



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:45 PM UTC

PDB ID : 8KAJ / pdb_00008kaj
Title : Crystal structure of SpyCas9-crRNA-tracrRNA complex bound to 16nt target DNA
Authors : Chen, Y.; Chen, J.; Liu, L.
Deposited on : 2023-08-03
Resolution : 3.42 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

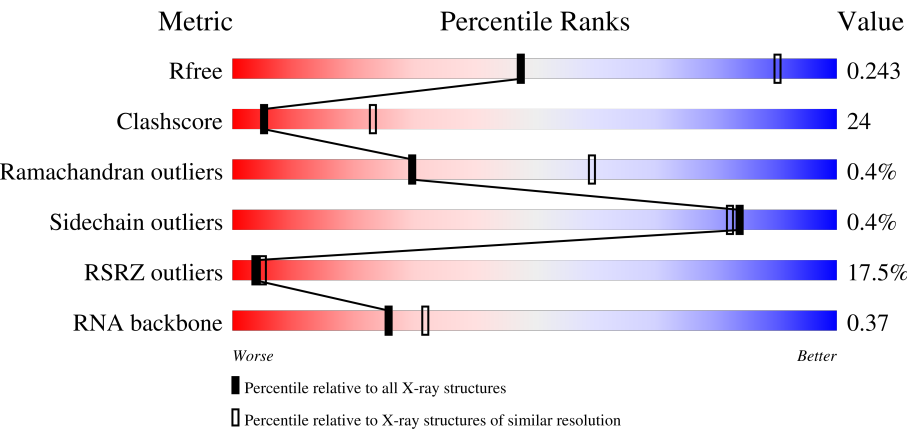
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.42 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	1210 (3.48-3.36)
Clashscore	190562	1234 (3.48-3.36)
Ramachandran outliers	187476	1222 (3.48-3.36)
Sidechain outliers	187428	1222 (3.48-3.36)
RSRZ outliers	180081	1210 (3.48-3.36)
RNA backbone	3983	1162 (3.84-3.00)

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 ≥ 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	9% 32% 38% 26% .
1	E	34	15% 26% 53% 12% 9%
2	B	1368	13% 55% 42% .
2	F	1368	23% 51% 45% ..

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Mol	Chain	Length	Quality of chain
3	C	24	8% 50% 50%
3	G	24	4% 67% 33%
4	D	11	18% 64% 36%
4	H	11	18% 73% 27%
5	I	65	5% 37% 48% 11% • •
5	J	65	8% 22% 55% 20% •

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 26963 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	31	Total	C	N	O	P	0	0	0
			663	297	118	217	31			

- 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
			10769	6854	1869	2024	22			
2	F	1327	Total	C	N	O	S	0	0	0
			10698	6816	1845	2014	23			

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 (5'-D(*CP*AP*AP*TP*AP*CP*CP*TP*TP*TP*TP*AP*TP*CP*CP*AP*TP*AP*AP*AP*TP*TP*CP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	24	Total	C	N	O	P	0	0	0
			481	234	81	143	23			
3	G	24	Total	C	N	O	P	0	0	0
			481	234	81	143	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 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

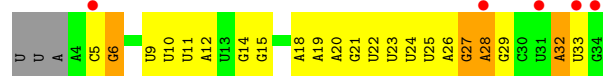
3 Residue-property plots [i](#)

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.

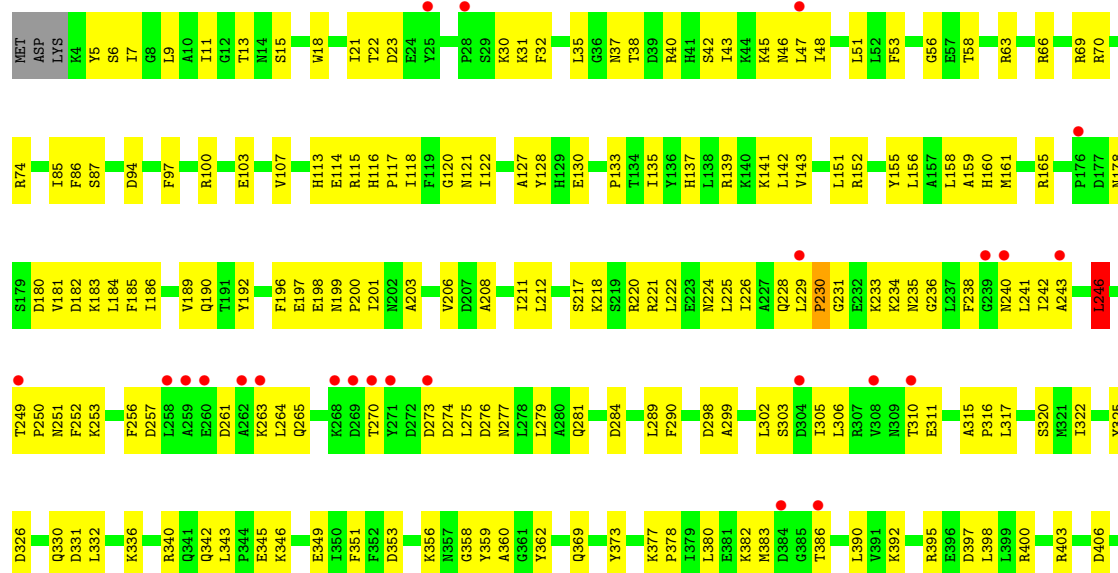
- Molecule 1: RNA (34-MER)

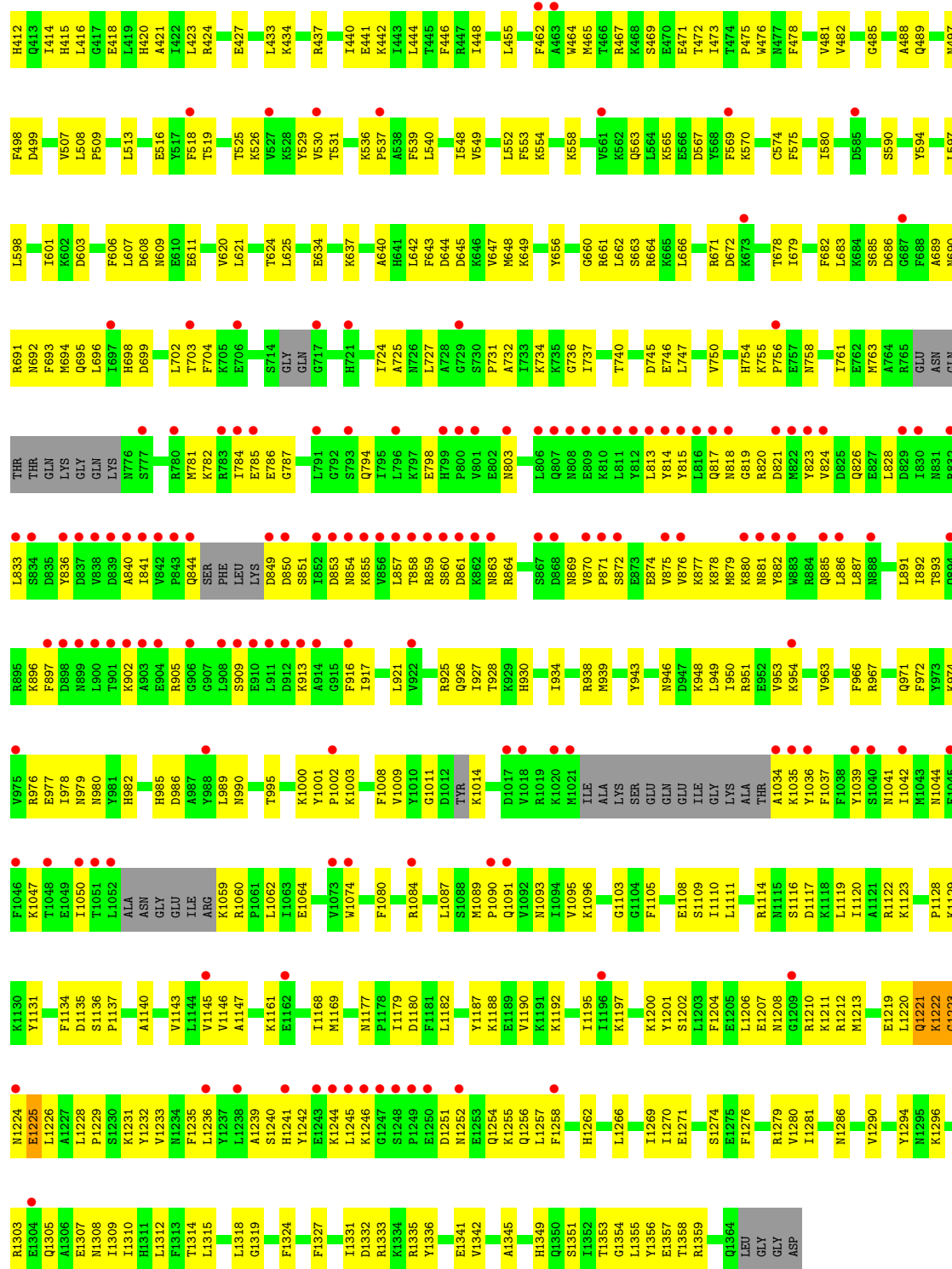


- Molecule 1: RNA (34-MER)



- Molecule 2: CRISPR-associated endonuclease Cas9/Csn1

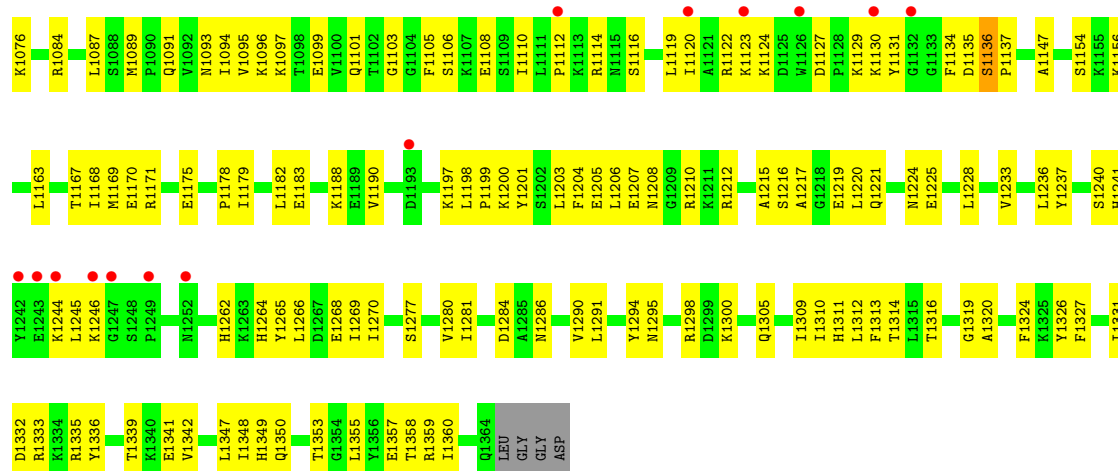




- Molecule 2: CRISPR-associated endonuclease Cas9/Csn1



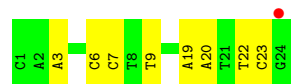




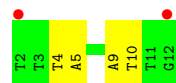
- Molecule 3: DNA (5'-D(*CP*AP*AP*TP*AP*CP*CP*TP*TP*TP*TP*AP*TP*CP*CP*AP*TP*AP*AP*AP*TP*TP*CP*G)-3')



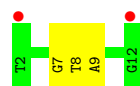
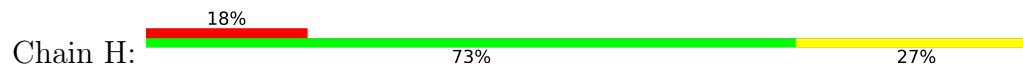
- Molecule 3: DNA (5'-D(*CP*AP*AP*TP*AP*CP*CP*TP*TP*TP*TP*AP*TP*CP*CP*AP*TP*AP*AP*AP*TP*TP*CP*G)-3')



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

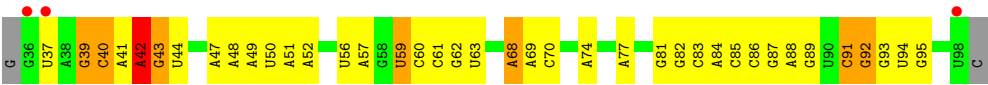


- Molecule 4: DNA (5'-D(*TP*TP*TP*AP*GP*GP*TP*AP*TP*TP*G)-3')

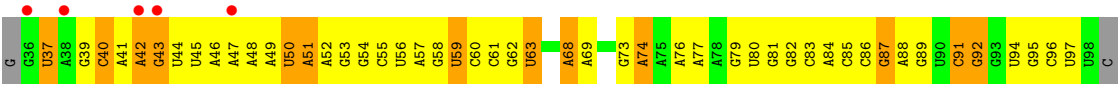


- Molecule 5: RNA (65-MER)





• 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	144.74Å 131.10Å 146.63Å 90.00° 103.68° 90.00°	Depositor
Resolution (Å)	48.03 – 3.42 48.03 – 3.42	Depositor EDS
% Data completeness (in resolution range)	69.1 (48.03-3.42) 79.6 (48.03-3.42)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.38 (at 3.40Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.237 , 0.246 0.237 , 0.243	Depositor DCC
R_{free} test set	1993 reflections (2.76%)	wwPDB-VP
Wilson B-factor (Å ²)	52.1	Xtriage
Anisotropy	0.048	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 46.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.034 for l,-k,h	Xtriage
F_o, F_c correlation	0.83	EDS
Total number of atoms	26963	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.92% 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 [i](#)

5.1 Standard geometry [i](#)

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	0.61	0/811	0.87	1/1261 (0.1%)
1	E	0.50	0/742	0.78	0/1154
2	B	0.57	2/10954 (0.0%)	0.84	4/14725 (0.0%)
2	F	0.57	1/10882 (0.0%)	0.84	3/14639 (0.0%)
3	C	0.71	0/537	0.93	0/825
3	G	0.61	0/537	0.84	0/825
4	D	0.76	0/251	0.81	0/387
4	H	0.69	0/251	0.81	0/387
5	I	0.57	0/1509	0.81	1/2350 (0.0%)
5	J	0.55	0/1509	0.81	0/2350
All	All	0.57	3/27983 (0.0%)	0.84	9/38903 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1103	GLY	C-O	11.25	1.39	1.23
2	F	1136	SER	C-O	-9.43	1.19	1.23
2	B	1103	GLY	C-N	-5.88	1.27	1.33

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1223	GLY	N-CA-C	9.74	125.24	112.77
2	F	1001	TYR	CB-CA-C	-9.16	103.03	111.00
2	F	1043	MET	CB-CG-SD	-6.91	91.97	112.70
2	B	246	LEU	N-CA-C	-5.89	102.20	110.50
1	A	27	G	C4'-C3'-O3'	5.72	121.58	113.00
2	B	1222	LYS	CA-C-N	5.57	126.13	120.00
2	B	1222	LYS	C-N-CA	5.57	126.13	120.00
5	I	42	A	C2'-C3'-O3'	5.52	121.98	113.70
2	F	246	LEU	CA-CB-CG	5.05	133.99	116.30

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	21	0
1	E	663	0	331	26	0
2	B	10769	0	10864	522	0
2	F	10698	0	10745	619	0
3	C	481	0	275	11	0
3	G	481	0	275	10	0
4	D	225	0	129	3	0
4	H	225	0	129	7	0
5	I	1348	0	678	43	0
5	J	1348	0	678	67	0
All	All	26963	0	24466	1245	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 24.

