



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:58 PM UTC

PDB ID : 4XLR / pdb_00004xlr
Title : Crystal structure of T.aquaticus transcription initiation complex with CarD containing bubble promoter and RNA
Authors : Bae, B.; Darst, S.A.
Deposited on : 2015-01-13
Resolution : 4.30 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

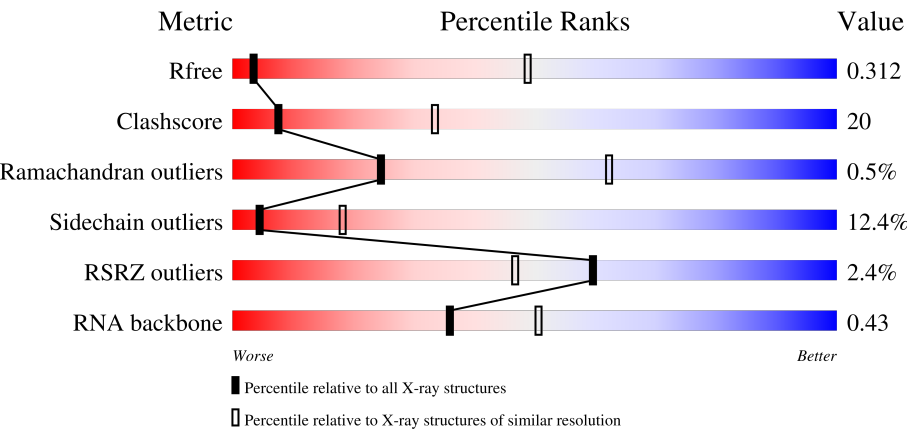
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	1052 (4.70-3.90)
Clashscore	190562	1097 (4.70-3.90)
Ramachandran outliers	187476	1001 (4.70-3.90)
Sidechain outliers	187428	1007 (4.72-3.88)
RSRZ outliers	180081	1049 (4.70-3.90)
RNA backbone	3983	1036 (5.50-3.10)

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

Mol	Chain	Length	Quality of chain
1	A	314	37% 31% • 28%
1	B	314	40% 27% 5% 28%
1	G	314	37% 30% • 28%
1	H	314	41% 26% 5% 28%

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Mol	Chain	Length	Quality of chain
2	C	1119	
2	I	1119	
3	D	1524	
3	J	1524	
4	E	99	
4	K	99	
5	F	347	
5	L	347	
6	M	164	
6	N	164	
7	O	48	
7	R	48	
8	P	48	
8	S	48	
9	Q	4	
9	T	4	

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 60854 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 DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	227	Total	C	N	O	S	0	0	0
			1770	1130	303	334	3			
1	B	227	Total	C	N	O	S	0	0	0
			1770	1130	303	334	3			
1	G	227	Total	C	N	O	S	0	0	0
			1770	1130	303	334	3			
1	H	227	Total	C	N	O	S	0	0	0
			1770	1130	303	334	3			

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1117	Total	C	N	O	S	0	0	0
			8762	5544	1558	1637	23			
2	I	1117	Total	C	N	O	S	0	0	0
			8762	5544	1558	1637	23			

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1490	Total	C	N	O	S	0	0	0
			11761	7439	2088	2196	38			
3	J	1367	Total	C	N	O	S	0	0	0
			10779	6810	1923	2010	36			

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	93	Total	C	N	O	S	0	0	0
			768	490	136	138	4			
4	K	93	Total	C	N	O	S	0	0	0
			768	490	136	138	4			

- Molecule 5 is a protein called RNA polymerase sigma factor SigA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	345	Total	C	N	O	S	0	0	0
			2787	1758	502	523	4			
5	L	345	Total	C	N	O	S	0	0	0
			2787	1758	502	523	4			

- Molecule 6 is a protein called CarD-like transcriptional regulator.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	M	158	Total	C	N	O	S	0	0	0
			1239	787	229	221	2			
6	N	158	Total	C	N	O	S	0	0	0
			1239	787	229	221	2			

- Molecule 7 is a DNA chain called DNA (48-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	O	48	Total	C	N	O	P	0	0	0
			988	472	182	287	47			
7	R	48	Total	C	N	O	P	0	0	0
			988	472	182	287	47			

- Molecule 8 is a DNA chain called DNA (48-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	P	48	Total	C	N	O	P	0	0	0
			985	471	183	284	47			
8	S	48	Total	C	N	O	P	0	0	0
			985	471	183	284	47			

- Molecule 9 is a RNA chain called RNA (5'-R(P*UP*CP*GP*A)-3').

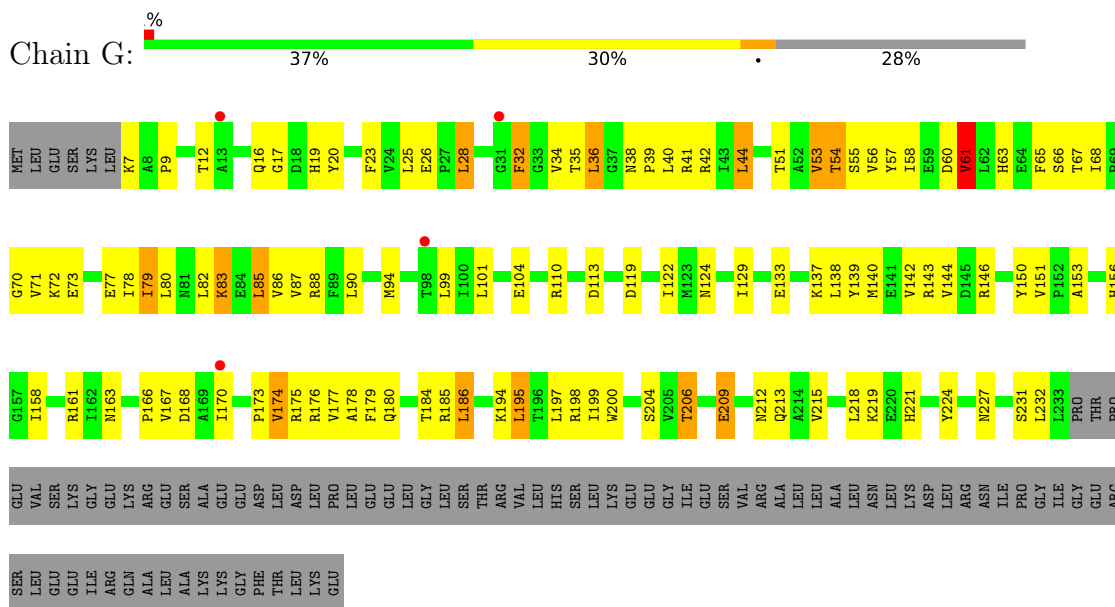
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	Q	4	Total	C	N	O	P	0	0	0
			85	38	15	28	4			
9	T	4	Total	C	N	O	P	0	0	0
			85	38	15	28	4			

- Molecule 10 is ZINC ION (CCD ID: ZN) (formula: Zn).

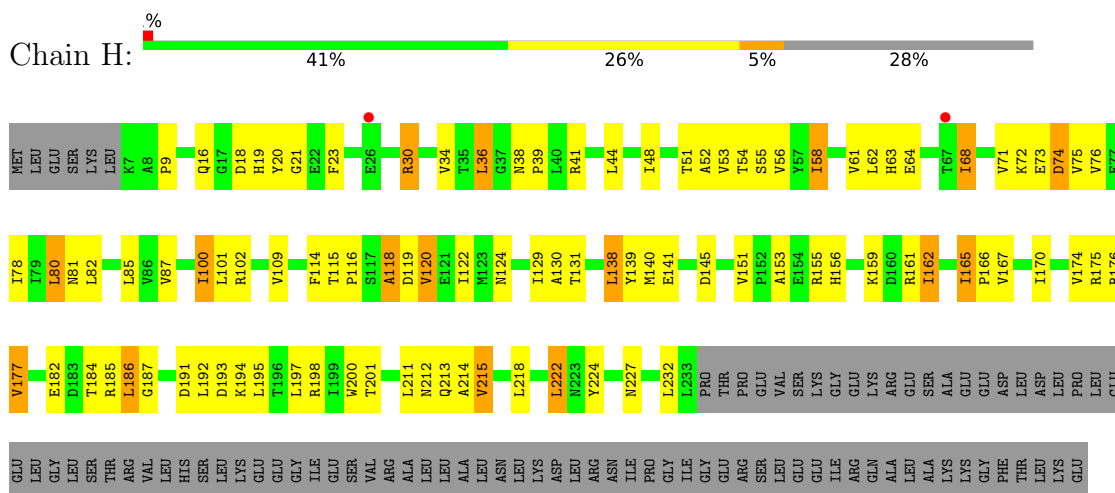
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	D	2	Total 2	Zn 2	0	0
10	J	2	Total 2	Zn 2	0	0

- Molecule 11 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

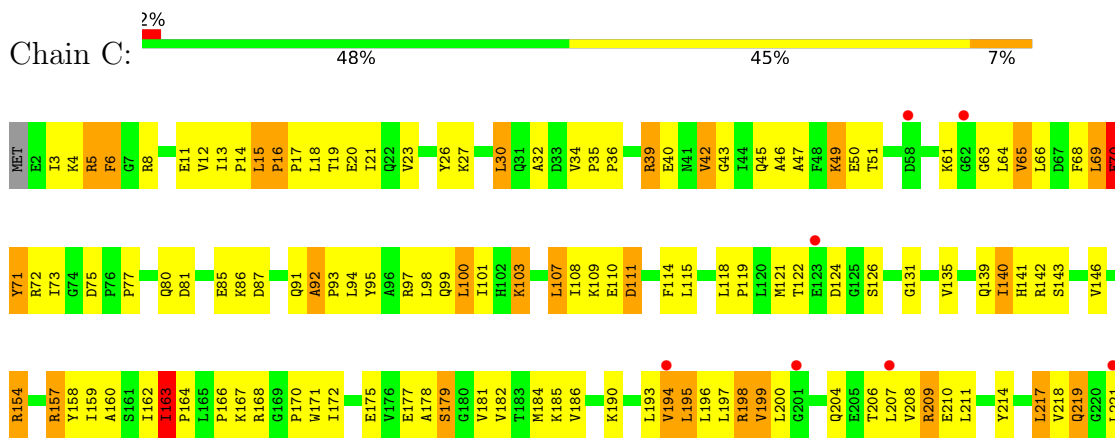
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	D	1	Total 1	Mg 1	0	0
11	J	1	Total 1	Mg 1	0	0

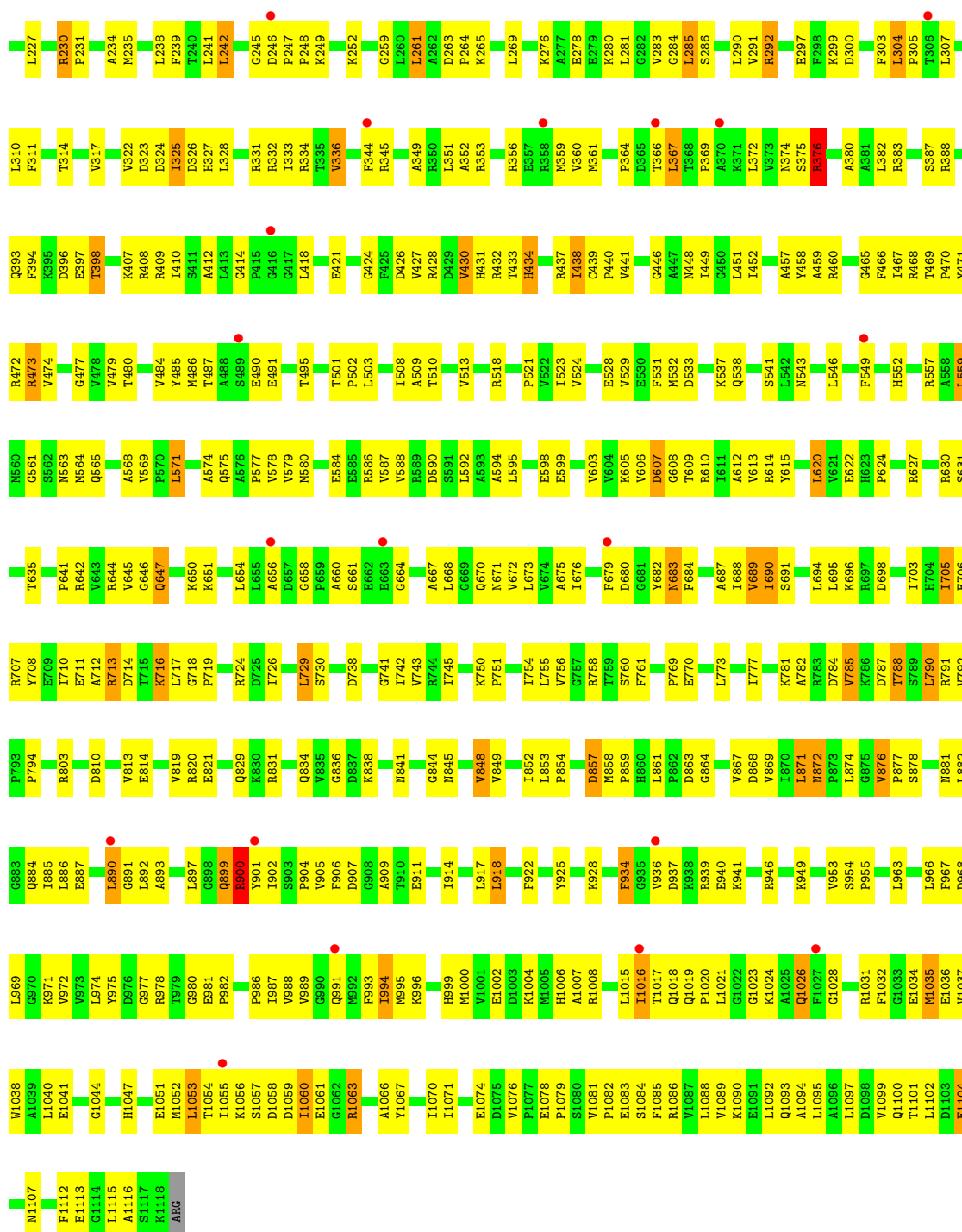


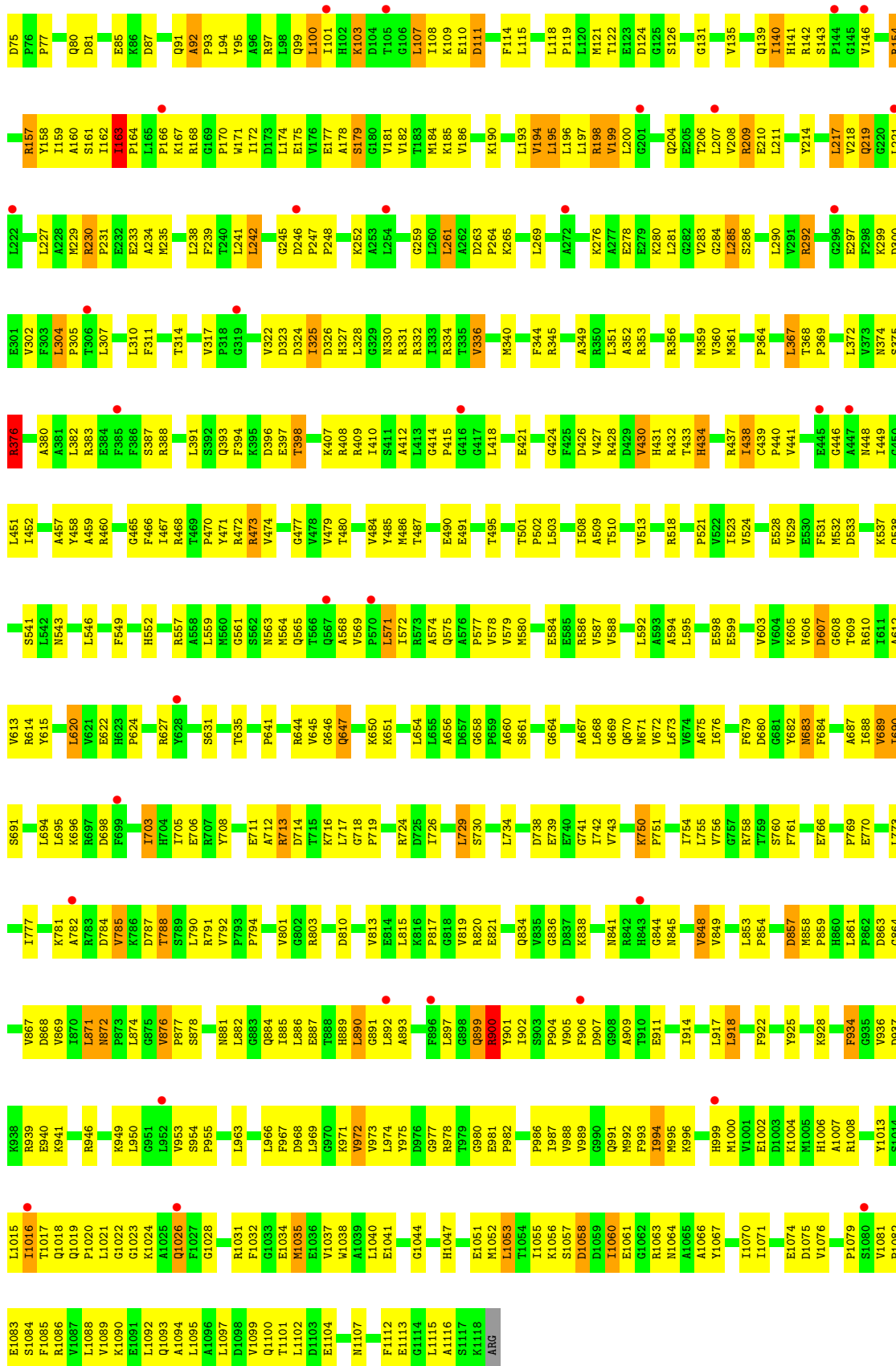
- Molecule 1: DNA-directed RNA polymerase subunit alpha



- Molecule 2: DNA-directed RNA polymerase subunit beta

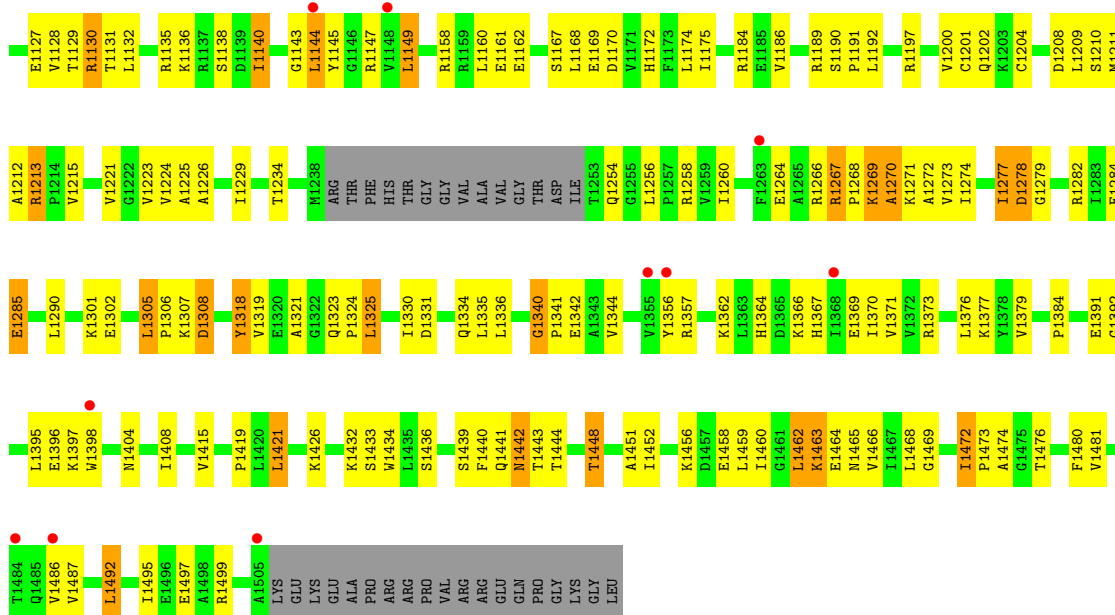




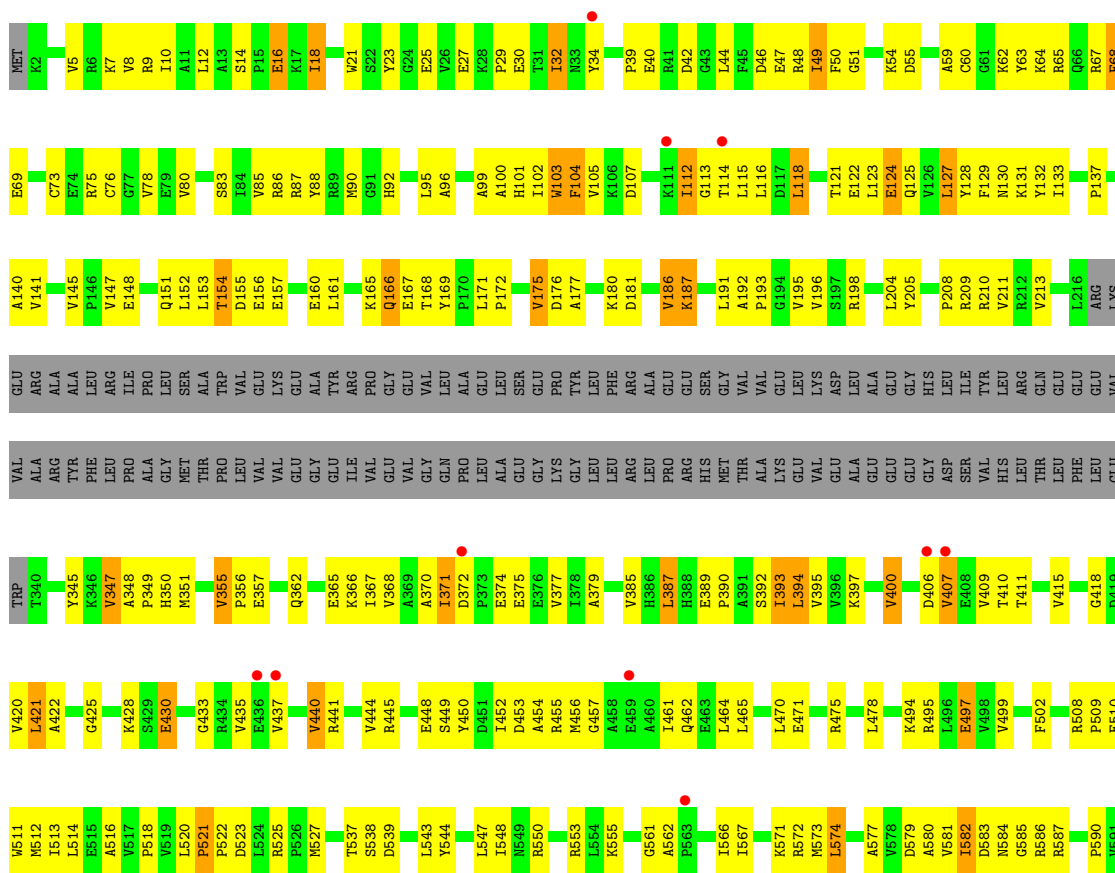


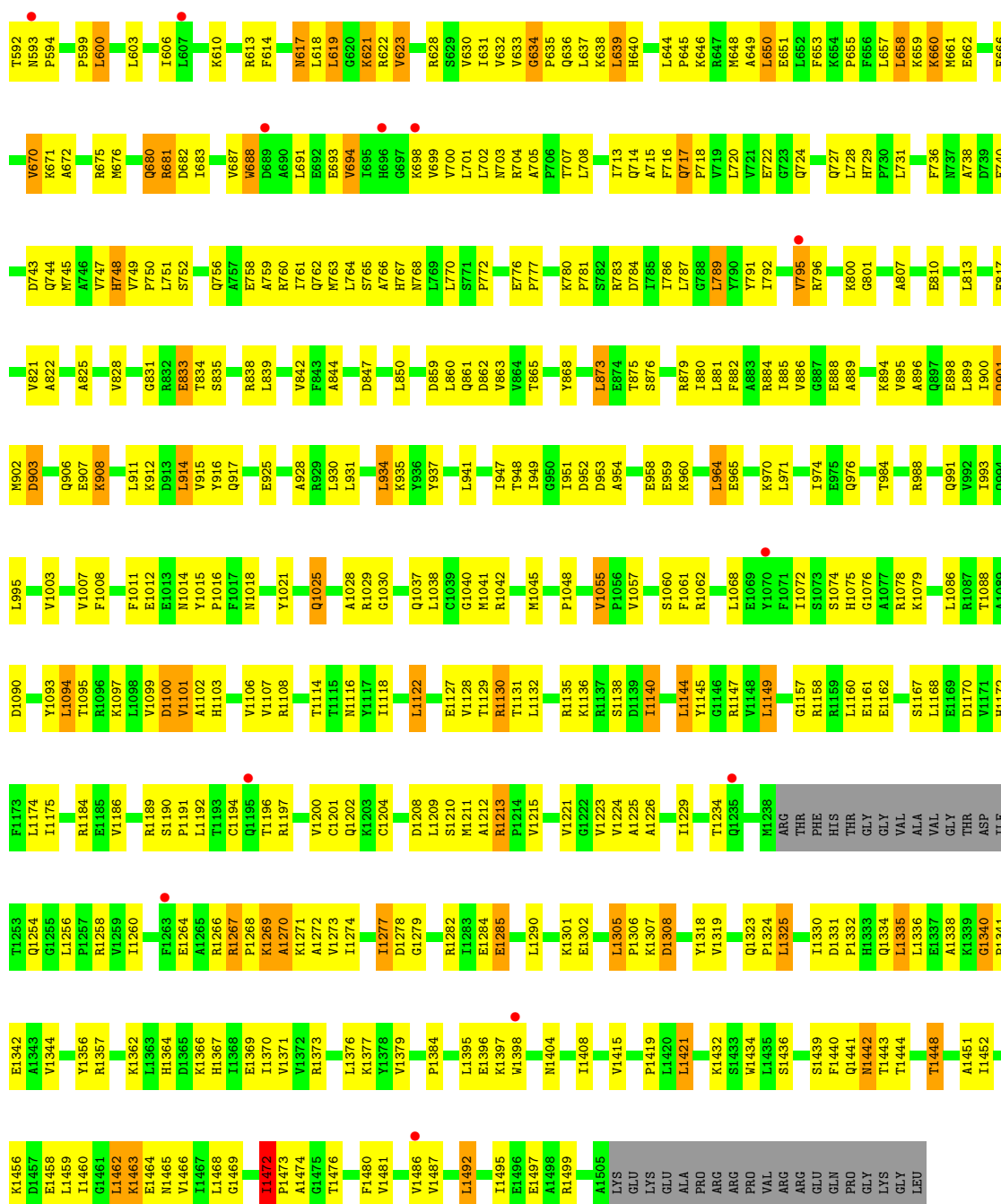
- Molecule 3: DNA-directed RNA polymerase subunit beta'



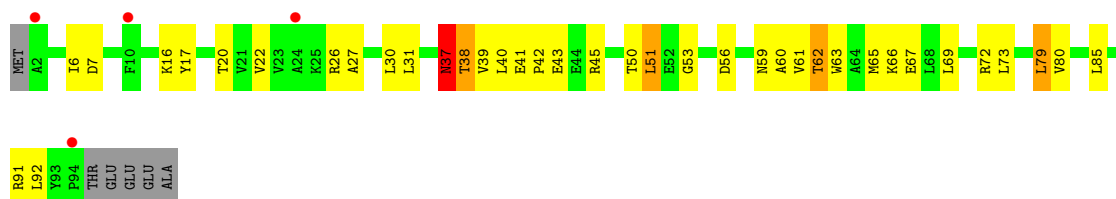


- Molecule 3: DNA-directed RNA polymerase subunit beta'

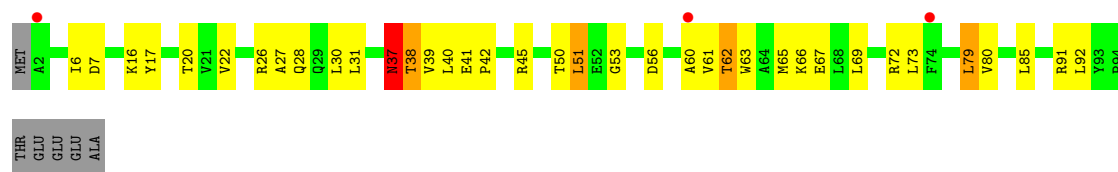




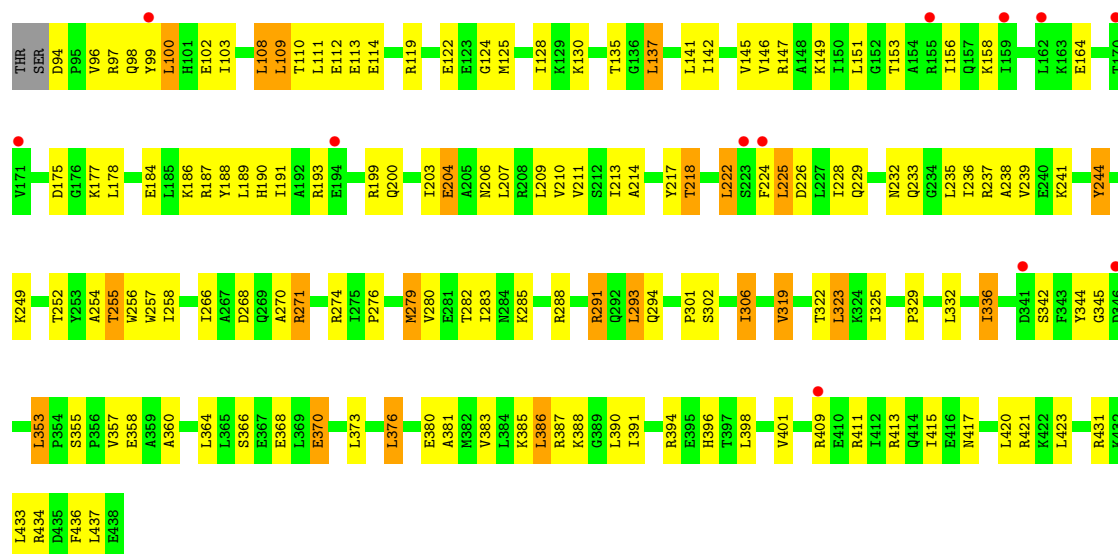
• Molecule 4: DNA-directed RNA polymerase subunit omega



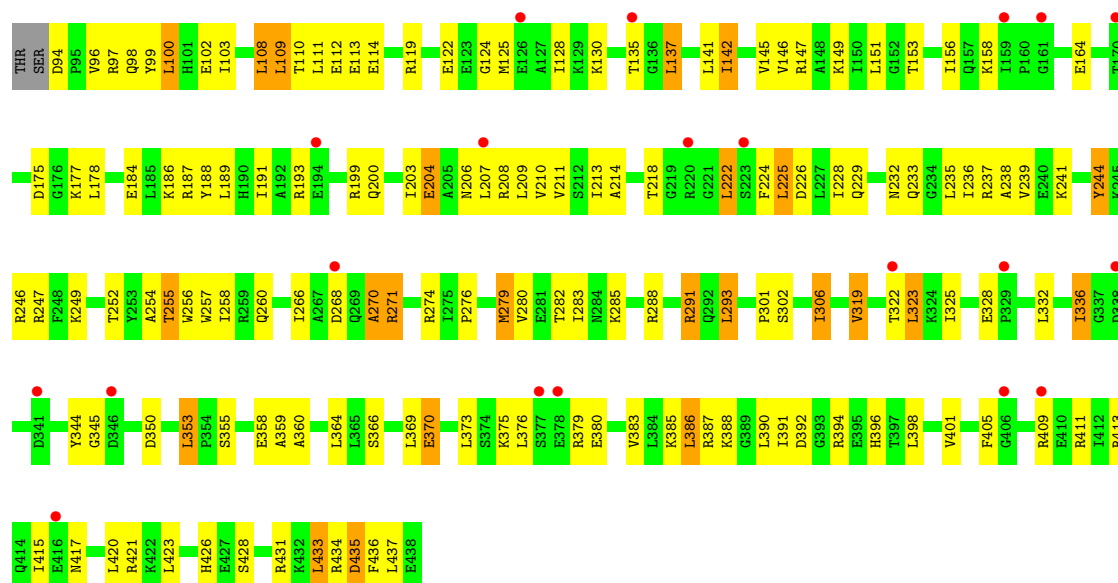
• Molecule 4: DNA-directed RNA polymerase subunit omega



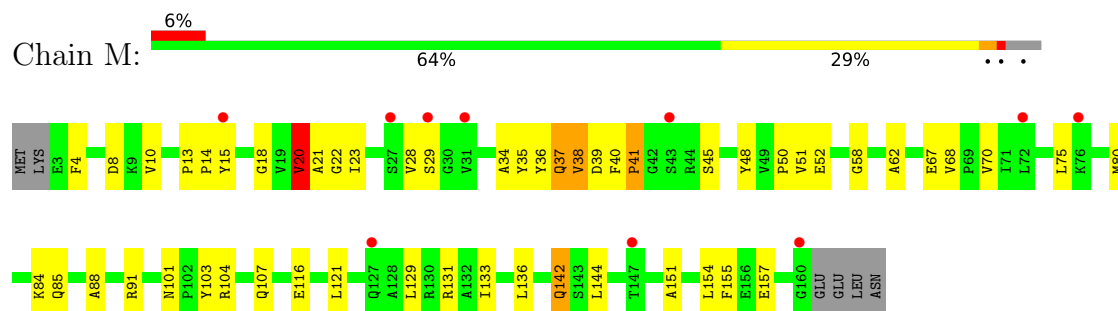
• Molecule 5: RNA polymerase sigma factor SigA



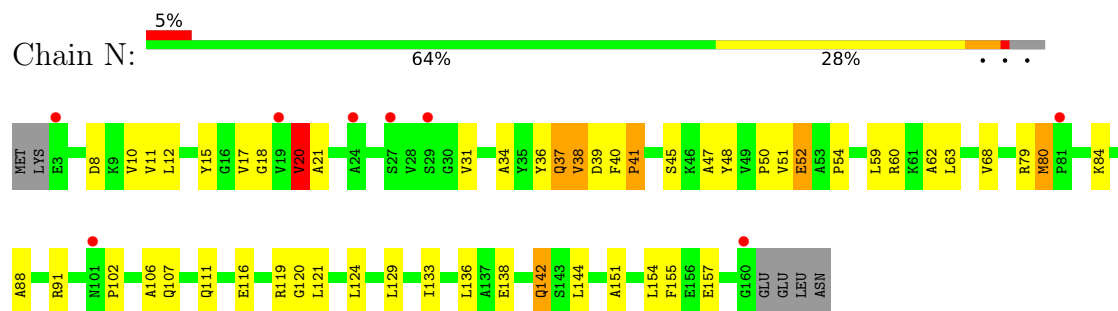
• Molecule 5: RNA polymerase sigma factor SigA



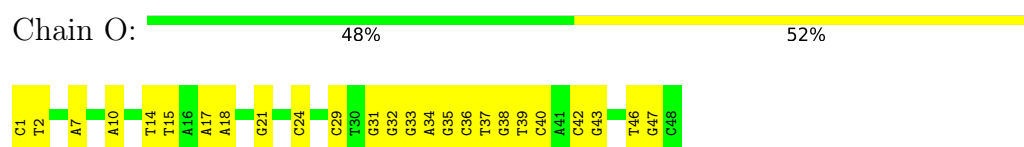
- Molecule 6: CarD-like transcriptional regulator



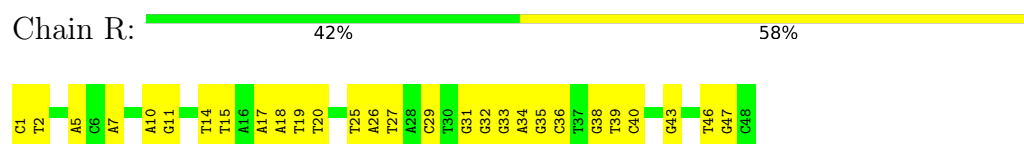
- Molecule 6: CarD-like transcriptional regulator



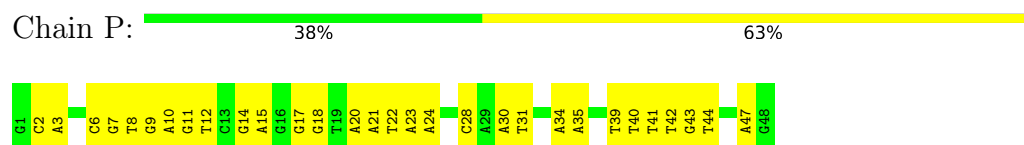
- Molecule 7: DNA (48-MER)



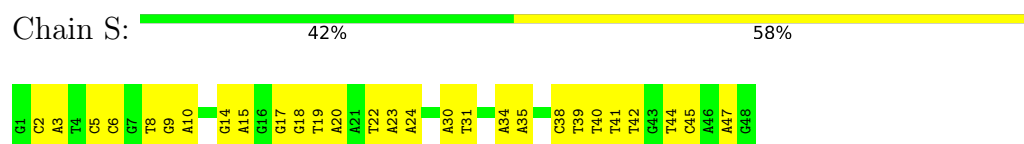
- Molecule 7: DNA (48-MER)



- Molecule 8: DNA (48-MER)



- Molecule 8: DNA (48-MER)



- Molecule 9: RNA (5'-R(P*UP*CP*GP*A)-3')

Chain Q:  25% 75%

 U1
C2
G3
A4

- Molecule 9: RNA (5'-R(P*UP*CP*GP*A)-3')

Chain T:  50% 50%

 U1
C2
G3
A4

4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	289.84Å 289.84Å 536.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.56 – 4.30 39.56 – 4.30	Depositor EDS
% Data completeness (in resolution range)	94.8 (39.56-4.30) 94.6 (39.56-4.30)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.11 (at 4.28Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1839)	Depositor
R, R_{free}	0.275 , 0.310 0.277 , 0.312	Depositor DCC
R_{free} test set	7337 reflections (4.18%)	wwPDB-VP
Wilson B-factor (Å ²)	165.1	Xtriage
Anisotropy	0.026	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 165.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.36$, $\langle L^2 \rangle = 0.19$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	60854	wwPDB-VP
Average B, all atoms (Å ²)	179.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.81% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG

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	0.39	0/1804	0.88	0/2455
1	B	0.37	0/1804	0.84	0/2455
1	G	0.40	0/1804	0.88	0/2455
1	H	0.38	0/1804	0.84	2/2455 (0.1%)
2	C	0.40	0/8929	0.89	32/12074 (0.3%)
2	I	0.39	0/8929	0.89	32/12074 (0.3%)
3	D	0.38	0/11963	0.84	15/16165 (0.1%)
3	J	0.37	0/10959	0.82	12/14802 (0.1%)
4	E	0.34	0/783	0.85	3/1054 (0.3%)
4	K	0.33	0/783	0.85	3/1054 (0.3%)
5	F	0.44	0/2829	0.85	3/3804 (0.1%)
5	L	0.44	0/2829	0.85	4/3804 (0.1%)
6	M	0.48	0/1267	0.94	6/1719 (0.3%)
6	N	0.48	0/1267	0.92	3/1719 (0.2%)
7	O	0.23	0/1109	0.41	0/1712
7	R	0.22	0/1109	0.41	0/1712
8	P	0.27	0/1106	0.43	0/1706
8	S	0.25	0/1106	0.45	0/1706
9	Q	0.14	0/94	0.28	0/144
9	T	0.13	0/94	0.29	0/144
All	All	0.38	0/62372	0.83	115/85213 (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
2	C	0	2
2	I	0	2
3	D	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
3	J	0	1
6	M	0	2
6	N	0	2
All	All	0	10

There are no bond length outliers.

