



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:28 AM UTC

PDB ID : 8KAH / pdb_00008kah
Title : Crystal structure of SpyCas9-crRNA-tracrRNA complex bound to 18nt target DNA
Authors : Chen, Y.; Chen, J.; Liu, L.
Deposited on : 2023-08-03
Resolution : 3.36 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

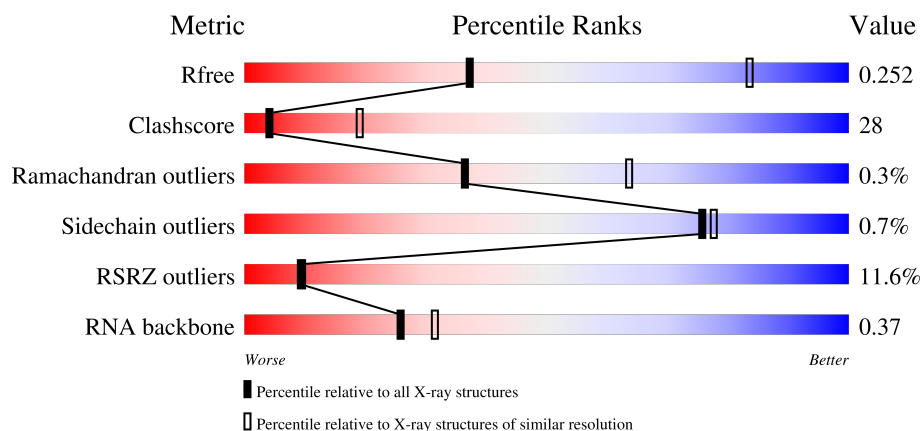
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.36 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1099 (3.40-3.32)
Clashscore	190562	1116 (3.40-3.32)
Ramachandran outliers	187476	1101 (3.40-3.32)
Sidechain outliers	187428	1101 (3.40-3.32)
RSRZ outliers	180081	1099 (3.40-3.32)
RNA backbone	3983	1110 (3.72-3.00)

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 ≥ 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	34	3% 29% 41% 29%
1	E	34	3% 21% 53% 21% 6%
2	B	1368	8% 53% 43% ..
2	F	1368	16% 51% 45% ..

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Mol	Chain	Length	Quality of chain
3	C	26	4% 46% 54%
3	G	26	4% 42% 58%
4	D	11	18% 55% 45%
4	H	11	9% 45% 55%
5	I	65	2% 38% 40% 17% • •
5	J	65	5% 28% 52% 17% •

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 27025 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 (34-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	34	Total	C	N	O	P	0	0	0
			725	325	127	239	34			
1	E	32	Total	C	N	O	P	0	0	0
			685	307	123	223	32			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1322	Total	C	N	O	S	0	0	0
			10732	6827	1864	2019	22			
2	F	1327	Total	C	N	O	S	0	0	0
			10695	6814	1845	2014	22			

There are 4 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
F	10	ALA	ASP	engineered mutation	UNP Q99ZW2
F	840	ALA	HIS	engineered mutation	UNP Q99ZW2

- Molecule 3 is a DNA chain called DNA (26-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	26	Total	C	N	O	P	0	0	0
			521	254	85	157	25			
3	G	26	Total	C	N	O	P	0	0	0
			521	254	85	157	25			

- 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 225	C 110	N 37	O 68	P 10	0	0	0
4	H	11	Total 225	C 110	N 37	O 68	P 10	0	0	0

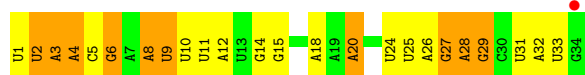
- Molecule 5 is a RNA chain called RNA (65-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	I	63	Total 1348	C 603	N 245	O 437	P 63	0	0	0
5	J	63	Total 1348	C 603	N 245	O 437	P 63	0	0	0

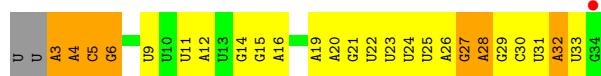
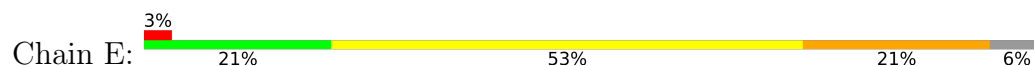
3 Residue-property plots

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

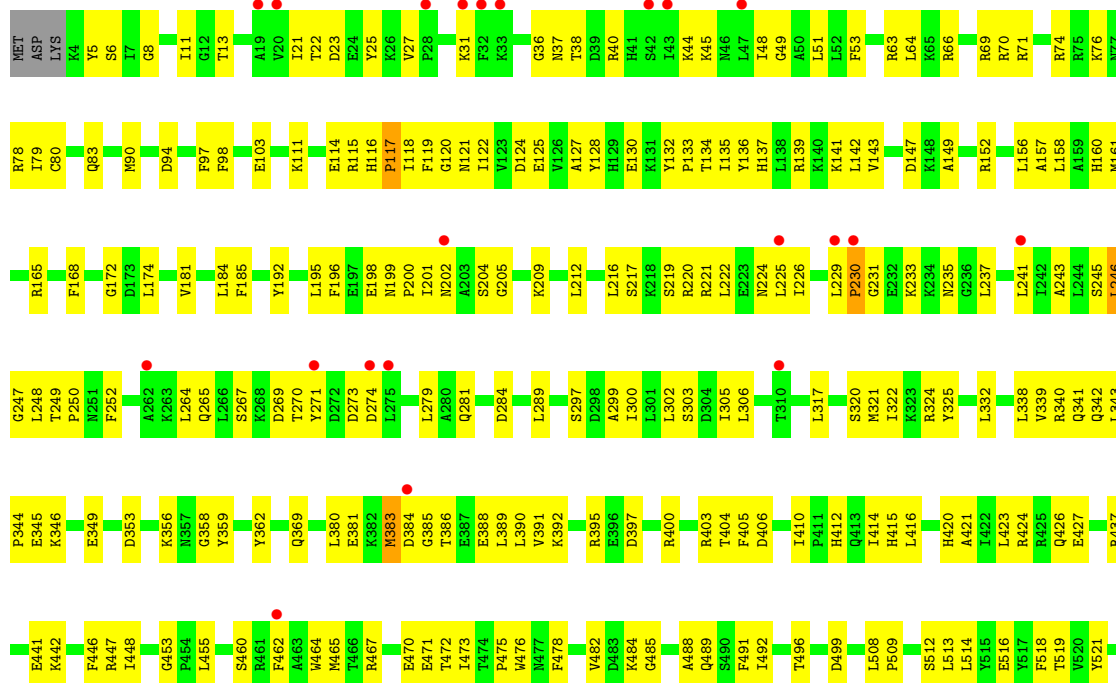
- Molecule 1: RNA (34-MER)

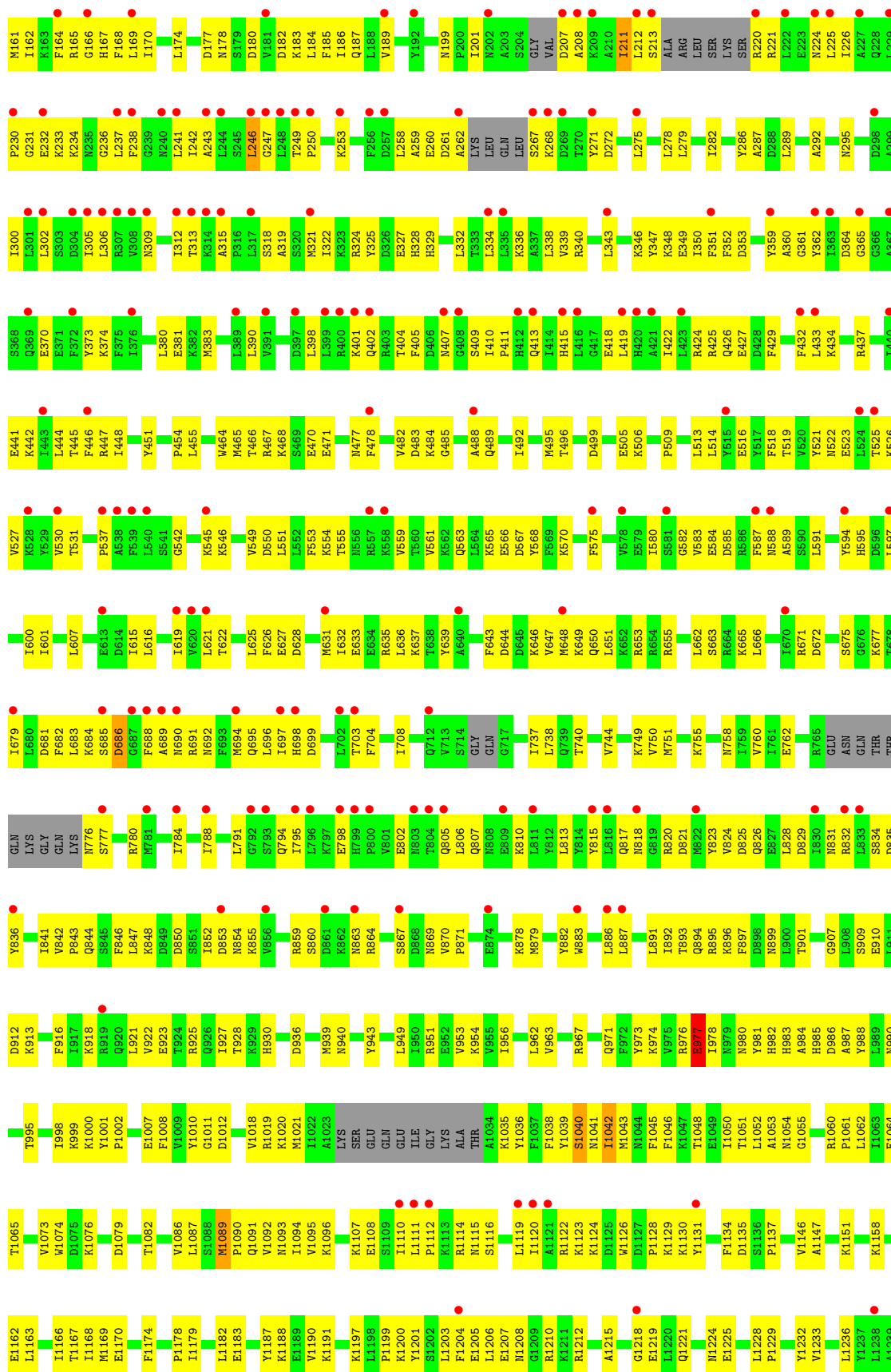


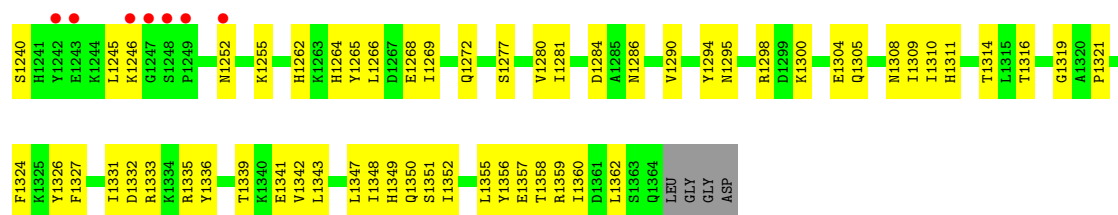
- Molecule 1: RNA (34-MER)



- Molecule 2: CRISPR-associated endonuclease Cas9/Csn1



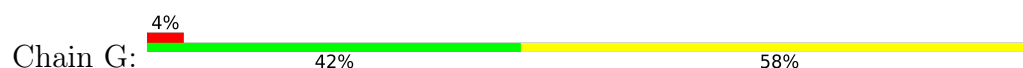




• Molecule 3: DNA (26-MER)



• Molecule 3: DNA (26-MER)



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



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

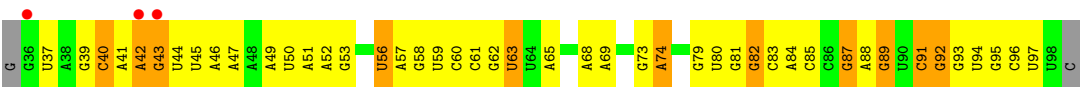


• Molecule 5: RNA (65-MER)



• Molecule 5: RNA (65-MER)





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	145.21Å 130.60Å 148.73Å 90.00° 104.08° 90.00°	Depositor
Resolution (Å)	48.23 – 3.36 48.23 – 3.36	Depositor EDS
% Data completeness (in resolution range)	59.4 (48.23-3.36) 73.8 (48.23-3.36)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.34 (at 3.33Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.230 , 0.255 0.229 , 0.252	Depositor DCC
R_{free} test set	1990 reflections (2.58%)	wwPDB-VP
Wilson B-factor (Å ²)	56.7	Xtriage
Anisotropy	0.207	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 47.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.069 for l,-k,h	Xtriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	27025	wwPDB-VP
Average B, all atoms (Å ²)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.53% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.59	0/811	0.92	0/1261
1	E	0.54	0/767	0.83	0/1193
2	B	0.56	2/10915 (0.0%)	0.85	6/14673 (0.0%)
2	F	0.56	1/10879 (0.0%)	0.84	7/14636 (0.0%)
3	C	0.67	0/581	0.89	1/893 (0.1%)
3	G	0.59	0/581	0.86	0/893
4	D	0.74	0/251	0.85	0/387
4	H	0.70	0/251	0.82	0/387
5	I	0.57	0/1509	0.82	1/2350 (0.0%)
5	J	0.52	0/1509	0.80	0/2350
All	All	0.57	3/28054 (0.0%)	0.84	15/39023 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	1089	MET	C-N	-9.60	1.24	1.34
2	B	1320	ALA	C-N	5.30	1.40	1.33
2	B	1321	PRO	N-CD	5.21	1.55	1.47

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1223	GLY	N-CA-C	9.95	125.51	112.77
2	B	246	LEU	N-CA-C	-7.58	99.81	110.50
2	F	211	ILE	N-CA-C	7.55	118.32	110.62
2	B	1320	ALA	CA-C-N	-6.56	113.00	119.76
2	B	1320	ALA	C-N-CA	-6.56	113.00	119.76
2	F	1040	SER	CA-C-N	-5.87	112.46	122.56
2	F	1040	SER	C-N-CA	-5.87	112.46	122.56
2	F	977	GLU	N-CA-C	5.85	117.66	111.28
2	F	160	HIS	N-CA-C	-5.59	105.18	111.28
5	I	42	A	C2'-C3'-O3'	5.51	121.97	113.70
2	B	582	GLY	N-CA-C	5.38	118.99	112.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	172	GLY	N-CA-C	-5.36	104.50	111.52
3	C	12	DA	O5'-C5'-C4'	5.28	118.72	110.80
2	F	246	LEU	CA-CB-CG	5.17	134.39	116.30
2	F	155	TYR	N-CA-C	-5.02	105.81	111.28

There are no chirality outliers.

There are no planarity outliers.

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	725	0	362	40	0
1	E	685	0	342	44	0
2	B	10732	0	10828	538	1
2	F	10695	0	10736	719	0
3	C	521	0	299	20	0
3	G	521	0	299	20	0
4	D	225	0	129	3	0
4	H	225	0	129	10	0
5	I	1348	0	678	40	0
5	J	1348	0	678	62	0
All	All	27025	0	24480	1411	1

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 28.

All (1411) 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:F:142:LEU:CD1	2:F:154:ILE:HG12	1.37	1.54
2:F:142:LEU:HD11	2:F:154:ILE:CG1	1.39	1.51
2:F:142:LEU:CD2	2:F:154:ILE:HD11	1.41	1.48
2:F:142:LEU:CD2	2:F:154:ILE:CD1	1.94	1.45
2:B:1222:LYS:O	2:B:1318:LEU:CD2	1.66	1.42
2:F:142:LEU:HD21	2:F:154:ILE:CD1	1.49	1.38

