.6
2	B	453	GLY	2.5
2	B	415	HIS	2.5
2	B	43	ILE	2.5
2	B	235	ASN	2.5
2	B	366	GLY	2.5
2	B	118	ILE	2.5
2	B	1213	MET	2.5
2	B	1110	ILE	2.5
2	B	918	LYS	2.5
2	B	181	VAL	2.5
2	B	75	ARG	2.4
2	B	939	MET	2.4
2	B	792	GLY	2.4
1	A	58	G	2.4
1	A	81	G	2.4
2	B	83	GLN	2.4
2	B	143	VAL	2.4
2	B	737	ILE	2.4
2	B	1042	ILE	2.4
1	A	52	A	2.4
2	B	163	LYS	2.4
2	B	1119	LEU	2.4
2	B	1164	LEU	2.4
2	B	161	MET	2.4
2	B	783	ARG	2.4
1	A	51	A	2.4
2	B	386	THR	2.4
2	B	426	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	862	LYS	2.3
2	B	1109	SER	2.3
2	B	724	ILE	2.3
2	B	238	PHE	2.3
2	B	1336	TYR	2.3
4	D	2	DT	2.3
2	B	822	MET	2.3
2	B	475	PRO	2.3
2	B	785	GLU	2.3
1	A	68	A	2.3
2	B	654	ARG	2.3
2	B	1267	ASP	2.3
2	B	1335	ARG	2.3
2	B	828	LEU	2.3
2	B	1266	LEU	2.3
1	A	62	G	2.3
2	B	713	VAL	2.3
2	B	329	HIS	2.3
2	B	365	GLY	2.3
4	D	6	DG	2.3
2	B	743	VAL	2.2
2	B	744	VAL	2.2
2	B	129	HIS	2.2
2	B	159	ALA	2.2
2	B	683	LEU	2.2
2	B	20	VAL	2.2
1	A	15	U	2.2
1	A	48	A	2.2
2	B	1203	LEU	2.2
2	B	1347	LEU	2.2
2	B	749	LYS	2.2
2	B	836	TYR	2.2
2	B	331	ASP	2.2
2	B	260	GLU	2.2
1	A	45	U	2.2
1	A	98	C	2.2
2	B	899	ASN	2.2
1	A	87	G	2.2
4	D	3	DT	2.2
2	B	729	GLY	2.2
2	B	1092	VAL	2.2
2	B	1153	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	759	ILE	2.1
2	B	32	PHE	2.1
1	A	6	G	2.1
2	B	173	ASP	2.1
2	B	417	GLY	2.1
1	A	26	A	2.1
2	B	35	LEU	2.1
2	B	451	TYR	2.1
2	B	697	ILE	2.1
2	B	233	LYS	2.1
1	A	13	A	2.1
2	B	176	PRO	2.1
2	B	89	GLU	2.1
2	B	990	ASN	2.1
2	B	411	PRO	2.1
2	B	795	ILE	2.1
1	A	65	A	2.1
2	B	34	VAL	2.1
2	B	625	LEU	2.1
2	B	850	ASP	2.1
2	B	698	HIS	2.1
2	B	761	ILE	2.1
2	B	543	GLU	2.1
2	B	977	GLU	2.1
2	B	459	ASN	2.1
1	A	76	A	2.0
1	A	5	C	2.0
2	B	466	THR	2.0
2	B	622	THR	2.0
2	B	553	PHE	2.0
2	B	970	PHE	2.0
2	B	293	ALA	2.0
2	B	1357	GLU	2.0
3	C	15	DT	2.0
3	C	19	DA	2.0
3	C	2	DA	2.0
2	B	509	PRO	2.0
2	B	1128	PRO	2.0
2	B	1214	LEU	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 monosaccharides 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.