



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 27, 2023 – 09:08 PM EDT

PDB ID : 3GUT
Title : Crystal structure of a higher-order complex of p50:RelA bound to the HIV-1 LTR
Authors : Stroud, J.C.; Oltman, A.J.; Han, A.; Bates, D.L.; Chen, L.
Deposited on : 2009-03-30
Resolution : 3.59 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 : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.35
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35

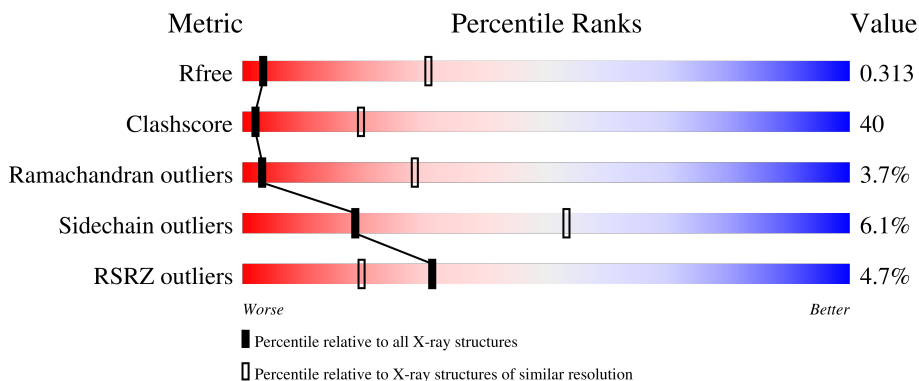
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.59 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}	130704	1257 (3.70-3.50)
Clashscore	141614	1353 (3.70-3.50)
Ramachandran outliers	138981	1307 (3.70-3.50)
Sidechain outliers	138945	1307 (3.70-3.50)
RSRZ outliers	127900	1161 (3.70-3.50)

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	273	
1	C	273	
1	E	273	
1	G	273	
2	B	312	

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Mol	Chain	Length	Quality of chain
2	D	312	<p>5% 47% 46% 5%</p>
2	F	312	<p>6% 47% 49%</p>
2	H	312	<p>7% 46% 47% 5%</p>
3	I	26	<p>42% 54%</p>
3	X	26	<p>35% 58% 8%</p>
4	J	26	<p>12% 73% 15%</p>
4	Y	26	<p>12% 73% 15%</p>

2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 20640 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 protein called Transcription factor p65.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	273	2176	1356	401	408	11	0	0	0
1	C	273	2176	1356	401	408	11	0	0	0
1	E	273	2176	1356	401	408	11	0	0	0
1	G	273	2176	1356	401	408	11	0	0	0

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	19	ALA	-	expression tag	UNP Q04206
A	99	TYR	PHE	SEE REMARK 999	UNP Q04206
A	103	ASP	GLU	SEE REMARK 999	UNP Q04206
A	109	SER	CYS	SEE REMARK 999	UNP Q04206
A	142	HIS	GLN	SEE REMARK 999	UNP Q04206
A	169	ALA	SER	SEE REMARK 999	UNP Q04206
A	174	LEU	ARG	SEE REMARK 999	UNP Q04206
A	176	THR	PRO	SEE REMARK 999	UNP Q04206
C	19	ALA	-	expression tag	UNP Q04206
C	99	TYR	PHE	SEE REMARK 999	UNP Q04206
C	103	ASP	GLU	SEE REMARK 999	UNP Q04206
C	109	SER	CYS	SEE REMARK 999	UNP Q04206
C	142	HIS	GLN	SEE REMARK 999	UNP Q04206
C	169	ALA	SER	SEE REMARK 999	UNP Q04206
C	174	LEU	ARG	SEE REMARK 999	UNP Q04206
C	176	THR	PRO	SEE REMARK 999	UNP Q04206
E	19	ALA	-	expression tag	UNP Q04206
E	99	TYR	PHE	SEE REMARK 999	UNP Q04206
E	103	ASP	GLU	SEE REMARK 999	UNP Q04206
E	109	SER	CYS	SEE REMARK 999	UNP Q04206
E	142	HIS	GLN	SEE REMARK 999	UNP Q04206

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Chain	Residue	Modelled	Actual	Comment	Reference
E	169	ALA	SER	SEE REMARK 999	UNP Q04206
E	174	LEU	ARG	SEE REMARK 999	UNP Q04206
E	176	THR	PRO	SEE REMARK 999	UNP Q04206
G	19	ALA	-	expression tag	UNP Q04206
G	99	TYR	PHE	SEE REMARK 999	UNP Q04206
G	103	ASP	GLU	SEE REMARK 999	UNP Q04206
G	109	SER	CYS	SEE REMARK 999	UNP Q04206
G	142	HIS	GLN	SEE REMARK 999	UNP Q04206
G	169	ALA	SER	SEE REMARK 999	UNP Q04206
G	174	LEU	ARG	SEE REMARK 999	UNP Q04206
G	176	THR	PRO	SEE REMARK 999	UNP Q04206

- Molecule 2 is a protein called Nuclear factor NF-kappa-B p105 subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	312	2454	1554	428	460	12	0	0	0
2	D	312	2454	1554	428	460	12	0	0	0
2	F	312	2454	1554	428	460	12	0	0	0
2	H	312	2454	1554	428	460	12	0	0	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	420	VAL	ILE	SEE REMARK 999	UNP P19838
B	471	SER	PRO	SEE REMARK 999	UNP P19838
B	487	THR	GLY	SEE REMARK 999	UNP P19838
B	493	ILE	LEU	SEE REMARK 999	UNP P19838
B	499	VAL	LEU	SEE REMARK 999	UNP P19838
B	619	VAL	ILE	SEE REMARK 999	UNP P19838
D	420	VAL	ILE	SEE REMARK 999	UNP P19838
D	471	SER	PRO	SEE REMARK 999	UNP P19838
D	487	THR	GLY	SEE REMARK 999	UNP P19838
D	493	ILE	LEU	SEE REMARK 999	UNP P19838
D	499	VAL	LEU	SEE REMARK 999	UNP P19838
D	619	VAL	ILE	SEE REMARK 999	UNP P19838
F	420	VAL	ILE	SEE REMARK 999	UNP P19838
F	471	SER	PRO	SEE REMARK 999	UNP P19838
F	487	THR	GLY	SEE REMARK 999	UNP P19838

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Chain	Residue	Modelled	Actual	Comment	Reference
F	493	ILE	LEU	SEE REMARK 999	UNP P19838
F	499	VAL	LEU	SEE REMARK 999	UNP P19838
F	619	VAL	ILE	SEE REMARK 999	UNP P19838
H	420	VAL	ILE	SEE REMARK 999	UNP P19838
H	471	SER	PRO	SEE REMARK 999	UNP P19838
H	487	THR	GLY	SEE REMARK 999	UNP P19838
H	493	ILE	LEU	SEE REMARK 999	UNP P19838
H	499	VAL	LEU	SEE REMARK 999	UNP P19838
H	619	VAL	ILE	SEE REMARK 999	UNP P19838

- Molecule 3 is a DNA chain called HIV-LTR Core Forward Strand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	X	26	Total	C	N	O	P	0	0	0
			530	253	95	157	25			
3	I	26	Total	C	N	O	P	0	0	0
			530	253	95	157	25			

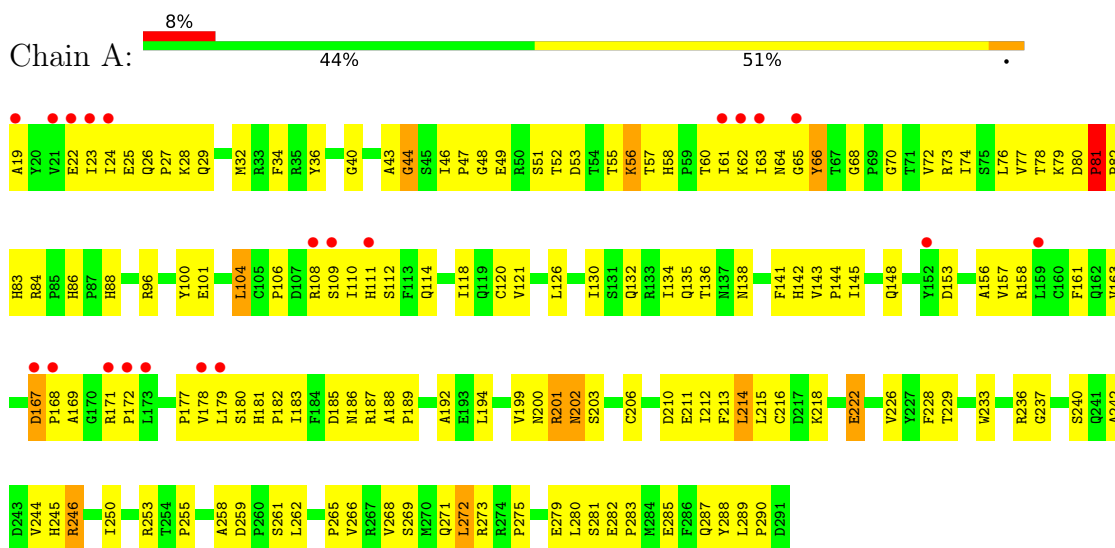
- Molecule 4 is a DNA chain called HIV-LTR Core Reverse Strand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	Y	26	Total	C	N	O	P	0	0	0
			530	252	102	151	25			
4	J	26	Total	C	N	O	P	0	0	0
			530	252	102	151	25			

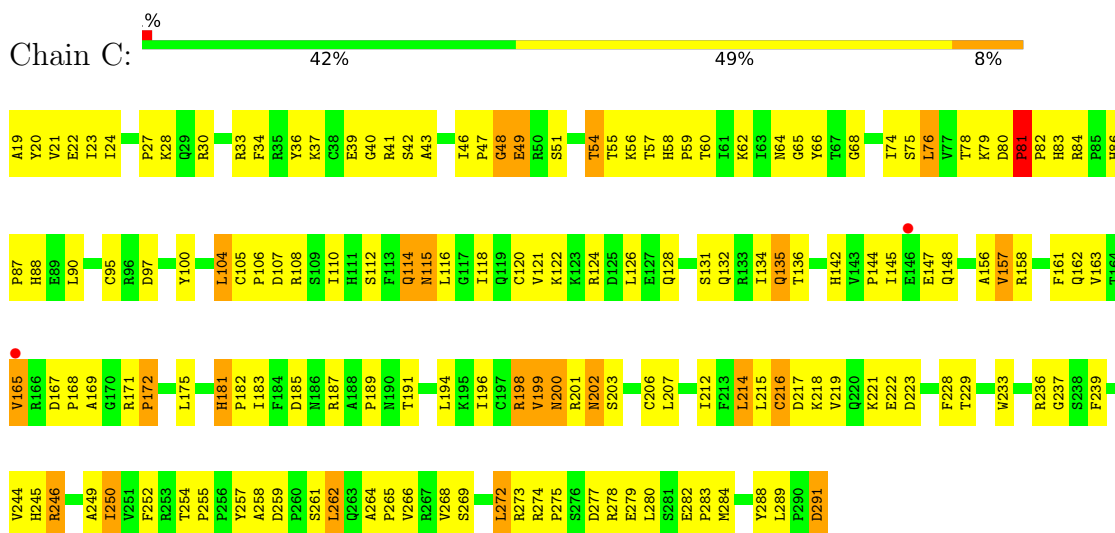
3 Residue-property plots i

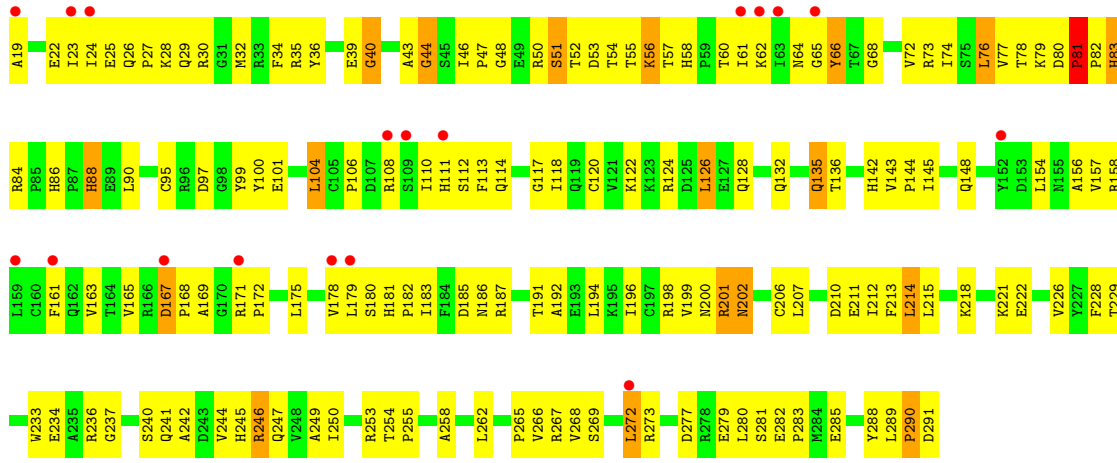
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Transcription factor p65

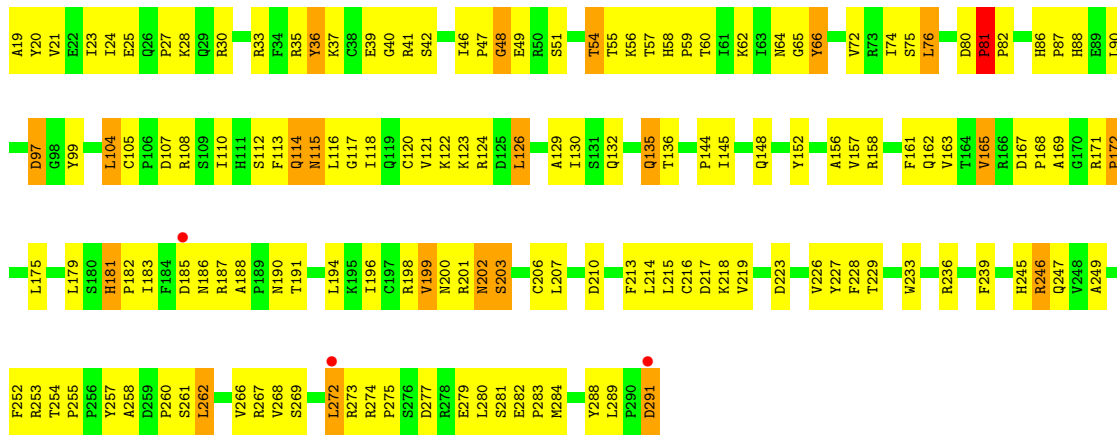


- Molecule 1: Transcription factor p65

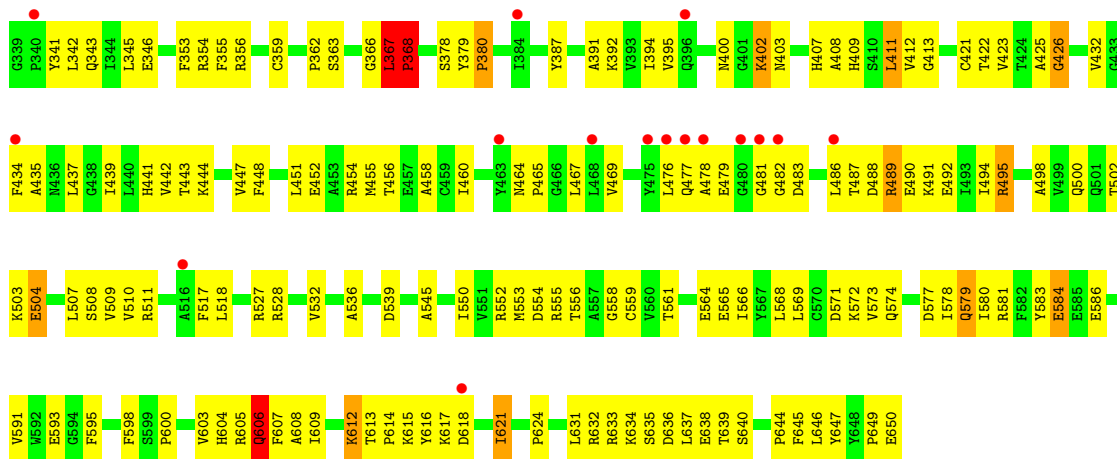




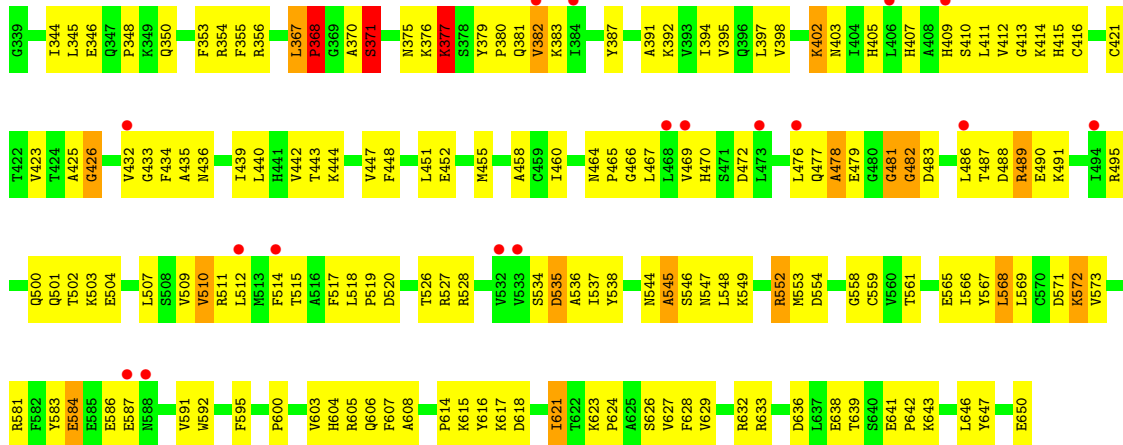
• Molecule 1: Transcription factor p65



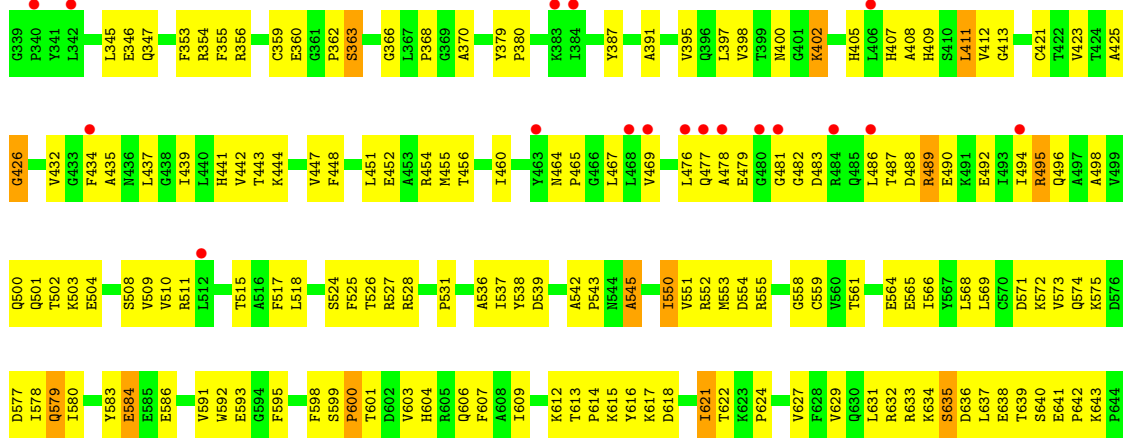
• Molecule 2: Nuclear factor NF-kappa-B p105 subunit



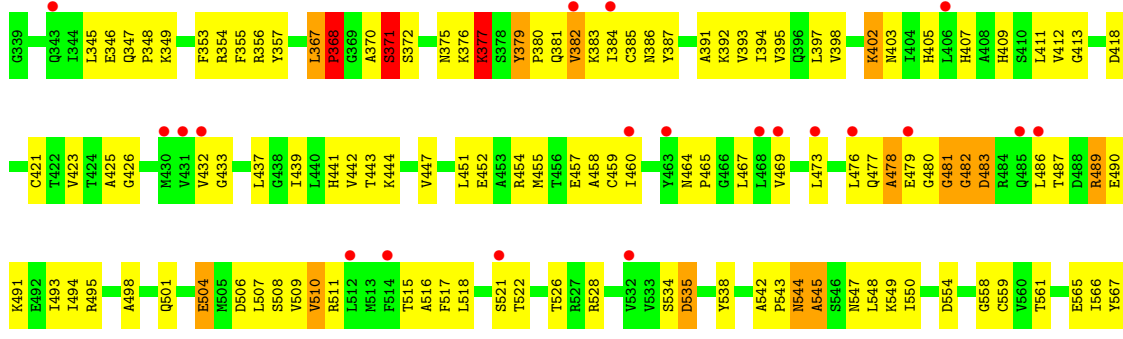
• Molecule 2: Nuclear factor NF-kappa-B p105 subunit



• Molecule 2: Nuclear factor NF-kappa-B p105 subunit

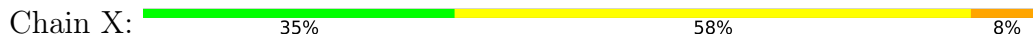


• Molecule 2: Nuclear factor NF-kappa-B p105 subunit

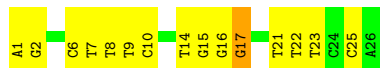




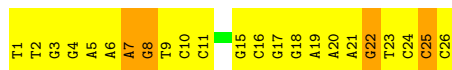
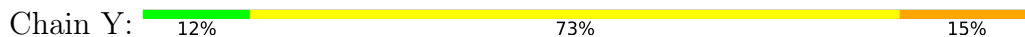
● Molecule 3: HIV-LTR Core Forward Strand