All (1245) 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:243:ALA:CA	2:B:246:LEU:HD23	1.44	1.38
2:B:243:ALA:HA	2:B:246:LEU:CD2	1.64	1.28
2:B:980:ASN:HB2	2:B:1225:GLU:OE2	1.39	1.21
2:F:1207:GLU:OE2	2:F:1210:ARG:NH1	1.79	1.14
2:B:243:ALA:CA	2:B:246:LEU:CD2	2.22	1.13
2:B:525:THR:HG23	2:B:690:ASN:HB3	1.12	1.12
2:F:525:THR:HG23	2:F:690:ASN:HB2	1.22	1.11
2:F:249:THR:HG1	2:F:267:SER:N	1.48	1.11
2:B:525:THR:CG2	2:B:690:ASN:HB3	1.89	1.02
2:B:1224:ASN:HB2	2:B:1280:VAL:HG11	1.38	1.02
2:B:270:THR:OG1	2:B:274:ASP:OD2	1.78	1.00
2:F:1060:ARG:HH11	2:F:1060:ARG:HB3	1.23	0.98
2:B:539:PHE:HB3	2:B:690:ASN:ND2	1.80	0.97
2:F:545:LYS:HZ2	2:F:690:ASN:HD22	1.11	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1123:LYS:HD2	5:J:53:G:OP1	1.66	0.95
2:B:1120:ILE:HD11	2:B:1137:PRO:HG3	1.49	0.95
2:F:1045:PHE:HB2	2:F:1064:GLU:HG2	1.46	0.95
2:F:226:ILE:HG13	2:F:232:GLU:HG2	1.49	0.94
2:B:539:PHE:HB3	2:B:690:ASN:HD22	1.32	0.94
2:F:63:ARG:HA	2:F:66:ARG:HG3	1.49	0.94
2:F:962:LEU:HB3	2:F:1043:MET:HE1	1.50	0.94
2:F:380:LEU:HD11	2:F:390:LEU:HG	1.51	0.93
2:F:1210:ARG:NH2	2:F:1341:GLU:OE1	2.01	0.93
2:F:425:ARG:HG3	2:F:426:GLN:HG2	1.51	0.93
2:F:485:GLY:HA3	2:F:631:MET:HG3	1.49	0.91
2:B:465:MET:HE3	2:B:467:ARG:HG2	1.53	0.90
1:A:2:U:H3	1:A:4:A:H3'	1.37	0.89
2:F:978:ILE:HD12	2:F:1228:LEU:HD23	1.52	0.89
2:B:1308:ASN:HD22	2:B:1327:PHE:H	1.19	0.89
2:F:525:THR:CG2	2:F:690:ASN:HB2	2.02	0.88
2:B:980:ASN:CB	2:B:1225:GLU:OE2	2.20	0.88
2:F:70:ARG:NE	5:J:61:C:OP2	2.07	0.87
2:F:545:LYS:HZ2	2:F:690:ASN:ND2	1.72	0.87
2:F:184:LEU:HD13	2:F:295:ASN:HB3	1.54	0.87
2:F:142:LEU:HD22	2:F:422:ILE:HG23	1.57	0.87
2:F:1294:TYR:HE1	2:F:1305:GLN:HE21	1.21	0.87
2:F:978:ILE:HD13	2:F:1233:VAL:HG22	1.59	0.85
2:F:1060:ARG:HH11	2:F:1060:ARG:CB	1.89	0.84
2:F:221:ARG:HA	2:F:224:ASN:HB2	1.58	0.84
2:B:46:ASN:ND2	2:B:1091:GLN:OE1	2.10	0.84
2:B:1207:GLU:CD	2:B:1210:ARG:HH11	1.85	0.83
1:E:15:G:OP1	2:F:66:ARG:NH2	2.10	0.83
2:B:530:VAL:HG22	2:B:537:PRO:HB3	1.60	0.83
2:B:246:LEU:H	2:B:246:LEU:HD22	1.44	0.83
2:B:548:ILE:HG23	2:B:552:LEU:HD12	1.60	0.82
5:J:46:A:H2'	5:J:47:A:C8	2.15	0.82
2:F:525:THR:OG1	2:F:545:LYS:NZ	2.13	0.82
2:F:1212:ARG:NH2	2:F:1280:VAL:O	2.13	0.81
2:F:70:ARG:NH2	5:J:61:C:OP1	2.13	0.81
2:F:451:TYR:O	2:F:464:TRP:NE1	2.14	0.80
2:B:243:ALA:C	2:B:246:LEU:HD23	2.05	0.80
2:B:725:ALA:O	2:B:734:LYS:NZ	2.14	0.80
2:F:1045:PHE:O	2:F:1076:LYS:NZ	2.14	0.80
2:F:777:SER:HA	2:F:807:GLN:HE21	1.46	0.79
2:F:545:LYS:NZ	2:F:690:ASN:HD22	1.81	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:137:HIS:HA	2:B:322:ILE:HD11	1.64	0.79
2:F:826:GLN:OE1	2:F:859:ARG:NH1	2.15	0.79
2:F:829:ASP:OD1	2:F:832:ARG:N	2.10	0.79
2:B:1210:ARG:NH2	2:B:1341:GLU:OE1	2.17	0.78
2:B:1211:LYS:O	2:B:1223:GLY:HA3	1.83	0.78
2:F:525:THR:HG23	2:F:690:ASN:CB	2.09	0.78
2:F:1091:GLN:HG3	5:J:91:C:H5''	1.66	0.78
2:B:9:LEU:HD12	2:B:761:ILE:HG22	1.64	0.78
2:B:220:ARG:O	2:B:224:ASN:ND2	2.14	0.77
2:B:539:PHE:CD2	2:B:689:ALA:HA	2.18	0.77
2:B:823:TYR:HA	2:B:875:VAL:HG11	1.66	0.77
2:F:249:THR:OG1	2:F:267:SER:N	2.18	0.77
1:E:27:G:N2	5:J:44:U:OP2	2.17	0.77
1:A:27:G:H5'	1:A:28:A:H5''	1.67	0.77
2:F:1266:LEU:HD12	2:F:1309:ILE:HD12	1.67	0.77
2:B:902:LYS:HA	2:B:905:ARG:HE	1.50	0.76
2:F:1051:THR:HG22	2:F:1053:ALA:H	1.50	0.76
2:F:467:ARG:HA	2:F:482:VAL:HG22	1.67	0.76
2:B:270:THR:O	2:B:274:ASP:OD2	2.03	0.76
2:F:672:ASP:OD1	2:F:703:THR:HG22	1.85	0.76
2:F:886:LEU:HA	2:F:891:LEU:HD21	1.68	0.76
2:F:522:ASN:OD1	2:F:692:ASN:ND2	2.19	0.76
2:F:253:LYS:HB2	2:F:262:ALA:H	1.49	0.76
2:F:94:ASP:HB3	2:F:97:PHE:HB2	1.67	0.75
2:B:342:GLN:HE22	2:B:383:MET:HA	1.51	0.75
2:F:844:GLN:HG3	2:F:848:LYS:HD2	1.67	0.75
2:B:114:GLU:HG3	2:B:116:HIS:H	1.50	0.75
2:F:878:LYS:HB3	2:F:879:MET:SD	2.26	0.75
2:B:1147:ALA:HB2	2:B:1190:VAL:HA	1.67	0.75
2:B:727:LEU:HD12	2:B:927:ILE:HD12	1.69	0.75
1:E:32:A:N6	5:J:37:U:O4	2.20	0.74
2:F:527:VAL:HA	2:F:582:GLY:HA3	1.67	0.74
2:B:1135:ASP:OD1	2:B:1136:SER:N	2.20	0.74
2:B:400:ARG:NH2	2:B:406:ASP:OD2	2.20	0.74
2:B:1110:ILE:HD12	2:B:1122:ARG:HD2	1.69	0.73
2:F:145:SER:O	2:F:425:ARG:NH1	2.21	0.73
2:F:918:LYS:HZ3	2:F:1007:GLU:CD	1.97	0.73
2:B:540:LEU:O	2:B:690:ASN:ND2	2.20	0.73
2:B:909:SER:O	2:B:913:LYS:N	2.21	0.73
2:B:913:LYS:HA	2:B:916:PHE:HD2	1.54	0.73
2:F:143:VAL:O	2:F:425:ARG:CZ	2.37	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:262:ALA:HB1	2:F:278:LEU:HG	1.70	0.72
2:F:892:ILE:HB	2:F:896:LYS:HE2	1.71	0.72
2:B:601:ILE:HD11	2:B:607:LEU:HD21	1.70	0.72
2:F:178:ASN:ND2	2:F:295:ASN:OD1	2.22	0.72
2:B:1357:GLU:OE1	2:B:1359:ARG:NH1	2.22	0.72
2:F:1041:ASN:O	2:F:1043:MET:N	2.17	0.72
2:B:1037:PHE:CE1	2:B:1039:TYR:CD2	2.78	0.72
2:F:841:ILE:HD12	2:F:854:ASN:HA	1.72	0.72
2:B:763:MET:SD	2:B:928:THR:HG22	2.30	0.71
2:F:1124:LYS:N	5:J:53:G:OP1	2.16	0.71
2:B:229:LEU:HB2	2:B:230:PRO:HD2	1.71	0.71
2:F:1108:GLU:HB2	3:G:9:DT:H5"	1.72	0.71
2:F:646:LYS:O	2:F:650:GLN:NE2	2.17	0.71
2:B:243:ALA:HA	2:B:246:LEU:HD23	0.74	0.71
2:F:180:ASP:HB2	2:F:184:LEU:HG	1.73	0.71
2:B:644:ASP:HB3	2:B:647:VAL:HG23	1.71	0.70
2:F:90:MET:HA	2:F:151:LEU:HD21	1.71	0.70
2:F:121:ASN:HB2	2:F:123:VAL:HG12	1.72	0.70
2:B:249:THR:HG22	2:B:265:GLN:HB2	1.73	0.70
2:B:860:SER:OG	2:B:863:ASN:OD1	2.08	0.70
2:B:1037:PHE:HE1	2:B:1039:TYR:CD2	2.10	0.70
2:B:1241:HIS:CE1	2:B:1244:LYS:HA	2.26	0.70
2:F:893:THR:HG23	2:F:896:LYS:H	1.57	0.70
1:E:23:U:H5"	2:F:1112:PRO:HG3	1.72	0.70
2:F:165:ARG:HD2	2:F:168:PHE:HE1	1.56	0.70
2:F:913:LYS:HG3	2:F:1040:SER:HB3	1.74	0.70
2:F:531:THR:HG21	2:F:575:PHE:CE1	2.26	0.70
2:F:89:GLU:OE2	2:F:92:LYS:NZ	2.21	0.70
2:F:545:LYS:HD2	2:F:690:ASN:ND2	2.07	0.69
2:F:1060:ARG:HB3	2:F:1060:ARG:NH1	2.04	0.69
2:B:1333:ARG:NH1	2:B:1335:ARG:HD2	2.07	0.69
2:F:918:LYS:NZ	2:F:1018:VAL:CG1	2.55	0.69
2:F:978:ILE:CD1	2:F:1233:VAL:HG22	2.22	0.69
1:A:14:G:OP2	2:B:63:ARG:NH1	2.25	0.69
2:B:1041:ASN:HB2	2:B:1044:ASN:HD21	1.57	0.69
2:B:558:LYS:HE3	2:B:590:SER:HB3	1.75	0.69
2:F:675:SER:CB	2:F:682:PHE:HZ	2.06	0.69
2:F:174:LEU:HD11	2:F:302:LEU:HD21	1.73	0.68
2:B:45:LYS:NZ	2:B:1357:GLU:OE2	2.22	0.68
2:B:1207:GLU:OE2	2:B:1210:ARG:NH1	2.26	0.68
2:B:1207:GLU:CD	2:B:1210:ARG:NH1	2.51	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:15:G:P	2:F:66:ARG:HH22	2.17	0.68
2:F:776:ASN:O	2:F:780:ARG:HG2	1.92	0.68
2:F:1236:LEU:HD11	2:F:1269:ILE:HD13	1.76	0.68
2:F:818:ASN:ND2	2:F:818:ASN:O	2.26	0.68
2:F:1312:LEU:HD21	2:F:1326:TYR:HD1	1.59	0.68
2:B:22:THR:HG22	2:B:23:ASP:H	1.59	0.68
2:B:242:ILE:HG22	2:B:246:LEU:HD21	1.75	0.68
2:F:649:LYS:O	2:F:653:ARG:NE	2.27	0.68
2:B:516:GLU:O	2:B:519:THR:HG22	1.94	0.67
5:J:44:U:O2'	5:J:45:U:H5'	1.94	0.67
2:B:94:ASP:OD2	2:B:100:ARG:NH2	2.27	0.67
2:B:1258:PHE:HE1	2:B:1262:HIS:CD2	2.13	0.67
3:C:22:DT:H2''	3:C:23:DC:O5'	1.94	0.67
2:F:137:HIS:HA	2:F:322:ILE:HD11	1.76	0.67
2:B:526:LYS:HE2	2:B:692:ASN:HB2	1.76	0.67
2:F:967:ARG:NH1	2:F:974:LYS:HE3	2.10	0.67
2:B:982:HIS:HA	2:B:985:HIS:HB2	1.77	0.67
1:E:18:A:N7	2:F:71:ARG:NH2	2.43	0.67
2:F:737:ILE:O	2:F:740:THR:HG22	1.95	0.67
5:J:73:G:H5'	5:J:74:A:OP2	1.95	0.67
2:F:1215:ALA:HB2	2:F:1221:GLN:HG3	1.77	0.67
2:B:1179:ILE:HD11	2:B:1192:LYS:HD2	1.77	0.67
2:F:999:LYS:HB3	2:F:1073:VAL:HG12	1.77	0.66
2:F:413:GLN:O	2:F:417:GLY:N	2.22	0.66
2:F:821:ASP:HB2	2:F:828:LEU:HD21	1.77	0.66
2:B:1037:PHE:HD1	2:B:1039:TYR:H	1.43	0.66
2:F:1097:LYS:HD3	2:F:1099:GLU:OE2	1.95	0.66
1:A:1:U:H5	2:B:661:ARG:HH12	1.43	0.66
2:B:746:GLU:OE2	2:B:1353:THR:OG1	2.09	0.66
2:F:1207:GLU:CD	2:F:1210:ARG:NH1	2.54	0.66
2:F:46:ASN:ND2	2:F:1089:MET:SD	2.69	0.66
2:F:302:LEU:HD22	2:F:306:LEU:HD22	1.78	0.66
2:F:846:PHE:O	2:F:1040:SER:OG	2.08	0.66
2:B:662:LEU:HD23	2:B:666:LEU:HD22	1.78	0.66
2:B:1109:SER:OG	3:C:9:DT:OP2	2.09	0.66
2:B:679:ILE:O	2:B:683:LEU:HD13	1.96	0.66
2:B:1236:LEU:HD11	2:B:1269:ILE:HD13	1.77	0.66
1:E:25:U:H5'	2:F:107:VAL:HG12	1.77	0.65
2:F:545:LYS:HD2	2:F:690:ASN:HD21	1.61	0.65
2:B:1333:ARG:CZ	2:B:1335:ARG:HD2	2.26	0.65
2:F:998:ILE:HG22	2:F:1008:PHE:HE1	1.59	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:936:ASP:OD1	2:F:940:ASN:ND2	2.29	0.65
2:B:594:TYR:OH	2:B:608:ASP:OD1	2.15	0.65
2:B:70:ARG:NH2	5:I:61:C:OP1	2.29	0.65
2:B:243:ALA:C	2:B:246:LEU:CD2	2.69	0.65
2:F:545:LYS:NZ	2:F:683:LEU:O	2.29	0.65
2:B:70:ARG:HH21	5:I:61:C:P	2.19	0.65
2:B:226:ILE:HA	2:B:229:LEU:HG	1.78	0.65
2:B:787:GLY:HA3	2:B:891:LEU:HD21	1.78	0.65
2:B:824:VAL:HG11	2:B:859:ARG:HH12	1.61	0.65
2:B:69:ARG:HD3	5:I:62:G:N7	2.12	0.64
2:B:1226:LEU:HB2	2:B:1276:PHE:CE2	2.32	0.64
5:J:94:U:H2'	5:J:95:G:C8	2.32	0.64
2:F:139:ARG:NH2	2:F:418:GLU:OE1	2.25	0.64
2:F:1206:LEU:HD11	2:F:1210:ARG:NH2	2.12	0.64
2:B:823:TYR:HD2	2:B:858:THR:HG21	1.62	0.64
2:B:1356:TYR:HB3	5:I:81:G:C6	2.33	0.64
2:F:332:LEU:HD11	2:F:336:LYS:HE3	1.79	0.64
2:B:317:LEU:HB2	2:B:414:ILE:HD12	1.80	0.64
2:F:44:LYS:HD3	5:J:92:G:N7	2.13	0.64
2:F:918:LYS:HZ2	2:F:1018:VAL:HG11	1.62	0.64
2:B:967:ARG:HE	2:B:974:LYS:HB2	1.63	0.64
2:F:63:ARG:HG3	2:F:66:ARG:NH1	2.11	0.64
2:F:760:VAL:HG22	2:F:956:ILE:HD12	1.80	0.64
2:F:328:HIS:NE2	2:F:359:TYR:OH	2.30	0.64
2:F:666:LEU:HD21	2:F:693:PHE:CZ	2.33	0.64
1:A:22:U:O2'	2:B:1110:ILE:HB	1.97	0.63
2:F:505:GLU:HG3	2:F:665:LYS:HB2	1.80	0.63
2:F:530:VAL:HG22	2:F:537:PRO:HB3	1.80	0.63
2:F:1203:LEU:HD23	2:F:1348:ILE:HB	1.80	0.63
2:B:640:ALA:HA	2:B:648:MET:HE3	1.81	0.63
2:B:1271:GLU:O	2:B:1274:SER:OG	2.16	0.63
2:F:189:VAL:HG13	2:F:201:ILE:HG22	1.79	0.63
2:F:226:ILE:CG1	2:F:232:GLU:HG2	2.25	0.63
2:B:116:HIS:CE1	2:B:122:ILE:HG12	2.33	0.63
2:B:818:ASN:O	2:B:818:ASN:ND2	2.32	0.63
2:F:309:ASN:OD1	2:F:312:ILE:HG23	1.99	0.63
2:F:234:LYS:H	2:F:234:LYS:HD3	1.62	0.63
2:F:972:PHE:CE1	2:F:1084:ARG:HG2	2.34	0.63
1:E:14:G:OP2	2:F:63:ARG:HD3	1.99	0.63
2:F:601:ILE:HD11	2:F:607:LEU:HD11	1.81	0.63
2:B:183:LYS:NZ	2:B:311:GLU:OE2	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1216:SER:OG	4:H:7:DG:OP1	2.16	0.63
2:F:138:LEU:HD21	2:F:153:LEU:HD21	1.81	0.62
2:F:272:ASP:HA	2:F:275:LEU:HB3	1.80	0.62
2:B:781:MET:HG3	2:B:803:ASN:ND2	2.14	0.62
2:F:158:LEU:HA	2:F:161:MET:SD	2.40	0.62
2:B:1224:ASN:CB	2:B:1280:VAL:HG11	2.22	0.62
2:F:70:ARG:HH21	5:J:61:C:P	2.22	0.62
2:F:745:ASP:OD2	2:F:938:ARG:NH2	2.33	0.62
2:F:1241:HIS:CE1	2:F:1244:LYS:HA	2.35	0.62
2:B:5:TYR:CE2	2:B:756:PRO:HB3	2.35	0.62
2:B:930:HIS:O	2:B:934:ILE:HG13	1.98	0.62
2:F:867:SER:HB2	2:F:1053:ALA:C	2.25	0.62
2:B:745:ASP:OD2	2:B:938:ARG:NH2	2.33	0.61
2:B:1147:ALA:HB1	2:B:1188:LYS:O	2.00	0.61
2:F:626:PHE:CE1	2:F:635:ARG:NH1	2.68	0.61
2:B:281:GLN:OE1	2:B:281:GLN:N	2.27	0.61
2:B:353:ASP:CG	2:B:356:LYS:HG2	2.25	0.61
2:B:1000:LYS:HB3	2:B:1001:TYR:CE2	2.36	0.61
2:F:35:LEU:HB2	2:F:1358:THR:HG22	1.80	0.61
2:F:918:LYS:HE3	2:F:1018:VAL:HG11	1.81	0.61
2:F:1207:GLU:CD	2:F:1210:ARG:HH11	2.08	0.61
2:F:635:ARG:HG3	2:F:635:ARG:HH11	1.64	0.61
2:F:671:ARG:H	2:F:671:ARG:HD3	1.65	0.61
2:F:918:LYS:NZ	2:F:1018:VAL:HG11	2.14	0.61
2:F:163:LYS:HG2	2:F:164:PHE:CE1	2.36	0.61
2:F:380:LEU:HD11	2:F:390:LEU:CG	2.29	0.61
5:I:88:A:N6	5:I:91:C:H42	1.99	0.61
2:F:258:LEU:HD22	2:F:260:GLU:H	1.65	0.61
2:F:671:ARG:HD3	2:F:671:ARG:N	2.16	0.61
2:B:472:THR:HG23	5:I:59:U:OP2	2.01	0.61
2:B:926:GLN:HG2	3:C:20:DA:P	2.40	0.61
2:F:867:SER:HB2	2:F:1054:ASN:N	2.16	0.61
2:B:340:ARG:HH21	5:I:41:A:P	2.24	0.61
2:B:1308:ASN:HD22	2:B:1327:PHE:N	1.96	0.61
2:F:139:ARG:HG3	2:F:139:ARG:HH11	1.65	0.60
2:F:1167:THR:HG23	2:F:1170:GLU:H	1.66	0.60
2:F:1326:TYR:HE2	2:F:1327:PHE:HD2	1.47	0.60
2:B:448:ILE:HD13	2:B:455:LEU:HD13	1.83	0.60
2:F:824:VAL:HG12	2:F:825:ASP:H	1.65	0.60
2:F:841:ILE:HD11	2:F:896:LYS:HG3	1.82	0.60
2:B:554:LYS:HG2	2:B:594:TYR:CE2	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:342:GLN:HG3	2:F:383:MET:HE2	1.83	0.60
2:F:918:LYS:NZ	2:F:1018:VAL:HG12	2.15	0.60
2:B:893:THR:HG23	2:B:896:LYS:H	1.65	0.60
2:B:1002:PRO:HD2	2:B:1036:TYR:OH	2.01	0.60
2:B:539:PHE:HD2	2:B:689:ALA:HA	1.67	0.60
2:F:985:HIS:CD2	2:F:1087:LEU:HD22	2.37	0.60
2:B:1211:LYS:C	2:B:1223:GLY:HA3	2.27	0.60
2:F:514:LEU:HD21	2:F:664:ARG:HH21	1.66	0.60
2:F:1206:LEU:HD11	2:F:1210:ARG:HH22	1.66	0.60
2:B:694:MET:HG3	2:B:698:HIS:CD2	2.37	0.60
2:B:813:LEU:HD11	2:B:855:LYS:HB3	1.84	0.60
2:B:1286:ASN:ND2	2:B:1332:ASP:O	2.34	0.60
2:F:690:ASN:OD1	2:F:690:ASN:N	2.35	0.60
5:I:52:A:OP2	5:I:62:G:N2	2.34	0.60
2:B:879:MET:HG3	2:B:882:TYR:HB3	1.81	0.60
2:F:489:GLN:HG3	2:F:625:LEU:HD21	1.83	0.60
2:F:853:ASP:OD1	2:F:893:THR:HG21	2.01	0.60
2:F:632:ILE:O	2:F:636:LEU:HD13	2.01	0.59
5:J:88:A:C2	5:J:91:C:N3	2.70	0.59
2:B:620:VAL:HG13	2:B:656:TYR:HD2	1.67	0.59
2:B:881:ASN:OD1	2:B:885:GLN:NE2	2.27	0.59
2:B:1236:LEU:HA	2:B:1239:ALA:HB3	1.83	0.59
2:F:165:ARG:HD2	2:F:168:PHE:CE1	2.36	0.59
2:F:180:ASP:HB3	2:F:183:LYS:HD2	1.85	0.59
2:F:958:LEU:HD22	2:F:962:LEU:HD12	1.84	0.59
2:F:1061:PRO:O	2:F:1076:LYS:HE2	2.02	0.59
2:B:386:THR:O	2:B:386:THR:HG22	2.01	0.59
2:B:427:GLU:HB2	2:B:434:LYS:HB2	1.83	0.59
2:F:1347:LEU:N	2:F:1360:ILE:O	2.34	0.59
2:B:794:GLN:HG2	2:B:798:GLU:HG3	1.84	0.59
2:B:1037:PHE:CE1	2:B:1039:TYR:CG	2.90	0.59
2:B:1207:GLU:HG3	2:B:1208:ASN:H	1.67	0.59
2:B:21:ILE:HD11	2:B:995:THR:HG21	1.83	0.59
2:B:1108:GLU:N	3:C:9:DT:OP1	2.31	0.59
2:F:40:ARG:NE	2:F:43:ILE:HD11	2.18	0.59
2:B:212:LEU:O	2:B:221:ARG:HD2	2.02	0.59
2:B:1356:TYR:HB3	5:I:81:G:N1	2.17	0.59
2:F:755:LYS:HD3	2:F:939:MET:HE3	1.84	0.59
2:F:923:GLU:HG2	2:F:928:THR:HG21	1.85	0.59
2:F:939:MET:HE2	2:F:953:VAL:HG21	1.83	0.59
2:F:1110:ILE:HD13	2:F:1122:ARG:CZ	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1120:ILE:HD11	2:F:1137:PRO:HD3	1.84	0.59
2:F:1236:LEU:O	2:F:1240:SER:OG	2.14	0.59
5:J:40:C:H2'	5:J:41:A:C8	2.38	0.59
2:B:380:LEU:O	2:B:386:THR:HG21	2.02	0.59
2:F:149:ALA:H	2:F:426:GLN:HE22	1.51	0.58
2:F:794:GLN:H	2:F:794:GLN:CD	2.10	0.58
2:F:1224:ASN:HB2	2:F:1280:VAL:HG11	1.85	0.58