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:212:LEU:CD1	2:F:300:ILE:HG12	1.55	1.35
2:F:139:ARG:CG	2:F:157:ALA:HB1	1.56	1.34
2:F:138:LEU:CD1	2:F:153:LEU:HD21	1.58	1.32
2:F:165:ARG:HD2	2:F:168:PHE:CE1	1.65	1.31
2:F:138:LEU:CD1	2:F:153:LEU:CD2	2.10	1.30
2:F:90:MET:HE1	2:F:151:LEU:CD2	1.63	1.29
1:E:4:A:C2	1:E:5:C:C5	2.20	1.27
2:F:139:ARG:HG2	2:F:157:ALA:CB	1.63	1.27
2:F:208:ALA:CA	2:F:211:ILE:HD12	1.63	1.26
2:F:138:LEU:HD11	2:F:153:LEU:CD2	1.66	1.25
2:F:921:LEU:HD12	2:F:1008:PHE:CE2	1.71	1.22
2:F:208:ALA:HA	2:F:211:ILE:CD1	1.71	1.21
2:F:142:LEU:HD21	2:F:154:ILE:CG1	1.72	1.19
2:F:249:THR:HG1	2:F:267:SER:N	1.43	1.17
2:B:392:LYS:HG2	2:B:395:ARG:NH1	1.61	1.14
2:F:207:ASP:O	2:F:211:ILE:HG13	1.49	1.12
2:F:142:LEU:HD13	2:F:154:ILE:HG23	1.21	1.11
2:F:142:LEU:HD22	2:F:154:ILE:CD1	1.71	1.11
2:F:90:MET:HE1	2:F:151:LEU:HD21	1.21	1.11
2:F:90:MET:CE	2:F:151:LEU:HD21	1.80	1.10
2:F:138:LEU:CD2	2:F:153:LEU:HD21	1.80	1.10
2:F:142:LEU:HD11	2:F:154:ILE:CB	1.81	1.10
2:F:164:PHE:O	2:F:415:HIS:CD2	2.03	1.10
2:F:165:ARG:HD2	2:F:168:PHE:CZ	1.90	1.06
2:B:392:LYS:HG2	2:B:395:ARG:HH12	0.91	1.05
2:F:212:LEU:HD12	2:F:300:ILE:HG12	1.29	1.05
2:F:142:LEU:CG	2:F:154:ILE:HG12	1.86	1.05
3:G:24:DG:H2'	3:G:25:DT:H5'	1.10	1.04
2:B:545:LYS:NZ	2:B:690:ASN:OD1	1.92	1.03
2:B:558:LYS:HE3	2:B:590:SER:HB3	1.36	1.03
2:F:142:LEU:CD1	2:F:154:ILE:CG1	2.11	1.03
2:F:139:ARG:HD3	2:F:157:ALA:C	1.84	1.03
2:B:1221:GLN:HG2	2:B:1319:GLY:O	1.59	1.02
2:F:151:LEU:HD13	2:F:152:ARG:H	1.22	1.02
2:F:180:ASP:HB3	2:F:183:LYS:HB2	1.39	1.02
2:B:1222:LYS:O	2:B:1318:LEU:HD21	1.60	1.00
2:F:138:LEU:CG	2:F:153:LEU:HD21	1.93	0.99
2:F:139:ARG:HD3	2:F:157:ALA:O	1.63	0.99
2:F:1210:ARG:NH2	2:F:1341:GLU:OE1	1.95	0.99
2:F:138:LEU:HD13	2:F:153:LEU:HD21	1.42	0.99
2:B:1222:LYS:O	2:B:1318:LEU:HD23	1.59	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:381:GLU:HG2	2:B:390:LEU:HD11	1.43	0.98
2:F:138:LEU:CD2	2:F:153:LEU:CD2	2.42	0.98
2:B:951:ARG:NH2	2:B:1011:GLY:HA2	1.80	0.97
2:F:90:MET:CE	2:F:151:LEU:CD2	2.42	0.97
2:F:142:LEU:HD22	2:F:154:ILE:HD13	1.45	0.97
2:F:142:LEU:CD2	2:F:154:ILE:CG1	2.39	0.96
3:G:24:DG:C2'	3:G:25:DT:H5'	1.96	0.96
2:B:1211:LYS:O	2:B:1223:GLY:HA3	1.65	0.95
2:B:137:HIS:HA	2:B:322:ILE:HD11	1.47	0.95
2:F:686:ASP:CG	2:F:690:ASN:HA	1.91	0.95
2:F:212:LEU:CD1	2:F:300:ILE:CG1	2.44	0.95
2:B:1222:LYS:O	2:B:1318:LEU:HD22	1.67	0.94
2:F:921:LEU:HD12	2:F:1008:PHE:HE2	1.15	0.94
1:A:4:A:O2'	1:A:5:C:O5'	1.83	0.94
3:G:24:DG:H2'	3:G:25:DT:C5'	1.97	0.94
2:B:220:ARG:O	2:B:224:ASN:ND2	2.00	0.94
2:F:142:LEU:HD13	2:F:154:ILE:CG2	1.97	0.94
2:F:212:LEU:HD11	2:F:300:ILE:HG12	1.48	0.94
2:F:165:ARG:HD2	2:F:168:PHE:HE1	1.15	0.93
2:F:142:LEU:CD1	2:F:154:ILE:HG23	1.98	0.93
1:A:3:A:O2'	1:A:4:A:O5'	1.85	0.93
2:F:142:LEU:HD22	2:F:154:ILE:HD11	1.38	0.93
2:F:626:PHE:O	2:F:655:ARG:NH1	2.01	0.93
1:E:4:A:N3	1:E:5:C:C6	2.38	0.92
2:F:149:ALA:HB3	2:F:154:ILE:CD1	2.00	0.92
2:F:138:LEU:HD13	2:F:153:LEU:CD2	1.97	0.91
2:F:777:SER:HA	2:F:807:GLN:HE21	1.35	0.91
2:F:138:LEU:HD11	2:F:153:LEU:HD22	1.51	0.91
2:F:485:GLY:HA3	2:F:631:MET:HG3	1.52	0.91
2:F:142:LEU:HD21	2:F:154:ILE:HD11	1.00	0.90
2:B:601:ILE:HD11	2:B:607:LEU:HD21	1.53	0.90
2:F:142:LEU:HD11	2:F:154:ILE:CA	2.02	0.90
2:F:978:ILE:HD12	2:F:1233:VAL:HG22	1.53	0.90
2:F:138:LEU:HD21	2:F:153:LEU:CD2	2.03	0.89
2:F:686:ASP:CB	2:F:690:ASN:HA	2.02	0.89
2:F:142:LEU:HD11	2:F:154:ILE:HA	1.54	0.89
2:F:138:LEU:CD1	2:F:153:LEU:HD22	2.02	0.88
1:E:4:A:N3	1:E:5:C:C5	2.40	0.88
2:F:380:LEU:HD11	2:F:390:LEU:HG	1.53	0.88
2:B:392:LYS:CG	2:B:395:ARG:HH12	1.84	0.87
1:E:4:A:C2	1:E:5:C:C6	2.63	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:142:LEU:CD2	2:F:154:ILE:HG12	2.04	0.87
2:F:467:ARG:HA	2:F:482:VAL:HG22	1.57	0.87
2:F:249:THR:OG1	2:F:267:SER:N	2.08	0.86
2:F:142:LEU:CD1	2:F:154:ILE:HA	2.06	0.85
2:B:921:LEU:HD21	2:B:1042:ILE:HG21	1.57	0.85
2:B:967:ARG:HE	2:B:974:LYS:HB2	1.42	0.85
2:F:893:THR:HG23	2:F:896:LYS:H	1.40	0.84
2:F:279:LEU:HD21	2:F:287:ALA:HB2	1.59	0.84
2:F:226:ILE:HG13	2:F:232:GLU:HG2	1.59	0.84
2:F:139:ARG:HH21	2:F:160:HIS:CD2	1.95	0.84
2:F:208:ALA:HA	2:F:211:ILE:HD12	0.88	0.84
2:B:455:LEU:HD23	2:B:473:ILE:HD12	1.60	0.84
2:F:451:TYR:O	2:F:464:TRP:NE1	2.10	0.84
5:J:46:A:H2'	5:J:47:A:C8	2.13	0.83
1:A:2:U:H3	1:A:4:A:H3'	1.42	0.83
3:G:1:DC:N4	4:H:12:DG:O6	2.11	0.83
2:F:1045:PHE:HA	2:F:1060:ARG:HH11	1.43	0.83
2:B:1110:ILE:HD12	2:B:1122:ARG:HD2	1.60	0.83
2:F:151:LEU:HD13	2:F:152:ARG:N	1.93	0.82
1:A:14:G:OP2	2:B:63:ARG:NH1	2.12	0.82
2:B:1236:LEU:HD11	2:B:1269:ILE:HD13	1.62	0.82
2:B:384:ASP:OD1	2:B:385:GLY:N	2.12	0.82
2:F:1045:PHE:HB2	2:F:1064:GLU:HG2	1.62	0.82
3:G:25:DT:H2''	3:G:26:DT:OP2	1.80	0.81
2:F:138:LEU:HD21	2:F:153:LEU:HD23	1.59	0.81
2:F:151:LEU:HD22	2:F:152:ARG:N	1.95	0.81
2:F:164:PHE:O	2:F:415:HIS:HD2	1.58	0.81
1:E:4:A:C2	1:E:5:C:C4	2.68	0.81
2:F:1120:ILE:HD11	2:F:1137:PRO:HD3	1.62	0.81
2:B:212:LEU:O	2:B:221:ARG:NH1	2.14	0.81
2:F:165:ARG:CD	2:F:168:PHE:CE1	2.56	0.81
2:F:1212:ARG:NH2	2:F:1280:VAL:O	2.15	0.80
2:F:142:LEU:CD1	2:F:154:ILE:CB	2.52	0.80
2:F:1041:ASN:O	2:F:1043:MET:N	2.13	0.80
2:F:425:ARG:HG3	2:F:426:GLN:HG2	1.63	0.79
2:F:139:ARG:CD	2:F:157:ALA:O	2.29	0.79
2:F:165:ARG:CD	2:F:168:PHE:HE1	1.92	0.79
2:F:135:ILE:HD11	2:F:156:LEU:HB3	1.64	0.79
2:F:686:ASP:HB3	2:F:690:ASN:HA	1.63	0.79
2:B:823:TYR:HA	2:B:875:VAL:HG11	1.64	0.79
2:F:89:GLU:OE2	2:F:92:LYS:NZ	2.15	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:90:MET:SD	2:F:151:LEU:HD21	2.22	0.79
2:B:116:HIS:CE1	2:B:122:ILE:HG12	2.17	0.78
2:F:166:GLY:HA3	2:F:410:ILE:HG22	1.64	0.78
2:B:404:THR:HG22	2:B:405:PHE:CD1	2.19	0.78
2:F:886:LEU:HA	2:F:891:LEU:HD21	1.64	0.78
2:F:142:LEU:CD1	2:F:154:ILE:CG2	2.59	0.78
2:B:442:LYS:HE3	2:B:476:TRP:HA	1.65	0.78
2:B:725:ALA:O	2:B:734:LYS:NZ	2.17	0.77
2:F:522:ASN:OD1	2:F:692:ASN:ND2	2.16	0.77
2:F:962:LEU:HB3	2:F:1043:MET:HE1	1.63	0.77
2:B:338:LEU:O	2:B:383:MET:HE1	1.84	0.77
2:B:1222:LYS:HE3	2:B:1317:ASN:O	1.85	0.77
2:F:94:ASP:HB3	2:F:97:PHE:HB2	1.65	0.77
2:F:846:PHE:O	2:F:1040:SER:OG	2.02	0.77
2:F:70:ARG:NH2	5:J:61:C:OP1	2.16	0.77
2:F:63:ARG:HA	2:F:66:ARG:HG3	1.65	0.77
1:A:27:G:H5'	1:A:28:A:H5''	1.67	0.77
2:F:649:LYS:O	2:F:653:ARG:NE	2.17	0.77
2:B:1147:ALA:HB2	2:B:1190:VAL:HA	1.67	0.77
3:G:6:DC:N4	4:H:7:DG:O6	2.18	0.77
2:B:279:LEU:HD11	2:B:284:ASP:HA	1.68	0.76
2:F:142:LEU:HD11	2:F:154:ILE:HG12	0.76	0.76
2:B:913:LYS:HA	2:B:916:PHE:HD2	1.50	0.76
2:B:201:ILE:HG22	2:B:202:ASN:H	1.51	0.76
2:B:524:LEU:HD12	2:B:587:PHE:HE2	1.50	0.76
1:E:15:G:OP1	2:F:66:ARG:NH2	2.19	0.76
2:F:921:LEU:HD21	2:F:1042:ILE:HG21	1.67	0.76
2:B:586:ARG:NH1	3:C:26:DT:O2	2.19	0.76
2:F:128:TYR:CE1	2:F:153:LEU:HD11	2.21	0.76
2:F:1045:PHE:HA	2:F:1060:ARG:NH1	2.01	0.76
2:F:999:LYS:HB3	2:F:1073:VAL:HG12	1.66	0.75
2:F:139:ARG:HG2	2:F:157:ALA:HB1	0.79	0.75
2:F:139:ARG:CG	2:F:157:ALA:CB	2.40	0.75
2:F:149:ALA:CB	2:F:154:ILE:CD1	2.65	0.74
2:F:446:PHE:HZ	2:F:478:PHE:HD1	1.34	0.74
2:B:45:LYS:NZ	2:B:1357:GLU:OE2	2.15	0.74
2:B:864:ARG:NH2	2:B:869:ASN:O	2.19	0.74
2:F:1215:ALA:HB2	2:F:1221:GLN:HG3	1.68	0.74
2:F:168:PHE:HB2	2:F:447:ARG:HH11	1.52	0.74
2:F:844:GLN:OE1	2:F:848:LYS:NZ	2.15	0.74
2:B:74:ARG:HH21	5:I:60:C:P	2.10	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1211:LYS:O	2:B:1223:GLY:CA	2.34	0.74
2:F:842:VAL:HG12	2:F:854:ASN:OD1	1.87	0.74
2:F:148:LYS:CB	2:F:429:PHE:CD2	2.70	0.73
2:F:446:PHE:CZ	2:F:478:PHE:HD1	2.06	0.73
1:A:20:A:OP2	2:B:403:ARG:NH1	2.21	0.73
2:F:199:ASN:O	2:F:201:ILE:HD11	1.87	0.73
2:B:939:MET:HE2	2:B:953:VAL:HG21	1.70	0.73
2:F:138:LEU:HD22	2:F:153:LEU:HD21	1.69	0.73
2:F:142:LEU:HD21	2:F:149:ALA:CB	2.17	0.73
2:F:149:ALA:CB	2:F:154:ILE:HG13	2.18	0.73
2:F:913:LYS:HG3	2:F:1040:SER:HB3	1.69	0.73
3:C:25:DT:C2	3:C:26:DT:H72	2.24	0.73
1:E:27:G:N2	5:J:44:U:OP2	2.22	0.73
2:F:149:ALA:CB	2:F:154:ILE:HD11	2.18	0.73
2:F:151:LEU:HD22	2:F:151:LEU:C	2.14	0.72
2:F:370:GLU:OE2	2:F:374:LYS:NZ	2.22	0.72
2:B:279:LEU:CD1	2:B:284:ASP:HA	2.19	0.72
2:B:1210:ARG:NH2	2:B:1341:GLU:OE1	2.22	0.72
2:F:923:GLU:HG2	2:F:928:THR:HG21	1.72	0.72
2:B:619:ILE:O	2:B:623:LEU:HB2	1.90	0.72
2:F:530:VAL:HG22	2:F:537:PRO:HB3	1.70	0.72
1:E:19:A:O2'	2:F:405:PHE:O	2.07	0.72
2:F:253:LYS:HG3	2:F:261:ASP:HA	1.72	0.72
2:B:1210:ARG:HB2	2:B:1280:VAL:HG13	1.72	0.71
2:F:1205:GLU:OE1	2:F:1359:ARG:NH2	2.22	0.71
2:B:21:ILE:HD11	2:B:995:THR:HG21	1.71	0.71
2:B:217:SER:HB2	2:B:220:ARG:H	1.56	0.71
2:B:1220:LEU:HD11	2:B:1339:THR:HA	1.70	0.71
2:F:128:TYR:HE1	2:F:153:LEU:HD11	1.55	0.71
2:B:165:ARG:NH2	2:B:446:PHE:O	2.24	0.71
2:B:787:GLY:HA3	2:B:891:LEU:HD21	1.71	0.71
2:B:299:ALA:O	2:B:303:SER:OG	2.07	0.71
2:F:527:VAL:HA	2:F:582:GLY:HA3	1.73	0.71
3:C:25:DT:N3	3:C:26:DT:C4	2.59	0.70
2:F:505:GLU:HG3	2:F:665:LYS:HB2	1.72	0.70
2:F:1207:GLU:OE2	2:F:1210:ARG:NH1	2.24	0.70
2:B:530:VAL:HG22	2:B:537:PRO:HB3	1.72	0.70
2:F:139:ARG:CD	2:F:157:ALA:HB1	2.21	0.70
2:F:153:LEU:HD23	2:F:153:LEU:C	2.16	0.70
2:F:921:LEU:HD21	2:F:1042:ILE:HD13	1.73	0.70
2:B:874:GLU:HA	2:B:877:LYS:HE3	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1135:ASP:OD1	2:B:1136:SER:N	2.24	0.70
2:B:650:GLN:OE1	2:B:653:ARG:NH2	2.25	0.70
2:B:951:ARG:CZ	2:B:1011:GLY:HA2	2.21	0.70
2:F:128:TYR:CE1	2:F:153:LEU:CD1	2.75	0.70
3:G:24:DG:C2'	3:G:25:DT:C5'	2.65	0.70
2:B:69:ARG:HD3	5:I:62:G:N7	2.07	0.70
2:F:936:ASP:OD1	2:F:940:ASN:ND2	2.24	0.70
2:B:1119:LEU:HD23	2:B:1128:PRO:HB2	1.73	0.69
2:B:1333:ARG:NH1	2:B:1335:ARG:HD2	2.06	0.69
2:F:921:LEU:HD12	2:F:1008:PHE:CZ	2.25	0.69
2:F:1206:LEU:HD11	2:F:1210:ARG:CZ	2.21	0.69
2:B:51:LEU:HD13	2:B:1095:VAL:HG23	1.74	0.69
2:F:199:ASN:O	2:F:201:ILE:CD1	2.41	0.69
2:F:90:MET:HE1	2:F:151:LEU:HD23	1.71	0.69
2:F:20:VAL:HG11	2:F:751:MET:HE3	1.75	0.69
2:F:446:PHE:HZ	2:F:478:PHE:CD1	2.11	0.69
2:F:892:ILE:HB	2:F:896:LYS:HE3	1.74	0.69
2:B:345:GLU:N	2:B:345:GLU:OE1	2.26	0.69
5:J:40:C:H2'	5:J:41:A:C8	2.28	0.68
2:B:465:MET:HE3	2:B:467:ARG:HG2	1.76	0.68
2:B:243:ALA:O	2:B:248:LEU:HB2	1.93	0.68
2:F:471:GLU:OE1	2:F:477:ASN:ND2	2.26	0.68
2:F:1091:GLN:HG3	5:J:91:C:H5''	1.76	0.68
2:F:1219:GLU:OE1	2:F:1335:ARG:NH2	2.22	0.68
2:B:745:ASP:OD2	2:B:938:ARG:NH2	2.27	0.68
2:B:369:GLN:HE22	2:B:400:ARG:HD2	1.57	0.68
