



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 08:36 am GMT

PDB ID : 4S20  
Title : Structural basis for transcription reactivation by RapA  
Authors : Liu, B.; Zuo, Y.; Steitz, T.A.  
Deposited on : 2015-01-16  
Resolution : 4.70 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28683  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

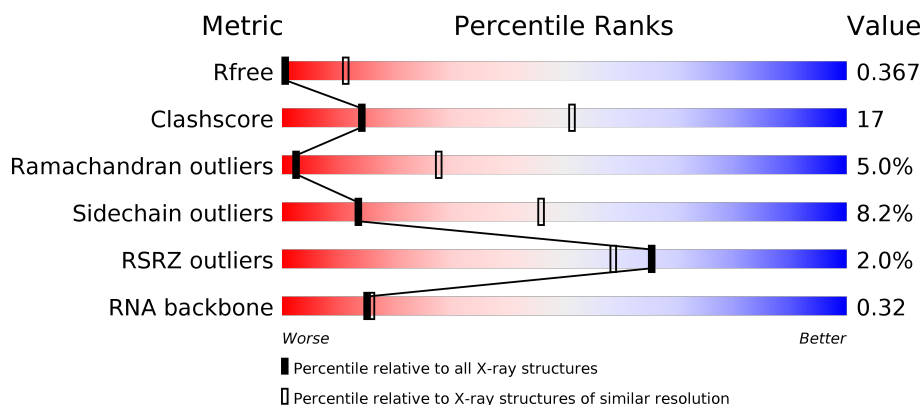
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 4.70 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))
$R_{free}$	100719	1010 (5.70-3.66)
Clashscore	112137	1059 (5.70-3.70)
Ramachandran outliers	110173	1004 (5.70-3.68)
Sidechain outliers	110143	1026 (5.70-3.66)
RSRZ outliers	101464	1019 (5.70-3.66)
RNA backbone	2435	1040 (6.46-2.90)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	329	
1	B	329	
1	F	329	
1	G	329	

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Mol	Chain	Length	Quality of chain
2	C	1342	
2	H	1342	
3	D	1416	
3	I	1416	
4	E	90	
4	J	90	
5	K	974	
5	L	974	
6	M	15	
6	O	15	
7	N	9	
7	P	9	

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 61154 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
			1759	1096	311	346	6			
1	B	227	Total	C	N	O	S	0	0	0
			1759	1096	311	346	6			
1	F	227	Total	C	N	O	S	0	0	0
			1759	1096	311	346	6			
1	G	227	Total	C	N	O	S	0	0	0
			1759	1096	311	346	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1179	Total	C	N	O	S	0	0	0
			9285	5828	1620	1798	39			
2	H	1173	Total	C	N	O	S	0	0	0
			9235	5799	1609	1788	39			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1149	Total	C	N	O	S	0	0	0
			8990	5649	1614	1681	46			
3	I	1160	Total	C	N	O	S	0	0	0
			9068	5701	1626	1695	46			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	1408	LEU	-	EXPRESSION TAG	UNP K0BCS5
D	1409	GLU	-	EXPRESSION TAG	UNP K0BCS5
D	1410	VAL	-	EXPRESSION TAG	UNP K0BCS5
D	1411	HIS	-	EXPRESSION TAG	UNP K0BCS5

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Chain	Residue	Modelled	Actual	Comment	Reference
D	1412	HIS	-	EXPRESSION TAG	UNP K0BCS5
D	1413	HIS	-	EXPRESSION TAG	UNP K0BCS5
D	1414	HIS	-	EXPRESSION TAG	UNP K0BCS5
D	1415	HIS	-	EXPRESSION TAG	UNP K0BCS5
D	1416	HIS	-	EXPRESSION TAG	UNP K0BCS5
I	1408	LEU	-	EXPRESSION TAG	UNP K0BCS5
I	1409	GLU	-	EXPRESSION TAG	UNP K0BCS5
I	1410	VAL	-	EXPRESSION TAG	UNP K0BCS5
I	1411	HIS	-	EXPRESSION TAG	UNP K0BCS5
I	1412	HIS	-	EXPRESSION TAG	UNP K0BCS5
I	1413	HIS	-	EXPRESSION TAG	UNP K0BCS5
I	1414	HIS	-	EXPRESSION TAG	UNP K0BCS5
I	1415	HIS	-	EXPRESSION TAG	UNP K0BCS5
I	1416	HIS	-	EXPRESSION TAG	UNP K0BCS5