2:F:1290:VAL:HG22	2:F:1331:ILE:HD13	1.85	0.58
2:B:107:VAL:HG22	2:B:1131:TYR:OH	2.02	0.58
2:B:979:ASN:OD1	2:B:980:ASN:N	2.35	0.58
2:B:317:LEU:HD22	2:B:414:ILE:HD11	1.84	0.58
2:B:1120:ILE:HB	2:B:1134:PHE:HB2	1.84	0.58
2:F:189:VAL:HG13	2:F:201:ILE:CG2	2.32	0.58
2:F:918:LYS:HZ2	2:F:1018:VAL:CG1	2.15	0.58
2:B:853:ASP:CG	2:B:893:THR:HG21	2.28	0.58
2:B:1011:GLY:O	2:B:1014:LYS:N	2.36	0.58
2:F:11:ILE:HB	2:F:763:MET:HE3	1.85	0.58
2:F:14:ASN:OD1	2:F:55:SER:OG	2.19	0.58
1:A:2:U:N3	1:A:4:A:H3'	2.13	0.58
2:B:48:ILE:O	2:B:1093:ASN:ND2	2.33	0.58
2:F:207:ASP:O	2:F:211:ILE:HG12	2.03	0.58
2:F:954:LYS:HZ3	2:F:998:ILE:HD13	1.67	0.58
2:F:1219:GLU:OE1	2:F:1335:ARG:NH2	2.28	0.58
2:B:5:TYR:OH	2:B:754:HIS:O	2.21	0.58
2:F:967:ARG:NH1	2:F:986:ASP:OD1	2.36	0.58
5:J:40:C:H2'	5:J:41:A:H8	1.68	0.58
2:B:1123:LYS:NZ	5:I:52:A:OP1	2.37	0.58
2:B:1206:LEU:HB3	2:B:1345:ALA:HB2	1.84	0.58
2:F:821:ASP:HA	2:F:828:LEU:HD11	1.86	0.58
2:B:621:LEU:O	2:B:625:LEU:HB2	2.03	0.58
2:F:25:TYR:O	2:F:988:TYR:OH	2.21	0.58
2:F:860:SER:OG	2:F:863:ASN:OD1	2.20	0.58
2:B:181:VAL:O	2:B:185:PHE:N	2.31	0.58
2:B:305:ILE:HG13	2:B:306:LEU:N	2.19	0.57
2:B:343:LEU:HD21	2:B:346:LYS:HG3	1.85	0.57
2:B:620:VAL:HG13	2:B:656:TYR:CD2	2.39	0.57
2:F:954:LYS:NZ	2:F:998:ILE:HD13	2.19	0.57
2:B:118:ILE:O	2:B:152:ARG:HD2	2.04	0.57
2:B:1251:ASP:HB3	2:B:1255:LYS:HE2	1.85	0.57
2:B:1256:GLN:O	2:B:1256:GLN:NE2	2.38	0.57
2:F:178:ASN:HB3	2:F:184:LEU:HD11	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:220:ARG:O	2:F:224:ASN:N	2.32	0.57
2:B:233:LYS:HG2	2:B:235:ASN:H	1.69	0.57
2:F:48:ILE:HG12	2:F:984:ALA:HB1	1.86	0.57
2:F:258:LEU:HD12	2:F:281:GLN:HE22	1.68	0.57
2:F:794:GLN:HE21	2:F:798:GLU:CD	2.13	0.57
1:A:27:G:H5'	1:A:28:A:C5'	2.33	0.57
2:B:1235:PHE:O	2:B:1239:ALA:N	2.32	0.57
2:F:63:ARG:HG3	2:F:66:ARG:HH12	1.69	0.57
2:F:697:ILE:HD11	2:F:708:ILE:HG13	1.86	0.57
1:A:12:A:H61	3:C:17:DT:H3	1.51	0.57
2:F:843:PRO:HG3	2:F:864:ARG:HH22	1.68	0.57
5:J:91:C:O2'	5:J:92:G:P	2.63	0.57
2:B:143:VAL:HG13	2:B:421:ALA:CB	2.33	0.57
2:B:699:ASP:HB3	2:B:702:LEU:HD12	1.87	0.57
2:B:823:TYR:HA	2:B:875:VAL:CG1	2.31	0.57
2:B:184:LEU:HD12	2:B:299:ALA:HB2	1.86	0.57
2:B:525:THR:CG2	2:B:690:ASN:CB	2.75	0.57
2:B:1140:ALA:HB2	2:B:1168:ILE:HG12	1.85	0.57
2:F:1096:LYS:HG2	2:F:1201:TYR:CD2	2.40	0.57
2:B:373:TYR:OH	2:B:398:LEU:N	2.31	0.57
2:F:979:ASN:OD1	2:F:981:TYR:N	2.31	0.57
2:B:686:ASP:HB3	2:B:690:ASN:HA	1.86	0.57
2:B:939:MET:HE2	2:B:953:VAL:HG21	1.86	0.57
2:B:1074:TRP:HZ2	2:B:1080:PHE:CE2	2.23	0.57
2:F:165:ARG:O	2:F:415:HIS:HD2	1.87	0.57
2:B:977:GLU:N	2:B:977:GLU:OE1	2.38	0.56
2:F:312:ILE:HG13	2:F:313:THR:N	2.19	0.56
2:F:646:LYS:HG3	2:F:650:GLN:NE2	2.20	0.56
2:F:918:LYS:CE	2:F:1018:VAL:HG11	2.35	0.56
2:B:1315:LEU:HB2	2:B:1324:PHE:CE1	2.40	0.56
2:F:1060:ARG:HH11	2:F:1060:ARG:CG	2.16	0.56
2:B:978:ILE:HD12	2:B:1233:VAL:HG22	1.85	0.56
2:B:1200:LYS:HG2	2:B:1201:TYR:CD1	2.40	0.56
2:F:737:ILE:HA	2:F:740:THR:HG22	1.87	0.56
2:F:750:VAL:HG21	2:F:1355:LEU:HD12	1.87	0.56
2:B:634:GLU:OE2	2:B:637:LYS:NZ	2.38	0.56
2:F:199:ASN:O	2:F:201:ILE:CD1	2.53	0.56
2:F:1108:GLU:N	3:G:9:DT:OP1	2.30	0.56
3:G:3:DA:N6	4:H:9:DA:H61	2.04	0.56
2:B:985:HIS:ND1	2:B:1087:LEU:HD13	2.20	0.56
2:B:1314:THR:HG21	2:B:1324:PHE:HB3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:643:PHE:HD1	2:F:647:VAL:HG11	1.71	0.56
2:F:886:LEU:HD22	2:F:891:LEU:HD11	1.88	0.56
2:F:446:PHE:HE2	2:F:448:ILE:HD13	1.70	0.56
2:B:672:ASP:HA	2:B:703:THR:HG22	1.88	0.56
2:B:864:ARG:HB2	2:B:871:PRO:HA	1.88	0.56
2:B:1116:SER:OG	2:B:1117:ASP:N	2.38	0.56
2:B:1228:LEU:HD12	2:B:1229:PRO:HD2	1.88	0.56
2:F:841:ILE:CD1	2:F:896:LYS:HG3	2.36	0.56
2:F:1095:VAL:HG13	2:F:1350:GLN:OE1	2.06	0.56
2:F:1326:TYR:HE2	2:F:1327:PHE:CD2	2.23	0.56
2:F:621:LEU:O	2:F:625:LEU:HB2	2.05	0.56
2:F:644:ASP:HB3	2:F:647:VAL:HG23	1.88	0.56
2:B:358:GLY:O	2:B:362:TYR:N	2.34	0.56
2:B:1177:ASN:ND2	2:B:1180:ASP:OD2	2.38	0.56
2:B:45:LYS:NZ	2:B:1354:GLY:O	2.36	0.55
2:B:315:ALA:HB1	2:B:418:GLU:OE2	2.06	0.55
2:F:535:ARG:HD2	2:F:535:ARG:H	1.71	0.55
2:F:633:GLU:O	2:F:637:LYS:N	2.38	0.55
2:F:1205:GLU:CD	2:F:1359:ARG:HH22	2.14	0.55
2:B:427:GLU:OE1	2:B:437:ARG:NH1	2.38	0.55
1:E:19:A:H4'	2:F:407:ASN:C	2.31	0.55
2:F:1349:HIS:CE1	5:J:69:A:H5'	2.40	0.55
2:F:139:ARG:HG3	2:F:139:ARG:NH1	2.21	0.55
2:F:839:ASP:OD2	2:F:864:ARG:HD2	2.06	0.55
2:B:565:LYS:HE2	2:B:580:ILE:HG12	1.88	0.55
2:F:321:MET:HE1	2:F:324:ARG:CZ	2.35	0.55
2:F:448:ILE:HD12	2:F:455:LEU:HD11	1.88	0.55
2:F:468:LYS:HE3	2:F:483:ASP:HB3	1.88	0.55
2:B:30:LYS:HD3	5:I:83:C:P	2.46	0.55
2:B:302:LEU:HA	2:B:305:ILE:HG12	1.88	0.55
2:F:939:MET:HG3	2:F:953:VAL:HG11	1.89	0.55
2:F:1264:HIS:O	2:F:1268:GLU:HG3	2.07	0.55
5:J:88:A:C6	5:J:91:C:N4	2.72	0.55
2:F:853:ASP:CG	2:F:893:THR:HG21	2.31	0.55
2:F:1270:ILE:HG13	2:F:1294:TYR:CD2	2.42	0.55
2:B:672:ASP:HA	2:B:703:THR:CG2	2.37	0.55
2:B:489:GLN:HG3	2:B:625:LEU:HD21	1.87	0.55
2:F:369:GLN:HG2	2:F:373:TYR:HE2	1.71	0.55
2:F:977:GLU:HG3	2:F:1310:ILE:CG2	2.37	0.55
2:F:675:SER:HB2	2:F:682:PHE:HZ	1.71	0.55
3:G:6:DC:H2''	3:G:7:DC:O5'	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:887:LEU:HD21	2:F:894:GLN:HG2	1.88	0.55
2:B:833:LEU:HD22	2:B:857:LEU:HD21	1.89	0.54
2:F:20:VAL:HG11	2:F:751:MET:HE3	1.89	0.54
2:F:199:ASN:O	2:F:201:ILE:HD11	2.06	0.54
2:F:972:PHE:HE1	2:F:1084:ARG:HG2	1.71	0.54
5:J:83:C:H2'	5:J:84:A:H8	1.72	0.54
2:F:918:LYS:HZ1	2:F:1018:VAL:HG12	1.72	0.54
2:B:139:ARG:NH2	2:B:161:MET:HG2	2.22	0.54
2:B:1060:ARG:NH1	2:B:1064:GLU:OE2	2.40	0.54
2:B:1222:LYS:NZ	2:B:1315:LEU:O	2.34	0.54
2:F:943:TYR:CE2	2:F:949:LEU:HD13	2.42	0.54
2:F:1135:ASP:OD1	2:F:1136:SER:N	2.40	0.54
2:F:1347:LEU:HB3	2:F:1360:ILE:HB	1.88	0.54
2:B:978:ILE:CD1	2:B:1233:VAL:HG22	2.37	0.54
2:F:618:ASP:HB3	2:F:639:TYR:OH	2.08	0.54
2:B:218:LYS:H	2:B:218:LYS:HD2	1.73	0.54
2:B:345:GLU:N	2:B:345:GLU:OE1	2.39	0.54
2:F:350:ILE:O	2:F:359:TYR:N	2.40	0.54
2:B:531:THR:HG21	2:B:575:PHE:CE2	2.43	0.54
2:B:814:TYR:CE2	2:B:819:GLY:HA2	2.43	0.54
2:B:116:HIS:HE1	2:B:122:ILE:HG12	1.70	0.54
1:E:6:G:H1	3:G:23:DC:H42	1.55	0.54
2:F:672:ASP:HB3	2:F:675:SER:HB2	1.88	0.54
2:F:1147:ALA:HB2	2:F:1190:VAL:HA	1.89	0.54
2:B:1062:LEU:HD23	2:B:1062:LEU:H	1.72	0.54
2:F:140:LYS:HE3	2:F:313:THR:OG1	2.07	0.54
2:B:118:ILE:HG12	2:B:156:LEU:HD11	1.90	0.54
2:B:1105:PHE:CG	2:B:1169:MET:HG3	2.43	0.54
2:F:90:MET:SD	2:F:151:LEU:HD23	2.47	0.54
2:F:324:ARG:O	2:F:327:GLU:HB2	2.08	0.54
2:F:868:ASP:O	2:F:869:ASN:HB2	2.08	0.54
2:F:1207:GLU:HG3	2:F:1208:ASN:H	1.72	0.54
2:F:1347:LEU:HD23	2:F:1348:ILE:N	2.23	0.54
1:A:8:A:H2'	1:A:9:U:C6	2.43	0.53
2:F:226:ILE:HD11	2:F:232:GLU:CD	2.32	0.53
2:F:1019:ARG:O	2:F:1021:MET:N	2.35	0.53
2:B:233:LYS:HB3	2:B:236:GLY:H	1.74	0.53
2:B:240:ASN:HB3	2:B:252:PHE:CE2	2.44	0.53
2:F:1106:SER:HA	2:F:1137:PRO:HA	1.91	0.53
2:F:1169:MET:HE3	5:J:52:A:N3	2.23	0.53
2:B:38:THR:HG22	2:B:40:ARG:H	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:165:ARG:NH2	2:B:446:PHE:O	2.40	0.53
2:B:305:ILE:HD11	2:B:414:ILE:HG21	1.91	0.53
2:B:597:LEU:O	2:B:601:ILE:HG12	2.07	0.53
2:F:971:GLN:HG2	2:F:973:TYR:CE2	2.43	0.53
2:B:1206:LEU:HD11	2:B:1210:ARG:NH2	2.24	0.53
2:F:351:PHE:HD1	5:J:43:G:O6	1.91	0.53
2:F:923:GLU:OE2	2:F:925:ARG:NH1	2.41	0.53
2:F:1205:GLU:OE1	2:F:1359:ARG:NH2	2.36	0.53
2:B:526:LYS:NZ	2:B:690:ASN:O	2.28	0.53
2:B:951:ARG:NH2	2:B:1011:GLY:HA2	2.23	0.53
2:F:1123:LYS:HD2	5:J:53:G:P	2.49	0.53
2:B:279:LEU:HD11	2:B:284:ASP:HA	1.91	0.53
2:F:174:LEU:CD1	2:F:302:LEU:HD21	2.39	0.53
2:B:165:ARG:O	2:B:415:HIS:HD2	1.91	0.53
2:F:167:HIS:CD2	2:F:169:LEU:HB2	2.43	0.53
2:F:323:LYS:HE3	2:F:327:GLU:OE2	2.08	0.53
5:J:94:U:H2'	5:J:95:G:H8	1.73	0.53
2:B:263:LYS:C	2:B:264:LEU:HD12	2.34	0.53
2:B:455:LEU:HD23	2:B:473:ILE:HD12	1.91	0.53
2:B:755:LYS:NZ	2:B:939:MET:O	2.29	0.53
2:B:1236:LEU:O	2:B:1240:SER:OG	2.23	0.53
2:B:1266:LEU:O	2:B:1270:ILE:HG12	2.09	0.53
2:F:154:ILE:HG23	2:F:158:LEU:HG	1.89	0.53
2:F:554:LYS:HB3	2:F:594:TYR:CE2	2.44	0.53
2:F:1286:ASN:O	2:F:1290:VAL:HG23	2.08	0.53
2:B:143:VAL:HG13	2:B:421:ALA:HB1	1.90	0.53
2:B:273:ASP:N	2:B:273:ASP:OD1	2.37	0.53
2:F:167:HIS:HD2	2:F:169:LEU:H	1.57	0.53
2:F:563:GLN:O	2:F:567:ASP:HB2	2.08	0.53
2:F:1326:TYR:CE2	2:F:1327:PHE:HD2	2.26	0.53
2:F:911:LEU:HD12	2:F:911:LEU:H	1.74	0.53
2:B:203:ALA:O	2:B:206:VAL:HG22	2.08	0.52
2:B:530:VAL:CG2	2:B:537:PRO:HB3	2.36	0.52
2:B:531:THR:HG21	2:B:575:PHE:HE2	1.73	0.52
2:B:784:ILE:HD13	2:B:815:TYR:HB3	1.91	0.52
2:B:1114:ARG:NH1	4:D:9:DA:OP1	2.42	0.52
2:F:1221:GLN:NE2	2:F:1320:ALA:HB2	2.24	0.52
5:I:83:C:H2'	5:I:84:A:H8	1.74	0.52
2:B:251:ASN:HD21	2:B:253:LYS:HB3	1.74	0.52
2:B:1169:MET:HE3	5:I:52:A:N3	2.24	0.52
2:B:94:ASP:HB3	2:B:97:PHE:HB2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:925:ARG:HB3	2:B:928:THR:HG23	1.91	0.52
2:F:226:ILE:HD11	2:F:232:GLU:OE1	2.09	0.52
2:F:253:LYS:HG3	2:F:261:ASP:HA	1.91	0.52
2:F:1002:PRO:HD2	2:F:1036:TYR:OH	2.09	0.52
2:F:699:ASP:OD1	2:F:701:SER:OG	2.27	0.52
2:F:1326:TYR:CE2	2:F:1327:PHE:CD2	2.97	0.52
2:F:1167:THR:CG2	2:F:1170:GLU:HG3	2.40	0.52
5:J:96:C:C4	5:J:97:U:C4	2.97	0.52
1:A:25:U:H2'	1:A:26:A:H8	1.74	0.52
2:B:736:GLY:O	2:B:740:THR:N	2.32	0.52
2:F:90:MET:HA	2:F:151:LEU:CD2	2.39	0.52
2:F:795:ILE:HA	2:F:798:GLU:HB2	1.91	0.52
2:B:217:SER:HB2	2:B:220:ARG:HG2	1.92	0.52
2:B:727:LEU:HD12	2:B:927:ILE:CD1	2.37	0.52
2:F:1054:ASN:C	2:F:1056:GLU:H	2.17	0.52
2:B:737:ILE:O	2:B:740:THR:HG22	2.09	0.52
1:E:11:U:C2	1:E:12:A:C8	2.97	0.52
1:E:18:A:OP2	2:F:71:ARG:HD2	2.09	0.52
2:F:820:ARG:HG3	2:F:826:GLN:O	2.09	0.52
2:B:186:ILE:O	2:B:190:GLN:N	2.37	0.52
2:B:946:ASN:HB3	2:B:948:LYS:HD2	1.92	0.52
2:B:1241:HIS:ND1	2:B:1244:LYS:HA	2.25	0.52
2:F:923:GLU:CG	2:F:928:THR:HG21	2.39	0.52
2:B:180:ASP:HB3	2:B:183:LYS:HB2	1.92	0.52
2:B:369:GLN:HE22	2:B:400:ARG:HD2	1.74	0.52
2:F:1212:ARG:CZ	2:F:1336:TYR:HE2	2.23	0.52
3:G:3:DA:H61	4:H:9:DA:N6	2.07	0.52
2:B:137:HIS:HE1	2:B:325:TYR:CD2	2.28	0.51
2:B:416:LEU:HB2	2:B:444:LEU:HD22	1.92	0.51
2:F:38:THR:HG22	2:F:40:ARG:H	1.75	0.51
2:F:869:ASN:HD21	2:F:907:GLY:HA3	1.75	0.51
2:B:473:ILE:HG12	2:B:481:VAL:HG11	1.92	0.51
2:F:122:ILE:O	2:F:126:VAL:HG23	2.11	0.51
2:F:918:LYS:HE3	2:F:1018:VAL:CG1	2.39	0.51
2:F:1313:PHE:O	2:F:1316:THR:N	2.43	0.51
5:J:85:C:H2'	5:J:86:C:C6	2.45	0.51
5:J:91:C:HO2'	5:J:92:G:P	2.33	0.51
1:E:27:G:H5'	1:E:28:A:C5'	2.41	0.51
2:B:256:PHE:O	2:B:257:ASP:OD1	2.29	0.51
2:F:619:ILE:HD11	2:F:651:LEU:HD11	1.92	0.51
2:F:1205:GLU:HB2	2:F:1348:ILE:HD11	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:3:DA:H61	4:H:9:DA:H61	1.58	0.51
2:B:643:PHE:HB2	2:B:648:MET:HE2	1.91	0.51
2:B:1037:PHE:HE2	2:B:1060:ARG:HH21	1.53	0.51
3:C:19:DA:H2'	3:C:20:DA:C8	2.45	0.51
2:F:138:LEU:CD2	2:F:153:LEU:HD11	2.41	0.51
2:F:226:ILE:CG2	2:F:230:PRO:HA	2.41	0.51
2:B:943:TYR:CZ	2:B:949:LEU:HD13	2.46	0.51
2:F:275:LEU:O	2:F:279:LEU:N	2.42	0.51
5:J:79:G:O2'	5:J:80:U:H5'	2.10	0.51
2:F:1207:GLU:HG3	2:F:1208:ASN:N	2.26	0.51
2:F:74:ARG:O	2:F:78:ARG:HG3	2.11	0.51
2:F:137:HIS:HA	2:F:322:ILE:CD1	2.39	0.51
2:F:998:ILE:HG22	2:F:1008:PHE:CE1	2.45	0.51
2:F:666:LEU:HD21	2:F:693:PHE:CE1	2.46	0.51
2:F:694:MET:HE3	2:F:698:HIS:NE2	2.26	0.51
2:F:1312:LEU:HD21	2:F:1326:TYR:CD1	2.44	0.51
1:A:16:A:H4'	2:B:448:ILE:O	2.11	0.51
2:B:135:ILE:HG21	2:B:160:HIS:NE2	2.25	0.51
2:B:325:TYR:HD1	5:I:44:U:C2	2.28	0.51
2:B:724:ILE:O	2:B:727:LEU:HB2	2.11	0.51
2:F:511:HIS:O	2:F:593:THR:OG1	2.26	0.51
2:F:671:ARG:H	2:F:671:ARG:CD	2.21	0.51
2:F:135:ILE:HG21	5:J:46:A:H5'	1.92	0.50
2:F:338:LEU:HD13	2:F:386:THR:HG22	1.93	0.50
2:F:620:VAL:O	2:F:624:THR:N	2.37	0.50
2:F:1347:LEU:HD22	2:F:1349:HIS:CD2	2.46	0.50
2:B:1041:ASN:HB2	2:B:1044:ASN:ND2	2.23	0.50
2:B:1208:ASN:OD1	2:B:1279:ARG:HG3	2.10	0.50
2:F:334:LEU:O	2:F:338:LEU:HG	2.11	0.50
2:F:508:LEU:HD11	2:F:664:ARG:HB2	1.94	0.50
2:F:1357:GLU:O	5:J:81:G:N2	2.38	0.50
2:F:1060:ARG:NH1	2:F:1060:ARG:CG	2.73	0.50
2:F:1135:ASP:OD1	4:H:8:DT:H5''	2.11	0.50
2:B:473:ILE:HD13	2:B:482:VAL:HG23	1.92	0.50
2:F:442:LYS:HB3	2:F:476:TRP:CD1	2.46	0.50
2:F:1241:HIS:ND1	2:F:1244:LYS:HA	2.26	0.50
5:J:91:C:O2'	5:J:92:G:O5'	2.29	0.50
2:B:249:THR:HG22	2:B:265:GLN:CB	2.39	0.50
2:F:108:GLU:HG3	2:F:115:ARG:HD3	1.94	0.50
2:F:138:LEU:HD22	2:F:153:LEU:HD11	1.94	0.50
2:F:165:ARG:C	2:F:415:HIS:HD2	2.19	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:7:DC:O2	4:H:7:DG:N2	2.45	0.50
5:I:42:A:H8	5:I:42:A:H5''	1.77	0.50
5:I:83:C:H2'	5:I:84:A:C8	2.47	0.50
5:J:96:C:H2'	5:J:97:U:O4'	2.12	0.50
1:A:31:U:N3	1:A:32:A:N7	2.59	0.50
2:B:331:ASP:OD2	2:B:392:LYS:NZ	2.41	0.50
1:E:27:G:H5'	1:E:28:A:O5'	2.10	0.50
2:F:979:ASN:OD1	2:F:980:ASN:N	2.44	0.50
2:F:853:ASP:HB3	2:F:895:ARG:HD3	1.93	0.50
2:F:867:SER:C	2:F:869:ASN:H	2.20	0.50
2:B:661:ARG:HB2	2:B:662:LEU:HD12	1.93	0.50
2:B:939:MET:HG3	2:B:953:VAL:HG11	1.94	0.50
2:F:226:ILE:HG23	2:F:230:PRO:HA	1.93	0.50
2:F:465:MET:SD	2:F:482:VAL:HG21	2.51	0.50
2:F:884:ARG:HG3	2:F:884:ARG:HH11	1.76	0.50
2:F:1198:LEU:HD21	2:F:1347:LEU:HD11	1.92	0.50
2:B:1240:SER:HB2	2:B:1242:TYR:CD1	2.47	0.50
2:F:167:HIS:HD2	2:F:169:LEU:HB2	1.77	0.50
2:F:923:GLU:HA	2:F:923:GLU:OE1	2.12	0.50
2:F:961:LYS:HA	2:F:964:SER:HB3	1.94	0.50
2:B:761:ILE:HG13	2:B:761:ILE:O	2.11	0.49
2:B:874:GLU:HA	2:B:877:LYS:HE3	1.94	0.49
2:F:566:GLU:O	2:F:570:LYS:HB3	2.11	0.49
2:B:198:GLU:HG2	2:B:199:ASN:N	2.27	0.49
2:B:917:ILE:HD11	2:B:1042:ILE:HG22	1.95	0.49
2:B:40:ARG:NE	2:B:43:ILE:HD11	2.27	0.49
2:B:310:THR:OG1	2:B:316:PRO:HB3	2.13	0.49
2:B:943:TYR:CE1	2:B:949:LEU:HD13	2.47	0.49
2:B:982:HIS:H	2:B:982:HIS:HD1	1.59	0.49
2:F:271:TYR:O	2:F:275:LEU:N	2.42	0.49
2:B:1037:PHE:HE1	2:B:1039:TYR:CG	2.27	0.49
2:F:180:ASP:HB3	2:F:183:LYS:CD	2.41	0.49
2:F:1333:ARG:CZ	2:F:1335:ARG:HD2	2.41	0.49