2:F:697:ILE:HD11	2:F:708:ILE:HG13	1.76	0.67
5:J:40:C:H2'	5:J:41:A:H8	1.59	0.67
2:B:557:ARG:NH2	2:B:596:ASP:OD1	2.27	0.67
2:F:686:ASP:OD2	2:F:690:ASN:HA	1.93	0.67
2:B:565:LYS:HE2	2:B:580:ILE:HG12	1.77	0.67
2:B:818:ASN:O	2:B:818:ASN:ND2	2.28	0.67
2:B:860:SER:OG	2:B:863:ASN:OD1	2.11	0.67
2:F:208:ALA:HA	2:F:211:ILE:CG1	2.24	0.67
2:F:328:HIS:NE2	2:F:359:TYR:OH	2.24	0.67
2:F:148:LYS:HB3	2:F:429:PHE:CD2	2.30	0.67
2:B:229:LEU:HB2	2:B:230:PRO:HD2	1.76	0.67
2:B:1241:HIS:CE1	2:B:1244:LYS:HA	2.29	0.67
2:F:870:VAL:HG12	2:F:871:PRO:HD2	1.77	0.67
2:B:1318:LEU:HD13	2:B:1319:GLY:N	2.09	0.67
2:F:791:LEU:HD23	2:F:818:ASN:OD1	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:826:GLN:OE1	2:F:859:ARG:NH1	2.28	0.67
1:A:27:G:H5'	1:A:28:A:C5'	2.25	0.66
2:B:70:ARG:NH2	5:I:61:C:OP1	2.28	0.66
2:F:70:ARG:NE	5:J:61:C:OP2	2.19	0.66
2:F:967:ARG:NH1	2:F:986:ASP:OD1	2.27	0.66
2:B:585:ASP:OD1	2:B:586:ARG:N	2.28	0.66
1:E:19:A:H4'	2:F:407:ASN:C	2.20	0.66
2:F:672:ASP:OD1	2:F:703:THR:HG22	1.95	0.66
2:B:5:TYR:CE2	2:B:756:PRO:HB3	2.30	0.66
2:F:139:ARG:NE	2:F:157:ALA:O	2.28	0.66
2:F:165:ARG:CD	2:F:168:PHE:CZ	2.73	0.66
2:B:967:ARG:NE	2:B:974:LYS:HB2	2.09	0.66
2:F:46:ASN:HD21	5:J:88:A:H61	1.44	0.66
2:F:892:ILE:HB	2:F:896:LYS:CE	2.25	0.66
2:F:40:ARG:NE	2:F:43:ILE:HD11	2.11	0.66
2:B:1318:LEU:HD13	2:B:1318:LEU:C	2.20	0.66
2:F:633:GLU:O	2:F:637:LYS:N	2.27	0.66
2:B:317:LEU:HD22	2:B:414:ILE:HD11	1.78	0.66
2:F:1206:LEU:HD11	2:F:1210:ARG:NH2	2.11	0.66
2:B:5:TYR:OH	2:B:754:HIS:O	2.13	0.66
2:F:340:ARG:HG3	2:F:347:TYR:CE1	2.31	0.66
2:F:686:ASP:HB3	2:F:690:ASN:OD1	1.96	0.66
2:B:544:GLN:O	2:B:548:ILE:N	2.18	0.65
2:F:142:LEU:HD21	2:F:154:ILE:HG12	1.64	0.65
2:B:524:LEU:HD12	2:B:587:PHE:CE2	2.30	0.65
2:B:549:VAL:HA	2:B:553:PHE:HD2	1.61	0.65
2:B:989:LEU:HD21	2:B:1087:LEU:HD21	1.78	0.65
2:B:404:THR:HG22	2:B:405:PHE:H	1.61	0.65
2:F:853:ASP:HB3	2:F:895:ARG:HH11	1.61	0.65
2:B:823:TYR:HD2	2:B:858:THR:HG21	1.61	0.65
2:F:212:LEU:O	2:F:221:ARG:CB	2.45	0.65
2:F:686:ASP:HB3	2:F:690:ASN:CA	2.26	0.65
2:F:867:SER:HB2	2:F:1054:ASN:N	2.11	0.65
2:B:181:VAL:O	2:B:185:PHE:N	2.28	0.65
3:C:22:DT:H2''	3:C:23:DC:O5'	1.95	0.65
2:F:986:ASP:O	2:F:990:ASN:ND2	2.30	0.65
3:C:25:DT:N3	3:C:26:DT:O4	2.29	0.65
2:F:153:LEU:HD23	2:F:153:LEU:O	1.96	0.65
2:F:422:ILE:O	2:F:425:ARG:HG2	1.97	0.65
2:F:978:ILE:CD1	2:F:1233:VAL:HG22	2.25	0.65
2:F:1197:LYS:O	2:F:1199:PRO:HD3	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1304:GLU:O	2:F:1308:ASN:ND2	2.29	0.65
2:B:742:LYS:NZ	5:I:67:C:OP1	2.21	0.65
2:B:516:GLU:O	2:B:519:THR:HG22	1.98	0.64
2:B:824:VAL:HG22	2:B:863:ASN:HD22	1.61	0.64
2:F:167:HIS:HD2	2:F:169:LEU:HB2	1.60	0.64
2:F:221:ARG:O	2:F:225:LEU:N	2.22	0.64
1:A:5:C:O2'	1:A:6:G:O5'	2.16	0.64
2:B:879:MET:HG3	2:B:882:TYR:HB3	1.78	0.64
2:F:887:LEU:HD21	2:F:894:GLN:HG2	1.80	0.64
2:F:1357:GLU:O	5:J:81:G:N2	2.29	0.64
2:F:923:GLU:OE2	2:F:925:ARG:NH1	2.29	0.64
1:E:3:A:C4	1:E:4:A:N7	2.66	0.64
2:F:149:ALA:HB3	2:F:154:ILE:HG13	1.80	0.64
2:F:760:VAL:HG22	2:F:956:ILE:HD12	1.79	0.64
2:B:1120:ILE:HD11	2:B:1137:PRO:HG3	1.79	0.64
2:F:149:ALA:HB3	2:F:154:ILE:CG1	2.28	0.64
2:F:1110:ILE:HD13	2:F:1122:ARG:CZ	2.28	0.64
2:F:1286:ASN:ND2	2:F:1332:ASP:O	2.31	0.64
2:F:89:GLU:HG3	2:F:432:PHE:HD2	1.62	0.63
2:F:165:ARG:HG2	2:F:166:GLY:O	1.98	0.63
2:F:184:LEU:HD13	2:F:295:ASN:HB3	1.79	0.63
2:F:853:ASP:HB3	2:F:895:ARG:NH1	2.12	0.63
2:F:1147:ALA:HB2	2:F:1190:VAL:HA	1.79	0.63
2:B:1312:LEU:HD21	2:B:1326:TYR:HD1	1.63	0.63
1:A:2:U:O2	1:A:3:A:H2'	1.97	0.63
2:F:135:ILE:HG21	5:J:46:A:H5'	1.80	0.63
2:F:189:VAL:HG13	2:F:201:ILE:HG22	1.80	0.63
1:A:2:U:O2	1:A:3:A:C2'	2.46	0.63
2:F:168:PHE:HB2	2:F:447:ARG:NH1	2.14	0.63
2:F:373:TYR:OH	2:F:398:LEU:N	2.30	0.63
2:B:121:ASN:OD1	2:B:124:ASP:HB2	1.99	0.63
2:B:270:THR:O	2:B:274:ASP:HB2	1.98	0.63
1:E:19:A:OP1	2:F:164:PHE:HD1	1.82	0.63
2:B:103:GLU:OE2	2:B:111:LYS:HG2	1.99	0.62
2:F:121:ASN:OD1	2:F:124:ASP:N	2.31	0.62
2:F:601:ILE:CD1	2:F:607:LEU:HD21	2.28	0.62
2:F:646:LYS:O	2:F:650:GLN:NE2	2.22	0.62
2:F:921:LEU:CD1	2:F:1008:PHE:HE2	2.02	0.62
2:F:963:VAL:HG21	2:F:990:ASN:OD1	1.99	0.62
2:B:70:ARG:HH22	2:B:462:PHE:HD2	1.47	0.62
2:B:139:ARG:HD3	2:B:161:MET:HE2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:89:GLU:HG3	2:F:432:PHE:CD2	2.34	0.62
2:F:139:ARG:HH21	2:F:160:HIS:HD2	1.45	0.62
2:F:168:PHE:CB	2:F:447:ARG:HH11	2.12	0.62
2:F:182:ASP:O	2:F:186:ILE:HD12	1.99	0.62
1:E:3:A:H2'	1:E:4:A:H8	1.64	0.62
2:F:918:LYS:O	2:F:922:VAL:HG22	2.00	0.62
2:F:1266:LEU:HB3	2:F:1294:TYR:OH	1.99	0.62
2:F:1294:TYR:HE1	2:F:1305:GLN:HE21	1.45	0.62
2:F:1311:HIS:O	2:F:1314:THR:HG22	2.00	0.62
1:A:5:C:H2'	1:A:6:G:H8	1.64	0.62
2:F:114:GLU:HG2	2:F:120:GLY:HA2	1.81	0.62
2:B:893:THR:HG23	2:B:896:LYS:H	1.63	0.62
2:F:841:ILE:HD12	2:F:854:ASN:HA	1.82	0.62
2:B:823:TYR:HA	2:B:875:VAL:CG1	2.30	0.62
2:F:189:VAL:HG13	2:F:201:ILE:CG2	2.30	0.62
2:F:207:ASP:O	2:F:211:ILE:CG1	2.39	0.62
2:F:977:GLU:HG3	2:F:1310:ILE:CG2	2.30	0.62
2:F:1300:LYS:NZ	2:F:1304:GLU:OE1	2.33	0.62
2:B:118:ILE:HD13	2:B:128:TYR:CD2	2.35	0.62
2:F:184:LEU:O	2:F:187:GLN:OE1	2.18	0.62
2:B:233:LYS:HG2	2:B:235:ASN:H	1.65	0.61
2:B:247:GLY:O	2:B:248:LEU:HG	2.00	0.61
2:B:810:LYS:HG2	2:B:838:VAL:HG23	1.82	0.61
2:B:184:LEU:HD12	2:B:299:ALA:HB2	1.82	0.61
2:F:183:LYS:H	2:F:183:LYS:HD2	1.65	0.61
2:B:174:LEU:HD23	2:B:302:LEU:HD23	1.81	0.61
2:F:208:ALA:N	2:F:211:ILE:HD12	2.15	0.61
2:B:332:LEU:HD13	2:B:359:TYR:CE1	2.35	0.61
2:F:212:LEU:HD11	2:F:300:ILE:CG1	2.19	0.61
5:J:83:C:H2'	5:J:84:A:H8	1.65	0.61
5:I:83:C:H2'	5:I:84:A:H8	1.64	0.61
2:F:1064:GLU:OE1	2:F:1065:THR:N	2.31	0.61
2:B:525:THR:HA	2:B:545:LYS:HE2	1.83	0.61
2:B:1000:LYS:HE2	2:B:1066:ASN:HA	1.83	0.61
2:F:35:LEU:HB2	2:F:1358:THR:HG22	1.83	0.61
2:F:841:ILE:CD1	2:F:896:LYS:HG3	2.30	0.61
2:F:275:LEU:O	2:F:279:LEU:N	2.34	0.61
2:F:818:ASN:ND2	2:F:818:ASN:O	2.32	0.61
5:J:44:U:O2'	5:J:45:U:H5'	1.99	0.61
2:B:168:PHE:CD2	2:B:447:ARG:HD3	2.35	0.61
2:B:114:GLU:HG2	2:B:120:GLY:HA2	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:U:H1'	5:I:39:G:N2	2.15	0.60
2:F:755:LYS:HD3	2:F:939:MET:HE3	1.82	0.60
2:F:1062:LEU:O	2:F:1062:LEU:HG	2.01	0.60
2:F:1206:LEU:CD1	2:F:1210:ARG:NH1	2.64	0.60
2:B:1123:LYS:NZ	5:I:52:A:OP1	2.34	0.60
2:F:70:ARG:HH21	5:J:61:C:P	2.24	0.60
2:F:149:ALA:CB	2:F:154:ILE:CG1	2.79	0.60
1:A:2:U:O2	1:A:4:A:H8	1.83	0.60
2:B:917:ILE:HD11	2:B:1042:ILE:HG22	1.82	0.60
2:F:692:ASN:O	2:F:696:LEU:HG	2.01	0.60
2:B:909:SER:O	2:B:913:LYS:N	2.26	0.60
2:F:737:ILE:O	2:F:740:THR:HG22	2.01	0.60
2:F:1120:ILE:HB	2:F:1134:PHE:HB2	1.84	0.60
2:B:27:VAL:HG12	2:B:1086:VAL:HG22	1.83	0.60
2:B:250:PRO:HD2	2:B:264:LEU:O	2.01	0.60
2:B:420:HIS:ND1	2:B:441:GLU:OE2	2.35	0.60
2:F:69:ARG:NH2	5:J:63:U:OP2	2.35	0.60
2:F:545:LYS:NZ	2:F:683:LEU:O	2.35	0.60
2:F:142:LEU:HD21	2:F:149:ALA:HB2	1.83	0.60
2:B:541:SER:N	2:B:544:GLN:OE1	2.34	0.59
2:B:670:ILE:HG22	2:B:704:PHE:HE1	1.67	0.59
2:B:1305:GLN:O	2:B:1309:ILE:HG13	2.02	0.59
2:F:821:ASP:HB2	2:F:828:LEU:HD21	1.83	0.59
2:B:902:LYS:HA	2:B:905:ARG:HE	1.67	0.59
2:F:138:LEU:HD11	2:F:153:LEU:HD23	1.74	0.59
2:F:694:MET:HE3	2:F:698:HIS:NE2	2.17	0.59
2:B:158:LEU:HD11	2:B:423:LEU:HD21	1.84	0.59
2:B:386:THR:O	2:B:386:THR:HG22	2.01	0.59
2:B:1062:LEU:HD23	2:B:1062:LEU:H	1.67	0.59
2:F:137:HIS:HA	2:F:322:ILE:HD11	1.83	0.59
2:F:138:LEU:HD21	2:F:153:LEU:O	2.01	0.59
2:F:149:ALA:HB2	2:F:154:ILE:HD11	1.82	0.59
2:F:677:LYS:HB3	2:F:682:PHE:CD2	2.36	0.59
1:A:10:U:H2'	1:A:11:U:C6	2.37	0.59
3:C:25:DT:H2'	3:C:25:DT:O2	2.01	0.59
2:F:643:PHE:HB2	2:F:648:MET:HE3	1.84	0.59
2:B:979:ASN:OD1	2:B:980:ASN:N	2.35	0.59
2:B:358:GLY:O	2:B:362:TYR:N	2.33	0.59
2:B:644:ASP:HB3	2:B:647:VAL:HG23	1.85	0.59
2:F:253:LYS:HB2	2:F:262:ALA:H	1.66	0.59
2:F:686:ASP:OD2	2:F:691:ARG:N	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1252:ASN:HD22	2:B:1255:LYS:HD2	1.66	0.59
2:F:531:THR:HG21	2:F:575:PHE:CE1	2.38	0.59
2:B:828:LEU:HD22	2:B:836:TYR:CE2	2.37	0.59
2:F:853:ASP:CG	2:F:893:THR:HG21	2.27	0.59
2:F:943:TYR:CE2	2:F:949:LEU:HD13	2.38	0.59
2:B:971:GLN:O	2:B:971:GLN:HG2	2.01	0.59
2:B:1308:ASN:HD22	2:B:1327:PHE:H	1.51	0.59
2:F:601:ILE:HD11	2:F:607:LEU:HD21	1.83	0.59
2:B:1258:PHE:HE1	2:B:1262:HIS:CD2	2.21	0.59
2:B:1290:VAL:HG22	2:B:1331:ILE:HD13	1.85	0.59
2:B:980:ASN:HB2	2:B:1225:GLU:CD	2.28	0.58
2:F:1326:TYR:CE2	2:F:1327:PHE:HD2	2.21	0.58
2:B:565:LYS:HA	2:B:569:PHE:HB2	1.84	0.58
2:F:1206:LEU:HD11	2:F:1210:ARG:NH1	2.16	0.58
2:B:563:GLN:O	2:B:567:ASP:HB2	2.03	0.58
2:B:971:GLN:O	2:B:1234:ASN:ND2	2.35	0.58
2:F:1019:ARG:C	2:F:1021:MET:H	2.11	0.58
2:B:671:ARG:HG3	2:B:678:THR:HG22	1.84	0.58
2:B:1146:VAL:HG11	2:B:1194:LEU:HD12	1.86	0.58
2:F:466:THR:O	2:F:482:VAL:HG13	2.04	0.58
2:F:681:ASP:HA	2:F:684:LYS:HZ3	1.68	0.58
2:B:135:ILE:HG21	2:B:160:HIS:CD2	2.39	0.58
5:J:53:G:C4	5:J:62:G:N2	2.72	0.58
2:F:208:ALA:O	2:F:211:ILE:HB	2.04	0.58
2:F:448:ILE:HD12	2:F:455:LEU:HD11	1.86	0.58
2:F:135:ILE:HD13	2:F:156:LEU:HD23	1.85	0.58
2:F:139:ARG:NH1	2:F:418:GLU:OE2	2.37	0.58
2:B:243:ALA:O	2:B:246:LEU:O	2.21	0.58
2:F:844:GLN:HA	2:F:847:LEU:O	2.04	0.58
2:B:119:PHE:HD1	2:B:152:ARG:NH1	2.01	0.58
2:B:1041:ASN:O	2:B:1044:ASN:ND2	2.36	0.58
2:F:149:ALA:HB3	2:F:154:ILE:HD12	1.82	0.58
2:F:226:ILE:CG1	2:F:232:GLU:HG2	2.30	0.58
2:B:544:GLN:HA	2:B:547:ALA:HB3	1.86	0.57
2:F:305:ILE:HG13	2:F:306:LEU:HD13	1.86	0.57
2:F:499:ASP:HB2	2:F:663:SER:HB3	1.85	0.57
2:B:245:SER:HA	2:B:297:SER:HB2	1.85	0.57
2:B:687:GLY:O	2:B:690:ASN:ND2	2.38	0.57
2:F:677:LYS:HB3	2:F:682:PHE:CE2	2.39	0.57
1:E:3:A:N6	1:E:4:A:H62	2.01	0.57
2:F:78:ARG:CZ	2:F:165:ARG:NH2	2.67	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:226:ILE:HD11	2:F:232:GLU:CD	2.30	0.57
2:F:1286:ASN:O	2:F:1290:VAL:HG23	2.04	0.57
2:F:135:ILE:CG2	5:J:46:A:H5'	2.33	0.57
2:F:1019:ARG:O	2:F:1021:MET:N	2.31	0.57
2:B:76:LYS:HE3	2:B:80:CYS:SG	2.44	0.57
2:B:229:LEU:O	2:B:231:GLY:N	2.38	0.57
2:B:485:GLY:HA3	2:B:631:MET:SD	2.44	0.57
2:B:954:LYS:HG3	2:B:1009:VAL:HG11	1.86	0.57
2:B:1211:LYS:C	2:B:1223:GLY:HA3	2.28	0.57
1:E:14:G:OP2	2:F:63:ARG:HD3	2.04	0.57
1:E:4:A:O2'	1:E:5:C:O5'	2.21	0.57
2:F:886:LEU:HD22	2:F:891:LEU:HD11	1.87	0.57
2:B:11:ILE:HB	2:B:763:MET:HG2	1.87	0.57
2:B:70:ARG:HH21	5:I:61:C:P	2.27	0.57