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	75	Total	C	N	O	S	0	0	0
			600	365	114	120	1			
4	J	75	Total	C	N	O	S	0	0	0
			600	365	114	120	1			

- Molecule 5 is a protein called RNA polymerase-associated protein RapA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	K	961	Total	C	N	O	S	0	0	0
			7665	4797	1370	1468	30			
5	L	961	Total	C	N	O	S	0	0	0
			7665	4797	1370	1468	30			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	-5	HIS	-	EXPRESSION TAG	UNP P60240
K	-4	HIS	-	EXPRESSION TAG	UNP P60240
K	-3	HIS	-	EXPRESSION TAG	UNP P60240
K	-2	HIS	-	EXPRESSION TAG	UNP P60240
K	-1	HIS	-	EXPRESSION TAG	UNP P60240
K	0	HIS	-	EXPRESSION TAG	UNP P60240
K	350	CYS	ARG	ENGINEERED MUTATION	UNP P60240
L	-5	HIS	-	EXPRESSION TAG	UNP P60240

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Chain	Residue	Modelled	Actual	Comment	Reference
L	-4	HIS	-	EXPRESSION TAG	UNP P60240
L	-3	HIS	-	EXPRESSION TAG	UNP P60240
L	-2	HIS	-	EXPRESSION TAG	UNP P60240
L	-1	HIS	-	EXPRESSION TAG	UNP P60240
L	0	HIS	-	EXPRESSION TAG	UNP P60240
L	350	CYS	ARG	ENGINEERED MUTATION	UNP P60240

- Molecule 6 is a DNA chain called 5'-D(P\*AP\*CP\*GP\*AP\*CP\*TP\*GP\*AP\*GP\*CP\*CP\*GP\*AP\*TP\*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	M	15	Total	C	N	O	P	0	0	0
			311	146	61	89	15			
6	O	15	Total	C	N	O	P	0	0	0
			311	146	61	89	15			

- Molecule 7 is a RNA chain called 5'-R(P\*AP\*UP\*CP\*GP\*GP\*CP\*UP\*CP\*A)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	N	9	Total	C	N	O	P	0	0	0
			191	85	33	64	9			
7	P	9	Total	C	N	O	P	0	0	0
			191	85	33	64	9			

- Molecule 8 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	I	2	Total	Zn	0	0
			2	2		
8	D	2	Total	Zn	0	0
			2	2		

- Molecule 9 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	I	1	Total	Mg	0	0
			1	1		
9	D	1	Total	Mg	0	0
			1	1		



- Molecule 1: DNA-directed RNA polymerase subunit alpha



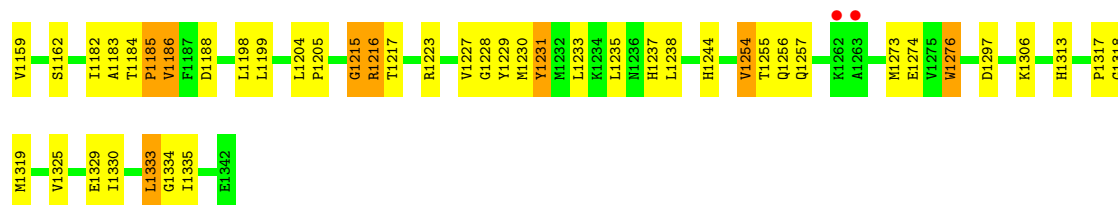
App Type	Percentage
Shopping app	62%
Social media app	7%
Productivity app	31%