2:B:121:ASN:H	2:B:121:ASN:ND2	2.10	0.49
2:B:448:ILE:HD13	2:B:455:LEU:CD1	2.41	0.49
2:B:679:ILE:HD13	2:B:704:PHE:CE2	2.48	0.49
2:B:841:ILE:HD11	2:B:896:LYS:HG3	1.94	0.49
2:F:9:LEU:HD13	2:F:740:THR:OG1	2.12	0.49
2:F:19:ALA:HB2	2:F:48:ILE:HG13	1.93	0.49
2:F:32:PHE:CE1	2:F:1355:LEU:HB3	2.47	0.49
2:F:362:TYR:OH	2:F:401:LYS:HG3	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:420:HIS:ND1	2:B:441:GLU:OE2	2.46	0.49
2:B:31:LYS:HG2	2:B:42:SER:OG	2.12	0.49
2:B:336:LYS:NZ	5:I:43:G:O6	2.46	0.49
2:B:603:ASP:OD1	2:B:606:PHE:N	2.40	0.49
2:F:925:ARG:HB3	2:F:928:THR:HG22	1.94	0.49
2:F:1216:SER:HB3	2:F:1219:GLU:H	1.77	0.49
2:B:967:ARG:NE	2:B:974:LYS:HB2	2.26	0.49
2:B:1290:VAL:HG22	2:B:1331:ILE:HD13	1.94	0.49
2:B:1305:GLN:O	2:B:1309:ILE:HG13	2.12	0.49
2:F:473:ILE:HG12	2:F:481:VAL:HG11	1.93	0.49
2:F:692:ASN:O	2:F:696:LEU:HG	2.13	0.49
2:B:465:MET:CE	2:B:467:ARG:HG2	2.35	0.49
2:B:1314:THR:CG2	2:B:1324:PHE:HB3	2.43	0.49
2:F:139:ARG:NH2	2:F:161:MET:HG3	2.27	0.49
2:F:628:ASP:O	2:F:632:ILE:HG13	2.13	0.49
2:B:182:ASP:O	2:B:186:ILE:HG12	2.12	0.49
2:F:221:ARG:HA	2:F:224:ASN:CB	2.38	0.49
2:F:601:ILE:CD1	2:F:607:LEU:HD21	2.43	0.49
5:J:42:A:O2'	5:J:43:G:OP1	2.26	0.49
1:A:31:U:C2	1:A:32:A:C8	3.00	0.48
2:F:471:GLU:OE2	2:F:481:VAL:HG22	2.13	0.48
2:F:641:HIS:CD2	2:F:642:LEU:HG	2.48	0.48
2:F:755:LYS:NZ	2:F:939:MET:O	2.35	0.48
2:F:1311:HIS:O	2:F:1314:THR:HG22	2.12	0.48
1:A:20:A:OP2	2:B:403:ARG:NH1	2.46	0.48
2:B:499:ASP:OD2	2:B:663:SER:N	2.39	0.48
2:F:467:ARG:HH21	2:F:473:ILE:HD11	1.79	0.48
2:F:583:VAL:HG22	2:F:584:GLU:N	2.27	0.48
2:F:918:LYS:CE	2:F:1018:VAL:CG1	2.92	0.48
2:B:253:LYS:O	2:B:257:ASP:N	2.43	0.48
2:B:380:LEU:HB3	2:B:386:THR:HG21	1.94	0.48
2:B:645:ASP:O	2:B:649:LYS:HE2	2.14	0.48
2:F:336:LYS:HG2	2:F:351:PHE:CE1	2.49	0.48
2:B:139:ARG:CD	2:B:161:MET:HE2	2.43	0.48
2:F:629:ARG:HH11	2:F:629:ARG:HG2	1.79	0.48
2:F:1019:ARG:C	2:F:1021:MET:H	2.21	0.48
2:F:1245:LEU:HA	2:F:1245:LEU:HD23	1.59	0.48
2:B:1179:ILE:HD11	2:B:1192:LYS:CD	2.43	0.48
2:F:36:GLY:HA3	2:F:1359:ARG:O	2.13	0.48
2:F:963:VAL:HG21	2:F:990:ASN:OD1	2.13	0.48
5:J:48:A:H2'	5:J:49:A:C8	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:63:ARG:HG3	2:B:66:ARG:HH21	1.79	0.48
2:B:971:GLN:O	2:B:971:GLN:HG2	2.13	0.48
1:A:25:U:H2'	1:A:26:A:C8	2.49	0.48
2:B:840:ALA:HA	2:B:854:ASN:O	2.12	0.48
2:B:1207:GLU:HG3	2:B:1208:ASN:N	2.29	0.48
1:E:21:G:H2'	1:E:22:U:O4'	2.14	0.48
2:F:652:LYS:HE3	2:F:652:LYS:HB2	1.62	0.48
2:F:828:LEU:HD22	2:F:836:TYR:CE2	2.49	0.48
2:B:570:LYS:O	2:B:574:CYS:HA	2.14	0.48
2:B:1336:TYR:N	2:B:1336:TYR:CD1	2.81	0.48
2:F:143:VAL:HG22	2:F:422:ILE:HG12	1.95	0.48
2:F:891:LEU:H	2:F:891:LEU:HD23	1.79	0.48
2:F:1284:ASP:OD1	2:F:1284:ASP:N	2.35	0.48
2:B:35:LEU:HB2	2:B:1358:THR:HG22	1.96	0.48
2:B:229:LEU:O	2:B:231:GLY:N	2.47	0.48
2:B:563:GLN:O	2:B:567:ASP:HB2	2.14	0.48
1:E:25:U:H2'	1:E:26:A:H8	1.79	0.48
2:F:63:ARG:CA	2:F:66:ARG:HG3	2.33	0.48
2:B:275:LEU:O	2:B:279:LEU:N	2.35	0.48
2:B:977:GLU:HG3	2:B:1310:ILE:HG23	1.96	0.48
2:F:545:LYS:CD	2:F:690:ASN:ND2	2.77	0.48
2:B:241:LEU:HD11	2:B:289:LEU:HD21	1.96	0.47
2:F:316:PRO:O	2:F:320:SER:N	2.46	0.47
2:F:359:TYR:CE1	2:F:399:LEU:HD13	2.49	0.47
2:F:746:GLU:HG2	2:F:1353:THR:CG2	2.44	0.47
5:J:53:G:N3	5:J:62:G:C2	2.82	0.47
2:B:1035:LYS:HA	2:B:1035:LYS:HD3	1.71	0.47
2:B:1041:ASN:O	2:B:1044:ASN:ND2	2.47	0.47
2:F:22:THR:HG22	2:F:28:PRO:HG3	1.95	0.47
2:F:180:ASP:HB3	2:F:183:LYS:HB2	1.96	0.47
2:F:691:ARG:HG2	2:F:695:GLN:NE2	2.29	0.47
2:F:882:TYR:CD2	2:F:883:TRP:CD1	3.02	0.47
2:B:844:GLN:C	2:B:1041:ASN:OD1	2.58	0.47
2:F:164:PHE:CZ	2:F:403:ARG:NH2	2.83	0.47
2:B:199:ASN:N	2:B:200:PRO:HD3	2.29	0.47
2:F:514:LEU:H	2:F:514:LEU:HD12	1.79	0.47
2:B:351:PHE:C	2:B:360:ALA:HB2	2.39	0.47
2:B:967:ARG:HB3	2:B:972:PHE:O	2.15	0.47
1:E:18:A:N7	2:F:71:ARG:CZ	2.78	0.47
2:F:114:GLU:HG2	2:F:120:GLY:HA2	1.96	0.47
2:F:410:ILE:HG21	2:F:415:HIS:NE2	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:943:TYR:HE2	2:F:949:LEU:HD13	1.80	0.47
2:B:325:TYR:CD1	5:I:44:U:C2	3.03	0.47
2:B:1349:HIS:HB3	5:I:68:A:N3	2.30	0.47
3:C:1:DC:H2'	3:C:2:DA:C8	2.49	0.47
2:F:5:TYR:CZ	2:F:751:MET:HG3	2.50	0.47
2:F:466:THR:O	2:F:482:VAL:HG13	2.15	0.47
2:F:531:THR:HG22	2:F:534:MET:HG2	1.96	0.47
2:F:1182:LEU:HD13	2:F:1190:VAL:HG11	1.96	0.47
2:B:6:SER:HB3	2:B:758:ASN:HB2	1.97	0.47
2:B:277:ASN:O	2:B:281:GLN:NE2	2.43	0.47
2:B:369:GLN:NE2	2:B:400:ARG:HD2	2.28	0.47
2:B:1050:ILE:HG12	2:B:1059:LYS:N	2.29	0.47
2:F:137:HIS:HA	2:F:322:ILE:CG1	2.45	0.47
2:F:143:VAL:HG22	2:F:422:ILE:CG1	2.44	0.47
2:F:297:SER:HA	2:F:300:ILE:HD12	1.96	0.47
2:F:784:ILE:HD13	2:F:815:TYR:HB3	1.95	0.47
2:F:824:VAL:HG12	2:F:825:ASP:N	2.30	0.47
2:F:921:LEU:HD21	2:F:1008:PHE:HE2	1.79	0.47
2:F:949:LEU:HD23	2:F:951:ARG:HH22	1.79	0.47
5:J:85:C:C2	5:J:86:C:C5	3.02	0.47
2:B:107:VAL:HG13	2:B:1131:TYR:CE1	2.49	0.47
2:B:208:ALA:O	2:B:212:LEU:HD23	2.15	0.47
2:B:671:ARG:HG3	2:B:678:THR:HG22	1.97	0.47
2:B:917:ILE:O	2:B:921:LEU:HG	2.15	0.47
2:B:1003:LYS:HE3	2:B:1034:ALA:HB1	1.97	0.47
2:B:1251:ASP:O	2:B:1254:GLN:HG3	2.15	0.47
2:F:328:HIS:ND1	5:J:44:U:C2	2.83	0.47
2:F:813:LEU:O	2:F:817:GLN:HG3	2.14	0.47
2:F:1221:GLN:HB3	2:F:1319:GLY:O	2.15	0.47
2:B:22:THR:HG22	2:B:23:ASP:N	2.29	0.47
2:B:249:THR:HG22	2:B:265:GLN:CG	2.45	0.47
2:F:212:LEU:HD13	2:F:300:ILE:HG12	1.97	0.47
2:F:223:GLU:O	2:F:227:ALA:N	2.48	0.47
2:F:307:ARG:HG2	2:F:307:ARG:HH11	1.80	0.47
2:F:427:GLU:OE1	2:F:434:LYS:HA	2.14	0.47
2:F:597:LEU:O	2:F:601:ILE:HG12	2.15	0.47
2:F:1035:LYS:HA	2:F:1035:LYS:HD3	1.71	0.47
5:I:85:C:H42	5:I:93:G:H1	1.62	0.47
2:B:139:ARG:O	2:B:143:VAL:HG23	2.15	0.47
2:B:141:LYS:HD3	2:B:142:LEU:HD23	1.97	0.47
2:B:155:TYR:CE1	2:B:159:ALA:HB2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:252:PHE:CE1	2:B:290:PHE:HE2	2.32	0.47
2:B:724:ILE:HA	2:B:727:LEU:HD23	1.98	0.47
2:B:813:LEU:O	2:B:817:GLN:HG3	2.15	0.47
2:B:1270:ILE:HG13	2:B:1294:TYR:CE2	2.50	0.47
2:F:465:MET:SD	2:F:482:VAL:HG11	2.55	0.47
2:F:720:LEU:HD13	2:F:938:ARG:HD2	1.97	0.47
2:B:823:TYR:CD2	2:B:858:THR:HG21	2.46	0.46
2:B:1204:PHE:CG	2:B:1342:VAL:HG13	2.50	0.46
1:E:27:G:H5'	1:E:28:A:H5''	1.96	0.46
2:F:478:PHE:HE2	2:F:482:VAL:HB	1.80	0.46
2:F:679:ILE:HG12	2:F:704:PHE:CE2	2.51	0.46
2:F:889:ALA:HB3	2:F:891:LEU:CD2	2.45	0.46
2:F:1270:ILE:HG13	2:F:1294:TYR:CE2	2.50	0.46
2:B:114:GLU:HG2	2:B:120:GLY:O	2.15	0.46
2:B:624:THR:HA	2:B:656:TYR:O	2.15	0.46
5:I:69:A:H2'	5:I:70:C:C6	2.51	0.46
2:B:58:THR:HG22	2:B:731:PRO:CG	2.46	0.46
2:B:925:ARG:HG2	2:B:927:ILE:HG22	1.98	0.46
2:F:119:PHE:CD2	2:F:124:ASP:HB3	2.50	0.46
2:F:467:ARG:HD3	2:F:470:GLU:HA	1.97	0.46
2:F:978:ILE:CD1	2:F:1233:VAL:CG2	2.92	0.46
5:J:43:G:O2'	5:J:44:U:H5'	2.14	0.46
2:B:74:ARG:HH21	5:I:60:C:P	2.39	0.46
2:B:525:THR:O	2:B:690:ASN:HB2	2.14	0.46
2:B:1119:LEU:HD12	2:B:1119:LEU:HA	1.75	0.46
2:F:143:VAL:O	2:F:425:ARG:NH1	2.48	0.46
2:F:338:LEU:HB3	2:F:383:MET:HE3	1.98	0.46
2:F:921:LEU:HG	2:F:1008:PHE:HD2	1.79	0.46
2:F:969:ASP:HB2	2:F:970:PHE:CD2	2.49	0.46
2:F:1286:ASN:ND2	2:F:1332:ASP:O	2.48	0.46
5:J:45:U:C2	5:J:46:A:C8	3.02	0.46
1:A:8:A:H2'	1:A:9:U:H6	1.79	0.46
2:B:976:ARG:HD3	2:B:982:HIS:NE2	2.31	0.46
2:B:1145:VAL:HG11	2:B:1187:TYR:CD2	2.51	0.46
2:B:1357:GLU:O	5:I:81:G:N2	2.40	0.46
3:C:2:DA:H2'	3:C:3:DA:C8	2.51	0.46
3:C:2:DA:H2''	3:C:3:DA:OP1	2.14	0.46
2:F:138:LEU:HD11	2:F:153:LEU:HD21	1.98	0.46
2:F:253:LYS:HA	2:F:256:PHE:HD2	1.80	0.46
2:F:1042:ILE:HD12	2:F:1042:ILE:HA	1.66	0.46
2:F:1094:ILE:HG21	2:F:1225:GLU:OE2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:45:U:H2'	5:J:46:A:O4'	2.15	0.46
2:B:516:GLU:HA	2:B:519:THR:HG22	1.97	0.46
2:B:1296:LYS:HA	2:B:1296:LYS:HD3	1.82	0.46
2:F:137:HIS:HE1	2:F:325:TYR:HB3	1.80	0.46
2:F:1314:THR:HG21	2:F:1324:PHE:HB3	1.98	0.46
5:I:47:A:H2'	5:I:48:A:H8	1.81	0.46
2:F:1127:ASP:HB3	2:F:1130:LYS:HE2	1.97	0.46
2:B:332:LEU:HD13	2:B:359:TYR:CE1	2.51	0.46
2:F:243:ALA:O	2:F:246:LEU:HB3	2.16	0.46
2:F:1000:LYS:HB2	2:F:1073:VAL:HG21	1.98	0.46
2:F:1087:LEU:HD23	2:F:1087:LEU:HA	1.57	0.46
5:J:91:C:H6	5:J:91:C:H2'	1.44	0.46
2:B:86:PHE:O	2:B:87:SER:C	2.59	0.46
2:B:349:GLU:HG3	2:B:356:LYS:HG3	1.98	0.46
2:B:509:PRO:HB3	2:B:624:THR:HG21	1.98	0.46
2:B:530:VAL:HG22	2:B:537:PRO:CB	2.40	0.46
2:B:913:LYS:O	2:B:916:PHE:HB2	2.16	0.46
2:B:1312:LEU:O	2:B:1315:LEU:HB3	2.16	0.46
2:F:855:LYS:NZ	2:F:1246:LYS:O	2.41	0.46
2:F:1219:GLU:CD	2:F:1335:ARG:HH21	2.21	0.46
2:F:1291:LEU:HA	2:F:1291:LEU:HD23	1.75	0.46
2:F:1349:HIS:ND1	5:J:69:A:H5'	2.31	0.46
2:F:258:LEU:HB3	2:F:260:GLU:O	2.16	0.46
2:F:373:TYR:O	2:F:376:ILE:HG22	2.15	0.46
2:F:553:PHE:CD2	2:F:559:VAL:HG21	2.51	0.46
2:F:1046:PHE:C	2:F:1076:LYS:HZ2	2.24	0.46
2:F:1062:LEU:O	2:F:1062:LEU:HG	2.14	0.46
5:J:96:C:H2'	5:J:97:U:C6	2.51	0.46
2:B:192:TYR:O	2:B:196:PHE:HB2	2.16	0.45
2:B:1111:LEU:HD12	2:B:1135:ASP:HB2	1.98	0.45
2:B:1143:VAL:HG13	2:B:1195:ILE:HG23	1.98	0.45
2:F:40:ARG:HD3	2:F:43:ILE:HD11	1.98	0.45
2:F:167:HIS:CD2	2:F:169:LEU:H	2.34	0.45
2:F:510:LYS:HG2	2:F:511:HIS:CD2	2.51	0.45
2:F:626:PHE:O	2:F:655:ARG:NH1	2.49	0.45
2:F:1219:GLU:O	2:F:1220:LEU:HD23	2.16	0.45
2:B:18:TRP:HZ2	2:B:1353:THR:O	1.99	0.45
2:B:1105:PHE:CD1	2:B:1169:MET:HG3	2.51	0.45
2:F:167:HIS:HD2	2:F:169:LEU:CB	2.29	0.45
2:F:289:LEU:O	2:F:292:ALA:HB3	2.15	0.45
2:F:684:LYS:C	2:F:685:SER:HG	2.21	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:802:GLU:HB2	2:F:805:GLN:HG3	1.97	0.45
2:B:340:ARG:NH2	5:I:41:A:P	2.87	0.45
2:B:666:LEU:HD21	2:B:693:PHE:CZ	2.51	0.45
2:B:989:LEU:HD21	2:B:1087:LEU:HD21	1.98	0.45
2:B:1089:MET:HA	2:B:1090:PRO:HD3	1.71	0.45
1:E:10:U:C4	1:E:11:U:C4	3.05	0.45
2:F:111:LYS:HD3	2:F:115:ARG:HA	1.97	0.45
2:F:1205:GLU:CB	2:F:1348:ILE:HD11	2.46	0.45
2:F:1212:ARG:CZ	2:F:1336:TYR:CE2	2.99	0.45
2:B:1254:GLN:HA	2:B:1257:LEU:HB2	1.97	0.45
4:D:4:DT:H2''	4:D:5:DA:C8	2.52	0.45
2:F:549:VAL:HA	2:F:553:PHE:HB2	1.98	0.45
2:F:897:PHE:CZ	2:F:901:THR:HG21	2.51	0.45
2:F:1167:THR:OG1	2:F:1168:ILE:N	2.48	0.45
2:B:13:THR:O	2:B:53:PHE:HE1	1.99	0.45
2:B:15:SER:HA	2:B:51:LEU:O	2.16	0.45
2:B:85:ILE:HD12	2:B:440:ILE:HG12	1.98	0.45
2:B:963:VAL:HG21	2:B:990:ASN:OD1	2.17	0.45
2:B:1119:LEU:HD23	2:B:1128:PRO:HB2	1.97	0.45
1:E:25:U:O2'	2:F:111:LYS:NZ	2.50	0.45
2:F:339:VAL:HG12	2:F:347:TYR:HB2	1.99	0.45
2:B:317:LEU:O	2:B:320:SER:HB3	2.17	0.45
2:F:562:LYS:O	2:F:566:GLU:HB2	2.17	0.45
2:F:731:PRO:HA	2:F:734:LYS:HE3	1.99	0.45
2:B:114:GLU:HG3	2:B:116:HIS:N	2.27	0.45
2:B:158:LEU:HD11	2:B:423:LEU:HD21	1.98	0.45
2:B:558:LYS:HD3	2:B:558:LYS:HA	1.76	0.45
2:B:949:LEU:HD12	2:B:950:ILE:H	1.81	0.45
2:F:478:PHE:CE2	2:F:482:VAL:HB	2.52	0.45
2:F:1038:PHE:CD2	2:F:1039:TYR:CE1	3.05	0.45
5:J:53:G:C4	5:J:62:G:N2	2.85	0.45
5:J:85:C:H2'	5:J:86:C:H6	1.81	0.45
1:A:10:U:H2'	1:A:11:U:C6	2.51	0.45
2:B:378:PRO:O	2:B:382:LYS:NZ	2.36	0.45
2:B:1003:LYS:HG2	2:B:1036:TYR:OH	2.16	0.45
2:F:583:VAL:HG22	2:F:584:GLU:H	1.81	0.45
2:B:103:GLU:OE2	2:B:113:HIS:N	2.47	0.45
2:B:864:ARG:NH2	2:B:869:ASN:O	2.50	0.45
2:B:874:GLU:O	2:B:878:LYS:HG3	2.16	0.45
2:F:143:VAL:HG21	2:F:315:ALA:HB2	1.98	0.45
2:F:411:PRO:HB2	2:F:413:GLN:OE1	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:135:ILE:CG2	5:J:46:A:H5'	2.47	0.45
2:F:615:ILE:HG23	2:F:639:TYR:CE1	2.52	0.45
2:F:823:TYR:CD2	2:F:858:THR:HG21	2.52	0.45
5:I:85:C:H2'	5:I:86:C:C6	2.52	0.45
5:J:95:G:C6	5:J:96:C:N4	2.85	0.45
2:B:640:ALA:HA	2:B:648:MET:CE	2.46	0.44
2:F:51:LEU:HD12	2:F:1095:VAL:HB	2.00	0.44
2:F:803:ASN:OD1	2:F:803:ASN:N	2.50	0.44
2:F:842:VAL:HG23	2:F:908:LEU:HD11	1.99	0.44
5:J:95:G:H2'	5:J:96:C:C6	2.52	0.44
2:B:824:VAL:HG11	2:B:859:ARG:NH1	2.30	0.44
2:B:977:GLU:HG3	2:B:1310:ILE:CG2	2.47	0.44
2:B:1318:LEU:HD23	2:B:1319:GLY:N	2.32	0.44
2:F:118:ILE:HG21	2:F:128:TYR:HE2	1.82	0.44
2:F:369:GLN:HG2	2:F:373:TYR:CE2	2.51	0.44
2:F:1120:ILE:HB	2:F:1134:PHE:HB2	1.98	0.44
2:B:135:ILE:HG21	2:B:160:HIS:CD2	2.52	0.44
2:B:887:LEU:HD12	2:B:897:PHE:CG	2.52	0.44
2:B:1232:TYR:HA	2:B:1235:PHE:HB3	1.99	0.44
2:B:1308:ASN:ND2	2:B:1327:PHE:H	2.01	0.44
2:B:1349:HIS:ND1	5:I:69:A:H4'	2.33	0.44
2:F:873:GLU:H	2:F:873:GLU:CD	2.25	0.44
2:F:1167:THR:HG22	2:F:1170:GLU:HG3	1.99	0.44
2:F:1171:ARG:O	2:F:1175:GLU:HG3	2.16	0.44
5:I:92:G:H2'	5:I:93:G:C8	2.52	0.44
5:J:86:C:C4	5:J:87:G:C8	3.04	0.44
2:B:189:VAL:HG22	2:B:238:PHE:HZ	1.83	0.44
2:B:724:ILE:HD13	2:B:934:ILE:HD13	1.99	0.44
2:B:954:LYS:HG2	2:B:1009:VAL:HG21	1.99	0.44
2:B:1146:VAL:HG23	2:B:1161:LYS:HB2	1.98	0.44
2:B:1226:LEU:HD13	2:B:1276:PHE:CG	2.53	0.44
2:F:110:ASP:OD2	2:F:1131:TYR:OH	2.34	0.44
2:F:328:HIS:C	2:F:328:HIS:CD2	2.95	0.44
2:F:481:VAL:HG12	2:F:482:VAL:HG23	1.99	0.44
2:F:727:LEU:N	2:F:727:LEU:HD23	2.32	0.44
2:F:844:GLN:CG	2:F:848:LYS:HD2	2.43	0.44
2:F:5:TYR:CE2	2:F:751:MET:HG3	2.52	0.44
2:F:103:GLU:OE2	2:F:113:HIS:N	2.47	0.44
2:F:201:ILE:N	2:F:201:ILE:HD12	2.33	0.44
2:F:256:PHE:CD1	2:F:282:ILE:HD11	2.52	0.44
2:F:398:LEU:CD1	2:F:399:LEU:HG	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:553:PHE:HZ	2:F:587:PHE:CD2	2.36	0.44
2:F:600:ILE:HD13	2:F:651:LEU:HA	2.00	0.44
2:F:649:LYS:HB3	2:F:653:ARG:HH21	1.83	0.44
2:F:1265:TYR:O	2:F:1268:GLU:N	2.50	0.44
2:B:1201:TYR:CD1	2:B:1201:TYR:N	2.85	0.44
2:F:1200:LYS:HG2	2:F:1201:TYR:CD1	2.51	0.44
2:B:118:ILE:HD13	2:B:128:TYR:CD2	2.53	0.44
2:B:377:LYS:N	2:B:378:PRO:HD2	2.33	0.44
2:B:850:ASP:HB3	2:B:855:LYS:NZ	2.33	0.44
2:B:872:SER:O	2:B:876:VAL:HG23	2.18	0.44
2:B:967:ARG:NH1	2:B:989:LEU:HD12	2.33	0.44
2:B:972:PHE:HE1	2:B:1084:ARG:HB2	1.82	0.44
2:F:83:GLN:O	2:F:87:SER:HB3	2.17	0.44
2:F:112:LYS:O	2:F:113:HIS:ND1	2.39	0.44
2:F:425:ARG:HE	2:F:425:ARG:HB3	1.62	0.44
2:F:1084:ARG:CZ	2:F:1084:ARG:HB3	2.46	0.44
2:F:1114:ARG:O	2:F:1129:LYS:HA	2.18	0.44
2:B:11:ILE:O	2:B:763:MET:HA	2.18	0.44
2:B:609:ASN:CG	2:B:611:GLU:HG3	2.43	0.44