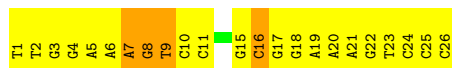
● Molecule 3: HIV-LTR Core Forward Strand



● Molecule 4: HIV-LTR Core Reverse Strand



● Molecule 4: HIV-LTR Core Reverse Strand



4 Data and refinement statistics i

Property	Value	Source
Space group	P 42	Depositor
Cell constants a, b, c, α , β , γ	167.49Å 167.49Å 172.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.45 – 3.59 46.89 – 3.59	Depositor EDS
% Data completeness (in resolution range)	81.2 (46.45-3.59) 91.9 (46.89-3.59)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.26 (at 3.57Å)	Xtrriage
Refinement program	CNS	Depositor
R, R_{free}	0.245 , 0.301 0.259 , 0.313	Depositor DCC
R_{free} test set	5648 reflections (10.14%)	wwPDB-VP
Wilson B-factor (Å ²)	118.8	Xtrriage
Anisotropy	0.196	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 83.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.011 for -h,-l,-k 0.005 for -h,l,k 0.006 for l,-k,h 0.012 for -l,-k,-h 0.438 for h,-k,-l	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	20640	wwPDB-VP
Average B, all atoms (Å ²)	150.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 40.03 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.9062e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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	0.50	0/2228	0.75	1/3021 (0.0%)
1	C	0.54	0/2228	0.79	0/3021
1	E	0.50	0/2228	0.76	0/3021
1	G	0.52	0/2228	0.79	0/3021
2	B	0.67	3/2506 (0.1%)	0.94	6/3384 (0.2%)
2	D	0.63	3/2506 (0.1%)	0.97	11/3384 (0.3%)
2	F	0.54	0/2506	0.72	0/3384
2	H	0.65	3/2506 (0.1%)	0.98	12/3384 (0.4%)
3	I	0.87	0/593	0.97	0/914
3	X	0.89	0/593	1.00	0/914
4	J	0.91	1/595 (0.2%)	0.98	0/916
4	Y	0.95	2/595 (0.3%)	0.98	0/916
All	All	0.62	12/21312 (0.1%)	0.86	30/29280 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	G	0	1
2	B	0	1
2	D	0	1
2	H	0	1
3	I	0	2
3	X	0	2
4	J	0	3
4	Y	0	2
All	All	0	13

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	367	LEU	CG-CD2	-10.36	1.13	1.51
2	B	368	PRO	N-CD	8.14	1.59	1.47
2	H	370	ALA	C-O	6.68	1.36	1.23
2	D	370	ALA	CA-C	-6.58	1.35	1.52
2	H	370	ALA	CA-C	-6.19	1.36	1.52
2	D	370	ALA	C-O	6.04	1.34	1.23
2	B	368	PRO	CA-CB	-5.93	1.41	1.53
2	D	371	SER	CB-OG	-5.77	1.34	1.42
2	H	371	SER	CB-OG	-5.74	1.34	1.42
4	J	8	DG	C2-N2	-5.60	1.28	1.34
4	Y	8	DG	C2-N2	-5.39	1.29	1.34
4	Y	22	DG	C2-N2	-5.20	1.29	1.34

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	367	LEU	C-N-CD	-25.69	64.09	120.60
2	H	371	SER	N-CA-CB	17.03	136.04	110.50
2	D	371	SER	N-CA-CB	17.00	136.00	110.50
2	H	370	ALA	CA-C-N	-12.45	89.82	117.20
2	D	370	ALA	CA-C-N	-12.13	90.51	117.20
2	B	368	PRO	CA-N-CD	-12.01	94.69	111.50
2	H	370	ALA	O-C-N	9.70	138.22	122.70
2	D	370	ALA	O-C-N	9.56	138.00	122.70
2	B	367	LEU	C-N-CA	8.73	158.66	122.00
2	D	370	ALA	N-CA-CB	8.43	121.89	110.10
2	H	370	ALA	N-CA-CB	8.28	121.69	110.10
2	D	367	LEU	C-N-CD	-8.06	102.87	120.60
2	B	367	LEU	CB-CG-CD1	8.01	124.62	111.00
2	H	367	LEU	C-N-CD	-7.86	103.30	120.60
2	B	367	LEU	N-CA-CB	7.76	125.93	110.40
2	D	371	SER	CA-C-O	7.40	135.63	120.10
2	H	371	SER	CA-C-O	7.35	135.53	120.10
2	D	371	SER	CA-C-N	-7.18	101.41	117.20
2	H	371	SER	CA-C-N	-7.12	101.53	117.20
2	H	371	SER	CA-CB-OG	-6.71	93.08	111.20
2	D	371	SER	CA-CB-OG	-6.69	93.13	111.20
2	D	377	LYS	N-CA-C	6.03	127.29	111.00
2	H	377	LYS	N-CA-C	6.02	127.25	111.00
2	B	367	LEU	CB-CG-CD2	-5.95	100.89	111.00
2	H	370	ALA	CA-C-O	5.34	131.31	120.10
1	A	216	CYS	CA-CB-SG	-5.26	104.53	114.00
2	H	368	PRO	N-CA-CB	-5.23	96.85	102.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	368	PRO	N-CA-CB	-5.22	96.86	102.60
2	D	379	TYR	CA-CB-CG	5.20	123.28	113.40
2	H	379	TYR	CA-CB-CG	5.04	122.98	113.40

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	367	LEU	Mainchain
2	D	371	SER	Mainchain
1	G	227	TYR	Sidechain
2	H	371	SER	Mainchain
3	I	17	DG	Sidechain
3	I	25	DC	Sidechain
4	J	16	DC	Sidechain
4	J	7	DA	Sidechain
4	J	9	DT	Sidechain
3	X	16	DG	Sidechain
3	X	17	DG	Sidechain
4	Y	25	DC	Sidechain
4	Y	7	DA	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2176	0	2137	194	0
1	C	2176	0	2137	183	0
1	E	2176	0	2137	222	0
1	G	2176	0	2137	184	0
2	B	2454	0	2451	164	0
2	D	2454	0	2450	172	0
2	F	2454	0	2451	176	0
2	H	2454	0	2450	166	0
3	I	530	0	295	28	0
3	X	530	0	295	39	0
4	J	530	0	290	74	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	Y	530	0	288	71	0
All	All	20640	0	19518	1596	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 40.