Category	Percentage
Very good	1%
Good	63%
Not good	22%
Very bad	12%

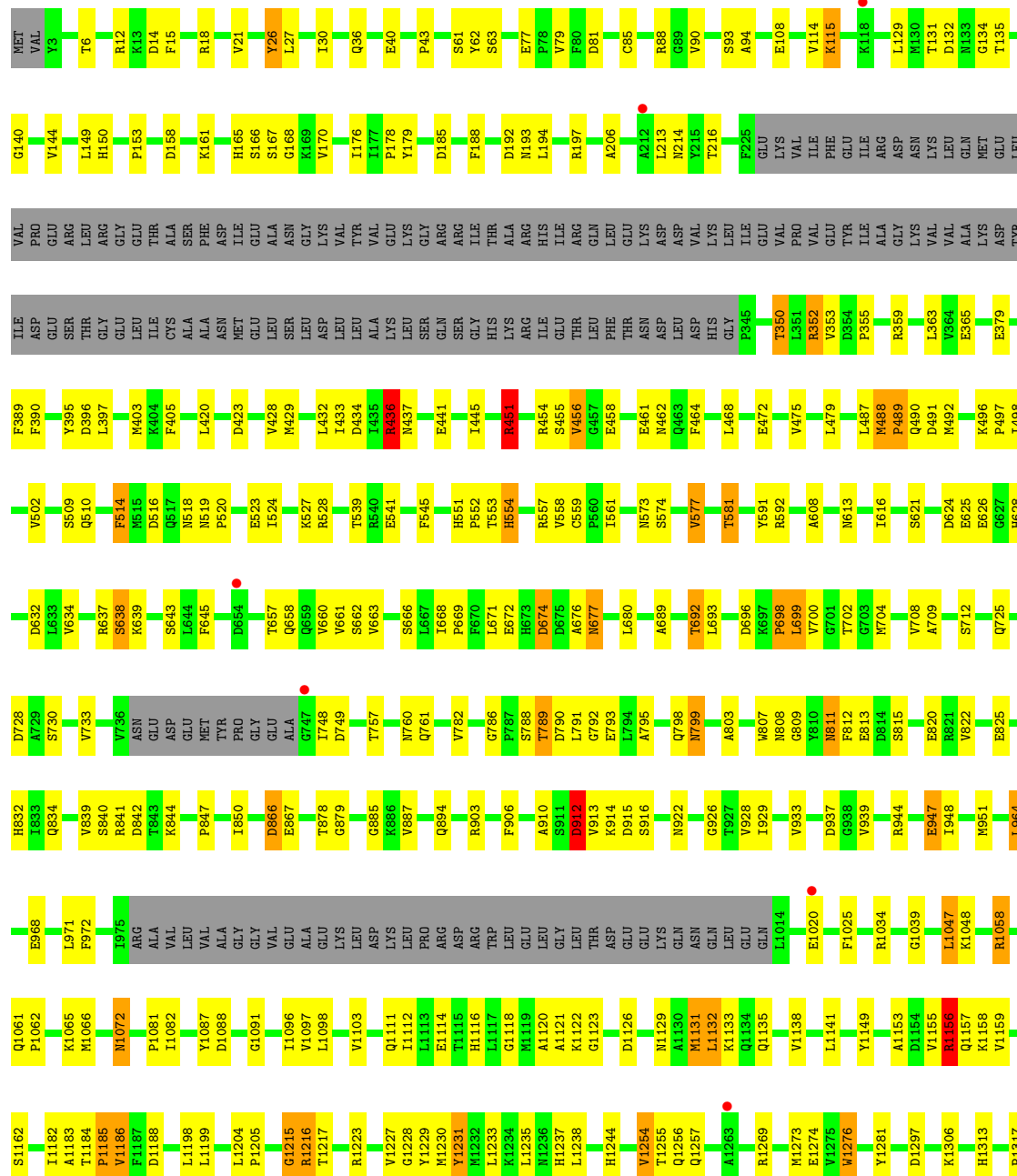




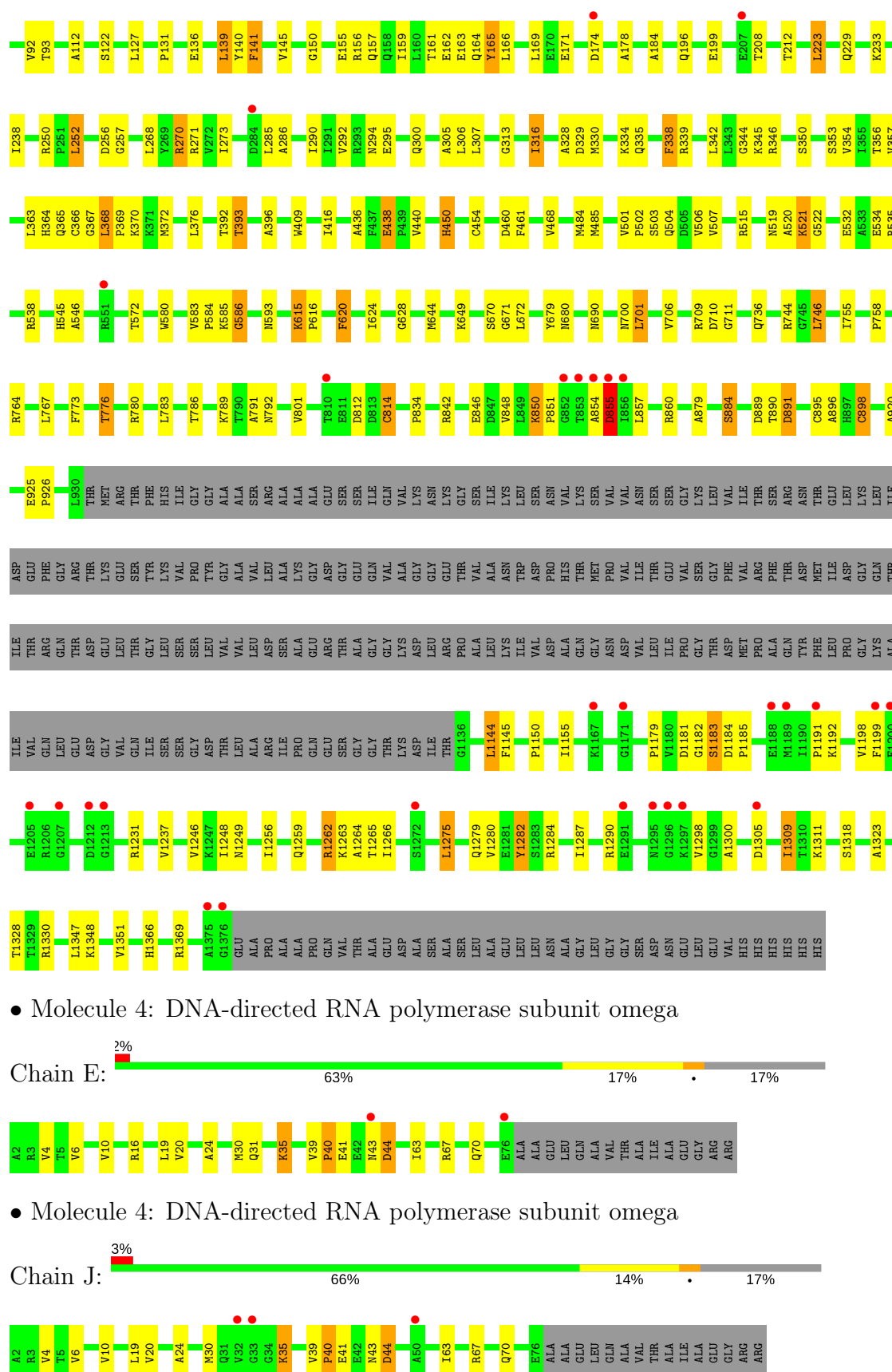