All (115) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	302	VAL	N-CA-C	10.23	120.15	110.53
2	C	163	ILE	CA-C-N	9.31	131.48	119.84
2	C	163	ILE	C-N-CA	9.31	131.48	119.84
2	I	163	ILE	CA-C-N	9.23	131.38	119.84
2	I	163	ILE	C-N-CA	9.23	131.38	119.84
3	D	169	TYR	CA-C-N	9.02	128.87	120.21
3	D	169	TYR	C-N-CA	9.02	128.87	120.21
2	C	70	GLU	N-CA-C	8.76	122.09	110.53
2	I	70	GLU	N-CA-C	8.09	121.21	110.53
2	C	6	PHE	N-CA-C	7.91	118.42	108.45
2	I	6	PHE	N-CA-C	7.87	118.65	108.34
2	I	750	LYS	CA-C-N	-7.64	110.29	119.84
2	I	750	LYS	C-N-CA	-7.64	110.29	119.84
2	C	750	LYS	CA-C-N	-7.50	110.47	119.84
2	C	750	LYS	C-N-CA	-7.50	110.47	119.84
2	I	414	GLY	CA-C-N	6.57	128.05	119.84
2	I	414	GLY	C-N-CA	6.57	128.05	119.84
2	I	35	PRO	CA-C-N	6.55	126.24	119.56
2	I	35	PRO	C-N-CA	6.55	126.24	119.56
2	C	414	GLY	CA-C-N	6.45	127.91	119.84
2	C	414	GLY	C-N-CA	6.45	127.91	119.84
2	C	35	PRO	CA-C-N	6.39	126.07	119.56
2	C	35	PRO	C-N-CA	6.39	126.07	119.56
5	L	270	ALA	CB-CA-C	-6.36	109.23	116.54
3	J	521	PRO	CA-C-N	6.20	125.93	119.05
3	J	521	PRO	C-N-CA	6.20	125.93	119.05
3	D	521	PRO	CA-C-N	6.18	125.91	119.05
3	D	521	PRO	C-N-CA	6.18	125.91	119.05
6	N	37	GLN	N-CA-C	-6.17	100.70	109.96
3	D	406	ASP	CB-CA-C	-6.11	109.51	116.54
5	L	94	ASP	CA-C-N	6.09	125.71	119.56
5	L	94	ASP	C-N-CA	6.09	125.71	119.56
2	C	718	GLY	CA-C-N	6.05	126.39	119.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	718	GLY	C-N-CA	6.05	126.39	119.92
5	F	94	ASP	CA-C-N	6.01	125.63	119.56
5	F	94	ASP	C-N-CA	6.01	125.63	119.56
6	N	38	VAL	CA-C-N	-5.99	112.31	122.67
6	N	38	VAL	C-N-CA	-5.99	112.31	122.67
4	E	38	THR	N-CA-C	5.98	118.01	110.24
2	I	177	GLU	CA-C-N	-5.96	112.81	122.34
2	I	177	GLU	C-N-CA	-5.96	112.81	122.34
4	K	38	THR	N-CA-C	5.93	117.95	110.24
3	D	1340	GLY	CA-C-N	5.92	125.63	119.05
3	D	1340	GLY	C-N-CA	5.92	125.63	119.05
2	C	177	GLU	CA-C-N	-5.91	112.89	122.34
2	C	177	GLU	C-N-CA	-5.91	112.89	122.34
3	J	1340	GLY	CA-C-N	5.89	125.59	119.05
3	J	1340	GLY	C-N-CA	5.89	125.59	119.05
6	M	37	GLN	N-CA-C	-5.89	101.33	110.10
2	I	718	GLY	CA-C-N	5.84	126.17	119.92
2	I	718	GLY	C-N-CA	5.84	126.17	119.92
2	C	376	ARG	CA-C-N	-5.82	112.92	118.97
2	C	376	ARG	C-N-CA	-5.82	112.92	118.97
2	I	376	ARG	CA-C-N	-5.76	112.98	118.97
2	I	376	ARG	C-N-CA	-5.76	112.98	118.97
6	M	38	VAL	CA-C-N	-5.76	112.45	122.64
6	M	38	VAL	C-N-CA	-5.76	112.45	122.64
3	J	634	GLY	N-CA-C	5.71	123.99	112.34
3	D	243	ALA	CB-CA-C	-5.70	109.01	115.79
3	J	1030	GLY	N-CA-C	5.70	118.31	110.56
3	J	617	ASN	N-CA-C	5.69	120.50	113.50
3	D	634	GLY	N-CA-C	5.69	123.94	112.34
3	D	1030	GLY	N-CA-C	5.63	118.21	110.56
3	D	617	ASN	N-CA-C	5.59	120.38	113.50
2	I	900	ARG	N-CA-C	-5.51	101.85	110.17
2	C	34	VAL	CA-C-N	5.51	123.68	119.66
2	C	34	VAL	C-N-CA	5.51	123.68	119.66
3	D	1055	VAL	N-CA-C	5.49	113.87	107.89
2	C	900	ARG	N-CA-C	-5.49	101.88	110.17
3	J	1055	VAL	N-CA-C	5.46	113.85	107.89
3	J	670	VAL	CA-C-N	-5.41	113.03	120.28
3	J	670	VAL	C-N-CA	-5.41	113.03	120.28
2	I	34	VAL	CA-C-N	5.35	123.56	119.66
2	I	34	VAL	C-N-CA	5.35	123.56	119.66
3	D	670	VAL	CA-C-N	-5.34	113.12	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	670	VAL	C-N-CA	-5.34	113.12	120.28
2	I	1084	SER	N-CA-C	-5.32	105.53	112.23
2	C	1084	SER	N-CA-C	-5.31	105.54	112.23
2	C	75	ASP	CA-C-N	-5.30	114.92	120.38
2	C	75	ASP	C-N-CA	-5.30	114.92	120.38
2	I	92	ALA	CA-C-N	5.30	125.22	119.76
2	I	92	ALA	C-N-CA	5.30	125.22	119.76
6	M	29	SER	CB-CA-C	-5.22	110.14	117.23
2	C	4	LYS	O-C-N	5.20	129.08	123.10
2	I	4	LYS	O-C-N	5.19	129.06	123.10
2	I	16	PRO	O-C-N	5.18	123.69	121.31
2	I	1058	ASP	N-CA-C	5.16	120.21	113.30
2	C	92	ALA	CA-C-N	5.14	125.06	119.76
2	C	92	ALA	C-N-CA	5.14	125.06	119.76
2	I	4	LYS	CA-C-N	5.14	130.58	122.36
2	I	4	LYS	C-N-CA	5.14	130.58	122.36
5	F	218	THR	N-CA-C	5.13	117.48	110.24
2	C	16	PRO	O-C-N	5.12	123.67	121.31
2	C	4	LYS	CA-C-N	5.11	130.54	122.36
2	C	4	LYS	C-N-CA	5.11	130.54	122.36
4	K	37	ASN	CA-C-N	5.10	128.32	120.82
4	K	37	ASN	C-N-CA	5.10	128.32	120.82
3	J	1472	ILE	CA-C-N	5.08	124.80	119.82
3	J	1472	ILE	C-N-CA	5.08	124.80	119.82
3	D	1143	GLY	N-CA-C	5.06	118.61	112.49
2	I	75	ASP	CA-C-N	-5.06	115.17	120.38
2	I	75	ASP	C-N-CA	-5.06	115.17	120.38
6	M	20	VAL	CA-C-N	-5.05	114.89	122.47
6	M	20	VAL	C-N-CA	-5.05	114.89	122.47
1	H	165	ILE	CA-C-N	5.04	125.04	119.90
1	H	165	ILE	C-N-CA	5.04	125.04	119.90
4	E	37	ASN	CA-C-N	5.04	128.22	120.82
4	E	37	ASN	C-N-CA	5.04	128.22	120.82
2	C	899	GLN	CA-C-N	-5.03	113.74	122.64
2	C	899	GLN	C-N-CA	-5.03	113.74	122.64
2	C	1078	GLU	CA-C-N	5.01	124.99	120.03
2	C	1078	GLU	C-N-CA	5.01	124.99	120.03
2	I	899	GLN	CA-C-N	-5.01	113.77	122.64
2	I	899	GLN	C-N-CA	-5.01	113.77	122.64
5	L	218	THR	N-CA-C	5.01	117.30	110.24

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	360	VAL	Peptide
2	C	71	TYR	Mainchain
3	D	1270	ALA	Peptide
2	I	360	VAL	Peptide
2	I	71	TYR	Mainchain
3	J	1270	ALA	Peptide
6	M	20	VAL	Mainchain,Peptide
6	N	20	VAL	Mainchain,Peptide

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	1770	0	1799	90	0
1	B	1770	0	1799	68	0
1	G	1770	0	1799	90	0
1	H	1770	0	1799	65	0
2	C	8762	0	8854	451	0
2	I	8762	0	8854	453	0
3	D	11761	0	11976	552	0
3	J	10779	0	10993	506	0
4	E	768	0	784	38	0
4	K	768	0	784	36	0
5	F	2787	0	2866	123	0
5	L	2787	0	2866	128	0
6	M	1239	0	1259	39	0
6	N	1239	0	1259	40	0
7	O	988	0	544	30	0
7	R	988	0	544	38	0
8	P	985	0	543	36	0
8	S	985	0	543	30	0
9	Q	85	0	43	1	0
9	T	85	0	43	2	0
10	D	2	0	0	0	0
10	J	2	0	0	0	0
11	D	1	0	0	0	0
11	J	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	60854	0	59951	2434	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 20.