2:F:174:LEU:HD13	2:F:174:LEU:O	2.18	0.44
5:J:58:G:C6	5:J:60:C:C2	3.06	0.44
2:B:875:VAL:HA	2:B:878:LYS:HD2	2.00	0.44
2:F:44:LYS:HG2	5:J:91:C:C5	2.53	0.44
2:F:551:LEU:O	2:F:555:THR:OG1	2.20	0.44
2:F:809:GLU:OE2	2:F:1246:LYS:HG3	2.17	0.44
2:F:958:LEU:HA	2:F:958:LEU:HD23	1.70	0.44
2:F:967:ARG:CZ	2:F:974:LYS:HB2	2.48	0.44
3:G:22:DT:H2''	3:G:23:DC:O5'	2.18	0.44
5:I:39:G:H5'	5:I:40:C:OP2	2.18	0.44
2:B:6:SER:HB2	2:B:21:ILE:CG1	2.48	0.43
2:B:133:PRO:HG2	2:B:137:HIS:ND1	2.33	0.43
2:B:342:GLN:CD	2:B:383:MET:HB3	2.43	0.43
2:B:943:TYR:HA	2:B:950:ILE:HG13	2.00	0.43
2:B:1145:VAL:HG11	2:B:1187:TYR:CE2	2.52	0.43
1:E:25:U:O4	1:E:26:A:N6	2.51	0.43
2:F:90:MET:SD	2:F:151:LEU:CD2	3.06	0.43
2:F:154:ILE:CG2	2:F:158:LEU:HG	2.47	0.43
2:F:342:GLN:HB2	2:F:383:MET:HG2	1.99	0.43
5:I:92:G:H2'	5:I:93:G:H8	1.82	0.43
2:B:165:ARG:O	2:B:412:HIS:HA	2.18	0.43
2:B:276:ASP:HA	2:B:279:LEU:HB3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:526:LYS:NZ	2:B:695:GLN:OE1	2.29	0.43
2:B:1202:SER:O	2:B:1213:MET:HA	2.17	0.43
2:F:430:TYR:HB3	2:F:432:PHE:CE2	2.53	0.43
2:F:650:GLN:O	2:F:653:ARG:HG2	2.17	0.43
2:F:742:LYS:NZ	5:J:68:A:OP1	2.51	0.43
2:B:406:ASP:OD1	2:B:406:ASP:N	2.47	0.43
2:B:782:LYS:O	2:B:786:GLU:HG3	2.18	0.43
2:B:917:ILE:HD12	2:B:917:ILE:HA	1.82	0.43
2:B:1047:LYS:HB2	2:B:1050:ILE:HG22	1.99	0.43
5:J:51:A:C2	5:J:62:G:H2'	2.53	0.43
1:A:20:A:P	2:B:403:ARG:NH1	2.92	0.43
2:B:594:TYR:O	2:B:598:LEU:N	2.48	0.43
2:F:514:LEU:CD2	2:F:664:ARG:HH21	2.31	0.43
2:F:1277:SER:O	2:F:1281:ILE:N	2.46	0.43
2:B:497:ASN:OD1	2:B:498:PHE:N	2.51	0.43
2:B:1200:LYS:HG2	2:B:1201:TYR:CE1	2.53	0.43
1:E:25:U:H6	1:E:25:U:O5'	2.00	0.43
1:E:32:A:N6	5:J:37:U:C4	2.84	0.43
2:F:140:LYS:HB3	2:F:322:ILE:HD12	2.00	0.43
2:F:274:ASP:O	2:F:277:ASN:OD1	2.36	0.43
2:F:475:PRO:HG3	5:J:59:U:O4	2.17	0.43
2:F:647:VAL:O	2:F:651:LEU:HB2	2.18	0.43
2:F:972:PHE:HE1	2:F:1084:ARG:CG	2.31	0.43
5:I:47:A:H2'	5:I:48:A:C8	2.54	0.43
2:B:682:PHE:CB	2:B:696:LEU:HD11	2.49	0.43
2:B:781:MET:O	2:B:785:GLU:HB2	2.18	0.43
2:B:1246:LYS:HB2	2:B:1246:LYS:HE2	1.79	0.43
2:B:1280:VAL:HG12	2:B:1281:ILE:HD13	2.01	0.43
2:F:161:MET:HE2	2:F:419:LEU:HA	2.00	0.43
2:F:282:ILE:HG22	2:F:286:TYR:CD1	2.54	0.43
2:F:438:GLU:HA	2:F:441:GLU:OE1	2.19	0.43
2:F:836:TYR:HB2	2:F:857:LEU:HD11	2.01	0.43
2:F:1204:PHE:CG	2:F:1342:VAL:HG13	2.53	0.43
2:B:158:LEU:CD1	2:B:423:LEU:HD21	2.48	0.43
2:B:197:GLU:HA	2:B:200:PRO:HG3	2.01	0.43
2:B:201:ILE:HD12	2:B:238:PHE:CD1	2.53	0.43
2:B:836:TYR:N	2:B:836:TYR:CD1	2.86	0.43
2:B:1270:ILE:HG13	2:B:1294:TYR:CD2	2.54	0.43
2:F:8:GLY:O	2:F:987:ALA:HB1	2.19	0.43
2:F:523:GLU:OE1	2:F:589:ALA:N	2.51	0.43
2:F:749:LYS:O	2:F:750:VAL:C	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:978:ILE:HD12	2:F:1228:LEU:CD2	2.37	0.43
2:B:299:ALA:O	2:B:303:SER:OG	2.31	0.43
2:B:373:TYR:HH	2:B:398:LEU:H	1.59	0.43
2:B:540:LEU:HA	2:B:540:LEU:HD12	1.54	0.43
2:B:861:ASP:O	2:B:864:ARG:HG2	2.18	0.43
2:B:913:LYS:HA	2:B:916:PHE:CD2	2.44	0.43
2:F:275:LEU:HD13	2:F:279:LEU:HG	2.01	0.43
2:F:821:ASP:OD1	2:F:823:TYR:N	2.40	0.43
2:F:1178:PRO:O	2:F:1182:LEU:HG	2.18	0.43
1:A:5:C:H42	3:C:24:DG:H1	1.67	0.43
2:B:7:ILE:HD13	2:B:747:LEU:HD12	2.00	0.43
2:B:37:ASN:OD1	2:B:37:ASN:N	2.52	0.43
2:B:485:GLY:O	2:B:488:ALA:N	2.52	0.43
2:B:644:ASP:HB3	2:B:647:VAL:CG2	2.44	0.43
2:F:623:LEU:HD11	2:F:654:ARG:O	2.18	0.43
2:F:1154:SER:OG	2:F:1156:LYS:HE2	2.18	0.43
5:J:52:A:N7	5:J:53:G:H1'	2.34	0.43
2:B:246:LEU:CD2	2:B:246:LEU:H	2.19	0.43
2:B:469:SER:C	2:B:471:GLU:H	2.27	0.43
2:B:475:PRO:HG3	5:I:59:U:O4	2.19	0.43
2:B:886:LEU:HD22	2:B:891:LEU:HD12	2.01	0.43
2:B:892:ILE:HB	2:B:896:LYS:HD3	2.01	0.43
2:F:332:LEU:HD13	2:F:359:TYR:CE1	2.54	0.43
2:F:977:GLU:HG3	2:F:1310:ILE:HG22	2.00	0.43
2:B:464:TRP:CD1	2:B:464:TRP:C	2.97	0.42
2:B:1111:LEU:HD12	2:B:1135:ASP:CB	2.49	0.42
2:F:531:THR:HG21	2:F:575:PHE:HE1	1.76	0.42
2:F:842:VAL:HG12	2:F:854:ASN:OD1	2.19	0.42
2:F:1147:ALA:HB1	2:F:1188:LYS:O	2.19	0.42
2:F:1156:LYS:HE2	2:F:1156:LYS:HB2	1.78	0.42
2:F:1197:LYS:O	2:F:1199:PRO:HD3	2.19	0.42
2:B:32:PHE:CZ	2:B:1355:LEU:HD13	2.54	0.42
2:B:340:ARG:NH2	5:I:41:A:OP2	2.52	0.42
2:B:1074:TRP:HZ2	2:B:1080:PHE:CD2	2.37	0.42
1:E:27:G:H22	5:J:44:U:P	2.42	0.42
2:F:66:ARG:NH2	2:F:462:PHE:CG	2.87	0.42
2:F:258:LEU:HD23	2:F:259:ALA:H	1.84	0.42
2:F:338:LEU:HD22	2:F:383:MET:HE1	2.01	0.42
5:J:49:A:H2'	5:J:50:U:O4'	2.19	0.42
2:B:1219:GLU:HG3	2:B:1220:LEU:N	2.34	0.42
2:F:40:ARG:CD	2:F:43:ILE:HD11	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:140:LYS:HB3	2:F:322:ILE:CD1	2.49	0.42
2:F:649:LYS:HB2	2:F:650:GLN:NE2	2.33	0.42
2:F:746:GLU:HG2	2:F:1353:THR:HG23	2.01	0.42
1:A:29:G:C4	5:I:41:A:C2	3.07	0.42
2:B:69:ARG:HE	2:B:69:ARG:HB2	1.53	0.42
2:B:395:ARG:NH2	2:B:397:ASP:OD2	2.52	0.42
2:F:237:LEU:HD12	2:F:238:PHE:N	2.35	0.42
2:F:291:LEU:HD12	2:F:291:LEU:HA	1.88	0.42
2:F:561:VAL:HG12	2:F:565:LYS:HD3	2.00	0.42
2:F:1103:GLY:HA2	5:J:63:U:H1'	2.01	0.42
2:B:275:LEU:O	2:B:279:LEU:HB2	2.19	0.42
2:B:876:VAL:O	2:B:880:LYS:N	2.50	0.42
2:B:1143:VAL:HG22	2:B:1197:LYS:HG3	2.01	0.42
2:F:134:THR:O	2:F:137:HIS:HB2	2.19	0.42
2:F:139:ARG:O	2:F:143:VAL:HG23	2.19	0.42
2:F:258:LEU:CD1	2:F:281:GLN:HE22	2.29	0.42
2:F:761:ILE:HG21	2:F:761:ILE:HD13	1.85	0.42
2:F:883:TRP:HB3	2:F:897:PHE:HD1	1.84	0.42
2:F:1060:ARG:HA	2:F:1060:ARG:HD2	1.87	0.42
2:F:909:SER:N	2:F:912:ASP:HB2	2.34	0.42
2:F:958:LEU:CD2	2:F:962:LEU:HD12	2.47	0.42
2:B:32:PHE:N	2:B:43:ILE:O	2.38	0.42
2:B:217:SER:HB2	2:B:220:ARG:H	1.84	0.42
2:B:390:LEU:HD23	2:B:390:LEU:HA	1.72	0.42
2:B:507:VAL:HG12	2:B:508:LEU:O	2.20	0.42
2:B:516:GLU:C	2:B:519:THR:HG22	2.44	0.42
2:F:165:ARG:O	2:F:412:HIS:HA	2.20	0.42
2:F:323:LYS:O	2:F:327:GLU:HG2	2.19	0.42
2:F:739:GLN:NE2	2:F:1097:LYS:HE3	2.35	0.42
2:F:980:ASN:HB2	2:F:1225:GLU:OE2	2.19	0.42
2:F:1093:ASN:O	2:F:1094:ILE:HD13	2.19	0.42
1:A:24:U:H2'	1:A:25:U:O4'	2.19	0.42
2:B:686:ASP:OD1	2:B:691:ARG:HB2	2.20	0.42
2:B:727:LEU:HD21	2:B:934:ILE:HD11	2.01	0.42
2:B:1000:LYS:O	2:B:1000:LYS:HD3	2.19	0.42
2:B:1212:ARG:CZ	2:B:1336:TYR:CE2	3.03	0.42
2:B:1235:PHE:CE1	2:B:1239:ALA:HB2	2.54	0.42
2:F:93:VAL:HG11	2:F:150:ASP:OD1	2.20	0.42
2:F:168:PHE:CB	2:F:447:ARG:HH11	2.33	0.42
2:F:645:ASP:O	2:F:649:LYS:HG2	2.20	0.42
2:B:51:LEU:HD13	2:B:1095:VAL:HG23	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:141:LYS:HD3	2:B:141:LYS:C	2.45	0.42
2:B:252:PHE:CD1	2:B:264:LEU:HD13	2.55	0.42
2:B:507:VAL:HG11	2:B:660:GLY:O	2.20	0.42
2:B:1228:LEU:HD12	2:B:1229:PRO:CD	2.50	0.42
2:F:5:TYR:OH	2:F:756:PRO:HG3	2.20	0.42
2:F:20:VAL:HG11	2:F:751:MET:CE	2.50	0.42
2:F:305:ILE:HG13	2:F:306:LEU:HD13	2.02	0.42
2:F:491:PHE:O	2:F:494:ARG:HG2	2.19	0.42
2:F:922:VAL:HG12	2:F:1007:GLU:HB3	2.01	0.42
2:F:976:ARG:HA	2:F:982:HIS:CD2	2.55	0.42
2:F:1064:GLU:OE1	2:F:1065:THR:N	2.51	0.42
2:F:1101:GLN:O	2:F:1168:ILE:HD11	2.19	0.42
5:J:43:G:H3'	5:J:44:U:H6	1.85	0.42
2:B:30:LYS:HD3	5:I:83:C:OP1	2.19	0.42
2:B:165:ARG:O	2:B:415:HIS:CD2	2.71	0.42
2:B:225:LEU:HD13	2:B:242:ILE:HG21	2.01	0.42
2:B:869:ASN:OD1	2:B:870:VAL:N	2.52	0.42
2:B:980:ASN:HB2	2:B:1225:GLU:CD	2.32	0.42
2:F:44:LYS:NZ	5:J:85:C:H42	2.18	0.42
2:F:47:LEU:HD11	2:F:750:VAL:HG11	2.02	0.42
2:B:58:THR:HG22	2:B:731:PRO:HG3	2.00	0.41
2:B:114:GLU:HG3	2:B:115:ARG:N	2.33	0.41
2:B:526:LYS:NZ	2:B:691:ARG:HA	2.35	0.41
2:B:821:ASP:HB3	2:B:828:LEU:HD11	2.02	0.41
2:B:1212:ARG:HA	2:B:1212:ARG:HD3	1.87	0.41
2:B:1231:LYS:HE3	2:B:1232:TYR:CE2	2.54	0.41
2:F:32:PHE:HD1	2:F:45:LYS:HD3	1.84	0.41
2:F:106:LEU:HD22	2:F:1131:TYR:OH	2.19	0.41
2:F:108:GLU:CD	2:F:115:ARG:HD3	2.45	0.41
2:F:546:LYS:HE3	2:F:546:LYS:HB3	1.84	0.41
2:B:47:LEU:HD11	2:B:750:VAL:HG11	2.02	0.41
2:B:508:LEU:HD21	2:B:664:ARG:HB2	2.02	0.41
2:B:849:ASP:OD1	2:B:851:SER:OG	2.38	0.41
2:B:966:PHE:CD2	2:B:966:PHE:C	2.97	0.41
2:B:1241:HIS:HD1	2:B:1244:LYS:HA	1.85	0.41
2:B:1303:ARG:O	2:B:1307:GLU:HG2	2.19	0.41
2:B:1349:HIS:CE1	5:I:69:A:H4'	2.55	0.41
3:C:4:DT:H2''	3:C:5:DA:O5'	2.20	0.41
4:D:10:DT:H6	4:D:10:DT:H2'	1.73	0.41
2:F:258:LEU:HD23	2:F:259:ALA:N	2.35	0.41
2:F:882:TYR:HD2	2:F:883:TRP:CD1	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1262:HIS:HB3	2:F:1265:TYR:CD2	2.55	0.41
2:B:70:ARG:HH22	2:B:462:PHE:HD2	1.68	0.41
2:B:518:PHE:CD2	2:B:518:PHE:C	2.98	0.41
2:F:18:TRP:CZ2	2:F:49:GLY:HA3	2.55	0.41
2:F:427:GLU:HA	2:F:433:LEU:HB2	2.02	0.41
2:F:795:ILE:O	2:F:795:ILE:HG13	2.20	0.41
2:F:939:MET:CE	2:F:953:VAL:HG21	2.50	0.41
5:I:48:A:O2'	5:I:49:A:H5'	2.20	0.41
2:B:151:LEU:HD12	2:B:151:LEU:HA	1.77	0.41
2:B:549:VAL:HA	2:B:553:PHE:HD2	1.85	0.41
2:B:594:TYR:CE1	2:B:607:LEU:HB3	2.55	0.41
2:B:986:ASP:O	2:B:990:ASN:ND2	2.53	0.41
2:B:1096:LYS:HG2	2:B:1201:TYR:CD2	2.55	0.41
2:B:1182:LEU:HD23	2:B:1182:LEU:HA	1.94	0.41
2:F:328:HIS:CG	5:J:44:U:C2	3.08	0.41
2:F:646:LYS:O	2:F:650:GLN:HG2	2.21	0.41
2:F:748:VAL:HG13	2:F:754:HIS:O	2.21	0.41
2:F:971:GLN:HG2	2:F:973:TYR:CZ	2.56	0.41
3:G:19:DA:H2'	3:G:20:DA:C8	2.55	0.41
5:I:94:U:H2'	5:I:95:G:H8	1.86	0.41
2:B:56:GLY:O	2:B:732:ALA:HB2	2.21	0.41
2:B:241:LEU:HA	2:B:241:LEU:HD23	1.81	0.41
2:B:442:LYS:HE3	2:B:476:TRP:HA	2.02	0.41
2:B:921:LEU:HB3	2:B:1008:PHE:HZ	1.84	0.41
2:B:1000:LYS:HB3	2:B:1001:TYR:CD2	2.54	0.41
2:B:1231:LYS:H	2:B:1231:LYS:HG2	1.71	0.41
2:B:1251:ASP:O	2:B:1255:LYS:HG3	2.20	0.41
2:F:140:LYS:HE3	2:F:313:THR:CB	2.50	0.41
2:F:1300:LYS:HG3	2:F:1327:PHE:CZ	2.56	0.41
2:B:326:ASP:O	2:B:330:GLN:HG3	2.20	0.41
2:B:954:LYS:HB2	2:B:954:LYS:HE3	1.71	0.41
2:B:1351:SER:HA	5:I:68:A:N7	2.35	0.41
2:F:499:ASP:OD2	2:F:663:SER:HB3	2.20	0.41
2:F:1105:PHE:CD1	2:F:1169:MET:HG3	2.55	0.41
2:B:253:LYS:HD3	2:B:261:ASP:HA	2.02	0.41
2:B:642:LEU:HB2	2:B:643:PHE:CD2	2.55	0.41
2:B:1114:ARG:O	2:B:1129:LYS:HA	2.20	0.41
2:B:1208:ASN:CG	2:B:1208:ASN:O	2.63	0.41
2:F:89:GLU:HG3	2:F:432:PHE:CD2	2.55	0.41
2:F:140:LYS:CB	2:F:322:ILE:HD12	2.50	0.41
2:F:622:THR:HG23	2:F:626:PHE:CD1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1017:ASP:CB	2:F:1020:LYS:HZ3	2.34	0.41
2:F:1116:SER:HB3	2:F:1119:LEU:HB2	2.02	0.41
2:B:661:ARG:CB	2:B:662:LEU:HD12	2.50	0.41
2:B:794:GLN:HE21	2:B:798:GLU:CD	2.28	0.41
2:B:1206:LEU:H	2:B:1206:LEU:HD23	1.86	0.41
2:B:1221:GLN:HG2	2:B:1319:GLY:O	2.20	0.41
2:F:308:VAL:HG11	2:F:316:PRO:O	2.21	0.41
2:F:335:LEU:O	2:F:339:VAL:HG23	2.20	0.41
2:F:921:LEU:HG	2:F:1008:PHE:CD2	2.56	0.41
2:F:1266:LEU:O	2:F:1270:ILE:HG12	2.20	0.41
2:B:35:LEU:HD23	2:B:35:LEU:HA	1.80	0.41
2:B:127:ALA:O	2:B:130:GLU:HB2	2.20	0.41
2:B:178:ASN:O	2:B:302:LEU:HD11	2.20	0.41
2:B:424:ARG:NH1	2:B:437:ARG:CZ	2.83	0.41
2:B:478:PHE:CE1	2:B:482:VAL:HG21	2.56	0.41
2:B:820:ARG:HA	2:B:826:GLN:O	2.21	0.41
2:B:824:VAL:HG22	2:B:863:ASN:HD22	1.85	0.41
2:B:1226:LEU:HB2	2:B:1276:PHE:CZ	2.56	0.41
2:B:1252:ASN:HA	2:B:1255:LYS:HD2	2.03	0.41
1:E:25:U:C4	1:E:26:A:N7	2.89	0.41
2:F:32:PHE:O	2:F:42:SER:HA	2.21	0.41
2:F:35:LEU:HB2	2:F:1358:THR:CG2	2.50	0.41
2:F:199:ASN:O	2:F:201:ILE:HD12	2.21	0.41
2:F:429:PHE:N	2:F:429:PHE:CD1	2.87	0.41
2:F:449:PRO:HB2	2:F:452:VAL:HG23	2.03	0.41
2:F:455:LEU:O	5:J:60:C:H5'	2.21	0.41
2:F:510:LYS:HG2	2:F:511:HIS:HD2	1.86	0.41
2:F:724:ILE:O	2:F:727:LEU:HG	2.20	0.41
2:F:973:TYR:CG	2:F:1237:TYR:HD1	2.38	0.41
2:F:1163:LEU:HD23	2:F:1163:LEU:HA	1.90	0.41
2:F:1179:ILE:O	2:F:1183:GLU:HG3	2.21	0.41
2:F:1295:ASN:OD1	2:F:1298:ARG:NH1	2.46	0.41
5:I:84:A:C2	5:I:85:C:C2	3.09	0.41
2:B:30:LYS:HD3	5:I:83:C:OP2	2.21	0.41
2:B:529:TYR:CD2	2:B:569:PHE:HE1	2.39	0.41
2:B:666:LEU:HD21	2:B:693:PHE:CE1	2.56	0.41
5:J:46:A:C2	5:J:47:A:C5	3.09	0.41
5:J:76:A:C5	5:J:77:A:H1'	2.55	0.41
2:B:222:LEU:HD21	2:B:234:LYS:HG3	2.03	0.40
2:B:298:ASP:O	2:B:302:LEU:HG	2.21	0.40
2:B:513:LEU:HA	2:B:513:LEU:HD23	1.83	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:951:ARG:HH21	2:B:1011:GLY:HA2	1.84	0.40
2:B:1245:LEU:HD12	2:B:1245:LEU:O	2.22	0.40
2:F:97:PHE:HE1	2:F:118:ILE:HA	1.86	0.40
2:B:536:LYS:HG2	2:B:537:PRO:O	2.21	0.40
2:B:1307:GLU:O	2:B:1310:ILE:HB	2.20	0.40
2:F:140:LYS:O	2:F:140:LYS:HE2	2.22	0.40
2:F:223:GLU:HA	2:F:226:ILE:HB	2.03	0.40
2:F:342:GLN:CG	2:F:383:MET:HE2	2.49	0.40
2:F:359:TYR:HE1	2:F:399:LEU:HD13	1.86	0.40
2:F:666:LEU:O	2:F:679:ILE:HD12	2.21	0.40
2:F:782:LYS:HA	2:F:785:GLU:HB2	2.03	0.40
2:F:962:LEU:CB	2:F:1043:MET:HE1	2.36	0.40
2:F:975:VAL:CG1	2:F:978:ILE:CG2	2.98	0.40
2:F:975:VAL:HG11	2:F:978:ILE:HG22	2.03	0.40
5:I:94:U:H2'	5:I:95:G:C8	2.57	0.40
5:J:46:A:C2	5:J:47:A:C6	3.09	0.40
1:E:27:G:H1'	2:F:129:HIS:CD2	2.56	0.40
2:F:136:TYR:CZ	2:F:160:HIS:NE2	2.88	0.40
2:F:465:MET:HE1	2:F:473:ILE:CD1	2.51	0.40
2:F:998:ILE:CG2	2:F:1008:PHE:HE1	2.30	0.40
4:H:7:DG:H2''	4:H:8:DT:O5'	2.22	0.40
2:B:211:ILE:HD11	2:B:228:GLN:HG3	2.03	0.40
2:B:380:LEU:C	2:B:386:THR:HG21	2.45	0.40
2:F:64:LEU:O	2:F:67:THR:HB	2.21	0.40
2:F:101:LEU:HD12	2:F:117:PRO:HB2	2.04	0.40
2:F:317:LEU:HD21	2:F:410:ILE:HD13	2.04	0.40
2:F:478:PHE:HD2	2:F:478:PHE:O	2.03	0.40
2:F:506:LYS:H	2:F:506:LYS:HG2	1.48	0.40
2:F:1110:ILE:HG21	2:F:1122:ARG:NH2	2.37	0.40
2:F:1336:TYR:N	2:F:1336:TYR:CD1	2.89	0.40
5:I:47:A:C5	5:I:48:A:N7	2.89	0.40
2:B:142:LEU:HD23	2:B:142:LEU:HA	1.78	0.40
2:B:433:LEU:HD23	2:B:433:LEU:HA	1.78	0.40
2:B:539:PHE:CB	2:B:690:ASN:ND2	2.68	0.40
2:B:882:TYR:O	2:B:886:LEU:HG	2.21	0.40
2:F:169:LEU:O	2:F:170:ILE:HD12	2.22	0.40
2:F:258:LEU:CD2	2:F:260:GLU:H	2.33	0.40
2:F:275:LEU:CD1	2:F:279:LEU:HG	2.52	0.40
2:F:632:ILE:HG22	2:F:636:LEU:HD22	2.04	0.40
2:F:1200:LYS:HG2	2:F:1201:TYR:CE1	2.57	0.40
2:F:1217:ALA:O	2:F:1339:THR:HG21	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:54:G:C6	5:J:55:C:N4	2.89	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	1312/1368 (96%)	1275 (97%)	34 (3%)	3 (0%)	43	71
2	F	1313/1368 (96%)	1265 (96%)	40 (3%)	8 (1%)	21	49
All	All	2625/2736 (96%)	2540 (97%)	74 (3%)	11 (0%)	30	59