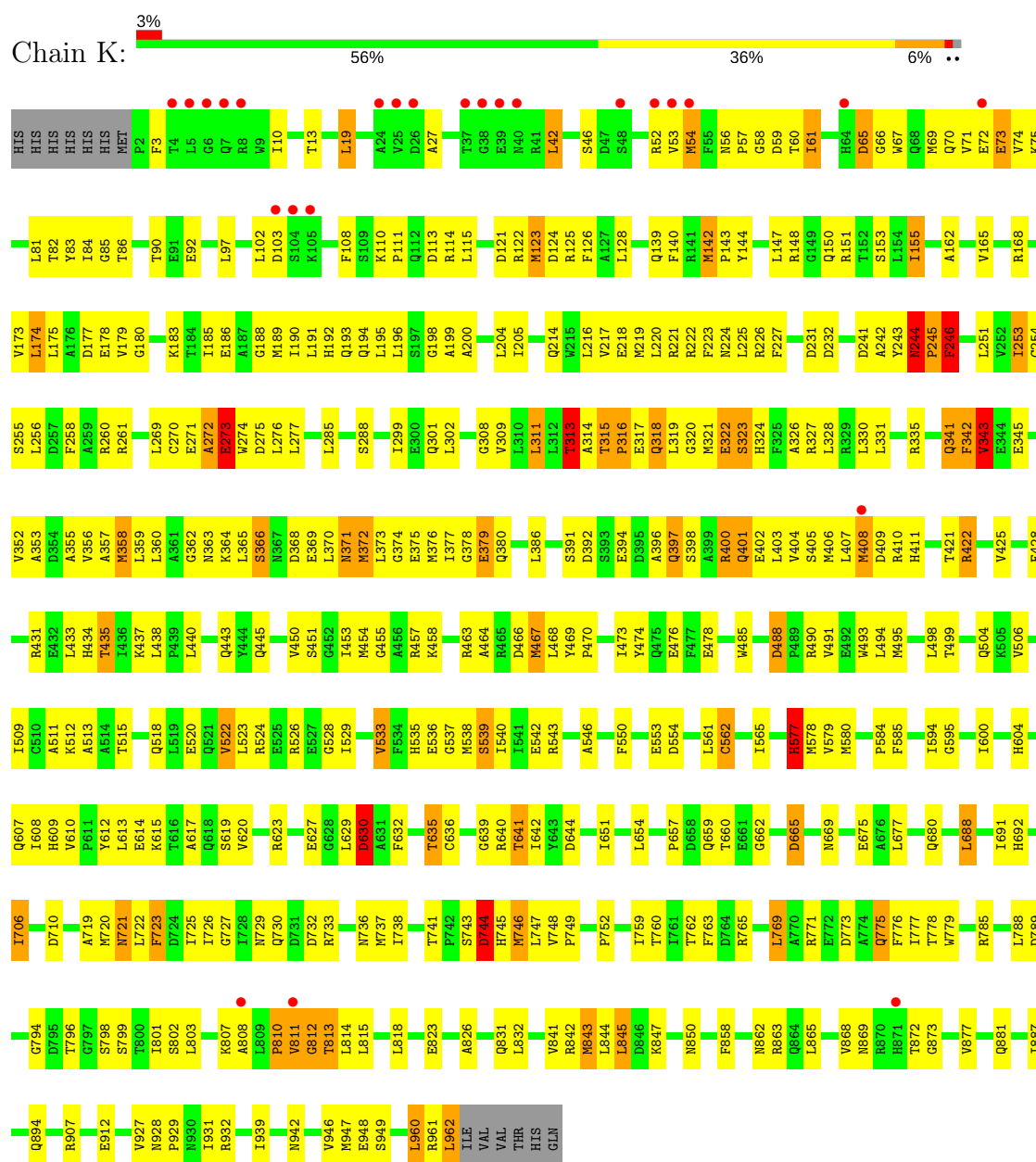
● Molecule 2: DNA-directed RNA polymerase subunit beta