2:B:321:MET:HE1	2:B:324:ARG:HH21	1.70	0.57
2:B:51:LEU:CD1	2:B:1095:VAL:HG23	2.35	0.57
2:B:816:LEU:HD12	2:B:891:LEU:HA	1.86	0.57
4:H:11:DT:H2''	4:H:12:DG:C8	2.39	0.57
2:F:212:LEU:HA	2:F:221:ARG:CB	2.35	0.57
2:F:921:LEU:HD21	2:F:1042:ILE:CD1	2.35	0.57
2:F:1179:ILE:O	2:F:1183:GLU:HG3	2.05	0.57
2:B:22:THR:HG22	2:B:23:ASP:H	1.69	0.56
2:B:45:LYS:NZ	2:B:1354:GLY:O	2.34	0.56
2:B:756:PRO:O	2:B:953:VAL:HG22	2.05	0.56
2:F:514:LEU:H	2:F:514:LEU:HD12	1.70	0.56
2:B:40:ARG:NH2	5:I:92:G:OP1	2.37	0.56
2:B:127:ALA:HA	2:B:130:GLU:HB2	1.87	0.56
2:B:1220:LEU:CD1	2:B:1338:SER:O	2.53	0.56
2:F:272:ASP:HA	2:F:275:LEU:HB3	1.86	0.56
2:F:867:SER:HB2	2:F:1053:ALA:C	2.30	0.56
2:F:1114:ARG:HD2	2:F:1116:SER:HB2	1.88	0.56
2:B:139:ARG:O	2:B:143:VAL:HG23	2.05	0.56
2:B:583:VAL:HG22	2:B:584:GLU:N	2.19	0.56
2:B:1000:LYS:O	2:B:1000:LYS:HD3	2.05	0.56
2:B:1349:HIS:HB3	5:I:68:A:N3	2.20	0.56
2:F:149:ALA:HB1	2:F:154:ILE:HG13	1.86	0.56
2:F:167:HIS:CD2	2:F:169:LEU:HB2	2.40	0.56
2:F:258:LEU:HD22	2:F:260:GLU:H	1.69	0.56
2:F:925:ARG:HB3	2:F:928:THR:HG22	1.87	0.56
5:J:94:U:H2'	5:J:95:G:C8	2.40	0.56
2:B:6:SER:HB2	2:B:21:ILE:HG13	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1228:LEU:HD12	2:B:1229:PRO:HD2	1.86	0.56
2:F:94:ASP:CB	2:F:97:PHE:HB2	2.36	0.56
2:F:551:LEU:O	2:F:555:THR:OG1	2.14	0.56
2:F:870:VAL:HG11	2:F:899:ASN:O	2.05	0.56
2:F:1326:TYR:HE2	2:F:1327:PHE:HD2	1.54	0.56
5:J:91:C:O2'	5:J:92:G:P	2.64	0.56
2:B:321:MET:HE1	2:B:324:ARG:NH2	2.20	0.56
2:B:114:GLU:HG3	2:B:116:HIS:H	1.70	0.56
2:B:489:GLN:HG3	2:B:625:LEU:HD21	1.88	0.56
2:F:135:ILE:HG21	2:F:160:HIS:ND1	2.21	0.56
2:F:332:LEU:HD21	2:F:336:LYS:HE3	1.85	0.56
2:F:681:ASP:HA	2:F:684:LYS:NZ	2.20	0.56
2:B:543:GLU:O	2:B:547:ALA:N	2.38	0.56
2:B:956:ILE:HG12	2:B:1009:VAL:HG22	1.88	0.56
2:F:820:ARG:HG3	2:F:826:GLN:O	2.06	0.56
2:F:1205:GLU:CD	2:F:1359:ARG:HH22	2.13	0.56
2:B:369:GLN:NE2	2:B:400:ARG:HD2	2.21	0.56
2:B:755:LYS:NZ	2:B:939:MET:O	2.19	0.56
2:F:829:ASP:OD1	2:F:831:ASN:N	2.39	0.56
2:F:1114:ARG:NH1	4:H:9:DA:OP1	2.38	0.56
1:A:5:C:C2'	1:A:6:G:O5'	2.54	0.56
2:B:321:MET:O	2:B:324:ARG:N	2.39	0.56
2:B:353:ASP:CG	2:B:356:LYS:HG2	2.30	0.56
2:B:8:GLY:HA3	2:B:991:ALA:HB2	1.88	0.55
2:B:38:THR:HG22	2:B:40:ARG:H	1.71	0.55
2:B:395:ARG:NH2	2:B:397:ASP:OD2	2.38	0.55
2:F:185:PHE:O	2:F:189:VAL:HG23	2.07	0.55
2:F:1266:LEU:HG	2:F:1309:ILE:CD1	2.36	0.55
2:B:620:VAL:O	2:B:624:THR:HG22	2.06	0.55
2:B:875:VAL:HA	2:B:878:LYS:HD2	1.88	0.55
4:D:5:DA:H1'	4:D:6:DG:C8	2.41	0.55
2:F:51:LEU:HD13	2:F:1352:ILE:HG13	1.87	0.55
2:F:162:ILE:HG12	2:F:444:LEU:HD12	1.88	0.55
2:F:516:GLU:O	2:F:519:THR:HG22	2.06	0.55
2:B:1041:ASN:HB2	2:B:1044:ASN:HD21	1.72	0.55
1:E:25:U:H5'	2:F:107:VAL:HG12	1.87	0.55
2:F:478:PHE:HE2	2:F:482:VAL:HB	1.71	0.55
2:F:336:LYS:HE2	2:F:351:PHE:CE1	2.41	0.55
2:F:243:ALA:HB3	2:F:250:PRO:HG3	1.88	0.55
2:F:671:ARG:HD3	2:F:671:ARG:N	2.21	0.55
2:B:1207:GLU:HG2	2:B:1210:ARG:HH11	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:122:ILE:O	2:F:126:VAL:HG23	2.05	0.55
2:F:1224:ASN:HB2	2:F:1280:VAL:HG11	1.87	0.55
2:F:106:LEU:HD22	2:F:1131:TYR:OH	2.06	0.55
2:F:46:ASN:HD22	2:F:1089:MET:CE	2.20	0.55
2:F:151:LEU:HD13	2:F:151:LEU:N	2.21	0.55
2:B:325:TYR:HD1	5:I:44:U:C2	2.24	0.55
2:B:595:HIS:HB3	2:B:599:LYS:NZ	2.22	0.55
2:F:234:LYS:H	2:F:234:LYS:HD3	1.71	0.55
2:F:309:ASN:OD1	2:F:312:ILE:HG23	2.07	0.55
2:F:794:GLN:H	2:F:794:GLN:CD	2.15	0.55
2:F:1349:HIS:CE1	5:J:69:A:H5'	2.41	0.55
2:B:824:VAL:HG11	2:B:859:ARG:HH12	1.72	0.55
2:B:1120:ILE:HB	2:B:1134:PHE:HB2	1.89	0.55
2:F:160:HIS:CD2	2:F:160:HIS:C	2.85	0.55
2:F:427:GLU:HA	2:F:433:LEU:HB2	1.87	0.55
2:F:523:GLU:OE1	2:F:589:ALA:N	2.38	0.55
2:F:672:ASP:HB3	2:F:675:SER:HB2	1.89	0.55
2:F:921:LEU:HD11	2:F:1042:ILE:HD13	1.89	0.55
2:F:1262:HIS:HB3	2:F:1265:TYR:CD2	2.41	0.55
2:B:971:GLN:HA	2:B:973:TYR:CE2	2.42	0.54
2:F:155:TYR:C	2:F:155:TYR:CD1	2.84	0.54
2:F:583:VAL:HG22	2:F:584:GLU:H	1.72	0.54
2:B:139:ARG:CD	2:B:161:MET:HE2	2.37	0.54
2:B:212:LEU:HD21	2:B:225:LEU:HD12	1.90	0.54
2:B:1318:LEU:HD22	2:B:1319:GLY:H	1.72	0.54
3:G:3:DA:N6	4:H:9:DA:H61	2.04	0.54
4:H:11:DT:H2''	4:H:12:DG:H8	1.72	0.54
2:B:117:PRO:HD2	2:B:125:GLU:OE2	2.07	0.54
2:B:930:HIS:O	2:B:934:ILE:HG13	2.06	0.54
2:B:217:SER:O	2:B:221:ARG:HG3	2.08	0.54
2:B:545:LYS:CE	2:B:690:ASN:OD1	2.55	0.54
2:F:1169:MET:HE3	5:J:52:A:N3	2.22	0.54
2:B:212:LEU:O	2:B:221:ARG:HD2	2.08	0.54
2:F:90:MET:CE	2:F:151:LEU:HD23	2.33	0.54
2:F:662:LEU:HD22	2:F:666:LEU:HD23	1.89	0.54
2:B:824:VAL:HG22	2:B:863:ASN:ND2	2.23	0.54
2:F:140:LYS:HD3	2:F:319:ALA:HB2	1.90	0.54
2:F:1108:GLU:HB2	3:G:9:DT:H5''	1.90	0.54
2:B:265:GLN:HG2	2:B:267:SER:H	1.72	0.54
5:J:96:C:C4	5:J:97:U:C4	2.96	0.54
2:B:219:SER:O	2:B:222:LEU:HB3	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:302:LEU:HA	2:B:305:ILE:HG12	1.90	0.54
2:F:869:ASN:HD21	2:F:907:GLY:HA3	1.72	0.54
2:F:922:VAL:CG1	2:F:1007:GLU:HG3	2.38	0.54
2:F:750:VAL:HG21	2:F:1355:LEU:HD12	1.90	0.54
2:B:137:HIS:HE1	2:B:325:TYR:CD2	2.25	0.54
2:B:521:TYR:CE2	2:B:549:VAL:HG21	2.43	0.54
2:B:621:LEU:O	2:B:625:LEU:HB2	2.08	0.54
1:E:27:G:H5'	1:E:28:A:O5'	2.07	0.54
2:F:343:LEU:HD11	2:F:383:MET:HB2	1.90	0.54
2:F:489:GLN:HG3	2:F:625:LEU:HD21	1.89	0.54
2:B:464:TRP:CZ2	2:B:491:PHE:HD1	2.26	0.53
2:F:362:TYR:OH	2:F:401:LYS:HG3	2.08	0.53
1:A:3:A:H2'	1:A:3:A:N3	2.23	0.53
2:B:94:ASP:OD2	2:B:152:ARG:HD3	2.08	0.53
2:B:338:LEU:O	2:B:383:MET:CE	2.53	0.53
2:B:1207:GLU:HG3	2:B:1208:ASN:N	2.22	0.53
1:E:27:G:H5'	1:E:28:A:C5'	2.39	0.53
2:F:5:TYR:CE2	2:F:751:MET:HG3	2.44	0.53
2:F:212:LEU:CD1	2:F:300:ILE:CD1	2.87	0.53
5:I:37:U:H2'	5:I:38:A:C8	2.43	0.53
5:J:45:U:C2	5:J:46:A:C8	2.97	0.53
2:F:32:PHE:O	2:F:42:SER:HA	2.08	0.53
2:F:220:ARG:O	2:F:224:ASN:N	2.37	0.53
2:F:841:ILE:HD11	2:F:896:LYS:HG3	1.89	0.53
2:F:1124:LYS:N	5:J:53:G:OP1	2.33	0.53
3:G:3:DA:H61	4:H:9:DA:N6	2.07	0.53
2:B:1147:ALA:HB1	2:B:1188:LYS:O	2.08	0.53
2:B:1207:GLU:HG3	2:B:1208:ASN:H	1.74	0.53
1:E:27:G:H1'	2:F:129:HIS:CD2	2.44	0.53
2:F:1295:ASN:HA	2:F:1298:ARG:NH1	2.24	0.53
1:A:2:U:N3	1:A:4:A:H3'	2.19	0.53
2:B:1232:TYR:HA	2:B:1235:PHE:HB3	1.89	0.53
2:F:468:LYS:HE3	2:F:483:ASP:HB3	1.91	0.53
2:F:976:ARG:HA	2:F:982:HIS:CD2	2.43	0.53
2:B:642:LEU:HB2	2:B:643:PHE:CD2	2.43	0.53
2:B:972:PHE:HE1	2:B:1084:ARG:HB2	1.73	0.53
2:F:48:ILE:HG12	2:F:984:ALA:HB1	1.90	0.53
2:F:137:HIS:HA	2:F:322:ILE:CD1	2.39	0.53
2:F:271:TYR:O	2:F:275:LEU:N	2.34	0.53
2:B:118:ILE:HD13	2:B:128:TYR:HD2	1.71	0.53
2:B:672:ASP:HA	2:B:703:THR:HG22	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:849:ASP:OD2	2:B:895:ARG:NH1	2.40	0.53
3:C:25:DT:C2	3:C:26:DT:C5	2.96	0.53
2:F:649:LYS:HB3	2:F:653:ARG:HH21	1.74	0.53
5:I:69:A:H2'	5:I:70:C:C6	2.44	0.53
2:B:273:ASP:N	2:B:273:ASP:OD1	2.36	0.53
2:B:595:HIS:HB3	2:B:599:LYS:HZ2	1.72	0.53
2:F:312:ILE:HG13	2:F:313:THR:N	2.24	0.53
2:F:1048:THR:HA	2:F:1076:LYS:HD3	1.91	0.53
2:B:672:ASP:HA	2:B:703:THR:CG2	2.39	0.53
2:F:164:PHE:O	2:F:415:HIS:NE2	2.41	0.53
2:F:860:SER:OG	2:F:863:ASN:OD1	2.27	0.53
2:B:380:LEU:O	2:B:386:THR:HG21	2.07	0.52
2:B:879:MET:HE3	2:B:882:TYR:CG	2.44	0.52
2:F:66:ARG:HA	2:F:69:ARG:NH1	2.24	0.52
2:F:1272:GLN:CD	5:J:89:G:H1	2.18	0.52
2:B:1047:LYS:HB2	2:B:1050:ILE:HG22	1.90	0.52
2:B:1106:SER:HB2	2:B:1135:ASP:O	2.09	0.52
2:B:1241:HIS:ND1	2:B:1244:LYS:HA	2.25	0.52
2:F:139:ARG:O	2:F:143:VAL:HG23	2.09	0.52
2:F:977:GLU:HG3	2:F:1310:ILE:HG21	1.90	0.52
2:F:1351:SER:OG	2:F:1356:TYR:HB2	2.09	0.52
3:G:3:DA:H61	4:H:9:DA:H61	1.57	0.52
2:B:233:LYS:HG2	2:B:235:ASN:N	2.25	0.52
2:B:1002:PRO:HA	2:B:1005:GLU:HG3	1.90	0.52
2:F:167:HIS:HD2	2:F:169:LEU:CB	2.23	0.52
2:F:1050:ILE:HG13	2:F:1050:ILE:O	2.09	0.52
1:A:2:U:O2	1:A:3:A:O2'	2.27	0.52
1:A:10:U:H2'	1:A:11:U:H6	1.75	0.52
2:F:962:LEU:HB3	2:F:1043:MET:CE	2.35	0.52
2:F:38:THR:HG22	2:F:40:ARG:H	1.74	0.52
2:F:140:LYS:HB3	2:F:322:ILE:CD1	2.40	0.52
2:F:922:VAL:HG11	2:F:1007:GLU:HG3	1.90	0.52
2:B:391:VAL:O	2:B:395:ARG:HG3	2.09	0.52
2:B:427:GLU:OE1	2:B:437:ARG:NH1	2.42	0.52
2:F:151:LEU:HD22	2:F:152:ARG:CA	2.40	0.52
4:H:6:DG:H2''	4:H:7:DG:H5''	1.91	0.52
2:B:1231:LYS:HD2	2:B:1265:TYR:OH	2.10	0.52
2:F:844:GLN:HG3	2:F:848:LYS:HD2	1.91	0.52
2:F:151:LEU:N	2:F:151:LEU:CD1	2.73	0.52
2:F:776:ASN:O	2:F:780:ARG:HG2	2.08	0.52
2:F:980:ASN:HB2	2:F:1225:GLU:OE2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:39:G:H5'	5:I:40:C:OP2	2.10	0.52
2:B:737:ILE:O	2:B:740:THR:HG22	2.09	0.51
2:B:1074:TRP:HZ2	2:B:1080:PHE:CD2	2.28	0.51
2:B:1243:GLU:HG3	2:B:1246:LYS:NZ	2.26	0.51
2:F:262:ALA:HB1	2:F:278:LEU:HG	1.91	0.51
2:F:867:SER:HB2	2:F:1054:ASN:CA	2.40	0.51
2:F:1000:LYS:HG3	2:F:1001:TYR:CD2	2.46	0.51
1:A:5:C:O2'	1:A:6:G:C5'	2.58	0.51
2:B:201:ILE:HG22	2:B:202:ASN:N	2.22	0.51
2:B:849:ASP:OD1	2:B:851:SER:OG	2.25	0.51
2:F:40:ARG:HE	2:F:43:ILE:HD11	1.75	0.51
2:F:542:GLY:HA3	2:F:685:SER:HA	1.92	0.51
2:F:878:LYS:HB3	2:F:879:MET:SD	2.51	0.51
2:F:1167:THR:HG23	2:F:1170:GLU:H	1.74	0.51
5:J:45:U:H2'	5:J:46:A:C8	2.45	0.51
2:F:551:LEU:HD23	2:F:568:TYR:HD1	1.75	0.51
1:A:29:G:N3	5:I:41:A:C2	2.78	0.51
2:F:134:THR:O	2:F:137:HIS:HB2	2.11	0.51
2:F:650:GLN:O	2:F:653:ARG:HG2	2.11	0.51
2:B:686:ASP:HB3	2:B:690:ASN:HA	1.92	0.51
2:B:921:LEU:HB3	2:B:1008:PHE:CZ	2.45	0.51
2:F:349:GLU:O	2:F:353:ASP:HB3	2.11	0.51
3:G:22:DT:H2''	3:G:23:DC:O5'	2.09	0.51
2:B:492:ILE:O	2:B:496:THR:HG23	2.10	0.51
2:B:1060:ARG:NH1	2:B:1064:GLU:OE2	2.42	0.51
2:B:1074:TRP:HZ2	2:B:1080:PHE:CE2	2.28	0.51
2:F:142:LEU:CD1	2:F:154:ILE:CD1	2.85	0.51
2:F:44:LYS:NZ	5:J:92:G:O6	2.21	0.51
2:F:410:ILE:HG21	2:F:415:HIS:NE2	2.26	0.51
1:A:25:U:H2'	1:A:26:A:C8	2.46	0.51
2:B:325:TYR:CD1	5:I:44:U:C2	2.99	0.51
2:B:640:ALA:HA	2:B:648:MET:HE2	1.92	0.51
2:B:677:LYS:HD3	2:B:682:PHE:CZ	2.45	0.51
2:B:1232:TYR:O	2:B:1236:LEU:N	2.29	0.51
2:B:1308:ASN:HD22	2:B:1327:PHE:N	2.07	0.51
2:F:167:HIS:N	2:F:410:ILE:O	2.41	0.51
2:F:1051:THR:HG22	2:F:1053:ALA:H	1.76	0.51
2:B:66:ARG:HD2	2:B:462:PHE:CE2	2.46	0.51
2:B:853:ASP:CG	2:B:893:THR:HG21	2.36	0.51
2:F:465:MET:SD	2:F:482:VAL:HG21	2.51	0.51
5:J:83:C:H2'	5:J:84:A:C8	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:137:HIS:HA	2:F:322:ILE:CG1	2.41	0.51
2:F:226:ILE:CG2	2:F:231:GLY:H	2.24	0.51
2:F:971:GLN:HG2	2:F:973:TYR:CE2	2.47	0.51