All (2434) 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)
3:D:73:CYS:HB3	3:D:76:CYS:SG	1.97	1.04
3:J:73:CYS:HB3	3:J:76:CYS:SG	1.97	1.04
3:D:105:VAL:HA	3:D:112:ILE:HD11	1.55	0.89
3:D:412:GLY:HA2	3:D:434:ARG:HD3	1.55	0.89
3:J:105:VAL:HA	3:J:112:ILE:HD11	1.55	0.88
1:A:42:ARG:HH12	2:C:857:ASP:HB3	1.38	0.86
3:D:208:PRO:HA	3:D:390:PRO:HA	1.56	0.85
1:G:42:ARG:HH12	2:I:857:ASP:HB3	1.38	0.85
3:J:210:ARG:HG2	3:J:389:GLU:HB3	1.58	0.85
2:I:679:PHE:H	2:I:683:ASN:HD21	1.25	0.85
2:C:858:MET:H	2:C:977:GLY:HA3	1.40	0.84
2:I:374:ASN:HD21	5:L:291:ARG:HE	1.22	0.84
2:I:858:MET:H	2:I:977:GLY:HA3	1.42	0.84
5:L:203:ILE:HG12	5:L:239:VAL:HG21	1.60	0.84
1:G:55:SER:HB3	1:G:143:ARG:HB2	1.61	0.83
2:C:679:PHE:H	2:C:683:ASN:HD21	1.26	0.82
2:C:374:ASN:HD21	5:F:291:ARG:HE	1.26	0.82
5:F:203:ILE:HG12	5:F:239:VAL:HG21	1.61	0.82
2:I:364:PRO:HA	2:I:367:LEU:HD12	1.61	0.82
2:I:537:LYS:HZ3	2:I:905:VAL:H	1.26	0.82
2:C:364:PRO:HA	2:C:367:LEU:HD12	1.61	0.82
6:N:20:VAL:HA	6:N:38:VAL:HA	1.60	0.81
2:C:836:GLY:H	2:C:849:VAL:HB	1.44	0.81
2:C:537:LYS:HZ3	2:C:905:VAL:H	1.28	0.81
3:D:954:ALA:O	3:D:1062:ARG:NH1	2.12	0.81
3:J:208:PRO:HB3	3:J:387:LEU:HD21	1.60	0.81
2:I:836:GLY:H	2:I:849:VAL:HB	1.45	0.80
1:A:55:SER:HB3	1:A:143:ARG:HB2	1.61	0.80
2:C:603:VAL:HB	2:C:646:GLY:HA2	1.63	0.80
2:I:292:ARG:HH11	2:I:292:ARG:H	1.29	0.80
2:I:603:VAL:HA	2:I:613:VAL:HG12	1.63	0.80
6:M:20:VAL:HA	6:M:38:VAL:HA	1.63	0.80
2:C:71:TYR:HA	2:C:95:TYR:O	1.81	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:712:ALA:HB3	2:C:821:GLU:H	1.47	0.80
2:C:603:VAL:HA	2:C:613:VAL:HG12	1.64	0.80
3:D:73:CYS:CB	3:D:76:CYS:SG	2.65	0.80
8:P:30:DA:H2"	8:P:31:DT:H5"	1.64	0.80
2:C:292:ARG:HH11	2:C:292:ARG:H	1.30	0.80
3:D:1103:HIS:HB2	3:D:1462:LEU:HD11	1.64	0.79
2:C:1102:LEU:HB2	3:D:7:LYS:HB2	1.63	0.79
3:J:73:CYS:CB	3:J:76:CYS:SG	2.64	0.79
2:I:71:TYR:HA	2:I:95:TYR:O	1.83	0.79
3:J:954:ALA:O	3:J:1062:ARG:NH1	2.15	0.79
2:I:603:VAL:HB	2:I:646:GLY:HA2	1.63	0.79
2:I:1102:LEU:HB2	3:J:7:LYS:HB2	1.63	0.78
3:D:1189:ARG:NH2	3:D:1204:CYS:SG	2.55	0.78
7:R:7:DA:H61	8:S:42:DT:H3	1.30	0.78
3:D:130:ASN:HD22	5:F:98:GLN:HE22	1.31	0.78
3:J:1103:HIS:HB2	3:J:1462:LEU:HD11	1.66	0.78
2:I:63:GLY:HA3	2:I:103:LYS:HB2	1.67	0.77
2:C:374:ASN:HD21	5:F:291:ARG:NE	1.83	0.77
3:D:715:ALA:HB3	3:D:764:LEU:HA	1.65	0.77
2:I:154:ARG:HD3	2:I:178:ALA:HB2	1.65	0.77
2:I:1063:ARG:HH22	5:L:353:LEU:HD11	1.49	0.77
2:I:712:ALA:HB3	2:I:821:GLU:H	1.48	0.77
3:D:953:ASP:O	3:D:1018:ASN:ND2	2.17	0.77
8:S:30:DA:H2"	8:S:31:DT:H5"	1.65	0.77
3:D:367:ILE:HG22	3:D:368:VAL:HG23	1.67	0.77
3:J:953:ASP:O	3:J:1018:ASN:ND2	2.16	0.77
2:C:63:GLY:HA3	2:C:103:LYS:HB2	1.67	0.77
3:J:951:ILE:O	3:J:1062:ARG:NH1	2.18	0.76
3:D:323:GLU:HB3	3:D:334:THR:H	1.49	0.76
2:C:154:ARG:HD3	2:C:178:ALA:HB2	1.66	0.76
5:F:218:THR:O	8:P:23:DA:N6	2.19	0.76
3:D:462:GLN:HB2	3:D:513:ILE:HG21	1.68	0.76
2:I:427:VAL:HG22	7:R:38:DG:H21	1.51	0.76
3:J:48:ARG:HA	3:J:78:VAL:HG22	1.68	0.75
3:J:462:GLN:HB2	3:J:513:ILE:HG21	1.67	0.75
3:J:1189:ARG:NH2	3:J:1204:CYS:SG	2.56	0.75
3:D:423:ASP:HB3	3:D:426:LYS:HB3	1.69	0.75
3:J:130:ASN:HD22	5:L:98:GLN:HE22	1.31	0.75
3:D:951:ILE:O	3:D:1062:ARG:NH1	2.19	0.75
4:K:79:LEU:HG	4:K:80:VAL:HG22	1.69	0.75
3:D:48:ARG:HA	3:D:78:VAL:HG22	1.69	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:911:GLU:OE1	3:J:1062:ARG:NH2	2.20	0.75
1:G:53:VAL:HG23	1:G:144:VAL:HG22	1.69	0.74
3:J:715:ALA:HB3	3:J:764:LEU:HA	1.67	0.74
5:F:398:LEU:HB3	5:F:409:ARG:HB2	1.67	0.74
2:I:694:LEU:HD11	2:I:868:ASP:HB3	1.68	0.74
2:C:876:VAL:HG11	2:C:885:ILE:HD11	1.70	0.74
4:E:79:LEU:HG	4:E:80:VAL:HG22	1.69	0.74
2:I:167:LYS:HD3	7:R:35:DG:H5'	1.69	0.74
5:L:428:SER:HA	5:L:434:ARG:HH22	1.52	0.74
3:D:1379:VAL:HG12	3:D:1419:PRO:HA	1.69	0.74
3:J:67:ARG:HD2	5:L:394:ARG:HD3	1.67	0.74
5:L:332:LEU:HD22	5:L:345:GLY:HA2	1.70	0.74
3:D:760:ARG:HH22	4:E:62:THR:HG23	1.50	0.74
2:I:876:VAL:HG11	2:I:885:ILE:HD11	1.70	0.74
2:C:694:LEU:HD11	2:C:868:ASP:HB3	1.69	0.74
1:A:53:VAL:HG23	1:A:144:VAL:HG22	1.68	0.74
3:D:188:GLY:N	3:D:197:SER:O	2.20	0.74
3:J:760:ARG:HH22	4:K:62:THR:HG23	1.51	0.74
3:D:214:ASP:HA	3:D:342:PRO:HA	1.69	0.74
2:I:3:ILE:HG23	2:I:900:ARG:HB2	1.70	0.73
2:I:108:ILE:HB	6:N:48:TYR:HB2	1.70	0.73
3:D:792:ILE:HG21	3:D:941:LEU:HD22	1.70	0.73
3:J:786:ILE:HD13	3:J:908:LYS:HG2	1.69	0.73
3:J:1254:GLN:HB2	3:J:1258:ARG:HB2	1.70	0.73
5:L:398:LEU:HB3	5:L:409:ARG:HB2	1.69	0.73
3:J:1379:VAL:HG12	3:J:1419:PRO:HA	1.71	0.73
2:C:3:ILE:HG23	2:C:900:ARG:HB2	1.71	0.73
3:J:792:ILE:HG21	3:J:941:LEU:HD22	1.71	0.72
5:L:235:LEU:HB2	5:L:258:ILE:HD11	1.70	0.72
2:C:427:VAL:HG22	7:O:38:DG:H21	1.55	0.72
3:D:786:ILE:HD13	3:D:908:LYS:HG2	1.69	0.72
3:J:670:VAL:HB	5:L:364:LEU:HD11	1.70	0.72
5:F:235:LEU:HB2	5:F:258:ILE:HD11	1.70	0.72
2:C:911:GLU:OE1	3:D:1062:ARG:NH2	2.23	0.71
2:I:72:ARG:HB2	2:I:95:TYR:HB2	1.71	0.71
2:I:1019:GLN:HG3	3:J:617:ASN:HD22	1.54	0.71
2:C:366:THR:HA	6:M:14:PRO:HG3	1.72	0.71
3:J:18:ILE:HG12	3:J:518:PRO:HG3	1.72	0.71
2:C:72:ARG:HB2	2:C:95:TYR:HB2	1.72	0.71
1:A:179:PHE:HB3	1:A:197:LEU:HD12	1.73	0.71
3:D:1436:SER:HB2	3:D:1464:GLU:HG2	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:971:LYS:HB2	2:C:986:PRO:HB2	1.72	0.71
3:D:917:GLN:HE22	3:D:1168:LEU:HD11	1.57	0.70
3:D:1254:GLN:HB2	3:D:1258:ARG:HB2	1.71	0.70
3:D:1135:ARG:HH21	3:D:1357:ARG:HH12	1.39	0.70
2:I:14:PRO:HB3	2:I:586:ARG:HH22	1.57	0.70
3:D:226:PRO:HA	3:D:330:SER:HA	1.73	0.70
1:A:175:ARG:N	1:A:200:TRP:O	2.25	0.70
1:G:175:ARG:N	1:G:200:TRP:O	2.24	0.70
2:I:214:TYR:HB2	2:I:217:LEU:HD11	1.74	0.70
3:D:165:LYS:HB3	3:D:397:LYS:HE2	1.72	0.70
5:F:293:LEU:HD11	5:F:306:ILE:HD13	1.74	0.70
2:C:217:LEU:HD13	2:C:311:PHE:HD2	1.57	0.69
3:D:1472:ILE:HG13	3:D:1474:ALA:H	1.56	0.69
2:I:971:LYS:HB2	2:I:986:PRO:HB2	1.72	0.69
1:B:175:ARG:HB3	3:D:847:ASP:HB3	1.73	0.69
2:C:214:TYR:HB2	2:C:217:LEU:HD11	1.74	0.69
2:C:472:ARG:HD3	2:C:479:VAL:HG13	1.74	0.69
2:I:230:ARG:HH21	2:I:231:PRO:HD2	1.57	0.69
3:D:18:ILE:HG12	3:D:518:PRO:HG3	1.74	0.69
1:H:175:ARG:HB3	3:J:847:ASP:HB3	1.74	0.69
3:J:1135:ARG:HH21	3:J:1357:ARG:HH12	1.40	0.69
2:I:472:ARG:HD3	2:I:479:VAL:HG13	1.73	0.69
5:L:293:LEU:HD11	5:L:306:ILE:HD13	1.74	0.69
1:A:34:VAL:HG11	2:C:981:GLU:HG2	1.74	0.69
2:C:230:ARG:HH21	2:C:231:PRO:HD2	1.57	0.69
3:D:628:ARG:NH2	3:D:744:GLN:OE1	2.24	0.69
1:G:179:PHE:HB3	1:G:197:LEU:HD12	1.74	0.69
3:J:658:LEU:HD22	3:J:670:VAL:HG13	1.74	0.69
2:C:50:GLU:HA	2:C:265:LYS:HZ2	1.57	0.69
2:C:872:ASN:HD21	2:C:874:LEU:HG	1.57	0.69
5:F:411:ARG:HD3	7:O:1:DC:H2'	1.75	0.69
2:I:324:ASP:HB3	2:I:327:HIS:HB2	1.75	0.69
2:I:484:VAL:HG21	2:I:531:PHE:HE1	1.57	0.69
2:I:872:ASN:HD21	2:I:874:LEU:HG	1.58	0.69
3:J:1472:ILE:HG13	3:J:1474:ALA:H	1.57	0.69
2:C:304:LEU:HB3	2:C:305:PRO:HD3	1.74	0.69
2:C:484:VAL:HG21	2:C:531:PHE:HE1	1.56	0.69
3:D:835:SER:HB3	3:D:838:ARG:HG3	1.75	0.69
2:C:502:PRO:HB2	2:C:509:ALA:HB3	1.74	0.69
3:D:704:ARG:HG2	3:D:738:ALA:HB2	1.75	0.69
2:I:304:LEU:HB3	2:I:305:PRO:HD3	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:917:GLN:HE22	3:J:1168:LEU:HD11	1.57	0.69
3:D:9:ARG:HG3	3:D:1456:LYS:HB3	1.75	0.68
1:A:41:ARG:HG3	1:A:177:VAL:HB	1.76	0.68
3:J:1122:LEU:HD23	3:J:1140:ILE:HG21	1.75	0.68
6:M:88:ALA:HA	6:M:91:ARG:HD2	1.76	0.68
5:F:288:ARG:NH1	8:P:24:DA:OP1	2.26	0.68
1:G:34:VAL:HG11	2:I:981:GLU:HG2	1.74	0.68
1:G:41:ARG:HG3	1:G:177:VAL:HB	1.75	0.68
3:J:356:PRO:HB3	3:J:441:ARG:HA	1.75	0.68
3:J:628:ARG:NH2	3:J:744:GLN:OE1	2.25	0.68
3:J:835:SER:HB3	3:J:838:ARG:HG3	1.75	0.68
7:O:7:DA:H61	8:P:42:DT:H3	1.39	0.68
2:C:1063:ARG:HH22	5:F:353:LEU:HD11	1.59	0.68
3:J:704:ARG:HG2	3:J:738:ALA:HB2	1.75	0.68
2:C:264:PRO:HG2	2:C:265:LYS:HE2	1.75	0.68
3:D:1122:LEU:HD23	3:D:1140:ILE:HG21	1.75	0.68
2:I:502:PRO:HB2	2:I:509:ALA:HB3	1.74	0.68
3:J:572:ARG:NH1	5:L:98:GLN:HE21	1.92	0.68
5:L:124:GLY:HA2	5:L:191:ILE:HG22	1.76	0.68
7:R:2:DT:H3	8:S:47:DA:H2	1.40	0.68
2:C:6:PHE:HE1	2:C:901:TYR:HD1	1.42	0.68
3:D:743:ASP:HA	9:Q:4:A:H4'	1.75	0.68
2:I:217:LEU:HD13	2:I:311:PHE:HD2	1.57	0.68
2:C:108:ILE:HB	6:M:48:TYR:HB2	1.76	0.67
2:C:902:ILE:HG22	2:C:904:PRO:HD3	1.75	0.67
2:I:711:GLU:O	2:I:758:ARG:NH1	2.27	0.67
2:I:6:PHE:HE1	2:I:901:TYR:HD1	1.42	0.67
2:C:328:LEU:HD22	2:C:437:ARG:HD2	1.75	0.67
2:C:711:GLU:O	2:C:758:ARG:NH1	2.27	0.67
5:F:103:ILE:HG21	5:F:211:VAL:HG21	1.76	0.67
3:J:67:ARG:HG3	5:L:392:ASP:HB2	1.77	0.67
2:C:1008:ARG:HH11	2:C:1028:GLY:HA2	1.59	0.67
2:C:14:PRO:HB3	2:C:586:ARG:HH22	1.58	0.67
3:D:102:ILE:HD11	3:D:587:ARG:HG3	1.77	0.67
2:I:12:VAL:HG11	2:I:472:ARG:HH12	1.59	0.67
3:J:9:ARG:HG3	3:J:1456:LYS:HB3	1.77	0.67
3:J:12:LEU:HD11	3:J:1452:ILE:HA	1.77	0.67
2:C:487:THR:O	2:C:491:GLU:N	2.28	0.66
3:D:572:ARG:NH1	5:F:98:GLN:HE21	1.92	0.66
2:I:902:ILE:HG22	2:I:904:PRO:HD3	1.75	0.66
2:I:487:THR:O	2:I:491:GLU:N	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:743:ASP:HA	9:T:4:A:H4'	1.77	0.66
2:I:211:LEU:HD11	2:I:221:LEU:HB3	1.78	0.66
2:I:770:GLU:HG2	5:L:366:SER:HA	1.76	0.66
7:R:10:DA:H2	8:S:39:DT:H3	1.43	0.66
2:C:770:GLU:HG2	5:F:366:SER:HA	1.76	0.66
5:F:383:VAL:HG13	5:F:401:VAL:HG11	1.78	0.66
2:C:12:VAL:HG11	2:C:472:ARG:HH12	1.60	0.66
3:D:543:LEU:HG	3:D:600:LEU:HD23	1.78	0.66
5:F:124:GLY:HA2	5:F:191:ILE:HG22	1.76	0.66
2:I:328:LEU:HD22	2:I:437:ARG:HD2	1.76	0.66
2:I:468:ARG:HB3	2:I:485:TYR:O	1.96	0.66
2:I:1008:ARG:HH11	2:I:1028:GLY:HA2	1.59	0.66
3:D:191:LEU:HD11	3:D:197:SER:HB2	1.76	0.66
3:D:349:PRO:HB3	5:F:112:GLU:HG2	1.77	0.66
2:I:264:PRO:HG2	2:I:265:LYS:HE2	1.76	0.66
3:D:12:LEU:HD11	3:D:1452:ILE:HA	1.78	0.66
5:F:332:LEU:HD22	5:F:345:GLY:HA2	1.75	0.66
2:I:859:PRO:HB2	2:I:974:LEU:HD23	1.76	0.66
6:M:21:ALA:O	6:M:37:GLN:HB3	1.96	0.66
1:B:176:ARG:HD2	3:D:884:ARG:HH22	1.61	0.66
3:D:178:LEU:HD21	3:D:190:GLU:HB3	1.78	0.66
4:E:30:LEU:HA	4:E:37:ASN:HD21	1.60	0.66
2:I:100:LEU:HB2	2:I:369:PRO:HD3	1.76	0.66
2:C:199:VAL:HA	2:C:231:PRO:HB3	1.77	0.66
3:J:543:LEU:HG	3:J:600:LEU:HD23	1.76	0.66
1:H:55:SER:HB2	1:H:166:PRO:HA	1.78	0.65
2:I:199:VAL:HA	2:I:231:PRO:HB3	1.77	0.65
2:I:595:LEU:HB2	2:I:656:ALA:HB3	1.76	0.65
5:L:103:ILE:HG21	5:L:211:VAL:HG21	1.77	0.65
2:C:100:LEU:HB2	2:C:369:PRO:HD3	1.77	0.65
2:C:630:ARG:HA	2:C:705:ILE:HD13	1.77	0.65
3:D:1331:ASP:HB3	3:D:1334:GLN:HB2	1.78	0.65
2:I:1095:LEU:HD11	3:J:603:LEU:HB3	1.77	0.65
3:J:102:ILE:HD11	3:J:587:ARG:HG3	1.77	0.65
2:C:468:ARG:HB3	2:C:485:TYR:O	1.96	0.65
5:F:222:LEU:HB3	5:F:226:ASP:HB3	1.78	0.65
7:R:39:DT:H2''	7:R:40:DC:H5'	1.77	0.65
2:C:859:PRO:HB2	2:C:974:LEU:HD23	1.78	0.65
3:D:561:GLY:HA3	5:F:147:ARG:HD3	1.77	0.65
2:I:458:TYR:HB3	2:I:470:PRO:HG2	1.78	0.65
4:K:30:LEU:HA	4:K:37:ASN:HD21	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:55:SER:HB2	1:B:166:PRO:HA	1.78	0.65
3:D:973:GLN:HG2	3:J:831:GLY:HA2	1.78	0.65
3:J:1331:ASP:HB3	3:J:1334:GLN:HB2	1.79	0.65
8:P:17:DG:H2''	8:P:18:DG:O4'	1.97	0.65
7:O:39:DT:H2''	7:O:40:DC:H5'	1.77	0.65
2:C:211:LEU:HD11	2:C:221:LEU:HB3	1.77	0.65
3:J:411:THR:HG22	3:J:437:VAL:H	1.62	0.65
3:D:1042:ARG:HD3	3:D:1045:MET:HE1	1.78	0.65
3:D:1088:THR:HG22	3:D:1234:THR:HG23	1.78	0.65
2:I:158:TYR:HB2	2:I:314:THR:HG22	1.79	0.65
1:A:53:VAL:HG22	1:A:54:THR:H	1.61	0.65
2:C:595:LEU:HB2	2:C:656:ALA:HB3	1.78	0.65
3:D:759:ALA:HA	3:D:763:MET:HB3	1.78	0.65
3:D:1045:MET:HE2	3:D:1057:VAL:HG11	1.78	0.64
2:I:751:PRO:HD2	3:J:681:ARG:HD2	1.78	0.64
1:H:176:ARG:HD2	3:J:884:ARG:HH22	1.62	0.64
3:D:1434:TRP:CD1	3:D:1434:TRP:H	2.15	0.64
3:J:1045:MET:HE2	3:J:1057:VAL:HG11	1.79	0.64
5:L:222:LEU:HB3	5:L:226:ASP:HB3	1.78	0.64
2:C:143:SER:H	2:C:331:ARG:HA	1.63	0.64
3:J:561:GLY:HA3	5:L:147:ARG:HD3	1.79	0.64
7:R:46:DT:H3	8:S:3:DA:H61	1.45	0.64
2:C:374:ASN:ND2	5:F:291:ARG:HE	1.94	0.64
2:I:36:PRO:HB2	2:I:70:GLU:HG2	1.79	0.64
1:A:73:GLU:HB3	1:A:77:GLU:HB3	1.80	0.64
3:D:1138:SER:HB3	3:D:1362:LYS:HD3	1.80	0.64
3:D:1486:VAL:HG11	4:E:22:VAL:HG13	1.79	0.64
2:C:324:ASP:HB3	2:C:327:HIS:HB2	1.80	0.64
3:D:32:ILE:HG22	3:D:39:PRO:HA	1.80	0.64
2:I:374:ASN:HD21	5:L:291:ARG:NE	1.95	0.64
3:J:1042:ARG:HD3	3:J:1045:MET:HE1	1.78	0.64
1:A:219:LYS:HB2	1:B:222:LEU:HD22	1.79	0.64
2:I:874:LEU:HD13	3:J:783:ARG:HB3	1.80	0.64
2:I:966:LEU:HD11	2:I:986:PRO:HG3	1.80	0.64
3:J:1434:TRP:CD1	3:J:1434:TRP:H	2.15	0.64
2:C:36:PRO:HB2	2:C:70:GLU:HG2	1.80	0.64
3:J:1486:VAL:HG11	4:K:22:VAL:HG13	1.80	0.64
5:L:383:VAL:HG13	5:L:401:VAL:HG11	1.79	0.64
2:C:157:ARG:HH22	2:C:314:THR:HB	1.62	0.63
2:C:1095:LEU:HD11	3:D:603:LEU:HB3	1.79	0.63
3:J:759:ALA:HA	3:J:763:MET:HB3	1.78	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:229:ALA:HA	3:D:245:LEU:H	1.63	0.63
6:N:18:GLY:HA2	6:N:41:PRO:HD3	1.78	0.63
8:S:14:DG:H1	9:T:2:C:H42	1.46	0.63
2:C:458:TYR:HB3	2:C:470:PRO:HG2	1.78	0.63
1:G:219:LYS:HB2	1:H:222:LEU:HD22	1.79	0.63
2:I:124:ASP:O	2:I:407:LYS:NZ	2.31	0.63
3:J:168:THR:HA	3:J:394:LEU:HG	1.81	0.63
1:B:184:THR:HG23	1:B:192:LEU:HB2	1.81	0.63
3:D:637:LEU:O	3:D:935:LYS:NZ	2.32	0.63
3:D:1459:LEU:HD21	3:D:1468:LEU:HG	1.80	0.63
1:G:53:VAL:HG22	1:G:54:THR:H	1.63	0.63
2:I:42:VAL:HA	2:I:46:ALA:HB2	1.81	0.63
2:I:914:ILE:HA	2:I:917:LEU:HD12	1.81	0.63
3:D:1432:LYS:HG3	3:D:1460:ILE:HD11	1.81	0.63
3:J:1138:SER:HB3	3:J:1362:LYS:HD3	1.80	0.63
3:D:1038:LEU:O	3:D:1060:SER:OG	2.17	0.63
1:G:73:GLU:HB3	1:G:77:GLU:HB3	1.79	0.63
3:J:192:ALA:HB1	3:J:193:PRO:HD2	1.81	0.63
2:C:158:TYR:HB2	2:C:314:THR:HG22	1.80	0.63
4:E:41:GLU:HB3	4:E:42:PRO:HD2	1.81	0.63
2:I:157:ARG:HH22	2:I:314:THR:HB	1.63	0.63
3:J:1432:LYS:HG3	3:J:1460:ILE:HD11	1.80	0.63
5:L:409:ARG:NH2	7:R:5:DA:H61	1.95	0.63
3:D:291:LEU:HD23	3:D:303:PRO:HB2	1.80	0.63
1:H:184:THR:HG23	1:H:192:LEU:HB2	1.81	0.63
2:I:437:ARG:NH1	2:I:467:ILE:O	2.32	0.63
7:O:47:DG:N2	8:P:2:DC:N3	2.46	0.63
3:D:675:ARG:HH12	5:F:437:LEU:HG	1.64	0.63
2:I:675:ALA:HA	2:I:989:VAL:HG12	1.81	0.63
1:B:186:LEU:HD13	4:E:51:LEU:HD13	1.80	0.62
2:I:1064:ASN:HD22	5:L:359:ALA:HB2	1.64	0.62
3:J:1038:LEU:O	3:J:1060:SER:OG	2.17	0.62
5:L:431:ARG:HG3	5:L:434:ARG:HE	1.64	0.62
2:C:42:VAL:HA	2:C:46:ALA:HB2	1.81	0.62
2:C:1034:GLU:HG2	3:D:619:LEU:HB3	1.82	0.62
3:D:658:LEU:HD22	3:D:670:VAL:HG13	1.81	0.62
3:D:1323:GLN:HG2	3:D:1324:PRO:HD2	1.81	0.62
2:I:245:GLY:HA2	5:L:97:ARG:HD2	1.81	0.62
6:N:20:VAL:HA	6:N:38:VAL:CA	2.29	0.62
3:J:1323:GLN:HG2	3:J:1324:PRO:HD2	1.81	0.62
3:D:264:LEU:HG	3:D:316:HIS:HE2	1.63	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:876:VAL:HG13	2:I:884:GLN:HE21	1.65	0.62
3:J:1088:THR:HG22	3:J:1234:THR:HG23	1.80	0.62
2:C:914:ILE:HA	2:C:917:LEU:HD12	1.81	0.62
2:C:1055:ILE:HD11	2:C:1079:PRO:HD3	1.82	0.62
3:J:32:ILE:HG22	3:J:39:PRO:HA	1.81	0.62
3:J:1201:CYS:SG	3:J:1204:CYS:HB2	2.40	0.62
2:C:118:LEU:HD12	2:C:119:PRO:HD2	1.82	0.62
2:C:874:LEU:HD13	3:D:783:ARG:HB3	1.81	0.62
3:D:30:GLU:HB2	5:F:274:ARG:HB2	1.82	0.62
3:J:680:GLN:O	3:J:682:ASP:N	2.29	0.62
4:K:41:GLU:HB3	4:K:42:PRO:HD2	1.81	0.62
3:D:1201:CYS:SG	3:D:1204:CYS:HB2	2.39	0.62
3:J:125:GLN:NE2	3:J:130:ASN:OD1	2.33	0.62
3:J:462:GLN:HA	3:J:513:ILE:HG13	1.82	0.62
2:C:876:VAL:HG13	2:C:884:GLN:HE21	1.65	0.62
1:H:186:LEU:HD13	4:K:51:LEU:HD13	1.80	0.62
2:I:143:SER:H	2:I:331:ARG:HA	1.64	0.61
2:C:164:PRO:HB3	2:C:269:LEU:HG	1.82	0.61
2:C:437:ARG:NH1	2:C:467:ILE:O	2.33	0.61
7:R:11:DG:N2	8:S:38:DC:O2	2.32	0.61
3:D:8:VAL:HG21	3:D:1468:LEU:HD21	1.82	0.61
3:J:30:GLU:HB2	5:L:274:ARG:HB2	1.80	0.61
2:C:1060:ILE:HG13	2:C:1061:GLU:H	1.65	0.61
3:J:700:VAL:HG22	3:J:718:PRO:HG3	1.82	0.61
3:J:1436:SER:HB2	3:J:1464:GLU:HG2	1.82	0.61
3:D:770:LEU:HB2	3:D:1210:SER:HA	1.81	0.61
3:J:1106:VAL:HB	3:J:1108:ARG:HH22	1.66	0.61
3:D:356:PRO:HG2	3:D:359:ALA:HB2	1.82	0.61
2:I:1100:GLN:HB2	3:J:9:ARG:HB3	1.82	0.61
2:C:71:TYR:HA	2:C:95:TYR:C	2.26	0.61
2:C:966:LEU:HD11	2:C:986:PRO:HG3	1.82	0.61
3:D:417:PRO:HA	3:D:430:GLU:HA	1.82	0.61
3:D:661:MET:HG2	3:D:666:PHE:CZ	2.35	0.61
6:N:21:ALA:O	6:N:37:GLN:HB3	2.00	0.61
3:D:700:VAL:HG22	3:D:718:PRO:HG3	1.82	0.61
1:G:175:ARG:HB3	1:G:200:TRP:HB3	1.83	0.61
2:I:15:LEU:HD21	2:I:457:ALA:HB1	1.83	0.61
2:C:197:LEU:HD23	2:C:200:LEU:HD23	1.81	0.61
3:J:770:LEU:HB2	3:J:1210:SER:HA	1.83	0.61
3:J:1384:PRO:HA	3:J:1415:VAL:HG13	1.83	0.61
3:J:1459:LEU:HD21	3:J:1468:LEU:HG	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:14:THR:HG1	1:B:231:SER:HG	1.48	0.61
2:I:383:ARG:HH21	2:I:388:ARG:NH2	1.99	0.61
2:C:15:LEU:HD21	2:C:457:ALA:HB1	1.83	0.60
2:C:383:ARG:HH21	2:C:388:ARG:NH2	1.99	0.60
3:D:125:GLN:NE2	3:D:130:ASN:OD1	2.33	0.60
2:I:1060:ILE:HG13	2:I:1061:GLU:H	1.65	0.60
3:J:191:LEU:HB2	3:J:195:VAL:HG11	1.81	0.60
3:J:1465:ASN:O	3:J:1468:LEU:N	2.34	0.60
3:D:101:HIS:NE2	3:D:582:ILE:HG21	2.17	0.60
2:I:71:TYR:HA	2:I:95:TYR:C	2.27	0.60
2:I:139:GLN:HB3	2:I:334:ARG:HB2	1.83	0.60
2:I:486:MET:HE3	2:I:491:GLU:HA	1.83	0.60
3:J:1149:LEU:HB3	3:J:1162:GLU:HA	1.83	0.60
1:A:175:ARG:HB3	1:A:200:TRP:HB3	1.84	0.60
3:D:462:GLN:HA	3:D:513:ILE:HG13	1.82	0.60
3:D:699:VAL:HG13	3:D:760:ARG:HD3	1.83	0.60
3:J:100:ALA:HA	3:J:513:ILE:HA	1.83	0.60
3:J:637:LEU:O	3:J:935:LYS:NZ	2.34	0.60
4:K:37:ASN:N	4:K:37:ASN:OD1	2.34	0.60
2:C:994:ILE:HG22	2:C:995:MET:H	1.65	0.60
3:D:260:GLU:HB3	3:D:271:TYR:HB2	1.84	0.60
3:D:1106:VAL:HB	3:D:1108:ARG:HH22	1.66	0.60
3:D:1149:LEU:HB3	3:D:1162:GLU:HA	1.83	0.60
4:E:37:ASN:OD1	4:E:37:ASN:N	2.34	0.60
1:A:40:LEU:O	1:A:44:LEU:HB2	2.02	0.60
3:D:644:LEU:HD12	3:D:645:PRO:HD2	1.82	0.60
2:I:276:LYS:HD3	2:I:466:PHE:HZ	1.67	0.60
3:D:162:ARG:HG2	3:D:414:ARG:HH22	1.67	0.60
3:D:960:LYS:O	3:D:964:LEU:HB3	2.02	0.60
2:I:714:ASP:HA	2:I:719:PRO:HA	1.84	0.60
3:D:100:ALA:HA	3:D:513:ILE:HA	1.84	0.60
2:I:549:PHE:HZ	2:I:890:LEU:HD12	1.67	0.60
3:J:729:HIS:HE1	3:J:731:LEU:HD23	1.66	0.60
3:D:213:VAL:HG22	3:D:385:VAL:HG12	1.82	0.60
3:D:1465:ASN:O	3:D:1468:LEU:N	2.34	0.60
3:J:433:GLY:HA2	3:J:449:SER:H	1.67	0.60
3:J:644:LEU:HD12	3:J:645:PRO:HD2	1.83	0.60
7:O:32:DG:H2'	7:O:33:DG:C8	2.37	0.60
1:A:32:PHE:O	1:A:35:THR:OG1	2.16	0.59
2:C:139:GLN:HB3	2:C:334:ARG:HB2	1.82	0.59
4:K:67:GLU:HB3	4:K:73:LEU:HD11	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:M:18:GLY:HA2	6:M:41:PRO:HD3	1.84	0.59
2:C:532:MET:HG2	2:C:533:ASP:H	1.68	0.59
2:C:675:ALA:HA	2:C:989:VAL:HG12	1.83	0.59
3:D:1384:PRO:HA	3:D:1415:VAL:HG13	1.84	0.59
1:G:215:VAL:HG13	1:H:222:LEU:HD23	1.84	0.59
1:H:18:ASP:O	1:H:201:THR:OG1	2.11	0.59
2:I:994:ILE:HG22	2:I:995:MET:H	1.66	0.59
3:J:699:VAL:HG13	3:J:760:ARG:HD3	1.83	0.59
4:E:38:THR:HG21	4:E:63:TRP:HZ3	1.67	0.59
2:I:197:LEU:HD23	2:I:200:LEU:HD23	1.83	0.59
3:J:729:HIS:CE1	3:J:731:LEU:HD23	2.37	0.59
3:J:960:LYS:O	3:J:964:LEU:HB3	2.01	0.59
5:L:210:VAL:HA	5:L:213:ILE:HD12	1.85	0.59
1:A:14:THR:OG1	1:B:231:SER:OG	2.19	0.59
2:I:853:LEU:HB3	2:I:858:MET:HE1	1.85	0.59
2:C:15:LEU:HD13	2:C:16:PRO:HD2	1.84	0.59
2:C:182:VAL:HG21	2:C:193:LEU:HD12	1.85	0.59
2:C:238:LEU:HD23	2:C:241:LEU:HD12	1.84	0.59
2:C:575:GLN:HB3	2:C:670:GLN:HG3	1.84	0.59
2:C:1100:GLN:HB2	3:D:9:ARG:HB3	1.82	0.59
3:D:680:GLN:C	3:D:682:ASP:H	2.10	0.59
3:D:729:HIS:HE1	3:D:731:LEU:HD23	1.66	0.59
2:I:163:ILE:HD13	2:I:171:TRP:CD1	2.37	0.59
2:I:193:LEU:HD21	2:I:307:LEU:HD11	1.84	0.59
3:J:421:LEU:H	3:J:428:LYS:HA	1.67	0.59
3:J:127:LEU:HG	3:J:461:ILE:HG13	1.85	0.59
3:J:1197:ARG:HE	3:J:1398:TRP:HB3	1.66	0.59
6:N:106:ALA:HA	6:N:136:LEU:HD11	1.85	0.59
1:A:215:VAL:HG13	1:B:222:LEU:HD23	1.84	0.59
2:C:886:LEU:HD21	3:D:951:ILE:HD13	1.84	0.59
2:C:1019:GLN:HG3	3:D:617:ASN:HD22	1.67	0.59
2:C:1056:LYS:HE2	3:D:751:LEU:HG	1.84	0.59
1:G:40:LEU:O	1:G:44:LEU:HB2	2.02	0.59
2:I:238:LEU:HD23	2:I:241:LEU:HD12	1.84	0.59
2:I:575:GLN:HB3	2:I:670:GLN:HG3	1.83	0.59
3:J:101:HIS:NE2	3:J:582:ILE:HG21	2.17	0.59
2:C:714:ASP:HA	2:C:719:PRO:HA	1.85	0.59
2:I:754:ILE:HG12	2:I:791:ARG:HD3	1.85	0.59
2:I:886:LEU:HD21	3:J:951:ILE:HD13	1.85	0.59
6:N:88:ALA:HA	6:N:91:ARG:HD2	1.84	0.59
2:C:261:LEU:HB3	2:C:290:LEU:HD12	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:181:ASP:HB3	3:D:357:GLU:HG2	1.85	0.59
2:I:1034:GLU:HG2	3:J:619:LEU:HB3	1.85	0.59
3:J:186:VAL:HG12	3:J:187:LYS:H	1.67	0.59
2:I:118:LEU:HD12	2:I:119:PRO:HD2	1.84	0.58
2:I:1056:LYS:HE2	3:J:751:LEU:HG	1.84	0.58
3:J:355:VAL:HG12	3:J:356:PRO:HD2	1.85	0.58
4:K:38:THR:HG21	4:K:63:TRP:HZ3	1.68	0.58
2:C:14:PRO:HB3	2:C:586:ARG:NH2	2.18	0.58
3:D:977:ALA:HB2	3:J:831:GLY:HA3	1.85	0.58
3:D:1201:CYS:SG	3:D:1204:CYS:CB	2.91	0.58
1:B:18:ASP:O	1:B:201:THR:OG1	2.11	0.58
2:C:163:ILE:HD13	2:C:171:TRP:CD1	2.37	0.58
3:D:729:HIS:CE1	3:D:731:LEU:HD23	2.37	0.58
2:I:164:PRO:HB3	2:I:269:LEU:HG	1.83	0.58
7:O:10:DA:H2	8:P:39:DT:H3	1.51	0.58
2:I:532:MET:HG2	2:I:533:ASP:H	1.68	0.58
3:D:1197:ARG:HE	3:D:1398:TRP:HB3	1.66	0.58
3:J:1336:LEU:HD22	3:J:1421:LEU:HB3	1.86	0.58
5:L:364:LEU:HD22	5:L:436:PHE:HZ	1.68	0.58
1:A:53:VAL:HA	1:A:144:VAL:HG13	1.85	0.58
2:C:486:MET:HE3	2:C:491:GLU:HA	1.84	0.58
3:D:245:LEU:HD11	3:D:249:TYR:HB3	1.85	0.58
2:I:15:LEU:HD13	2:I:16:PRO:HD2	1.84	0.58
2:I:182:VAL:HG21	2:I:193:LEU:HD12	1.86	0.58
2:I:261:LEU:HB3	2:I:290:LEU:HD12	1.85	0.58
2:I:1082:PRO:HG3	3:J:1469:GLY:HA3	1.86	0.58
4:K:91:ARG:HH21	4:K:92:LEU:HG	1.68	0.58
6:M:151:ALA:HA	6:M:154:LEU:HD12	1.86	0.58
7:O:32:DG:H2''	7:O:33:DG:H5'	1.86	0.58
2:C:239:PHE:HA	2:C:242:LEU:HD12	1.85	0.58
3:D:127:LEU:HG	3:D:461:ILE:HG13	1.85	0.58
4:E:67:GLU:HB3	4:E:73:LEU:HD11	1.84	0.58
3:J:1201:CYS:SG	3:J:1204:CYS:CB	2.91	0.58
6:M:20:VAL:HA	6:M:38:VAL:CA	2.32	0.58
2:C:549:PHE:HZ	2:C:890:LEU:HD12	1.68	0.58
2:C:773:LEU:HD13	5:F:388:LYS:HG3	1.86	0.58
5:F:210:VAL:HA	5:F:213:ILE:HD12	1.85	0.58
5:L:417:ASN:HD22	5:L:421:ARG:HH12	1.52	0.58
2:C:432:ARG:HH12	2:C:518:ARG:HH21	1.52	0.58
3:D:1336:LEU:HD22	3:D:1421:LEU:HB3	1.86	0.58
2:I:14:PRO:HB3	2:I:586:ARG:NH2	2.17	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:371:ILE:HD12	5:L:247:ARG:HE	1.68	0.58
6:M:116:GLU:HB2	6:M:121:LEU:HD22	1.84	0.58
7:O:2:DT:H3	8:P:47:DA:H2	1.52	0.58
2:C:754:ILE:HG12	2:C:791:ARG:HD3	1.86	0.58
2:C:1047:HIS:O	2:C:1051:GLU:HG2	2.04	0.58
5:F:252:THR:HA	7:O:29:DC:H5	1.69	0.58
2:I:949:LYS:HD2	3:J:796:ARG:HH11	1.69	0.58
3:J:1042:ARG:HH11	3:J:1045:MET:HE1	1.69	0.58
2:C:1057:SER:HB3	3:D:623:VAL:HG13	1.86	0.57
2:I:239:PHE:HA	2:I:242:LEU:HD12	1.85	0.57
2:I:1017:THR:HG21	3:J:617:ASN:ND2	2.18	0.57
5:L:151:LEU:HD23	5:L:156:ILE:HD12	1.86	0.57
1:A:36:LEU:HB2	1:A:195:LEU:HD12	1.86	0.57
2:C:86:LYS:HE2	2:C:814:GLU:H	1.68	0.57
3:D:672:ALA:O	3:D:676:MET:HB2	2.04	0.57
3:D:60:CYS:SG	3:D:76:CYS:HB3	2.44	0.57
3:D:520:LEU:HB3	3:D:525:ARG:HD3	1.86	0.57
3:D:527:MET:HG3	3:D:537:THR:HB	1.86	0.57
5:F:100:LEU:HD13	7:O:31:DG:H21	1.69	0.57
3:D:44:LEU:HB3	3:D:525:ARG:HH22	1.70	0.57
1:G:53:VAL:HA	1:G:144:VAL:HG13	1.87	0.57
1:A:224:TYR:CE1	1:B:9:PRO:HG2	2.39	0.57
3:D:1462:LEU:HD12	3:D:1463:LYS:H	1.69	0.57
3:J:527:MET:HG3	3:J:537:THR:HB	1.87	0.57
3:J:661:MET:HG2	3:J:666:PHE:CZ	2.39	0.57
1:B:72:LYS:HG3	1:B:131:THR:HB	1.86	0.57
3:D:236:TYR:HB2	3:D:319:ALA:HB3	1.85	0.57
4:E:91:ARG:HH21	4:E:92:LEU:HG	1.69	0.57
3:J:60:CYS:SG	3:J:76:CYS:HB3	2.45	0.57
2:C:167:LYS:HD3	7:O:35:DG:H5'	1.86	0.57
2:I:1057:SER:HB3	3:J:623:VAL:HG13	1.87	0.57
3:J:1097:LYS:HE2	3:J:1440:PHE:HZ	1.69	0.57
2:C:690:ILE:HD11	2:C:849:VAL:HG22	1.87	0.57
1:H:72:LYS:HG3	1:H:131:THR:HB	1.86	0.57
2:I:773:LEU:HD13	5:L:388:LYS:HG3	1.85	0.57
2:C:163:ILE:HD13	2:C:171:TRP:HD1	1.69	0.57
2:C:949:LYS:HD2	3:D:796:ARG:HH11	1.69	0.57
3:D:229:ALA:HB1	3:D:243:ALA:HB1	1.86	0.57
3:D:703:ASN:HB2	3:D:713:ILE:HG12	1.87	0.57
2:I:285:LEU:HD23	2:I:286:SER:H	1.70	0.57
2:I:660:ALA:HB1	2:I:667:ALA:O	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:141:VAL:HG12	3:J:450:TYR:HE2	1.69	0.57
3:J:1462:LEU:HD12	3:J:1463:LYS:H	1.69	0.57
2:C:193:LEU:HD21	2:C:307:LEU:HD11	1.86	0.57
1:G:178:ALA:HB2	2:I:864:GLY:HA3	1.87	0.57
3:J:1045:MET:HB2	3:J:1072:ILE:HG22	1.86	0.57
2:C:93:PRO:HB3	2:C:114:PHE:HE1	1.69	0.56
2:C:439:CYS:HB2	2:C:541:SER:HB3	1.87	0.56
5:F:252:THR:HA	7:O:29:DC:C5	2.40	0.56
2:I:432:ARG:HH12	2:I:518:ARG:HH21	1.53	0.56
3:J:672:ALA:O	3:J:676:MET:HB2	2.04	0.56
3:J:703:ASN:HB2	3:J:713:ILE:HG12	1.87	0.56
3:J:828:VAL:HA	3:J:833:GLU:HA	1.87	0.56
1:A:153:ALA:HB1	1:A:166:PRO:HB2	1.86	0.56
2:C:194:VAL:HA	2:C:197:LEU:HD12	1.88	0.56
1:G:36:LEU:HB2	1:G:195:LEU:HD12	1.86	0.56
1:G:224:TYR:CE1	1:H:9:PRO:HG2	2.40	0.56
2:I:93:PRO:HB3	2:I:114:PHE:HE1	1.70	0.56
2:I:194:VAL:HA	2:I:197:LEU:HD12	1.87	0.56
1:A:67:THR:HG21	2:C:627:ARG:HG3	1.87	0.56
2:C:87:ASP:HA	2:C:131:GLY:HA3	1.87	0.56
2:C:376:ARG:HH22	5:F:294:GLN:HG3	1.70	0.56
2:C:853:LEU:HB3	2:C:858:MET:HE1	1.86	0.56
3:D:886:VAL:HG11	3:D:900:ILE:HD11	1.86	0.56
3:D:1045:MET:HB2	3:D:1072:ILE:HG22	1.86	0.56
4:E:38:THR:HG21	4:E:63:TRP:CZ3	2.40	0.56
5:F:151:LEU:HD23	5:F:156:ILE:HD12	1.87	0.56
2:I:26:TYR:HB2	2:I:336:VAL:HB	1.87	0.56
2:I:69:LEU:HB2	2:I:97:ARG:O	2.05	0.56
2:I:163:ILE:HD13	2:I:171:TRP:HD1	1.69	0.56
3:J:349:PRO:HB3	5:L:112:GLU:HG2	1.85	0.56
3:J:613:ARG:HD3	3:J:617:ASN:OD1	2.05	0.56
3:J:628:ARG:HH12	8:S:14:DG:H2"	1.69	0.56
3:J:886:VAL:HG11	3:J:900:ILE:HD11	1.86	0.56
3:J:901:GLN:HG2	3:J:906:GLN:HE22	1.70	0.56
3:J:1042:ARG:HE	3:J:1061:PHE:HE2	1.53	0.56
3:J:1377:LYS:O	3:J:1397:LYS:N	2.38	0.56
1:A:62:LEU:HD13	2:C:745:ILE:HG21	1.88	0.56
2:I:853:LEU:HD12	2:I:854:PRO:HD2	1.86	0.56
3:J:86:ARG:O	3:J:521:PRO:HB3	2.06	0.56
5:L:252:THR:HA	7:R:29:DC:C5	2.41	0.56
7:R:47:DG:N2	8:S:2:DC:N3	2.54	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:437:ARG:HB3	2:C:467:ILE:HG21	1.88	0.56
2:I:606:VAL:HG23	2:I:645:VAL:HA	1.87	0.56
2:I:690:ILE:HD11	2:I:849:VAL:HG22	1.87	0.56
3:J:916:TYR:HE2	3:J:1168:LEU:HD22	1.71	0.56
3:J:1068:LEU:H	3:J:1068:LEU:HD12	1.70	0.56
3:D:1042:ARG:HH11	3:D:1045:MET:HE1	1.71	0.56
3:D:1042:ARG:HE	3:D:1061:PHE:HE2	1.54	0.56
2:C:473:ARG:O	2:C:480:THR:OG1	2.17	0.56
2:C:606:VAL:HG23	2:C:645:VAL:HA	1.87	0.56
2:C:1066:ALA:HA	2:C:1076:VAL:HG12	1.87	0.56
3:D:439:LEU:HD22	3:D:439:LEU:H	1.70	0.56
1:G:67:THR:HG21	2:I:627:ARG:HG3	1.87	0.56
2:I:458:TYR:HD1	2:I:538:GLN:HB3	1.70	0.56
3:J:208:PRO:HA	3:J:390:PRO:HA	1.88	0.56
2:C:146:VAL:HG21	2:C:281:LEU:HD11	1.88	0.56
2:C:374:ASN:ND2	2:C:375:SER:H	2.04	0.56
3:D:613:ARG:HD3	3:D:617:ASN:OD1	2.06	0.56
5:F:417:ASN:HD22	5:F:421:ARG:HH12	1.53	0.56
1:G:32:PHE:O	1:G:35:THR:OG1	2.18	0.56
1:G:153:ALA:HB1	1:G:166:PRO:HB2	1.87	0.56
2:I:473:ARG:O	2:I:480:THR:OG1	2.19	0.56
2:I:1047:HIS:O	2:I:1051:GLU:HG2	2.05	0.56
3:J:470:LEU:HD22	3:J:499:VAL:HG13	1.88	0.56
3:J:572:ARG:HH12	5:L:98:GLN:HE21	1.54	0.56
5:L:252:THR:HG23	7:R:29:DC:H41	1.71	0.56
1:A:178:ALA:HB2	2:C:864:GLY:HA3	1.86	0.56
2:C:571:LEU:HB2	2:C:574:ALA:HB2	1.88	0.56
2:C:660:ALA:HB1	2:C:667:ALA:O	2.05	0.56
3:D:317:MET:HB3	3:D:337:LEU:HD21	1.86	0.56
3:D:800:LYS:HB3	3:D:822:ALA:HB2	1.88	0.56
2:I:146:VAL:HG21	2:I:281:LEU:HD11	1.88	0.56
3:J:44:LEU:HB3	3:J:525:ARG:HH22	1.71	0.56
2:C:546:LEU:HB2	2:C:565:GLN:HE22	1.71	0.56
3:D:638:LYS:HG2	3:D:639:LEU:H	1.70	0.56
5:L:99:TYR:HA	5:L:102:GLU:HB2	1.88	0.56
2:C:245:GLY:HA2	5:F:97:ARG:HD2	1.88	0.55
2:C:328:LEU:HD21	2:C:438:ILE:HD11	1.88	0.55
2:C:605:LYS:HG2	2:C:612:ALA:HB3	1.88	0.55
2:C:853:LEU:HD12	2:C:854:PRO:HD2	1.87	0.55
3:D:203:ALA:HB2	3:D:395:VAL:HB	1.87	0.55
3:D:470:LEU:HD22	3:D:499:VAL:HG13	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:828:VAL:HA	3:D:833:GLU:HA	1.88	0.55
3:D:901:GLN:HG2	3:D:906:GLN:HE22	1.70	0.55
3:D:1100:ASP:CG	3:D:1440:PHE:HB2	2.31	0.55
2:I:1066:ALA:HA	2:I:1076:VAL:HG12	1.88	0.55
3:J:171:LEU:HD12	3:J:393:ILE:HD11	1.88	0.55
3:J:758:GLU:HG2	3:J:1476:THR:HG21	1.87	0.55
2:C:69:LEU:HB2	2:C:97:ARG:O	2.06	0.55
2:C:428:ARG:HH11	2:C:451:LEU:HD21	1.71	0.55
3:D:234:GLU:HA	3:D:322:VAL:HB	1.88	0.55
3:D:453:ASP:OD2	3:D:455:ARG:NE	2.37	0.55
2:I:23:VAL:HA	2:I:121:MET:SD	2.47	0.55
3:J:407:VAL:HA	3:J:422:ALA:HB1	1.87	0.55
3:J:800:LYS:HB3	3:J:822:ALA:HB2	1.87	0.55
6:N:151:ALA:HA	6:N:154:LEU:HD12	1.88	0.55
2:C:124:ASP:O	2:C:407:LYS:NZ	2.38	0.55
3:D:1458:GLU:HB2	3:D:1460:ILE:HG23	1.89	0.55
3:J:1272:ALA:HB3	3:J:1330:ILE:HD13	1.88	0.55
2:C:26:TYR:HB2	2:C:336:VAL:HB	1.88	0.55
3:D:758:GLU:HG2	3:D:1476:THR:HG21	1.88	0.55
3:D:1444:THR:O	3:D:1448:THR:OG1	2.24	0.55
2:I:328:LEU:H	2:I:328:LEU:HD12	1.72	0.55
3:J:371:ILE:HG23	3:J:372:ASP:H	1.72	0.55
3:J:520:LEU:HB3	3:J:525:ARG:HD3	1.87	0.55
3:J:1404:ASN:O	3:J:1408:ILE:HG12	2.06	0.55
4:K:38:THR:HG21	4:K:63:TRP:CZ3	2.41	0.55
2:C:278:GLU:HG3	2:C:284:GLY:HA2	1.89	0.55
2:C:458:TYR:HD1	2:C:538:GLN:HB3	1.69	0.55
3:D:421:LEU:H	3:D:421:LEU:HD12	1.71	0.55
5:F:99:TYR:HA	5:F:102:GLU:HB2	1.88	0.55
2:I:344:PHE:HA	2:I:382:LEU:HD21	1.89	0.55
3:J:140:ALA:HB1	3:J:161:LEU:HD21	1.88	0.55
3:J:680:GLN:C	3:J:682:ASP:H	2.12	0.55
2:C:71:TYR:HD1	2:C:94:LEU:HD11	1.71	0.55
2:C:172:ILE:HA	2:C:186:VAL:HG22	1.89	0.55
3:D:288:MET:HE2	3:D:307:GLY:HA3	1.88	0.55
5:F:235:LEU:HD12	5:F:254:ALA:HB1	1.89	0.55
2:I:428:ARG:HH11	2:I:451:LEU:HD21	1.71	0.55
2:I:897:LEU:HB3	2:I:899:GLN:HE21	1.72	0.55
3:J:633:VAL:HG13	3:J:635:PRO:HD3	1.87	0.55
3:J:699:VAL:HA	3:J:718:PRO:HD3	1.89	0.55
2:I:439:CYS:HB2	2:I:541:SER:HB3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:176:ASP:OD1	3:J:177:ALA:N	2.40	0.55
3:J:1444:THR:O	3:J:1448:THR:OG1	2.25	0.55
5:L:235:LEU:HD12	5:L:254:ALA:HB1	1.88	0.55
7:R:46:DT:H2''	7:R:47:DG:C8	2.41	0.55
2:C:897:LEU:HB3	2:C:899:GLN:HE21	1.71	0.55
2:I:259:GLY:HA2	2:I:263:ASP:HB2	1.89	0.55
2:I:605:LYS:HG2	2:I:612:ALA:HB3	1.89	0.55
3:J:130:ASN:HD22	5:L:98:GLN:NE2	2.04	0.55
3:J:1011:PHE:HD1	3:J:1021:TYR:HB2	1.71	0.55
2:C:328:LEU:H	2:C:328:LEU:HD12	1.72	0.55
2:C:344:PHE:HA	2:C:382:LEU:HD21	1.89	0.55
3:D:792:ILE:HG12	3:D:941:LEU:HD13	1.88	0.55
3:D:1404:ASN:O	3:D:1408:ILE:HG12	2.07	0.55
3:J:1273:VAL:HG23	3:J:1325:LEU:HB2	1.89	0.55
3:D:258:VAL:HG22	3:D:273:ARG:HG2	1.88	0.55
3:D:976:GLN:HG2	3:J:807:ALA:HB1	1.87	0.55
3:D:1377:LYS:O	3:D:1397:LYS:N	2.37	0.55
2:I:546:LEU:HB2	2:I:565:GLN:HE22	1.72	0.55
2:I:571:LEU:HB2	2:I:574:ALA:HB2	1.89	0.55
2:C:988:VAL:H	3:D:948:THR:HG21	1.73	0.54
2:C:1067:TYR:CZ	5:F:357:VAL:HG12	2.41	0.54
3:D:1068:LEU:H	3:D:1068:LEU:HD12	1.71	0.54
2:I:328:LEU:HD21	2:I:438:ILE:HD11	1.88	0.54
2:I:584:GLU:HA	2:I:587:VAL:HB	1.89	0.54
3:J:792:ILE:HG12	3:J:941:LEU:HD13	1.89	0.54
2:C:607:ASP:OD2	2:C:610:ARG:NH1	2.40	0.54
3:D:1011:PHE:HD1	3:D:1021:TYR:HB2	1.72	0.54
5:F:302:SER:O	5:F:306:ILE:HG22	2.08	0.54
1:G:221:HIS:HA	1:G:224:TYR:CD1	2.42	0.54
3:J:453:ASP:OD2	3:J:455:ARG:NE	2.38	0.54
2:C:584:GLU:HA	2:C:587:VAL:HB	1.89	0.54
3:D:535:PHE:O	5:F:329:PRO:HA	2.06	0.54
3:D:634:GLY:O	3:D:637:LEU:N	2.40	0.54
3:D:1290:LEU:HD12	3:D:1307:LYS:HG2	1.90	0.54
1:H:78:ILE:HA	1:H:81:ASN:HD22	1.72	0.54
2:I:195:LEU:HD12	2:I:198:ARG:HH11	1.71	0.54
3:J:418:GLY:H	3:J:430:GLU:HA	1.72	0.54
7:R:14:DT:H1'	7:R:15:DT:H5''	1.89	0.54
1:A:184:THR:HB	1:A:194:LYS:HB3	1.90	0.54
3:D:1209:LEU:O	3:D:1212:ALA:N	2.36	0.54
3:D:1272:ALA:HB3	3:D:1330:ILE:HD13	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:44:LEU:O	1:G:174:VAL:HG11	2.06	0.54
3:J:8:VAL:HG23	3:J:1459:LEU:HD11	1.89	0.54
3:J:573:MET:SD	5:L:229:GLN:HG3	2.47	0.54
5:L:204:GLU:O	5:L:207:LEU:HB3	2.07	0.54
3:D:8:VAL:HG23	3:D:1459:LEU:HD11	1.89	0.54
3:D:29:PRO:HB3	3:D:548:ILE:HB	1.90	0.54
3:D:573:MET:SD	5:F:229:GLN:HG3	2.47	0.54
3:D:1256:LEU:O	3:D:1260:ILE:HG13	2.08	0.54
3:D:1472:ILE:HD12	3:D:1473:PRO:HD2	1.90	0.54
2:I:278:GLU:HG3	2:I:284:GLY:HA2	1.89	0.54
2:I:437:ARG:HB3	2:I:467:ILE:HG21	1.89	0.54
3:J:1093:TYR:HD1	8:S:10:DA:H5"	1.71	0.54
7:O:43:DG:H1	8:P:6:DC:H42	1.55	0.54
3:D:916:TYR:HE2	3:D:1168:LEU:HD22	1.72	0.54
2:I:71:TYR:HD1	2:I:94:LEU:HD11	1.71	0.54
2:I:172:ILE:HA	2:I:186:VAL:HG22	1.88	0.54
3:J:147:VAL:HG21	3:J:153:LEU:HD21	1.89	0.54
2:C:969:LEU:HG	3:D:952:ASP:HB2	1.90	0.54
3:D:140:ALA:HB1	3:D:161:LEU:HD21	1.89	0.54
3:D:414:ARG:HG3	3:D:451:ASP:HB2	1.89	0.54
3:D:572:ARG:HH12	5:F:98:GLN:HE21	1.54	0.54
3:D:699:VAL:HA	3:D:718:PRO:HD3	1.89	0.54
3:D:1048:PRO:HD3	3:D:1075:HIS:HB3	1.90	0.54
1:G:38:ASN:HB2	2:I:980:GLY:HA3	1.90	0.54
3:J:704:ARG:NE	3:J:705:ALA:O	2.41	0.54
3:J:1202:GLN:NE2	3:J:1215:VAL:O	2.32	0.54
5:L:100:LEU:HD13	7:R:31:DG:H21	1.73	0.54
1:A:38:ASN:HB2	2:C:980:GLY:HA3	1.90	0.54
1:B:58:ILE:HB	1:B:61:VAL:HB	1.90	0.54
2:C:276:LYS:HD3	2:C:466:PHE:HZ	1.73	0.54
2:C:283:VAL:HG11	2:C:305:PRO:HG3	1.90	0.54
1:G:184:THR:HB	1:G:194:LYS:HB3	1.90	0.54
2:I:1035:MET:HG3	3:J:707:THR:HB	1.89	0.54
3:J:101:HIS:HB3	3:J:104:PHE:CE2	2.43	0.54
3:J:881:LEU:O	3:J:885:ILE:HG13	2.08	0.54
3:J:1290:LEU:HD12	3:J:1307:LYS:HG2	1.89	0.54
1:A:44:LEU:O	1:A:174:VAL:HG11	2.07	0.54
1:B:151:VAL:HG13	1:B:155:ARG:HB2	1.89	0.54
3:D:1273:VAL:HG23	3:D:1325:LEU:HB2	1.89	0.54
5:F:204:GLU:O	5:F:207:LEU:HB3	2.06	0.54
1:H:58:ILE:HB	1:H:61:VAL:HB	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:936:VAL:HB	2:I:941:LYS:HE2	1.90	0.54
3:J:8:VAL:HG21	3:J:1468:LEU:HD21	1.89	0.54
2:C:195:LEU:HD12	2:C:198:ARG:HH11	1.73	0.54
3:D:633:VAL:HG13	3:D:635:PRO:HD3	1.88	0.54
1:G:35:THR:HG22	1:H:39:PRO:HA	1.89	0.54
2:I:47:ALA:HA	2:I:345:ARG:HG2	1.90	0.54
2:I:111:ASP:HA	6:N:45:SER:HB2	1.89	0.54
2:C:285:LEU:HD23	2:C:286:SER:H	1.71	0.53
2:C:1023:GLY:HA2	8:P:15:DA:OP2	2.08	0.53
3:D:225:ILE:O	3:D:331:VAL:HG12	2.08	0.53
3:D:628:ARG:HH22	8:P:14:DG:H2"	1.73	0.53
3:D:977:ALA:HB2	3:J:831:GLY:N	2.24	0.53
3:D:1147:ARG:HH12	3:D:1190:SER:HA	1.73	0.53
1:H:151:VAL:HG13	1:H:155:ARG:HB2	1.90	0.53
4:K:27:ALA:HB1	4:K:60:ALA:HB1	1.90	0.53
2:C:829:GLN:HE21	2:C:831:ARG:HH21	1.57	0.53
3:D:147:VAL:HG21	3:D:153:LEU:HD21	1.90	0.53
3:D:192:ALA:HB1	3:D:193:PRO:HD2	1.89	0.53
3:D:245:LEU:HB2	3:D:311:LEU:HD21	1.90	0.53
3:D:810:GLU:HA	3:D:813:LEU:HD12	1.89	0.53
3:D:1202:GLN:NE2	3:D:1215:VAL:O	2.32	0.53
4:E:27:ALA:HB1	4:E:60:ALA:HB1	1.89	0.53
5:F:217:TYR:O	8:P:23:DA:N6	2.41	0.53
6:N:119:ARG:HG3	6:N:120:GLY:H	1.72	0.53
1:A:79:ILE:HA	1:A:82:LEU:HD12	1.90	0.53
3:D:407:VAL:HG22	3:D:409:VAL:H	1.73	0.53
2:I:142:ARG:HG3	2:I:331:ARG:HG2	1.89	0.53
3:J:211:VAL:HG12	3:J:345:TYR:HB2	1.89	0.53
3:J:351:MET:HE2	3:J:368:VAL:HG12	1.90	0.53
3:J:1256:LEU:O	3:J:1260:ILE:HG13	2.08	0.53
3:J:1274:ILE:HD11	3:J:1334:GLN:HG2	1.90	0.53
2:C:1017:THR:HG21	3:D:617:ASN:ND2	2.24	0.53
2:C:1035:MET:HG3	3:D:707:THR:HB	1.90	0.53
5:F:110:THR:HG23	5:F:113:GLU:H	1.74	0.53
2:I:124:ASP:HA	2:I:592:LEU:HD12	1.90	0.53
2:I:988:VAL:HG22	3:J:948:THR:OG1	2.09	0.53
5:L:302:SER:O	5:L:306:ILE:HG22	2.07	0.53
2:C:259:GLY:HA2	2:C:263:ASP:HB2	1.90	0.53
2:C:1037:VAL:O	2:C:1041:GLU:HG3	2.07	0.53
3:D:223:LEU:HB2	3:D:251:PHE:HZ	1.74	0.53
2:I:742:ILE:HD12	2:I:803:ARG:HD2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:357:GLU:HG2	3:J:387:LEU:HB2	1.91	0.53
2:C:47:ALA:HA	2:C:345:ARG:HG2	1.90	0.53
2:C:668:LEU:HB2	2:C:993:PHE:HZ	1.73	0.53
3:D:231:VAL:HB	3:D:243:ALA:H	1.73	0.53
3:D:371:ILE:HG23	3:D:372:ASP:H	1.73	0.53
2:I:502:PRO:HG3	2:I:510:THR:HG22	1.89	0.53
2:I:552:HIS:HB3	2:I:882:LEU:HB2	1.91	0.53
2:I:668:LEU:HB2	2:I:993:PHE:HZ	1.74	0.53
2:I:969:LEU:HG	3:J:952:ASP:HB2	1.90	0.53
1:A:221:HIS:HA	1:A:224:TYR:CD1	2.43	0.53
1:B:78:ILE:HA	1:B:81:ASN:HD22	1.72	0.53
2:C:878:SER:HB3	3:D:1029:ARG:HG3	1.91	0.53
3:D:801:GLY:HA2	3:D:821:VAL:HA	1.90	0.53
3:D:1269:LYS:HD3	3:D:1269:LYS:H	1.74	0.53
5:F:210:VAL:HG11	5:F:232:ASN:HA	1.91	0.53
1:G:58:ILE:HG22	1:G:60:ASP:H	1.74	0.53
2:I:1037:VAL:O	2:I:1041:GLU:HG3	2.09	0.53
3:J:638:LYS:HG2	3:J:639:LEU:H	1.72	0.53
3:J:1209:LEU:O	3:J:1212:ALA:N	2.37	0.53
3:D:101:HIS:HB3	3:D:104:PHE:CE2	2.44	0.53
2:I:374:ASN:ND2	2:I:375:SER:H	2.07	0.53
2:I:577:PRO:HG2	2:I:580:MET:HB3	1.90	0.53
2:I:607:ASP:OD2	2:I:610:ARG:NH1	2.41	0.53
3:J:421:LEU:HD21	3:J:444:VAL:HG11	1.90	0.53
1:B:68:ILE:HG23	1:B:71:VAL:HB	1.91	0.53
1:B:118:ALA:O	1:B:120:VAL:N	2.42	0.53
2:C:388:ARG:NH2	8:P:20:DA:O5'	2.42	0.53
2:C:552:HIS:HB3	2:C:882:LEU:HB2	1.90	0.53
2:C:859:PRO:HA	2:C:975:TYR:O	2.09	0.53
2:C:936:VAL:HB	2:C:941:LYS:HE2	1.91	0.53
3:D:881:LEU:O	3:D:885:ILE:HG13	2.09	0.53
2:I:374:ASN:ND2	5:L:291:ARG:HE	2.00	0.53
2:I:878:SER:HB3	3:J:1029:ARG:HG3	1.90	0.53
8:S:17:DG:H2''	8:S:18:DG:O4'	2.08	0.53
2:C:142:ARG:HG3	2:C:331:ARG:HG2	1.90	0.53
2:C:502:PRO:HG3	2:C:510:THR:HG22	1.90	0.53