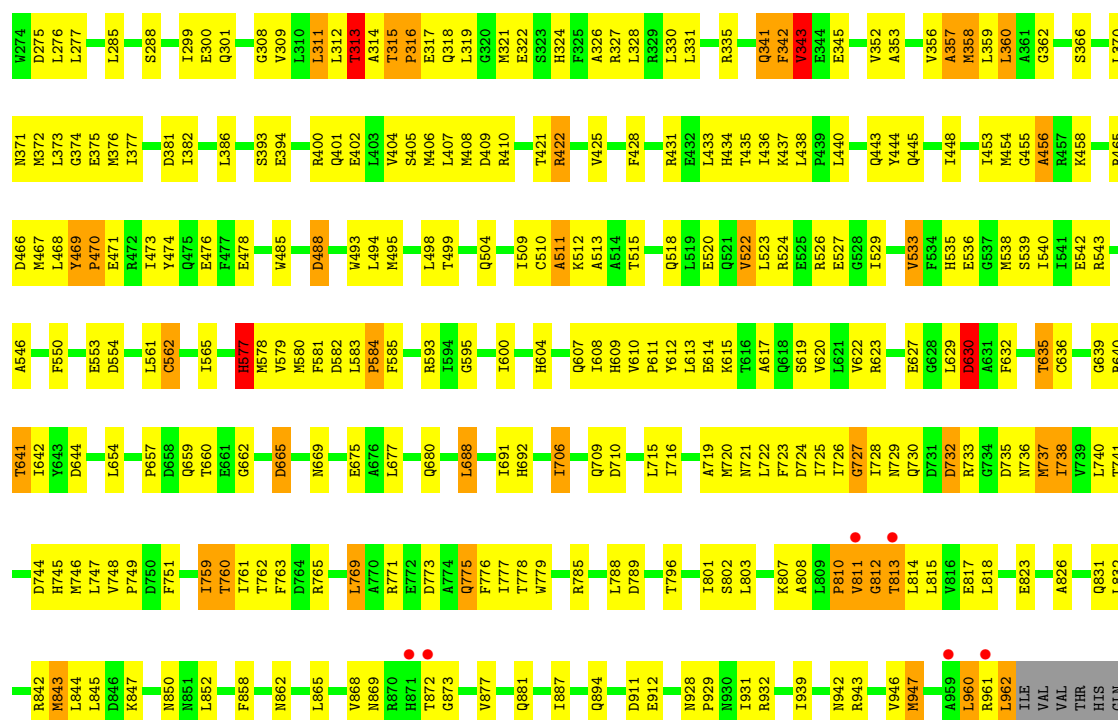
Chain H: 62% 22% 13%







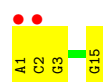
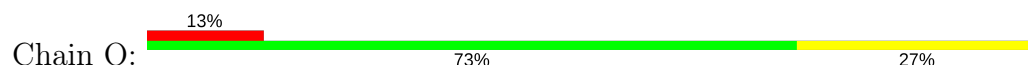




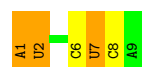
• Molecule 6: 5'-D(P\*AP\*CP\*GP\*AP\*CP\*TP\*GP\*AP\*GP\*CP\*CP\*GP\*AP\*TP\*G)-3'



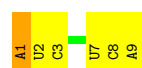
• Molecule 6: 5'-D(P\*AP\*CP\*GP\*AP\*CP\*TP\*GP\*AP\*GP\*CP\*CP\*GP\*AP\*TP\*G)-3'



• Molecule 7: 5'-R(P\*AP\*UP\*CP\*GP\*GP\*CP\*UP\*CP\*A)-3'



• Molecule 7: 5'-R(P\*AP\*UP\*CP\*GP\*GP\*CP\*UP\*CP\*A)-3'