2:B:509:PRO:HB3	2:B:624:THR:HG21	1.93	0.50
2:B:977:GLU:N	2:B:977:GLU:OE1	2.44	0.50
1:A:1:U:H5	2:B:661:ARG:HH12	1.59	0.50
2:B:823:TYR:CD2	2:B:858:THR:HG21	2.45	0.50
2:B:1081:ALA:O	2:B:1085:LYS:HG3	2.11	0.50
2:F:148:LYS:HB2	2:F:429:PHE:CD2	2.46	0.50
2:B:281:GLN:OE1	2:B:281:GLN:N	2.38	0.50
2:B:1356:TYR:HB3	5:I:81:G:N1	2.27	0.50
2:F:128:TYR:CE1	2:F:153:LEU:HD12	2.45	0.50
2:F:601:ILE:HD11	2:F:607:LEU:HD11	1.93	0.50
2:F:1045:PHE:CA	2:F:1060:ARG:NH1	2.73	0.50
2:B:448:ILE:HD13	2:B:455:LEU:HD13	1.93	0.50
2:B:1105:PHE:CG	2:B:1169:MET:HG3	2.46	0.50
3:C:24:DG:H5"	3:C:25:DT:OP2	2.11	0.50
2:F:43:ILE:HG22	2:F:45:LYS:HG3	1.91	0.50
2:B:69:ARG:HD3	5:I:62:G:C8	2.47	0.50
2:B:1047:LYS:CB	2:B:1050:ILE:HG22	2.42	0.50
1:E:23:U:H5"	2:F:1112:PRO:HG3	1.93	0.50
2:F:762:GLU:OE1	2:F:990:ASN:ND2	2.39	0.50
2:F:810:LYS:HZ2	2:F:834:SER:HA	1.76	0.50
5:J:95:G:C6	5:J:96:C:N4	2.79	0.50
2:B:670:ILE:HG22	2:B:704:PHE:CE1	2.45	0.50
2:F:1333:ARG:CZ	2:F:1335:ARG:HD2	2.41	0.50
2:B:195:LEU:HB3	2:B:196:PHE:HD1	1.77	0.50
2:B:460:SER:OG	5:I:61:C:OP1	2.28	0.50
2:B:813:LEU:O	2:B:817:GLN:HG3	2.11	0.50
2:B:1207:GLU:CG	2:B:1208:ASN:H	2.25	0.50
2:F:8:GLY:O	2:F:987:ALA:HB1	2.11	0.50
2:F:74:ARG:O	2:F:78:ARG:HG3	2.12	0.50
2:F:531:THR:HG1	2:F:575:PHE:HD1	1.58	0.50
2:B:339:VAL:HA	2:B:383:MET:HE1	1.94	0.50
2:B:606:PHE:O	2:B:612:ASN:ND2	2.44	0.50
2:B:913:LYS:O	2:B:916:PHE:HB2	2.12	0.50
2:B:1226:LEU:HB2	2:B:1276:PHE:CE2	2.47	0.50
2:F:237:LEU:HD12	2:F:238:PHE:N	2.27	0.50
2:B:1220:LEU:HD12	2:B:1338:SER:O	2.12	0.50
2:F:27:VAL:HG12	2:F:1086:VAL:HG22	1.92	0.50
2:F:616:LEU:HA	2:F:619:ILE:HG22	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:74:ARG:NH2	5:I:60:C:OP1	2.44	0.49
2:B:514:LEU:HD11	2:B:667:ILE:HG21	1.94	0.49
2:B:1096:LYS:HG2	2:B:1201:TYR:CD2	2.47	0.49
2:F:427:GLU:OE1	2:F:434:LYS:HA	2.12	0.49
2:F:981:TYR:O	2:F:983:HIS:N	2.45	0.49
2:B:1235:PHE:O	2:B:1239:ALA:N	2.33	0.49
2:F:410:ILE:HD13	2:F:415:HIS:NE2	2.27	0.49
2:F:695:GLN:O	2:F:699:ASP:HB2	2.12	0.49
2:F:985:HIS:CD2	2:F:1087:LEU:HD22	2.47	0.49
2:F:1147:ALA:HB1	2:F:1188:LYS:O	2.11	0.49
2:F:1206:LEU:HD12	2:F:1210:ARG:HH12	1.76	0.49
2:F:1228:LEU:HD12	2:F:1229:PRO:HD2	1.94	0.49
2:B:961:LYS:HA	2:B:964:SER:HB3	1.94	0.49
2:F:628:ASP:O	2:F:632:ILE:HG13	2.12	0.49
2:F:918:LYS:CE	2:F:1018:VAL:HG11	2.43	0.49
2:B:784:ILE:HG21	2:B:815:TYR:HD2	1.77	0.49
2:F:334:LEU:O	2:F:338:LEU:HG	2.12	0.49
2:F:566:GLU:O	2:F:570:LYS:HB3	2.11	0.49
2:F:583:VAL:HG22	2:F:584:GLU:N	2.26	0.49
2:F:1351:SER:OG	2:F:1356:TYR:O	2.19	0.49
2:B:809:GLU:OE1	2:B:855:LYS:HE2	2.12	0.49
2:B:850:ASP:HB3	2:B:855:LYS:NZ	2.27	0.49
2:F:433:LEU:O	2:F:437:ARG:HB2	2.12	0.49
2:F:795:ILE:HA	2:F:798:GLU:HB2	1.94	0.49
2:F:1114:ARG:HG2	2:F:1115:ASN:N	2.28	0.49
5:J:88:A:C6	5:J:91:C:N4	2.76	0.49
2:F:253:LYS:CG	2:F:261:ASP:HA	2.43	0.49
2:F:268:LYS:O	2:F:271:TYR:HD2	1.95	0.49
2:F:850:ASP:O	2:F:855:LYS:HD2	2.11	0.49
2:F:1300:LYS:HG3	2:F:1327:PHE:CZ	2.48	0.49
2:B:1111:LEU:HD12	2:B:1135:ASP:HB2	1.95	0.49
2:B:1252:ASN:ND2	2:B:1255:LYS:HD2	2.27	0.49
2:F:158:LEU:O	2:F:161:MET:N	2.46	0.49
2:F:324:ARG:O	2:F:327:GLU:HB2	2.12	0.49
2:F:981:TYR:O	2:F:984:ALA:N	2.45	0.49
2:F:1206:LEU:CD1	2:F:1210:ARG:HH12	2.25	0.49
2:B:252:PHE:CE1	2:B:264:LEU:HD13	2.47	0.49
2:F:784:ILE:HG21	2:F:815:TYR:HD1	1.78	0.49
2:F:791:LEU:CD2	2:F:818:ASN:OD1	2.59	0.49
2:B:149:ALA:H	2:B:426:GLN:HE22	1.59	0.49
2:B:455:LEU:HD12	2:B:455:LEU:N	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:512:SER:O	2:B:516:GLU:HG2	2.13	0.49
2:B:1204:PHE:CG	2:B:1342:VAL:HG13	2.48	0.49
2:B:1357:GLU:O	5:I:81:G:N2	2.46	0.49
2:F:758:ASN:HD22	2:F:995:THR:HG22	1.78	0.49
2:F:939:MET:HE2	2:F:953:VAL:HG21	1.95	0.49
2:F:1046:PHE:O	2:F:1076:LYS:NZ	2.45	0.49
5:J:79:G:C2'	5:J:80:U:H5'	2.43	0.49
2:B:478:PHE:HE2	2:B:484:LYS:HE2	1.78	0.49
1:E:3:A:N6	1:E:4:A:N6	2.60	0.49
2:F:411:PRO:HB2	2:F:413:GLN:OE1	2.13	0.49
2:F:632:ILE:O	2:F:636:LEU:HD13	2.13	0.49
2:F:843:PRO:HG3	2:F:864:ARG:HH22	1.77	0.49
2:F:1002:PRO:HD2	2:F:1036:TYR:OH	2.13	0.49
2:F:1314:THR:HG21	2:F:1324:PHE:HB3	1.94	0.49
5:J:94:U:H2'	5:J:95:G:H8	1.77	0.49
2:B:83:GLN:HG2	2:B:98:PHE:CE1	2.48	0.48
2:B:850:ASP:O	2:B:855:LYS:HD2	2.13	0.48
2:B:1062:LEU:O	2:B:1075:ASP:HA	2.13	0.48
3:C:25:DT:C2	3:C:26:DT:C7	2.94	0.48
2:F:923:GLU:CG	2:F:928:THR:HG21	2.40	0.48
2:B:241:LEU:HD11	2:B:289:LEU:HD11	1.96	0.48
2:B:531:THR:HG21	2:B:575:PHE:HE2	1.78	0.48
2:B:1208:ASN:CG	2:B:1208:ASN:O	2.55	0.48
2:F:140:LYS:HB3	2:F:322:ILE:HD12	1.96	0.48
2:B:736:GLY:O	2:B:740:THR:HB	2.14	0.48
2:F:346:LYS:O	2:F:350:ILE:N	2.42	0.48
1:A:3:A:H2'	1:A:4:A:H8	1.78	0.48
2:B:83:GLN:HG2	2:B:98:PHE:CZ	2.49	0.48
2:B:525:THR:CG2	2:B:690:ASN:HB3	2.43	0.48
2:B:540:LEU:HD12	2:B:540:LEU:HA	1.52	0.48
2:F:844:GLN:HG3	2:F:848:LYS:HA	1.95	0.48
2:F:1162:GLU:OE2	2:F:1187:TYR:OH	2.16	0.48
2:B:157:ALA:O	2:B:161:MET:HG3	2.14	0.48
2:F:138:LEU:HD22	2:F:153:LEU:CD2	2.34	0.48
2:F:142:LEU:HD12	2:F:154:ILE:HA	1.93	0.48
2:F:563:GLN:O	2:F:567:ASP:HB2	2.14	0.48
5:J:95:G:H2'	5:J:96:C:C6	2.49	0.48
2:B:472:THR:HG23	5:I:59:U:OP2	2.14	0.48
2:B:697:ILE:HG22	2:B:698:HIS:ND1	2.29	0.48
2:B:985:HIS:O	2:B:989:LEU:HG	2.13	0.48
2:F:208:ALA:CA	2:F:211:ILE:CD1	2.53	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:373:TYR:HE1	2:F:398:LEU:HB3	1.77	0.48
2:F:780:ARG:HB2	2:F:806:LEU:HD12	1.95	0.48
5:J:49:A:O5'	5:J:49:A:H8	1.96	0.48
2:B:525:THR:HG23	2:B:690:ASN:HB3	1.95	0.48
2:F:361:GLY:HA2	2:F:365:GLY:HA3	1.96	0.48
2:F:446:PHE:CZ	2:F:478:PHE:CD1	2.92	0.48
2:F:467:ARG:HD3	2:F:470:GLU:HA	1.95	0.48
2:F:1038:PHE:CD2	2:F:1039:TYR:HE1	2.31	0.48
1:A:2:U:O2	1:A:4:A:C8	2.67	0.48
2:B:90:MET:HE3	2:B:97:PHE:CD2	2.48	0.48
2:B:345:GLU:H	2:B:345:GLU:CD	2.21	0.48
2:F:44:LYS:HD3	5:J:92:G:N7	2.29	0.48
2:F:151:LEU:CD1	2:F:151:LEU:H	2.27	0.48
2:F:404:THR:HG22	2:F:405:PHE:CD1	2.48	0.48
2:F:1119:LEU:HD23	2:F:1128:PRO:HB2	1.94	0.48
2:F:1205:GLU:CB	2:F:1348:ILE:HD11	2.44	0.48
2:B:63:ARG:O	2:B:66:ARG:N	2.47	0.48
2:B:181:VAL:HG21	2:B:209:LYS:HA	1.96	0.48
2:B:597:LEU:O	2:B:601:ILE:HG12	2.14	0.48
2:B:980:ASN:HB2	2:B:1225:GLU:OE1	2.14	0.48
2:F:143:VAL:HG21	2:F:315:ALA:HB2	1.96	0.48
2:F:1115:ASN:OD1	2:F:1129:LYS:HE3	2.14	0.48
2:F:1200:LYS:HG2	2:F:1201:TYR:CD1	2.49	0.48
2:B:530:VAL:CG2	2:B:537:PRO:HB3	2.42	0.47
1:E:19:A:O3'	2:F:407:ASN:HB2	2.14	0.47
2:F:137:HIS:HA	2:F:322:ILE:HG12	1.95	0.47
2:F:373:TYR:CE1	2:F:398:LEU:HB3	2.49	0.47
2:F:1266:LEU:HG	2:F:1309:ILE:HD12	1.96	0.47
2:B:66:ARG:HD2	2:B:462:PHE:HE2	1.78	0.47
2:B:269:ASP:O	2:B:271:TYR:N	2.41	0.47
2:B:531:THR:HG23	2:B:534:MET:HG3	1.96	0.47
2:B:644:ASP:OD2	2:B:646:LYS:HB2	2.14	0.47
2:B:1179:ILE:HD11	2:B:1192:LYS:HD2	1.94	0.47
2:B:1208:ASN:OD1	2:B:1279:ARG:HG3	2.14	0.47
2:B:1333:ARG:CZ	2:B:1335:ARG:HD2	2.45	0.47
1:E:6:G:C2	3:G:24:DG:N2	2.82	0.47
2:F:282:ILE:HG22	2:F:286:TYR:CD1	2.49	0.47
2:F:795:ILE:HG13	2:F:795:ILE:O	2.15	0.47
2:B:1109:SER:OG	3:C:9:DT:OP2	2.27	0.47
2:F:1019:ARG:C	2:F:1021:MET:N	2.73	0.47
3:G:6:DC:H2''	3:G:7:DC:O5'	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1122:ARG:O	5:I:52:A:H5'	2.14	0.47
2:B:1251:ASP:O	2:B:1255:LYS:HG3	2.13	0.47
2:F:853:ASP:OD1	2:F:893:THR:HG21	2.14	0.47
1:A:25:U:H2'	1:A:26:A:H8	1.78	0.47
2:B:136:TYR:CG	2:B:321:MET:HG3	2.49	0.47
2:B:217:SER:HB2	2:B:220:ARG:HG2	1.96	0.47
2:B:985:HIS:ND1	2:B:1087:LEU:HD13	2.29	0.47
2:B:1235:PHE:CE1	2:B:1239:ALA:HB2	2.50	0.47
2:B:1243:GLU:HG3	2:B:1246:LYS:HZ1	1.78	0.47
1:E:31:U:N3	1:E:32:A:N7	2.62	0.47
2:F:167:HIS:ND1	2:F:410:ILE:O	2.39	0.47
2:F:455:LEU:O	5:J:60:C:H5'	2.15	0.47
2:F:671:ARG:HD3	2:F:671:ARG:H	1.78	0.47
2:F:1326:TYR:CE2	2:F:1327:PHE:CD2	3.03	0.47
2:B:48:ILE:HG12	2:B:984:ALA:HB1	1.97	0.47
2:B:121:ASN:H	2:B:121:ASN:ND2	2.12	0.47
2:B:570:LYS:NZ	2:B:571:LYS:HG2	2.30	0.47
2:B:620:VAL:HG13	2:B:656:TYR:HD2	1.80	0.47
2:B:1000:LYS:HB3	2:B:1001:TYR:CE2	2.50	0.47
2:B:1110:ILE:HD13	2:B:1134:PHE:HE1	1.79	0.47
2:B:1286:ASN:ND2	2:B:1332:ASP:O	2.47	0.47
1:E:3:A:C5	1:E:4:A:N7	2.83	0.47
1:E:15:G:P	2:F:66:ARG:HH22	2.37	0.47
2:F:180:ASP:CB	2:F:183:LYS:HB2	2.28	0.47
2:F:258:LEU:HD23	2:F:259:ALA:H	1.80	0.47
2:B:49:GLY:HA2	2:B:1092:VAL:CG1	2.45	0.47
2:B:114:GLU:HG2	2:B:120:GLY:CA	2.45	0.47
2:B:939:MET:HG3	2:B:953:VAL:HG11	1.97	0.47
1:E:21:G:H2'	1:E:22:U:O4'	2.15	0.47
2:B:721:HIS:O	2:B:725:ALA:N	2.39	0.47
2:B:1114:ARG:O	2:B:1129:LYS:HA	2.15	0.47
2:B:1177:ASN:ND2	2:B:1180:ASP:OD2	2.47	0.47
2:F:424:ARG:HH12	2:F:437:ARG:NE	2.13	0.47
2:F:103:GLU:OE2	2:F:111:LYS:HG2	2.14	0.47
2:F:237:LEU:HD12	2:F:238:PHE:H	1.80	0.47
2:F:321:MET:HE1	2:F:324:ARG:CZ	2.45	0.47
2:F:1205:GLU:HB2	2:F:1348:ILE:HD11	1.96	0.47
5:J:73:G:H5'	5:J:74:A:OP2	2.14	0.47
2:B:343:LEU:HD21	2:B:346:LYS:HG3	1.98	0.46
2:B:478:PHE:CE1	2:B:482:VAL:HG21	2.51	0.46
2:B:1089:MET:HA	2:B:1090:PRO:HD3	1.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1163:LEU:HG	2:B:1343:LEU:HD21	1.97	0.46
2:F:832:ARG:HD2	2:F:835:ASP:OD2	2.15	0.46
2:B:74:ARG:O	2:B:78:ARG:HG3	2.15	0.46
2:B:143:VAL:HG13	2:B:421:ALA:HB1	1.97	0.46
2:B:970:PHE:HZ	2:B:1047:LYS:HG2	1.80	0.46
5:I:37:U:H2'	5:I:38:A:H8	1.79	0.46
2:B:133:PRO:HD2	2:B:137:HIS:CG	2.50	0.46
2:B:453:GLY:O	2:B:455:LEU:HD12	2.15	0.46
3:C:7:DC:H2'	3:C:8:DT:C6	2.50	0.46
2:F:553:PHE:HZ	2:F:587:PHE:CD2	2.34	0.46
2:F:794:GLN:HE21	2:F:798:GLU:CD	2.24	0.46
5:J:91:C:HO2'	5:J:92:G:P	2.38	0.46
1:A:11:U:C2	1:A:12:A:C8	3.03	0.46
1:E:16:A:H5''	2:F:74:ARG:HH12	1.79	0.46
2:F:521:TYR:CE2	2:F:549:VAL:HG21	2.49	0.46
2:F:1232:TYR:CE1	2:F:1265:TYR:CD1	3.04	0.46
2:B:1294:TYR:HE1	2:B:1305:GLN:HE21	1.62	0.46
1:E:27:G:H5'	1:E:28:A:H5''	1.97	0.46
2:F:142:LEU:CD1	2:F:154:ILE:CA	2.72	0.46
2:F:142:LEU:CD2	2:F:149:ALA:HB2	2.46	0.46
2:F:258:LEU:HB3	2:F:260:GLU:O	2.16	0.46
2:F:404:THR:HG22	2:F:405:PHE:H	1.80	0.46
2:F:842:VAL:CG1	2:F:854:ASN:OD1	2.61	0.46
2:F:1038:PHE:CD2	2:F:1039:TYR:CE1	3.04	0.46
2:F:1045:PHE:O	2:F:1076:LYS:NZ	2.49	0.46
3:G:25:DT:C2'	3:G:26:DT:OP2	2.55	0.46
2:B:221:ARG:NH1	2:B:246:LEU:HD22	2.30	0.46
2:B:1141:TYR:C	2:B:1141:TYR:CD1	2.94	0.46
1:E:3:A:H8	1:E:3:A:O5'	1.99	0.46
2:F:22:THR:HG23	2:F:26:LYS:O	2.15	0.46
2:F:468:LYS:HD2	2:F:483:ASP:N	2.29	0.46
2:F:1232:TYR:HE1	2:F:1265:TYR:CD1	2.33	0.46
2:B:718:ASP:H	2:B:723:HIS:HE1	1.64	0.46