2:C:684:PHE:HE1	3:D:783:ARG:HB2	1.74	0.53
3:D:313:LEU:HG	3:D:314:PRO:HD2	1.91	0.53
2:I:352:ALA:HB1	2:I:356:ARG:NH1	2.23	0.53
2:I:971:LYS:HA	2:I:988:VAL:HA	1.91	0.53
3:J:49:ILE:HG13	3:J:50:PHE:H	1.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:99:ALA:HB2	3:J:574:LEU:HD21	1.91	0.53
3:J:577:ALA:O	3:J:581:VAL:HG23	2.09	0.53
3:J:810:GLU:HA	3:J:813:LEU:HD12	1.90	0.53
6:N:80:MET:HB3	6:N:107:GLN:HG2	1.90	0.53
2:C:23:VAL:HA	2:C:121:MET:SD	2.49	0.52
2:C:988:VAL:HG22	3:D:948:THR:OG1	2.08	0.52
2:C:988:VAL:HG21	3:D:949:ILE:O	2.09	0.52
3:D:49:ILE:HG13	3:D:50:PHE:H	1.73	0.52
3:D:704:ARG:NE	3:D:705:ALA:O	2.42	0.52
3:D:1145:TYR:O	3:D:1364:HIS:NE2	2.37	0.52
2:I:204:GLN:HB2	2:I:227:LEU:HD21	1.92	0.52
2:I:577:PRO:HA	2:I:671:ASN:HD21	1.74	0.52
2:I:1013:TYR:O	5:L:350:ASP:N	2.42	0.52
3:J:801:GLY:HA2	3:J:821:VAL:HA	1.90	0.52
3:J:1145:TYR:O	3:J:1364:HIS:NE2	2.37	0.52
6:N:20:VAL:CA	6:N:38:VAL:HA	2.35	0.52
8:S:22:DT:H2"	8:S:23:DA:C8	2.44	0.52
2:C:577:PRO:HG2	2:C:580:MET:HB3	1.90	0.52
3:D:99:ALA:HB2	3:D:574:LEU:HD21	1.92	0.52
3:D:1060:SER:OG	3:D:1061:PHE:N	2.42	0.52
2:I:87:ASP:HA	2:I:131:GLY:HA3	1.92	0.52
3:J:180:LYS:HA	3:J:205:TYR:CZ	2.45	0.52
5:L:398:LEU:HD21	5:L:413:ARG:HB2	1.91	0.52
8:P:8:DT:H1'	8:P:9:DG:H5"	1.89	0.52
2:C:742:ILE:HD12	2:C:803:ARG:HD2	1.91	0.52
1:H:118:ALA:O	1:H:120:VAL:N	2.43	0.52
3:J:29:PRO:HB3	3:J:548:ILE:HB	1.92	0.52
1:A:104:GLU:HG3	1:A:137:LYS:HG2	1.91	0.52
2:I:457:ALA:HB3	2:I:538:GLN:HA	1.92	0.52
2:I:644:ARG:HG2	2:I:647:GLN:HG2	1.92	0.52
2:I:988:VAL:H	3:J:948:THR:HG21	1.73	0.52
3:J:699:VAL:HG22	3:J:760:ARG:HG2	1.92	0.52
3:J:1060:SER:OG	3:J:1061:PHE:N	2.42	0.52
3:J:1273:VAL:HG21	3:J:1305:LEU:HD22	1.91	0.52
2:C:374:ASN:HD22	2:C:375:SER:H	1.58	0.52
2:C:457:ALA:HB3	2:C:538:GLN:HA	1.92	0.52
2:C:694:LEU:O	2:C:698:ASP:N	2.42	0.52
2:C:971:LYS:HA	2:C:988:VAL:HA	1.91	0.52
3:D:10:ILE:HG23	3:D:1451:ALA:HA	1.92	0.52
3:D:577:ALA:O	3:D:581:VAL:HG23	2.09	0.52
5:L:210:VAL:HG11	5:L:232:ASN:HA	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:M:68:VAL:HG21	6:M:144:LEU:HD21	1.92	0.52
1:G:79:ILE:HA	1:G:82:LEU:HD12	1.92	0.52
1:G:104:GLU:HG3	1:G:137:LYS:HG2	1.90	0.52
1:H:68:ILE:HG23	1:H:71:VAL:HB	1.91	0.52
2:I:283:VAL:HG11	2:I:305:PRO:HG3	1.92	0.52
2:I:988:VAL:HG21	3:J:949:ILE:O	2.10	0.52
3:J:367:ILE:HD11	3:J:379:ALA:HB2	1.92	0.52
3:J:1269:LYS:HD3	3:J:1269:LYS:H	1.75	0.52
3:D:27:GLU:H	3:D:42:ASP:HB3	1.75	0.52
3:D:650:LEU:HD12	3:D:688:TRP:HZ3	1.74	0.52
5:F:398:LEU:HD21	5:F:413:ARG:HB2	1.90	0.52
2:C:352:ALA:HB1	2:C:356:ARG:NH1	2.24	0.52
3:D:104:PHE:CG	3:D:512:MET:HE2	2.45	0.52
3:D:977:ALA:HB2	3:J:831:GLY:CA	2.39	0.52
5:F:285:LYS:O	5:F:288:ARG:HB3	2.10	0.52
5:F:385:LYS:HA	5:F:390:LEU:HD12	1.91	0.52
2:I:332:ARG:HB2	2:I:465:GLY:HA3	1.91	0.52
3:J:1048:PRO:HD3	3:J:1075:HIS:HB3	1.90	0.52
3:J:1436:SER:O	3:J:1439:SER:OG	2.23	0.52
5:L:411:ARG:HD3	7:R:1:DC:C6	2.45	0.52
7:O:46:DT:H2"	7:O:47:DG:C8	2.44	0.52
3:D:1021:TYR:O	3:D:1025:GLN:HB2	2.10	0.52
1:G:16:GLN:HB3	1:G:20:TYR:O	2.10	0.52
1:G:42:ARG:NH1	2:I:978:ARG:HA	2.25	0.52
2:I:431:HIS:H	2:I:434:HIS:CE1	2.28	0.52
2:I:448:ASN:HA	2:I:451:LEU:HD23	1.92	0.52
2:I:694:LEU:O	2:I:698:ASP:N	2.43	0.52
2:C:292:ARG:H	2:C:292:ARG:NH1	2.04	0.52
2:C:448:ASN:HA	2:C:451:LEU:HD23	1.92	0.52
3:D:86:ARG:O	3:D:521:PRO:HB3	2.10	0.52
3:D:1426:LYS:HE3	7:O:43:DG:H5"	1.91	0.52
2:I:859:PRO:HA	2:I:975:TYR:O	2.09	0.52
2:I:974:LEU:HD13	2:I:987:ILE:HB	1.92	0.52
1:A:35:THR:HG22	1:B:39:PRO:HA	1.92	0.51
2:C:204:GLN:HB2	2:C:227:LEU:HD21	1.92	0.51
2:C:966:LEU:HD21	2:C:986:PRO:HB3	1.92	0.51
3:D:699:VAL:HG22	3:D:760:ARG:HG2	1.92	0.51
3:J:96:ALA:HB2	3:J:555:LYS:HG2	1.92	0.51
3:J:104:PHE:CG	3:J:512:MET:HE2	2.45	0.51
8:S:34:DA:H1'	8:S:35:DA:H5'	1.92	0.51
1:B:161:ARG:HG2	1:B:162:ILE:H	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:27:LYS:HA	2:C:30:LEU:HD22	1.92	0.51
2:C:644:ARG:HG2	2:C:647:GLN:HG2	1.92	0.51
3:D:1273:VAL:HG21	3:D:1305:LEU:HD22	1.91	0.51
5:F:130:LYS:HD3	5:F:188:TYR:CZ	2.45	0.51
2:I:376:ARG:HD2	5:L:291:ARG:CZ	2.40	0.51
3:J:1147:ARG:HH12	3:J:1190:SER:HA	1.74	0.51
5:L:336:ILE:HB	8:S:17:DG:H21	1.75	0.51
3:D:96:ALA:HB2	3:D:555:LYS:HG2	1.93	0.51
4:E:26:ARG:HH22	4:E:37:ASN:HB2	1.76	0.51
1:G:9:PRO:HB2	1:G:25:LEU:HD21	1.91	0.51
3:J:27:GLU:H	3:J:42:ASP:HB3	1.75	0.51
3:J:650:LEU:HD12	3:J:688:TRP:HZ3	1.76	0.51
4:K:26:ARG:HH22	4:K:37:ASN:HB2	1.76	0.51
5:L:130:LYS:HD3	5:L:188:TYR:CZ	2.45	0.51
6:N:62:ALA:HB1	6:N:142:GLN:HE22	1.75	0.51
3:D:260:GLU:HA	3:D:294:GLU:HG3	1.92	0.51
2:I:65:VAL:HG13	2:I:101:ILE:HB	1.92	0.51
2:I:557:ARG:O	2:I:844:GLY:HA3	2.10	0.51
2:I:684:PHE:HE1	3:J:783:ARG:HB2	1.76	0.51
3:J:175:VAL:HG11	3:J:193:PRO:HG3	1.92	0.51
3:J:640:HIS:O	3:J:717:GLN:HB2	2.09	0.51
3:J:1458:GLU:HB2	3:J:1460:ILE:HG23	1.92	0.51
5:L:206:ASN:HB3	5:L:235:LEU:HD11	1.92	0.51
1:A:42:ARG:NH1	2:C:978:ARG:HA	2.26	0.51
2:C:937:ASP:HB3	2:C:940:GLU:HG3	1.92	0.51
3:D:675:ARG:HH22	5:F:437:LEU:HG	1.76	0.51
5:F:186:LYS:O	5:F:189:LEU:HB3	2.10	0.51
5:F:387:ARG:HD3	5:F:398:LEU:HD12	1.93	0.51
2:I:64:LEU:HB3	2:I:359:MET:HE3	1.93	0.51
3:J:628:ARG:NH1	8:S:14:DG:H2"	2.26	0.51
3:J:1021:TYR:O	3:J:1025:GLN:HB2	2.11	0.51
5:L:285:LYS:O	5:L:288:ARG:HB3	2.10	0.51
5:L:387:ARG:HD3	5:L:398:LEU:HD12	1.93	0.51
6:M:62:ALA:HB1	6:M:142:GLN:HE22	1.76	0.51
1:A:218:LEU:HB3	1:B:222:LEU:HD21	1.93	0.51
1:B:153:ALA:HA	1:B:156:HIS:CE1	2.46	0.51
2:C:172:ILE:HG23	2:C:184:MET:HE3	1.93	0.51
2:C:332:ARG:HB2	2:C:465:GLY:HA3	1.93	0.51
3:D:465:LEU:HD22	3:D:509:PRO:HB2	1.93	0.51
3:D:592:THR:HG22	3:D:599:PRO:HA	1.93	0.51
5:L:110:THR:HG23	5:L:113:GLU:H	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:N:37:GLN:HA	6:N:47:ALA:O	2.10	0.51
1:A:16:GLN:HB3	1:A:20:TYR:O	2.10	0.51
1:A:32:PHE:O	1:A:36:LEU:HG	2.11	0.51
1:B:184:THR:OG1	1:B:185:ARG:N	2.44	0.51
2:C:65:VAL:HG13	2:C:101:ILE:HB	1.92	0.51
2:C:124:ASP:HA	2:C:592:LEU:HD12	1.92	0.51
3:D:493:ARG:HD3	3:D:1392:GLY:O	2.11	0.51
4:E:40:LEU:HD21	4:E:67:GLU:HA	1.93	0.51
5:F:413:ARG:HD2	8:P:44:DT:H72	1.92	0.51
1:H:48:ILE:HA	1:H:213:GLN:HE22	1.76	0.51
3:J:137:PRO:HA	3:J:452:ILE:HG13	1.92	0.51
2:C:577:PRO:HA	2:C:671:ASN:HD21	1.75	0.51
3:D:67:ARG:HD2	5:F:394:ARG:HD3	1.92	0.51
3:D:699:VAL:HG12	3:D:717:GLN:HG2	1.92	0.51
1:G:63:HIS:HE2	2:I:801:VAL:HG13	1.76	0.51
3:J:367:ILE:HG22	3:J:368:VAL:HG23	1.91	0.51
7:O:46:DT:H3	8:P:3:DA:H61	1.58	0.51
1:B:177:VAL:HG12	1:B:197:LEU:HD11	1.92	0.51
2:C:471:TYR:N	2:C:484:VAL:O	2.37	0.51
2:C:974:LEU:HD13	2:C:987:ILE:HB	1.92	0.51
3:D:680:GLN:O	3:D:682:ASP:N	2.31	0.51
3:D:1442:ASN:N	8:P:9:DG:OP1	2.42	0.51
5:F:199:ARG:O	5:F:203:ILE:HG13	2.11	0.51
2:I:292:ARG:H	2:I:292:ARG:NH1	2.04	0.51
2:I:966:LEU:HD21	2:I:986:PRO:HB3	1.92	0.51
3:J:1472:ILE:HD12	3:J:1473:PRO:HD2	1.92	0.51
6:M:20:VAL:CA	6:M:38:VAL:HA	2.36	0.51
3:D:750:PRO:HG2	3:D:756:GLN:NE2	2.26	0.51
3:D:1274:ILE:HD11	3:D:1334:GLN:HG2	1.92	0.51
1:G:218:LEU:HB3	1:H:222:LEU:HD21	1.93	0.51
1:H:153:ALA:HA	1:H:156:HIS:CE1	2.46	0.51
3:J:1003:VAL:O	3:J:1007:VAL:HG23	2.11	0.51
5:L:385:LYS:HA	5:L:390:LEU:HD12	1.93	0.51
1:B:198:ARG:NH1	3:D:937:TYR:OH	2.42	0.50
2:C:431:HIS:H	2:C:434:HIS:CE1	2.28	0.50
3:D:137:PRO:HA	3:D:452:ILE:HG13	1.92	0.50
3:D:188:GLY:HA2	3:D:196:VAL:HG23	1.93	0.50
2:I:1032:PHE:HZ	2:I:1040:LEU:HD13	1.76	0.50
3:J:592:THR:HG22	3:J:599:PRO:HA	1.92	0.50
3:J:900:ILE:HB	3:J:902:MET:HE3	1.94	0.50
3:J:1194:CYS:SG	3:J:1196:THR:OG1	2.69	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:1279:GLY:H	3:J:1319:VAL:HG23	1.75	0.50
5:L:214:ALA:HB3	5:L:228:ILE:HG13	1.91	0.50
1:G:232:LEU:HD23	1:H:16:GLN:HG3	1.93	0.50
2:I:27:LYS:HA	2:I:30:LEU:HD22	1.93	0.50
2:I:50:GLU:HA	2:I:265:LYS:HZ1	1.77	0.50
3:J:121:THR:HA	3:J:124:GLU:HB3	1.93	0.50
3:J:636:GLN:HG2	3:J:637:LEU:HD12	1.93	0.50
3:J:699:VAL:HG12	3:J:717:GLN:HG2	1.92	0.50
3:J:1042:ARG:HB3	3:J:1057:VAL:HG21	1.93	0.50
1:A:151:VAL:HG22	1:A:156:HIS:HD2	1.77	0.50
2:C:688:ILE:HG22	2:C:689:VAL:H	1.76	0.50
3:D:272:LEU:O	3:D:279:VAL:N	2.42	0.50
3:D:636:GLN:HG2	3:D:637:LEU:HD12	1.94	0.50
3:D:1003:VAL:O	3:D:1007:VAL:HG23	2.11	0.50
2:I:18:LEU:HD12	2:I:408:ARG:NE	2.26	0.50
2:I:758:ARG:HB3	2:I:788:THR:HB	1.93	0.50
1:A:232:LEU:HD23	1:B:16:GLN:HG3	1.92	0.50
3:D:1042:ARG:HB3	3:D:1057:VAL:HG21	1.94	0.50
3:J:420:VAL:HG21	3:J:425:GLY:HA2	1.94	0.50
3:J:634:GLY:O	3:J:637:LEU:N	2.41	0.50
2:C:758:ARG:HB3	2:C:788:THR:HB	1.93	0.50
3:D:121:THR:HA	3:D:124:GLU:HB3	1.94	0.50
3:D:791:TYR:CD1	3:D:947:ILE:HD11	2.46	0.50
1:G:32:PHE:O	1:G:36:LEU:HG	2.12	0.50
1:H:184:THR:OG1	1:H:185:ARG:N	2.44	0.50
1:A:39:PRO:HG3	1:B:39:PRO:HG3	1.93	0.50
1:A:218:LEU:HD23	1:B:222:LEU:HD21	1.94	0.50
2:C:18:LEU:HD12	2:C:408:ARG:NE	2.26	0.50
2:C:690:ILE:HG22	2:C:691:SER:H	1.76	0.50
2:C:1082:PRO:HG3	3:D:1469:GLY:HA3	1.94	0.50
3:D:537:THR:O	5:F:332:LEU:N	2.43	0.50
3:D:628:ARG:HB2	3:D:745:MET:O	2.12	0.50
3:D:645:PRO:HB2	3:D:648:MET:HB3	1.93	0.50
3:D:1279:GLY:H	3:D:1319:VAL:HG23	1.76	0.50
5:F:206:ASN:HB3	5:F:235:LEU:HD11	1.92	0.50
2:I:110:GLU:O	6:N:45:SER:HB2	2.12	0.50
2:I:743:VAL:HG11	2:I:755:LEU:HD22	1.94	0.50
2:I:937:ASP:HB3	2:I:940:GLU:HG3	1.92	0.50
3:J:10:ILE:HG23	3:J:1451:ALA:HA	1.94	0.50
3:J:660:LYS:HD3	3:J:693:GLU:HB3	1.93	0.50
3:J:1100:ASP:CG	3:J:1440:PHE:HB2	2.37	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:319:VAL:O	5:L:323:LEU:HB2	2.11	0.50
7:O:34:DA:H2''	7:O:35:DG:O4'	2.12	0.50
1:B:48:ILE:HA	1:B:213:GLN:HE22	1.76	0.50
2:C:714:ASP:OD1	2:C:820:ARG:HB2	2.12	0.50
2:C:1032:PHE:HZ	2:C:1040:LEU:HD13	1.76	0.50
3:D:714:GLN:HB2	3:D:736:PHE:HZ	1.76	0.50
1:G:68:ILE:HG21	1:G:138:LEU:HD13	1.93	0.50
2:I:162:ILE:HB	2:I:172:ILE:HB	1.94	0.50
2:I:568:ALA:HB1	2:I:995:MET:HE2	1.93	0.50
3:J:1037:GLN:HB3	3:J:1042:ARG:HG3	1.93	0.50
3:J:1201:CYS:SG	3:J:1204:CYS:N	2.84	0.50
4:K:40:LEU:HD21	4:K:67:GLU:HA	1.93	0.50
1:A:63:HIS:CE1	1:A:65:PHE:HB2	2.47	0.50
1:A:68:ILE:HG21	1:A:138:LEU:HD13	1.93	0.50
1:B:185:ARG:NH1	1:B:187:GLY:O	2.45	0.50
3:D:413:ASP:O	3:D:435:VAL:HG22	2.11	0.50
1:H:80:LEU:HD11	3:J:842:VAL:HG12	1.94	0.50
2:I:1060:ILE:HG23	2:I:1083:GLU:HB2	1.93	0.50
3:J:87:ARG:HG2	3:J:523:ASP:HB3	1.94	0.50
3:J:750:PRO:HG2	3:J:756:GLN:NE2	2.26	0.50
1:B:80:LEU:HD11	3:D:842:VAL:HG12	1.93	0.50
2:C:64:LEU:HB3	2:C:359:MET:HE3	1.94	0.50
3:D:900:ILE:HB	3:D:902:MET:HE3	1.94	0.50
3:D:1018:ASN:HB3	3:D:1021:TYR:HB3	1.94	0.50
5:F:206:ASN:O	5:F:210:VAL:HG23	2.12	0.50
2:I:172:ILE:HG23	2:I:184:MET:HE3	1.92	0.50
2:I:766:GLU:OE2	3:J:64:LYS:HB3	2.12	0.50
3:J:137:PRO:HG3	3:J:148:GLU:HA	1.93	0.50
3:J:1285:GLU:HB3	3:J:1290:LEU:HG	1.94	0.50
6:N:12:LEU:HD13	6:N:59:LEU:HD13	1.93	0.50
6:N:12:LEU:HB3	6:N:40:PHE:HE1	1.76	0.50
2:C:841:ASN:HD21	2:C:845:ASN:HB3	1.77	0.49
3:D:137:PRO:HG3	3:D:148:GLU:HA	1.93	0.49
3:D:1037:GLN:HB3	3:D:1042:ARG:HG3	1.93	0.49
2:I:750:LYS:HD3	3:J:681:ARG:HG3	1.93	0.49
3:J:465:LEU:HD22	3:J:509:PRO:HB2	1.92	0.49
3:J:1462:LEU:HD12	3:J:1463:LYS:N	2.26	0.49
1:A:101:LEU:HB3	1:A:140:MET:HB3	1.94	0.49
2:C:1031:ARG:HB3	3:D:622:ARG:HD3	1.93	0.49
3:D:1462:LEU:HD12	3:D:1463:LYS:N	2.26	0.49
1:G:151:VAL:HG22	1:G:156:HIS:HD2	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:198:ARG:NH1	3:J:937:TYR:OH	2.41	0.49
2:I:167:LYS:HD3	7:R:35:DG:C5'	2.42	0.49
2:I:369:PRO:HA	2:I:372:LEU:HB3	1.94	0.49
3:J:789:LEU:O	3:J:792:ILE:HG13	2.13	0.49
5:L:186:LYS:O	5:L:189:LEU:HB3	2.11	0.49
2:C:162:ILE:HB	2:C:172:ILE:HB	1.93	0.49
2:C:557:ARG:O	2:C:844:GLY:HA3	2.12	0.49
3:D:1094:LEU:HD21	3:D:1260:ILE:HG12	1.93	0.49
1:H:161:ARG:HG2	1:H:162:ILE:H	1.77	0.49
3:J:461:ILE:HG22	3:J:465:LEU:HD12	1.95	0.49
3:J:1099:VAL:HG22	3:J:1226:ALA:HB1	1.94	0.49
3:J:1264:GLU:HB3	3:J:1266:ARG:HG3	1.93	0.49
3:J:1448:THR:O	3:J:1452:ILE:HG12	2.12	0.49
6:N:18:GLY:HA3	6:N:40:PHE:HA	1.94	0.49
8:S:19:DT:OP1	8:S:19:DT:H4'	2.12	0.49
1:A:70:GLY:HA2	1:A:133:GLU:HG2	1.94	0.49
2:C:94:LEU:HD23	2:C:115:LEU:HD12	1.93	0.49
3:D:900:ILE:HG12	3:D:914:LEU:HD11	1.94	0.49
5:F:214:ALA:HB3	5:F:228:ILE:HG13	1.93	0.49
1:H:185:ARG:NH1	1:H:187:GLY:O	2.45	0.49
3:J:348:ALA:HB1	3:J:350:HIS:ND1	2.28	0.49
3:J:1094:LEU:HD21	3:J:1260:ILE:HG12	1.94	0.49
5:L:199:ARG:O	5:L:203:ILE:HG13	2.12	0.49
8:S:8:DT:H1'	8:S:9:DG:H5''	1.93	0.49
2:C:568:ALA:HB1	2:C:995:MET:HE2	1.93	0.49
2:C:1115:LEU:HD13	3:D:88:TYR:CG	2.48	0.49
1:G:39:PRO:HG3	1:H:39:PRO:HG3	1.93	0.49
1:G:63:HIS:CE1	1:G:65:PHE:HB2	2.47	0.49
1:G:218:LEU:HD23	1:H:222:LEU:HD21	1.93	0.49
1:H:177:VAL:HG12	1:H:197:LEU:HD11	1.94	0.49
6:M:101:ASN:HD22	6:M:104:ARG:H	1.57	0.49
1:A:88:ARG:HB2	1:A:204:SER:HA	1.94	0.49
2:C:170:PRO:HB3	7:O:36:DC:H42	1.76	0.49
2:C:610:ARG:HA	2:C:624:PRO:HA	1.94	0.49
2:C:743:VAL:HG11	2:C:755:LEU:HD22	1.94	0.49
2:C:874:LEU:O	2:C:877:PRO:HD2	2.12	0.49
3:D:562:ALA:HB3	3:D:567:ILE:HD11	1.94	0.49
5:F:319:VAL:O	5:F:323:LEU:HB2	2.12	0.49
1:H:78:ILE:O	1:H:82:LEU:HG	2.12	0.49
2:I:217:LEU:HD13	2:I:311:PHE:CD2	2.43	0.49
2:I:231:PRO:O	2:I:235:MET:HB2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1075:ASP:OD1	4:K:28:GLN:NE2	2.45	0.49
3:J:16:GLU:H	3:J:16:GLU:CD	2.19	0.49
3:J:791:TYR:CD1	3:J:947:ILE:HD11	2.47	0.49
5:L:254:ALA:O	5:L:258:ILE:HG12	2.13	0.49
1:A:90:LEU:HB2	1:A:119:ASP:HA	1.94	0.49
2:C:387:SER:HB2	2:C:388:ARG:HH11	1.77	0.49
3:D:16:GLU:H	3:D:16:GLU:CD	2.20	0.49
3:D:347:VAL:HG23	3:D:368:VAL:HG11	1.94	0.49
3:D:1099:VAL:HG22	3:D:1226:ALA:HB1	1.94	0.49
2:I:207:LEU:HD21	2:I:221:LEU:O	2.13	0.49
2:I:714:ASP:OD1	2:I:820:ARG:HB2	2.13	0.49
2:I:874:LEU:O	2:I:877:PRO:HD2	2.13	0.49
2:I:1053:LEU:HG	3:J:621:LYS:HD3	1.94	0.49
3:J:351:MET:HE1	3:J:377:VAL:HG23	1.95	0.49
5:L:224:PHE:HZ	7:R:33:DG:H5'	1.76	0.49
1:A:58:ILE:HG22	1:A:60:ASP:H	1.76	0.49
1:A:133:GLU:OE1	2:C:606:VAL:N	2.46	0.49
1:B:36:LEU:C	1:B:39:PRO:HD2	2.37	0.49
3:D:264:LEU:HD23	3:D:317:MET:HE2	1.93	0.49
5:F:224:PHE:HE1	7:O:32:DG:H21	1.59	0.49
5:F:235:LEU:O	5:F:239:VAL:HG23	2.13	0.49
1:G:70:GLY:HA2	1:G:133:GLU:HG2	1.94	0.49
1:G:101:LEU:HB3	1:G:140:MET:HB3	1.94	0.49
2:I:437:ARG:HA	2:I:459:ALA:HB2	1.95	0.49
2:I:688:ILE:HG22	2:I:689:VAL:H	1.77	0.49
3:J:351:MET:HE3	3:J:370:ALA:HB2	1.95	0.49
3:J:907:GLU:O	3:J:911:LEU:HG	2.13	0.49
3:J:1225:ALA:HB2	3:J:1370:ILE:HD12	1.94	0.49
5:L:280:VAL:HA	5:L:283:ILE:HD12	1.95	0.49
2:C:369:PRO:HA	2:C:372:LEU:HB3	1.94	0.49
2:C:684:PHE:CE1	3:D:783:ARG:HB2	2.47	0.49
3:D:489:ARG:HD3	3:D:1391:GLU:OE2	2.12	0.49
3:D:660:LYS:HD3	3:D:693:GLU:HB3	1.93	0.49
3:D:761:ILE:HD13	4:E:20:THR:HA	1.95	0.49
3:D:1225:ALA:HB2	3:D:1370:ILE:HD12	1.95	0.49
2:I:387:SER:HB2	2:I:388:ARG:HH11	1.77	0.49
2:I:690:ILE:HG22	2:I:691:SER:H	1.77	0.49
2:I:742:ILE:HG22	2:I:756:VAL:HG13	1.95	0.49
3:J:628:ARG:HB2	3:J:745:MET:O	2.12	0.49
3:J:761:ILE:HD13	4:K:20:THR:HA	1.94	0.49
3:J:1011:PHE:CD1	3:J:1021:TYR:HB2	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:434:HIS:CD2	2:C:438:ILE:HD13	2.48	0.49
2:C:437:ARG:HA	2:C:459:ALA:HB2	1.95	0.49
2:C:1060:ILE:HG23	2:C:1083:GLU:HB2	1.94	0.49
3:D:671:LYS:HG3	5:F:436:PHE:CE2	2.47	0.49
1:G:57:TYR:HD1	1:G:163:ASN:O	1.96	0.49
1:G:133:GLU:OE1	2:I:606:VAL:N	2.46	0.49
2:I:166:PRO:C	2:I:168:ARG:H	2.21	0.49
2:I:610:ARG:HA	2:I:624:PRO:HA	1.94	0.49
3:J:129:PHE:O	3:J:572:ARG:NH2	2.46	0.49
2:C:995:MET:HE3	2:C:996:LYS:O	2.13	0.48
3:D:130:ASN:HD22	5:F:98:GLN:NE2	2.04	0.48
3:D:423:ASP:HB2	3:D:427:VAL:HG12	1.93	0.48
3:D:1495:ILE:HD12	4:E:85:LEU:HA	1.94	0.48
2:I:135:VAL:HG21	2:I:407:LYS:HG2	1.95	0.48
3:J:645:PRO:HB2	3:J:648:MET:HB3	1.94	0.48
3:J:1018:ASN:HB3	3:J:1021:TYR:HB3	1.93	0.48
4:K:61:VAL:O	4:K:65:MET:HG2	2.12	0.48
6:M:34:ALA:HB3	6:M:51:VAL:HG21	1.94	0.48
1:A:9:PRO:HB2	1:A:25:LEU:HD21	1.94	0.48
1:B:78:ILE:O	1:B:82:LEU:HG	2.12	0.48
2:C:231:PRO:O	2:C:235:MET:HB2	2.13	0.48
3:D:129:PHE:O	3:D:572:ARG:NH2	2.46	0.48
3:D:706:PRO:HG3	8:P:11:DG:N2	2.27	0.48
3:D:789:LEU:O	3:D:792:ILE:HG13	2.13	0.48
4:E:61:VAL:O	4:E:65:MET:HG2	2.11	0.48
1:G:218:LEU:HG	1:H:222:LEU:HD11	1.95	0.48
2:I:434:HIS:CD2	2:I:438:ILE:HD13	2.48	0.48
2:I:471:TYR:N	2:I:484:VAL:O	2.37	0.48
3:J:1495:ILE:HD12	4:K:85:LEU:HA	1.94	0.48
4:K:26:ARG:HH12	4:K:37:ASN:HD22	1.60	0.48
1:A:72:LYS:HG3	2:C:606:VAL:HG11	1.96	0.48
2:C:166:PRO:C	2:C:168:ARG:H	2.22	0.48
2:C:571:LEU:HD23	2:C:668:LEU:O	2.14	0.48
5:F:280:VAL:HA	5:F:283:ILE:HD12	1.95	0.48
1:G:72:LYS:HG3	2:I:606:VAL:HG11	1.96	0.48
2:I:280:LYS:HD3	2:I:323:ASP:OD2	2.13	0.48
2:I:352:ALA:HB1	2:I:356:ARG:HH12	1.78	0.48
2:I:607:ASP:O	2:I:609:THR:N	2.47	0.48
2:I:1097:LEU:HB3	3:J:10:ILE:HD11	1.95	0.48
3:J:900:ILE:HG12	3:J:914:LEU:HD11	1.94	0.48
3:J:970:LYS:O	3:J:974:ILE:HG13	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:1462:LEU:O	3:J:1466:VAL:HG23	2.13	0.48
2:C:437:ARG:HH11	2:C:467:ILE:HG22	1.79	0.48
2:C:607:ASP:O	2:C:609:THR:N	2.46	0.48
3:D:203:ALA:HA	3:D:395:VAL:HA	1.95	0.48
3:D:238:PRO:HB3	3:D:315:ARG:O	2.13	0.48
3:D:1448:THR:O	3:D:1452:ILE:HG12	2.13	0.48
3:D:1462:LEU:O	3:D:1466:VAL:HG23	2.14	0.48
5:F:142:ILE:O	5:F:146:VAL:HG23	2.13	0.48
2:I:1115:LEU:HD13	3:J:88:TYR:CG	2.47	0.48
3:J:14:SER:HB3	3:J:511:TRP:CE2	2.49	0.48
3:J:357:GLU:HG2	3:J:387:LEU:CB	2.43	0.48
3:J:822:ALA:HB3	3:J:825:ALA:HB2	1.96	0.48
1:A:173:PRO:HB3	1:A:204:SER:HB2	1.96	0.48
1:A:176:ARG:HG3	1:A:200:TRP:CE3	2.49	0.48
2:C:110:GLU:O	6:M:45:SER:HB2	2.14	0.48
2:C:280:LYS:HD3	2:C:323:ASP:OD2	2.13	0.48
2:C:397:GLU:HB3	2:C:631:SER:HB2	1.94	0.48
2:C:742:ILE:HG22	2:C:756:VAL:HG13	1.96	0.48
3:D:699:VAL:HB	3:D:716:PHE:O	2.13	0.48
3:D:1285:GLU:HB3	3:D:1290:LEU:HG	1.94	0.48
3:D:1433:SER:HB3	3:D:1464:GLU:CD	2.39	0.48
3:D:1440:PHE:CE1	3:D:1441:GLN:HG2	2.49	0.48
3:D:1487:VAL:HG21	3:D:1492:LEU:HD23	1.95	0.48
2:I:94:LEU:HD23	2:I:115:LEU:HD12	1.94	0.48
2:I:397:GLU:HB3	2:I:631:SER:HB2	1.95	0.48
2:I:706:GLU:HB3	2:I:708:TYR:HE1	1.78	0.48
3:J:1442:ASN:N	8:S:9:DG:OP1	2.45	0.48
5:L:235:LEU:O	5:L:239:VAL:HG23	2.13	0.48
2:C:683:ASN:C	2:C:687:ALA:HB3	2.39	0.48
3:D:253:ALA:HB2	3:D:304:LEU:HG	1.95	0.48
3:D:255:GLU:OE2	3:D:256:SER:N	2.45	0.48
3:D:761:ILE:O	3:D:767:HIS:ND1	2.47	0.48
3:D:1201:CYS:SG	3:D:1204:CYS:N	2.85	0.48
3:D:1476:THR:HA	4:E:17:TYR:HB3	1.95	0.48
4:E:39:VAL:HB	4:E:72:ARG:HD2	1.95	0.48
2:I:684:PHE:CE1	3:J:783:ARG:HB2	2.48	0.48
3:J:714:GLN:HB3	3:J:765:SER:HB3	1.96	0.48
3:J:714:GLN:HB2	3:J:736:PHE:HZ	1.78	0.48
3:D:714:GLN:HB3	3:D:765:SER:HB3	1.96	0.48
3:D:764:LEU:HB3	3:D:767:HIS:CD2	2.49	0.48
3:D:1127:GLU:C	3:D:1129:THR:H	2.22	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:199:ARG:HE	5:F:200:GLN:NE2	2.12	0.48
2:I:706:GLU:HB3	2:I:708:TYR:CE1	2.49	0.48
2:I:1035:MET:HA	2:I:1038:TRP:CE3	2.49	0.48
2:I:1094:ALA:HB2	3:J:520:LEU:HD13	1.96	0.48
6:N:91:ARG:NH1	7:R:27:DT:OP1	2.46	0.48
7:R:32:DG:H2'	7:R:33:DG:C8	2.48	0.48
2:C:706:GLU:HB3	2:C:708:TYR:HE1	1.79	0.48
3:D:907:GLU:O	3:D:911:LEU:HG	2.14	0.48
3:D:1095:THR:O	3:D:1099:VAL:HG23	2.14	0.48
1:G:173:PRO:HB3	1:G:204:SER:HB2	1.96	0.48
2:I:374:ASN:HD22	2:I:375:SER:H	1.61	0.48
2:I:857:ASP:OD1	2:I:857:ASP:N	2.42	0.48
2:I:995:MET:HE3	2:I:996:LYS:O	2.14	0.48
2:I:1008:ARG:NH2	2:I:1020:PRO:HB3	2.29	0.48
3:J:900:ILE:HA	3:J:914:LEU:HD21	1.96	0.48
3:J:1487:VAL:HG21	3:J:1492:LEU:HD23	1.94	0.48
8:P:34:DA:H1'	8:P:35:DA:H5'	1.96	0.48
1:B:156:HIS:O	1:B:156:HIS:ND1	2.47	0.48
2:C:658:GLY:H	2:C:661:SER:HB3	1.79	0.48
2:C:1035:MET:HA	2:C:1038:TRP:CE3	2.48	0.48
3:D:263:ASP:HB3	3:D:268:HIS:CD2	2.49	0.48
3:D:461:ILE:HG22	3:D:465:LEU:HD12	1.95	0.48
5:F:398:LEU:HD13	8:P:43:DG:OP2	2.13	0.48
1:G:88:ARG:HB2	1:G:204:SER:HA	1.94	0.48
2:I:299:LYS:HG3	2:I:300:ASP:H	1.79	0.48
4:K:39:VAL:HB	4:K:72:ARG:HD2	1.95	0.48
2:C:409:ARG:HG2	2:C:452:ILE:HG22	1.96	0.48
2:C:430:VAL:HG12	2:C:434:HIS:CD2	2.49	0.48
2:C:892:LEU:HD23	2:C:918:LEU:HD11	1.96	0.48
3:D:14:SER:HB3	3:D:511:TRP:CE2	2.49	0.48
3:D:87:ARG:HG2	3:D:523:ASP:HB3	1.94	0.48
2:I:658:GLY:H	2:I:661:SER:HB3	1.77	0.48
3:J:622:ARG:HH12	8:S:14:DG:H5'	1.79	0.48
3:J:1364:HIS:CE1	3:J:1366:LYS:HG3	2.48	0.48
7:O:14:DT:H1'	7:O:15:DT:H5''	1.96	0.48
2:C:430:VAL:HG12	2:C:434:HIS:HD2	1.79	0.47
3:D:900:ILE:HA	3:D:914:LEU:HD21	1.97	0.47
3:D:1341:PRO:O	3:D:1344:VAL:HB	2.14	0.47
3:D:1364:HIS:CE1	3:D:1366:LYS:HG3	2.49	0.47
1:G:90:LEU:HB2	1:G:119:ASP:HA	1.96	0.47
2:I:430:VAL:HG12	2:I:434:HIS:CD2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:63:TYR:HE2	3:J:73:CYS:HA	1.79	0.47
3:J:131:LYS:HG2	3:J:153:LEU:O	2.14	0.47
3:J:537:THR:C	5:L:332:LEU:HG	2.39	0.47
3:J:761:ILE:O	3:J:767:HIS:ND1	2.47	0.47
5:L:252:THR:HA	7:R:29:DC:H5	1.78	0.47
1:A:218:LEU:HG	1:B:222:LEU:HD11	1.96	0.47
1:B:186:LEU:HD22	4:E:51:LEU:HD22	1.96	0.47
2:C:49:LYS:NZ	2:C:50:GLU:HG3	2.29	0.47
2:C:726:ILE:HB	2:C:729:LEU:HB2	1.96	0.47
2:C:1053:LEU:HG	3:D:621:LYS:HD3	1.94	0.47
3:D:762:GLN:HB3	4:E:16:LYS:HE2	1.96	0.47
3:D:822:ALA:HB3	3:D:825:ALA:HB2	1.97	0.47
3:D:1144:LEU:HD21	3:D:1186:VAL:HG11	1.96	0.47
3:D:1264:GLU:HB3	3:D:1266:ARG:HG3	1.94	0.47
1:G:65:PHE:CE1	2:I:703:ILE:HG21	2.49	0.47
2:I:521:PRO:HG2	3:J:1055:VAL:HG21	1.96	0.47
2:I:892:LEU:HD23	2:I:918:LEU:HD11	1.95	0.47
2:I:1067:TYR:CE1	3:J:655:PRO:HG3	2.49	0.47
3:J:762:GLN:HB3	4:K:16:LYS:HE2	1.97	0.47
3:J:1476:THR:HA	4:K:17:TYR:HB3	1.96	0.47
5:L:137:LEU:HB3	5:L:141:LEU:HD23	1.96	0.47
5:L:206:ASN:O	5:L:210:VAL:HG23	2.13	0.47
1:A:26:GLU:HG3	1:A:186:LEU:HD12	1.96	0.47
2:C:508:ILE:HD11	2:C:529:VAL:HG11	1.96	0.47
2:C:1097:LEU:HB3	3:D:10:ILE:HD11	1.96	0.47
3:D:1097:LYS:HE2	3:D:1440:PHE:HZ	1.79	0.47
1:G:26:GLU:HG3	1:G:186:LEU:HD12	1.96	0.47
3:J:10:ILE:HB	3:J:1434:TRP:CH2	2.50	0.47
3:J:743:ASP:OD1	3:J:743:ASP:N	2.47	0.47
3:J:764:LEU:HB3	3:J:767:HIS:CD2	2.48	0.47
3:J:1127:GLU:C	3:J:1129:THR:H	2.22	0.47
4:K:65:MET:O	4:K:69:LEU:HG	2.13	0.47
5:L:119:ARG:HA	5:L:244:TYR:CE1	2.49	0.47
6:M:75:LEU:HD11	6:M:136:LEU:HD13	1.96	0.47
1:A:17:GLY:HA3	1:A:19:HIS:CE1	2.49	0.47
1:A:198:ARG:HD2	2:C:934:PHE:CE1	2.49	0.47
2:C:18:LEU:HD12	2:C:408:ARG:HE	1.80	0.47
3:D:585:GLY:HA2	3:D:590:PRO:HG3	1.96	0.47
3:D:646:LYS:HA	3:D:720:LEU:HD22	1.96	0.47
2:I:430:VAL:HG12	2:I:434:HIS:HD2	1.79	0.47
2:I:437:ARG:HH11	2:I:467:ILE:HG22	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:971:LYS:HD2	2:I:986:PRO:HG2	1.96	0.47
2:I:1031:ARG:HB3	3:J:622:ARG:HD3	1.95	0.47
3:J:165:LYS:H	3:J:397:LYS:HE2	1.79	0.47
5:L:271:ARG:HG2	5:L:328:GLU:HB3	1.96	0.47
1:A:57:TYR:HD1	1:A:163:ASN:O	1.97	0.47
2:C:352:ALA:HB1	2:C:356:ARG:HH12	1.79	0.47
2:C:706:GLU:HB3	2:C:708:TYR:CE1	2.49	0.47
4:E:26:ARG:HH12	4:E:37:ASN:HD22	1.61	0.47
2:I:140:ILE:HG12	2:I:141:HIS:N	2.30	0.47
2:I:185:LYS:HD3	2:I:190:LYS:HB3	1.96	0.47
2:I:817:PRO:HB3	5:L:323:LEU:HB3	1.96	0.47
3:J:140:ALA:HA	3:J:450:TYR:CD2	2.50	0.47
2:C:682:TYR:HA	3:D:633:VAL:HG11	1.95	0.47
3:D:131:LYS:HG2	3:D:153:LEU:O	2.15	0.47
3:D:141:VAL:HG12	3:D:450:TYR:HE2	1.80	0.47
3:D:639:LEU:HD22	3:D:766:ALA:HA	1.97	0.47
1:H:36:LEU:C	1:H:39:PRO:HD2	2.38	0.47
1:H:186:LEU:HD22	4:K:51:LEU:HD22	1.97	0.47
2:I:1112:PHE:HB3	2:I:1115:LEU:HB2	1.97	0.47
3:J:630:VAL:HG22	3:J:631:ILE:H	1.79	0.47
8:P:9:DG:H2''	8:P:10:DA:H5'	1.97	0.47
2:C:1026:GLN:HE21	2:C:1026:GLN:HB2	1.50	0.47
3:D:273:ARG:HB3	3:D:278:VAL:HG12	1.95	0.47
3:D:471:GLU:O	3:D:475:ARG:HG2	2.15	0.47
3:D:630:VAL:HG22	3:D:631:ILE:H	1.79	0.47
3:D:772:PRO:O	3:D:1209:LEU:HD12	2.14	0.47
5:F:137:LEU:HB3	5:F:141:LEU:HD23	1.97	0.47
5:F:368:GLU:HB3	5:F:433:LEU:HD21	1.97	0.47
1:H:52:ALA:HB3	1:H:145:ASP:O	2.15	0.47
2:I:18:LEU:HD12	2:I:408:ARG:HE	1.80	0.47
2:I:36:PRO:CB	2:I:70:GLU:HG2	2.45	0.47
2:I:163:ILE:HD12	2:I:164:PRO:HD2	1.96	0.47
2:I:424:GLY:H	2:I:427:VAL:CG2	2.28	0.47
2:I:508:ILE:HD11	2:I:529:VAL:HG11	1.96	0.47
2:I:683:ASN:C	2:I:687:ALA:HB3	2.40	0.47
3:J:367:ILE:HB	3:J:377:VAL:HB	1.97	0.47
3:J:1341:PRO:O	3:J:1344:VAL:HB	2.15	0.47
6:M:136:LEU:HB3	6:M:155:PHE:CZ	2.50	0.47
6:N:68:VAL:HG21	6:N:144:LEU:HD21	1.96	0.47
1:A:53:VAL:HA	1:A:144:VAL:HA	1.97	0.47
2:C:135:VAL:HG21	2:C:407:LYS:HG2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:398:THR:HA	2:C:635:THR:HG21	1.97	0.47
3:D:638:LYS:C	3:D:729:HIS:HD2	2.22	0.47
2:I:68:PHE:O	2:I:69:LEU:HD13	2.14	0.47
2:I:409:ARG:HG2	2:I:452:ILE:HG22	1.97	0.47
2:I:708:TYR:HE2	2:I:792:VAL:HG23	1.79	0.47
2:I:922:PHE:HB2	2:I:967:PHE:CD2	2.50	0.47
3:J:646:LYS:HA	3:J:720:LEU:HD22	1.96	0.47
3:J:1267:ARG:H	3:J:1267:ARG:NE	2.13	0.47
2:C:1112:PHE:HB3	2:C:1115:LEU:HB2	1.97	0.47
3:D:151:GLN:HG2	3:D:152:LEU:H	1.80	0.47
3:D:704:ARG:HB2	3:D:745:MET:HG2	1.97	0.47
3:D:1089:ALA:O	8:P:11:DG:H5'	2.15	0.47
1:G:176:ARG:HG3	1:G:200:TRP:CE3	2.50	0.47
1:G:198:ARG:HD2	2:I:934:PHE:CE1	2.49	0.47
1:H:30:ARG:HB3	1:H:191:ASP:O	2.15	0.47
1:H:156:HIS:ND1	1:H:156:HIS:O	2.48	0.47
3:J:167:GLU:OE2	3:J:198:ARG:NH2	2.48	0.47
3:J:699:VAL:HB	3:J:716:PHE:O	2.14	0.47
2:C:68:PHE:O	2:C:69:LEU:HD13	2.15	0.47
2:C:207:LEU:HD21	2:C:221:LEU:O	2.15	0.47
3:D:83:SER:O	3:D:86:ARG:HB2	2.15	0.47
3:D:970:LYS:O	3:D:974:ILE:HG13	2.15	0.47
2:I:101:ILE:HG12	2:I:108:ILE:HG23	1.95	0.47
2:I:549:PHE:HE1	2:I:909:ALA:HB3	1.80	0.47
2:I:726:ILE:HB	2:I:729:LEU:HB2	1.96	0.47
3:J:112:ILE:HD12	3:J:113:GLY:N	2.29	0.47
3:J:538:SER:HA	5:L:332:LEU:HB2	1.97	0.47
3:J:1364:HIS:CD2	3:J:1366:LYS:HE2	2.49	0.47
6:N:34:ALA:HB3	6:N:51:VAL:HG21	1.96	0.47
2:C:922:PHE:HB2	2:C:967:PHE:CD2	2.50	0.46
3:D:10:ILE:HB	3:D:1434:TRP:CH2	2.50	0.46
3:D:339:TRP:HE1	3:D:341:GLU:HG3	1.79	0.46
3:D:628:ARG:NH2	8:P:14:DG:H2''	2.30	0.46
3:D:881:LEU:HG	3:D:885:ILE:HD11	1.96	0.46
3:D:1364:HIS:CD2	3:D:1366:LYS:HE2	2.49	0.46
3:D:1436:SER:O	3:D:1439:SER:OG	2.24	0.46
5:F:276:PRO:O	5:F:280:VAL:HG23	2.15	0.46
5:F:342:SER:OG	8:P:17:DG:N2	2.48	0.46
5:F:386:LEU:HB3	5:F:396:HIS:HB2	1.98	0.46
1:G:94:MET:O	1:G:146:ARG:HD3	2.16	0.46
2:I:42:VAL:HG12	2:I:43:GLY:H	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:841:ASN:HD21	2:I:845:ASN:HB3	1.78	0.46
3:J:585:GLY:HA2	3:J:590:PRO:HG3	1.96	0.46
3:J:896:ALA:O	3:J:900:ILE:HG13	2.15	0.46
5:L:142:ILE:O	5:L:146:VAL:HG23	2.15	0.46
5:L:411:ARG:HD3	7:R:1:DC:H6	1.78	0.46
5:L:413:ARG:HE	8:S:44:DT:H2'	1.80	0.46
2:C:470:PRO:HG3	2:C:485:TYR:CZ	2.50	0.46
2:C:874:LEU:O	3:D:1029:ARG:HG2	2.15	0.46
2:C:893:ALA:HB2	2:C:918:LEU:HD22	1.97	0.46
2:C:1094:ALA:HB2	3:D:520:LEU:HD13	1.96	0.46
2:I:893:ALA:HB2	2:I:918:LEU:HD22	1.97	0.46
3:J:34:TYR:HD1	5:L:325:ILE:HG21	1.80	0.46
3:J:166:GLN:HE21	3:J:166:GLN:HB2	1.52	0.46
3:J:508:ARG:HB3	3:J:510:GLU:CD	2.40	0.46
3:J:657:LEU:HB2	3:J:691:LEU:HD13	1.97	0.46
3:J:1144:LEU:HD21	3:J:1186:VAL:HG11	1.98	0.46
3:J:1440:PHE:CE1	3:J:1441:GLN:HG2	2.50	0.46
5:L:187:ARG:O	5:L:191:ILE:HG13	2.15	0.46
2:C:971:LYS:HD2	2:C:986:PRO:HG2	1.97	0.46
3:D:34:TYR:HD1	5:F:325:ILE:HG21	1.80	0.46
3:D:63:TYR:HE2	3:D:73:CYS:HA	1.80	0.46
3:D:682:ASP:C	3:D:684:LYS:H	2.24	0.46
3:D:1042:ARG:HD3	3:D:1045:MET:CE	2.45	0.46
5:F:254:ALA:O	5:F:258:ILE:HG12	2.15	0.46
1:G:9:PRO:HG3	1:H:224:TYR:CZ	2.50	0.46
1:G:133:GLU:OE1	2:I:607:ASP:HB2	2.15	0.46
3:J:881:LEU:HG	3:J:885:ILE:HD11	1.96	0.46
2:C:101:ILE:HG12	2:C:108:ILE:HG23	1.97	0.46
2:C:140:ILE:HG12	2:C:141:HIS:N	2.30	0.46
2:C:163:ILE:HD12	2:C:164:PRO:HD2	1.97	0.46
2:C:708:TYR:HE2	2:C:792:VAL:HG23	1.80	0.46
2:C:882:LEU:HD21	3:D:1038:LEU:HD22	1.97	0.46
2:C:1008:ARG:NH2	2:C:1020:PRO:HB3	2.30	0.46
3:D:169:TYR:CZ	3:D:197:SER:HA	2.50	0.46
3:D:229:ALA:HA	3:D:244:GLU:HB2	1.97	0.46
3:D:259:VAL:HG23	3:D:294:GLU:HA	1.98	0.46
3:D:363:ALA:HA	3:D:381:ALA:O	2.16	0.46
3:D:671:LYS:H	5:F:364:LEU:HD11	1.81	0.46
1:H:78:ILE:HD12	1:H:130:ALA:HB2	1.97	0.46
1:H:80:LEU:HD12	3:J:844:ALA:HB2	1.98	0.46
2:I:438:ILE:HD12	2:I:438:ILE:H	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:874:LEU:O	3:J:1029:ARG:HG2	2.14	0.46
3:J:638:LYS:C	3:J:729:HIS:HD2	2.22	0.46
3:J:772:PRO:O	3:J:1209:LEU:HD12	2.15	0.46
5:L:369:LEU:HD23	5:L:433:LEU:HD13	1.96	0.46
1:B:52:ALA:HB3	1:B:145:ASP:O	2.16	0.46
2:C:185:LYS:HD3	2:C:190:LYS:HB3	1.97	0.46
2:C:521:PRO:HG2	3:D:1055:VAL:HG21	1.98	0.46
3:D:729:HIS:CE1	3:D:935:LYS:HD3	2.50	0.46
3:D:889:ALA:HB1	3:D:930:LEU:HA	1.97	0.46
1:H:74:ASP:O	1:H:78:ILE:HG12	2.15	0.46
2:I:107:LEU:HD12	6:N:50:PRO:HD2	1.98	0.46
3:J:562:ALA:HB3	3:J:567:ILE:HD11	1.96	0.46
3:J:606:ILE:HG22	3:J:613:ARG:HB2	1.98	0.46
5:L:199:ARG:HE	5:L:200:GLN:NE2	2.13	0.46
5:L:355:SER:HB3	5:L:358:GLU:HG3	1.97	0.46
5:L:360:ALA:O	5:L:364:LEU:HB2	2.16	0.46
2:C:42:VAL:HG12	2:C:43:GLY:H	1.79	0.46
2:C:418:LEU:HD11	7:O:38:DG:C4	2.50	0.46
2:C:472:ARG:HB3	2:C:532:MET:HB3	1.97	0.46
2:C:1083:GLU:HA	2:C:1086:ARG:HG3	1.98	0.46
3:D:1267:ARG:H	3:D:1267:ARG:NE	2.13	0.46
4:E:65:MET:O	4:E:69:LEU:HG	2.14	0.46
5:F:149:LYS:HB3	5:F:193:ARG:HH12	1.81	0.46
1:G:83:LYS:HD3	1:G:83:LYS:H	1.81	0.46
2:I:49:LYS:NZ	2:I:50:GLU:HG3	2.29	0.46
2:I:571:LEU:HD23	2:I:668:LEU:O	2.15	0.46
2:I:607:ASP:O	2:I:610:ARG:N	2.49	0.46
5:L:411:ARG:HB2	7:R:1:DC:H2'	1.97	0.46
1:B:20:TYR:HD1	1:B:21:GLY:H	1.64	0.46
2:C:588:VAL:HG21	2:C:664:GLY:HA2	1.98	0.46
2:C:1104:GLU:H	2:C:1104:GLU:HG2	1.52	0.46
3:D:1011:PHE:CD1	3:D:1021:TYR:HB2	2.49	0.46
5:F:364:LEU:HD22	5:F:436:PHE:HZ	1.81	0.46
2:I:140:ILE:HG23	2:I:412:ALA:HA	1.98	0.46
3:J:440:VAL:HG13	3:J:441:ARG:HD2	1.98	0.46
3:J:580:ALA:O	3:J:584:ASN:HB2	2.16	0.46
3:J:639:LEU:HD22	3:J:766:ALA:HA	1.98	0.46
3:J:1192:LEU:HD23	3:J:1373:ARG:HB2	1.98	0.46
3:J:1282:ARG:NH1	3:J:1284:GLU:OE2	2.49	0.46
6:N:20:VAL:HG22	6:N:38:VAL:HG22	1.96	0.46
2:C:86:LYS:HE2	2:C:813:VAL:HA	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1038:TRP:O	3:D:1223:VAL:HG11	2.16	0.46
3:D:233:LYS:HB3	3:D:236:TYR:CZ	2.51	0.46
3:D:263:ASP:HA	3:D:268:HIS:HA	1.97	0.46
3:D:508:ARG:HB3	3:D:510:GLU:CD	2.41	0.46
3:D:539:ASP:HB3	3:D:600:LEU:HG	1.97	0.46
3:D:606:ILE:HG22	3:D:613:ARG:HB2	1.98	0.46
3:D:657:LEU:HB2	3:D:691:LEU:HD13	1.98	0.46
3:D:896:ALA:O	3:D:900:ILE:HG13	2.16	0.46
3:D:1192:LEU:HD23	3:D:1373:ARG:HB2	1.98	0.46
5:F:119:ARG:HA	5:F:244:TYR:CE1	2.50	0.46
5:F:122:GLU:HA	5:F:125:MET:HE2	1.97	0.46
1:G:17:GLY:HA3	1:G:19:HIS:CE1	2.50	0.46
2:I:163:ILE:HA	2:I:164:PRO:HD2	1.75	0.46
2:I:398:THR:HA	2:I:635:THR:HG21	1.97	0.46
2:I:682:TYR:HA	3:J:633:VAL:HG11	1.96	0.46
3:J:151:GLN:HG2	3:J:152:LEU:H	1.80	0.46
3:J:1095:THR:O	3:J:1099:VAL:HG23	2.15	0.46
1:B:64:GLU:HG3	1:B:165:ILE:HG21	1.98	0.46
2:C:332:ARG:HH11	2:C:334:ARG:HD2	1.81	0.46
2:C:438:ILE:HD12	2:C:438:ILE:H	1.81	0.46
5:F:431:ARG:HG3	5:F:434:ARG:CZ	2.46	0.46
2:I:472:ARG:HB3	2:I:532:MET:HB3	1.98	0.46
3:J:729:HIS:CE1	3:J:935:LYS:HD3	2.51	0.46
5:L:413:ARG:NH2	8:S:45:DC:OP2	2.48	0.46
6:N:10:VAL:HB	6:N:60:ARG:O	2.16	0.46
7:R:34:DA:H2''	7:R:35:DG:O4'	2.16	0.46
2:C:15:LEU:HD11	2:C:457:ALA:O	2.16	0.46
2:C:424:GLY:H	2:C:427:VAL:CG2	2.29	0.46
2:C:607:ASP:O	2:C:610:ARG:N	2.49	0.46
2:C:620:LEU:H	2:C:620:LEU:HD12	1.81	0.46
2:C:1102:LEU:HD21	3:D:9:ARG:HB2	1.97	0.46
3:D:132:TYR:CZ	3:D:456:MET:HE3	2.51	0.46
3:D:783:ARG:HD3	3:D:1028:ALA:O	2.16	0.46
3:D:834:THR:HG21	3:D:839:LEU:HD21	1.98	0.46
5:F:244:TYR:CD2	5:F:244:TYR:N	2.84	0.46
1:H:20:TYR:HD1	1:H:21:GLY:H	1.64	0.46
1:H:20:TYR:HD1	1:H:21:GLY:N	2.14	0.46
2:I:676:ILE:HA	2:I:871:LEU:O	2.16	0.46
5:L:276:PRO:O	5:L:280:VAL:HG23	2.16	0.46
5:L:386:LEU:HB3	5:L:396:HIS:HB2	1.98	0.46
8:P:6:DC:H2''	8:P:7:DG:H5'	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:GLU:OE1	2:C:607:ASP:HB2	2.15	0.45
1:A:185:ARG:HG2	1:A:185:ARG:O	2.16	0.45
2:C:409:ARG:NH2	2:C:563:ASN:OD1	2.49	0.45
2:C:939:ARG:HB3	2:C:982:PRO:HG3	1.98	0.45
2:I:1083:GLU:HA	2:I:1086:ARG:HG3	1.98	0.45
2:I:1102:LEU:HD21	3:J:9:ARG:HB2	1.97	0.45
3:J:132:TYR:CZ	3:J:456:MET:HE3	2.51	0.45
3:J:862:ASP:O	3:J:876:SER:HA	2.16	0.45
3:J:889:ALA:HB1	3:J:930:LEU:HA	1.98	0.45
6:M:23:ILE:HA	6:M:35:TYR:O	2.16	0.45
2:C:954:SER:HA	2:C:955:PRO:HD3	1.85	0.45
3:D:112:ILE:HD12	3:D:113:GLY:N	2.30	0.45
3:D:156:GLU:O	3:D:160:GLU:HB2	2.16	0.45
3:D:406:ASP:HB3	3:D:407:VAL:H	1.50	0.45
3:D:1318:TYR:N	3:J:1157:GLY:O	2.49	0.45
5:F:252:THR:O	5:F:255:THR:OG1	2.25	0.45
1:G:53:VAL:HA	1:G:144:VAL:HA	1.97	0.45
1:H:138:LEU:HD22	1:H:139:TYR:N	2.31	0.45
2:I:167:LYS:HD2	2:I:167:LYS:O	2.15	0.45
2:I:620:LEU:H	2:I:620:LEU:HD12	1.80	0.45
2:C:204:GLN:HA	2:C:227:LEU:HD11	1.98	0.45
2:C:1016:ILE:HG13	2:C:1017:THR:H	1.82	0.45
3:D:859:ASP:HB2	3:D:862:ASP:OD2	2.17	0.45
3:D:1040:GLY:O	3:D:1060:SER:HB2	2.16	0.45
2:I:109:LYS:HG2	6:N:15:TYR:OH	2.16	0.45
2:I:276:LYS:HD3	2:I:466:PHE:CZ	2.48	0.45
3:J:521:PRO:HA	3:J:522:PRO:HD3	1.77	0.45
3:J:539:ASP:HB3	3:J:600:LEU:HG	1.97	0.45
3:J:783:ARG:HD3	3:J:1028:ALA:O	2.15	0.45
1:A:71:VAL:HG11	1:A:78:ILE:HD11	1.99	0.45
1:B:20:TYR:HD1	1:B:21:GLY:N	2.13	0.45
1:B:214:ALA:O	1:B:218:LEU:HD13	2.16	0.45
2:C:676:ILE:HA	2:C:871:LEU:O	2.15	0.45
2:C:1083:GLU:OE1	3:D:88:TYR:OH	2.34	0.45
3:D:743:ASP:N	3:D:743:ASP:OD1	2.48	0.45
3:D:1197:ARG:NE	3:D:1398:TRP:HB3	2.32	0.45
2:I:204:GLN:HA	2:I:227:LEU:HD11	1.96	0.45
2:I:769:PRO:HB3	5:L:390:LEU:HA	1.98	0.45
2:I:1086:ARG:HD2	2:I:1112:PHE:CD2	2.52	0.45
3:J:169:TYR:O	3:J:392:SER:OG	2.34	0.45
3:J:675:ARG:HH12	5:L:437:LEU:HB3	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:699:VAL:HG21	3:J:764:LEU:HD13	1.99	0.45
3:J:1269:LYS:HG2	3:J:1270:ALA:N	2.31	0.45
7:R:15:DT:H6	7:R:15:DT:H5'	1.81	0.45
1:A:9:PRO:HG3	1:B:224:TYR:CZ	2.51	0.45
1:B:30:ARG:HB3	1:B:191:ASP:O	2.16	0.45
1:B:138:LEU:HD22	1:B:139:TYR:N	2.32	0.45
2:C:167:LYS:HD2	2:C:167:LYS:O	2.17	0.45
2:C:729:LEU:HD13	2:C:730:SER:O	2.16	0.45
3:D:59:ALA:HB2	3:D:78:VAL:HG21	1.99	0.45
3:D:1282:ARG:NH1	3:D:1284:GLU:OE2	2.49	0.45
2:I:332:ARG:HH11	2:I:334:ARG:HD2	1.81	0.45
2:I:470:PRO:HG3	2:I:485:TYR:CZ	2.51	0.45
2:I:588:VAL:HG21	2:I:664:GLY:HA2	1.98	0.45
2:I:939:ARG:HB3	2:I:982:PRO:HG3	1.97	0.45
2:I:1026:GLN:HE21	2:I:1026:GLN:HB2	1.51	0.45
3:J:859:ASP:HB2	3:J:862:ASP:OD2	2.17	0.45
3:J:1040:GLY:O	3:J:1060:SER:HB2	2.16	0.45
3:J:1129:THR:C	3:J:1131:THR:H	2.25	0.45
6:M:4:PHE:HE1	6:M:10:VAL:HG11	1.82	0.45
7:R:32:DG:H2''	7:R:33:DG:O4'	2.17	0.45
1:B:63:HIS:CD2	1:B:64:GLU:H	2.35	0.45
2:C:549:PHE:HE1	2:C:909:ALA:HB3	1.81	0.45
2:C:724:ARG:HD3	2:C:741:GLY:N	2.32	0.45
3:D:186:VAL:HG13	3:D:200:ASP:OD1	2.17	0.45
3:D:217:ARG:HH12	3:D:381:ALA:CB	2.29	0.45
3:D:580:ALA:O	3:D:584:ASN:HB2	2.16	0.45
3:D:699:VAL:HG21	3:D:764:LEU:HD13	1.99	0.45
3:D:973:GLN:CG	3:J:831:GLY:HA2	2.46	0.45
3:D:1072:ILE:O	3:D:1075:HIS:HB2	2.17	0.45
5:F:355:SER:HB3	5:F:358:GLU:HG3	1.99	0.45
2:I:15:LEU:HD11	2:I:457:ALA:O	2.16	0.45
2:I:521:PRO:HB2	3:J:1055:VAL:HG11	1.98	0.45
2:I:1089:VAL:HG13	2:I:1099:VAL:HG11	1.98	0.45
3:J:83:SER:O	3:J:86:ARG:HB2	2.17	0.45
3:J:704:ARG:HB2	3:J:745:MET:HG2	1.97	0.45
3:J:903:ASP:OD1	3:J:903:ASP:N	2.49	0.45
7:R:39:DT:C2'	7:R:40:DC:H5'	2.43	0.45
2:C:299:LYS:HG3	2:C:300:ASP:H	1.81	0.45
2:C:642:ARG:HD3	2:C:642:ARG:HA	1.55	0.45
2:C:751:PRO:HA	2:C:792:VAL:HG13	1.99	0.45
2:C:1089:VAL:O	2:C:1093:GLN:HG2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:101:HIS:CE1	3:D:103:TRP:HB2	2.52	0.45
3:D:102:ILE:HB	3:D:579:ASP:HB3	1.99	0.45
3:D:764:LEU:HD23	3:D:767:HIS:CD2	2.52	0.45
5:F:96:VAL:HA	5:F:225:LEU:HD11	1.97	0.45
5:F:124:GLY:O	5:F:128:ILE:HG13	2.17	0.45
2:I:409:ARG:NH2	2:I:563:ASN:OD1	2.49	0.45
2:I:569:VAL:H	2:I:995:MET:HE2	1.81	0.45
2:I:658:GLY:N	2:I:661:SER:HB3	2.32	0.45
3:J:118:LEU:HD12	3:J:123:LEU:HB2	1.99	0.45
8:S:19:DT:H5'	8:S:20:DA:OP1	2.16	0.45
1:B:78:ILE:HD12	1:B:130:ALA:HB2	1.98	0.45
1:B:80:LEU:HD12	3:D:844:ALA:HB2	1.99	0.45
2:C:521:PRO:HB2	3:D:1055:VAL:HG11	1.99	0.45
2:C:905:VAL:HG12	2:C:906:PHE:CD2	2.52	0.45
2:C:1086:ARG:HD2	2:C:1112:PHE:CD2	2.52	0.45
3:D:862:ASP:O	3:D:876:SER:HA	2.16	0.45
2:I:882:LEU:HD21	3:J:1038:LEU:HD22	1.97	0.45
2:I:1083:GLU:OE1	3:J:88:TYR:OH	2.34	0.45
3:J:101:HIS:CE1	3:J:103:TRP:HB2	2.52	0.45
4:K:31:LEU:HG	4:K:60:ALA:HB2	1.98	0.45
5:L:96:VAL:HA	5:L:225:LEU:HD11	1.97	0.45
5:L:122:GLU:HA	5:L:125:MET:HE2	1.98	0.45
6:M:20:VAL:HG22	6:M:38:VAL:HG22	1.98	0.45
6:N:84:LYS:HE2	6:N:84:LYS:HB2	1.75	0.45
1:A:53:VAL:HG22	1:A:54:THR:N	2.29	0.45
1:A:158:ILE:HG13	1:A:166:PRO:HG3	1.99	0.45
1:B:74:ASP:O	1:B:78:ILE:HG12	2.17	0.45
2:C:217:LEU:HD13	2:C:311:PHE:CD2	2.43	0.45
3:D:633:VAL:C	3:D:635:PRO:HD3	2.42	0.45
3:D:880:ILE:H	3:D:880:ILE:HG12	1.42	0.45
3:D:1208:ASP:N	3:D:1213:ARG:O	2.47	0.45