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	1042	ILE
2	F	585	ASP
2	F	869	ASN
2	F	1020	LYS
2	F	1055	GLY
2	F	202	ASN
2	F	117	PRO
2	F	868	ASP
2	B	117	PRO
2	B	250	PRO
2	B	230	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	1173/1225 (96%)	1169 (100%)	4 (0%)	86	84
2	F	1156/1225 (94%)	1150 (100%)	6 (0%)	81	80
All	All	2329/2450 (95%)	2319 (100%)	10 (0%)	84	82

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	246	LEU
2	B	685	SER
2	B	1221	GLN
2	B	1225	GLU
2	F	686	ASP
2	F	690	ASN
2	F	977	GLU
2	F	978	ILE
2	F	979	ASN
2	F	1060	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	137	HIS
2	B	178	ASN
2	B	342	GLN
2	B	712	GLN
2	B	739	GLN
2	B	818	ASN
2	B	844	GLN
2	B	933	GLN
2	B	1044	ASN
2	B	1066	ASN
2	B	1252	ASN
2	B	1256	GLN
2	B	1262	HIS
2	B	1305	GLN
2	B	1308	ASN
2	B	1350	GLN
2	F	121	ASN

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Mol	Chain	Res	Type
2	F	167	HIS
2	F	178	ASN
2	F	281	GLN
2	F	394	ASN
2	F	415	HIS
2	F	426	GLN
2	F	544	GLN
2	F	612	ASN
2	F	690	ASN
2	F	726	ASN
2	F	758	ASN
2	F	807	GLN
2	F	817	GLN
2	F	881	ASN
2	F	885	GLN
2	F	982	HIS
2	F	985	HIS
2	F	1252	ASN
2	F	1256	GLN
2	F	1317	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	33/34 (97%)	10 (30%)	3 (9%)
1	E	30/34 (88%)	9 (30%)	1 (3%)
5	I	62/65 (95%)	19 (30%)	1 (1%)
5	J	62/65 (95%)	18 (29%)	1 (1%)
All	All	187/198 (94%)	56 (29%)	6 (3%)