All (1596) 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:572:LYS:NZ	2:B:606:GLN:HG2	1.45	1.32
2:F:572:LYS:NZ	2:F:606:GLN:HG2	1.53	1.23
2:H:572:LYS:NZ	2:H:606:GLN:HG2	1.59	1.18
3:I:15:DG:H2''	3:I:16:DG:H5''	1.17	1.15
4:Y:9:DT:H2''	4:Y:10:DC:H5''	1.14	1.13
4:J:9:DT:H2''	4:J:10:DC:H5''	1.27	1.12
3:X:15:DG:H2''	3:X:16:DG:H5''	1.17	1.10
2:D:572:LYS:NZ	2:D:606:GLN:HG2	1.67	1.10
1:A:51:SER:HB2	1:A:57:THR:CG2	1.82	1.09
4:Y:18:DG:H2''	4:Y:19:DA:H5''	1.30	1.08
4:Y:9:DT:H2''	4:Y:10:DC:C5'	1.84	1.07
4:Y:15:DG:H2''	4:Y:16:DC:H5''	1.33	1.06
4:J:18:DG:H2''	4:J:19:DA:H5''	1.33	1.06
2:F:572:LYS:HZ1	2:F:606:GLN:HG2	1.06	1.05
1:A:52:THR:HG22	1:A:53:ASP:H	1.20	1.05
3:X:15:DG:C2'	3:X:16:DG:H5''	1.86	1.04
1:C:24:ILE:HD11	1:C:62:LYS:HB2	1.38	1.04
1:G:282:GLU:HG2	1:G:283:PRO:HD2	1.34	1.04
1:G:24:ILE:HD11	1:G:62:LYS:HB2	1.35	1.03
3:I:15:DG:C2'	3:I:16:DG:H5''	1.88	1.03
4:Y:9:DT:C2'	4:Y:10:DC:H5''	1.88	1.02
1:E:51:SER:HB2	1:E:57:THR:CG2	1.90	1.02
1:E:262:LEU:HD21	1:E:266:VAL:HG12	1.43	1.00
1:A:46:ILE:HD11	1:A:118:ILE:HD11	1.43	0.98
4:J:15:DG:H2''	4:J:16:DC:H5''	1.43	0.97
1:A:211:GLU:O	1:A:212:ILE:HD13	1.66	0.96
2:H:367:LEU:HD11	2:H:439:ILE:HD11	1.48	0.95
2:D:367:LEU:HD11	2:D:439:ILE:HD11	1.46	0.94
1:E:211:GLU:O	1:E:212:ILE:HD13	1.68	0.94
2:D:489:ARG:O	2:D:489:ARG:HD3	1.69	0.93
2:B:572:LYS:HZ2	2:B:606:GLN:HG2	1.33	0.93
4:J:16:DC:H2''	4:J:17:DG:H5''	1.51	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:52:THR:HG22	1:E:53:ASP:H	1.34	0.92
1:G:74:ILE:HD12	1:G:161:PHE:CD2	2.04	0.92
4:Y:18:DG:H2''	4:Y:19:DA:C5'	1.99	0.92
4:J:9:DT:H2''	4:J:10:DC:C5'	2.01	0.91
1:A:262:LEU:HD21	1:A:266:VAL:HG12	1.52	0.91
2:D:487:THR:OG1	2:D:490:GLU:HG3	1.70	0.91
4:J:9:DT:C2'	4:J:10:DC:H5''	1.98	0.91
3:X:15:DG:H2''	3:X:16:DG:C5'	2.01	0.91
1:C:74:ILE:HD12	1:C:161:PHE:CD2	2.06	0.91
3:I:15:DG:H2''	3:I:16:DG:C5'	2.01	0.91
2:F:402:LYS:N	2:F:402:LYS:HE3	1.86	0.90
2:H:572:LYS:HZ1	2:H:606:GLN:HG2	1.19	0.90
1:A:51:SER:HB2	1:A:57:THR:CB	2.02	0.89
1:G:88:HIS:CE1	1:G:120:CYS:HB2	2.06	0.89
3:X:7:DT:O2	4:Y:22:DG:N2	2.06	0.89
4:Y:18:DG:C2'	4:Y:19:DA:H5''	2.02	0.89
1:E:46:ILE:HD11	1:E:118:ILE:HD11	1.51	0.89
1:E:48:GLY:H	1:E:57:THR:HG21	1.37	0.89
1:A:48:GLY:H	1:A:57:THR:CG2	1.86	0.89
1:E:51:SER:HB2	1:E:57:THR:HB	1.53	0.89
1:E:51:SER:HB2	1:E:57:THR:CB	2.01	0.89
2:D:572:LYS:HZ1	2:D:606:GLN:HG2	1.35	0.89
4:Y:15:DG:C2'	4:Y:16:DC:H5''	2.03	0.89
1:C:282:GLU:HG2	1:C:283:PRO:HD2	1.55	0.88
2:B:572:LYS:HZ3	2:B:606:GLN:HG2	1.13	0.88
2:D:397:LEU:HD21	2:D:411:LEU:HD13	1.57	0.87
1:E:48:GLY:H	1:E:57:THR:CG2	1.87	0.87
1:G:236:ARG:HH11	1:G:236:ARG:HG3	1.40	0.87
1:A:167:ASP:HB2	1:A:168:PRO:HD2	1.54	0.86
2:B:367:LEU:HD12	2:B:367:LEU:O	1.74	0.86
2:B:402:LYS:HE3	2:B:402:LYS:N	1.90	0.86
2:F:402:LYS:HE3	2:F:402:LYS:H	1.38	0.86
2:F:621:ILE:HD13	2:F:649:PRO:HB3	1.57	0.86
1:C:21:VAL:HG21	1:C:163:VAL:HG21	1.58	0.86
4:Y:24:DC:H2''	4:Y:25:DC:H5'	1.54	0.86
2:B:621:ILE:HD13	2:B:649:PRO:HB3	1.54	0.86
1:E:167:ASP:OD1	1:E:169:ALA:HB3	1.75	0.86
2:D:382:VAL:HG12	2:D:383:LYS:H	1.39	0.86
2:F:423:VAL:HG21	2:F:432:VAL:HG11	1.58	0.85
2:D:345:LEU:HB2	2:D:381:GLN:O	1.76	0.85
4:J:18:DG:C2'	4:J:19:DA:H5''	2.06	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:ASP:OD1	1:A:169:ALA:HB3	1.76	0.85
2:F:366:GLY:O	2:F:368:PRO:HD3	1.76	0.85
2:F:489:ARG:O	2:F:489:ARG:HD3	1.76	0.85
3:I:22:DT:O2	4:J:7:DA:H2	1.59	0.85
2:F:487:THR:OG1	2:F:490:GLU:HG3	1.76	0.84
4:J:18:DG:H2''	4:J:19:DA:C5'	2.06	0.84
1:E:77:VAL:HG23	1:E:158:ARG:HB2	1.60	0.84
2:F:561:THR:O	2:F:615:LYS:HG3	1.77	0.84
2:H:382:VAL:HG12	2:H:383:LYS:H	1.43	0.84
2:H:487:THR:OG1	2:H:490:GLU:HG3	1.77	0.84
4:J:16:DC:C2'	4:J:17:DG:H5''	2.07	0.83
1:A:51:SER:HB2	1:A:57:THR:HB	1.58	0.83
2:H:489:ARG:O	2:H:489:ARG:HD3	1.78	0.83
2:F:391:ALA:HB3	2:F:425:ALA:HB3	1.59	0.83
2:H:409:HIS:HD2	2:H:442:VAL:HG22	1.44	0.83
2:B:489:ARG:O	2:B:489:ARG:HD3	1.79	0.82
1:C:196:ILE:HG13	1:C:272:LEU:HD22	1.61	0.82
1:G:229:THR:HG23	1:G:269:SER:HB3	1.60	0.82
1:A:236:ARG:HG3	1:A:236:ARG:HH11	1.44	0.82
2:B:395:VAL:HB	2:B:421:CYS:HB3	1.60	0.82
2:B:460:ILE:HG12	2:B:486:LEU:HD13	1.62	0.82
2:F:550:ILE:HD12	2:F:550:ILE:N	1.94	0.82
2:H:407:HIS:ND1	2:H:510:VAL:HG23	1.93	0.82
1:A:19:ALA:HA	1:A:64:ASN:O	1.80	0.82
1:E:167:ASP:HB2	1:E:168:PRO:HD2	1.60	0.82
2:D:387:TYR:CE1	2:D:518:LEU:HD13	2.15	0.81
2:H:409:HIS:CD2	2:H:442:VAL:HG22	2.15	0.81
4:J:15:DG:C2'	4:J:16:DC:H5''	2.10	0.81
1:C:86:HIS:ND1	1:C:87:PRO:HD2	1.96	0.81
1:C:88:HIS:CE1	1:C:120:CYS:HB2	2.15	0.81
2:B:407:HIS:HD2	2:B:409:HIS:H	1.25	0.81
2:H:603:VAL:HG22	2:H:609:ILE:HG12	1.63	0.81
4:J:23:DT:H2''	4:J:24:DC:H5''	1.63	0.81
1:G:30:ARG:HE	1:G:191:THR:HB	1.46	0.81
1:G:262:LEU:HD21	1:G:266:VAL:HG12	1.62	0.81
3:X:23:DT:O2	4:Y:6:DA:H2	1.64	0.80
1:A:202:ASN:HD22	1:A:202:ASN:H	1.29	0.80
2:D:624:PRO:HB2	2:D:646:LEU:HD11	1.63	0.80
2:B:342:LEU:HD13	2:B:343:GLN:N	1.96	0.80
2:F:572:LYS:HZ1	2:F:606:GLN:CG	1.91	0.80
2:H:636:ASP:OD2	2:H:638:GLU:HG2	1.82	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:545:ALA:HA	2:D:633:ARG:NH2	1.96	0.80
1:E:236:ARG:HG3	1:E:236:ARG:HH11	1.47	0.80
4:J:15:DG:H2''	4:J:16:DC:C5'	2.11	0.80
2:B:367:LEU:O	2:B:367:LEU:CD1	2.30	0.80
2:B:391:ALA:HB3	2:B:425:ALA:HB3	1.63	0.80
2:B:402:LYS:HE3	2:B:402:LYS:H	1.44	0.80
2:F:452:GLU:OE2	2:F:495:ARG:HG3	1.80	0.80
4:J:24:DC:H2''	4:J:25:DC:H5'	1.63	0.80
2:H:353:PHE:HE2	2:H:439:ILE:HG12	1.47	0.80
4:Y:15:DG:H2''	4:Y:16:DC:C5'	2.11	0.80
3:I:6:DC:H42	4:J:22:DG:H1	1.29	0.80
1:E:55:THR:HA	2:H:375:ASN:OD1	1.81	0.79
3:I:8:DT:H2''	3:I:9:DT:OP2	1.82	0.79
1:A:51:SER:HB2	1:A:57:THR:HG21	1.61	0.79
2:D:402:LYS:HE3	2:D:402:LYS:H	1.46	0.79
1:A:237:GLY:HA2	1:A:255:PRO:HD3	1.65	0.79
2:F:402:LYS:H	2:F:402:LYS:CE	1.94	0.79
2:F:477:GLN:O	2:F:479:GLU:HG2	1.83	0.79
2:F:550:ILE:HD12	2:F:550:ILE:H	1.46	0.79
2:F:572:LYS:NZ	2:F:606:GLN:CG	2.43	0.79
1:G:51:SER:CB	1:G:57:THR:H	1.95	0.79
2:B:477:GLN:O	2:B:479:GLU:HG2	1.81	0.79
1:C:236:ARG:HG3	1:C:236:ARG:HH11	1.46	0.79
1:C:262:LEU:HD21	1:C:266:VAL:HG12	1.63	0.79
1:E:27:PRO:O	1:E:181:HIS:HE1	1.66	0.79
4:Y:23:DT:H2''	4:Y:24:DC:H5''	1.63	0.78
1:C:19:ALA:O	1:C:175:LEU:HD22	1.84	0.78
2:H:595:PHE:O	2:H:614:PRO:HB3	1.82	0.78
1:A:74:ILE:HG12	1:A:100:TYR:CD1	2.19	0.78
2:D:387:TYR:CE2	2:D:518:LEU:HD22	2.18	0.78
2:H:565:GLU:C	2:H:566:ILE:HD12	2.04	0.77
1:E:202:ASN:HD22	1:E:202:ASN:H	1.31	0.77
2:H:345:LEU:HB2	2:H:381:GLN:O	1.84	0.77
1:A:27:PRO:O	1:A:181:HIS:HE1	1.67	0.77
1:E:51:SER:HB2	1:E:57:THR:HG21	1.64	0.77
1:E:82:PRO:O	1:E:84:ARG:HG3	1.85	0.77
1:C:30:ARG:HE	1:C:191:THR:HB	1.48	0.77
1:E:273:ARG:HD2	1:E:280:LEU:HD21	1.67	0.77
1:A:36:TYR:CE2	3:X:8:DT:H2'	2.19	0.77
1:C:81:PRO:HB2	1:C:82:PRO:HD3	1.65	0.77
1:C:229:THR:HG23	1:C:269:SER:HB3	1.67	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:572:LYS:NZ	2:B:606:GLN:CG	2.39	0.77
2:H:387:TYR:CE2	2:H:518:LEU:HD22	2.20	0.77
1:E:25:GLU:OE2	1:E:50:ARG:HG2	1.85	0.76
3:X:8:DT:H2''	3:X:9:DT:OP2	1.83	0.76
1:G:196:ILE:HG12	1:G:272:LEU:HD22	1.65	0.76
4:J:16:DC:H2''	4:J:17:DG:C5'	2.15	0.76
4:Y:4:DG:H2''	4:Y:5:DA:H5''	1.67	0.76
2:B:423:VAL:HG21	2:B:432:VAL:HG11	1.67	0.76
2:D:402:LYS:HE3	2:D:402:LYS:N	2.01	0.76
2:D:409:HIS:HD2	2:D:442:VAL:HG22	1.50	0.76
1:E:48:GLY:HA3	1:E:57:THR:OG1	1.86	0.76
3:X:7:DT:C2	4:Y:22:DG:N2	2.53	0.76
2:F:460:ILE:HG12	2:F:486:LEU:HD13	1.68	0.76
2:H:542:ALA:HB3	2:H:545:ALA:HB3	1.68	0.76
1:A:82:PRO:O	1:A:84:ARG:HG3	1.86	0.76
2:B:487:THR:OG1	2:B:490:GLU:HG3	1.85	0.76
2:D:409:HIS:CD2	2:D:442:VAL:HG22	2.21	0.76
2:D:595:PHE:O	2:D:614:PRO:HB3	1.85	0.75
1:E:229:THR:HG23	1:E:269:SER:HB3	1.67	0.75
1:G:202:ASN:H	1:G:202:ASN:HD22	1.34	0.75
3:I:21:DT:C2	4:J:8:DG:N2	2.54	0.75
1:A:77:VAL:HG23	1:A:158:ARG:HB2	1.66	0.75
2:F:409:HIS:CD2	2:F:441:HIS:HA	2.22	0.75
2:F:603:VAL:HG22	2:F:609:ILE:HG12	1.67	0.75
1:G:218:LYS:NZ	1:G:218:LYS:HB3	2.02	0.75
2:H:572:LYS:HD3	2:H:573:VAL:N	2.02	0.75
1:G:196:ILE:CG1	1:G:272:LEU:HD22	2.17	0.75
1:A:48:GLY:H	1:A:57:THR:HG21	1.50	0.75
1:E:210:ASP:O	1:E:253:ARG:HA	1.87	0.75
1:C:24:ILE:CD1	1:C:62:LYS:HB2	2.15	0.75
2:B:366:GLY:O	2:B:368:PRO:HD3	1.86	0.74
1:E:81:PRO:HB2	1:E:82:PRO:HD3	1.69	0.74
1:C:51:SER:HB3	1:C:57:THR:H	1.51	0.74
1:C:76:LEU:HD13	1:C:90:LEU:HD13	1.70	0.74
1:A:60:THR:OG1	1:A:112:SER:HB3	1.88	0.74
2:B:613:THR:HG22	2:B:614:PRO:O	1.87	0.74
1:A:56:LYS:HB3	2:D:375:ASN:HD21	1.52	0.74
2:H:559:CYS:SG	2:H:650:GLU:HB2	2.28	0.74
4:J:19:DA:H2''	4:J:20:DA:C8	2.23	0.74
2:F:613:THR:HG23	2:F:614:PRO:HD2	1.69	0.74
2:H:545:ALA:HA	2:H:633:ARG:NH2	2.02	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:621:ILE:HD11	2:F:649:PRO:HD3	1.70	0.73
2:H:624:PRO:HB2	2:H:646:LEU:HD11	1.70	0.73
1:G:81:PRO:HB2	1:G:82:PRO:HD3	1.70	0.73
1:A:229:THR:HG23	1:A:269:SER:HB3	1.68	0.73
4:Y:17:DG:H4'	4:Y:17:DG:OP1	1.88	0.73
1:E:158:ARG:HD3	1:E:179:LEU:HD23	1.71	0.73
4:Y:19:DA:C2	4:Y:20:DA:C2	2.77	0.73
1:E:104:LEU:HD21	1:E:163:VAL:HG13	1.71	0.73
1:G:30:ARG:HH21	1:G:191:THR:HB	1.52	0.73
1:G:185:ASP:OD2	1:G:187:ARG:HB3	1.89	0.73
1:A:27:PRO:HG2	1:A:183:ILE:HD11	1.71	0.73
1:C:198:ARG:O	1:C:199:VAL:HG23	1.89	0.73
1:E:27:PRO:HG2	1:E:183:ILE:HD11	1.71	0.73
1:E:36:TYR:CE2	3:I:8:DT:H2'	2.24	0.73
2:F:467:LEU:N	2:F:467:LEU:HD12	2.04	0.73
2:B:451:LEU:O	2:B:455:MET:HG3	1.87	0.73
1:C:114:GLN:HE21	1:E:241:GLN:HB2	1.53	0.73
1:G:167:ASP:OD1	1:G:169:ALA:HB3	1.89	0.73
2:B:394:ILE:HG22	2:B:422:THR:OG1	1.89	0.72
2:D:387:TYR:CZ	2:D:518:LEU:HD22	2.24	0.72
1:E:23:ILE:HD12	1:E:23:ILE:H	1.53	0.72
1:E:233:TRP:HZ3	1:E:268:VAL:HG11	1.54	0.72
1:A:52:THR:HG22	1:A:53:ASP:N	2.00	0.72
2:D:572:LYS:CE	2:D:606:GLN:HG2	2.19	0.72
1:E:215:LEU:HB3	2:F:604:HIS:CD2	2.24	0.72
4:J:23:DT:H2''	4:J:24:DC:C5'	2.20	0.72
1:G:74:ILE:CD1	1:G:161:PHE:CD2	2.72	0.72
1:C:51:SER:CB	1:C:57:THR:H	2.03	0.72
3:X:8:DT:O2	4:Y:21:DA:H2	1.72	0.72
4:J:24:DC:H2''	4:J:25:DC:C5'	2.19	0.72
3:X:22:DT:O2	4:Y:7:DA:H2	1.72	0.72
2:H:377:LYS:O	2:H:377:LYS:HG3	1.90	0.72
1:A:74:ILE:HB	1:A:100:TYR:HB3	1.70	0.72
1:C:21:VAL:HG21	1:C:163:VAL:CG2	2.19	0.72
1:E:207:LEU:HD12	1:E:291:ASP:OD2	1.89	0.72
2:F:409:HIS:CD2	2:F:442:VAL:H	2.08	0.72
2:B:552:ARG:HG3	2:B:553:MET:H	1.55	0.72
1:C:196:ILE:CG1	1:C:272:LEU:HD22	2.20	0.72
1:E:185:ASP:C	1:E:187:ARG:H	1.93	0.72
1:G:80:ASP:HB3	1:G:81:PRO:HD2	1.72	0.72
2:D:377:LYS:O	2:D:377:LYS:HG3	1.89	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:565:GLU:C	2:D:566:ILE:HD12	2.11	0.71
1:A:273:ARG:HD2	1:A:280:LEU:HD21	1.71	0.71
1:E:229:THR:CG2	1:E:269:SER:HB3	2.20	0.71
1:G:185:ASP:O	1:G:187:ARG:N	2.21	0.71
1:G:24:ILE:CD1	1:G:62:LYS:HB2	2.16	0.71
1:A:32:MET:HG3	1:A:47:PRO:CD	2.21	0.71
1:C:185:ASP:OD2	1:C:187:ARG:HB3	1.91	0.71
1:E:25:GLU:HG2	1:E:58:HIS:O	1.90	0.71
2:F:451:LEU:O	2:F:455:MET:HG3	1.91	0.71
1:G:185:ASP:C	1:G:187:ARG:H	1.92	0.71
1:A:201:ARG:HB3	1:A:212:ILE:HD12	1.73	0.71
1:C:236:ARG:O	1:C:255:PRO:HB3	1.90	0.71
1:G:23:ILE:H	1:G:23:ILE:HD12	1.55	0.71
1:A:48:GLY:H	1:A:57:THR:HG23	1.54	0.71
1:G:223:ASP:OD2	1:G:274:ARG:HG3	1.91	0.71
1:C:80:ASP:HB3	1:C:81:PRO:HD2	1.70	0.71
2:D:452:GLU:OE2	2:D:495:ARG:HG3	1.90	0.71
2:F:363:SER:CB	3:X:26:DA:H3'	2.21	0.70
1:G:132:GLN:O	1:G:136:THR:HG22	1.91	0.70
1:A:185:ASP:C	1:A:187:ARG:H	1.93	0.70
2:F:402:LYS:H	2:F:402:LYS:CD	2.04	0.70
1:A:244:VAL:HG22	1:A:250:ILE:CD1	2.20	0.70
1:E:19:ALA:HA	1:E:64:ASN:O	1.90	0.70
1:A:222:GLU:CD	1:A:222:GLU:H	1.94	0.70
4:Y:16:DC:C2''	4:Y:17:DG:H5''	2.21	0.70
1:G:51:SER:HB3	1:G:57:THR:H	1.54	0.70
2:H:477:GLN:O	2:H:479:GLU:HG2	1.90	0.70
2:H:509:VAL:HG22	2:H:538:TYR:CD1	2.26	0.70
2:H:544:ASN:OD1	2:H:544:ASN:N	2.25	0.70
2:D:402:LYS:H	2:D:402:LYS:CE	2.05	0.70
2:H:626:SER:OG	2:H:646:LEU:HD23	1.92	0.70
4:Y:16:DC:H2''	4:Y:17:DG:H5''	1.73	0.70
2:F:572:LYS:CE	2:F:606:GLN:HG2	2.20	0.70
1:A:114:GLN:O	1:A:114:GLN:HG2	1.92	0.69
1:A:23:ILE:HD12	1:A:23:ILE:H	1.58	0.69
1:A:200:ASN:O	1:A:201:ARG:HB2	1.91	0.69
4:Y:17:DG:H5''	4:Y:17:DG:H8	1.57	0.69
2:D:509:VAL:HG22	2:D:538:TYR:HD1	1.56	0.69
2:H:353:PHE:CE2	2:H:439:ILE:HG12	2.27	0.69
2:F:559:CYS:SG	2:F:561:THR:HG23	2.33	0.69
1:G:229:THR:CG2	1:G:269:SER:HB3	2.22	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:214:LEU:HD23	1:E:214:LEU:O	1.93	0.69
2:F:618:ASP:OD2	2:F:621:ILE:HG22	1.92	0.69
1:G:114:GLN:O	1:G:115:ASN:ND2	2.24	0.69
1:A:46:ILE:CD1	1:A:118:ILE:HD11	2.23	0.69
1:A:57:THR:HG23	1:A:57:THR:O	1.92	0.69
2:B:580:ILE:HD13	2:B:598:PHE:CE2	2.27	0.69
2:D:387:TYR:CD1	2:D:518:LEU:HD13	2.26	0.69
1:E:226:VAL:HG12	1:E:228:PHE:CE1	2.27	0.69
2:H:566:ILE:HD12	2:H:566:ILE:N	2.08	0.69
4:J:17:DG:H4'	4:J:17:DG:OP1	1.91	0.69
1:A:104:LEU:HD21	1:A:163:VAL:HG13	1.74	0.69
1:G:198:ARG:O	1:G:199:VAL:HG23	1.93	0.69
4:J:25:DC:H2''	4:J:26:DC:C5	2.28	0.69
2:B:561:THR:O	2:B:615:LYS:HG3	1.92	0.69
2:B:618:ASP:OD2	2:B:621:ILE:HG22	1.93	0.69
2:D:572:LYS:NZ	2:D:606:GLN:CG	2.53	0.69
1:E:60:THR:HG22	1:E:61:ILE:N	2.08	0.68
1:G:188:ALA:HB1	1:G:190:ASN:HD21	1.57	0.68
2:H:348:PRO:HA	2:H:368:PRO:O	1.94	0.68
2:F:646:LEU:HD13	2:F:646:LEU:C	2.14	0.68
3:X:21:DT:C2	4:Y:8:DG:N2	2.61	0.68
1:A:210:ASP:O	1:A:253:ARG:HA	1.94	0.68
2:B:452:GLU:OE2	2:B:495:ARG:HG3	1.94	0.68
2:B:621:ILE:HD11	2:B:649:PRO:HD3	1.74	0.68
1:C:114:GLN:NE2	1:E:241:GLN:HB2	2.09	0.68
2:H:572:LYS:HD3	2:H:573:VAL:H	1.58	0.68
2:D:348:PRO:HA	2:D:368:PRO:O	1.93	0.68
1:A:215:LEU:HB3	2:B:604:HIS:CD2	2.28	0.68
1:C:23:ILE:HD12	1:C:23:ILE:H	1.58	0.68
1:C:76:LEU:CD1	1:C:90:LEU:HD13	2.24	0.68
2:F:407:HIS:HD2	2:F:409:HIS:H	1.39	0.68
1:G:187:ARG:O	1:G:187:ARG:HG2	1.94	0.68
2:D:548:LEU:HD11	2:D:633:ARG:HG3	1.76	0.67
1:G:74:ILE:CD1	1:G:161:PHE:HD2	2.07	0.67
1:G:202:ASN:H	1:G:202:ASN:ND2	1.91	0.67
1:C:114:GLN:HE22	1:E:241:GLN:H	1.40	0.67
1:A:202:ASN:HD22	1:A:202:ASN:N	1.91	0.67
1:C:229:THR:CG2	1:C:269:SER:HB3	2.25	0.67
1:E:211:GLU:C	1:E:212:ILE:HD13	2.15	0.67
2:H:387:TYR:CZ	2:H:518:LEU:HD22	2.30	0.67
1:A:23:ILE:HD12	1:A:23:ILE:N	2.10	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:550:ILE:HG23	2:F:568:LEU:HD11	1.76	0.67
2:F:584:GLU:O	2:F:591:VAL:HG23	1.95	0.67
1:C:132:GLN:O	1:C:136:THR:HG22	1.95	0.67
1:G:236:ARG:O	1:G:255:PRO:HB3	1.95	0.67
1:A:194:LEU:HD22	1:A:279:GLU:HG3	1.75	0.67
2:B:402:LYS:H	2:B:402:LYS:CE	2.08	0.67
1:C:86:HIS:CE1	1:C:87:PRO:HD2	2.30	0.67
1:A:233:TRP:CD1	1:A:258:ALA:HB2	2.29	0.66
1:A:171:ARG:HE	1:A:171:ARG:HA	1.59	0.66
1:A:262:LEU:HD21	1:A:266:VAL:CG1	2.24	0.66
2:B:504:GLU:HA	2:B:504:GLU:OE1	1.94	0.66
1:C:74:ILE:CD1	1:C:161:PHE:CD2	2.78	0.66
2:F:363:SER:HB2	3:X:26:DA:H3'	1.77	0.66
3:X:1:DA:H2''	3:X:2:DG:O5'	1.95	0.66
1:C:23:ILE:HD12	1:C:23:ILE:N	2.11	0.66
1:G:21:VAL:HG21	1:G:163:VAL:HG21	1.78	0.66
2:H:402:LYS:CD	2:H:402:LYS:H	2.09	0.66
1:E:244:VAL:HG22	1:E:250:ILE:HD12	1.76	0.66
2:F:434:PHE:HB3	2:F:437:LEU:HD22	1.77	0.66
1:A:74:ILE:HG12	1:A:100:TYR:HD1	1.61	0.66
1:G:66:TYR:CE2	1:G:165:VAL:HB	2.31	0.66
3:I:14:DT:H2''	3:I:15:DG:H5'	1.78	0.66
3:I:23:DT:O2	4:J:6:DA:H2	1.79	0.66
1:A:80:ASP:HB3	1:A:81:PRO:HD2	1.78	0.65
1:E:77:VAL:HG21	1:E:179:LEU:HD11	1.78	0.65
2:H:572:LYS:CE	2:H:606:GLN:HG2	2.24	0.65
1:A:81:PRO:HB2	1:A:82:PRO:HD3	1.78	0.65
2:F:580:ILE:HD13	2:F:598:PHE:CE2	2.31	0.65
1:C:54:THR:OG1	1:C:55:THR:HG23	1.97	0.65
1:E:199:VAL:CG1	1:E:201:ARG:O	2.45	0.65
1:C:239:PHE:HB3	1:C:252:PHE:CB	2.27	0.65
1:A:79:LYS:O	1:A:158:ARG:NE	2.30	0.65
4:Y:23:DT:H2''	4:Y:24:DC:C5'	2.27	0.65
3:I:7:DT:C2	4:J:22:DG:N2	2.65	0.65
1:E:222:GLU:CD	1:E:222:GLU:H	1.99	0.65
1:G:86:HIS:ND1	1:G:87:PRO:HD2	2.11	0.65
2:F:395:VAL:HB	2:F:421:CYS:HB3	1.77	0.65
2:B:467:LEU:N	2:B:467:LEU:HD12	2.12	0.65
1:C:202:ASN:H	1:C:202:ASN:ND2	1.95	0.65
1:G:215:LEU:HB3	2:H:604:HIS:CD2	2.32	0.65
2:H:572:LYS:HZ3	2:H:606:GLN:HG2	1.60	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:32:MET:SD	1:E:47:PRO:HD3	2.37	0.64
3:X:23:DT:O2	4:Y:6:DA:C2	2.50	0.64
1:E:171:ARG:HE	1:E:171:ARG:HA	1.60	0.64
2:D:636:ASP:OD2	2:D:638:GLU:HG2	1.96	0.64
1:C:202:ASN:H	1:C:202:ASN:HD22	1.42	0.64
1:E:108:ARG:HD2	1:E:110:ILE:O	1.98	0.64
2:D:554:ASP:OD2	2:D:567:TYR:HB2	1.98	0.64
2:F:550:ILE:HD11	2:F:640:SER:OG	1.97	0.64
1:A:68:GLY:HA2	1:A:106:PRO:O	1.98	0.64
2:D:592:TRP:CD1	2:D:617:LYS:HB3	2.33	0.64
1:E:118:ILE:N	1:E:118:ILE:HD12	2.13	0.64
1:A:199:VAL:CG1	1:A:201:ARG:O	2.45	0.64
2:B:621:ILE:CD1	2:B:649:PRO:HB3	2.28	0.64
2:D:407:HIS:ND1	2:D:510:VAL:HG23	2.13	0.64
1:C:27:PRO:CG	1:C:183:ILE:HD11	2.28	0.64
1:A:218:LYS:NZ	1:A:218:LYS:HB3	2.13	0.63
2:B:603:VAL:HG22	2:B:609:ILE:HG12	1.78	0.63
1:E:60:THR:OG1	1:E:112:SER:HB3	1.97	0.63
2:D:402:LYS:H	2:D:402:LYS:CD	2.11	0.63
2:F:451:LEU:CD1	2:F:498:ALA:HA	2.27	0.63
2:F:572:LYS:HD3	2:F:606:GLN:HB3	1.79	0.63
2:F:613:THR:HG22	2:F:614:PRO:O	1.99	0.63
4:J:2:DT:H1'	4:J:3:DG:H5''	1.81	0.63
1:C:60:THR:OG1	1:C:112:SER:HB3	1.99	0.63
2:F:580:ILE:N	2:F:580:ILE:HD12	2.14	0.63
1:G:21:VAL:HG21	1:G:163:VAL:CG2	2.28	0.63
1:A:77:VAL:HG21	1:A:179:LEU:HD11	1.80	0.63
2:H:543:PRO:HD2	2:H:544:ASN:OD1	1.98	0.63
2:H:572:LYS:NZ	2:H:606:GLN:CG	2.50	0.63
4:Y:20:DA:N1	4:Y:21:DA:C6	2.66	0.63
1:A:60:THR:HG22	1:A:61:ILE:N	2.14	0.63
1:E:68:GLY:HA2	1:E:106:PRO:O	1.99	0.63
1:E:185:ASP:OD2	1:E:187:ARG:HB2	1.98	0.63
1:E:244:VAL:HG22	1:E:250:ILE:CD1	2.29	0.63
4:Y:17:DG:H5''	4:Y:17:DG:C8	2.34	0.63
2:H:633:ARG:NH1	2:H:638:GLU:HB2	2.14	0.63
4:Y:20:DA:C6	4:Y:21:DA:N6	2.66	0.63
2:B:451:LEU:C	2:B:451:LEU:HD13	2.19	0.63
2:D:566:ILE:HD12	2:D:566:ILE:N	2.13	0.63