3:D:1269:LYS:HG2	3:D:1270:ALA:N	2.32	0.45
1:H:211:LEU:O	1:H:215:VAL:HG13	2.16	0.45
2:I:211:LEU:HD22	2:I:218:VAL:HA	1.99	0.45
2:I:729:LEU:HD13	2:I:730:SER:O	2.16	0.45
3:J:123:LEU:HG	3:J:127:LEU:HD12	1.98	0.45
3:J:550:ARG:HG3	3:J:553:ARG:HH21	1.82	0.45
3:J:764:LEU:HD23	3:J:767:HIS:CD2	2.52	0.45
5:L:244:TYR:CD2	5:L:244:TYR:N	2.83	0.45
1:A:83:LYS:H	1:A:83:LYS:HD3	1.82	0.45
2:C:247:PRO:HA	2:C:248:PRO:HD3	1.76	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:569:VAL:H	2:C:995:MET:HE2	1.80	0.45
2:C:726:ILE:HG23	2:C:787:ASP:HB2	1.99	0.45
2:C:829:GLN:NE2	2:C:831:ARG:HH21	2.14	0.45
2:C:1054:THR:OG1	2:C:1079:PRO:HG3	2.17	0.45
3:D:245:LEU:HA	3:D:245:LEU:HD23	1.66	0.45
3:D:369:ALA:HA	3:D:376:GLU:HG2	1.99	0.45
2:I:160:ALA:HB2	2:I:310:LEU:HD13	1.99	0.45
2:I:368:THR:HB	6:N:15:TYR:HE2	1.82	0.45
3:J:102:ILE:HB	3:J:579:ASP:HB3	1.99	0.45
3:J:156:GLU:O	3:J:160:GLU:HB2	2.16	0.45
3:J:160:GLU:CD	3:J:165:LYS:HD3	2.42	0.45
3:J:633:VAL:C	3:J:635:PRO:HD3	2.42	0.45
1:A:28:LEU:HD13	1:A:36:LEU:HD11	1.99	0.44
1:A:56:VAL:HG22	1:A:142:VAL:HG12	1.99	0.44
2:C:209:ARG:HG3	2:C:210:GLU:N	2.32	0.44
2:C:891:GLY:HA3	2:C:991:GLN:O	2.17	0.44
3:D:521:PRO:HA	3:D:522:PRO:HD3	1.78	0.44
3:D:1129:THR:C	3:D:1131:THR:H	2.24	0.44
3:D:1340:GLY:O	3:D:1344:VAL:HG23	2.17	0.44
1:G:71:VAL:HG11	1:G:78:ILE:HD11	1.98	0.44
1:H:214:ALA:O	1:H:218:LEU:HD13	2.16	0.44
2:I:8:ARG:H	2:I:907:ASP:CG	2.25	0.44
2:I:1102:LEU:HA	2:I:1107:ASN:O	2.17	0.44
3:J:365:GLU:HG2	3:J:366:LYS:H	1.82	0.44
7:O:39:DT:C2'	7:O:40:DC:H5'	2.44	0.44
3:D:1170:ASP:O	3:D:1174:LEU:HG	2.18	0.44
5:F:187:ARG:O	5:F:191:ILE:HG13	2.16	0.44
1:G:56:VAL:HG22	1:G:142:VAL:HG12	1.99	0.44
1:H:63:HIS:CD2	1:H:64:GLU:H	2.35	0.44
1:H:73:GLU:HB2	1:H:78:ILE:HD11	1.99	0.44
2:I:111:ASP:HA	6:N:45:SER:CB	2.47	0.44
2:I:446:GLY:O	2:I:449:ILE:HG13	2.18	0.44
2:I:1008:ARG:NH1	2:I:1028:GLY:HA2	2.31	0.44
2:I:1089:VAL:O	2:I:1093:GLN:HG2	2.16	0.44
5:L:336:ILE:HD11	5:L:344:TYR:HD2	1.82	0.44
6:M:18:GLY:HA3	6:M:40:PHE:HA	1.99	0.44
2:C:36:PRO:CB	2:C:70:GLU:HG2	2.46	0.44
2:C:327:HIS:O	2:C:331:ARG:HG3	2.17	0.44
2:C:838:LYS:HD3	2:C:999:HIS:HB2	1.99	0.44
3:D:248:PRO:HA	3:D:307:GLY:O	2.17	0.44
3:D:1221:VAL:HA	3:D:1224:VAL:HB	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:360:ALA:O	5:F:364:LEU:HB2	2.17	0.44
1:G:28:LEU:HD13	1:G:36:LEU:HD11	2.00	0.44
2:I:64:LEU:HD11	2:I:100:LEU:HD11	2.00	0.44
2:I:1066:ALA:O	2:I:1070:ILE:HD12	2.17	0.44
3:J:1042:ARG:HD3	3:J:1045:MET:CE	2.45	0.44
5:L:149:LYS:HB3	5:L:193:ARG:HH12	1.81	0.44
1:B:211:LEU:O	1:B:215:VAL:HG13	2.17	0.44
2:C:484:VAL:HG12	2:C:486:MET:H	1.82	0.44
2:C:1019:GLN:OE1	3:D:621:LYS:HE3	2.18	0.44
2:C:1035:MET:SD	8:P:12:DT:H4'	2.57	0.44
3:D:470:LEU:HD11	3:D:502:PHE:HB3	2.00	0.44
3:D:550:ARG:HG3	3:D:553:ARG:HH21	1.82	0.44
3:D:566:ILE:HG23	5:F:229:GLN:HE22	1.83	0.44
4:E:41:GLU:O	4:E:45:ARG:HG2	2.18	0.44
1:H:101:LEU:HD22	1:H:102:ARG:H	1.82	0.44
2:I:708:TYR:CE2	2:I:792:VAL:HG23	2.52	0.44
2:I:1038:TRP:O	3:J:1223:VAL:HG11	2.17	0.44
3:J:702:LEU:HG	3:J:747:VAL:HG22	1.99	0.44
3:J:1003:VAL:HG21	3:J:1041:MET:HB3	1.99	0.44
3:J:1170:ASP:O	3:J:1174:LEU:HG	2.17	0.44
6:N:17:VAL:HG13	6:N:138:GLU:HB3	1.98	0.44
1:A:133:GLU:OE1	2:C:605:LYS:HB2	2.17	0.44
1:B:87:VAL:HG12	1:B:122:ILE:HG12	2.00	0.44
2:C:658:GLY:N	2:C:661:SER:HB3	2.33	0.44
2:C:1054:THR:C	2:C:1059:ASP:HB2	2.43	0.44
3:D:32:ILE:HA	3:D:40:GLU:HG2	2.00	0.44
3:D:894:LYS:H	3:D:894:LYS:HG2	1.53	0.44
3:D:1003:VAL:HG21	3:D:1041:MET:HB3	1.99	0.44
3:D:1190:SER:HB2	3:D:1369:GLU:OE1	2.18	0.44
3:D:1209:LEU:HD23	3:D:1209:LEU:HA	1.73	0.44
2:I:484:VAL:HG12	2:I:486:MET:H	1.83	0.44
2:I:946:ARG:HH12	3:J:860:LEU:HD13	1.82	0.44
3:J:59:ALA:HB2	3:J:78:VAL:HG21	1.98	0.44
3:J:205:TYR:CD2	3:J:387:LEU:HD22	2.53	0.44
3:J:566:ILE:HG23	5:L:229:GLN:HE22	1.82	0.44
3:J:1172:HIS:O	3:J:1175:ILE:HB	2.18	0.44
6:N:11:VAL:HG22	6:N:17:VAL:HG12	1.98	0.44
7:O:17:DA:H1'	7:O:18:DA:H5''	1.98	0.44
7:O:21:DG:N2	8:P:28:DC:O2	2.51	0.44
1:A:94:MET:O	1:A:146:ARG:HD3	2.17	0.44
2:C:683:ASN:HB2	2:C:872:ASN:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:154:THR:HG22	3:D:157:GLU:CD	2.43	0.44
3:D:314:PRO:HB2	3:D:317:MET:HG3	2.00	0.44
2:I:549:PHE:CE1	2:I:909:ALA:HB3	2.53	0.44
2:I:773:LEU:HD22	5:L:390:LEU:HD11	1.99	0.44
2:I:838:LYS:HD3	2:I:999:HIS:HB2	2.00	0.44
3:J:101:HIS:HB3	3:J:104:PHE:CZ	2.52	0.44
3:J:1197:ARG:NE	3:J:1398:TRP:HB3	2.32	0.44
3:J:1495:ILE:HD13	4:K:80:VAL:HG21	1.99	0.44
5:L:252:THR:O	5:L:256:TRP:HD1	2.01	0.44
5:L:266:ILE:O	5:L:270:ALA:HB2	2.18	0.44
8:P:40:DT:H1'	8:P:41:DT:H5'	1.99	0.44
2:C:154:ARG:HB2	2:C:157:ARG:HB2	1.99	0.44
2:C:200:LEU:HD12	2:C:200:LEU:HA	1.82	0.44
2:C:561:GLY:HA2	2:C:564:MET:HE3	2.00	0.44
2:C:857:ASP:O	2:C:858:MET:HE2	2.17	0.44
3:D:353:VAL:HG22	3:D:355:VAL:H	1.82	0.44
3:D:1122:LEU:H	3:D:1122:LEU:HD12	1.82	0.44
3:J:465:LEU:HD12	3:J:513:ILE:HD11	1.99	0.44
3:J:471:GLU:O	3:J:475:ARG:HG2	2.17	0.44
3:J:911:LEU:O	3:J:915:VAL:HG23	2.17	0.44
6:M:84:LYS:HB2	6:M:84:LYS:HE2	1.79	0.44
2:C:650:LYS:HG2	2:C:651:LYS:H	1.82	0.44
2:C:708:TYR:CE2	2:C:792:VAL:HG23	2.53	0.44
3:D:520:LEU:HD12	3:D:521:PRO:HD2	1.99	0.44
3:D:675:ARG:HH12	5:F:437:LEU:H	1.65	0.44
3:D:1093:TYR:HD1	8:P:10:DA:H5''	1.82	0.44
1:H:156:HIS:NE2	1:H:167:VAL:O	2.51	0.44
2:I:324:ASP:O	2:I:330:ASN:ND2	2.51	0.44
2:I:440:PRO:HB2	3:J:1074:SER:OG	2.18	0.44
2:I:724:ARG:HD3	2:I:741:GLY:N	2.33	0.44
3:J:834:THR:HG21	3:J:839:LEU:HD21	1.98	0.44
1:A:82:LEU:O	1:A:85:LEU:HB3	2.18	0.44
2:C:72:ARG:N	2:C:95:TYR:O	2.49	0.44
2:C:716:LYS:H	2:C:716:LYS:HG2	1.59	0.44
2:C:1102:LEU:CD2	3:D:9:ARG:HB2	2.48	0.44
2:C:1116:ALA:HA	3:D:23:TYR:OH	2.18	0.44
3:D:895:VAL:O	3:D:898:GLU:HB3	2.18	0.44
3:D:1090:ASP:O	3:D:1093:TYR:HB3	2.18	0.44
3:D:1495:ILE:HD13	4:E:80:VAL:HG21	1.99	0.44
5:F:336:ILE:HD11	5:F:344:TYR:HD2	1.81	0.44
1:G:133:GLU:OE1	2:I:605:LYS:HB2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:209:GLU:HA	1:G:212:ASN:HB2	2.00	0.44
2:I:46:ALA:O	2:I:50:GLU:HB2	2.18	0.44
2:I:501:THR:O	2:I:503:LEU:HG	2.18	0.44
2:I:1019:GLN:OE1	3:J:621:LYS:HE3	2.18	0.44
5:L:375:LYS:HD2	5:L:426:HIS:ND1	2.32	0.44
2:C:211:LEU:HD22	2:C:218:VAL:HA	2.00	0.43
2:C:328:LEU:HD21	2:C:434:HIS:HA	2.00	0.43
2:C:446:GLY:O	2:C:449:ILE:HG13	2.17	0.43
2:C:673:LEU:H	2:C:673:LEU:HD12	1.83	0.43
2:C:1067:TYR:CE2	5:F:357:VAL:HA	2.53	0.43
3:D:171:LEU:HD21	3:D:175:VAL:O	2.17	0.43
3:D:622:ARG:NH1	8:P:14:DG:OP2	2.51	0.43
3:D:670:VAL:HB	5:F:364:LEU:HD11	2.00	0.43
2:I:72:ARG:N	2:I:95:TYR:O	2.49	0.43
2:I:230:ARG:NH2	2:I:231:PRO:HD2	2.28	0.43
2:I:561:GLY:HA2	2:I:564:MET:HE3	2.00	0.43
2:I:874:LEU:HD22	3:J:1029:ARG:HB2	2.00	0.43
3:J:129:PHE:CE1	3:J:457:GLY:HA3	2.53	0.43
3:J:154:THR:HG22	3:J:157:GLU:CD	2.43	0.43
3:J:400:VAL:HG12	3:J:445:ARG:HG2	1.99	0.43
3:J:1267:ARG:HE	3:J:1267:ARG:HB2	1.63	0.43
1:A:206:THR:HG23	1:A:209:GLU:OE2	2.17	0.43
2:C:160:ALA:HB2	2:C:310:LEU:HD13	1.99	0.43
2:C:751:PRO:HD2	3:D:681:ARG:HD2	2.00	0.43
2:C:946:ARG:HH12	3:D:860:LEU:HD13	1.83	0.43
3:D:439:LEU:HD11	5:F:190:HIS:CB	2.48	0.43
3:D:762:GLN:CB	4:E:16:LYS:HE2	2.48	0.43
3:D:1172:HIS:O	3:D:1175:ILE:HB	2.18	0.43
5:F:266:ILE:O	5:F:270:ALA:HB2	2.18	0.43
2:I:3:ILE:HG13	2:I:900:ARG:HG3	2.00	0.43
2:I:892:LEU:HD13	2:I:989:VAL:HG23	2.00	0.43
2:I:905:VAL:HG12	2:I:906:PHE:CD2	2.53	0.43
2:I:1081:VAL:HG21	2:I:1086:ARG:CZ	2.48	0.43
3:J:1072:ILE:O	3:J:1075:HIS:HB2	2.18	0.43
3:J:1208:ASP:HB3	3:J:1211:MET:HB2	2.00	0.43
4:K:30:LEU:HD11	4:K:67:GLU:OE2	2.17	0.43
4:K:42:PRO:HA	4:K:45:ARG:HG3	1.99	0.43
5:L:124:GLY:O	5:L:128:ILE:HG13	2.18	0.43
1:A:179:PHE:HD1	1:A:195:LEU:HD21	1.84	0.43
2:C:769:PRO:HB3	5:F:390:LEU:HA	1.99	0.43
2:C:773:LEU:HD22	5:F:390:LEU:HD11	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1006:HIS:HB2	2:C:1024:LYS:HG3	2.00	0.43
2:C:1066:ALA:O	2:C:1070:ILE:HD12	2.18	0.43
3:D:123:LEU:HG	3:D:127:LEU:HD12	1.99	0.43
3:D:716:PHE:CZ	3:D:728:LEU:HD11	2.54	0.43
3:D:1225:ALA:HA	3:D:1367:HIS:HB3	2.00	0.43
1:G:206:THR:HG23	1:G:209:GLU:OE2	2.19	0.43
1:H:87:VAL:HG12	1:H:122:ILE:HG12	2.00	0.43
2:I:327:HIS:O	2:I:331:ARG:HG3	2.17	0.43
2:I:351:LEU:HD11	2:I:374:ASN:H	1.84	0.43
2:I:376:ARG:O	2:I:380:ALA:HB3	2.19	0.43
2:I:857:ASP:O	2:I:858:MET:HE2	2.18	0.43
3:J:675:ARG:HD3	5:L:435:ASP:OD2	2.18	0.43
3:J:1225:ALA:HA	3:J:1367:HIS:HB3	2.00	0.43
4:K:45:ARG:HD2	4:K:63:TRP:CH2	2.54	0.43
6:M:67:GLU:OE2	6:M:103:TYR:OH	2.36	0.43
1:A:63:HIS:CE1	1:A:66:SER:HB2	2.53	0.43
2:C:166:PRO:HA	7:O:37:DT:H71	2.01	0.43
2:C:440:PRO:HB2	3:D:1074:SER:OG	2.18	0.43
3:D:465:LEU:HD12	3:D:513:ILE:HD11	2.00	0.43
3:D:475:ARG:O	3:D:478:LEU:HB2	2.19	0.43
3:D:702:LEU:HG	3:D:747:VAL:HG22	1.99	0.43
3:D:781:PRO:O	3:D:908:LYS:NZ	2.50	0.43
4:E:31:LEU:HG	4:E:60:ALA:HB2	2.00	0.43
4:E:42:PRO:HA	4:E:45:ARG:HG3	1.99	0.43
1:G:71:VAL:HG21	1:G:138:LEU:HD22	2.01	0.43
1:G:158:ILE:HG13	1:G:166:PRO:HG3	2.00	0.43
2:I:20:GLU:O	2:I:24:GLU:N	2.44	0.43
2:I:181:VAL:HG22	2:I:182:VAL:H	1.83	0.43
2:I:683:ASN:HB2	2:I:872:ASN:HB3	1.99	0.43
3:J:895:VAL:O	3:J:898:GLU:HB3	2.18	0.43
3:J:1090:ASP:O	3:J:1093:TYR:HB3	2.19	0.43
3:J:1208:ASP:N	3:J:1213:ARG:O	2.47	0.43
1:B:101:LEU:HD22	1:B:102:ARG:N	2.33	0.43
2:C:219:GLN:H	2:C:219:GLN:HG3	1.60	0.43
2:C:1008:ARG:NH1	2:C:1028:GLY:HA2	2.31	0.43
2:C:1067:TYR:CE1	3:D:655:PRO:HG3	2.53	0.43
3:D:107:ASP:HA	3:D:586:ARG:HH21	1.84	0.43
3:D:1167:SER:H	3:D:1170:ASP:HB2	1.83	0.43
1:G:53:VAL:HG22	1:G:54:THR:N	2.31	0.43
1:G:63:HIS:CE1	1:G:66:SER:HB2	2.53	0.43
1:G:110:ARG:HA	1:G:129:ILE:HG12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:140:MET:HE3	1:G:140:MET:HB2	1.85	0.43
2:I:427:VAL:HG22	7:R:38:DG:N2	2.26	0.43
2:I:650:LYS:HG2	2:I:651:LYS:H	1.83	0.43
2:I:781:LYS:HE2	2:I:782:ALA:O	2.19	0.43
2:I:1044:GLY:HA3	4:K:17:TYR:CE1	2.53	0.43
5:L:238:ALA:HB2	5:L:257:TRP:CG	2.54	0.43
5:L:252:THR:O	5:L:255:THR:OG1	2.26	0.43
8:P:24:DA:H3'	8:P:24:DA:P	2.58	0.43
1:B:174:VAL:HA	1:B:200:TRP:O	2.19	0.43
2:C:5:ARG:HB2	2:C:902:ILE:HB	2.01	0.43
2:C:140:ILE:HG23	2:C:412:ALA:HA	1.99	0.43
2:C:501:THR:O	2:C:503:LEU:HG	2.19	0.43
2:C:781:LYS:HE2	2:C:782:ALA:O	2.18	0.43
3:D:132:TYR:HB3	3:D:454:ALA:HB1	2.00	0.43
3:D:439:LEU:HD11	5:F:190:HIS:HB3	2.01	0.43
3:D:897:GLN:HE21	3:D:897:GLN:HB3	1.66	0.43
5:F:241:LYS:HE2	7:O:24:DC:H3'	1.99	0.43
1:G:58:ILE:HG22	1:G:60:ASP:N	2.33	0.43
1:H:64:GLU:HG3	1:H:165:ILE:HG21	1.98	0.43
1:H:101:LEU:HD22	1:H:102:ARG:N	2.32	0.43
2:I:577:PRO:HG2	2:I:580:MET:HE2	2.01	0.43
2:I:754:ILE:HA	2:I:791:ARG:HA	2.01	0.43
2:I:1023:GLY:HA2	8:S:15:DA:P	2.58	0.43
2:I:1055:ILE:HD11	2:I:1079:PRO:HD3	2.01	0.43
3:J:44:LEU:HD21	3:J:544:TYR:HB3	2.01	0.43
3:J:362:GLN:HB2	3:J:365:GLU:HB2	2.00	0.43
3:J:561:GLY:HA2	5:L:151:LEU:HD22	2.00	0.43
3:J:762:GLN:CB	4:K:16:LYS:HE2	2.49	0.43
6:M:22:GLY:O	6:M:36:TYR:HA	2.19	0.43
2:C:46:ALA:O	2:C:50:GLU:HB2	2.18	0.43
2:C:760:SER:O	2:C:785:VAL:HA	2.19	0.43
3:D:372:ASP:HB3	3:D:374:GLU:HG3	2.00	0.43
3:D:475:ARG:HG2	3:D:475:ARG:H	1.67	0.43
3:D:930:LEU:O	3:D:934:LEU:HD12	2.19	0.43
2:I:999:HIS:CD2	2:I:1004:LYS:HE3	2.54	0.43
2:I:1102:LEU:CD2	3:J:9:ARG:HB2	2.49	0.43
3:J:406:ASP:CG	3:J:407:VAL:H	2.25	0.43
3:J:508:ARG:HB2	3:J:511:TRP:CE2	2.53	0.43
6:M:80:MET:HB3	6:M:107:GLN:HG2	1.99	0.43
6:M:85:GLN:H	6:M:85:GLN:HG2	1.58	0.43
1:A:110:ARG:HA	1:A:129:ILE:HG12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:276:LYS:HD3	2:C:466:PHE:CZ	2.54	0.43
2:C:549:PHE:HB3	2:C:552:HIS:CD2	2.53	0.43
2:C:946:ARG:NH2	3:D:860:LEU:H	2.17	0.43
2:C:1044:GLY:HA3	4:E:17:TYR:CE1	2.53	0.43
2:C:1102:LEU:HA	2:C:1107:ASN:O	2.17	0.43
3:D:51:GLY:HA3	3:D:85:VAL:HG23	2.00	0.43
3:D:54:LYS:HD3	3:D:55:ASP:N	2.34	0.43
3:D:129:PHE:CE1	3:D:457:GLY:HA3	2.54	0.43
3:D:646:LYS:HD2	3:D:722:GLU:OE1	2.18	0.43
3:D:911:LEU:O	3:D:915:VAL:HG23	2.18	0.43
3:D:1191:PRO:O	3:D:1373:ARG:HD3	2.19	0.43
2:I:751:PRO:HA	2:I:792:VAL:HG13	2.00	0.43
2:I:1007:ALA:HB2	3:J:648:MET:HG3	2.01	0.43
2:I:1016:ILE:HG13	2:I:1017:THR:H	1.83	0.43
4:K:41:GLU:O	4:K:45:ARG:HG2	2.18	0.43
6:M:18:GLY:CA	6:M:41:PRO:HD3	2.47	0.43
7:R:43:DG:H1	8:S:6:DC:H42	1.67	0.43
2:C:1018:GLN:HB2	2:C:1058:ASP:HB2	2.00	0.43
2:C:1081:VAL:HG21	2:C:1086:ARG:CZ	2.49	0.43
2:C:1092:LEU:HD22	2:C:1097:LEU:HD13	2.00	0.43
3:D:248:PRO:HG3	3:D:308:LYS:HD3	2.00	0.43
3:D:632:VAL:O	3:D:727:GLN:HA	2.19	0.43
1:G:179:PHE:HD1	1:G:195:LEU:HD21	1.83	0.43
1:H:38:ASN:CG	1:H:39:PRO:HD3	2.44	0.43
2:I:64:LEU:HD22	2:I:359:MET:SD	2.59	0.43
2:I:208:VAL:HA	2:I:211:LEU:HB2	2.00	0.43
2:I:726:ILE:HG23	2:I:787:ASP:HB2	2.00	0.43
2:I:874:LEU:HD23	2:I:874:LEU:HA	1.91	0.43
2:I:1090:LYS:HA	2:I:1090:LYS:HD2	1.72	0.43
3:J:409:VAL:HG23	3:J:437:VAL:HG22	2.01	0.43
3:J:587:ARG:HE	3:J:587:ARG:HB3	1.62	0.43
5:L:137:LEU:HD11	5:L:178:LEU:HD11	2.00	0.43
2:C:351:LEU:HD11	2:C:374:ASN:H	1.84	0.43
2:C:874:LEU:HD22	3:D:1029:ARG:HB2	2.01	0.43
2:C:892:LEU:HD13	2:C:989:VAL:HG23	2.01	0.43
3:D:101:HIS:HB3	3:D:104:PHE:CZ	2.54	0.43
3:D:903:ASP:OD1	3:D:903:ASP:N	2.51	0.43
3:D:1480:PHE:CD2	3:D:1481:VAL:HG13	2.54	0.43
5:F:238:ALA:HB2	5:F:257:TRP:CG	2.54	0.43
1:H:109:VAL:HG12	1:H:129:ILE:HB	2.01	0.43
2:I:159:ILE:HG13	2:I:175:GLU:HA	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:328:LEU:HD21	2:I:434:HIS:HA	2.01	0.43
2:I:1081:VAL:HG21	2:I:1086:ARG:NE	2.34	0.43
3:J:583:ASP:OD1	3:J:586:ARG:HB2	2.18	0.43
3:J:671:LYS:HG3	5:L:436:PHE:CE2	2.54	0.43
3:J:1014:ASN:C	3:J:1016:PRO:HD3	2.44	0.43
3:J:1167:SER:H	3:J:1170:ASP:HB2	1.84	0.43
3:J:1221:VAL:HA	3:J:1224:VAL:HB	2.01	0.43
6:N:36:TYR:HE2	6:N:54:PRO:HG3	1.83	0.43
6:N:52:GLU:H	6:N:52:GLU:HG2	1.52	0.43
1:A:42:ARG:NH1	2:C:857:ASP:HB3	2.19	0.42
1:A:231:SER:C	1:A:232:LEU:HD12	2.44	0.42
1:B:38:ASN:CG	1:B:39:PRO:HD3	2.44	0.42
2:C:109:LYS:HE2	6:M:40:PHE:CZ	2.53	0.42
2:C:376:ARG:O	2:C:380:ALA:HB3	2.19	0.42
2:C:1089:VAL:HG13	2:C:1099:VAL:HG11	2.00	0.42
3:D:698:LYS:HB3	3:D:756:GLN:NE2	2.34	0.42
3:D:1267:ARG:HE	3:D:1267:ARG:HB2	1.62	0.42
1:H:182:GLU:HG3	1:H:194:LYS:HB3	2.01	0.42
2:I:418:LEU:HD11	7:R:38:DG:C4	2.54	0.42
2:I:572:ILE:HD11	2:I:703:ILE:HD11	2.00	0.42
2:I:925:TYR:O	2:I:928:LYS:HB3	2.19	0.42
2:I:1038:TRP:CE3	3:J:1099:VAL:HG21	2.54	0.42
3:J:51:GLY:HA3	3:J:85:VAL:HG23	1.99	0.42
3:J:470:LEU:HD11	3:J:502:PHE:HB3	2.01	0.42
3:J:716:PHE:CZ	3:J:728:LEU:HD11	2.53	0.42
3:J:1093:TYR:CD1	8:S:10:DA:H5''	2.52	0.42
3:J:1122:LEU:H	3:J:1122:LEU:HD12	1.84	0.42
7:R:32:DG:H2''	7:R:33:DG:H5'	2.01	0.42
1:A:48:ILE:HA	1:A:49:PRO:HD3	1.91	0.42
1:A:209:GLU:HA	1:A:212:ASN:HB2	2.02	0.42
2:C:8:ARG:H	2:C:907:ASP:CG	2.27	0.42
2:C:64:LEU:HD11	2:C:100:LEU:HD11	2.01	0.42
2:C:122:THR:OG1	2:C:126:SER:O	2.35	0.42
2:C:159:ILE:HG13	2:C:175:GLU:HA	2.01	0.42
3:D:212:ARG:HG2	3:D:344:ASP:HB3	2.01	0.42
3:D:230:TRP:CD1	3:D:232:GLU:H	2.37	0.42
3:D:561:GLY:HA2	5:F:151:LEU:HD22	2.02	0.42
3:D:691:LEU:HA	3:D:694:VAL:HG23	2.01	0.42
5:F:279:MET:O	5:F:283:ILE:HG13	2.19	0.42
5:F:431:ARG:HG3	5:F:434:ARG:NE	2.34	0.42
1:G:23:PHE:HE2	1:G:199:ILE:HD12	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:185:ARG:O	1:G:185:ARG:HG2	2.18	0.42
2:I:549:PHE:HB3	2:I:552:HIS:CD2	2.54	0.42
2:I:760:SER:O	2:I:785:VAL:HA	2.20	0.42
2:I:946:ARG:NH2	3:J:860:LEU:H	2.17	0.42
2:I:992:MET:HE3	2:I:992:MET:HB3	1.89	0.42
2:I:1006:HIS:HB2	2:I:1024:LYS:HG3	2.00	0.42
2:I:1116:ALA:HA	3:J:23:TYR:OH	2.19	0.42
3:J:103:TRP:CH2	3:J:1444:THR:HA	2.54	0.42
3:J:107:ASP:HA	3:J:586:ARG:HH21	1.84	0.42
3:J:209:ARG:H	3:J:390:PRO:HA	1.83	0.42
3:J:1099:VAL:O	3:J:1103:HIS:HB3	2.19	0.42
1:B:101:LEU:HD22	1:B:102:ARG:H	1.84	0.42
2:C:477:GLY:HA2	2:C:508:ILE:HG13	2.02	0.42
2:C:1038:TRP:CE3	3:D:1099:VAL:HG21	2.54	0.42
3:D:583:ASP:OD1	3:D:586:ARG:HB2	2.18	0.42
3:D:706:PRO:HG3	8:P:11:DG:H21	1.83	0.42
5:F:137:LEU:HD11	5:F:178:LEU:HD11	2.00	0.42
2:I:647:GLN:HE21	2:I:647:GLN:HB2	1.52	0.42
2:I:1090:LYS:HD2	2:I:1093:GLN:HG3	2.01	0.42
3:J:68:PHE:CZ	5:L:394:ARG:HD2	2.54	0.42
3:J:752:SER:O	3:J:756:GLN:N	2.50	0.42
3:J:789:LEU:HD23	3:J:882:PHE:HE1	1.84	0.42
3:J:914:LEU:HD13	3:J:914:LEU:HA	1.84	0.42
3:J:1340:GLY:O	3:J:1344:VAL:HG23	2.18	0.42
5:L:108:LEU:O	5:L:109:LEU:HB3	2.19	0.42
5:L:199:ARG:HG3	5:L:239:VAL:HG11	2.02	0.42
8:S:40:DT:H1'	8:S:41:DT:H5'	2.02	0.42
1:A:54:THR:O	1:A:167:VAL:HG22	2.19	0.42
1:B:109:VAL:HG12	1:B:129:ILE:HB	2.01	0.42
1:B:176:ARG:HG2	1:B:177:VAL:N	2.34	0.42
2:C:16:PRO:HB2	2:C:460:ARG:NH2	2.34	0.42
2:C:111:ASP:HA	6:M:45:SER:HB2	2.00	0.42
2:C:208:VAL:HA	2:C:211:LEU:HB2	2.00	0.42
2:C:374:ASN:HD22	2:C:375:SER:N	2.17	0.42
2:C:614:ARG:HH21	2:C:620:LEU:HD23	1.84	0.42
2:C:881:ASN:OD1	2:C:884:GLN:NE2	2.52	0.42
2:C:1007:ALA:HB2	3:D:648:MET:HG3	2.02	0.42
2:C:1081:VAL:HG21	2:C:1086:ARG:NE	2.35	0.42
3:D:407:VAL:HG23	3:D:422:ALA:HB2	2.00	0.42
3:D:508:ARG:HB2	3:D:511:TRP:CE2	2.54	0.42
3:D:752:SER:O	3:D:756:GLN:N	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:795:VAL:HG13	3:D:879:ARG:NH2	2.34	0.42
3:D:970:LYS:O	3:D:973:GLN:HB3	2.20	0.42
3:D:1208:ASP:HB3	3:D:1211:MET:HB2	2.00	0.42
4:E:30:LEU:HD11	4:E:67:GLU:OE2	2.18	0.42
5:F:135:THR:HG21	5:F:177:LYS:HG2	2.01	0.42
1:G:36:LEU:HD12	1:G:195:LEU:HD12	2.01	0.42
1:G:54:THR:O	1:G:167:VAL:HG22	2.19	0.42
1:G:99:LEU:HB2	1:G:142:VAL:HG23	2.02	0.42
2:I:477:GLY:HA2	2:I:508:ILE:HG13	2.01	0.42
3:J:32:ILE:HA	3:J:40:GLU:HG2	2.01	0.42
3:J:132:TYR:HB3	3:J:454:ALA:HB1	2.00	0.42
3:J:141:VAL:HG12	3:J:450:TYR:CE2	2.52	0.42
3:J:475:ARG:O	3:J:478:LEU:HB2	2.19	0.42
3:J:658:LEU:HD21	3:J:670:VAL:O	2.20	0.42
3:J:691:LEU:HA	3:J:694:VAL:HG23	2.01	0.42
3:J:698:LYS:HB3	3:J:756:GLN:NE2	2.34	0.42
3:J:795:VAL:HG13	3:J:879:ARG:NH2	2.34	0.42
3:J:884:ARG:NE	3:J:888:GLU:OE2	2.52	0.42
3:J:1191:PRO:O	3:J:1373:ARG:HD3	2.20	0.42
5:L:135:THR:HG21	5:L:177:LYS:HG2	2.02	0.42
1:B:73:GLU:HB2	1:B:78:ILE:HD11	2.02	0.42
2:C:198:ARG:HG2	2:C:234:ALA:HB3	2.02	0.42
2:C:549:PHE:CE1	2:C:909:ALA:HB3	2.54	0.42
2:C:999:HIS:CD2	2:C:1004:LYS:HE3	2.54	0.42
2:C:1082:PRO:O	2:C:1083:GLU:HB3	2.18	0.42
3:D:44:LEU:HD21	3:D:544:TYR:HB3	2.01	0.42
3:D:118:LEU:HD12	3:D:123:LEU:HB2	2.01	0.42
3:D:720:LEU:HD23	3:D:720:LEU:HA	1.90	0.42
3:D:1114:THR:OG1	3:D:1116:ASN:ND2	2.48	0.42
5:F:380:GLU:HB2	5:F:415:ILE:HG23	2.02	0.42
2:I:77:PRO:HD3	2:I:92:ALA:HA	2.00	0.42
2:I:688:ILE:HG23	2:I:871:LEU:HD23	2.02	0.42
2:I:810:ASP:O	2:I:813:VAL:HG12	2.19	0.42
2:I:1092:LEU:HD22	2:I:1097:LEU:HD13	2.00	0.42
3:J:421:LEU:CD2	3:J:422:ALA:H	2.32	0.42
3:J:649:ALA:HB3	3:J:720:LEU:HD21	2.00	0.42
3:J:1190:SER:HB2	3:J:1369:GLU:OE1	2.20	0.42
3:J:1480:PHE:CD2	3:J:1481:VAL:HG13	2.54	0.42
6:N:129:LEU:O	6:N:133:ILE:HG12	2.19	0.42
1:A:71:VAL:HG21	1:A:138:LEU:HD22	2.01	0.42
1:B:100:ILE:HG22	1:B:141:GLU:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:39:ARG:HD3	2:C:45:GLN:OE1	2.20	0.42
2:C:179:SER:OG	2:C:181:VAL:HG12	2.20	0.42
2:C:925:TYR:O	2:C:928:LYS:HB3	2.19	0.42
2:C:1017:THR:OG1	2:C:1019:GLN:HG2	2.20	0.42
2:C:1056:LYS:HG3	3:D:751:LEU:HD11	2.02	0.42
3:D:171:LEU:HD23	3:D:172:PRO:O	2.19	0.42
3:D:181:ASP:HB2	3:D:205:TYR:CE2	2.54	0.42
3:D:288:MET:HE3	3:D:288:MET:HB2	1.96	0.42
5:F:199:ARG:HG3	5:F:239:VAL:HG11	2.02	0.42
2:I:99:GLN:HB3	2:I:110:GLU:HG3	2.01	0.42
2:I:247:PRO:HA	2:I:248:PRO:HD3	1.76	0.42
2:I:891:GLY:HA3	2:I:991:GLN:O	2.19	0.42
3:J:167:GLU:HB3	3:J:395:VAL:HG12	2.01	0.42
3:J:553:ARG:NH2	5:L:226:ASP:OD1	2.47	0.42
3:J:632:VAL:O	3:J:727:GLN:HA	2.19	0.42
4:K:50:THR:HB	4:K:53:GLY:O	2.20	0.42
1:B:182:GLU:HG3	1:B:194:LYS:HB3	2.01	0.42
2:C:77:PRO:HD3	2:C:92:ALA:HA	2.01	0.42
2:C:181:VAL:HG22	2:C:182:VAL:H	1.84	0.42
2:C:524:VAL:HB	2:C:528:GLU:HG3	2.01	0.42
2:C:1031:ARG:HA	3:D:622:ARG:HA	2.02	0.42
3:D:176:ASP:OD2	3:D:388:HIS:HB3	2.19	0.42
3:D:610:LYS:NZ	8:P:10:DA:OP2	2.28	0.42
5:F:252:THR:O	5:F:256:TRP:HD1	2.03	0.42
1:G:180:GLN:HB3	2:I:934:PHE:CZ	2.54	0.42
2:I:441:VAL:O	2:I:559:LEU:HD12	2.20	0.42
2:I:524:VAL:HB	2:I:528:GLU:HG3	2.00	0.42
2:I:946:ARG:HH22	3:J:860:LEU:HD13	1.84	0.42
2:I:954:SER:HA	2:I:955:PRO:HD3	1.85	0.42
2:I:1082:PRO:O	2:I:1083:GLU:HB3	2.19	0.42
3:J:397:LYS:HE3	3:J:448:GLU:O	2.19	0.42
3:J:520:LEU:HD12	3:J:521:PRO:HD2	2.01	0.42
3:J:593:ASN:HA	3:J:594:PRO:HD3	1.91	0.42
3:J:1008:PHE:O	3:J:1012:GLU:HG3	2.20	0.42
3:J:1103:HIS:HE1	3:J:1464:GLU:HG3	1.84	0.42
1:A:180:GLN:HB3	2:C:934:PHE:CZ	2.55	0.42
3:D:176:ASP:CG	3:D:389:GLU:H	2.28	0.42
3:D:514:LEU:HD11	3:D:516:ALA:O	2.20	0.42
3:D:914:LEU:HA	3:D:914:LEU:HD13	1.84	0.42
5:F:114:GLU:OE1	5:F:249:LYS:HD2	2.20	0.42
2:I:848:VAL:HG22	3:J:740:PHE:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:610:LYS:NZ	8:S:10:DA:OP2	2.37	0.42
3:J:930:LEU:O	3:J:934:LEU:HD12	2.19	0.42
3:J:1268:PRO:HB2	3:J:1271:LYS:HB2	2.02	0.42
5:L:370:GLU:O	5:L:373:LEU:HB3	2.20	0.42
6:M:131:ARG:HD2	6:M:131:ARG:HA	1.89	0.42
1:B:76:VAL:O	1:B:80:LEU:HD22	2.20	0.42
2:C:99:GLN:HB3	2:C:110:GLU:HG3	2.00	0.42
2:C:109:LYS:HG2	6:M:15:TYR:OH	2.20	0.42
2:C:946:ARG:HH22	3:D:860:LEU:HD13	1.85	0.42
2:C:1056:LYS:HE3	2:C:1056:LYS:HB2	1.84	0.42
3:D:789:LEU:HD23	3:D:882:PHE:HE1	1.84	0.42
3:D:1014:ASN:C	3:D:1016:PRO:HD3	2.44	0.42
3:D:1462:LEU:H	3:D:1462:LEU:HG	1.71	0.42
4:E:45:ARG:HD2	4:E:63:TRP:CH2	2.55	0.42
1:H:58:ILE:HG23	1:H:140:MET:HB3	2.02	0.42
1:H:174:VAL:HA	1:H:200:TRP:O	2.19	0.42
2:I:122:THR:OG1	2:I:126:SER:O	2.38	0.42
2:I:179:SER:OG	2:I:181:VAL:HG12	2.20	0.42
2:I:1019:GLN:HE21	3:J:617:ASN:HB3	1.85	0.42
2:I:1031:ARG:HA	3:J:622:ARG:HA	2.02	0.42
3:J:720:LEU:HD23	3:J:720:LEU:HA	1.90	0.42
5:L:376:LEU:HD21	5:L:423:LEU:HG	2.02	0.42
8:S:24:DA:H3'	8:S:24:DA:OP1	2.20	0.42
1:A:58:ILE:HG22	1:A:60:ASP:N	2.34	0.42
2:C:72:ARG:CB	2:C:95:TYR:HB2	2.46	0.42
2:C:91:GLN:HA	2:C:119:PRO:HA	2.02	0.42
2:C:349:ALA:O	2:C:353:ARG:HG2	2.19	0.42
2:C:848:VAL:HG22	3:D:740:PHE:O	2.20	0.42
2:C:1090:LYS:HD2	2:C:1093:GLN:HG3	2.00	0.42
3:D:494:LYS:O	3:D:497:GLU:HB3	2.19	0.42
3:D:658:LEU:HD21	3:D:670:VAL:O	2.20	0.42
4:E:50:THR:HB	4:E:53:GLY:O	2.20	0.42
2:I:16:PRO:HB2	2:I:460:ARG:NH2	2.34	0.42
2:I:70:GLU:CD	2:I:70:GLU:H	2.23	0.42
2:I:200:LEU:HD12	2:I:200:LEU:HA	1.83	0.42
2:I:552:HIS:ND1	3:J:1061:PHE:O	2.50	0.42
2:I:934:PHE:HD2	2:I:934:PHE:HA	1.62	0.42
3:J:62:LYS:HD2	3:J:75:ARG:HD2	2.02	0.42
3:J:161:LEU:HD12	3:J:161:LEU:HA	1.78	0.42
3:J:623:VAL:HB	3:J:748:HIS:CE1	2.55	0.42
4:K:39:VAL:HG21	4:K:72:ARG:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:111:LEU:H	5:L:111:LEU:HD22	1.85	0.42
5:L:206:ASN:O	5:L:209:LEU:HB3	2.20	0.42
6:N:116:GLU:HB2	6:N:121:LEU:HD22	2.02	0.42
8:P:22:DT:H4'	8:P:23:DA:OP1	2.19	0.42
1:B:85:LEU:HD12	1:B:124:ASN:HB3	2.01	0.41
2:C:441:VAL:O	2:C:559:LEU:HD12	2.20	0.41
2:C:577:PRO:HG2	2:C:580:MET:HE2	2.02	0.41
2:C:1115:LEU:HD23	3:D:85:VAL:HG12	2.01	0.41
3:D:585:GLY:CA	3:D:590:PRO:HG3	2.50	0.41
3:D:640:HIS:H	3:D:640:HIS:CD2	2.38	0.41
3:D:660:LYS:HD2	3:D:694:VAL:HG22	2.02	0.41
5:F:388:LYS:HD3	5:F:388:LYS:HA	1.73	0.41
2:I:39:ARG:HD3	2:I:45:GLN:OE1	2.20	0.41
2:I:91:GLN:HA	2:I:119:PRO:HA	2.02	0.41
2:I:340:MET:HE3	2:I:340:MET:HB3	1.94	0.41
2:I:1023:GLY:HA2	8:S:15:DA:OP2	2.20	0.41
3:J:103:TRP:CE2	3:J:1444:THR:HG23	2.55	0.41
3:J:1014:ASN:O	3:J:1016:PRO:HD3	2.20	0.41
3:J:1331:ASP:HA	3:J:1332:PRO:HD3	1.90	0.41
6:N:12:LEU:HD23	6:N:40:PHE:CZ	2.55	0.41
6:N:136:LEU:HB3	6:N:155:PHE:CZ	2.55	0.41
1:A:23:PHE:HE2	1:A:199:ILE:HD12	1.85	0.41
1:A:36:LEU:HD12	1:A:195:LEU:HD12	2.01	0.41
1:B:115:THR:HA	1:B:116:PRO:HD3	1.90	0.41
1:B:176:ARG:HD2	3:D:884:ARG:NH2	2.30	0.41
2:C:594:ALA:HB1	2:C:654:LEU:HD11	2.01	0.41
2:C:688:ILE:HG23	2:C:871:LEU:HD23	2.02	0.41
3:D:260:GLU:O	3:D:270:ILE:HA	2.20	0.41
3:D:313:LEU:HG	3:D:314:PRO:CD	2.50	0.41
3:D:659:LYS:O	3:D:662:GLU:HB3	2.20	0.41
3:D:884:ARG:NE	3:D:888:GLU:OE2	2.53	0.41
3:D:976:GLN:HG2	3:J:807:ALA:CB	2.50	0.41
3:D:1008:PHE:O	3:D:1012:GLU:HG3	2.20	0.41
3:D:1099:VAL:O	3:D:1103:HIS:HB3	2.20	0.41
3:D:1268:PRO:HB2	3:D:1271:LYS:HB2	2.03	0.41
1:H:176:ARG:HG3	3:J:850:LEU:HD22	2.02	0.41
2:I:5:ARG:HB2	2:I:902:ILE:HB	2.02	0.41
2:I:198:ARG:HG2	2:I:234:ALA:HB3	2.02	0.41
2:I:724:ARG:NE	2:I:739:GLU:O	2.51	0.41
2:I:751:PRO:HB2	2:I:794:PRO:HA	2.02	0.41
5:L:380:GLU:HB2	5:L:415:ILE:HG23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:M:20:VAL:C	6:M:39:ASP:H	2.28	0.41
1:A:60:ASP:O	1:A:61:VAL:HB	2.20	0.41
2:C:3:ILE:HG13	2:C:900:ARG:HG3	2.02	0.41
2:C:40:GLU:C	2:C:42:VAL:H	2.28	0.41
2:C:108:ILE:HD11	6:M:28:VAL:HG21	2.02	0.41
3:D:103:TRP:CH2	3:D:1444:THR:HA	2.55	0.41
3:D:225:ILE:HG23	3:D:229:ALA:HB3	2.02	0.41
3:D:351:MET:HB3	3:D:368:VAL:HG12	2.02	0.41
2:I:325:ILE:HG23	2:I:326:ASP:H	1.84	0.41
2:I:376:ARG:H	2:I:376:ARG:HG2	1.58	0.41
2:I:599:GLU:HA	2:I:651:LYS:HB3	2.03	0.41
2:I:614:ARG:HH21	2:I:620:LEU:HD23	1.84	0.41
3:J:585:GLY:CA	3:J:590:PRO:HG3	2.50	0.41
3:J:653:PHE:HB2	3:J:691:LEU:HD11	2.02	0.41
3:J:680:GLN:C	3:J:682:ASP:N	2.76	0.41
3:J:1042:ARG:NE	3:J:1061:PHE:HE2	2.18	0.41
3:J:1209:LEU:HD23	3:J:1209:LEU:HA	1.72	0.41
4:K:66:LYS:HA	4:K:69:LEU:HB2	2.02	0.41
5:L:249:LYS:HG2	7:R:29:DC:OP2	2.19	0.41
1:B:48:ILE:HA	1:B:49:PRO:HD2	1.94	0.41
1:B:176:ARG:HG3	3:D:850:LEU:HD22	2.02	0.41
3:D:675:ARG:NH1	5:F:437:LEU:H	2.19	0.41
3:D:1306:PRO:HB2	3:D:1308:ASP:OD1	2.21	0.41
5:F:108:LEU:O	5:F:109:LEU:HB3	2.19	0.41
1:G:63:HIS:CE1	1:G:66:SER:H	2.38	0.41
2:I:209:ARG:HG3	2:I:210:GLU:N	2.33	0.41
2:I:513:VAL:O	2:I:524:VAL:HG22	2.20	0.41
2:I:881:ASN:OD1	2:I:884:GLN:NE2	2.53	0.41
3:J:213:VAL:HG13	3:J:385:VAL:HG12	2.02	0.41
3:J:660:LYS:HD2	3:J:694:VAL:HG22	2.01	0.41
3:J:758:GLU:OE1	3:J:1476:THR:OG1	2.36	0.41
1:B:156:HIS:NE2	1:B:167:VAL:O	2.52	0.41
2:C:107:LEU:HA	6:M:50:PRO:HD3	2.03	0.41
2:C:513:VAL:O	2:C:524:VAL:HG22	2.20	0.41
2:C:532:MET:HE2	2:C:533:ASP:O	2.21	0.41
3:D:62:LYS:HD2	3:D:75:ARG:HD2	2.03	0.41
3:D:129:PHE:CE1	3:D:571:LYS:HE2	2.56	0.41
3:D:186:VAL:HG12	3:D:187:LYS:N	2.36	0.41
3:D:298:VAL:HB	3:D:302:GLN:HG2	2.03	0.41
3:D:618:LEU:HD13	3:D:618:LEU:HA	1.87	0.41
3:D:623:VAL:HB	3:D:748:HIS:CE1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:984:THR:O	3:D:988:ARG:HB2	2.20	0.41
3:D:1076:GLY:O	3:D:1079:LYS:HB3	2.21	0.41
4:E:39:VAL:HG21	4:E:72:ARG:HB2	2.02	0.41
1:G:133:GLU:CD	2:I:605:LYS:HB2	2.45	0.41
1:G:170:ILE:HG23	2:I:696:LYS:HD3	2.02	0.41
1:H:100:ILE:HG22	1:H:141:GLU:HB3	2.02	0.41
2:I:1002:GLU:HA	3:J:724:GLN:OE1	2.20	0.41
5:L:279:MET:O	5:L:283:ILE:HG13	2.20	0.41
7:R:19:DT:H1'	7:R:20:DT:H5'	2.03	0.41
1:A:63:HIS:CE1	1:A:66:SER:H	2.37	0.41
2:C:872:ASN:OD1	2:C:874:LEU:HB2	2.20	0.41
2:C:1002:GLU:HA	3:D:724:GLN:OE1	2.21	0.41
3:D:638:LYS:HA	3:D:932:ASP:OD1	2.20	0.41
3:D:649:ALA:HB3	3:D:720:LEU:HD21	2.02	0.41
3:D:669:ASN:HD22	5:F:364:LEU:HD21	1.85	0.41
3:D:873:LEU:HD22	3:D:875:THR:HG23	2.02	0.41
5:F:370:GLU:O	5:F:373:LEU:HB3	2.21	0.41
5:F:381:ALA:O	5:F:385:LYS:HG3	2.20	0.41
1:G:82:LEU:O	1:G:85:LEU:HB3	2.20	0.41
1:H:76:VAL:O	1:H:80:LEU:HD22	2.21	0.41
1:H:85:LEU:HD12	1:H:124:ASN:HB3	2.02	0.41
2:I:349:ALA:O	2:I:353:ARG:HG2	2.20	0.41
2:I:594:ALA:HB1	2:I:654:LEU:HD11	2.01	0.41
2:I:1022:GLY:HA3	3:J:622:ARG:CZ	2.50	0.41
3:J:781:PRO:O	3:J:908:LYS:NZ	2.50	0.41
3:J:886:VAL:HG12	3:J:896:ALA:HB1	2.03	0.41
5:L:141:LEU:O	5:L:145:VAL:HG23	2.21	0.41
6:N:79:ARG:HB3	6:N:111:GLN:OE1	2.20	0.41
1:A:36:LEU:O	1:A:39:PRO:HD2	2.20	0.41
1:B:212:ASN:O	1:B:215:VAL:HG22	2.21	0.41
2:C:64:LEU:HD22	2:C:359:MET:SD	2.60	0.41
2:C:140:ILE:HB	2:C:333:ILE:HD13	2.03	0.41
2:C:325:ILE:HG23	2:C:326:ASP:H	1.86	0.41
2:C:754:ILE:HA	2:C:791:ARG:HA	2.02	0.41
2:C:1085:PHE:O	2:C:1089:VAL:HG23	2.21	0.41
3:D:1014:ASN:O	3:D:1016:PRO:HD3	2.20	0.41
5:F:206:ASN:O	5:F:209:LEU:HB3	2.21	0.41
2:I:161:SER:HA	2:I:172:ILE:O	2.21	0.41
2:I:1017:THR:OG1	2:I:1019:GLN:HG2	2.20	0.41
2:I:1018:GLN:HB2	2:I:1058:ASP:HB2	2.01	0.41
2:I:1052:MET:HE1	3:J:623:VAL:HG21	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1085:PHE:O	2:I:1089:VAL:HG23	2.20	0.41
3:J:129:PHE:CE1	3:J:571:LYS:HE2	2.55	0.41
3:J:171:LEU:HD23	3:J:172:PRO:O	2.21	0.41
3:J:646:LYS:HE3	3:J:688:TRP:HZ2	1.86	0.41
3:J:1335:LEU:HA	3:J:1338:ALA:HB3	2.03	0.41
5:L:233:GLN:HG3	5:L:236:ILE:HD12	2.03	0.41
6:M:13:PRO:HD2	6:M:58:GLY:O	2.20	0.41
6:M:21:ALA:N	6:M:37:GLN:O	2.54	0.41
6:M:129:LEU:O	6:M:133:ILE:HG12	2.21	0.41
6:M:142:GLN:HE21	6:M:142:GLN:HB3	1.66	0.41
1:A:133:GLU:CD	2:C:605:LYS:HB2	2.45	0.41
2:C:70:GLU:CD	2:C:70:GLU:H	2.24	0.41
2:C:230:ARG:NH2	2:C:231:PRO:HD2	2.29	0.41
2:C:598:GLU:HG2	2:C:615:TYR:CE2	2.56	0.41
2:C:1037:VAL:HG12	2:C:1041:GLU:OE2	2.20	0.41
3:D:354:ILE:HD11	3:D:369:ALA:HB2	2.02	0.41
3:D:430:GLU:O	3:D:431:ILE:HB	2.20	0.41
3:D:1278:ASP:OD2	3:D:1321:ALA:N	2.54	0.41
4:E:6:ILE:HG23	4:E:7:ASP:H	1.85	0.41
4:E:66:LYS:HA	4:E:69:LEU:HB2	2.02	0.41
1:G:150:TYR:HE1	1:G:168:ASP:HB3	1.86	0.41
2:I:66:LEU:HD11	2:I:372:LEU:HD23	2.03	0.41
2:I:872:ASN:OD1	2:I:874:LEU:HB2	2.21	0.41
3:J:181:ASP:HB3	3:J:357:GLU:HG3	2.02	0.41
3:J:494:LYS:O	3:J:497:GLU:HB3	2.19	0.41
3:J:514:LEU:HD11	3:J:516:ALA:O	2.21	0.41
3:J:659:LYS:O	3:J:662:GLU:HB3	2.20	0.41
3:J:894:LYS:H	3:J:894:LYS:HG2	1.54	0.41
3:J:1076:GLY:O	3:J:1079:LYS:HB3	2.21	0.41
5:L:208:ARG:HH21	7:R:31:DG:H8	1.69	0.41
1:A:122:ILE:HG13	1:A:124:ASN:H	1.86	0.41
2:C:206:THR:HG22	2:C:209:ARG:NH2	2.36	0.41
2:C:249:LYS:HE2	2:C:249:LYS:HB3	1.88	0.41
2:C:437:ARG:NH2	2:C:469:THR:HG22	2.36	0.41
2:C:751:PRO:HB2	2:C:794:PRO:HA	2.03	0.41
2:C:1035:MET:HG2	2:C:1036:GLU:N	2.36	0.41
2:C:1051:GLU:OE1	2:C:1055:ILE:HD12	2.21	0.41
2:C:1052:MET:HE1	3:D:623:VAL:HG21	2.03	0.41
3:D:7:LYS:HE3	3:D:1458:GLU:OE1	2.21	0.41
3:D:56:TYR:HE2	3:D:82:ARG:HE	1.69	0.41
3:D:103:TRP:CE2	3:D:1444:THR:HG23	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:122:GLU:HG2	3:D:152:LEU:HD21	2.03	0.41
3:D:206:ARG:HA	3:D:206:ARG:HD3	1.76	0.41
3:D:299:GLU:O	3:D:302:GLN:HB3	2.21	0.41
3:D:352:ASN:O	3:D:368:VAL:HG13	2.21	0.41
3:D:490:ALA:O	3:D:493:ARG:HB3	2.21	0.41
3:D:553:ARG:NH2	5:F:226:ASP:OD1	2.47	0.41
3:D:569:ASN:O	3:D:572:ARG:HB3	2.21	0.41
3:D:653:PHE:HB2	3:D:691:LEU:HD11	2.02	0.41
3:D:1072:ILE:H	3:D:1072:ILE:HG13	1.69	0.41
3:D:1130:ARG:CZ	3:D:1130:ARG:HB3	2.51	0.41
5:F:233:GLN:HG3	5:F:236:ILE:HD12	2.03	0.41
5:F:252:THR:HG23	7:O:29:DC:H41	1.86	0.41
5:F:376:LEU:HD21	5:F:423:LEU:HG	2.02	0.41
1:G:36:LEU:O	1:G:39:PRO:HD2	2.20	0.41
1:G:99:LEU:HD13	1:G:144:VAL:HG23	2.03	0.41
2:I:217:LEU:H	2:I:217:LEU:HG	1.58	0.41
2:I:229:MET:HE2	2:I:233:GLU:HG2	2.03	0.41
2:I:608:GLY:HA2	2:I:641:PRO:HG2	2.03	0.41
2:I:673:LEU:H	2:I:673:LEU:HD12	1.85	0.41
2:I:885:ILE:HG22	2:I:889:HIS:NE2	2.36	0.41
2:I:1082:PRO:CG	3:J:1469:GLY:HA3	2.50	0.41
2:I:1115:LEU:HD23	3:J:85:VAL:HG12	2.02	0.41
3:J:21:TRP:HE3	3:J:90:MET:HE1	1.86	0.41
3:J:39:PRO:HB3	3:J:46:ASP:HA	2.03	0.41
3:J:54:LYS:HD3	3:J:55:ASP:N	2.35	0.41
3:J:392:SER:C	3:J:393:ILE:HG13	2.46	0.41
3:J:770:LEU:HD23	3:J:777:PRO:HA	2.03	0.41
3:J:873:LEU:HD22	3:J:875:THR:HG23	2.01	0.41
3:J:984:THR:O	3:J:988:ARG:HB2	2.20	0.41
3:J:1101:VAL:HG13	3:J:1102:ALA:H	1.86	0.41
5:L:114:GLU:OE1	5:L:249:LYS:HD2	2.21	0.41
5:L:237:ARG:NH1	5:L:241:LYS:HD2	2.36	0.41
5:L:293:LEU:HD13	5:L:301:PRO:HG3	2.02	0.41
8:P:21:DA:H4'	8:P:22:DT:OP1	2.21	0.41
8:S:5:DC:H2'	8:S:6:DC:C5	2.56	0.41
2:C:6:PHE:HE1	2:C:901:TYR:CD1	2.30	0.41
2:C:552:HIS:ND1	3:D:1061:PHE:O	2.49	0.41
2:C:578:VAL:HG23	2:C:671:ASN:CG	2.45	0.41
2:C:1044:GLY:O	3:D:1476:THR:HG23	2.21	0.41
3:D:114:THR:O	3:D:495:ARG:HG3	2.20	0.41
3:D:440:VAL:HG13	3:D:441:ARG:H	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:970:LYS:HG2	3:D:995:LEU:HD13	2.03	0.41
3:D:1023:MET:HE3	3:D:1023:MET:HB2	1.90	0.41
3:D:1101:VAL:HG13	3:D:1102:ALA:H	1.85	0.41
5:F:293:LEU:HD13	5:F:301:PRO:HG3	2.02	0.41
1:G:231:SER:C	1:G:232:LEU:HD12	2.46	0.41
1:H:176:ARG:HD2	3:J:884:ARG:NH2	2.32	0.41
2:I:9:ILE:H	2:I:9:ILE:HG13	1.70	0.41
2:I:893:ALA:HB2	2:I:918:LEU:HD13	2.03	0.41
3:J:67:ARG:HH11	5:L:394:ARG:NH1	2.19	0.41
3:J:114:THR:O	3:J:495:ARG:HG3	2.21	0.41
3:J:122:GLU:HG2	3:J:152:LEU:HD21	2.03	0.41
3:J:646:LYS:HD2	3:J:722:GLU:OE1	2.20	0.41
3:J:970:LYS:HG2	3:J:995:LEU:HD13	2.03	0.41
3:J:1306:PRO:HB2	3:J:1308:ASP:OD1	2.20	0.41
5:L:246:ARG:HG3	7:R:26:DA:N1	2.35	0.41
6:N:20:VAL:C	6:N:39:ASP:H	2.29	0.41
8:P:42:DT:H2''	8:P:43:DG:C8	2.56	0.41
1:B:58:ILE:HG23	1:B:140:MET:HB3	2.03	0.40
2:C:32:ALA:HB1	2:C:73:ILE:HD13	2.03	0.40
2:C:66:LEU:HD22	2:C:98:LEU:HD12	2.03	0.40
2:C:599:GLU:HA	2:C:651:LYS:HB3	2.03	0.40
3:D:236:TYR:HB3	3:D:313:LEU:HD13	2.03	0.40
3:D:273:ARG:HE	3:D:278:VAL:HG12	1.86	0.40
1:H:212:ASN:O	1:H:215:VAL:HG22	2.22	0.40
3:J:176:ASP:HA	3:J:389:GLU:HA	2.03	0.40
3:J:683:ILE:H	3:J:683:ILE:HG12	1.67	0.40
3:J:1130:ARG:CZ	3:J:1130:ARG:HB3	2.51	0.40
5:L:379:ARG:HG3	5:L:405:PHE:CE2	2.56	0.40
7:R:17:DA:H1'	7:R:18:DA:H5''	2.03	0.40
1:A:99:LEU:HB2	1:A:142:VAL:HG23	2.03	0.40
2:C:690:ILE:HB	2:C:852:ILE:HG23	2.03	0.40
3:D:118:LEU:HD13	3:D:122:GLU:OE2	2.21	0.40
3:D:276:GLU:HG2	3:D:277:GLU:H	1.86	0.40
3:D:689:ASP:O	3:D:692:GLU:HB2	2.20	0.40
3:D:691:LEU:O	3:D:695:ILE:HG13	2.20	0.40
3:D:1266:ARG:CD	7:O:42:DC:H5''	2.51	0.40
5:F:111:LEU:H	5:F:111:LEU:HD22	1.86	0.40
1:G:60:ASP:O	1:G:61:VAL:HB	2.21	0.40
2:I:109:LYS:HE2	6:N:40:PHE:CZ	2.57	0.40
2:I:170:PRO:HB3	7:R:36:DC:H42	1.86	0.40
2:I:598:GLU:HG2	2:I:615:TYR:CE2	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:769:PRO:HD3	3:J:65:ARG:HH12	1.86	0.40
2:I:950:LEU:HD23	2:I:950:LEU:H	1.86	0.40
2:I:972:VAL:HG12	2:I:973:VAL:H	1.86	0.40
5:L:257:TRP:O	5:L:260:GLN:HB3	2.22	0.40
5:L:260:GLN:HB2	7:R:25:DT:O4	2.22	0.40
5:L:388:LYS:HA	5:L:388:LYS:HD3	1.73	0.40
1:A:170:ILE:HG23	2:C:696:LYS:HD3	2.03	0.40
2:C:608:GLY:HA2	2:C:641:PRO:HG2	2.03	0.40
2:C:710:ILE:HB	2:C:790:LEU:HD13	2.03	0.40
2:C:810:ASP:O	2:C:813:VAL:HG12	2.20	0.40
3:D:70:GLY:HA2	3:D:79:GLU:HG3	2.03	0.40
3:D:116:LEU:HD21	3:D:465:LEU:HG	2.03	0.40
3:D:161:LEU:HA	3:D:161:LEU:HD12	1.78	0.40
3:D:646:LYS:HE3	3:D:688:TRP:HZ2	1.86	0.40
3:D:731:LEU:HD13	3:D:731:LEU:HA	1.93	0.40
1:H:176:ARG:HG2	1:H:177:VAL:N	2.36	0.40
2:I:724:ARG:O	2:I:734:LEU:HD11	2.21	0.40
3:J:124:GLU:HG3	3:J:125:GLN:N	2.37	0.40
3:J:213:VAL:HG22	3:J:385:VAL:HG12	2.03	0.40
3:J:537:THR:O	5:L:332:LEU:N	2.54	0.40
6:N:63:LEU:HD11	6:N:102:PRO:HB2	2.04	0.40
1:B:44:LEU:HA	1:B:48:ILE:HD13	2.04	0.40
2:C:17:PRO:HA	2:C:590:ASP:OD1	2.21	0.40
2:C:630:ARG:HE	2:C:707:ARG:HH11	1.70	0.40
3:D:247:GLU:O	3:D:249:TYR:N	2.51	0.40
3:D:786:ILE:H	3:D:786:ILE:HG13	1.70	0.40
4:E:27:ALA:HB1	4:E:60:ALA:CB	2.51	0.40
4:E:41:GLU:HB2	4:E:43:GLU:OE2	2.22	0.40
5:F:141:LEU:O	5:F:145:VAL:HG23	2.21	0.40
5:F:237:ARG:NH1	5:F:241:LYS:HD2	2.37	0.40
1:G:58:ILE:HG23	1:G:139:TYR:O	2.21	0.40
1:H:115:THR:HA	1:H:116:PRO:HD3	1.90	0.40
2:I:72:ARG:CB	2:I:95:TYR:HB2	2.44	0.40
2:I:219:GLN:H	2:I:219:GLN:HG3	1.60	0.40
2:I:391:LEU:CD2	2:I:415:PRO:HD2	2.50	0.40
3:J:116:LEU:HD21	3:J:465:LEU:HG	2.03	0.40
3:J:928:ALA:HA	3:J:931:LEU:HD12	2.03	0.40
1:A:40:LEU:HD23	1:A:40:LEU:HA	1.91	0.40
2:C:64:LEU:HD13	2:C:359:MET:HB2	2.04	0.40
2:C:185:LYS:HG2	2:C:190:LYS:HA	2.04	0.40
2:C:291:VAL:HG13	2:C:303:PHE:HE1	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:713:ARG:HA	2:C:819:VAL:HA	2.03	0.40
3:D:318:THR:O	3:D:337:LEU:HG	2.22	0.40
3:D:626:SER:HB3	3:D:748:HIS:CE1	2.56	0.40
3:D:1135:ARG:O	3:D:1140:ILE:HD11	2.21	0.40
4:E:59:ASN:HD21	4:E:61:VAL:HG23	1.86	0.40
5:F:271:ARG:H	5:F:271:ARG:HE	1.69	0.40
1:G:122:ILE:HG13	1:G:124:ASN:H	1.86	0.40
1:H:44:LEU:HA	1:H:48:ILE:HD13	2.04	0.40
2:I:6:PHE:HE1	2:I:901:TYR:CD1	2.31	0.40
2:I:174:LEU:HD23	2:I:174:LEU:HA	1.84	0.40
2:I:206:THR:HG22	2:I:209:ARG:NH2	2.36	0.40
2:I:578:VAL:HG23	2:I:671:ASN:CG	2.46	0.40
2:I:669:GLY:HA3	2:I:994:ILE:O	2.22	0.40
2:I:713:ARG:HA	2:I:819:VAL:HA	2.03	0.40
3:J:209:ARG:HA	3:J:347:VAL:CG1	2.51	0.40
3:J:374:GLU:HG3	3:J:375:GLU:N	2.36	0.40
3:J:784:ASP:O	3:J:787:LEU:HB3	2.22	0.40
3:J:1107:VAL:HG23	3:J:1221:VAL:HG11	2.03	0.40
3:J:1114:THR:OG1	3:J:1116:ASN:ND2	2.47	0.40
3:J:1135:ARG:O	3:J:1140:ILE:HD11	2.21	0.40
4:K:6:ILE:HG23	4:K:7:ASP:H	1.87	0.40
6:M:75:LEU:HD23	6:M:75:LEU:HA	1.92	0.40
7:O:18:DA:H5'	7:O:18:DA:C8	2.56	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	225/314 (72%)	191 (85%)	32 (14%)	2 (1%)	14 49
1	B	225/314 (72%)	196 (87%)	27 (12%)	2 (1%)	14 49