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	336.09Å 158.93Å 255.01Å 90.00° 101.28° 90.00°	Depositor
Resolution (Å)	20.00 – 4.70 20.00 – 4.70	Depositor EDS
% Data completeness (in resolution range)	93.2 (20.00-4.70) 94.5 (20.00-4.70)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.21 (at 4.74Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, $R_{free}$	0.273 , 0.369 0.288 , 0.367	Depositor DCC
$R_{free}$ test set	3240 reflections (5.32%)	DCC
Wilson B-factor (Å <sup>2</sup> )	196.2	Xtriage
Anisotropy	0.118	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.19 , 247.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	61154	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	292.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.40% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

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	0.33	0/1781	0.54	0/2414
1	B	0.32	0/1781	0.55	0/2414
1	F	0.33	0/1781	0.54	0/2414
1	G	0.32	0/1781	0.55	0/2414
2	C	0.36	0/9435	0.60	1/12729 (0.0%)
2	H	0.35	0/9385	0.60	1/12662 (0.0%)
3	D	0.35	0/9128	0.58	1/12313 (0.0%)
3	I	0.35	0/9208	0.58	3/12426 (0.0%)
4	E	0.36	0/602	0.52	0/810
4	J	0.35	0/602	0.52	0/810
5	K	0.38	0/7808	0.65	2/10576 (0.0%)
5	L	0.38	0/7808	0.66	2/10576 (0.0%)
6	M	0.60	1/349 (0.3%)	0.70	0/535
6	O	0.61	1/349 (0.3%)	0.72	0/535
7	N	0.73	1/212 (0.5%)	0.63	0/326
7	P	0.72	1/212 (0.5%)	0.67	0/326
All	All	0.36	4/62222 (0.0%)	0.60	10/84280 (0.0%)

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
5	L	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	N	1	A	OP3-P	-10.19	1.49	1.61
6	O	1	DA	OP3-P	-10.18	1.49	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	P	1	A	OP3-P	-10.14	1.49	1.61
6	M	1	DA	OP3-P	-10.10	1.49	1.61

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	814	CYS	N-CA-C	-5.33	96.60	111.00
5	L	577	HIS	C-N-CA	-5.32	108.39	121.70
5	K	577	HIS	N-CA-C	-5.27	96.77	111.00
2	C	436	ARG	NE-CZ-NH1	5.24	122.92	120.30
3	I	850	LYS	C-N-CD	5.22	139.37	128.40
3	I	814	CYS	N-CA-C	-5.21	96.92	111.00
3	I	855	ASP	CB-CG-OD2	5.20	122.98	118.30
5	K	244	ASN	C-N-CD	5.16	139.24	128.40
5	L	469	TYR	C-N-CD	5.13	139.18	128.40
2	H	436	ARG	NE-CZ-NH1	5.10	122.85	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	L	148	ARG	Sidechain

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1759	0	1785	10	0
1	B	1759	0	1785	11	0
1	F	1759	0	1785	11	0
1	G	1759	0	1785	11	0
2	C	9285	0	9291	156	0
2	H	9235	0	9242	161	0
3	D	8990	0	9174	155	0
3	I	9068	0	9265	152	0
4	E	600	0	607	10	0
4	J	600	0	607	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	K	7665	0	7524	735	0
5	L	7665	0	7524	786	0
6	M	311	0	168	19	0
6	O	311	0	168	5	0
7	N	191	0	98	11	0
7	P	191	0	98	8	0
8	D	2	0	0	1	0
8	I	2	0	0	0	0
9	D	1	0	0	0	0
9	I	1	0	0	0	0
All	All	61154	0	60906	2127	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 17.