4:Y:19:DA:H2''	4:Y:20:DA:C8	2.33	0.63
1:A:233:TRP:HZ3	1:A:268:VAL:HG11	1.64	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:199:VAL:HG12	1:E:201:ARG:H	1.64	0.63
1:G:30:ARG:NE	1:G:191:THR:HB	2.14	0.63
4:J:19:DA:C2	4:J:20:DA:C2	2.87	0.63
2:B:580:ILE:HD12	2:B:580:ILE:N	2.14	0.62
1:C:74:ILE:CD1	1:C:161:PHE:HD2	2.12	0.62
1:C:105:CYS:SG	1:C:107:ASP:OD1	2.57	0.62
1:C:233:TRP:HZ3	1:C:268:VAL:HG11	1.64	0.62
4:Y:23:DT:C2'	4:Y:24:DC:H5''	2.29	0.62
1:E:51:SER:CB	1:E:57:THR:HB	2.27	0.62
1:E:214:LEU:HD23	1:E:214:LEU:C	2.18	0.62
1:G:46:ILE:HD11	1:G:118:ILE:HD13	1.81	0.62
2:H:473:LEU:HD13	2:H:493:ILE:HG21	1.81	0.62
1:C:40:GLY:C	1:C:42:SER:N	2.47	0.62
2:H:549:LYS:HB3	2:H:571:ASP:OD1	1.99	0.62
1:G:233:TRP:HZ3	1:G:268:VAL:HG11	1.65	0.62
2:B:454:ARG:HG2	2:B:454:ARG:HH11	1.64	0.62
2:B:559:CYS:SG	2:B:650:GLU:HB2	2.40	0.62
2:D:477:GLN:O	2:D:479:GLU:HG2	1.99	0.62
2:F:355:PHE:CD2	2:F:539:ASP:HB2	2.35	0.62
2:F:409:HIS:HD2	2:F:442:VAL:H	1.44	0.62
1:G:262:LEU:HD21	1:G:266:VAL:CG1	2.29	0.62
2:D:629:VAL:HG12	2:D:643:LYS:O	2.00	0.62
1:E:46:ILE:CD1	1:E:118:ILE:HD11	2.26	0.62
2:F:555:ARG:HG2	2:F:555:ARG:HH11	1.64	0.62
1:G:19:ALA:O	1:G:175:LEU:HD22	1.99	0.62
4:J:23:DT:C2'	4:J:24:DC:H5''	2.29	0.62
2:B:552:ARG:HG3	2:B:553:MET:N	2.13	0.62
2:B:342:LEU:HD13	2:B:343:GLN:H	1.63	0.62
2:B:613:THR:HG23	2:B:614:PRO:HD2	1.82	0.62
2:H:561:THR:O	2:H:615:LYS:HG3	2.00	0.62
2:H:618:ASP:OD2	2:H:621:ILE:HG22	2.00	0.62
1:A:132:GLN:O	1:A:136:THR:HG22	1.99	0.61
2:B:555:ARG:HH11	2:B:555:ARG:HG2	1.65	0.61
2:D:572:LYS:HZ3	2:D:606:GLN:HG2	1.64	0.61
1:E:80:ASP:HB3	1:E:81:PRO:HD2	1.81	0.61
1:A:214:LEU:HD23	1:A:214:LEU:O	2.00	0.61
1:C:88:HIS:NE2	1:C:120:CYS:HB2	2.15	0.61
1:C:262:LEU:HD21	1:C:266:VAL:CG1	2.30	0.61
1:A:199:VAL:HG12	1:A:201:ARG:H	1.64	0.61
1:C:88:HIS:CE1	1:C:121:VAL:H	2.18	0.61
2:D:518:LEU:O	2:D:527:ARG:HG3	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:573:VAL:HG22	2:F:606:GLN:O	2.00	0.61
2:F:551:VAL:HG12	2:F:552:ARG:N	2.14	0.61
1:A:52:THR:CG2	1:A:53:ASP:H	2.01	0.61
2:B:451:LEU:O	2:B:451:LEU:HD13	2.00	0.61
2:D:348:PRO:HG3	2:D:512:LEU:HD12	1.82	0.61
1:E:27:PRO:CG	1:E:183:ILE:HD11	2.30	0.61
1:G:108:ARG:HD2	1:G:110:ILE:O	2.01	0.61
1:C:30:ARG:HH21	1:C:191:THR:HB	1.64	0.61
4:Y:25:DC:H2 ⁷	4:Y:26:DC:C5	2.36	0.61
2:D:382:VAL:HG12	2:D:383:LYS:N	2.13	0.61
1:E:194:LEU:HD22	1:E:279:GLU:HG3	1.82	0.61
2:F:444:LYS:O	2:F:447:VAL:HG23	2.00	0.61
1:G:236:ARG:HH11	1:G:236:ARG:CG	2.12	0.61
2:H:646:LEU:HD13	2:H:646:LEU:C	2.21	0.61
4:J:20:DA:N1	4:J:21:DA:C6	2.68	0.61
1:C:28:LYS:N	1:C:48:GLY:O	2.34	0.61
2:H:443:THR:O	2:H:447:VAL:HG23	2.01	0.61
2:H:407:HIS:HD2	2:H:409:HIS:H	1.49	0.61
1:A:244:VAL:HG22	1:A:250:ILE:HD12	1.82	0.61
2:F:631:LEU:HB2	2:F:640:SER:HB3	1.83	0.61
1:G:282:GLU:HG2	1:G:283:PRO:CD	2.21	0.61
1:E:25:GLU:OE2	1:E:50:ARG:CG	2.49	0.60
1:A:185:ASP:OD2	1:A:187:ARG:HB2	2.01	0.60
2:D:391:ALA:HB3	2:D:425:ALA:HB3	1.81	0.60
3:I:22:DT:O2	4:J:7:DA:C2	2.48	0.60
1:A:229:THR:CG2	1:A:269:SER:HB3	2.31	0.60
2:B:572:LYS:HZ2	2:B:606:GLN:CG	2.06	0.60
1:C:217:ASP:O	1:C:219:VAL:HG13	2.01	0.60
1:E:23:ILE:HD12	1:E:23:ILE:N	2.16	0.60
2:F:624:PRO:HB2	2:F:646:LEU:HD11	1.83	0.60
2:B:366:GLY:O	2:B:367:LEU:C	2.36	0.60
1:E:88:HIS:NE2	1:E:120:CYS:HB3	2.16	0.60
2:H:476:LEU:HD22	2:H:483:ASP:HB2	1.84	0.60
1:E:57:THR:HG23	1:E:57:THR:O	2.01	0.60
1:E:58:HIS:HE1	1:E:114:GLN:NE2	2.00	0.60
1:A:48:GLY:HA3	1:A:57:THR:OG1	2.01	0.60
1:C:273:ARG:O	1:C:275:PRO:HD3	2.02	0.60
1:E:54:THR:HG22	1:E:54:THR:O	2.02	0.60
2:F:443:THR:HA	4:J:22:DG:OP2	2.01	0.60
1:G:185:ASP:C	1:G:187:ARG:N	2.55	0.60
1:E:77:VAL:HG22	1:E:158:ARG:O	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:48:GLY:HA3	1:G:57:THR:OG1	2.00	0.60
4:Y:17:DG:H8	4:Y:17:DG:C5'	2.13	0.60
1:A:58:HIS:HB3	1:A:112:SER:HB2	1.82	0.60
1:E:95:CYS:SG	1:E:100:TYR:HB2	2.41	0.60
2:B:636:ASP:OD2	2:B:638:GLU:HG2	2.02	0.59
1:E:158:ARG:NH1	1:E:182:PRO:HD3	2.16	0.59
2:H:509:VAL:HG22	2:H:538:TYR:HD1	1.66	0.59
1:A:55:THR:HG22	1:A:56:LYS:N	2.17	0.59
1:A:77:VAL:HG22	1:A:158:ARG:O	2.01	0.59
2:B:550:ILE:N	2:B:550:ILE:HD12	2.16	0.59
2:F:409:HIS:NE2	2:F:441:HIS:HA	2.17	0.59
1:G:88:HIS:CE1	1:G:120:CYS:CB	2.83	0.59
1:G:171:ARG:HE	1:G:172:PRO:CD	2.15	0.59
1:C:114:GLN:O	1:C:115:ASN:ND2	2.36	0.59
2:D:572:LYS:HD3	2:D:573:VAL:N	2.17	0.59
1:E:32:MET:HG3	1:E:47:PRO:CD	2.32	0.59
1:E:206:CYS:HA	1:E:288:TYR:CD1	2.38	0.59
2:H:571:ASP:O	2:H:573:VAL:HG13	2.02	0.59
2:D:380:PRO:O	2:D:433:GLY:HA2	2.03	0.59
2:F:646:LEU:HD13	2:F:647:TYR:N	2.16	0.59
3:X:5:DA:C2	3:X:6:DC:N3	2.70	0.59
1:G:20:TYR:CE1	1:G:64:ASN:HB2	2.38	0.59
4:Y:22:DG:H2'	4:Y:23:DT:OP2	2.03	0.59
1:A:88:HIS:CE1	1:A:120:CYS:HB2	2.38	0.59
2:D:458:ALA:O	2:D:465:PRO:HG3	2.01	0.59
3:X:8:DT:C2	4:Y:21:DA:H2	2.19	0.59
1:A:108:ARG:HD2	1:A:110:ILE:O	2.02	0.59
1:E:171:ARG:HE	1:E:172:PRO:CD	2.16	0.59
2:H:507:LEU:HD12	2:H:507:LEU:N	2.18	0.59
1:E:202:ASN:HD22	1:E:202:ASN:N	1.94	0.58
1:E:236:ARG:HH11	1:E:236:ARG:CG	2.16	0.58
1:G:88:HIS:ND1	1:G:120:CYS:HA	2.18	0.58
1:G:27:PRO:CG	1:G:183:ILE:HD11	2.33	0.58
1:A:32:MET:HG3	1:A:47:PRO:HD3	1.85	0.58
2:B:646:LEU:C	2:B:646:LEU:HD13	2.23	0.58
1:G:51:SER:HB2	1:G:56:LYS:HA	1.86	0.58
2:B:434:PHE:HB3	2:B:437:LEU:HD22	1.86	0.58
2:D:646:LEU:HD13	2:D:646:LEU:C	2.24	0.58
1:C:171:ARG:HE	1:C:172:PRO:CD	2.17	0.58
1:C:215:LEU:HB3	2:D:604:HIS:CD2	2.39	0.58
1:E:74:ILE:HD12	1:E:161:PHE:CD2	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:144:PRO:O	1:G:148:GLN:HG3	2.03	0.58
2:H:395:VAL:HB	2:H:421:CYS:HB3	1.85	0.58
1:A:214:LEU:HD23	1:A:214:LEU:C	2.23	0.58
2:F:444:LYS:HB2	4:J:22:DG:OP1	2.04	0.58
2:F:464:ASN:ND2	2:F:528:ARG:NH1	2.51	0.58
2:H:407:HIS:CE1	2:H:510:VAL:HG23	2.38	0.58
2:B:572:LYS:CE	2:B:606:GLN:HG2	2.32	0.58
1:C:206:CYS:HA	1:C:288:TYR:CD1	2.38	0.58
1:G:198:ARG:HD2	2:H:567:TYR:OH	2.04	0.58
2:H:380:PRO:O	2:H:433:GLY:HA2	2.03	0.58
3:I:1:DA:H2''	3:I:2:DG:O5'	2.03	0.58
2:H:632:ARG:HG3	2:H:639:THR:HG22	1.84	0.57
1:A:236:ARG:HH11	1:A:236:ARG:CG	2.12	0.57
1:E:84:ARG:HG2	1:E:143:VAL:HG11	1.85	0.57
1:G:30:ARG:NH2	1:G:191:THR:HB	2.17	0.57
1:G:88:HIS:NE2	1:G:120:CYS:HB2	2.19	0.57
2:H:625:ALA:O	2:H:646:LEU:HD22	2.05	0.57
3:I:6:DC:N4	4:J:22:DG:H1	2.01	0.57
1:A:84:ARG:HG2	1:A:143:VAL:HG11	1.86	0.57
1:E:185:ASP:O	1:E:187:ARG:N	2.35	0.57
2:H:382:VAL:HG12	2:H:383:LYS:N	2.16	0.57
3:X:22:DT:C2	4:Y:7:DA:H2	2.21	0.57
1:G:86:HIS:CE1	1:G:87:PRO:HD2	2.39	0.57
2:D:464:ASN:ND2	2:D:528:ARG:NH1	2.53	0.57
2:D:646:LEU:HD13	2:D:647:TYR:N	2.19	0.57
1:E:262:LEU:O	1:E:290:PRO:HB3	2.03	0.57
2:F:412:VAL:HG22	2:F:413:GLY:N	2.20	0.57
2:B:490:GLU:O	2:B:494:ILE:HG12	2.05	0.57
1:E:76:LEU:HD13	1:E:90:LEU:HD22	1.85	0.57
1:G:36:TYR:CD1	1:G:36:TYR:N	2.73	0.57
1:G:245:HIS:HB3	1:G:249:ALA:HB3	1.86	0.57
1:A:78:THR:O	1:A:158:ARG:HD2	2.04	0.57
2:B:454:ARG:HG2	2:B:454:ARG:NH1	2.18	0.57
2:F:504:GLU:OE1	2:F:504:GLU:HA	2.05	0.57
3:X:7:DT:N3	4:Y:22:DG:N2	2.53	0.57
1:C:156:ALA:O	1:C:157:VAL:HG13	2.05	0.57
2:F:500:GLN:O	2:F:503:LYS:HG2	2.05	0.57
1:G:219:VAL:O	1:G:247:GLN:HB3	2.05	0.57
2:D:353:PHE:HE2	2:D:439:ILE:HG12	1.68	0.57
1:E:26:GLN:HB3	1:E:181:HIS:NE2	2.19	0.57
2:H:354:ARG:HD2	2:H:356:ARG:HD3	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:THR:CG2	1:A:56:LYS:N	2.68	0.56
1:A:72:VAL:O	1:A:101:GLU:HA	2.05	0.56
1:C:58:HIS:HB3	1:C:59:PRO:HD2	1.86	0.56
2:D:489:ARG:HD3	2:D:489:ARG:C	2.25	0.56
1:E:52:THR:HG22	1:E:53:ASP:N	2.14	0.56
1:E:62:LYS:HE2	1:E:64:ASN:ND2	2.20	0.56
1:E:185:ASP:C	1:E:187:ARG:N	2.57	0.56
1:G:76:LEU:HD13	1:G:90:LEU:HD13	1.85	0.56
4:Y:5:DA:H2''	4:Y:6:DA:C8	2.39	0.56
4:J:19:DA:N3	4:J:20:DA:C5	2.73	0.56
1:E:74:ILE:HG12	1:E:100:TYR:CD1	2.39	0.56
1:E:262:LEU:HD21	1:E:266:VAL:CG1	2.27	0.56
2:B:355:PHE:CD2	2:B:539:ASP:HB2	2.41	0.56
2:B:550:ILE:HD11	2:B:640:SER:OG	2.06	0.56
1:C:167:ASP:HB2	1:C:168:PRO:HD2	1.86	0.56
1:E:48:GLY:N	1:E:57:THR:HG21	2.17	0.56
1:E:132:GLN:O	1:E:136:THR:HG22	2.06	0.56
1:G:46:ILE:HD11	1:G:118:ILE:CD1	2.36	0.56
1:G:86:HIS:CG	1:G:87:PRO:HD2	2.40	0.56
2:H:504:GLU:OE1	2:H:504:GLU:HA	2.04	0.56
2:H:583:TYR:HA	2:H:592:TRP:O	2.04	0.56
2:B:559:CYS:SG	2:B:561:THR:HG23	2.46	0.56
2:D:460:ILE:HG12	2:D:486:LEU:HD13	1.87	0.56
1:G:30:ARG:HH21	1:G:191:THR:CB	2.17	0.56
2:D:509:VAL:HG22	2:D:538:TYR:CD1	2.39	0.56
2:D:571:ASP:O	2:D:573:VAL:HG13	2.04	0.56
2:D:583:TYR:CD1	2:D:583:TYR:C	2.78	0.56
2:D:584:GLU:O	2:D:591:VAL:HG23	2.06	0.56
1:E:26:GLN:OE1	1:E:180:SER:HB2	2.04	0.56
2:F:451:LEU:HD11	2:F:498:ALA:HA	1.88	0.56
2:B:409:HIS:CD2	2:B:442:VAL:H	2.23	0.56
2:D:544:ASN:OD1	2:D:544:ASN:N	2.33	0.56
2:F:423:VAL:CG2	2:F:432:VAL:HG11	2.34	0.56
1:C:236:ARG:HG3	1:C:236:ARG:NH1	2.19	0.56
1:E:82:PRO:O	1:E:84:ARG:N	2.37	0.56
1:G:218:LYS:HB3	1:G:218:LYS:HZ2	1.69	0.56
2:H:646:LEU:HD13	2:H:647:TYR:N	2.21	0.56
2:D:500:GLN:HE21	2:D:503:LYS:HE2	1.71	0.56
2:H:482:GLY:O	2:H:483:ASP:HB2	2.06	0.56
4:Y:20:DA:C6	4:Y:21:DA:C6	2.94	0.56
1:A:288:TYR:O	1:A:289:LEU:HD23	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:464:ASN:N	2:B:465:PRO:HD3	2.20	0.56
1:E:72:VAL:O	1:E:101:GLU:HA	2.05	0.56
1:G:54:THR:OG1	1:G:55:THR:HG23	2.06	0.56
1:A:187:ARG:O	1:A:189:PRO:HD3	2.06	0.56
1:A:211:GLU:C	1:A:212:ILE:HD13	2.27	0.56
1:A:273:ARG:O	1:A:275:PRO:HD3	2.06	0.56
1:C:30:ARG:NE	1:C:191:THR:HB	2.20	0.56
1:C:36:TYR:N	1:C:36:TYR:CD1	2.74	0.56
2:D:451:LEU:C	2:D:451:LEU:HD13	2.27	0.56
1:G:47:PRO:O	1:G:48:GLY:O	2.24	0.56
1:G:181:HIS:HB2	1:G:182:PRO:HD2	1.88	0.56
1:G:194:LEU:HD22	1:G:279:GLU:HG3	1.87	0.56
3:X:6:DC:H42	4:Y:22:DG:H1	1.51	0.56
1:A:26:GLN:O	1:A:49:GLU:HB2	2.06	0.55
1:C:181:HIS:HB2	1:C:182:PRO:HD2	1.88	0.55
2:F:467:LEU:N	2:F:467:LEU:CD1	2.68	0.55
2:H:489:ARG:HD3	2:H:489:ARG:C	2.27	0.55
1:A:86:HIS:CG	1:A:157:VAL:HG12	2.40	0.55
1:A:88:HIS:CG	1:A:120:CYS:HA	2.41	0.55
2:D:571:ASP:O	2:D:572:LYS:C	2.45	0.55
2:F:550:ILE:H	2:F:550:ILE:CD1	2.17	0.55
1:G:24:ILE:N	1:G:60:THR:O	2.39	0.55
3:I:21:DT:H6	3:I:21:DT:H5'	1.69	0.55
1:A:282:GLU:HG2	1:A:283:PRO:HD2	1.87	0.55
2:B:511:ARG:HG2	2:B:536:ALA:HA	1.89	0.55
2:D:416:CYS:SG	2:D:421:CYS:HB2	2.46	0.55
1:E:30:ARG:HE	1:E:191:THR:HB	1.72	0.55
2:F:363:SER:HB3	3:X:26:DA:H3'	1.88	0.55
1:G:30:ARG:NE	1:G:191:THR:O	2.40	0.55
1:E:74:ILE:HB	1:E:100:TYR:HB3	1.89	0.55
1:G:27:PRO:HG2	1:G:183:ILE:HD11	1.89	0.55
3:I:23:DT:O2	4:J:6:DA:C2	2.58	0.55
1:A:60:THR:HG23	1:A:111:HIS:C	2.27	0.55
1:A:77:VAL:CG2	1:A:158:ARG:HB2	2.36	0.55
1:A:262:LEU:O	1:A:290:PRO:HB3	2.07	0.55
2:D:477:GLN:O	2:D:482:GLY:HA3	2.07	0.55
1:E:46:ILE:HG22	1:E:47:PRO:O	2.06	0.55
2:F:631:LEU:O	2:F:639:THR:HA	2.07	0.55
1:G:51:SER:HB2	1:G:57:THR:H	1.69	0.55
2:H:584:GLU:O	2:H:591:VAL:HG23	2.07	0.55
3:X:14:DT:H2''	3:X:15:DG:H5'	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Y:2:DT:H1'	4:Y:3:DG:H5''	1.89	0.55
1:A:82:PRO:O	1:A:84:ARG:N	2.39	0.55
1:C:187:ARG:O	1:C:187:ARG:HG2	2.06	0.55
2:F:464:ASN:N	2:F:465:PRO:HD3	2.21	0.55
2:F:632:ARG:HG3	2:F:639:THR:HG22	1.89	0.55
1:G:188:ALA:HB1	1:G:190:ASN:ND2	2.22	0.55
2:H:458:ALA:O	2:H:465:PRO:HG3	2.07	0.55
4:Y:24:DC:H2''	4:Y:25:DC:C5'	2.32	0.55
1:A:202:ASN:N	1:A:202:ASN:ND2	2.55	0.55
2:B:568:LEU:O	2:B:608:ALA:HA	2.06	0.55
1:E:158:ARG:HD3	1:E:179:LEU:CD2	2.37	0.55
1:E:237:GLY:HA2	1:E:255:PRO:HD3	1.89	0.55
1:A:27:PRO:CG	1:A:183:ILE:HD11	2.37	0.54
1:C:24:ILE:HD11	1:C:110:ILE:HG12	1.89	0.54
1:C:201:ARG:HB3	1:C:212:ILE:HD12	1.89	0.54
1:C:218:LYS:NZ	1:C:218:LYS:HB3	2.22	0.54
1:C:228:PHE:CZ	1:C:254:THR:HG22	2.42	0.54
2:D:353:PHE:CD2	2:D:367:LEU:HD21	2.41	0.54
1:E:60:THR:CG2	1:E:61:ILE:N	2.70	0.54
1:E:81:PRO:O	1:E:83:HIS:N	2.40	0.54
1:G:167:ASP:HB2	1:G:168:PRO:HD2	1.89	0.54
1:A:34:PHE:CD1	1:A:34:PHE:N	2.75	0.54
1:C:108:ARG:HD2	1:C:110:ILE:O	2.06	0.54
2:F:572:LYS:HZ3	2:F:606:GLN:HG2	1.63	0.54
2:F:633:ARG:O	2:F:637:LEU:HA	2.06	0.54
1:G:171:ARG:HE	1:G:171:ARG:HA	1.72	0.54
1:A:65:GLY:O	1:A:66:TYR:HB2	2.07	0.54
2:B:342:LEU:HD12	2:B:532:VAL:CG1	2.37	0.54
1:C:40:GLY:O	1:C:41:ARG:C	2.43	0.54
1:G:171:ARG:HE	1:G:172:PRO:HD2	1.72	0.54
1:C:59:PRO:O	1:C:112:SER:HA	2.07	0.54
2:F:550:ILE:N	2:F:550:ILE:CD1	2.66	0.54
2:H:393:VAL:HG21	2:H:432:VAL:HG21	1.89	0.54
2:H:402:LYS:H	2:H:402:LYS:HE3	1.73	0.54
1:A:51:SER:CB	1:A:57:THR:HB	2.32	0.54
1:A:144:PRO:O	1:A:148:GLN:HG3	2.07	0.54
1:A:246:ARG:HB3	2:B:607:PHE:CD2	2.41	0.54
1:C:58:HIS:HB3	1:C:59:PRO:CD	2.38	0.54
1:E:58:HIS:HB3	1:E:112:SER:HB2	1.90	0.54
1:E:282:GLU:HG2	1:E:283:PRO:HD2	1.90	0.54
4:Y:16:DC:H2''	4:Y:17:DG:C5'	2.35	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:HIS:CE1	1:A:120:CYS:CB	2.91	0.54
2:B:572:LYS:HD3	2:B:606:GLN:HB3	1.88	0.54
1:G:171:ARG:NE	1:G:172:PRO:HD2	2.23	0.54
2:H:397:LEU:HD21	2:H:411:LEU:HD13	1.88	0.54
4:J:4:DG:H2''	4:J:5:DA:H5''	1.90	0.54
1:A:88:HIS:CE1	1:A:121:VAL:H	2.25	0.54
2:B:425:ALA:O	2:B:426:GLY:O	2.25	0.54
2:B:443:THR:HA	4:Y:22:DG:OP2	2.08	0.54
1:C:27:PRO:O	1:C:181:HIS:HE1	1.91	0.54
2:D:559:CYS:SG	2:D:650:GLU:HB2	2.47	0.54
2:H:392:LYS:HB3	2:H:517:PHE:HB2	1.88	0.54
2:H:452:GLU:OE2	2:H:495:ARG:HG3	2.08	0.54
4:J:20:DA:C6	4:J:21:DA:N6	2.75	0.54
2:B:632:ARG:HG3	2:B:639:THR:HG22	1.89	0.54
2:D:414:LYS:O	2:D:415:HIS:HB2	2.08	0.54
2:F:448:PHE:HA	2:F:502:THR:HG21	1.89	0.54
2:F:583:TYR:CD1	2:F:583:TYR:C	2.80	0.54
1:A:26:GLN:HB3	1:A:181:HIS:NE2	2.23	0.54
1:A:185:ASP:C	1:A:187:ARG:N	2.57	0.54
2:D:398:VAL:HG23	2:D:511:ARG:HB2	1.90	0.54
1:G:40:GLY:C	1:G:42:SER:N	2.60	0.54
1:G:194:LEU:HB3	1:G:281:SER:HB3	1.89	0.54
2:H:587:GLU:HA	2:H:587:GLU:OE1	2.08	0.54
1:C:88:HIS:CE1	1:C:120:CYS:CB	2.88	0.53
1:C:171:ARG:HE	1:C:172:PRO:HD2	1.71	0.53
1:E:48:GLY:H	1:E:57:THR:HG23	1.69	0.53
1:G:257:TYR:CG	1:G:258:ALA:N	2.75	0.53
2:H:346:GLU:OE2	2:H:379:TYR:O	2.26	0.53
3:I:21:DT:H2''	3:I:22:DT:H5'	1.90	0.53
1:C:19:ALA:HA	1:C:64:ASN:O	2.08	0.53
1:C:236:ARG:HH11	1:C:236:ARG:CG	2.20	0.53
1:E:158:ARG:HG2	1:E:158:ARG:HH11	1.72	0.53
2:F:552:ARG:HG3	2:F:553:MET:N	2.24	0.53
1:G:51:SER:HA	1:G:57:THR:HG23	1.89	0.53
3:X:7:DT:H3	4:Y:22:DG:N2	2.06	0.53
2:B:402:LYS:H	2:B:402:LYS:CD	2.21	0.53
3:X:21:DT:H6	3:X:21:DT:H5'	1.73	0.53
1:C:86:HIS:CG	1:C:87:PRO:HD2	2.43	0.53
4:J:16:DC:H2'	4:J:17:DG:H5''	1.88	0.53
1:A:60:THR:HG21	1:A:110:ILE:HG23	1.90	0.53
2:D:572:LYS:HE2	2:D:606:GLN:HG2	1.88	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:375:ASN:O	2:H:376:LYS:CB	2.56	0.53
2:H:444:LYS:HA	2:H:447:VAL:HG23	1.90	0.53
4:J:17:DG:H5''	4:J:17:DG:H8	1.73	0.53
2:D:375:ASN:O	2:D:376:LYS:CB	2.57	0.53
4:J:1:DT:H2''	4:J:2:DT:O5'	2.08	0.53
4:Y:9:DT:H2''	4:Y:10:DC:H5'	1.85	0.53
1:A:194:LEU:HB3	1:A:281:SER:HB3	1.90	0.53
2:B:342:LEU:HD12	2:B:532:VAL:HG11	1.90	0.53
2:D:377:LYS:O	2:D:377:LYS:CG	2.57	0.53
1:E:132:GLN:O	1:E:132:GLN:HG2	2.07	0.53
1:E:215:LEU:N	1:E:215:LEU:HD23	2.24	0.53
2:H:558:GLY:O	2:H:647:TYR:HA	2.08	0.53
4:J:24:DC:H1'	4:J:25:DC:H5''	1.91	0.53
2:B:409:HIS:HD2	2:B:442:VAL:H	1.55	0.53
2:B:451:LEU:CD1	2:B:498:ALA:HA	2.39	0.53
1:C:27:PRO:HG2	1:C:183:ILE:HD11	1.90	0.53
2:D:616:TYR:CZ	2:D:617:LYS:HG2	2.44	0.53
1:E:65:GLY:O	1:E:66:TYR:HB2	2.09	0.53
4:J:17:DG:H2''	4:J:18:DG:H8	1.73	0.53
1:C:34:PHE:CD1	1:C:118:ILE:HG21	2.44	0.52
1:C:46:ILE:HD13	1:C:116:LEU:O	2.10	0.52
1:C:114:GLN:NE2	1:E:241:GLN:H	2.06	0.52
2:D:470:HIS:HD2	2:D:472:ASP:OD1	1.91	0.52
2:D:482:GLY:O	2:D:483:ASP:HB2	2.09	0.52
1:E:79:LYS:O	1:E:158:ARG:NE	2.24	0.52
1:E:273:ARG:CD	1:E:280:LEU:HD21	2.39	0.52
4:Y:17:DG:C8	4:Y:17:DG:C5'	2.92	0.52
4:J:22:DG:H2''	4:J:23:DT:OP2	2.09	0.52
2:D:545:ALA:CA	2:D:633:ARG:NH2	2.71	0.52
1:G:104:LEU:HD21	1:G:163:VAL:HG13	1.91	0.52
1:G:126:LEU:O	1:G:129:ALA:HB3	2.08	0.52
1:G:202:ASN:HD22	1:G:202:ASN:N	1.95	0.52
2:H:464:ASN:N	2:H:465:PRO:HD3	2.24	0.52
2:D:626:SER:OG	2:D:646:LEU:HD23	2.08	0.52
1:G:199:VAL:HG12	1:G:201:ARG:H	1.75	0.52
2:H:509:VAL:CG2	2:H:538:TYR:CD1	2.92	0.52
2:D:394:ILE:CG1	2:D:515:THR:HB	2.39	0.52
1:E:23:ILE:HD11	1:E:178:VAL:HG22	1.91	0.52
1:G:156:ALA:HA	1:G:183:ILE:O	2.10	0.52
1:G:198:ARG:HB3	2:H:567:TYR:OH	2.10	0.52
2:H:377:LYS:O	2:H:377:LYS:CG	2.57	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:402:LYS:H	2:H:402:LYS:CE	2.23	0.52
1:A:118:ILE:N	1:A:118:ILE:HD12	2.23	0.52
2:D:356:ARG:O	2:D:440:LEU:HD12	2.10	0.52
2:D:381:GLN:HA	2:D:432:VAL:O	2.10	0.52
2:D:621:ILE:HG12	2:D:623:LYS:O	2.10	0.52
1:G:196:ILE:HG12	1:G:272:LEU:CD2	2.39	0.52
3:X:15:DG:C3'	3:X:16:DG:H5''	2.39	0.52
1:C:75:SER:HB3	1:C:162:GLN:NE2	2.23	0.52
2:F:515:THR:OG1	2:F:531:PRO:HB3	2.09	0.52
4:J:17:DG:C2'	4:J:18:DG:H8	2.22	0.52
2:F:636:ASP:OD2	2:F:638:GLU:HG2	2.10	0.52
2:H:534:SER:O	2:H:535:ASP:O	2.28	0.52
2:B:578:ILE:HG12	2:B:579:GLN:N	2.25	0.52
1:C:30:ARG:NE	1:C:191:THR:O	2.42	0.52
1:C:144:PRO:O	1:C:148:GLN:HG3	2.10	0.52
1:C:156:ALA:O	1:C:157:VAL:CG1	2.58	0.52
2:F:500:GLN:HE21	2:F:503:LYS:HE2	1.74	0.52
1:E:60:THR:HG23	1:E:111:HIS:O	2.10	0.52
1:E:185:ASP:OD2	1:E:187:ARG:CB	2.58	0.52
2:F:615:LYS:N	2:F:615:LYS:HD2	2.24	0.52
2:F:632:ARG:HG3	2:F:638:GLU:O	2.10	0.52
1:G:30:ARG:HH21	1:G:191:THR:CG2	2.22	0.52
2:H:384:ILE:N	2:H:384:ILE:HD12	2.24	0.52
1:C:233:TRP:CZ2	1:C:257:TYR:HA	2.45	0.52
2:D:407:HIS:HD2	2:D:409:HIS:H	1.56	0.52
2:F:451:LEU:HD12	2:F:498:ALA:HA	1.92	0.52
2:H:548:LEU:HD11	2:H:633:ARG:HG3	1.91	0.52
4:Y:20:DA:C2	4:Y:21:DA:C6	2.98	0.52
1:C:37:LYS:HB2	1:C:37:LYS:NZ	2.25	0.51
1:C:88:HIS:ND1	1:C:120:CYS:HA	2.24	0.51
1:C:228:PHE:HZ	1:C:254:THR:HG22	1.74	0.51
2:F:387:TYR:CE2	2:F:518:LEU:HD22	2.44	0.51