2:F:151:LEU:CD1	2:F:152:ARG:N	2.73	0.46
2:F:600:ILE:HD13	2:F:651:LEU:HA	1.97	0.46
5:I:42:A:O3'	5:I:43:G:C8	2.69	0.46
1:A:3:A:H2'	1:A:4:A:C8	2.51	0.46
1:A:11:U:N3	1:A:12:A:N7	2.63	0.46
2:B:5:TYR:CD2	2:B:751:MET:HE2	2.51	0.46
2:B:448:ILE:HD13	2:B:455:LEU:CD1	2.46	0.46
2:B:780:ARG:HB2	2:B:806:LEU:HD12	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:963:VAL:HG21	2:B:990:ASN:OD1	2.16	0.46
3:C:1:DC:H2'	3:C:2:DA:C8	2.51	0.46
2:F:828:LEU:HD22	2:F:836:TYR:CE2	2.51	0.46
5:J:79:G:O2'	5:J:80:U:H5'	2.15	0.46
2:B:128:TYR:CE1	2:B:132:TYR:HB2	2.50	0.46
2:B:139:ARG:HH12	2:B:415:HIS:CD2	2.34	0.46
2:B:143:VAL:HG13	2:B:421:ALA:CB	2.46	0.46
2:B:343:LEU:HD13	2:B:383:MET:SD	2.56	0.46
2:B:818:ASN:HB3	2:B:882:TYR:OH	2.16	0.46
2:F:241:LEU:HD23	2:F:241:LEU:H	1.81	0.46
2:F:971:GLN:OE1	2:F:1255:LYS:HE3	2.16	0.46
2:F:978:ILE:HD13	2:F:1228:LEU:HD23	1.98	0.46
1:A:20:A:P	2:B:403:ARG:NH1	2.89	0.46
2:B:317:LEU:O	2:B:320:SER:HB3	2.16	0.46
2:B:692:ASN:O	2:B:696:LEU:HD23	2.16	0.46
2:B:978:ILE:HD12	2:B:1233:VAL:HG22	1.98	0.46
2:B:1115:ASN:HA	2:B:1129:LYS:HG2	1.98	0.46
2:F:1151:LYS:HD2	2:F:1158:LYS:HB3	1.97	0.46
2:B:548:ILE:HG23	2:B:552:LEU:CD1	2.46	0.45
2:B:1357:GLU:OE1	2:B:1359:ARG:NH1	2.49	0.45
2:F:151:LEU:CD2	2:F:151:LEU:C	2.86	0.45
2:F:238:PHE:O	2:F:242:ILE:HG12	2.15	0.45
2:F:1245:LEU:HD23	2:F:1245:LEU:HA	1.63	0.45
2:B:513:LEU:HD11	2:B:597:LEU:HD12	1.97	0.45
2:B:881:ASN:OD1	2:B:885:GLN:NE2	2.48	0.45
2:B:1146:VAL:HG13	2:B:1191:LYS:HB2	1.97	0.45
2:F:138:LEU:HD13	2:F:153:LEU:HD22	1.82	0.45
2:F:166:GLY:HA3	2:F:410:ILE:CG2	2.41	0.45
2:F:1096:LYS:HG2	2:F:1201:TYR:CD2	2.51	0.45
2:B:198:GLU:C	2:B:200:PRO:HD3	2.41	0.45
2:B:340:ARG:HA	2:B:344:PRO:HB3	1.97	0.45
2:B:640:ALA:HA	2:B:648:MET:CE	2.47	0.45
2:B:976:ARG:HB2	2:B:977:GLU:OE1	2.17	0.45
2:F:554:LYS:HB3	2:F:594:TYR:CE2	2.51	0.45
2:F:615:ILE:HG23	2:F:639:TYR:CD1	2.51	0.45
2:B:204:SER:HB2	2:B:205:GLY:H	1.47	0.45
2:B:392:LYS:CG	2:B:395:ARG:NH1	2.54	0.45
2:F:177:ASP:OD1	2:F:177:ASP:N	2.50	0.45
2:F:328:HIS:ND1	5:J:44:U:C2	2.85	0.45
5:J:82:G:N7	5:J:97:U:O2	2.50	0.45
2:B:1144:LEU:O	2:B:1195:ILE:HA	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1204:PHE:HE2	2:B:1214:LEU:HB2	1.80	0.45
3:C:25:DT:N1	3:C:26:DT:H72	2.32	0.45
2:F:151:LEU:CD2	2:F:152:ARG:N	2.75	0.45
2:F:321:MET:HE2	2:F:321:MET:HA	1.97	0.45
2:F:506:LYS:H	2:F:506:LYS:HG2	1.52	0.45
2:F:795:ILE:HA	2:F:798:GLU:OE1	2.15	0.45
2:F:855:LYS:NZ	2:F:1246:LYS:O	2.32	0.45
5:J:87:G:N3	5:J:87:G:H2'	2.31	0.45
2:B:1308:ASN:ND2	2:B:1327:PHE:H	2.15	0.45
3:C:25:DT:N3	3:C:26:DT:C5	2.85	0.45
3:C:25:DT:N3	3:C:26:DT:C7	2.80	0.45
2:F:139:ARG:HD3	2:F:157:ALA:CA	2.43	0.45
2:F:139:ARG:HD3	2:F:157:ALA:HB1	1.97	0.45
2:F:1079:ASP:HA	2:F:1082:THR:HG23	1.98	0.45
5:J:91:C:O2'	5:J:92:G:O5'	2.34	0.45
5:J:92:G:H2'	5:J:93:G:C8	2.51	0.45
2:B:269:ASP:OD1	2:B:270:THR:N	2.50	0.45
2:B:760:VAL:HG11	2:B:958:LEU:HD12	1.99	0.45
2:F:247:GLY:O	2:F:267:SER:HB3	2.16	0.45
2:F:551:LEU:HD12	2:F:551:LEU:HA	1.80	0.45
2:F:565:LYS:HD2	2:F:580:ILE:HG12	1.99	0.45
2:F:622:THR:HG21	2:F:635:ARG:CB	2.46	0.45
2:F:844:GLN:CG	2:F:848:LYS:HD2	2.47	0.45
2:B:36:GLY:HA3	2:B:1359:ARG:O	2.17	0.45
2:B:226:ILE:HA	2:B:229:LEU:HG	1.99	0.45
2:B:317:LEU:HD21	2:B:410:ILE:HD13	1.99	0.45
2:B:525:THR:HA	2:B:545:LYS:CE	2.47	0.45
2:F:137:HIS:HE1	2:F:325:TYR:CG	2.34	0.45
2:F:329:HIS:HB2	5:J:44:U:O4	2.17	0.45
2:F:913:LYS:O	2:F:916:PHE:HB2	2.17	0.45
2:F:1349:HIS:ND1	5:J:69:A:H5'	2.31	0.45
5:J:45:U:H2'	5:J:46:A:O4'	2.17	0.45
2:B:6:SER:HB2	2:B:21:ILE:CG1	2.47	0.45
2:B:94:ASP:HB3	2:B:97:PHE:HB2	1.99	0.45
2:B:116:HIS:NE2	2:B:122:ILE:HG23	2.32	0.45
2:B:165:ARG:O	2:B:412:HIS:HA	2.17	0.45
2:B:414:ILE:HG21	2:B:414:ILE:HD13	1.74	0.45
2:B:531:THR:HG21	2:B:575:PHE:CE2	2.52	0.45
2:F:328:HIS:CG	5:J:44:U:C2	3.05	0.45
2:F:909:SER:N	2:F:912:ASP:HB2	2.32	0.45
5:I:83:C:H2'	5:I:84:A:C8	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:467:ARG:NH2	2:B:471:GLU:O	2.50	0.45
2:B:1111:LEU:HD23	2:B:1111:LEU:HA	1.47	0.45
2:F:546:LYS:HE3	2:F:546:LYS:HB3	1.79	0.45
1:A:3:A:C2'	1:A:4:A:H8	2.30	0.44
2:B:719:SER:OG	2:B:720:LEU:N	2.49	0.44
2:B:864:ARG:HB2	2:B:871:PRO:HA	1.97	0.44
2:B:1113:LYS:HB2	2:B:1129:LYS:O	2.17	0.44
1:E:4:A:HO2'	1:E:5:C:C5'	2.29	0.44
2:F:788:ILE:HA	2:F:791:LEU:HB2	1.98	0.44
2:F:879:MET:HB3	2:F:882:TYR:HB3	1.99	0.44
2:F:954:LYS:NZ	2:F:998:ILE:HD13	2.32	0.44
2:F:1284:ASP:OD1	2:F:1284:ASP:N	2.43	0.44
2:B:115:ARG:HG3	2:B:116:HIS:CE1	2.53	0.44
2:B:118:ILE:HD12	2:B:125:GLU:OE2	2.17	0.44
2:B:662:LEU:HD23	2:B:666:LEU:HD22	1.98	0.44
2:B:958:LEU:HD22	2:B:962:LEU:HD12	1.99	0.44
2:B:1272:GLN:NE2	5:I:89:G:O6	2.31	0.44
1:E:3:A:O5'	1:E:3:A:C8	2.70	0.44
2:F:208:ALA:N	2:F:211:ILE:CD1	2.78	0.44
2:F:410:ILE:HD13	2:F:415:HIS:HE2	1.82	0.44
2:F:509:PRO:HG2	2:F:621:LEU:HA	1.98	0.44
2:F:518:PHE:C	2:F:518:PHE:CD2	2.94	0.44
2:F:615:ILE:HG23	2:F:639:TYR:CE1	2.52	0.44
2:F:1290:VAL:HG22	2:F:1331:ILE:HD13	2.00	0.44
2:B:264:LEU:HD23	2:B:271:TYR:CE1	2.52	0.44
2:B:390:LEU:HD23	2:B:390:LEU:HA	1.63	0.44
2:F:164:PHE:O	2:F:164:PHE:CD1	2.70	0.44
2:F:167:HIS:HD1	2:F:167:HIS:H	1.65	0.44
5:J:88:A:C2	5:J:91:C:N3	2.85	0.44
2:B:37:ASN:OD1	2:B:37:ASN:N	2.46	0.44
2:B:51:LEU:HD22	2:B:1352:ILE:HG13	1.98	0.44
2:B:192:TYR:HE1	2:B:237:LEU:HD23	1.82	0.44
2:B:548:ILE:HD13	2:B:564:LEU:HD11	1.98	0.44
2:F:233:LYS:HB3	2:F:236:GLY:H	1.82	0.44
2:F:883:TRP:HB3	2:F:897:PHE:HD1	1.82	0.44
2:F:1167:THR:OG1	2:F:1168:ILE:N	2.50	0.44
1:A:5:C:H2'	1:A:6:G:C8	2.47	0.44
2:B:147:ASP:O	2:B:426:GLN:NE2	2.51	0.44
2:F:30:LYS:HB2	2:F:30:LYS:HE3	1.81	0.44
2:F:821:ASP:HA	2:F:828:LEU:HD11	2.00	0.44
2:F:1212:ARG:HD2	2:F:1336:TYR:HD2	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8:A:H2'	1:A:9:U:C6	2.53	0.44
2:B:720:LEU:HD13	2:B:938:ARG:HH11	1.82	0.44
2:F:139:ARG:CD	2:F:157:ALA:C	2.73	0.44
2:F:672:ASP:OD2	2:F:675:SER:OG	2.31	0.44
2:F:867:SER:HB2	2:F:1054:ASN:HA	1.99	0.44
5:J:58:G:C6	5:J:60:C:C2	3.06	0.44
2:B:289:LEU:C	2:B:289:LEU:HD23	2.43	0.44
2:B:565:LYS:HD3	2:B:578:VAL:HG13	1.99	0.44
2:B:643:PHE:CD2	2:B:643:PHE:N	2.86	0.44
2:B:781:MET:HG3	2:B:803:ASN:ND2	2.33	0.44
1:E:4:A:C4	1:E:5:C:C5	3.05	0.44
2:F:158:LEU:HB2	2:F:419:LEU:HD12	1.99	0.44
2:F:823:TYR:HB3	2:F:863:ASN:HB3	1.99	0.44
2:F:1073:VAL:HG23	2:F:1074:TRP:N	2.32	0.44
2:B:90:MET:HE1	2:B:152:ARG:HA	2.00	0.44
2:B:141:LYS:HD3	2:B:142:LEU:HD23	2.00	0.44
2:B:400:ARG:HH22	2:B:406:ASP:CG	2.25	0.44
2:B:558:LYS:HA	2:B:558:LYS:HD3	1.68	0.44
2:B:601:ILE:HG21	2:B:643:PHE:HE1	1.83	0.44
2:B:628:ASP:OD1	2:B:630:GLU:HB3	2.17	0.44
2:B:829:ASP:OD1	2:B:831:ASN:N	2.50	0.44
1:E:25:U:H6	1:E:25:U:O5'	2.01	0.44
2:F:243:ALA:O	2:F:246:LEU:HB3	2.17	0.44
2:F:464:TRP:CD1	2:F:464:TRP:C	2.96	0.44
2:F:671:ARG:H	2:F:671:ARG:CD	2.30	0.44
2:B:13:THR:O	2:B:53:PHE:HE1	2.00	0.44
2:B:1276:PHE:CE2	2:B:1316:THR:HB	2.53	0.44
2:F:737:ILE:O	2:F:738:LEU:C	2.60	0.44
2:F:1095:VAL:HG13	2:F:1350:GLN:OE1	2.18	0.44
2:B:51:LEU:HD13	2:B:1095:VAL:CG2	2.44	0.43
2:B:134:THR:OG1	2:B:137:HIS:N	2.49	0.43
3:C:25:DT:C4	3:C:26:DT:O4	2.71	0.43
2:F:637:LYS:HB2	2:F:637:LYS:HE3	1.68	0.43
2:F:918:LYS:HZ1	2:F:1018:VAL:HG11	1.83	0.43
2:F:1212:ARG:CZ	2:F:1336:TYR:HE2	2.31	0.43
2:F:1347:LEU:HD22	2:F:1349:HIS:CD2	2.53	0.43
1:A:3:A:O2'	1:A:4:A:H8	2.00	0.43
2:B:921:LEU:HB3	2:B:1008:PHE:CE1	2.53	0.43
2:B:1200:LYS:HG2	2:B:1201:TYR:CD1	2.52	0.43
2:F:46:ASN:HD21	5:J:88:A:N6	2.13	0.43
2:F:63:ARG:HG3	2:F:66:ARG:NH1	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:156:LEU:HA	2:B:156:LEU:HD23	1.62	0.43
2:B:416:LEU:HD11	2:B:441:GLU:HG2	2.00	0.43
2:B:1345:ALA:O	2:B:1362:LEU:HG	2.19	0.43
2:F:57:GLU:HB2	5:J:65:A:OP1	2.18	0.43
2:F:1010:TYR:O	2:F:1012:ASP:N	2.51	0.43
2:F:1035:LYS:HD3	2:F:1035:LYS:HA	1.57	0.43
2:F:1123:LYS:HG3	5:J:53:G:OP1	2.18	0.43
5:J:84:A:C2	5:J:85:C:C2	3.06	0.43
2:B:79:ILE:HA	2:B:79:ILE:HD13	1.77	0.43
2:B:136:TYR:CD2	2:B:321:MET:HG3	2.53	0.43
2:B:220:ARG:HD3	2:B:220:ARG:HA	1.77	0.43
2:B:958:LEU:HA	2:B:958:LEU:HD23	1.63	0.43
2:B:978:ILE:CD1	2:B:1233:VAL:HG22	2.48	0.43
2:B:1325:LYS:HB3	2:B:1330:THR:HG22	2.00	0.43
2:F:631:MET:O	2:F:635:ARG:N	2.43	0.43
2:F:1126:TRP:N	2:F:1126:TRP:CD1	2.86	0.43
5:I:76:A:H2'	5:I:77:A:O4'	2.19	0.43
2:B:184:LEU:HD23	2:B:184:LEU:HA	1.78	0.43
2:B:64:LEU:HD13	2:B:64:LEU:HA	1.71	0.43
2:B:90:MET:HE3	2:B:97:PHE:CE2	2.53	0.43
2:B:305:ILE:HG13	2:B:306:LEU:N	2.33	0.43
2:B:341:GLN:HG2	2:B:342:GLN:HG3	1.99	0.43
2:B:926:GLN:HG2	3:C:20:DA:P	2.58	0.43
2:B:1120:ILE:HG21	2:B:1120:ILE:HD13	1.61	0.43
2:F:1166:ILE:HG13	2:F:1174:PHE:CE2	2.54	0.43
2:F:1356:TYR:HB3	5:J:81:G:C2	2.54	0.43
2:B:122:ILE:H	2:B:122:ILE:HG13	1.66	0.43
2:B:499:ASP:OD2	2:B:663:SER:N	2.37	0.43
2:B:839:ASP:N	2:B:856:VAL:O	2.33	0.43
2:B:886:LEU:HB3	2:B:891:LEU:HB2	2.01	0.43
2:F:164:PHE:CD1	2:F:164:PHE:C	2.94	0.43
2:F:981:TYR:C	2:F:983:HIS:N	2.77	0.43
2:F:1245:LEU:HD13	2:F:1252:ASN:CG	2.44	0.43
2:F:1277:SER:HA	2:F:1281:ILE:HG12	2.00	0.43
5:I:73:G:C2	5:I:77:A:C6	3.05	0.43
1:A:15:G:O5'	1:A:15:G:H8	2.02	0.43
2:B:508:LEU:HD21	2:B:664:ARG:HB2	2.00	0.43
2:B:524:LEU:CD2	2:B:545:LYS:HA	2.48	0.43
2:F:51:LEU:CD1	2:F:1352:ILE:HG13	2.49	0.43
2:F:777:SER:CA	2:F:807:GLN:HE21	2.18	0.43
1:E:5:C:O2	1:E:5:C:H2'	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:9:LEU:HD11	2:F:744:VAL:CG2	2.48	0.43
2:F:110:ASP:OD2	2:F:1130:LYS:HE3	2.18	0.43
2:F:212:LEU:HD13	2:F:300:ILE:CD1	2.49	0.43
2:F:226:ILE:CD1	2:F:232:GLU:HG2	2.49	0.43
2:F:561:VAL:HG12	2:F:565:LYS:HG3	2.00	0.43
2:F:597:LEU:O	2:F:601:ILE:HG12	2.19	0.43
2:F:627:GLU:HA	2:F:655:ARG:NH1	2.34	0.43
2:F:1052:LEU:HD12	2:F:1052:LEU:HA	1.86	0.43
2:B:216:LEU:HA	2:B:216:LEU:HD23	1.77	0.43
2:B:570:LYS:HE3	2:B:570:LYS:HB3	1.69	0.43
2:B:623:LEU:HD12	2:B:623:LEU:HA	1.70	0.43
2:B:946:ASN:HB3	2:B:948:LYS:HD2	2.00	0.43
1:E:15:G:H4'	2:F:454:PRO:HD3	2.01	0.43
2:F:137:HIS:CD2	2:F:322:ILE:HG23	2.54	0.43
2:F:339:VAL:HG12	2:F:347:TYR:HB2	2.00	0.43
2:F:829:ASP:OD1	2:F:832:ARG:N	2.36	0.43
5:J:96:C:H2'	5:J:97:U:O4'	2.19	0.43
2:F:5:TYR:CZ	2:F:751:MET:HG3	2.54	0.42
2:F:136:TYR:CZ	2:F:160:HIS:NE2	2.85	0.42
2:F:199:ASN:O	2:F:201:ILE:HD12	2.18	0.42
2:F:684:LYS:O	2:F:685:SER:OG	2.31	0.42
2:F:686:ASP:CB	2:F:690:ASN:CA	2.85	0.42
2:F:817:GLN:HB3	2:F:820:ARG:O	2.19	0.42