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	225/314 (72%)	190 (84%)	33 (15%)	2 (1%)	14	49
1	H	225/314 (72%)	196 (87%)	27 (12%)	2 (1%)	14	49
2	C	1115/1119 (100%)	974 (87%)	137 (12%)	4 (0%)	30	66
2	I	1115/1119 (100%)	974 (87%)	137 (12%)	4 (0%)	30	66
3	D	1486/1524 (98%)	1306 (88%)	171 (12%)	9 (1%)	21	58
3	J	1361/1524 (89%)	1200 (88%)	156 (12%)	5 (0%)	30	66
4	E	91/99 (92%)	82 (90%)	9 (10%)	0	100	100
4	K	91/99 (92%)	82 (90%)	9 (10%)	0	100	100
5	F	343/347 (99%)	301 (88%)	41 (12%)	1 (0%)	36	71
5	L	343/347 (99%)	300 (88%)	42 (12%)	1 (0%)	36	71
6	M	156/164 (95%)	143 (92%)	11 (7%)	2 (1%)	9	41
6	N	156/164 (95%)	142 (91%)	12 (8%)	2 (1%)	9	41
All	All	7157/7762 (92%)	6277 (88%)	844 (12%)	36 (0%)	24	62

All (36) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	53	VAL
3	D	681	ARG
3	D	683	ILE
3	D	1128	VAL
1	G	53	VAL
3	J	681	ARG
3	J	1128	VAL
2	C	738	ASP
3	D	431	ILE
3	D	666	PHE
2	I	738	ASP
6	M	20	VAL
6	N	20	VAL
2	C	61	LYS
2	I	61	LYS
1	B	118	ALA
1	B	119	ASP
2	C	607	ASP
3	D	680	GLN
1	H	118	ALA
2	I	607	ASP