All (56) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	2	U
1	A	4	A
1	A	5	C
1	A	6	G
1	A	9	U
1	A	20	A
1	A	28	A
1	A	29	G

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Mol	Chain	Res	Type
1	A	32	A
1	A	33	U
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	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	50	U
5	I	51	A
5	I	56	U
5	I	57	A
5	I	59	U
5	I	63	U
5	I	68	A
5	I	74	A
5	I	77	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

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Mol	Chain	Res	Type
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 (6) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	8	A
1	A	27	G
1	A	28	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%)	0.11	3 (8%) 15 14	7, 28, 140, 153	0
1	E	31/34 (91%)	0.99	5 (16%) 4 6	29, 64, 167, 193	0
2	B	1326/1368 (96%)	0.76	176 (13%) 7 8	4, 56, 173, 204	0
2	F	1327/1368 (97%)	1.16	311 (23%) 2 3	3, 82, 129, 161	0
3	C	24/24 (100%)	0.25	2 (8%) 17 15	16, 28, 79, 123	0
3	G	24/24 (100%)	0.33	1 (4%) 40 29	38, 48, 89, 139	0
4	D	11/11 (100%)	1.13	2 (18%) 3 5	24, 29, 129, 152	0
4	H	11/11 (100%)	0.69	2 (18%) 3 5	29, 48, 101, 160	0
5	I	63/65 (96%)	0.12	3 (4%) 35 26	6, 58, 102, 134	0
5	J	63/65 (96%)	0.35	5 (7%) 18 16	18, 40, 134, 165	0
All	All	2914/3004 (97%)	0.91	510 (17%) 4 5	3, 63, 149, 204	0