2:F:843:PRO:O	2:F:846:PHE:HB2	2.19	0.42
5:I:85:C:H42	5:I:93:G:H1	1.67	0.42
5:I:85:C:H2'	5:I:86:C:C6	2.54	0.42
1:A:3:A:O2'	1:A:4:A:P	2.77	0.42
2:B:814:TYR:CE2	2:B:819:GLY:HA2	2.54	0.42
1:E:26:A:C6	1:E:27:G:N7	2.87	0.42
2:F:484:LYS:H	2:F:484:LYS:CE	2.32	0.42
2:F:686:ASP:HB3	2:F:689:ALA:O	2.19	0.42
2:F:802:GLU:H	2:F:805:GLN:HG3	1.84	0.42
5:J:96:C:H2'	5:J:97:U:C6	2.54	0.42
2:B:594:TYR:OH	2:B:608:ASP:OD1	2.37	0.42
2:B:727:LEU:HD11	2:B:934:ILE:HD11	2.01	0.42
2:B:1163:LEU:HD23	2:B:1163:LEU:HA	1.71	0.42
2:B:1301:PRO:O	2:B:1305:GLN:HB2	2.20	0.42
2:B:1336:TYR:N	2:B:1336:TYR:CD1	2.87	0.42
1:E:19:A:OP1	2:F:164:PHE:CD1	2.68	0.42
2:F:165:ARG:CD	2:F:168:PHE:HZ	2.29	0.42
2:F:183:LYS:HD2	2:F:183:LYS:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:213:SER:O	2:F:213:SER:OG	2.32	0.42
2:F:350:ILE:O	2:F:359:TYR:N	2.52	0.42
2:F:848:LYS:HB3	2:F:848:LYS:HE3	1.55	0.42
2:F:1228:LEU:HD12	2:F:1228:LEU:HA	1.82	0.42
2:B:424:ARG:NE	2:B:427:GLU:OE2	2.52	0.42
2:B:913:LYS:HA	2:B:916:PHE:CD2	2.41	0.42
2:B:1110:ILE:CD1	2:B:1134:PHE:HE1	2.31	0.42
2:B:1246:LYS:HB2	2:B:1246:LYS:HE2	1.86	0.42
4:D:3:DT:H1'	4:D:4:DT:H5'	2.00	0.42
2:F:891:LEU:H	2:F:891:LEU:HD23	1.84	0.42
2:F:1266:LEU:HG	2:F:1309:ILE:HD11	2.00	0.42
3:G:23:DC:H2'	3:G:24:DG:O4'	2.19	0.42
2:B:609:ASN:ND2	2:B:611:GLU:OE1	2.45	0.42
2:B:840:ALA:HA	2:B:854:ASN:O	2.19	0.42
2:B:1082:THR:O	2:B:1086:VAL:HG23	2.19	0.42
1:E:15:G:H2'	1:E:16:A:O4'	2.19	0.42
2:F:824:VAL:HG12	2:F:825:ASP:H	1.83	0.42
2:F:1135:ASP:OD1	4:H:8:DT:H5''	2.20	0.42
1:A:4:A:O2'	1:A:5:C:C5'	2.68	0.42
2:B:665:LYS:O	2:B:670:ILE:HG12	2.19	0.42
2:B:986:ASP:O	2:B:990:ASN:ND2	2.52	0.42
2:B:1213:MET:O	2:B:1221:GLN:N	2.48	0.42
2:B:1244:LYS:HB2	2:B:1244:LYS:HE2	1.80	0.42
2:F:381:GLU:H	2:F:381:GLU:HG2	1.72	0.42
2:F:424:ARG:HH22	2:F:437:ARG:NH1	2.17	0.42
2:F:679:ILE:HG12	2:F:704:PHE:CZ	2.54	0.42
2:F:981:TYR:HE1	2:F:1225:GLU:HG3	1.84	0.42
2:F:985:HIS:CG	2:F:1087:LEU:HD22	2.55	0.42
2:F:988:TYR:CZ	2:F:1086:VAL:HG11	2.54	0.42
2:F:1111:LEU:HD23	2:F:1111:LEU:HA	1.64	0.42
2:F:1264:HIS:ND1	2:F:1268:GLU:OE2	2.49	0.42
5:J:42:A:O2'	5:J:43:G:OP1	2.30	0.42
2:B:25:TYR:O	2:B:988:TYR:OH	2.36	0.42
2:B:997:LEU:HD23	2:B:997:LEU:HA	1.87	0.42
1:E:11:U:C2	1:E:12:A:C8	3.07	0.42
2:F:165:ARG:CG	2:F:168:PHE:HE1	2.33	0.42
2:F:1089:MET:HA	2:F:1090:PRO:HD3	1.66	0.42
2:F:1178:PRO:O	2:F:1182:LEU:HG	2.19	0.42
2:B:8:GLY:O	2:B:987:ALA:HB1	2.20	0.42
2:B:1182:LEU:HD13	2:B:1190:VAL:HG11	2.01	0.42
2:F:226:ILE:HG22	2:F:230:PRO:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:813:LEU:O	2:F:817:GLN:HG3	2.20	0.42
2:F:1207:GLU:CD	2:F:1210:ARG:HH11	2.27	0.42
2:F:1321:PRO:HG2	2:F:1335:ARG:HA	2.02	0.42
2:B:1097:LYS:NZ	5:I:67:C:OP2	2.50	0.42
2:B:1318:LEU:C	2:B:1318:LEU:CD1	2.91	0.42
2:F:170:ILE:HG22	2:F:413:GLN:NE2	2.35	0.42
2:F:495:MET:HB3	3:G:17:DT:H1'	2.02	0.42
2:F:521:TYR:HE1	2:F:684:LYS:HD2	1.85	0.42
2:F:1096:LYS:HE2	2:F:1201:TYR:CE2	2.55	0.42
2:F:1218:GLY:C	2:F:1339:THR:HG23	2.44	0.42
2:B:1142:SER:O	2:B:1198:LEU:N	2.35	0.42
2:F:207:ASP:C	2:F:211:ILE:CD1	2.93	0.42
2:F:441:GLU:O	2:F:445:THR:HG22	2.20	0.42
2:F:591:LEU:O	2:F:595:HIS:ND1	2.48	0.42
2:F:644:ASP:HB3	2:F:647:VAL:HG23	2.02	0.42
2:F:823:TYR:CD2	2:F:863:ASN:HB2	2.55	0.42
2:B:570:LYS:O	2:B:574:CYS:HA	2.20	0.41
2:B:794:GLN:HG2	2:B:798:GLU:HG3	2.01	0.41
2:B:1191:LYS:HD2	2:B:1194:LEU:HD12	2.01	0.41
2:B:1229:PRO:HB2	2:B:1232:TYR:CE2	2.55	0.41
2:B:1258:PHE:CE1	2:B:1262:HIS:CD2	3.06	0.41
3:C:25:DT:N3	3:C:26:DT:H72	2.35	0.41
2:F:201:ILE:HD12	2:F:201:ILE:N	2.35	0.41
2:F:522:ASN:HA	2:F:683:LEU:HD13	2.01	0.41
2:F:523:GLU:OE1	2:F:588:ASN:HB2	2.20	0.41
2:F:910:GLU:OE1	2:F:910:GLU:N	2.51	0.41
2:F:1236:LEU:HD11	2:F:1269:ILE:HD13	2.01	0.41
5:J:53:G:C2	5:J:62:G:C2	3.08	0.41
2:B:40:ARG:HH22	5:I:92:G:P	2.43	0.41
2:B:300:ILE:HA	2:B:303:SER:OG	2.20	0.41
2:B:349:GLU:HG3	2:B:356:LYS:HG3	2.01	0.41
2:B:599:LYS:O	2:B:602:LYS:HG3	2.19	0.41
1:E:5:C:C2	1:E:6:G:C8	3.08	0.41
1:E:22:U:O2	2:F:1110:ILE:HD12	2.20	0.41
2:F:758:ASN:ND2	2:F:995:THR:HG22	2.36	0.41
2:F:1221:GLN:HB3	2:F:1319:GLY:O	2.20	0.41
1:A:18:A:OP2	2:B:71:ARG:HD2	2.20	0.41
1:A:18:A:OP1	2:B:165:ARG:HD3	2.19	0.41
2:B:325:TYR:HA	5:I:44:U:O2	2.20	0.41
2:B:820:ARG:HG2	2:B:879:MET:HE1	2.02	0.41
2:F:143:VAL:HG22	2:F:422:ILE:CG1	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:174:LEU:CD2	2:F:413:GLN:HB2	2.50	0.41
2:B:31:LYS:HG3	2:B:44:LYS:HG3	2.02	0.41
2:B:212:LEU:HD21	2:B:225:LEU:CD1	2.50	0.41
2:B:666:LEU:C	2:B:666:LEU:HD23	2.45	0.41
2:B:742:LYS:HB3	2:B:1352:ILE:HD13	2.02	0.41
2:B:1000:LYS:HE2	2:B:1065:THR:O	2.20	0.41
2:F:268:LYS:O	2:F:271:TYR:CD2	2.71	0.41
2:F:1087:LEU:HD23	2:F:1087:LEU:HA	1.76	0.41
2:F:1204:PHE:CE1	2:F:1347:LEU:HG	2.56	0.41
2:F:1245:LEU:HD13	2:F:1252:ASN:ND2	2.35	0.41
5:I:87:G:C2	5:I:92:G:C6	3.09	0.41
1:A:4:A:O2'	1:A:5:C:P	2.77	0.41
2:B:475:PRO:HG3	5:I:59:U:O4	2.21	0.41
2:B:680:LEU:HD12	2:B:680:LEU:HA	1.76	0.41
2:B:879:MET:HE3	2:B:882:TYR:CD2	2.55	0.41
2:B:1003:LYS:H	2:B:1003:LYS:HG2	1.54	0.41
2:B:1179:ILE:HD11	2:B:1192:LYS:CE	2.50	0.41
2:B:1207:GLU:HG2	2:B:1210:ARG:NH1	2.35	0.41
2:F:49:GLY:HA2	2:F:1092:VAL:CG1	2.50	0.41
2:F:174:LEU:HD22	2:F:413:GLN:HB2	2.02	0.41
2:F:289:LEU:O	2:F:292:ALA:HB3	2.19	0.41
2:F:302:LEU:HD23	2:F:305:ILE:HD11	2.02	0.41
2:F:409:SER:O	2:F:411:PRO:HD3	2.20	0.41
2:F:442:LYS:HE3	2:F:446:PHE:CD1	2.55	0.41
2:F:1228:LEU:HD12	2:F:1229:PRO:CD	2.51	0.41
2:F:1281:ILE:HG13	2:F:1316:THR:HG22	2.02	0.41
3:G:2:DA:H2''	3:G:3:DA:OP1	2.21	0.41
2:B:554:LYS:HG2	2:B:594:TYR:CE2	2.56	0.41
2:B:784:ILE:HD13	2:B:815:TYR:CB	2.51	0.41
2:B:841:ILE:HD11	2:B:896:LYS:HG3	2.02	0.41
2:B:1084:ARG:O	2:B:1084:ARG:HG2	2.18	0.41
2:F:143:VAL:HG21	2:F:315:ALA:CB	2.50	0.41
2:F:424:ARG:O	2:F:427:GLU:HG2	2.19	0.41
2:F:662:LEU:HD22	2:F:666:LEU:CD2	2.50	0.41
2:B:25:TYR:HE2	2:B:1074:TRP:CE3	2.38	0.41
2:B:534:MET:HE2	2:B:534:MET:HB3	1.93	0.41
2:B:650:GLN:CD	2:B:653:ARG:HH21	2.28	0.41
2:B:1220:LEU:HD21	2:B:1342:VAL:HG21	2.02	0.41
2:B:1318:LEU:HD22	2:B:1319:GLY:N	2.35	0.41
2:F:137:HIS:CD2	2:F:322:ILE:HG12	2.55	0.41
2:F:348:LYS:HA	2:F:352:PHE:HD2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:583:VAL:HG21	2:F:587:PHE:CD1	2.54	0.41
2:F:636:LEU:HA	2:F:639:TYR:HD2	1.84	0.41
2:F:649:LYS:CB	2:F:653:ARG:HH21	2.34	0.41
3:G:4:DT:H2''	3:G:5:DA:C5'	2.51	0.41
2:B:959:LYS:HB3	2:B:962:LEU:HG	2.02	0.41
3:C:2:DA:H2'	3:C:3:DA:C8	2.55	0.41
2:F:1061:PRO:O	2:F:1076:LYS:HE2	2.21	0.41
2:F:1203:LEU:HD23	2:F:1348:ILE:HD12	2.02	0.41
2:F:1343:LEU:O	2:F:1362:LEU:HB2	2.21	0.41
2:B:118:ILE:HG12	2:B:156:LEU:HD11	2.03	0.41
2:B:248:LEU:HA	2:B:248:LEU:HD23	1.72	0.41
2:B:447:ARG:HD3	2:B:447:ARG:HH11	1.76	0.41
2:B:524:LEU:HD23	2:B:545:LYS:HG2	2.02	0.41
2:B:535:ARG:HE	2:B:535:ARG:HB3	1.70	0.41
2:B:544:GLN:O	2:B:548:ILE:HG13	2.21	0.41
2:B:861:ASP:O	2:B:864:ARG:HG2	2.21	0.41
2:B:1119:LEU:HD12	2:B:1119:LEU:HA	1.93	0.41
2:B:1205:GLU:O	2:B:1345:ALA:HB1	2.21	0.41
2:F:4:LYS:HE2	2:F:4:LYS:HB2	1.54	0.41
2:F:97:PHE:CE1	2:F:118:ILE:HA	2.56	0.41
2:F:117:PRO:HD2	2:F:118:ILE:HD12	2.03	0.41
2:F:178:ASN:ND2	2:F:295:ASN:CG	2.79	0.41
2:F:336:LYS:HG2	2:F:351:PHE:CZ	2.55	0.41
2:F:513:LEU:HA	2:F:513:LEU:HD23	1.80	0.41
2:F:525:THR:OG1	2:F:545:LYS:NZ	2.30	0.41
2:F:546:LYS:NZ	2:F:550:ASP:OD2	2.53	0.41
2:F:553:PHE:CD2	2:F:559:VAL:HG21	2.56	0.41
2:F:632:ILE:O	2:F:636:LEU:N	2.39	0.41
2:F:852:ILE:O	2:F:896:LYS:HD3	2.21	0.41
2:F:853:ASP:OD2	2:F:895:ARG:HD3	2.21	0.41
2:F:878:LYS:HE3	2:F:878:LYS:HB2	1.84	0.41
2:F:897:PHE:CZ	2:F:901:THR:HG21	2.56	0.41
2:F:949:LEU:HD23	2:F:951:ARG:HH22	1.85	0.41
2:F:1163:LEU:HD23	2:F:1163:LEU:HA	1.91	0.41
2:F:1207:GLU:CG	2:F:1208:ASN:H	2.34	0.41
5:I:52:A:OP2	5:I:62:G:N2	2.51	0.41
5:I:82:G:N7	5:I:97:U:O2	2.53	0.41
5:I:92:G:H2'	5:I:93:G:C8	2.56	0.41
5:J:45:U:H2'	5:J:46:A:H8	1.86	0.41
5:J:56:U:O2	5:J:58:G:N2	2.46	0.41
2:B:383:MET:HE3	2:B:383:MET:HB3	1.82	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:423:LEU:HA	2:B:423:LEU:HD23	1.70	0.41
2:B:518:PHE:CD2	2:B:518:PHE:C	2.98	0.41
2:B:982:HIS:HA	2:B:985:HIS:HB2	2.02	0.41
2:B:1302:ILE:H	2:B:1302:ILE:HG13	1.71	0.41
2:F:318:SER:O	2:F:321:MET:HB2	2.21	0.41
2:F:1360:ILE:HD13	2:F:1360:ILE:HA	1.92	0.41
2:B:455:LEU:O	5:I:60:C:H5'	2.21	0.40
2:B:485:GLY:O	2:B:488:ALA:N	2.54	0.40
2:B:526:LYS:HD3	2:B:526:LYS:HA	1.91	0.40
2:B:788:ILE:HA	2:B:791:LEU:HB2	2.03	0.40
3:C:20:DA:C8	3:C:21:DT:H72	2.57	0.40
2:F:324:ARG:HB3	2:F:402:GLN:HE21	1.86	0.40
2:F:360:ALA:O	2:F:364:ASP:N	2.53	0.40
2:F:492:ILE:O	2:F:496:THR:HG23	2.21	0.40
5:J:46:A:H2'	5:J:47:A:H8	1.80	0.40
2:B:198:GLU:HG2	2:B:199:ASN:N	2.35	0.40
2:B:338:LEU:C	2:B:383:MET:HE1	2.44	0.40
2:B:455:LEU:N	2:B:455:LEU:CD1	2.84	0.40
2:B:966:PHE:CD2	2:B:966:PHE:C	2.99	0.40
2:B:1156:LYS:HE3	2:B:1156:LYS:HB2	1.91	0.40
1:E:15:G:O5'	1:E:15:G:H8	2.04	0.40
2:F:139:ARG:CG	2:F:157:ALA:CA	2.99	0.40
2:F:148:LYS:HA	2:F:429:PHE:CD2	2.56	0.40
2:F:451:TYR:CD1	2:F:488:ALA:HB2	2.56	0.40
2:F:749:LYS:O	2:F:750:VAL:C	2.64	0.40
2:F:967:ARG:NH1	2:F:974:LYS:HE3	2.36	0.40
2:F:1093:ASN:O	2:F:1094:ILE:HD13	2.22	0.40
2:F:1114:ARG:HG2	2:F:1115:ASN:H	1.85	0.40
2:B:424:ARG:CZ	2:B:437:ARG:NH1	2.85	0.40
2:B:821:ASP:OD2	2:B:828:LEU:HG	2.22	0.40
2:F:526:LYS:HA	2:F:526:LYS:HD3	1.68	0.40
2:F:927:ILE:O	2:F:930:HIS:N	2.54	0.40
2:F:1210:ARG:HB2	2:F:1280:VAL:HA	2.03	0.40
2:F:1236:LEU:O	2:F:1240:SER:OG	2.27	0.40
4:D:6:DG:H2''	4:D:7:DG:H5''	2.03	0.40
2:F:160:HIS:HE2	2:F:164:PHE:HD2	1.68	0.40
2:F:262:ALA:C	2:F:278:LEU:HD21	2.46	0.40
2:F:981:TYR:O	2:F:982:HIS:C	2.63	0.40
2:F:1053:ALA:C	2:F:1055:GLY:H	2.28	0.40
2:F:1107:LYS:HE2	3:G:8:DT:H1'	2.03	0.40
2:F:1146:VAL:O	2:F:1191:LYS:HG3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1204:PHE:CE2	2:F:1342:VAL:HG11	2.56	0.40
2:B:514:LEU:HD11	2:B:667:ILE:CG2	2.51	0.40
2:B:558:LYS:HD2	2:B:586:ARG:HD2	2.04	0.40
2:B:642:LEU:HB2	2:B:643:PHE:HD2	1.83	0.40
2:B:967:ARG:HH11	2:B:989:LEU:HD12	1.86	0.40
2:B:989:LEU:O	2:B:993:VAL:HG23	2.22	0.40
2:B:1228:LEU:HD12	2:B:1229:PRO:CD	2.51	0.40
1:E:14:G:O2'	1:E:15:G:H5'	2.22	0.40
2:F:57:GLU:HB2	5:J:65:A:P	2.62	0.40
2:F:1206:LEU:HD12	2:F:1210:ARG:NH1	2.35	0.40
2:F:1280:VAL:HG12	2:F:1281:ILE:HD13	2.03	0.40