1:G:36:TYR:CE1	1:G:120:CYS:SG	3.03	0.51
2:H:357:TYR:CE2	4:J:8:DG:H2'	2.45	0.51
4:J:5:DA:C2	4:J:6:DA:N1	2.79	0.51
1:A:171:ARG:HE	1:A:172:PRO:CD	2.23	0.51
1:C:261:SER:O	1:C:262:LEU:O	2.28	0.51
2:H:398:VAL:HG23	2:H:511:ARG:HB2	1.92	0.51
2:H:398:VAL:HG22	2:H:511:ARG:O	2.10	0.51
2:H:407:HIS:CG	2:H:510:VAL:HG23	2.44	0.51
4:J:19:DA:N3	4:J:20:DA:C4	2.78	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:581:ARG:HE	2:B:593:GLU:HG3	1.75	0.51
2:D:455:MET:SD	2:D:469:VAL:HG13	2.51	0.51
1:E:48:GLY:N	1:E:57:THR:CG2	2.67	0.51
1:E:88:HIS:CE1	1:E:120:CYS:CB	2.93	0.51
3:I:21:DT:H5'	3:I:21:DT:C6	2.45	0.51
2:B:409:HIS:CD2	2:B:441:HIS:HA	2.46	0.51
2:F:454:ARG:HG2	2:F:454:ARG:HH11	1.75	0.51
2:F:467:LEU:CD1	2:F:467:LEU:H	2.24	0.51
2:F:578:ILE:HG12	2:F:579:GLN:N	2.25	0.51
2:H:402:LYS:H	2:H:402:LYS:HD3	1.73	0.51
1:A:88:HIS:NE2	1:A:120:CYS:HB3	2.26	0.51
2:B:444:LYS:O	2:B:447:VAL:HG23	2.10	0.51
2:B:564:GLU:O	2:B:612:LYS:HA	2.10	0.51
1:C:239:PHE:HB3	1:C:252:PHE:HB3	1.92	0.51
2:D:618:ASP:OD2	2:D:621:ILE:HG22	2.10	0.51
1:G:58:HIS:HB3	1:G:59:PRO:CD	2.40	0.51
1:G:213:PHE:CE2	2:H:554:ASP:HB3	2.46	0.51
2:B:448:PHE:HA	2:B:502:THR:HG21	1.91	0.51
1:E:55:THR:CG2	1:E:56:LYS:N	2.74	0.51
1:G:261:SER:O	1:G:262:LEU:C	2.48	0.51
2:H:402:LYS:HE3	2:H:402:LYS:N	2.26	0.51
1:A:222:GLU:CD	1:A:222:GLU:N	2.64	0.51
2:B:583:TYR:CD1	2:B:583:TYR:C	2.84	0.51
1:C:79:LYS:HG2	1:C:80:ASP:OD1	2.11	0.51
1:E:78:THR:O	1:E:158:ARG:HD2	2.10	0.51
1:G:54:THR:OG1	1:G:55:THR:N	2.41	0.51
2:H:409:HIS:CD2	2:H:442:VAL:H	2.29	0.51
2:H:464:ASN:ND2	2:H:528:ARG:NH1	2.58	0.51
3:X:21:DT:H5'	3:X:21:DT:C6	2.45	0.51
4:J:17:DG:C2'	4:J:18:DG:C8	2.94	0.51
2:D:353:PHE:CE2	2:D:439:ILE:HG12	2.46	0.51
1:E:55:THR:HG22	1:E:56:LYS:N	2.26	0.51
1:E:226:VAL:CG1	1:E:228:PHE:CE1	2.94	0.51
2:B:632:ARG:HG3	2:B:639:THR:CG2	2.41	0.51
1:C:171:ARG:NE	1:C:172:PRO:HD2	2.27	0.51
1:C:202:ASN:ND2	1:C:202:ASN:N	2.55	0.51
1:E:24:ILE:HD11	1:E:62:LYS:HB2	1.92	0.51
2:F:451:LEU:HD13	2:F:451:LEU:C	2.30	0.51
1:A:36:TYR:CE2	3:X:8:DT:C2'	2.93	0.50
1:C:167:ASP:OD1	1:C:169:ALA:HB3	2.11	0.50
1:E:88:HIS:CG	1:E:120:CYS:HA	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:618:ASP:CG	2:F:621:ILE:HG22	2.31	0.50
2:B:573:VAL:HG22	2:B:606:GLN:O	2.11	0.50
1:C:49:GLU:O	1:C:49:GLU:HG2	2.11	0.50
1:E:202:ASN:H	1:E:202:ASN:ND2	2.05	0.50
1:E:202:ASN:N	1:E:202:ASN:ND2	2.59	0.50
2:F:489:ARG:HD3	2:F:489:ARG:C	2.32	0.50
4:Y:5:DA:C2	4:Y:6:DA:N1	2.79	0.50
1:A:132:GLN:O	1:A:132:GLN:HG2	2.11	0.50
2:B:624:PRO:HB2	2:B:646:LEU:HD11	1.94	0.50
2:D:375:ASN:O	2:D:376:LYS:HB2	2.11	0.50
2:D:568:LEU:C	2:D:568:LEU:HD23	2.30	0.50
1:E:90:LEU:HD12	1:E:117:GLY:O	2.11	0.50
1:E:95:CYS:SG	1:E:100:TYR:HA	2.52	0.50
1:G:236:ARG:CG	1:G:236:ARG:NH1	2.72	0.50
3:X:22:DT:N3	4:Y:7:DA:C2	2.78	0.50
2:B:423:VAL:CG2	2:B:432:VAL:HG11	2.40	0.50
2:B:508:SER:C	2:B:509:VAL:HG23	2.32	0.50
2:D:633:ARG:NH1	2:D:638:GLU:HB2	2.26	0.50
2:F:606:GLN:NE2	4:J:19:DA:OP2	2.44	0.50
2:B:550:ILE:HG23	2:B:568:LEU:HD11	1.93	0.50
2:B:572:LYS:HZ3	2:B:606:GLN:CG	2.04	0.50
2:B:646:LEU:HD13	2:B:647:TYR:N	2.27	0.50
2:D:407:HIS:CG	2:D:510:VAL:HG23	2.46	0.50
1:E:55:THR:CA	2:H:375:ASN:OD1	2.56	0.50
1:E:233:TRP:CZ3	1:E:268:VAL:HG11	2.39	0.50
1:G:25:GLU:O	1:G:59:PRO:HA	2.12	0.50
4:Y:1:DT:H2''	4:Y:2:DT:O5'	2.10	0.50
1:A:74:ILE:HD12	1:A:161:PHE:CD2	2.47	0.50
2:B:387:TYR:CE2	2:B:518:LEU:HD22	2.47	0.50
2:B:487:THR:O	2:B:491:LYS:HG3	2.11	0.50
2:D:486:LEU:HA	2:D:490:GLU:OE1	2.11	0.50
2:D:561:THR:O	2:D:615:LYS:HG3	2.11	0.50
2:F:545:ALA:C	2:F:633:ARG:NH2	2.64	0.50
2:F:559:CYS:SG	2:F:650:GLU:HB2	2.52	0.50
1:G:187:ARG:HG3	1:G:187:ARG:HH11	1.77	0.50
1:G:273:ARG:HD2	1:G:280:LEU:HD21	1.93	0.50
1:C:203:SER:OG	1:C:289:LEU:HD11	2.12	0.50
1:E:86:HIS:CE1	1:E:157:VAL:HG12	2.46	0.50
1:E:249:ALA:O	1:E:250:ILE:HD13	2.10	0.50
2:F:379:TYR:CD2	2:F:435:ALA:HB2	2.47	0.50
2:H:592:TRP:CD1	2:H:617:LYS:HB3	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:500:GLN:HE21	2:D:503:LYS:CE	2.25	0.50
2:H:412:VAL:HG22	2:H:413:GLY:N	2.27	0.50
3:X:21:DT:H2''	3:X:22:DT:H5'	1.93	0.50
1:A:48:GLY:N	1:A:57:THR:CG2	2.67	0.50
2:D:395:VAL:HB	2:D:421:CYS:HB3	1.93	0.50
1:G:23:ILE:HD12	1:G:23:ILE:N	2.26	0.50
1:G:37:LYS:HB2	1:G:37:LYS:NZ	2.27	0.50
1:G:229:THR:N	1:G:269:SER:O	2.42	0.50
2:D:583:TYR:HA	2:D:592:TRP:O	2.12	0.49
1:E:246:ARG:HB3	2:F:607:PHE:CD2	2.47	0.49
2:H:534:SER:C	2:H:535:ASP:O	2.50	0.49
2:H:632:ARG:CG	2:H:639:THR:HG22	2.41	0.49
2:B:455:MET:CE	2:B:469:VAL:HG13	2.43	0.49
2:B:460:ILE:HG12	2:B:486:LEU:CD1	2.38	0.49
1:C:48:GLY:HA3	1:C:57:THR:OG1	2.11	0.49
1:E:25:GLU:CG	1:E:58:HIS:O	2.60	0.49
2:H:353:PHE:CD2	2:H:367:LEU:HD21	2.48	0.49
2:H:375:ASN:O	2:H:376:LYS:HB2	2.11	0.49
1:C:187:ARG:O	1:C:189:PRO:HD3	2.12	0.49
1:E:218:LYS:NZ	1:E:218:LYS:HB3	2.27	0.49
1:E:226:VAL:HG12	1:E:228:PHE:HE1	1.74	0.49
1:C:156:ALA:HA	1:C:183:ILE:O	2.13	0.49
2:D:423:VAL:HG21	2:D:432:VAL:HG11	1.94	0.49
1:E:62:LYS:HE2	1:E:64:ASN:HD21	1.76	0.49
1:G:236:ARG:HG3	1:G:236:ARG:NH1	2.17	0.49
3:I:15:DG:C3'	3:I:16:DG:H5''	2.37	0.49
4:J:17:DG:C5'	4:J:17:DG:H8	2.24	0.49
4:J:20:DA:C6	4:J:21:DA:C6	3.00	0.49
2:B:460:ILE:CG1	2:B:486:LEU:HD13	2.40	0.49
2:B:467:LEU:N	2:B:467:LEU:CD1	2.75	0.49
2:B:550:ILE:HD12	2:B:550:ILE:H	1.77	0.49
1:C:51:SER:HB2	1:C:56:LYS:HA	1.94	0.49
2:D:439:ILE:N	2:D:439:ILE:HD13	2.26	0.49
2:D:558:GLY:O	2:D:647:TYR:HA	2.13	0.49
3:X:5:DA:C2	3:X:6:DC:C2	3.01	0.49
1:A:158:ARG:HD3	1:A:179:LEU:HD23	1.93	0.49
1:A:202:ASN:H	1:A:202:ASN:ND2	2.02	0.49
1:A:236:ARG:CG	1:A:236:ARG:NH1	2.72	0.49
2:D:412:VAL:HG22	2:D:413:GLY:H	1.77	0.49
2:D:552:ARG:HG3	2:D:553:MET:N	2.28	0.49
2:D:572:LYS:HD3	2:D:573:VAL:H	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:267:ARG:HG2	1:E:267:ARG:HH11	1.78	0.49
1:G:277:ASP:OD1	1:G:279:GLU:HB3	2.13	0.49
2:H:455:MET:SD	2:H:469:VAL:HG13	2.53	0.49
2:H:568:LEU:HD23	2:H:568:LEU:C	2.31	0.49
2:H:572:LYS:HZ1	2:H:606:GLN:CG	2.09	0.49
1:A:24:ILE:HG13	1:A:62:LYS:HB2	1.95	0.49
2:B:455:MET:HE1	2:B:469:VAL:HG13	1.94	0.49
2:H:583:TYR:CD1	2:H:583:TYR:C	2.85	0.49
1:A:51:SER:CB	1:A:57:THR:CG2	2.73	0.49
1:A:60:THR:OG1	1:A:112:SER:CB	2.57	0.49
1:C:24:ILE:CD1	1:C:110:ILE:HG12	2.42	0.49
1:C:132:GLN:O	1:C:132:GLN:HG2	2.13	0.49
2:D:487:THR:O	2:D:491:LYS:HG3	2.12	0.49
2:F:550:ILE:CG2	2:F:568:LEU:HD11	2.43	0.49
1:G:24:ILE:HD11	1:G:110:ILE:HG12	1.95	0.49
1:G:49:GLU:HG2	1:G:49:GLU:O	2.11	0.49
2:H:566:ILE:N	2:H:566:ILE:CD1	2.75	0.49
2:H:571:ASP:O	2:H:572:LYS:O	2.31	0.49
1:A:72:VAL:HB	1:A:104:LEU:HD13	1.94	0.49
1:A:185:ASP:OD2	1:A:187:ARG:CB	2.61	0.49
1:C:228:PHE:CZ	1:C:255:PRO:HD2	2.48	0.49
1:C:261:SER:O	1:C:262:LEU:C	2.51	0.49
2:D:464:ASN:N	2:D:465:PRO:HD3	2.28	0.49
1:E:51:SER:CB	1:E:57:THR:CG2	2.77	0.49
2:H:605:ARG:O	2:H:606:GLN:HB2	2.11	0.49
4:Y:10:DC:H2 [?]	4:Y:11:DC:O5 [?]	2.13	0.49
1:A:74:ILE:CB	1:A:100:TYR:HB3	2.42	0.48
2:B:346:GLU:OE1	2:B:378:SER:OG	2.29	0.48
2:F:477:GLN:O	2:F:479:GLU:N	2.46	0.48
2:F:517:PHE:HA	2:F:527:ARG:O	2.12	0.48
2:F:621:ILE:CD1	2:F:649:PRO:HB3	2.35	0.48
2:F:650:GLU:HG2	2:F:650:GLU:O	2.13	0.48
1:G:97:ASP:HB2	1:G:99:TYR:CE2	2.48	0.48
2:H:423:VAL:CG2	2:H:432:VAL:HG11	2.43	0.48
2:H:507:LEU:N	2:H:507:LEU:CD1	2.76	0.48
1:A:51:SER:HB2	1:A:57:THR:HG22	1.85	0.48
1:A:86:HIS:CE1	1:A:157:VAL:HG12	2.48	0.48
2:B:476:LEU:HD22	2:B:483:ASP:HB2	1.95	0.48
1:C:207:LEU:HG	1:C:291:ASP:OD1	2.13	0.48
4:J:20:DA:C2	4:J:21:DA:C6	3.02	0.48
1:A:236:ARG:HG3	1:A:236:ARG:NH1	2.21	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:608:ALA:O	2:B:609:ILE:HG13	2.13	0.48
2:B:631:LEU:O	2:B:639:THR:HA	2.13	0.48
2:D:354:ARG:HG2	2:D:355:PHE:N	2.27	0.48
1:E:194:LEU:HB3	1:E:281:SER:HB3	1.93	0.48
1:E:236:ARG:HG3	1:E:236:ARG:NH1	2.23	0.48
2:F:627:VAL:HG23	2:F:645:PHE:HB3	1.95	0.48
2:F:629:VAL:HG12	2:F:643:LYS:O	2.13	0.48
2:F:646:LEU:C	2:F:646:LEU:CD1	2.81	0.48
1:A:206:CYS:HA	1:A:288:TYR:CD1	2.48	0.48
2:B:477:GLN:O	2:B:479:GLU:N	2.46	0.48
2:B:552:ARG:CG	2:B:553:MET:N	2.76	0.48
1:C:34:PHE:CE2	1:C:185:ASP:HB2	2.48	0.48
1:C:104:LEU:HD21	1:C:163:VAL:HG13	1.96	0.48
1:C:273:ARG:HD2	1:C:280:LEU:HD21	1.94	0.48
1:E:88:HIS:CE1	1:E:120:CYS:HB2	2.49	0.48
3:I:7:DT:N3	4:J:22:DG:N2	2.61	0.48
1:A:229:THR:O	1:A:268:VAL:HG13	2.12	0.48
1:G:27:PRO:O	1:G:181:HIS:HE1	1.97	0.48
1:G:196:ILE:HG13	1:G:272:LEU:HD22	1.96	0.48
1:A:72:VAL:HB	1:A:104:LEU:CD1	2.43	0.48
1:E:222:GLU:CD	1:E:222:GLU:N	2.65	0.48
2:F:632:ARG:CG	2:F:639:THR:HG22	2.42	0.48
1:G:36:TYR:N	1:G:36:TYR:HD1	2.09	0.48
4:Y:19:DA:N3	4:Y:20:DA:C4	2.82	0.48
4:J:17:DG:H5''	4:J:17:DG:C8	2.48	0.48
1:A:57:THR:CG2	1:A:57:THR:O	2.61	0.48
2:B:615:LYS:HD2	2:B:615:LYS:N	2.28	0.48
1:G:207:LEU:HG	1:G:291:ASP:OD1	2.13	0.48
1:G:223:ASP:OD2	1:G:274:ARG:CG	2.59	0.48
1:G:228:PHE:CZ	1:G:254:THR:HG22	2.49	0.48
4:Y:16:DC:H2''	4:Y:17:DG:H5''	1.94	0.48
1:A:60:THR:CG2	1:A:61:ILE:N	2.75	0.48
1:A:88:HIS:NE2	1:A:120:CYS:CB	2.77	0.48
1:A:203:SER:OG	1:A:289:LEU:HD11	2.14	0.48
1:C:24:ILE:CG1	1:C:62:LYS:HB2	2.43	0.48
1:C:206:CYS:HA	1:C:288:TYR:HD1	1.78	0.48
2:D:467:LEU:N	2:D:467:LEU:HD12	2.28	0.48
1:E:60:THR:HG23	1:E:111:HIS:C	2.34	0.48
1:E:122:LYS:C	1:E:124:ARG:H	2.17	0.48
1:G:88:HIS:CE1	1:G:121:VAL:H	2.31	0.48
2:H:583:TYR:O	2:H:627:VAL:HB	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:8:DT:O2	4:Y:21:DA:C2	2.60	0.48
1:A:48:GLY:N	1:A:57:THR:HG21	2.24	0.48
1:C:222:GLU:CD	1:C:222:GLU:H	2.17	0.48
2:F:508:SER:C	2:F:509:VAL:HG23	2.34	0.48
2:F:599:SER:C	2:F:601:THR:H	2.17	0.48
1:G:28:LYS:N	1:G:48:GLY:O	2.47	0.48
1:G:262:LEU:CD2	1:G:266:VAL:HG12	2.39	0.48
1:A:185:ASP:O	1:A:187:ARG:N	2.42	0.48
1:C:36:TYR:CE1	1:C:120:CYS:SG	3.07	0.48
1:G:202:ASN:ND2	1:G:202:ASN:N	2.52	0.48
1:E:206:CYS:HA	1:E:288:TYR:HD1	1.77	0.47
2:F:577:ASP:OD1	2:F:634:LYS:HB2	2.13	0.47
1:G:203:SER:OG	1:G:289:LEU:HD11	2.13	0.47
1:A:167:ASP:CB	1:A:168:PRO:HD2	2.34	0.47
1:C:82:PRO:O	1:C:84:ARG:HG3	2.14	0.47
1:C:185:ASP:C	1:C:187:ARG:H	2.16	0.47
2:D:624:PRO:CB	2:D:646:LEU:HD11	2.39	0.47
2:D:632:ARG:HG3	2:D:639:THR:HG22	1.94	0.47
1:E:32:MET:HG3	1:E:47:PRO:HD3	1.96	0.47
1:E:88:HIS:NE2	1:E:120:CYS:CB	2.76	0.47
1:G:72:VAL:HB	1:G:104:LEU:HD11	1.95	0.47
1:E:236:ARG:CG	1:E:236:ARG:NH1	2.74	0.47
2:F:355:PHE:CE2	2:F:539:ASP:HB2	2.50	0.47
2:F:509:VAL:HA	2:F:537:ILE:O	2.13	0.47
2:F:578:ILE:O	2:F:598:PHE:HZ	1.97	0.47
1:C:30:ARG:HH21	1:C:191:THR:CG2	2.27	0.47
1:E:86:HIS:CG	1:E:157:VAL:HG12	2.50	0.47
2:F:405:HIS:HB3	2:F:501:GLN:OE1	2.15	0.47
1:C:51:SER:HA	1:C:57:THR:HG23	1.96	0.47
1:C:88:HIS:CE1	1:C:120:CYS:HA	2.50	0.47
1:C:199:VAL:HG12	1:C:201:ARG:H	1.78	0.47
2:D:534:SER:C	2:D:535:ASP:O	2.52	0.47
1:G:86:HIS:CG	1:G:87:PRO:CD	2.97	0.47
1:G:158:ARG:CZ	1:G:182:PRO:HD3	2.45	0.47
4:J:19:DA:H2''	4:J:20:DA:N7	2.29	0.47
2:B:402:LYS:HG2	2:B:403:ASN:OD1	2.14	0.47
2:B:456:THR:HG23	2:B:486:LEU:HD22	1.97	0.47
1:C:86:HIS:CG	1:C:87:PRO:CD	2.97	0.47
2:D:476:LEU:HD22	2:D:483:ASP:HB2	1.95	0.47
2:D:632:ARG:CG	2:D:639:THR:HG22	2.45	0.47
1:E:171:ARG:HE	1:E:172:PRO:HD3	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:226:VAL:CG1	1:E:228:PHE:HE1	2.27	0.47
3:X:8:DT:N3	4:Y:21:DA:C2	2.83	0.47
4:Y:19:DA:N3	4:Y:20:DA:C5	2.83	0.47
1:A:29:GLN:HG2	1:A:182:PRO:O	2.15	0.47
1:A:73:ARG:HA	1:A:100:TYR:O	2.14	0.47
2:B:508:SER:C	2:B:509:VAL:CG2	2.83	0.47
1:C:30:ARG:HH21	1:C:191:THR:CB	2.28	0.47
1:C:95:CYS:SG	1:C:100:TYR:HB2	2.55	0.47
1:C:200:ASN:O	1:C:201:ARG:HB2	2.14	0.47
2:D:583:TYR:CE1	2:D:628:PHE:HB2	2.50	0.47
2:F:454:ARG:HG2	2:F:454:ARG:NH1	2.30	0.47
1:G:65:GLY:O	1:G:66:TYR:HB2	2.14	0.47
2:H:550:ILE:HD11	2:H:640:SER:OG	2.13	0.47
1:C:86:HIS:CD2	1:C:157:VAL:HG12	2.50	0.47
1:E:74:ILE:HG12	1:E:100:TYR:HD1	1.78	0.47
1:E:200:ASN:O	1:E:201:ARG:HB2	2.15	0.47
1:E:265:PRO:HB3	1:E:289:LEU:HD23	1.97	0.47
1:G:105:CYS:SG	1:G:107:ASP:OD1	2.73	0.47
1:G:273:ARG:O	1:G:275:PRO:HD3	2.15	0.47
2:H:355:PHE:HB3	2:H:441:HIS:HB2	1.97	0.47
2:H:459:CYS:SG	2:H:494:ILE:HD11	2.55	0.47
2:H:571:ASP:O	2:H:572:LYS:C	2.52	0.47
3:I:8:DT:O2	4:J:21:DA:H2	1.98	0.47
4:J:5:DA:H2''	4:J:6:DA:C8	2.50	0.47
2:F:467:LEU:HD12	2:F:467:LEU:H	1.77	0.47
2:F:550:ILE:HD11	2:F:640:SER:HG	1.78	0.47
2:F:613:THR:HG23	2:F:614:PRO:CD	2.42	0.47
2:F:614:PRO:HG2	2:F:647:TYR:OH	2.14	0.47
1:G:25:GLU:HA	1:G:25:GLU:OE1	2.14	0.47
3:I:9:DT:H2''	3:I:10:DC:O5'	2.15	0.47
1:C:40:GLY:O	1:C:42:SER:N	2.48	0.47
1:E:158:ARG:HH12	1:E:182:PRO:HD3	1.77	0.47
2:H:478:ALA:O	2:H:526:THR:HB	2.14	0.47
4:Y:17:DG:OP1	4:Y:17:DG:C4'	2.61	0.47
1:E:113:PHE:CE2	1:E:161:PHE:HE2	2.33	0.46
2:F:552:ARG:HG3	2:F:553:MET:H	1.80	0.46
2:F:632:ARG:HG3	2:F:639:THR:CG2	2.45	0.46
1:G:66:TYR:CD2	1:G:165:VAL:HB	2.50	0.46
1:G:187:ARG:O	1:G:187:ARG:CG	2.61	0.46
2:H:405:HIS:HB3	2:H:501:GLN:OE1	2.14	0.46
2:H:467:LEU:HD12	2:H:467:LEU:N	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:8:DT:C2	4:Y:21:DA:C2	3.02	0.46
1:A:22:GLU:OE2	1:A:62:LYS:HD3	2.14	0.46
2:B:354:ARG:HD2	2:B:356:ARG:CZ	2.44	0.46
2:B:489:ARG:HD3	2:B:489:ARG:C	2.35	0.46
2:B:580:ILE:N	2:B:580:ILE:CD1	2.78	0.46
1:C:229:THR:N	1:C:269:SER:O	2.47	0.46
2:D:572:LYS:HZ3	2:D:606:GLN:CG	2.25	0.46
1:E:60:THR:CG2	1:E:61:ILE:H	2.26	0.46
2:B:555:ARG:HH11	2:B:555:ARG:CG	2.28	0.46
2:B:613:THR:CG2	2:B:614:PRO:N	2.79	0.46
1:C:194:LEU:HD22	1:C:279:GLU:HG3	1.96	0.46
1:E:233:TRP:CD1	1:E:258:ALA:HB2	2.49	0.46
2:F:593:GLU:HG2	2:F:595:PHE:CE1	2.50	0.46
1:G:74:ILE:HD11	1:G:161:PHE:HD2	1.76	0.46
1:G:210:ASP:O	1:G:253:ARG:HA	2.15	0.46
2:H:367:LEU:HG	2:H:437:LEU:O	2.16	0.46
1:E:58:HIS:CE1	1:E:114:GLN:NE2	2.81	0.46
2:F:398:VAL:HG23	2:F:511:ARG:HB2	1.96	0.46
2:F:400:ASN:CG	2:F:400:ASN:O	2.54	0.46
2:F:564:GLU:O	2:F:612:LYS:HA	2.16	0.46
4:J:2:DT:H2''	4:J:3:DG:H5'	1.96	0.46
2:B:451:LEU:HD11	2:B:498:ALA:HA	1.97	0.46
2:B:593:GLU:HG2	2:B:595:PHE:CE1	2.51	0.46
1:C:198:ARG:HD2	2:D:567:TYR:OH	2.16	0.46
2:D:520:ASP:HA	2:D:527:ARG:HD3	1.98	0.46
2:F:456:THR:HG23	2:F:486:LEU:HD22	1.98	0.46
2:F:508:SER:O	2:F:509:VAL:CG2	2.64	0.46
2:F:511:ARG:HG2	2:F:536:ALA:HA	1.98	0.46
1:G:239:PHE:HB3	1:G:252:PHE:CB	2.46	0.46
2:H:423:VAL:HG21	2:H:432:VAL:CG1	2.45	0.46
1:C:171:ARG:HE	1:C:171:ARG:HA	1.79	0.46
2:D:451:LEU:O	2:D:455:MET:HG3	2.15	0.46
1:E:273:ARG:HD2	1:E:280:LEU:CD2	2.41	0.46
2:F:490:GLU:O	2:F:494:ILE:HG12	2.16	0.46
2:H:574:GLN:HB3	2:H:577:ASP:HB3	1.98	0.46
1:A:213:PHE:CZ	2:B:554:ASP:HB3	2.51	0.46
2:B:605:ARG:HA	2:B:606:GLN:NE2	2.31	0.46
1:C:198:ARG:O	1:C:199:VAL:CG2	2.63	0.46
1:C:201:ARG:HB3	1:C:212:ILE:CD1	2.46	0.46
1:C:277:ASP:OD1	1:C:279:GLU:HB3	2.16	0.46
2:D:581:ARG:NH1	2:D:583:TYR:CD2	2.84	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:464:ASN:HD22	2:H:528:ARG:NH1	2.13	0.46
2:B:425:ALA:O	2:B:426:GLY:C	2.54	0.46
2:D:392:LYS:HB3	2:D:517:PHE:HB2	1.98	0.46
1:E:34:PHE:N	1:E:34:PHE:CD1	2.83	0.46
1:E:285:GLU:CD	1:E:285:GLU:H	2.19	0.46
1:G:46:ILE:HA	1:G:47:PRO:HD3	1.75	0.46
2:H:385:CYS:O	2:H:386:ASN:HB2	2.16	0.46
2:H:391:ALA:HB3	2:H:425:ALA:HB3	1.98	0.46
1:C:122:LYS:HG2	3:X:22:DT:H3'	1.98	0.46
1:E:29:GLN:NE2	1:E:181:HIS:HB2	2.30	0.46
2:F:500:GLN:HE21	2:F:503:LYS:CE	2.28	0.46
1:A:51:SER:CB	1:A:57:THR:HG21	2.39	0.46
1:A:265:PRO:HB3	1:A:287:GLN:OE1	2.16	0.46
2:B:354:ARG:HD2	2:B:356:ARG:NE	2.31	0.46
2:B:650:GLU:O	2:B:650:GLU:HG2	2.16	0.46
1:C:21:VAL:CG2	1:C:163:VAL:HG21	2.38	0.46
1:C:223:ASP:OD2	1:C:274:ARG:HG3	2.15	0.46
2:D:569:LEU:HD23	2:D:608:ALA:HB2	1.98	0.46
2:F:599:SER:O	2:F:601:THR:N	2.48	0.46
2:F:641:GLU:O	2:F:642:PRO:C	2.55	0.46
2:B:379:TYR:CD2	2:B:435:ALA:HB2	2.50	0.45
2:B:579:GLN:NE2	2:B:632:ARG:HE	2.15	0.45
2:B:584:GLU:O	2:B:591:VAL:HG23	2.16	0.45
1:C:30:ARG:NH2	1:C:191:THR:HB	2.30	0.45
2:D:353:PHE:CD2	2:D:367:LEU:CD2	2.98	0.45
1:E:26:GLN:HB3	1:E:181:HIS:CE1	2.50	0.45
2:F:565:GLU:C	2:F:566:ILE:HD12	2.36	0.45
2:F:580:ILE:N	2:F:580:ILE:CD1	2.79	0.45
1:G:132:GLN:HA	1:G:135:GLN:HG2	1.97	0.45
2:H:460:ILE:HG12	2:H:486:LEU:HD13	1.99	0.45
4:Y:20:DA:N1	4:Y:21:DA:N1	2.63	0.45
1:A:60:THR:HG23	1:A:111:HIS:O	2.17	0.45
1:C:46:ILE:HA	1:C:47:PRO:HD3	1.67	0.45
1:C:88:HIS:CE1	1:C:120:CYS:CA	2.99	0.45
1:C:237:GLY:HA2	1:C:255:PRO:HD3	1.98	0.45
2:D:464:ASN:ND2	2:D:528:ARG:HH11	2.14	0.45
2:D:509:VAL:CG2	2:D:538:TYR:CD1	2.99	0.45
2:D:509:VAL:CG2	2:D:538:TYR:HD1	2.27	0.45
2:F:408:ALA:O	2:F:442:VAL:HG11	2.16	0.45
2:D:387:TYR:OH	2:D:519:PRO:HD2	2.15	0.45
1:G:157:VAL:O	1:G:182:PRO:HA	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:214:LEU:O	1:G:249:ALA:HA	2.17	0.45
1:A:229:THR:N	1:A:269:SER:O	2.50	0.45
2:B:400:ASN:CG	2:B:400:ASN:O	2.55	0.45
1:C:268:VAL:HG12	1:C:269:SER:N	2.30	0.45
2:D:481:GLY:O	2:D:483:ASP:N	2.49	0.45
2:F:575:LYS:HD2	2:F:600:PRO:O	2.17	0.45
1:A:68:GLY:CA	1:A:106:PRO:O	2.64	0.45
1:A:141:PHE:CE1	1:A:177:PRO:HG2	2.52	0.45
2:B:556:THR:O	2:B:645:PHE:HA	2.16	0.45
1:E:171:ARG:HA	1:E:171:ARG:NE	2.28	0.45
2:F:568:LEU:C	2:F:568:LEU:HD23	2.37	0.45
1:G:258:ALA:O	1:G:260:PRO:HD3	2.16	0.45
2:H:349:LYS:NZ	2:H:372:SER:OG	2.37	0.45
2:H:487:THR:O	2:H:491:LYS:HG3	2.17	0.45
2:H:627:VAL:HG23	2:H:628:PHE:N	2.31	0.45
1:C:266:VAL:HG13	1:C:266:VAL:O	2.17	0.45
2:D:434:PHE:CE2	2:D:514:PHE:HE2	2.35	0.45
1:G:24:ILE:HD12	1:G:60:THR:HG22	1.97	0.45
1:G:59:PRO:O	1:G:112:SER:HA	2.16	0.45
1:E:25:GLU:HB3	1:E:60:THR:H	1.82	0.45
1:A:51:SER:H	1:A:57:THR:HB	1.82	0.45
2:B:500:GLN:HE21	2:B:503:LYS:HE2	1.82	0.45
1:C:23:ILE:H	1:C:23:ILE:CD1	2.29	0.45
1:C:259:ASP:HB3	1:C:262:LEU:HD13	1.99	0.45