All (510) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	1243	GLU	14.2
2	F	305	ILE	10.7
2	F	301	LEU	7.7
2	F	306	LEU	7.7
4	D	2	DT	7.3
2	B	900	LEU	7.3
2	B	841	ILE	6.7
2	F	413	GLN	6.6
2	B	833	LEU	6.6
2	B	813	LEU	6.5
2	F	156	LEU	6.4
2	B	810	LYS	6.4
2	B	881	ASN	6.2

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Mol	Chain	Res	Type	RSRZ
2	B	809	GLU	6.0
2	F	362	TYR	5.8
2	B	822	MET	5.8
2	F	402	GLN	5.8
2	F	400	ARG	5.7
2	F	1242	TYR	5.7
2	F	818	ASN	5.7
2	F	1246	LYS	5.7
2	F	142	LEU	5.7
2	B	842	VAL	5.6
2	B	834	SER	5.6
2	F	181	VAL	5.5
2	B	1052	LEU	5.4
2	F	796	LEU	5.3
2	B	817	GLN	5.3
2	B	812	TYR	5.3
2	F	128	TYR	5.3
2	F	697	ILE	5.2
2	B	858	THR	5.2
2	F	244	LEU	5.2
2	B	883	TRP	5.1
2	F	209	LYS	4.9
2	B	814	TYR	4.8
2	B	1045	PHE	4.8
2	F	82	LEU	4.8
2	F	287	ALA	4.7
2	B	857	LEU	4.7
2	B	914	ALA	4.7
2	F	246	LEU	4.7
2	B	801	VAL	4.7
2	B	910	GLU	4.7
2	F	39	ASP	4.7
2	B	823	TYR	4.7
2	B	1243	GLU	4.6
2	F	132	TYR	4.6
2	F	830	ILE	4.6
2	B	856	VAL	4.6
2	F	312	ILE	4.5
2	F	795	ILE	4.5
2	B	876	VAL	4.5
1	E	34	G	4.4
2	F	473	ILE	4.4

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Mol	Chain	Res	Type	RSRZ
2	F	863	ASN	4.4
2	B	852	ILE	4.3
2	B	894	GLN	4.3
2	F	788	ILE	4.3
2	B	867	SER	4.3
5	J	36	G	4.2
2	F	252	PHE	4.2
2	B	843	PRO	4.2
2	B	1050	ILE	4.2
2	F	141	LYS	4.2
2	F	877	LYS	4.2
2	B	824	VAL	4.2
2	F	267	SER	4.2
2	F	304	ASP	4.2
2	F	314	LYS	4.2
2	F	271	TYR	4.2
2	F	815	TYR	4.2
2	F	308	VAL	4.1
2	F	297	SER	4.1
2	F	224	ASN	4.1
2	B	871	PRO	4.1
2	F	1247	GLY	4.1
2	F	114	GLU	4.1
2	B	816	LEU	4.0
2	B	908	LEU	4.0
2	F	703	THR	4.0
2	F	284	ASP	4.0
2	F	207	ASP	4.0
2	F	152	ARG	4.0
2	F	679	ILE	4.0
2	F	73	THR	4.0
2	B	1073	VAL	3.9
2	F	158	LEU	3.9
2	F	286	TYR	3.9
2	F	702	LEU	3.9
2	F	886	LEU	3.9
2	F	81	TYR	3.8
2	F	643	PHE	3.8
2	F	225	LEU	3.8
2	F	698	HIS	3.8
2	B	243	ALA	3.8
2	B	830	ILE	3.8

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Mol	Chain	Res	Type	RSRZ
2	F	407	ASN	3.8
2	F	257	ASP	3.8
2	B	906	GLY	3.8
2	F	174	LEU	3.8
2	F	791	LEU	3.8
2	B	854	ASN	3.7
2	F	809	GLU	3.7
2	B	903	ALA	3.7
2	F	408	GLY	3.7
2	F	399	LEU	3.7
2	F	269	ASP	3.6
2	B	1021	MET	3.6
2	B	1051	THR	3.6
2	F	833	LEU	3.6
2	F	120	GLY	3.6
5	J	42	A	3.6
2	B	901	THR	3.6
2	F	281	GLN	3.6
2	B	1084	ARG	3.6
2	F	307	ARG	3.6
2	F	359	TYR	3.6
2	F	784	ILE	3.6
2	B	310	THR	3.6
2	F	483	ASP	3.6
2	F	166	GLY	3.5
2	B	885	GLN	3.5
2	F	145	SER	3.5
2	F	1123	LYS	3.5
2	B	886	LEU	3.5
5	J	43	G	3.5
2	B	463	ALA	3.5
2	F	683	LEU	3.5
2	B	259	ALA	3.5
2	F	243	ALA	3.5
2	B	859	ARG	3.5
2	B	902	LYS	3.4
2	F	302	LEU	3.4
2	F	133	PRO	3.4
2	F	249	THR	3.4
2	F	1252	ASN	3.4
2	F	794	GLN	3.4
2	F	799	HIS	3.4

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Mol	Chain	Res	Type	RSRZ
2	B	898	ASP	3.4
2	B	912	ASP	3.4
2	F	118	ILE	3.4
2	F	154	ILE	3.4
2	F	153	LEU	3.4
2	B	268	LYS	3.4
2	F	415	HIS	3.4
2	B	870	VAL	3.4
2	F	706	GLU	3.4
2	F	811	LEU	3.4
2	B	840	ALA	3.3
2	B	909	SER	3.3
2	F	824	VAL	3.3
2	B	855	LYS	3.3
2	F	211	ILE	3.3
2	F	443	ILE	3.3
2	F	478	PHE	3.3
2	B	808	ASN	3.3
2	F	210	ALA	3.3
2	B	836	TYR	3.3
2	F	423	LEU	3.3
2	F	806	LEU	3.3
2	F	155	TYR	3.2
2	F	694	MET	3.2
2	F	627	GLU	3.2
2	F	882	TYR	3.2
2	F	212	LEU	3.2
2	F	332	LEU	3.2
2	F	891	LEU	3.2
2	B	861	ASP	3.2
2	F	309	ASN	3.2
2	F	416	LEU	3.2
2	F	369	GLN	3.2
2	B	703	THR	3.2
2	F	440	ILE	3.2
2	F	800	PRO	3.2
1	A	1	U	3.1
2	F	247	GLY	3.1
2	B	849	ASP	3.1
2	F	119	PHE	3.1
2	F	136	TYR	3.1
2	F	421	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
2	F	317	LEU	3.1
2	F	445	THR	3.1
2	B	793	SER	3.1
2	B	384	ASP	3.1
2	F	873	GLU	3.1
2	B	462	PHE	3.1
2	F	196	PHE	3.1
2	F	135	ILE	3.1
2	F	781	MET	3.1
2	F	315	ALA	3.1
2	B	882	TYR	3.1
2	F	178	ASN	3.1
2	F	208	ALA	3.1
2	F	229	LEU	3.1
2	F	444	LEU	3.1
2	F	892	ILE	3.1
2	F	357	ASN	3.0
2	F	140	LYS	3.0
2	F	705	LYS	3.0
2	F	201	ILE	3.0
2	F	389	LEU	3.0
2	B	803	ASN	3.0
2	F	117	PRO	3.0
2	B	1245	LEU	3.0
2	F	331	ASP	3.0
2	B	916	PHE	3.0
2	F	351	PHE	3.0
2	F	691	ARG	3.0
2	F	149	ALA	3.0
2	F	777	SER	3.0
2	F	700	ASP	3.0
2	B	829	ASP	2.9
2	F	290	PHE	2.9
2	F	372	PHE	2.9
2	F	79	ILE	2.9
2	B	240	ASN	2.9
2	F	813	LEU	2.9
2	F	482	VAL	2.9
2	F	485	GLY	2.9
2	F	693	PHE	2.9
2	B	811	LEU	2.9
2	B	673	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
2	F	704	PHE	2.9
2	B	806	LEU	2.9
2	F	335	LEU	2.9
2	F	398	LEU	2.9
2	B	1246	LYS	2.9
2	F	836	TYR	2.9
2	B	815	TYR	2.9
2	F	321	MET	2.9
2	F	1126	TRP	2.8
2	F	874	GLU	2.8
2	F	883	TRP	2.8
2	B	784	ILE	2.8
2	F	122	ILE	2.8
2	F	651	LEU	2.8
2	F	192	TYR	2.8
2	F	701	SER	2.8
2	F	85	ILE	2.8
2	F	612	ASN	2.8
5	I	36	G	2.8
2	F	157	ALA	2.8
2	B	308	VAL	2.8
2	F	528	LYS	2.8
2	B	1048	THR	2.8
2	B	897	PHE	2.8
2	B	888	ASN	2.8
2	B	853	ASP	2.7
2	F	588	ASN	2.7
2	B	258	LEU	2.7
4	D	12	DG	2.7
2	B	1042	ILE	2.7
2	F	950	ILE	2.7
2	B	837	ASP	2.7
2	F	298	ASP	2.7
4	H	2	DT	2.7
2	B	25	TYR	2.7
2	B	818	ASN	2.7
2	B	1039	TYR	2.7
2	F	881	ASN	2.7
3	C	1	DC	2.7
2	F	248	LEU	2.7
2	B	904	GLU	2.7
2	B	868	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	E	33	U	2.7
2	B	304	ASP	2.7
2	F	412	HIS	2.7
3	C	24	DG	2.7
1	A	2	U	2.7
2	F	106	LEU	2.7
2	B	518	PHE	2.6
2	B	1046	PHE	2.6
2	B	1258	PHE	2.6
2	F	1132	GLY	2.6
2	F	804	THR	2.6
2	B	1248	SER	2.6
2	F	91	ALA	2.6
2	F	151	LEU	2.6
2	B	697	ILE	2.6
2	F	567	ASP	2.6
2	F	250	PRO	2.6
2	F	163	LYS	2.6
2	F	98	PHE	2.6
2	F	352	PHE	2.6
2	B	1034	ALA	2.6
1	E	28	A	2.6
2	F	172	GLY	2.6
2	F	193	ASN	2.6
2	F	202	ASN	2.6
2	F	636	LEU	2.6
2	F	530	VAL	2.6
2	F	789	LYS	2.6
2	F	878	LYS	2.6
2	B	721	HIS	2.6
2	B	1040	SER	2.6
2	F	256	PHE	2.6
2	B	796	LEU	2.6
2	B	838	VAL	2.6
2	F	452	VAL	2.6
2	B	270	THR	2.6
2	B	799	HIS	2.5
2	F	347	TYR	2.5
2	F	887	LEU	2.5
2	B	1018	VAL	2.5
2	F	143	VAL	2.5
2	F	708	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
2	B	687	GLY	2.5
2	F	390	LEU	2.5
2	F	123	VAL	2.5
2	F	227	ALA	2.5
2	F	449	PRO	2.5
2	F	1112	PRO	2.5
2	F	642	LEU	2.5
2	F	797	LYS	2.5
2	B	860	SER	2.5
2	F	538	ALA	2.5
2	F	441	GLU	2.5
2	F	240	ASN	2.5
2	F	876	VAL	2.5
2	F	581	SER	2.5
2	B	850	ASP	2.5
2	F	150	ASP	2.5
5	I	98	U	2.5
2	F	268	LYS	2.5
2	F	348	LYS	2.5
2	F	536	LYS	2.5
2	B	911	LEU	2.5
2	F	138	LEU	2.5
2	B	844	GLN	2.5
2	B	262	ALA	2.4
2	B	1196	ILE	2.4
2	F	219	SER	2.4
2	F	682	PHE	2.4
2	B	1017	ASP	2.4
2	F	99	HIS	2.4
2	F	801	VAL	2.4
2	F	709	GLN	2.4
2	F	322	ILE	2.4
2	B	273	ASP	2.4
2	B	756	PRO	2.4
2	B	530	VAL	2.4
2	B	717	GLY	2.4
2	F	162	ILE	2.4
2	F	414	ILE	2.4
2	B	260	GLU	2.4
2	F	606	PHE	2.4
2	F	527	VAL	2.4
2	B	1247	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
2	F	360	ALA	2.4
2	B	807	GLN	2.4
2	B	1244	LYS	2.4
2	F	426	GLN	2.4
2	B	706	GLU	2.4
2	F	802	GLU	2.4
5	I	37	U	2.4
2	F	685	SER	2.4
1	A	34	G	2.4
2	F	476	TRP	2.4
2	F	364	ASP	2.4
2	F	853	ASP	2.4
2	B	1020	LYS	2.4
2	F	604	LYS	2.4
2	F	1244	LYS	2.4
2	B	832	ARG	2.4
2	F	105	PHE	2.4
2	F	867	SER	2.4
2	B	239	GLY	2.3
2	B	585	ASP	2.3
2	F	169	LEU	2.3
2	F	194	GLN	2.3
2	B	28	PRO	2.3
2	B	872	SER	2.3
2	F	230	PRO	2.3
2	F	367	ALA	2.3
2	F	397	ASP	2.3
2	F	433	LEU	2.3
2	F	587	PHE	2.3
2	B	862	LYS	2.3
2	F	363	ILE	2.3
2	B	863	ASN	2.3
2	F	803	ASN	2.3
5	J	38	A	2.3
2	F	647	VAL	2.3
2	F	324	ARG	2.3
2	B	777	SER	2.3
2	F	793	SER	2.3
2	B	527	VAL	2.3
2	F	586	ARG	2.3
2	F	632	ILE	2.3
2	F	1249	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
2	F	621	LEU	2.3
2	F	356	LYS	2.3
2	F	484	LYS	2.3
2	F	100	ARG	2.3
2	B	47	LEU	2.2
2	B	263	LYS	2.2
2	F	430	TYR	2.2
2	F	814	TYR	2.2
2	F	834	SER	2.2
2	B	783	ARG	2.2
2	B	1145	VAL	2.2
2	F	885	GLN	2.2
2	F	144	ASP	2.2
2	F	613	GLU	2.2
2	F	350	ILE	2.2
2	F	448	ILE	2.2
2	F	1120	ILE	2.2
2	F	184	LEU	2.2
2	F	1011	GLY	2.2
2	F	375	PHE	2.2
2	F	466	THR	2.2
2	B	1036	TYR	2.2
2	F	557	ARG	2.2
2	F	817	GLN	2.2
2	F	785	GLU	2.2
2	B	839	ASP	2.2
2	F	947	ASP	2.2
2	F	1193	ASP	2.2
2	B	176	PRO	2.2
2	B	1074	TRP	2.2
2	F	405	PHE	2.2
2	F	139	ARG	2.2
2	F	638	THR	2.2
2	B	922	VAL	2.2
2	F	805	GLN	2.2
2	B	229	LEU	2.2
2	B	1236	LEU	2.2
2	B	1035	LYS	2.2
2	F	442	LYS	2.2
2	F	422	ILE	2.2
2	F	161	MET	2.2
2	F	798	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	800	PRO	2.2
2	B	1090	PRO	2.2
2	F	168	PHE	2.2
5	J	47	A	2.2
2	B	988	TYR	2.1
2	B	1002	PRO	2.1
2	F	431	PRO	2.1
3	G	24	DG	2.1
2	F	185	PHE	2.1
2	F	432	PHE	2.1
2	B	875	VAL	2.1
2	B	975	VAL	2.1
2	B	386	THR	2.1
2	F	334	LEU	2.1
2	F	571	LYS	2.1
2	B	1250	GLU	2.1
2	F	318	SER	2.1
2	F	497	ASN	2.1
2	F	126	VAL	2.1
1	E	31	U	2.1
2	B	791	LEU	2.1
2	B	913	LYS	2.1
2	F	101	LEU	2.1
2	F	222	LEU	2.1
2	F	594	TYR	2.1
2	B	729	GLY	2.1
2	B	1249	PRO	2.1
2	F	125	GLU	2.1
2	F	533	GLY	2.1
2	F	658	GLY	2.1
2	F	860	SER	2.1
2	F	880	LYS	2.1
2	F	943	TYR	2.1
2	B	1209	GLY	2.1
2	B	569	PHE	2.1
2	F	575	PHE	2.1
2	B	561	VAL	2.1
2	B	1252	ASN	2.1
2	F	199	ASN	2.1
2	F	1130	LYS	2.1
2	B	1238	LEU	2.1
2	F	598	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
2	F	601	ILE	2.1
2	B	1241	HIS	2.1
2	B	269	ASP	2.1
2	F	534	MET	2.1
2	B	271	TYR	2.1
2	F	488	ALA	2.1
4	H	12	DG	2.1
2	B	1162	GLU	2.1
2	F	391	VAL	2.0
2	F	393	LEU	2.0
2	F	690	ASN	2.0
2	F	852	ILE	2.0
2	B	821	ASP	2.0
2	F	628	ASP	2.0
2	B	1091	GLN	2.0
2	B	537	PRO	2.0
2	B	880	LYS	2.0
2	B	1304	GLU	2.0
2	F	130	GLU	2.0
2	F	189	VAL	2.0
2	B	899	ASN	2.0
2	B	1224	ASN	2.0
2	B	249	THR	2.0
2	F	451	TYR	2.0
2	F	353	ASP	2.0
2	B	954	LYS	2.0
2	F	316	PRO	2.0
2	F	475	PRO	2.0
2	F	503	PRO	2.0
2	F	526	LYS	2.0
2	B	785	GLU	2.0
2	F	311	GLU	2.0
2	B	780	ARG	2.0
2	F	783	ARG	2.0
1	E	5	C	2.0

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

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.