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Mol	Chain	Res	Type
3	J	680	GLN
5	F	391	ILE
1	H	119	ASP
3	J	868	TYR
5	L	391	ILE
1	A	61	VAL
2	C	1060	ILE
3	D	667	ALA
1	G	61	VAL
2	I	1060	ILE
6	M	41	PRO
6	N	41	PRO
3	D	1277	ILE
3	J	1277	ILE
3	D	238	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	194/270 (72%)	170 (88%)	24 (12%)	4	18
1	B	194/270 (72%)	163 (84%)	31 (16%)	2	13
1	G	194/270 (72%)	170 (88%)	24 (12%)	4	18
1	H	194/270 (72%)	163 (84%)	31 (16%)	2	13
2	C	931/936 (100%)	805 (86%)	126 (14%)	4	16
2	I	931/936 (100%)	806 (87%)	125 (13%)	4	16
3	D	1252/1281 (98%)	1090 (87%)	162 (13%)	4	17
3	J	1150/1281 (90%)	1004 (87%)	146 (13%)	4	17
4	E	83/88 (94%)	78 (94%)	5 (6%)	17	40
4	K	83/88 (94%)	78 (94%)	5 (6%)	17	40
5	F	296/299 (99%)	266 (90%)	30 (10%)	7	24
5	L	296/299 (99%)	264 (89%)	32 (11%)	6	22