2:D:354:ARG:HG2	2:D:355:PHE:O	2.17	0.45
1:A:259:ASP:HB3	1:A:262:LEU:HD13	1.98	0.45
2:B:518:LEU:O	2:B:527:ARG:HB2	2.17	0.45
2:B:568:LEU:C	2:B:568:LEU:HD23	2.37	0.45
1:C:132:GLN:HA	1:C:135:GLN:CG	2.47	0.45
2:D:603:VAL:O	2:D:603:VAL:HG12	2.16	0.45
1:G:213:PHE:CD2	2:H:554:ASP:HB3	2.51	0.45
2:B:500:GLN:O	2:B:503:LYS:HG2	2.16	0.45
2:B:613:THR:HG23	2:B:614:PRO:CD	2.47	0.45
1:C:214:LEU:HD22	1:C:250:ILE:HG13	1.99	0.45
2:D:629:VAL:O	2:D:629:VAL:HG13	2.16	0.45
1:E:22:GLU:OE2	1:E:62:LYS:HD3	2.16	0.45
1:E:126:LEU:HD21	1:E:154:LEU:HD21	1.99	0.45
2:B:379:TYR:O	2:B:380:PRO:C	2.54	0.44
2:B:517:PHE:HA	2:B:527:ARG:O	2.17	0.44
2:B:571:ASP:O	2:B:572:LYS:C	2.56	0.44
1:C:66:TYR:CE2	1:C:165:VAL:HB	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:23:ILE:H	1:E:23:ILE:CD1	2.28	0.44
1:E:201:ARG:HB3	1:E:212:ILE:HD12	1.99	0.44
2:F:354:ARG:HD2	2:F:356:ARG:HD3	1.98	0.44
2:F:571:ASP:O	2:F:573:VAL:HG13	2.17	0.44
1:G:116:LEU:HA	1:G:116:LEU:HD23	1.70	0.44
4:J:20:DA:C2	4:J:21:DA:C5	3.06	0.44
1:A:167:ASP:HB2	1:A:168:PRO:CD	2.38	0.44
2:B:411:LEU:HD12	2:B:411:LEU:HA	1.75	0.44
1:C:236:ARG:NH1	1:C:236:ARG:CG	2.79	0.44
1:E:122:LYS:C	1:E:124:ARG:N	2.69	0.44
1:E:213:PHE:CZ	2:F:554:ASP:HB3	2.52	0.44
1:E:229:THR:O	1:E:268:VAL:HG13	2.18	0.44
2:B:618:ASP:CG	2:B:621:ILE:HG22	2.37	0.44
1:C:66:TYR:CD1	1:C:66:TYR:C	2.90	0.44
1:C:233:TRP:CD1	1:C:258:ALA:HB2	2.52	0.44
2:D:344:ILE:O	2:D:344:ILE:HG22	2.17	0.44
1:E:46:ILE:CG1	1:E:118:ILE:HD11	2.46	0.44
1:G:130:ILE:CD1	1:G:152:TYR:HE1	2.30	0.44
2:H:454:ARG:HG2	2:H:454:ARG:HH11	1.82	0.44
4:J:16:DC:H6	4:J:16:DC:H5'	1.83	0.44
4:J:19:DA:C2	4:J:20:DA:C4	3.05	0.44
1:A:167:ASP:C	1:A:169:ALA:N	2.70	0.44
2:B:407:HIS:CD2	2:B:409:HIS:H	2.16	0.44
2:B:464:ASN:ND2	2:B:528:ARG:NH1	2.65	0.44
2:B:508:SER:O	2:B:509:VAL:CG2	2.65	0.44
2:B:555:ARG:HA	2:B:555:ARG:HD2	1.74	0.44
2:B:631:LEU:HB2	2:B:640:SER:HB3	1.99	0.44
1:C:34:PHE:CD1	1:C:118:ILE:CG2	3.01	0.44
2:D:367:LEU:HD23	2:D:367:LEU:HA	1.87	0.44
2:D:434:PHE:CE2	2:D:514:PHE:CE2	3.05	0.44
1:E:245:HIS:CD2	2:F:569:LEU:HB3	2.52	0.44
2:F:508:SER:C	2:F:509:VAL:CG2	2.86	0.44
2:B:409:HIS:CD2	2:B:442:VAL:HG22	2.52	0.44
1:C:76:LEU:HA	1:C:76:LEU:HD12	1.71	0.44
1:C:244:VAL:HG12	1:C:244:VAL:O	2.17	0.44
1:E:156:ALA:HA	1:E:183:ILE:O	2.18	0.44
2:F:347:GLN:O	2:F:370:ALA:N	2.50	0.44
4:Y:2:DT:H2''	4:Y:3:DG:H5'	1.99	0.44
4:Y:20:DA:C2	4:Y:21:DA:C2	3.05	0.44
1:A:48:GLY:N	1:A:57:THR:HG23	2.28	0.44
2:B:633:ARG:O	2:B:637:LEU:HA	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:274:ARG:NH2	1:C:279:GLU:HG2	2.33	0.44
1:G:30:ARG:CZ	1:G:191:THR:HB	2.48	0.44
1:A:24:ILE:CG1	1:A:62:LYS:HB2	2.48	0.44
2:D:504:GLU:HA	2:D:504:GLU:OE1	2.17	0.44
1:E:24:ILE:CD1	1:E:62:LYS:HB2	2.48	0.44
2:F:411:LEU:HD12	2:F:411:LEU:HA	1.77	0.44
1:G:114:GLN:H	1:G:114:GLN:HG2	1.57	0.44
1:G:206:CYS:HA	1:G:288:TYR:CD1	2.53	0.44
2:H:451:LEU:HD13	2:H:451:LEU:C	2.38	0.44
2:H:603:VAL:O	2:H:603:VAL:HG12	2.16	0.44
1:A:63:ILE:O	1:A:109:SER:OG	2.36	0.44
1:E:158:ARG:CZ	1:E:182:PRO:HD3	2.47	0.44
2:F:402:LYS:H	2:F:402:LYS:HD3	1.82	0.44
2:F:476:LEU:CD2	2:F:483:ASP:CG	2.86	0.44
3:X:8:DT:C2'	3:X:9:DT:OP2	2.61	0.44
1:A:226:VAL:HG12	1:A:228:PHE:CE1	2.53	0.44
1:C:214:LEU:O	1:C:249:ALA:HA	2.18	0.44
2:D:423:VAL:HG21	2:D:432:VAL:CG1	2.48	0.44
2:D:559:CYS:SG	2:D:650:GLU:CB	3.05	0.44
2:F:346:GLU:O	2:F:380:PRO:HA	2.18	0.44
2:F:489:ARG:NH1	2:F:489:ARG:HG2	2.32	0.44
1:G:60:THR:OG1	1:G:112:SER:HB3	2.17	0.44
1:G:88:HIS:CG	1:G:120:CYS:HA	2.53	0.44
2:H:394:ILE:CG1	2:H:515:THR:HB	2.48	0.44
1:A:74:ILE:N	1:A:100:TYR:O	2.50	0.43
1:C:75:SER:HB3	1:C:162:GLN:HE22	1.83	0.43
1:C:171:ARG:O	1:C:172:PRO:C	2.56	0.43
2:D:478:ALA:O	2:D:526:THR:HB	2.17	0.43
2:D:507:LEU:N	2:D:507:LEU:HD12	2.32	0.43
2:D:615:LYS:HD2	2:D:615:LYS:N	2.33	0.43
1:E:48:GLY:CA	1:E:57:THR:OG1	2.60	0.43
2:H:379:TYR:O	2:H:381:GLN:HG3	2.17	0.43
2:H:578:ILE:HG12	2:H:579:GLN:N	2.32	0.43
3:X:17:DG:H2''	3:X:18:DG:OP2	2.17	0.43
3:I:22:DT:C2	4:J:7:DA:H2	2.31	0.43
1:C:245:HIS:HB3	1:C:249:ALA:HB3	2.00	0.43
2:D:549:LYS:HB3	2:D:571:ASP:OD1	2.18	0.43
1:E:196:ILE:HG12	1:E:272:LEU:HD22	2.00	0.43
1:E:246:ARG:C	1:E:247:GLN:HG3	2.39	0.43
1:G:88:HIS:CE1	1:G:120:CYS:CA	3.01	0.43
2:H:423:VAL:HG21	2:H:432:VAL:HG11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:16:DG:H2''	3:I:17:DG:H8	1.84	0.43
2:D:581:ARG:HD2	2:D:632:ARG:NH1	2.33	0.43
2:F:464:ASN:HD21	2:F:528:ARG:NH1	2.16	0.43
2:F:554:ASP:C	2:F:554:ASP:OD1	2.57	0.43
2:H:381:GLN:HA	2:H:432:VAL:O	2.18	0.43
2:H:444:LYS:HA	2:H:447:VAL:CG2	2.48	0.43
1:A:240:SER:C	1:A:242:ALA:N	2.71	0.43
1:A:245:HIS:CD2	2:B:569:LEU:HB3	2.54	0.43
2:B:353:PHE:HE2	2:B:439:ILE:HG12	1.83	0.43
2:D:443:THR:O	2:D:447:VAL:HG23	2.18	0.43
1:E:126:LEU:HD13	1:E:126:LEU:O	2.17	0.43
2:F:425:ALA:O	2:F:426:GLY:O	2.36	0.43
2:F:634:LYS:O	2:F:635:SER:C	2.56	0.43
2:H:573:VAL:HG22	2:H:606:GLN:O	2.18	0.43
4:J:10:DC:H2''	4:J:11:DC:O5'	2.18	0.43
1:A:46:ILE:HG22	1:A:47:PRO:O	2.18	0.43
1:C:36:TYR:N	1:C:36:TYR:HD1	2.15	0.43
2:D:367:LEU:HA	2:D:368:PRO:HD3	1.69	0.43
2:D:587:GLU:OE1	2:D:587:GLU:HA	2.18	0.43
2:F:624:PRO:CB	2:F:646:LEU:HD11	2.48	0.43
2:H:646:LEU:C	2:H:646:LEU:CD1	2.87	0.43
1:A:29:GLN:NE2	1:A:181:HIS:HB2	2.34	0.43
1:A:86:HIS:CE1	1:A:157:VAL:CG1	3.01	0.43
2:B:469:VAL:HG11	2:B:494:ILE:HD13	2.01	0.43
2:H:480:GLY:H	2:H:526:THR:HG22	1.84	0.43
4:Y:1:DT:C6	4:Y:2:DT:H72	2.54	0.43
4:J:17:DG:C5'	4:J:17:DG:C8	3.02	0.43
2:B:508:SER:O	2:B:509:VAL:HG22	2.19	0.43
2:B:574:GLN:OE1	4:Y:20:DA:OP1	2.37	0.43
2:B:632:ARG:CG	2:B:639:THR:HG22	2.47	0.43
1:C:54:THR:OG1	1:C:55:THR:N	2.49	0.43
1:C:246:ARG:HB3	2:D:607:PHE:CD2	2.54	0.43
2:D:435:ALA:O	2:D:436:ASN:C	2.56	0.43
1:G:58:HIS:HB3	1:G:59:PRO:HD2	1.98	0.43
1:G:156:ALA:O	1:G:157:VAL:HG13	2.18	0.43
1:G:268:VAL:HG12	1:G:269:SER:N	2.33	0.43
2:H:477:GLN:O	2:H:479:GLU:N	2.52	0.43
4:J:23:DT:H1'	4:J:24:DC:H5''	2.00	0.43
1:A:34:PHE:N	1:A:34:PHE:HD1	2.16	0.43
2:B:412:VAL:HG22	2:B:413:GLY:N	2.34	0.43
1:C:20:TYR:CD1	1:C:20:TYR:N	2.87	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:354:ARG:HD2	2:D:356:ARG:HD3	2.01	0.43
2:D:409:HIS:CD2	2:D:442:VAL:H	2.37	0.43
2:D:633:ARG:HB2	2:D:636:ASP:OD1	2.18	0.43
1:E:51:SER:CB	1:E:57:THR:HG21	2.42	0.43
2:F:574:GLN:NE2	4:J:20:DA:OP1	2.51	0.43
2:H:476:LEU:HD22	2:H:483:ASP:CB	2.47	0.43
4:J:17:DG:H2"	4:J:18:DG:C8	2.52	0.43
1:A:23:ILE:H	1:A:23:ILE:CD1	2.28	0.43
1:A:43:ALA:O	1:A:44:GLY:O	2.37	0.43
1:A:130:ILE:O	1:A:134:ILE:HG12	2.19	0.43
1:C:156:ALA:C	1:C:157:VAL:HG13	2.39	0.43
2:D:464:ASN:HD22	2:D:528:ARG:NH1	2.17	0.43
1:G:75:SER:HB3	1:G:162:GLN:NE2	2.34	0.43
1:A:218:LYS:HB3	1:A:218:LYS:HZ2	1.80	0.43
1:E:86:HIS:ND1	1:E:157:VAL:HG12	2.34	0.43
1:G:35:ARG:NH2	1:G:39:GLU:OE2	2.45	0.43
1:G:122:LYS:C	1:G:124:ARG:N	2.71	0.43
2:H:354:ARG:HG2	2:H:355:PHE:N	2.33	0.43
2:H:506:ASP:C	2:H:508:SER:H	2.21	0.43
1:A:22:GLU:HG3	1:A:62:LYS:HB3	2.01	0.42
1:A:86:HIS:CD2	1:A:157:VAL:HG12	2.53	0.42
2:B:616:TYR:CG	2:B:617:LYS:N	2.87	0.42
2:D:464:ASN:HD21	2:D:528:ARG:HH11	1.67	0.42
2:F:621:ILE:HG12	2:F:622:THR:N	2.33	0.42
1:G:86:HIS:CD2	1:G:157:VAL:HG12	2.54	0.42
2:H:548:LEU:O	2:H:640:SER:HB2	2.19	0.42
3:X:22:DT:C2	4:Y:7:DA:C2	3.05	0.42
1:C:257:TYR:CG	1:C:258:ALA:N	2.87	0.42
2:D:444:LYS:O	2:D:447:VAL:HG23	2.19	0.42
1:E:61:ILE:HG21	1:E:161:PHE:CD2	2.54	0.42
1:E:240:SER:C	1:E:242:ALA:N	2.69	0.42
2:F:492:GLU:O	2:F:496:GLN:HG3	2.19	0.42
2:H:418:ASP:HB3	2:H:457:GLU:OE1	2.20	0.42
2:H:454:ARG:HG2	2:H:454:ARG:NH1	2.33	0.42
1:A:153:ASP:OD2	1:A:156:ALA:HB3	2.19	0.42
1:A:156:ALA:HA	1:A:183:ILE:O	2.18	0.42
2:B:444:LYS:HB2	4:Y:22:DG:OP1	2.19	0.42
2:D:425:ALA:O	2:D:426:GLY:O	2.36	0.42
1:E:144:PRO:O	1:E:148:GLN:HG3	2.19	0.42
1:E:165:VAL:HG22	1:E:175:LEU:HD21	2.00	0.42
2:F:583:TYR:HA	2:F:592:TRP:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:24:ILE:CD1	1:G:110:ILE:HG12	2.49	0.42
1:G:113:PHE:CD2	1:G:113:PHE:N	2.87	0.42
1:A:23:ILE:HD11	1:A:178:VAL:HG22	2.00	0.42
1:A:60:THR:CG2	1:A:61:ILE:H	2.33	0.42
2:D:646:LEU:C	2:D:646:LEU:CD1	2.87	0.42
2:F:425:ALA:O	2:F:426:GLY:C	2.58	0.42
2:F:455:MET:HE1	2:F:469:VAL:HG13	2.01	0.42
1:A:143:VAL:HA	1:A:144:PRO:HD3	1.83	0.42
2:B:341:TYR:N	2:B:341:TYR:CD1	2.87	0.42
2:B:574:GLN:NE2	4:Y:20:DA:OP1	2.53	0.42
1:C:24:ILE:HD12	1:C:60:THR:HG22	2.02	0.42
2:D:487:THR:N	2:D:490:GLU:OE1	2.44	0.42
2:F:353:PHE:HE2	2:F:439:ILE:HG12	1.83	0.42
2:F:555:ARG:HA	2:F:555:ARG:HD2	1.85	0.42
1:G:88:HIS:CE1	1:G:120:CYS:HA	2.53	0.42
3:X:5:DA:N1	4:Y:23:DT:O4	2.53	0.42
1:A:25:GLU:HB2	1:A:60:THR:H	1.85	0.42
1:A:55:THR:HA	2:D:375:ASN:OD1	2.20	0.42
1:E:213:PHE:CE1	2:F:554:ASP:HB3	2.55	0.42
2:F:362:PRO:O	2:F:363:SER:O	2.36	0.42
2:F:476:LEU:HD22	2:F:483:ASP:HB2	2.01	0.42
1:G:156:ALA:O	1:G:157:VAL:CG1	2.67	0.42
3:I:8:DT:O2	4:J:21:DA:C2	2.72	0.42
1:A:51:SER:N	1:A:57:THR:HB	2.34	0.42
1:A:200:ASN:O	1:A:201:ARG:CB	2.63	0.42
2:B:408:ALA:O	2:B:442:VAL:HG11	2.20	0.42
2:B:492:GLU:OE1	2:B:495:ARG:NH2	2.51	0.42
2:B:604:HIS:O	2:B:605:ARG:C	2.58	0.42
2:D:407:HIS:CE1	2:D:510:VAL:HG23	2.54	0.42
1:E:178:VAL:HG13	1:E:178:VAL:O	2.20	0.42
1:E:221:LYS:HG2	1:E:222:GLU:OE2	2.20	0.42
2:F:460:ILE:CG1	2:F:486:LEU:HD13	2.43	0.42
2:F:616:TYR:CG	2:F:617:LYS:N	2.87	0.42
1:G:171:ARG:O	1:G:172:PRO:C	2.58	0.42
2:H:387:TYR:CE2	2:H:518:LEU:CD2	2.99	0.42
1:A:55:THR:CG2	1:A:56:LYS:H	2.31	0.42
2:B:565:GLU:C	2:B:566:ILE:HD12	2.41	0.42
1:C:158:ARG:CZ	1:C:182:PRO:HD3	2.50	0.42
2:D:641:GLU:O	2:D:642:PRO:C	2.58	0.42
4:J:2:DT:H2''	4:J:3:DG:C5'	2.49	0.42
4:J:17:DG:OP1	4:J:17:DG:C4'	2.64	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:ALA:HA	1:A:189:PRO:HD3	1.85	0.42
1:C:24:ILE:N	1:C:60:THR:O	2.47	0.42
2:D:448:PHE:HA	2:D:502:THR:HG21	2.02	0.42
2:D:500:GLN:HE21	2:D:503:LYS:NZ	2.17	0.42
2:D:583:TYR:O	2:D:627:VAL:HB	2.20	0.42
1:E:165:VAL:CG2	1:E:175:LEU:HD21	2.50	0.42
1:E:254:THR:O	1:E:255:PRO:O	2.38	0.42
1:G:21:VAL:CG2	1:G:163:VAL:HG21	2.47	0.42
1:G:132:GLN:HA	1:G:135:GLN:CG	2.50	0.42
4:J:20:DA:H2''	4:J:21:DA:O5'	2.20	0.42
1:A:136:THR:HG23	1:A:138:ASN:HB2	2.01	0.42
2:D:546:SER:O	2:D:548:LEU:N	2.53	0.42
1:E:277:ASP:C	1:E:277:ASP:OD1	2.58	0.42
1:G:40:GLY:O	1:G:41:ARG:C	2.56	0.42
1:G:90:LEU:HA	1:G:117:GLY:O	2.20	0.42
1:A:32:MET:HG3	1:A:47:PRO:HD2	2.00	0.41
1:A:61:ILE:HG21	1:A:161:PHE:CD2	2.55	0.41
2:B:464:ASN:HD21	2:B:528:ARG:HH11	1.67	0.41
1:C:134:ILE:HD11	1:C:148:GLN:OE1	2.20	0.41
1:E:229:THR:HG22	1:E:269:SER:HB3	1.99	0.41
2:F:354:ARG:HD2	2:F:356:ARG:NE	2.34	0.41
2:F:524:SER:O	2:F:526:THR:HG23	2.20	0.41
1:G:21:VAL:HG23	1:G:175:LEU:HD12	2.01	0.41
1:G:122:LYS:O	1:G:123:LYS:C	2.58	0.41
2:H:572:LYS:HE2	2:H:606:GLN:HG2	2.02	0.41
2:B:409:HIS:HD2	2:B:442:VAL:HG22	1.85	0.41
1:E:54:THR:O	1:E:54:THR:CG2	2.66	0.41
1:E:158:ARG:NH1	1:E:158:ARG:HG2	2.33	0.41
2:F:464:ASN:HD21	2:F:528:ARG:HH11	1.67	0.41
1:G:40:GLY:O	1:G:42:SER:N	2.53	0.41
1:G:267:ARG:HG2	1:G:267:ARG:HH11	1.84	0.41
2:H:380:PRO:C	2:H:381:GLN:HG3	2.40	0.41
2:H:559:CYS:SG	2:H:650:GLU:CB	3.03	0.41
1:A:43:ALA:C	1:A:44:GLY:O	2.56	0.41
1:A:56:LYS:CB	2:D:375:ASN:HD21	2.25	0.41
1:A:60:THR:HG22	1:A:61:ILE:H	1.84	0.41
1:C:65:GLY:O	1:C:66:TYR:HB2	2.20	0.41
1:C:104:LEU:HD12	1:C:104:LEU:HA	1.87	0.41
2:D:423:VAL:CG2	2:D:432:VAL:HG11	2.50	0.41
1:E:95:CYS:HA	1:E:99:TYR:O	2.21	0.41
1:E:167:ASP:C	1:E:169:ALA:N	2.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:171:ARG:HE	1:E:172:PRO:HD2	1.85	0.41
2:F:558:GLY:O	2:F:647:TYR:HA	2.20	0.41
1:G:218:LYS:HB3	1:G:218:LYS:HZ3	1.80	0.41
2:H:521:SER:OG	2:H:522:THR:HG23	2.20	0.41
2:H:621:ILE:HG12	2:H:623:LYS:O	2.20	0.41
1:A:62:LYS:HE2	1:A:64:ASN:HD21	1.85	0.41
2:B:554:ASP:C	2:B:554:ASP:OD1	2.58	0.41
1:C:39:GLU:HB3	1:C:40:GLY:H	1.67	0.41
1:C:216:CYS:HB2	1:C:217:ASP:H	1.72	0.41
2:D:346:GLU:HB2	2:D:381:GLN:H	1.85	0.41
1:E:60:THR:HG22	1:E:61:ILE:H	1.78	0.41
1:G:130:ILE:HD13	1:G:152:TYR:HE1	1.86	0.41
1:G:226:VAL:O	1:G:236:ARG:HA	2.21	0.41
1:A:272:LEU:O	1:A:280:LEU:HA	2.21	0.41
2:B:392:LYS:HB3	2:B:517:PHE:HB2	2.03	0.41
2:B:458:ALA:O	2:B:465:PRO:HG3	2.20	0.41
1:C:78:THR:OG1	1:C:83:HIS:HA	2.21	0.41
2:D:466:GLY:HA2	2:D:470:HIS:O	2.20	0.41
1:E:39:GLU:O	1:E:40:GLY:O	2.39	0.41
2:H:347:GLN:OE1	2:H:348:PRO:HD2	2.20	0.41
2:H:392:LYS:O	2:H:516:ALA:HA	2.20	0.41
2:H:633:ARG:HB2	2:H:636:ASP:OD1	2.20	0.41
4:Y:2:DT:H2''	4:Y:3:DG:C5'	2.51	0.41
2:D:350:GLN:HB3	2:D:536:ALA:O	2.20	0.41
2:D:512:LEU:HB2	2:D:534:SER:OG	2.21	0.41
2:D:566:ILE:N	2:D:566:ILE:CD1	2.82	0.41
1:G:239:PHE:HB3	1:G:252:PHE:HB3	2.03	0.41
2:H:402:LYS:HG2	2:H:403:ASN:N	2.35	0.41
4:Y:22:DG:H1'	4:Y:23:DT:C5'	2.51	0.41
1:A:25:GLU:OE1	1:A:25:GLU:HA	2.21	0.41
1:A:86:HIS:ND1	1:A:157:VAL:HG12	2.36	0.41
1:A:272:LEU:HD12	1:A:272:LEU:HA	1.78	0.41
2:B:441:HIS:HE1	2:B:507:LEU:HD23	1.85	0.41
1:C:144:PRO:HB2	1:C:147:GLU:OE1	2.20	0.41
1:C:264:ALA:HA	1:C:265:PRO:HD3	1.94	0.41
2:D:605:ARG:O	2:D:606:GLN:HB2	2.20	0.41
2:F:397:LEU:HD12	2:F:409:HIS:O	2.21	0.41
2:F:508:SER:O	2:F:509:VAL:HG22	2.20	0.41
2:F:542:ALA:HA	2:F:543:PRO:HD3	1.94	0.41
1:G:122:LYS:O	1:G:124:ARG:N	2.54	0.41
1:G:246:ARG:C	1:G:247:GLN:HG3	2.40	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:613:THR:HG22	2:H:614:PRO:O	2.21	0.41
2:H:616:TYR:CZ	2:H:617:LYS:HG2	2.55	0.41
1:A:26:GLN:HB3	1:A:181:HIS:CE1	2.55	0.41
1:A:206:CYS:SG	1:A:290:PRO:HA	2.61	0.41
2:B:573:VAL:HG11	2:B:578:ILE:HD12	2.01	0.41
1:E:57:THR:CG2	1:E:57:THR:O	2.68	0.41
1:E:167:ASP:O	1:E:168:PRO:C	2.58	0.41
2:H:412:VAL:HG22	2:H:413:GLY:H	1.85	0.41
2:B:558:GLY:O	2:B:647:TYR:HA	2.21	0.41
1:C:22:GLU:HG2	1:C:64:ASN:OD1	2.20	0.41
1:C:185:ASP:C	1:C:187:ARG:N	2.74	0.41
1:C:277:ASP:O	1:C:278:ARG:HB2	2.21	0.41
2:D:425:ALA:O	2:D:426:GLY:C	2.58	0.41
2:D:616:TYR:CG	2:D:617:LYS:N	2.89	0.41
1:E:35:ARG:NH2	1:E:39:GLU:OE2	2.51	0.41
1:E:52:THR:CG2	1:E:53:ASP:H	2.14	0.41
1:E:54:THR:C	2:H:375:ASN:OD1	2.58	0.41
1:E:68:GLY:CA	1:E:106:PRO:O	2.68	0.41
1:E:126:LEU:HD22	1:E:126:LEU:HA	1.95	0.41
1:E:180:SER:O	1:E:181:HIS:C	2.59	0.41
1:E:229:THR:CG2	1:E:269:SER:CB	2.97	0.41
1:E:233:TRP:O	1:E:234:GLU:HB2	2.21	0.41
2:H:481:GLY:O	2:H:483:ASP:N	2.53	0.41
1:A:70:GLY:O	1:A:104:LEU:HB2	2.21	0.41
1:A:88:HIS:ND1	1:A:120:CYS:HA	2.35	0.41
1:E:95:CYS:SG	1:E:100:TYR:CA	3.09	0.41
1:E:221:LYS:CG	1:E:222:GLU:OE2	2.69	0.41
2:F:555:ARG:NH1	2:F:555:ARG:CG	2.84	0.41
1:G:268:VAL:CG1	1:G:269:SER:N	2.84	0.41
2:H:409:HIS:HA	2:H:442:VAL:HG13	2.03	0.41
4:Y:23:DT:H1'	4:Y:24:DC:H5''	2.03	0.41
4:Y:25:DC:H2''	4:Y:26:DC:C6	2.55	0.41
1:A:178:VAL:O	1:A:178:VAL:HG13	2.21	0.40
2:B:577:ASP:CG	2:B:577:ASP:O	2.58	0.40
2:B:634:LYS:O	2:B:635:SER:C	2.60	0.40
1:C:122:LYS:C	1:C:124:ARG:N	2.74	0.40
2:D:412:VAL:HG22	2:D:413:GLY:N	2.34	0.40
1:E:72:VAL:HB	1:E:104:LEU:CD1	2.50	0.40
2:F:356:ARG:HA	2:F:360:GLU:OE2	2.21	0.40
2:F:613:THR:CG2	2:F:614:PRO:N	2.84	0.40
1:G:76:LEU:HA	1:G:76:LEU:HD12	1.77	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:213:PHE:HD2	2:H:567:TYR:HB3	1.85	0.40
3:I:7:DT:H3	4:J:22:DG:N2	2.18	0.40
3:I:22:DT:C2	4:J:7:DA:C2	3.08	0.40
4:J:23:DT:H6	4:J:23:DT:H2'	1.75	0.40
2:B:346:GLU:OE2	2:B:378:SER:HB2	2.21	0.40
1:C:115:ASN:HD22	1:C:115:ASN:HA	1.51	0.40
1:C:128:GLN:O	1:C:131:SER:OG	2.30	0.40
2:D:405:HIS:HB3	2:D:501:GLN:OE1	2.21	0.40
2:F:538:TYR:CD2	2:F:538:TYR:N	2.89	0.40
1:G:24:ILE:CG1	1:G:62:LYS:HB2	2.52	0.40
2:H:479:GLU:C	2:H:481:GLY:N	2.74	0.40
3:X:12:DG:O5'	3:X:12:DG:H2'	2.21	0.40
4:J:20:DA:O5'	4:J:20:DA:H8	2.04	0.40
1:A:26:GLN:OE1	1:A:180:SER:HB2	2.22	0.40
1:C:221:LYS:HB3	1:C:244:VAL:HG11	2.02	0.40
1:C:223:ASP:OD2	1:C:274:ARG:CG	2.69	0.40
2:D:348:PRO:CB	2:D:537:ILE:HD11	2.51	0.40
2:D:402:LYS:HG2	2:D:403:ASN:OD1	2.21	0.40
2:D:500:GLN:NE2	2:D:503:LYS:NZ	2.69	0.40
1:E:23:ILE:HG22	1:E:25:GLU:O	2.21	0.40
1:E:73:ARG:HA	1:E:100:TYR:O	2.22	0.40
1:E:132:GLN:HA	1:E:135:GLN:HG2	2.03	0.40
2:F:412:VAL:CG2	2:F:413:GLY:N	2.84	0.40
2:F:525:PHE:CD1	2:F:525:PHE:N	2.89	0.40
2:F:572:LYS:HA	2:F:607:PHE:CE1	2.57	0.40
1:G:72:VAL:HB	1:G:104:LEU:CD1	2.51	0.40
1:G:199:VAL:C	1:G:201:ARG:H	2.24	0.40
2:H:451:LEU:CD1	2:H:498:ALA:HA	2.52	0.40
2:H:643:LYS:HA	2:H:644:PRO:HD3	1.97	0.40
1:A:261:SER:O	1:A:262:LEU:C	2.59	0.40
2:B:402:LYS:NZ	2:B:403:ASN:H	2.19	0.40
1:C:68:GLY:HA2	1:C:106:PRO:O	2.21	0.40
1:E:39:GLU:O	1:E:40:GLY:C	2.59	0.40
1:E:43:ALA:O	1:E:44:GLY:O	2.39	0.40
1:E:52:THR:CG2	1:E:53:ASP:N	2.81	0.40
1:E:95:CYS:SG	1:E:100:TYR:CB	3.07	0.40
1:E:171:ARG:NE	1:E:172:PRO:HD2	2.36	0.40
1:E:268:VAL:HG12	1:E:269:SER:N	2.37	0.40
1:G:228:PHE:HZ	1:G:254:THR:HG22	1.86	0.40
3:I:22:DT:H2''	3:I:23:DT:OP2	2.20	0.40
1:A:285:GLU:H	1:A:285:GLU:CD	2.25	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:613:THR:CG2	2:B:614:PRO:O	2.65	0.40
1:C:245:HIS:CD2	2:D:569:LEU:HB3	2.56	0.40
1:E:128:GLN:O	1:E:128:GLN:HG2	2.21	0.40
2:F:551:VAL:CG1	2:F:552:ARG:N	2.84	0.40
1:G:66:TYR:CD1	1:G:66:TYR:C	2.94	0.40
1:G:217:ASP:O	1:G:219:VAL:HG13	2.21	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	
1	A	271/273 (99%)	231 (85%)	29 (11%)	11 (4%)	3	26
1	C	271/273 (99%)	231 (85%)	29 (11%)	11 (4%)	3	26
1	E	271/273 (99%)	229 (84%)	31 (11%)	11 (4%)	3	26
1	G	271/273 (99%)	231 (85%)	31 (11%)	9 (3%)	4	31
2	B	310/312 (99%)	274 (88%)	25 (8%)	11 (4%)	3	30
2	D	310/312 (99%)	264 (85%)	34 (11%)	12 (4%)	3	27
2	F	310/312 (99%)	272 (88%)	29 (9%)	9 (3%)	4	33
2	H	310/312 (99%)	261 (84%)	36 (12%)	13 (4%)	3	25
All	All	2324/2340 (99%)	1993 (86%)	244 (10%)	87 (4%)	3	28