All (1) 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:202:ASN:OD1	2:B:541:SER:OG[2_545]	2.07	0.13

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	1308/1368 (96%)	1268 (97%)	36 (3%)	4 (0%)	36	63
2	F	1313/1368 (96%)	1267 (96%)	41 (3%)	5 (0%)	30	58
All	All	2621/2736 (96%)	2535 (97%)	77 (3%)	9 (0%)	36	63

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	1042	ILE
2	F	585	ASP

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Mol	Chain	Res	Type
2	F	1011	GLY
2	F	1020	LYS
2	B	1327	PHE
2	B	470	GLU
2	B	117	PRO
2	F	117	PRO
2	B	230	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	1170/1225 (96%)	1162 (99%)	8 (1%)	76	77
2	F	1155/1225 (94%)	1146 (99%)	9 (1%)	73	76
All	All	2325/2450 (95%)	2308 (99%)	17 (1%)	76	77

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	249	THR
2	B	383	MET
2	B	388	GLU
2	B	389	LEU
2	B	584	GLU
2	B	688	PHE
2	B	1221	GLN
2	B	1317	ASN
2	F	150	ASP
2	F	151	LEU
2	F	155	TYR
2	F	156	LEU
2	F	158	LEU
2	F	160	HIS
2	F	686	ASP
2	F	688	PHE

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Mol	Chain	Res	Type
2	F	977	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	137	HIS
2	B	235	ASN
2	B	255	ASN
2	B	436	ASN
2	B	511	HIS
2	B	1044	ASN
2	B	1252	ASN
2	B	1262	HIS
2	B	1308	ASN
2	B	1311	HIS
2	B	1350	GLN
2	B	1364	GLN
2	F	46	ASN
2	F	129	HIS
2	F	178	ASN
2	F	329	HIS
2	F	394	ASN
2	F	501	ASN
2	F	544	GLN
2	F	556	ASN
2	F	726	ASN
2	F	758	ASN
2	F	881	ASN
2	F	920	GLN
2	F	982	HIS
2	F	985	HIS
2	F	1208	ASN
2	F	1252	ASN
2	F	1311	HIS
2	F	1317	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	33/34 (97%)	11 (33%)	4 (12%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	E	32/34 (94%)	11 (34%)	2 (6%)
5	I	62/65 (95%)	19 (30%)	1 (1%)
5	J	62/65 (95%)	18 (29%)	1 (1%)
All	All	189/198 (95%)	59 (31%)	8 (4%)

All (59) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	2	U
1	A	3	A
1	A	4	A
1	A	6	G
1	A	9	U
1	A	20	A
1	A	24	U
1	A	28	A
1	A	29	G
1	A	32	A
1	A	33	U
1	E	4	A
1	E	5	C
1	E	6	G
1	E	9	U
1	E	20	A
1	E	24	U
1	E	28	A
1	E	29	G
1	E	30	C
1	E	32	A
1	E	33	U
5	I	37	U
5	I	39	G
5	I	40	C
5	I	42	A
5	I	43	G
5	I	44	U
5	I	50	U
5	I	51	A
5	I	56	U
5	I	57	A
5	I	59	U
5	I	63	U

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Mol	Chain	Res	Type
5	I	68	A
5	I	74	A
5	I	82	G
5	I	87	G
5	I	89	G
5	I	91	C
5	I	92	G
5	J	37	U
5	J	39	G
5	J	40	C
5	J	42	A
5	J	43	G
5	J	50	U
5	J	51	A
5	J	56	U
5	J	57	A
5	J	59	U
5	J	63	U
5	J	68	A
5	J	74	A
5	J	82	G
5	J	87	G
5	J	89	G
5	J	91	C
5	J	92	G

All (8) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	3	A
1	A	8	A
1	A	27	G
1	A	28	A
1	E	3	A
1	E	27	G
5	I	42	A
5	J	42	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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	34/34 (100%)	-0.21	1 (2%) 53 39	18, 45, 134, 169	0
1	E	32/34 (94%)	0.54	1 (3%) 51 38	38, 77, 181, 216	0
2	B	1322/1368 (96%)	0.51	111 (8%) 17 14	14, 71, 195, 218	0
2	F	1327/1368 (97%)	0.87	217 (16%) 4 5	13, 92, 149, 193	0
3	C	26/26 (100%)	0.01	1 (3%) 44 31	27, 50, 107, 115	0
3	G	26/26 (100%)	0.17	1 (3%) 44 31	45, 63, 112, 124	0
4	D	11/11 (100%)	0.45	2 (18%) 3 4	41, 53, 134, 168	0
4	H	11/11 (100%)	0.66	1 (9%) 15 13	41, 59, 110, 175	0
5	I	63/65 (96%)	-0.15	1 (1%) 70 55	20, 74, 126, 157	0
5	J	63/65 (96%)	-0.04	3 (4%) 35 25	36, 56, 156, 192	0
All	All	2915/3008 (96%)	0.63	339 (11%) 9 9	13, 77, 168, 218	0

All (339) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	305	ILE	9.8
1	E	34	G	8.9
2	F	1243	GLU	8.9
2	F	362	TYR	7.6
2	B	900	LEU	6.8
2	F	306	LEU	6.8
2	F	301	LEU	6.6
2	F	416	LEU	6.3
2	B	876	VAL	6.0
2	F	796	LEU	6.0
2	F	443	ILE	5.6
2	B	822	MET	5.5
2	F	815	TYR	5.5

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Mol	Chain	Res	Type	RSRZ
2	F	135	ILE	5.4
2	B	868	ASP	5.3
2	B	842	VAL	5.3
2	B	1051	THR	5.2
5	J	36	G	5.0
2	B	870	VAL	5.0
2	F	247	GLY	5.0
2	B	841	ILE	4.9
2	B	1045	PHE	4.8
2	B	1052	LEU	4.8
2	F	224	ASN	4.8
2	B	685	SER	4.7
2	B	42	SER	4.7
2	F	818	ASN	4.7
2	F	1246	LYS	4.5
2	B	867	SER	4.5
2	B	1046	PHE	4.5
2	F	1247	GLY	4.3
2	F	102	GLU	4.2
2	B	861	ASP	4.1
2	F	249	THR	4.1
2	F	244	LEU	4.1
2	F	181	VAL	4.0
2	F	400	ARG	4.0
2	B	843	PRO	4.0
2	F	557	ARG	4.0
2	B	815	TYR	4.0
2	F	367	ALA	4.0
2	F	103	GLU	4.0
2	F	621	LEU	4.0
2	B	871	PRO	4.0
2	F	81	TYR	3.9
2	F	267	SER	3.9
2	B	872	SER	3.9
2	F	1242	TYR	3.8
2	F	528	LYS	3.8
2	F	213	SER	3.8
2	F	581	SER	3.8
2	F	795	ILE	3.8
2	B	688	PHE	3.8
2	F	587	PHE	3.8
2	B	801	VAL	3.7

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Mol	Chain	Res	Type	RSRZ
2	F	207	ASP	3.7
4	H	2	DT	3.7
2	F	262	ALA	3.7
2	B	462	PHE	3.7
2	F	157	ALA	3.7
2	B	813	LEU	3.6
2	F	156	LEU	3.6
2	B	883	TRP	3.6
2	F	152	ARG	3.6
2	B	859	ARG	3.6
2	B	1040	SER	3.6
2	B	31	LYS	3.6
2	B	1039	TYR	3.6
2	F	413	GLN	3.5
2	F	597	LEU	3.5
2	F	359	TYR	3.5
2	B	811	LEU	3.5
2	F	335	LEU	3.5
2	F	136	TYR	3.5
2	F	613	GLU	3.4
2	F	415	HIS	3.4
2	F	154	ILE	3.4
2	B	810	LYS	3.4
2	F	229	LEU	3.4
2	F	412	HIS	3.4
2	B	906	GLY	3.3
2	B	1228	LEU	3.3
2	B	858	THR	3.3
2	F	119	PHE	3.3
2	F	142	LEU	3.3
2	B	809	GLU	3.3
2	F	538	ALA	3.3
2	F	697	ILE	3.3
2	B	32	PHE	3.3
2	B	897	PHE	3.3
2	F	334	LEU	3.3
2	B	817	GLN	3.3
2	F	246	LEU	3.2
2	F	524	LEU	3.2
2	F	402	GLN	3.2
2	F	98	PHE	3.2
2	F	679	ILE	3.2

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Mol	Chain	Res	Type	RSRZ
2	F	220	ARG	3.2
2	B	823	TYR	3.2
2	F	145	SER	3.2
2	B	824	VAL	3.2
2	F	164	PHE	3.2
2	B	1050	ILE	3.1
2	F	1252	ASN	3.1
2	B	902	LYS	3.1
2	F	132	TYR	3.1
2	F	369	GLN	3.1
2	F	440	ILE	3.0
2	F	537	PRO	3.0
4	D	2	DT	3.0
2	F	408	GLY	3.0
2	F	232	GLU	3.0
2	F	83	GLN	3.0
2	F	118	ILE	3.0
2	F	419	LEU	3.0
2	F	886	LEU	3.0
2	F	243	ALA	3.0
2	F	488	ALA	3.0
2	B	814	TYR	3.0
2	F	128	TYR	3.0
2	F	558	LYS	3.0
2	B	852	ILE	3.0
2	F	389	LEU	2.9
2	F	788	ILE	2.9
2	B	833	LEU	2.9
2	F	225	LEU	2.9
2	F	703	THR	2.9
2	B	869	ASN	2.9
2	F	478	PHE	2.9
2	F	784	ILE	2.9
2	B	796	LEU	2.9
2	F	159	ALA	2.9
2	F	302	LEU	2.9
2	B	901	THR	2.8
2	F	702	LEU	2.8
2	F	208	ALA	2.8
2	F	269	ASP	2.8
2	F	189	VAL	2.8
2	B	597	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
2	F	237	LEU	2.8
2	F	321	MET	2.8
2	F	777	SER	2.8
2	F	365	GLY	2.8
2	B	812	TYR	2.8
2	B	28	PRO	2.8
2	F	530	VAL	2.8
2	F	240	ASN	2.8
2	F	1249	PRO	2.8
2	B	899	ASN	2.7
2	F	155	TYR	2.7
2	F	304	ASP	2.7
2	F	227	ALA	2.7
2	F	317	LEU	2.7
2	F	688	PHE	2.7
2	F	202	ASN	2.7
2	F	811	LEU	2.7
2	F	800	PRO	2.7
2	B	903	ALA	2.7
2	F	689	ALA	2.7
2	F	160	HIS	2.7
2	B	857	LEU	2.6
2	F	141	LYS	2.6
2	F	407	ASN	2.6
2	F	792	GLY	2.6
2	B	1048	THR	2.6
2	F	248	LEU	2.6
2	B	1084	ARG	2.6
2	F	525	THR	2.6
2	F	804	THR	2.6
2	F	919	ARG	2.6
2	F	85	ILE	2.6
2	B	1242	TYR	2.6
2	B	860	SER	2.6
2	B	854	ASN	2.6
2	F	125	GLU	2.6
2	F	313	THR	2.6
2	F	363	ILE	2.5
2	F	539	PHE	2.5
2	B	908	LEU	2.5
2	F	781	MET	2.5
2	F	594	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
2	B	1073	VAL	2.5
2	F	257	ASP	2.5
2	F	863	ASN	2.5
2	F	575	PHE	2.5
2	B	836	TYR	2.5
2	F	117	PRO	2.5
2	F	836	TYR	2.5
2	F	158	LEU	2.5
2	F	253	LYS	2.5
2	F	1111	LEU	2.5
2	F	694	MET	2.5
2	F	372	PHE	2.5
2	B	855	LYS	2.5
2	B	830	ILE	2.5
2	B	856	VAL	2.5
2	B	844	GLN	2.5
2	B	912	ASP	2.4
2	B	816	LEU	2.4
5	J	43	G	2.4
2	F	307	ARG	2.4
2	B	43	ILE	2.4
2	F	1120	ILE	2.4
2	F	97	PHE	2.4
2	F	139	ARG	2.4
2	F	238	PHE	2.4
2	F	222	LEU	2.4
2	F	399	LEU	2.4
2	F	816	LEU	2.4
2	B	853	ASP	2.4
2	F	515	TYR	2.4
2	F	140	LYS	2.4
2	F	798	GLU	2.4
2	F	1248	SER	2.4
2	B	1090	PRO	2.4
2	F	93	VAL	2.4
2	B	881	ASN	2.4
2	F	588	ASN	2.4
2	B	829	ASP	2.4
2	F	545	LYS	2.4
2	F	698	HIS	2.3
2	F	78	ARG	2.3
2	F	271	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
5	I	82	G	2.3
2	B	241	LEU	2.3
2	B	1245	LEU	2.3
2	F	212	LEU	2.3
2	F	230	PRO	2.3
2	B	880	LYS	2.3
2	B	1310	ILE	2.3
2	F	420	HIS	2.3
2	F	853	ASP	2.3
2	B	47	LEU	2.3
2	F	423	LEU	2.3
2	F	209	LYS	2.3
2	F	1112	PRO	2.3
4	D	12	DG	2.3
2	B	795	ILE	2.3
2	F	631	MET	2.3
2	F	192	TYR	2.3
2	F	803	ASN	2.3
2	F	84	GLU	2.3
2	B	862	LYS	2.3
2	F	391	VAL	2.3
2	F	312	ILE	2.3
2	F	376	ILE	2.3
2	F	619	ILE	2.3
2	B	310	THR	2.3
2	B	1021	MET	2.3
2	F	833	LEU	2.3
2	F	712	GLN	2.3
2	F	861	ASP	2.3
2	B	877	LYS	2.3
2	B	1042	ILE	2.3
2	F	1218	GLY	2.3
2	B	229	LEU	2.3
2	B	832	ARG	2.3
2	B	864	ARG	2.3
2	F	308	VAL	2.3
2	F	670	ILE	2.2
2	F	421	ALA	2.2
2	F	883	TRP	2.2
2	F	256	PHE	2.2
2	F	432	PHE	2.2
2	B	271	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
2	F	805	GLN	2.2
2	B	978	ILE	2.2
2	B	1008	PHE	2.2
2	F	799	HIS	2.2
5	J	42	A	2.2
2	B	20	VAL	2.2
2	B	19	ALA	2.2
2	B	275	LEU	2.2
2	B	1249	PRO	2.2
2	F	822	MET	2.2
2	F	887	LEU	2.2
3	C	1	DC	2.2
2	F	446	PHE	2.2
2	F	620	VAL	2.2
2	F	856	VAL	2.2
2	F	309	ASN	2.2
2	F	82	LEU	2.2
2	F	648	MET	2.2
2	F	166	GLY	2.2
2	F	250	PRO	2.2
2	B	274	ASP	2.2
2	F	351	PHE	2.2
2	B	891	LEU	2.2
2	F	1238	LEU	2.2
2	F	133	PRO	2.2
2	F	578	VAL	2.1
2	F	1131	TYR	2.1
2	F	867	SER	2.1
2	F	144	ASP	2.1
2	F	298	ASP	2.1
2	F	397	ASP	2.1
2	F	169	LEU	2.1
3	G	26	DT	2.1
2	F	314	LYS	2.1
2	F	640	ALA	2.1
2	F	1121	ALA	2.1
2	B	230	PRO	2.1
2	F	687	GLY	2.1
2	F	809	GLU	2.1
2	F	874	GLU	2.1
2	B	202	ASN	2.1
2	F	690	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	225	LEU	2.1
2	F	106	LEU	2.1
2	F	268	LYS	2.1
2	B	631	MET	2.1
2	F	685	SER	2.1
2	F	793	SER	2.1
2	B	803	ASN	2.1
2	B	33	LYS	2.1
2	F	1110	ILE	2.1
2	F	832	ARG	2.1
2	B	785	GLU	2.1
2	F	1204	PHE	2.1
2	F	401	LYS	2.1
2	F	241	LEU	2.1
2	F	343	LEU	2.1
2	F	830	ILE	2.1
2	B	988	TYR	2.1
2	F	275	LEU	2.0
2	B	799	HIS	2.0
2	B	262	ALA	2.0
2	B	384	ASP	2.0
2	F	315	ALA	2.0
2	B	800	PRO	2.0
1	A	34	G	2.0
2	F	433	LEU	2.0
2	B	703	THR	2.0
2	B	1265	TYR	2.0
2	F	23	ASP	2.0
2	B	1038	PHE	2.0
2	B	1258	PHE	2.0
2	F	540	LEU	2.0
2	F	1119	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.