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	M	127/133 (96%)	122 (96%)	5 (4%)	28	50
6	N	127/133 (96%)	120 (94%)	7 (6%)	19	43
All	All	6052/6554 (92%)	5299 (88%)	753 (12%)	4	18

All (753) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LYS
1	A	12	THR
1	A	28	LEU
1	A	32	PHE
1	A	36	LEU
1	A	44	LEU
1	A	51	THR
1	A	54	THR
1	A	61	VAL
1	A	79	ILE
1	A	80	LEU
1	A	83	LYS
1	A	85	LEU
1	A	86	VAL
1	A	87	VAL
1	A	113	ASP
1	A	161	ARG
1	A	174	VAL
1	A	186	LEU
1	A	195	LEU
1	A	206	THR
1	A	209	GLU
1	A	213	GLN
1	A	227	ASN
1	B	19	HIS
1	B	23	PHE
1	B	30	ARG
1	B	34	VAL
1	B	36	LEU
1	B	41	ARG
1	B	51	THR
1	B	53	VAL
1	B	54	THR
1	B	56	VAL

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Mol	Chain	Res	Type
1	B	58	ILE
1	B	62	LEU
1	B	68	ILE
1	B	74	ASP
1	B	75	VAL
1	B	80	LEU
1	B	100	ILE
1	B	114	PHE
1	B	120	VAL
1	B	138	LEU
1	B	159	LYS
1	B	162	ILE
1	B	170	ILE
1	B	177	VAL
1	B	186	LEU
1	B	193	ASP
1	B	195	LEU
1	B	215	VAL
1	B	222	LEU
1	B	227	ASN
1	B	232	LEU
2	C	5	ARG
2	C	11	GLU
2	C	13	ILE
2	C	15	LEU
2	C	19	THR
2	C	20	GLU
2	C	21	ILE
2	C	30	LEU
2	C	39	ARG
2	C	42	VAL
2	C	49	LYS
2	C	51	THR
2	C	65	VAL
2	C	69	LEU
2	C	70	GLU
2	C	80	GLN
2	C	81	ASP
2	C	85	GLU
2	C	100	LEU
2	C	103	LYS
2	C	107	LEU

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Mol	Chain	Res	Type
2	C	111	ASP
2	C	140	ILE
2	C	154	ARG
2	C	157	ARG
2	C	163	ILE
2	C	179	SER
2	C	194	VAL
2	C	195	LEU
2	C	196	LEU
2	C	198	ARG
2	C	199	VAL
2	C	209	ARG
2	C	217	LEU
2	C	219	GLN
2	C	230	ARG
2	C	242	LEU
2	C	246	ASP
2	C	252	LYS
2	C	261	LEU
2	C	285	LEU
2	C	292	ARG
2	C	297	GLU
2	C	304	LEU
2	C	317	VAL
2	C	322	VAL
2	C	325	ILE
2	C	336	VAL
2	C	361	MET
2	C	367	LEU
2	C	376	ARG
2	C	393	GLN
2	C	394	PHE
2	C	396	ASP
2	C	398	THR
2	C	410	ILE
2	C	421	GLU
2	C	426	ASP
2	C	430	VAL
2	C	433	THR
2	C	434	HIS
2	C	438	ILE
2	C	473	ARG

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Mol	Chain	Res	Type
2	C	474	VAL
2	C	490	GLU
2	C	495	THR
2	C	523	ILE
2	C	543	ASN
2	C	559	LEU
2	C	571	LEU
2	C	579	VAL
2	C	620	LEU
2	C	622	GLU
2	C	647	GLN
2	C	672	VAL
2	C	680	ASP
2	C	683	ASN
2	C	689	VAL
2	C	690	ILE
2	C	695	LEU
2	C	703	ILE
2	C	705	ILE
2	C	713	ARG
2	C	716	LYS
2	C	717	LEU
2	C	729	LEU
2	C	761	PHE
2	C	777	ILE
2	C	784	ASP
2	C	785	VAL
2	C	788	THR
2	C	790	LEU
2	C	834	GLN
2	C	848	VAL
2	C	857	ASP
2	C	861	LEU
2	C	863	ASP
2	C	867	VAL
2	C	869	VAL
2	C	871	LEU
2	C	872	ASN
2	C	876	VAL
2	C	887	GLU
2	C	890	LEU
2	C	900	ARG

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Mol	Chain	Res	Type
2	C	918	LEU
2	C	934	PHE
2	C	953	VAL
2	C	963	LEU
2	C	968	ASP
2	C	972	VAL
2	C	994	ILE
2	C	1000	MET
2	C	1015	LEU
2	C	1016	ILE
2	C	1021	LEU
2	C	1026	GLN
2	C	1035	MET
2	C	1053	LEU
2	C	1063	ARG
2	C	1071	ILE
2	C	1074	GLU
2	C	1088	LEU
2	C	1101	THR
2	C	1104	GLU
2	C	1113	GLU
3	D	5	VAL
3	D	16	GLU
3	D	18	ILE
3	D	25	GLU
3	D	32	ILE
3	D	47	GLU
3	D	49	ILE
3	D	68	PHE
3	D	69	GLU
3	D	80	VAL
3	D	92	HIS
3	D	95	LEU
3	D	103	TRP
3	D	104	PHE
3	D	112	ILE
3	D	115	LEU
3	D	118	LEU
3	D	124	GLU
3	D	127	LEU
3	D	133	ILE
3	D	145	VAL

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Mol	Chain	Res	Type
3	D	154	THR
3	D	155	ASP
3	D	175	VAL
3	D	176	ASP
3	D	196	VAL
3	D	216	LEU
3	D	225	ILE
3	D	231	VAL
3	D	233	LYS
3	D	242	LEU
3	D	245	LEU
3	D	246	SER
3	D	258	VAL
3	D	261	LEU
3	D	281	ARG
3	D	289	THR
3	D	292	VAL
3	D	296	GLU
3	D	302	GLN
3	D	311	LEU
3	D	313	LEU
3	D	316	HIS
3	D	333	LEU
3	D	335	LEU
3	D	338	GLU
3	D	344	ASP
3	D	350	HIS
3	D	362	GLN
3	D	371	ILE
3	D	389	GLU
3	D	406	ASP
3	D	421	LEU
3	D	423	ASP
3	D	430	GLU
3	D	439	LEU
3	D	440	VAL
3	D	445	ARG
3	D	464	LEU
3	D	497	GLU
3	D	547	LEU
3	D	574	LEU
3	D	582	ILE

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Mol	Chain	Res	Type
3	D	600	LEU
3	D	614	PHE
3	D	618	LEU
3	D	619	LEU
3	D	621	LYS
3	D	623	VAL
3	D	639	LEU
3	D	650	LEU
3	D	651	GLU
3	D	658	LEU
3	D	660	LYS
3	D	687	VAL
3	D	688	TRP
3	D	694	VAL
3	D	701	LEU
3	D	708	LEU
3	D	717	GLN
3	D	748	HIS
3	D	749	VAL
3	D	768	ASN
3	D	776	GLU
3	D	780	LYS
3	D	789	LEU
3	D	795	VAL
3	D	817	GLU
3	D	833	GLU
3	D	850	LEU
3	D	861	GLN
3	D	863	VAL
3	D	865	THR
3	D	873	LEU
3	D	880	ILE
3	D	899	LEU
3	D	901	GLN
3	D	903	ASP
3	D	908	LYS
3	D	912	LYS
3	D	914	LEU
3	D	925	GLU
3	D	934	LEU
3	D	958	GLU
3	D	959	GLU

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Mol	Chain	Res	Type
3	D	964	LEU
3	D	965	GLU
3	D	971	LEU
3	D	976	GLN
3	D	991	GLN
3	D	993	ILE
3	D	1015	TYR
3	D	1025	GLN
3	D	1078	ARG
3	D	1086	LEU
3	D	1094	LEU
3	D	1100	ASP
3	D	1101	VAL
3	D	1118	ILE
3	D	1122	LEU
3	D	1130	ARG
3	D	1132	LEU
3	D	1136	LYS
3	D	1140	ILE
3	D	1144	LEU
3	D	1149	LEU
3	D	1158	ARG
3	D	1160	LEU
3	D	1161	GLU
3	D	1169	GLU
3	D	1184	ARG
3	D	1200	VAL
3	D	1213	ARG
3	D	1229	ILE
3	D	1267	ARG
3	D	1269	LYS
3	D	1277	ILE
3	D	1278	ASP
3	D	1285	GLU
3	D	1301	LYS
3	D	1302	GLU
3	D	1305	LEU
3	D	1308	ASP
3	D	1318	TYR
3	D	1325	LEU
3	D	1335	LEU
3	D	1342	GLU

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Mol	Chain	Res	Type
3	D	1356	TYR
3	D	1371	VAL
3	D	1376	LEU
3	D	1395	LEU
3	D	1396	GLU
3	D	1421	LEU
3	D	1442	ASN
3	D	1443	THR
3	D	1448	THR
3	D	1462	LEU
3	D	1463	LYS
3	D	1472	ILE
3	D	1492	LEU
3	D	1497	GLU
3	D	1499	ARG
4	E	37	ASN
4	E	51	LEU
4	E	56	ASP
4	E	62	THR
4	E	79	LEU
5	F	100	LEU
5	F	108	LEU
5	F	109	LEU
5	F	137	LEU
5	F	153	THR
5	F	158	LYS
5	F	164	GLU
5	F	175	ASP
5	F	184	GLU
5	F	204	GLU
5	F	222	LEU
5	F	225	LEU
5	F	244	TYR
5	F	255	THR
5	F	268	ASP
5	F	271	ARG
5	F	279	MET
5	F	282	THR
5	F	291	ARG
5	F	293	LEU
5	F	306	ILE
5	F	319	VAL

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Mol	Chain	Res	Type
5	F	322	THR
5	F	323	LEU
5	F	336	ILE
5	F	353	LEU
5	F	370	GLU
5	F	376	LEU
5	F	386	LEU
5	F	420	LEU
1	G	7	LYS
1	G	12	THR
1	G	28	LEU
1	G	32	PHE
1	G	36	LEU
1	G	44	LEU
1	G	51	THR
1	G	54	THR
1	G	61	VAL
1	G	79	ILE
1	G	80	LEU
1	G	83	LYS
1	G	85	LEU
1	G	86	VAL
1	G	87	VAL
1	G	113	ASP
1	G	161	ARG
1	G	174	VAL
1	G	186	LEU
1	G	195	LEU
1	G	206	THR
1	G	209	GLU
1	G	213	GLN
1	G	227	ASN
1	H	19	HIS
1	H	23	PHE
1	H	30	ARG
1	H	34	VAL
1	H	36	LEU
1	H	41	ARG
1	H	51	THR
1	H	53	VAL
1	H	54	THR
1	H	56	VAL

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Mol	Chain	Res	Type
1	H	58	ILE
1	H	62	LEU
1	H	68	ILE
1	H	74	ASP
1	H	75	VAL
1	H	80	LEU
1	H	100	ILE
1	H	114	PHE
1	H	120	VAL
1	H	138	LEU
1	H	159	LYS
1	H	162	ILE
1	H	170	ILE
1	H	177	VAL
1	H	186	LEU
1	H	193	ASP
1	H	195	LEU
1	H	215	VAL
1	H	222	LEU
1	H	227	ASN
1	H	232	LEU
2	I	5	ARG
2	I	11	GLU
2	I	13	ILE
2	I	15	LEU
2	I	19	THR
2	I	20	GLU
2	I	21	ILE
2	I	30	LEU
2	I	39	ARG
2	I	42	VAL
2	I	49	LYS
2	I	51	THR
2	I	65	VAL
2	I	69	LEU
2	I	70	GLU
2	I	80	GLN
2	I	81	ASP
2	I	85	GLU
2	I	100	LEU
2	I	103	LYS
2	I	107	LEU

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Mol	Chain	Res	Type
2	I	111	ASP
2	I	140	ILE
2	I	154	ARG
2	I	157	ARG
2	I	163	ILE
2	I	179	SER
2	I	194	VAL
2	I	195	LEU
2	I	196	LEU
2	I	198	ARG
2	I	199	VAL
2	I	209	ARG
2	I	217	LEU
2	I	219	GLN
2	I	230	ARG
2	I	242	LEU
2	I	246	ASP
2	I	252	LYS
2	I	261	LEU
2	I	285	LEU
2	I	292	ARG
2	I	297	GLU
2	I	304	LEU
2	I	317	VAL
2	I	322	VAL
2	I	325	ILE
2	I	336	VAL
2	I	361	MET
2	I	367	LEU
2	I	376	ARG
2	I	393	GLN
2	I	394	PHE
2	I	396	ASP
2	I	398	THR
2	I	410	ILE
2	I	421	GLU
2	I	426	ASP
2	I	430	VAL
2	I	433	THR
2	I	434	HIS
2	I	438	ILE
2	I	473	ARG

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Mol	Chain	Res	Type
2	I	474	VAL
2	I	490	GLU
2	I	495	THR
2	I	523	ILE
2	I	543	ASN
2	I	571	LEU
2	I	579	VAL
2	I	620	LEU
2	I	622	GLU
2	I	647	GLN
2	I	672	VAL
2	I	680	ASP
2	I	683	ASN
2	I	689	VAL
2	I	690	ILE
2	I	695	LEU
2	I	703	ILE
2	I	705	ILE
2	I	713	ARG
2	I	716	LYS
2	I	717	LEU
2	I	729	LEU
2	I	761	PHE
2	I	777	ILE
2	I	784	ASP
2	I	785	VAL
2	I	788	THR
2	I	790	LEU
2	I	815	LEU
2	I	834	GLN
2	I	848	VAL
2	I	857	ASP
2	I	861	LEU
2	I	863	ASP
2	I	867	VAL
2	I	869	VAL
2	I	871	LEU
2	I	872	ASN
2	I	876	VAL
2	I	887	GLU
2	I	890	LEU
2	I	900	ARG

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Mol	Chain	Res	Type
2	I	918	LEU
2	I	934	PHE
2	I	953	VAL
2	I	963	LEU
2	I	968	ASP
2	I	972	VAL
2	I	994	ILE
2	I	1000	MET
2	I	1015	LEU
2	I	1016	ILE
2	I	1021	LEU
2	I	1026	GLN
2	I	1035	MET
2	I	1053	LEU
2	I	1071	ILE
2	I	1074	GLU
2	I	1088	LEU
2	I	1101	THR
2	I	1104	GLU
2	I	1113	GLU
3	J	5	VAL
3	J	16	GLU
3	J	18	ILE
3	J	25	GLU
3	J	32	ILE
3	J	47	GLU
3	J	49	ILE
3	J	68	PHE
3	J	69	GLU
3	J	80	VAL
3	J	92	HIS
3	J	95	LEU
3	J	103	TRP
3	J	104	PHE
3	J	112	ILE
3	J	115	LEU
3	J	118	LEU
3	J	124	GLU
3	J	127	LEU
3	J	128	TYR
3	J	133	ILE
3	J	145	VAL

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Mol	Chain	Res	Type
3	J	154	THR
3	J	155	ASP
3	J	166	GLN
3	J	175	VAL
3	J	186	VAL
3	J	187	LYS
3	J	196	VAL
3	J	204	LEU
3	J	347	VAL
3	J	355	VAL
3	J	371	ILE
3	J	387	LEU
3	J	393	ILE
3	J	394	LEU
3	J	400	VAL
3	J	407	VAL
3	J	410	THR
3	J	415	VAL
3	J	421	LEU
3	J	430	GLU
3	J	435	VAL
3	J	440	VAL
3	J	464	LEU
3	J	497	GLU
3	J	547	LEU
3	J	574	LEU
3	J	582	ILE
3	J	600	LEU
3	J	614	PHE
3	J	618	LEU
3	J	619	LEU
3	J	621	LYS
3	J	623	VAL
3	J	639	LEU
3	J	650	LEU
3	J	651	GLU
3	J	658	LEU
3	J	660	LYS
3	J	687	VAL
3	J	688	TRP
3	J	694	VAL
3	J	701	LEU

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Mol	Chain	Res	Type
3	J	708	LEU
3	J	717	GLN
3	J	748	HIS
3	J	749	VAL
3	J	768	ASN
3	J	776	GLU
3	J	780	LYS
3	J	789	LEU
3	J	795	VAL
3	J	817	GLU
3	J	833	GLU
3	J	861	GLN
3	J	863	VAL
3	J	865	THR
3	J	873	LEU
3	J	880	ILE
3	J	899	LEU
3	J	901	GLN
3	J	903	ASP
3	J	908	LYS
3	J	912	LYS
3	J	914	LEU
3	J	925	GLU
3	J	934	LEU
3	J	958	GLU
3	J	959	GLU
3	J	964	LEU
3	J	965	GLU
3	J	971	LEU
3	J	976	GLN
3	J	991	GLN
3	J	993	ILE
3	J	1015	TYR
3	J	1025	GLN
3	J	1078	ARG
3	J	1086	LEU
3	J	1094	LEU
3	J	1100	ASP
3	J	1101	VAL
3	J	1118	ILE
3	J	1122	LEU
3	J	1130	ARG

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Mol	Chain	Res	Type
3	J	1132	LEU
3	J	1136	LYS
3	J	1140	ILE
3	J	1144	LEU
3	J	1149	LEU
3	J	1158	ARG
3	J	1160	LEU
3	J	1161	GLU
3	J	1184	ARG
3	J	1200	VAL
3	J	1213	ARG
3	J	1229	ILE
3	J	1267	ARG
3	J	1269	LYS
3	J	1277	ILE
3	J	1278	ASP
3	J	1285	GLU
3	J	1301	LYS
3	J	1302	GLU
3	J	1305	LEU
3	J	1308	ASP
3	J	1318	TYR
3	J	1325	LEU
3	J	1335	LEU
3	J	1342	GLU
3	J	1356	TYR
3	J	1371	VAL
3	J	1376	LEU
3	J	1395	LEU
3	J	1396	GLU
3	J	1421	LEU
3	J	1442	ASN
3	J	1443	THR
3	J	1448	THR
3	J	1462	LEU
3	J	1463	LYS
3	J	1472	ILE
3	J	1492	LEU
3	J	1497	GLU
3	J	1499	ARG
4	K	37	ASN
4	K	51	LEU

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Mol	Chain	Res	Type
4	K	56	ASP
4	K	62	THR
4	K	79	LEU
5	L	100	LEU
5	L	108	LEU
5	L	109	LEU
5	L	137	LEU
5	L	142	ILE
5	L	153	THR
5	L	158	LYS
5	L	164	GLU
5	L	175	ASP
5	L	184	GLU
5	L	204	GLU
5	L	222	LEU
5	L	225	LEU
5	L	244	TYR
5	L	255	THR
5	L	268	ASP
5	L	271	ARG
5	L	279	MET
5	L	282	THR
5	L	291	ARG
5	L	293	LEU
5	L	306	ILE
5	L	319	VAL
5	L	322	THR
5	L	323	LEU
5	L	336	ILE
5	L	353	LEU
5	L	370	GLU
5	L	386	LEU
5	L	420	LEU
5	L	433	LEU
5	L	435	ASP
6	M	8	ASP
6	M	52	GLU
6	M	70	VAL
6	M	142	GLN
6	M	157	GLU
6	N	8	ASP
6	N	31	VAL

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Mol	Chain	Res	Type
6	N	52	GLU
6	N	80	MET
6	N	124	LEU
6	N	142	GLN
6	N	157	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (144) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	GLN
1	A	19	HIS
1	A	128	HIS
1	A	156	HIS
1	A	188	GLN
1	A	213	GLN
1	B	63	HIS
1	B	81	ASN
1	B	180	GLN
1	B	213	GLN
1	B	223	ASN
2	C	80	GLN
2	C	99	GLN
2	C	102	HIS
2	C	187	ASN
2	C	204	GLN
2	C	374	ASN
2	C	434	HIS
2	C	565	GLN
2	C	647	GLN
2	C	670	GLN
2	C	683	ASN
2	C	765	GLN
2	C	829	GLN
2	C	834	GLN
2	C	899	GLN
2	C	930	GLN
2	C	999	HIS
2	C	1026	GLN
2	C	1050	GLN
2	C	1093	GLN
2	C	1107	ASN
3	D	66	GLN

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Mol	Chain	Res	Type
3	D	125	GLN
3	D	130	ASN
3	D	268	HIS
3	D	352	ASN
3	D	442	ASN
3	D	640	HIS
3	D	680	GLN
3	D	727	GLN
3	D	756	GLN
3	D	762	GLN
3	D	794	GLN
3	D	855	HIS
3	D	906	GLN
3	D	917	GLN
3	D	976	GLN
3	D	991	GLN
3	D	1103	HIS
3	D	1195	GLN
3	D	1235	GLN
3	D	1374	GLN
3	D	1442	ASN
4	E	29	GLN
4	E	37	ASN
5	F	98	GLN
5	F	200	GLN
5	F	229	GLN
5	F	233	GLN
5	F	263	ASN
5	F	269	GLN
5	F	294	GLN
5	F	295	GLN
5	F	417	ASN
5	F	426	HIS
1	G	16	GLN
1	G	19	HIS
1	G	128	HIS
1	G	156	HIS
1	G	188	GLN
1	G	212	ASN
1	G	213	GLN
1	H	63	HIS
1	H	81	ASN

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Mol	Chain	Res	Type
1	H	180	GLN
1	H	213	GLN
1	H	223	ASN
2	I	80	GLN
2	I	99	GLN
2	I	102	HIS
2	I	187	ASN
2	I	204	GLN
2	I	374	ASN
2	I	434	HIS
2	I	565	GLN
2	I	647	GLN
2	I	670	GLN
2	I	683	ASN
2	I	765	GLN
2	I	834	GLN
2	I	899	GLN
2	I	930	GLN
2	I	999	HIS
2	I	1018	GLN
2	I	1026	GLN
2	I	1050	GLN
2	I	1064	ASN
2	I	1093	GLN
3	J	66	GLN
3	J	125	GLN
3	J	130	ASN
3	J	166	GLN
3	J	362	GLN
3	J	714	GLN
3	J	727	GLN
3	J	756	GLN
3	J	762	GLN
3	J	794	GLN
3	J	855	HIS
3	J	906	GLN
3	J	917	GLN
3	J	976	GLN
3	J	991	GLN
3	J	1103	HIS
3	J	1235	GLN
3	J	1374	GLN

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Mol	Chain	Res	Type
3	J	1442	ASN
4	K	28	GLN
4	K	29	GLN
4	K	37	ASN
5	L	98	GLN
5	L	101	HIS
5	L	105	GLN
5	L	200	GLN
5	L	229	GLN
5	L	233	GLN
5	L	263	ASN
5	L	269	GLN
5	L	284	ASN
5	L	294	GLN
5	L	295	GLN
5	L	417	ASN
6	M	55	HIS
6	M	77	ASN
6	M	101	ASN
6	M	134	HIS
6	M	142	GLN
6	N	25	GLN
6	N	77	ASN
6	N	90	HIS
6	N	101	ASN
6	N	134	HIS
6	N	142	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
9	Q	3/4 (75%)	2 (66%)	0
9	T	3/4 (75%)	0	0
All	All	6/8 (75%)	2 (33%)	0

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
9	Q	2	C
9	Q	3	G

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	227/314 (72%)	0.25	3 (1%) 75 59	144, 176, 208, 241	0
1	B	227/314 (72%)	0.17	4 (1%) 67 53	143, 164, 196, 228	0
1	G	227/314 (72%)	0.32	4 (1%) 67 53	148, 188, 218, 252	0
1	H	227/314 (72%)	0.19	2 (0%) 81 66	145, 175, 207, 241	0
2	C	1117/1119 (99%)	0.33	26 (2%) 61 48	144, 172, 211, 253	0
2	I	1117/1119 (99%)	0.33	33 (2%) 52 40	144, 182, 221, 270	0
3	D	1490/1524 (97%)	0.29	29 (1%) 66 51	117, 162, 195, 251	0
3	J	1367/1524 (89%)	0.29	22 (1%) 70 55	120, 171, 204, 250	0
4	E	93/99 (93%)	0.55	4 (4%) 40 34	144, 165, 194, 217	0
4	K	93/99 (93%)	0.45	3 (3%) 50 39	144, 179, 206, 228	0
5	F	345/347 (99%)	0.33	12 (3%) 47 37	144, 179, 222, 245	0
5	L	345/347 (99%)	0.47	20 (5%) 29 28	145, 186, 225, 258	0
6	M	158/164 (96%)	0.53	10 (6%) 26 26	159, 207, 235, 243	0
6	N	158/164 (96%)	0.65	8 (5%) 33 30	171, 215, 240, 267	0
7	O	48/48 (100%)	0.35	0 100 100	157, 217, 256, 270	0
7	R	48/48 (100%)	0.26	0 100 100	163, 207, 251, 276	0
8	P	48/48 (100%)	0.42	0 100 100	161, 219, 260, 270	0
8	S	48/48 (100%)	0.46	0 100 100	161, 212, 250, 261	0
9	Q	4/4 (100%)	-0.01	0 100 100	175, 177, 186, 189	0
9	T	4/4 (100%)	-0.39	0 100 100	165, 183, 184, 196	0
All	All	7391/7962 (92%)	0.32	180 (2%) 59 47	117, 174, 219, 276	0

All (180) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	I	445	GLU	4.0
5	F	159	ILE	4.0
6	M	43	SER	3.8
6	N	160	GLY	3.8
2	C	306	THR	3.8
2	I	207	LEU	3.8
5	L	223	SER	3.7
2	I	101	ILE	3.6
5	F	223	SER	3.6
3	D	1097	LYS	3.5
2	I	221	LEU	3.5
3	J	436	GLU	3.4
4	E	24	ALA	3.4
5	F	194	GLU	3.3
5	F	341	ASP	3.3
2	I	306	THR	3.3
6	N	19	VAL	3.3
4	E	94	PRO	3.2
2	I	1080	SER	3.2
2	C	358	ARG	3.1
3	D	1486	VAL	3.1
2	I	628	TYR	3.0
1	G	13	ALA	3.0
2	C	489	SER	3.0
5	L	346	ASP	3.0
5	L	338	ASP	3.0
3	J	1195	GLN	3.0
3	D	513	ILE	3.0
2	I	166	PRO	3.0
2	C	549	PHE	2.9
2	C	201	GLY	2.9
4	K	2	ALA	2.9
2	I	570	PRO	2.9
5	F	170	THR	2.9
2	C	58	ASP	2.9
2	C	246	ASP	2.8
2	C	679	PHE	2.8
6	M	72	LEU	2.8
1	G	170	ILE	2.8
2	I	319	GLY	2.8
5	F	155	ARG	2.8
6	N	27	SER	2.8
4	E	2	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
5	F	346	ASP	2.8
5	F	162	LEU	2.7
6	M	147	THR	2.7
5	L	170	THR	2.7
5	L	207	LEU	2.7
3	D	538	SER	2.7
1	B	150	TYR	2.6
2	C	890	LEU	2.6
3	J	563	PRO	2.6
2	C	663	GLU	2.6
3	D	1263	PHE	2.6
5	L	161	GLY	2.6
2	I	222	LEU	2.6
5	L	406	GLY	2.6
2	C	123	GLU	2.6
5	L	194	GLU	2.6
3	J	593	ASN	2.6
2	I	1026	GLN	2.6
3	J	459	GLU	2.5
5	L	416	GLU	2.5
6	M	160	GLY	2.5
2	I	246	ASP	2.5
2	I	567	GLN	2.5
3	D	919	PHE	2.5
5	L	268	ASP	2.5
3	D	1484	THR	2.5
3	J	34	TYR	2.5
1	A	62	LEU	2.5
3	J	1263	PHE	2.5
1	A	56	VAL	2.5
2	C	366	THR	2.4
2	I	296	GLY	2.4
3	D	287	GLY	2.4
6	N	24	ALA	2.4
3	D	1062	ARG	2.4
3	J	1235	GLN	2.4
2	I	254	LEU	2.4
3	D	1144	LEU	2.4
6	M	27	SER	2.4
2	C	370	ALA	2.4
6	N	29	SER	2.4
2	I	272	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
2	C	194	VAL	2.4
6	M	127	GLN	2.3
2	I	105	THR	2.3
3	J	406	ASP	2.3
5	L	341	ASP	2.3
2	C	62	GLY	2.3
3	J	114	THR	2.3
3	J	437	VAL	2.3
1	B	233	LEU	2.3
3	J	1398	TRP	2.3
2	C	901	TYR	2.3
3	D	916	TYR	2.3
3	D	444	VAL	2.3
5	F	224	PHE	2.3
2	I	1016	ILE	2.3
5	F	171	VAL	2.3
3	D	648	MET	2.3
3	D	666	PHE	2.3
4	E	10	PHE	2.3
1	G	98	THR	2.2
1	G	31	GLY	2.2
2	C	207	LEU	2.2
3	D	607	LEU	2.2
3	J	1486	VAL	2.2
3	J	795	VAL	2.2
1	H	26	GLU	2.2
3	D	459	GLU	2.2
3	J	372	ASP	2.2
2	I	201	GLY	2.2
6	M	31	VAL	2.2
3	J	607	LEU	2.2
5	L	329	PRO	2.2
6	M	29	SER	2.2
2	I	906	PHE	2.2
3	J	1070	TYR	2.2
6	M	15	TYR	2.2
2	I	782	ALA	2.2
5	L	135	THR	2.2
2	I	952	LEU	2.2
3	D	159	ARG	2.2
2	C	416	GLY	2.2
2	I	146	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
3	D	1087	ARG	2.2
3	J	689	ASP	2.1
6	N	81	PRO	2.1
2	C	656	ALA	2.1
2	C	1055	ILE	2.1
2	C	936	VAL	2.1
5	L	377	SER	2.1
3	D	1355	VAL	2.1
3	D	445	ARG	2.1
3	D	1356	TYR	2.1
1	B	7	LYS	2.1
2	C	1016	ILE	2.1
5	L	220	ARG	2.1
5	L	409	ARG	2.1
4	K	60	ALA	2.1
5	L	159	ILE	2.1
5	F	409	ARG	2.1
5	L	322	THR	2.1
2	C	344	PHE	2.1
2	I	416	GLY	2.1
3	J	407	VAL	2.1
1	B	175	ARG	2.1
2	C	221	LEU	2.1
6	M	76	LYS	2.1
2	C	1027	PHE	2.1
2	I	447	ALA	2.1
2	I	896	PHE	2.1
3	D	1368	ILE	2.1
3	D	1505	ALA	2.1
6	N	101	ASN	2.1
3	J	111	LYS	2.0
5	F	99	TYR	2.0
2	I	999	HIS	2.0
3	D	1102	ALA	2.0
2	I	144	PRO	2.0
5	L	378	GLU	2.0
3	D	890	VAL	2.0
1	A	162	ILE	2.0
2	I	699	PHE	2.0
4	K	74	PHE	2.0
3	J	696	HIS	2.0
3	D	1398	TRP	2.0

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Mol	Chain	Res	Type	RSRZ
5	L	126	GLU	2.0
6	N	3	GLU	2.0
2	I	892	LEU	2.0
3	D	1122	LEU	2.0
3	J	698	LYS	2.0
3	D	1070	TYR	2.0
2	I	843	HIS	2.0
2	C	991	GLN	2.0
3	D	1148	VAL	2.0
1	H	67	THR	2.0
2	I	385	PHE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
11	MG	D	2003	1/1	0.84	0.08	283,283,283,283	0
11	MG	J	2003	1/1	0.92	0.06	270,270,270,270	0
10	ZN	J	2001	1/1	0.98	0.09	277,277,277,277	0
10	ZN	D	2002	1/1	0.99	0.07	237,237,237,237	0
10	ZN	J	2002	1/1	0.99	0.03	157,157,157,157	0
10	ZN	D	2001	1/1	1.00	0.06	116,116,116,116	0

6.5 Other polymers [i](#)

There are no such residues in this entry.