All (87) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	81	PRO
1	A	83	HIS
1	A	192	ALA
1	A	246	ARG

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Mol	Chain	Res	Type
2	B	363	SER
2	B	367	LEU
2	B	368	PRO
2	B	426	GLY
2	B	478	ALA
2	B	606	GLN
1	C	81	PRO
1	C	262	LEU
2	D	368	PRO
2	D	377	LYS
1	E	81	PRO
1	E	83	HIS
1	E	142	HIS
1	E	192	ALA
2	F	363	SER
2	F	478	ALA
1	G	81	PRO
2	H	368	PRO
2	H	377	LYS
2	H	478	ALA
2	H	482	GLY
2	H	535	ASP
2	H	572	LYS
1	A	142	HIS
1	A	201	ARG
2	B	359	CYS
2	B	482	GLY
1	C	199	VAL
2	D	371	SER
2	D	426	GLY
2	D	478	ALA
2	D	482	GLY
2	D	535	ASP
2	D	545	ALA
2	D	547	ASN
1	E	40	GLY
1	E	246	ARG
2	F	359	CYS
2	F	426	GLY
1	G	48	GLY
1	G	199	VAL
1	G	200	ASN

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Mol	Chain	Res	Type
2	H	371	SER
2	H	426	GLY
2	H	545	ALA
2	H	547	ASN
1	A	40	GLY
1	A	66	TYR
1	C	48	GLY
2	D	572	LYS
1	E	66	TYR
1	E	186	ASN
2	F	600	PRO
1	G	186	ASN
1	G	262	LEU
1	A	96	ARG
1	C	142	HIS
1	C	172	PRO
1	E	51	SER
2	F	482	GLY
2	F	635	SER
1	A	186	ASN
2	B	545	ALA
1	C	49	GLU
1	C	200	ASN
1	E	201	ARG
1	G	66	TYR
1	G	165	VAL
1	G	172	PRO
2	H	483	ASP
2	B	600	PRO
1	C	43	ALA
2	F	545	ALA
1	C	165	VAL
2	H	481	GLY
2	D	481	GLY
1	E	44	GLY
2	D	382	VAL
2	H	382	VAL
1	A	44	GLY
1	C	157	VAL
2	F	481	GLY
2	B	481	GLY

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	
1	A	242/242 (100%)	228 (94%)	14 (6%)	20	55
1	C	242/242 (100%)	221 (91%)	21 (9%)	10	41
1	E	242/242 (100%)	226 (93%)	16 (7%)	16	51
1	G	242/242 (100%)	221 (91%)	21 (9%)	10	41
2	B	268/268 (100%)	250 (93%)	18 (7%)	16	50
2	D	268/268 (100%)	257 (96%)	11 (4%)	30	64
2	F	268/268 (100%)	256 (96%)	12 (4%)	27	62
2	H	268/268 (100%)	257 (96%)	11 (4%)	30	64
All	All	2040/2040 (100%)	1916 (94%)	124 (6%)	18	53

All (124) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	LYS
1	A	56	LYS
1	A	76	LEU
1	A	81	PRO
1	A	104	LEU
1	A	126	LEU
1	A	135	GLN
1	A	145	ILE
1	A	167	ASP
1	A	202	ASN
1	A	214	LEU
1	A	222	GLU
1	A	271	GLN
1	A	272	LEU
2	B	345	LEU
2	B	362	PRO
2	B	367	LEU
2	B	380	PRO
2	B	402	LYS

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Mol	Chain	Res	Type
2	B	411	LEU
2	B	488	ASP
2	B	489	ARG
2	B	495	ARG
2	B	504	GLU
2	B	510	VAL
2	B	579	GLN
2	B	584	GLU
2	B	586	GLU
2	B	606	GLN
2	B	612	LYS
2	B	621	ILE
2	B	644	PRO
1	C	33	ARG
1	C	54	THR
1	C	76	LEU
1	C	81	PRO
1	C	97	ASP
1	C	104	LEU
1	C	114	GLN
1	C	115	ASN
1	C	126	LEU
1	C	135	GLN
1	C	145	ILE
1	C	181	HIS
1	C	198	ARG
1	C	202	ASN
1	C	214	LEU
1	C	216	CYS
1	C	246	ARG
1	C	250	ILE
1	C	272	LEU
1	C	284	MET
1	C	291	ASP
2	D	402	LYS
2	D	410	SER
2	D	488	ASP
2	D	489	ARG
2	D	510	VAL
2	D	552	ARG
2	D	568	LEU
2	D	584	GLU

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Mol	Chain	Res	Type
2	D	586	GLU
2	D	600	PRO
2	D	621	ILE
1	E	28	LYS
1	E	56	LYS
1	E	76	LEU
1	E	81	PRO
1	E	88	HIS
1	E	97	ASP
1	E	104	LEU
1	E	126	LEU
1	E	135	GLN
1	E	145	ILE
1	E	167	ASP
1	E	198	ARG
1	E	202	ASN
1	E	214	LEU
1	E	272	LEU
1	E	290	PRO
2	F	345	LEU
2	F	402	LYS
2	F	411	LEU
2	F	488	ASP
2	F	489	ARG
2	F	495	ARG
2	F	510	VAL
2	F	550	ILE
2	F	579	GLN
2	F	584	GLU
2	F	586	GLU
2	F	621	ILE
1	G	33	ARG
1	G	36	TYR
1	G	54	THR
1	G	76	LEU
1	G	81	PRO
1	G	97	ASP
1	G	104	LEU
1	G	114	GLN
1	G	115	ASN
1	G	126	LEU
1	G	135	GLN

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Mol	Chain	Res	Type
1	G	145	ILE
1	G	179	LEU
1	G	181	HIS
1	G	202	ASN
1	G	203	SER
1	G	216	CYS
1	G	246	ARG
1	G	272	LEU
1	G	284	MET
1	G	291	ASP
2	H	402	LYS
2	H	489	ARG
2	H	504	GLU
2	H	510	VAL
2	H	544	ASN
2	H	584	GLU
2	H	586	GLU
2	H	600	PRO
2	H	602	ASP
2	H	612	LYS
2	H	621	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (71) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	GLN
1	A	58	HIS
1	A	111	HIS
1	A	115	ASN
1	A	128	GLN
1	A	137	ASN
1	A	155	ASN
1	A	162	GLN
1	A	181	HIS
1	A	202	ASN
1	A	271	GLN
2	B	407	HIS
2	B	409	HIS
2	B	436	ASN
2	B	464	ASN
2	B	470	HIS
2	B	500	GLN

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Mol	Chain	Res	Type
2	B	574	GLN
2	B	579	GLN
2	B	606	GLN
1	C	114	GLN
1	C	115	ASN
1	C	128	GLN
1	C	137	ASN
1	C	155	ASN
1	C	162	GLN
1	C	202	ASN
1	C	271	GLN
2	D	375	ASN
2	D	396	GLN
2	D	407	HIS
2	D	409	HIS
2	D	436	ASN
2	D	464	ASN
2	D	470	HIS
2	D	500	GLN
2	D	547	ASN
1	E	29	GLN
1	E	58	HIS
1	E	111	HIS
1	E	114	GLN
1	E	115	ASN
1	E	128	GLN
1	E	137	ASN
1	E	155	ASN
1	E	162	GLN
1	E	181	HIS
1	E	202	ASN
1	E	271	GLN
2	F	407	HIS
2	F	436	ASN
2	F	464	ASN
2	F	470	HIS
2	F	500	GLN
2	F	574	GLN
2	F	579	GLN
2	F	606	GLN
1	G	115	ASN
1	G	128	GLN

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Mol	Chain	Res	Type
1	G	137	ASN
1	G	155	ASN
1	G	162	GLN
1	G	202	ASN
2	H	396	GLN
2	H	407	HIS
2	H	409	HIS
2	H	436	ASN
2	H	464	ASN
2	H	470	HIS
2	H	500	GLN
2	H	547	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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 monosaccharides 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	273/273 (100%)	0.18	21 (7%) 13 8	76, 176, 199, 200	0
1	C	273/273 (100%)	-0.08	2 (0%) 87 78	67, 142, 189, 199	0
1	E	273/273 (100%)	0.11	18 (6%) 18 10	77, 177, 199, 200	0
1	G	273/273 (100%)	-0.04	3 (1%) 80 68	66, 144, 190, 200	0
2	B	312/312 (100%)	0.11	16 (5%) 28 17	75, 155, 198, 200	0
2	D	312/312 (100%)	0.17	17 (5%) 25 16	75, 164, 199, 200	0
2	F	312/312 (100%)	0.09	18 (5%) 23 13	66, 156, 199, 200	0
2	H	312/312 (100%)	0.22	21 (6%) 17 10	74, 169, 199, 200	0
3	I	26/26 (100%)	-0.14	0 100 100	84, 106, 119, 122	0
3	X	26/26 (100%)	-0.15	0 100 100	90, 103, 116, 130	0
4	J	26/26 (100%)	-0.18	0 100 100	85, 108, 118, 127	0
4	Y	26/26 (100%)	-0.16	0 100 100	79, 104, 115, 129	0
All	All	2444/2444 (100%)	0.09	116 (4%) 31 19	66, 157, 199, 200	0

All (116) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	167	ASP	7.5
2	D	468	LEU	7.3
1	E	61	ILE	6.5
2	F	480	GLY	6.0
1	A	171	ARG	6.0
1	A	108	ARG	5.5
2	F	478	ALA	5.4
2	H	468	LEU	4.9
2	D	473	LEU	4.7
2	D	469	VAL	4.7
2	F	468	LEU	4.5

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Mol	Chain	Res	Type	RSRZ
1	E	171	ARG	4.4
1	A	61	ILE	4.2
1	E	167	ASP	4.2
2	B	468	LEU	4.1
1	E	111	HIS	4.1
1	E	19	ALA	4.1
1	A	65	GLY	3.9
2	F	486	LEU	3.9
2	D	432	VAL	3.9
2	D	406	LEU	3.8
2	D	486	LEU	3.8
2	D	588	ASN	3.8
2	F	494	ILE	3.7
1	A	23	ILE	3.7
2	D	382	VAL	3.7
2	D	494	ILE	3.6
2	H	473	LEU	3.6
1	E	63	ILE	3.5
1	E	179	LEU	3.5
2	B	480	GLY	3.5
2	H	469	VAL	3.5
1	A	19	ALA	3.4
2	B	463	TYR	3.4
1	E	109	SER	3.4
2	D	384	ILE	3.3
1	A	159	LEU	3.3
2	B	486	LEU	3.2
1	A	172	PRO	3.2
2	H	486	LEU	3.1
1	A	179	LEU	3.1
1	A	111	HIS	3.0
2	H	476	LEU	3.0
1	A	62	LYS	3.0
1	E	178	VAL	3.0
2	F	477	GLN	2.9
2	B	476	LEU	2.9
1	A	178	VAL	2.9
1	E	23	ILE	2.9
2	H	460	ILE	2.9
1	E	62	LYS	2.9
2	H	343	GLN	2.8
2	B	618	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
2	D	512	LEU	2.8
2	B	340	PRO	2.8
2	B	384	ILE	2.8
2	B	478	ALA	2.8
2	D	532	VAL	2.8
2	B	516	ALA	2.8
1	A	22	GLU	2.7
2	H	384	ILE	2.7
2	H	382	VAL	2.7
2	B	481	GLY	2.7
1	E	108	ARG	2.7
1	A	168	PRO	2.6
1	E	272	LEU	2.6
2	D	476	LEU	2.6
2	H	521	SER	2.6
2	B	434	PHE	2.6
2	F	340	PRO	2.6
2	B	396	GLN	2.6
1	G	185	ASP	2.6
1	A	109	SER	2.6
2	D	514	PHE	2.6
1	A	24	ILE	2.6
2	F	481	GLY	2.5
1	A	63	ILE	2.5
2	F	463	TYR	2.5
2	B	477	GLN	2.5
2	F	476	LEU	2.5
2	H	479	GLU	2.4
2	D	409	HIS	2.4
2	H	512	LEU	2.4
1	E	24	ILE	2.4
2	H	432	VAL	2.4
1	E	65	GLY	2.3
2	B	475	TYR	2.3
2	H	430	MET	2.3
2	F	342	LEU	2.3
1	A	173	LEU	2.3
2	H	485	GLN	2.3
2	H	532	VAL	2.3
1	C	165	VAL	2.2
1	C	146	GLU	2.2
2	D	587	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
2	H	406	LEU	2.2
1	E	159	LEU	2.2
2	F	406	LEU	2.2
1	G	272	LEU	2.2
2	F	383	LYS	2.2
2	D	533	VAL	2.2
1	A	152	TYR	2.2
2	B	482	GLY	2.1
1	A	21	VAL	2.1
2	F	384	ILE	2.1
2	F	434	PHE	2.1
2	H	514	PHE	2.1
2	F	512	LEU	2.1
2	H	588	ASN	2.1
2	F	484	ARG	2.1
2	F	469	VAL	2.1
2	H	463	TYR	2.1
1	E	152	TYR	2.0
2	H	431	VAL	2.0
1	E	161	PHE	2.0
1	G	291	ASP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.