All (2127) 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)
5:L:720:MET:HE3	5:L:723:PHE:CE2	1.20	1.64
5:K:69:MET:CG	5:K:97:LEU:HD22	1.28	1.61
5:L:184:THR:HG22	5:L:312:LEU:CD2	1.17	1.61
5:L:219:MET:HG2	5:L:227:PHE:CE1	1.37	1.60
5:L:468:LEU:HA	5:L:617:ALA:CB	1.24	1.59
5:L:720:MET:CE	5:L:723:PHE:HE2	1.17	1.57
5:L:434:HIS:CD2	5:L:436:ILE:HD11	1.39	1.51
5:L:737:MET:HB3	5:L:738:ILE:CG2	1.06	1.49
3:D:77:ARG:CD	5:L:747:LEU:HB2	1.41	1.49
5:K:578:MET:SD	5:K:608:ILE:HG12	1.50	1.49
5:L:737:MET:CB	5:L:738:ILE:HG22	1.44	1.48
5:L:123:MET:CG	5:L:865:LEU:HB2	1.43	1.47
5:L:494:LEU:CD1	5:L:523:LEU:HD21	1.44	1.45
5:L:494:LEU:CD2	5:L:523:LEU:HD22	1.48	1.41
5:L:219:MET:SD	5:L:227:PHE:CD1	2.14	1.40
5:L:74:VAL:CG1	5:L:81:LEU:HD11	1.51	1.39
5:K:376:MET:O	5:K:377:ILE:HG12	1.24	1.36
5:L:737:MET:CB	5:L:738:ILE:CG2	1.94	1.36
5:K:407:LEU:HD11	5:K:408:MET:CE	1.53	1.35
5:K:468:LEU:HD21	5:K:469:TYR:CD2	1.60	1.35
5:L:139:GLN:O	5:L:142:MET:HB2	1.17	1.34
5:L:139:GLN:O	5:L:142:MET:CB	1.75	1.34
5:L:185:ILE:HG13	5:L:222:ARG:CZ	1.55	1.34

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:727:GLY:HA3	5:L:746:MET:N	1.41	1.33
5:K:69:MET:HG3	5:K:97:LEU:CD2	1.58	1.33
5:K:69:MET:CG	5:K:97:LEU:CD2	2.06	1.32
5:L:244:ASN:HB3	5:L:245:PRO:CD	1.56	1.31
5:L:216:LEU:HA	5:L:219:MET:SD	1.71	1.31
5:L:61:ILE:HG23	5:L:70:GLN:NE2	1.45	1.30
3:D:77:ARG:NE	5:L:747:LEU:HB2	1.47	1.29
5:K:843:MET:HE2	5:K:850:ASN:ND2	1.47	1.28
3:D:814:CYS:SG	3:D:898:CYS:SG	1.29	1.28
5:L:434:HIS:HD2	5:L:436:ILE:CD1	1.47	1.28
5:L:219:MET:CG	5:L:227:PHE:CE1	2.16	1.28
5:K:468:LEU:CD2	5:K:469:TYR:CD2	2.16	1.28
6:M:15:DG:N1	7:N:1:A:C2	2.02	1.28
5:K:52:ARG:HG3	5:K:54:MET:SD	1.74	1.27
5:L:468:LEU:CA	5:L:617:ALA:CB	2.12	1.27
3:I:814:CYS:SG	3:I:898:CYS:SG	1.28	1.27
3:D:77:ARG:HE	5:L:747:LEU:CB	1.46	1.27
5:L:184:THR:CG2	5:L:312:LEU:CD2	2.13	1.27
5:L:727:GLY:CA	5:L:746:MET:H	1.48	1.27
5:K:123:MET:HG3	5:K:865:LEU:CD1	1.63	1.26
5:L:737:MET:CA	5:L:738:ILE:HB	1.67	1.25
5:L:353:ALA:HA	5:L:356:VAL:CG2	1.66	1.24
6:M:15:DG:C2	7:N:1:A:H2	1.55	1.24
3:D:77:ARG:NE	5:L:747:LEU:CB	2.01	1.23
5:L:148:ARG:NH1	5:L:709:GLN:HB3	1.50	1.23
5:L:185:ILE:CG1	5:L:222:ARG:CZ	2.16	1.23
5:L:726:ILE:O	5:L:746:MET:CG	1.86	1.23
5:K:720:MET:HB3	5:K:730:GLN:OE1	1.39	1.22
5:L:220:LEU:O	5:L:224:ASN:HA	1.38	1.21
5:L:728:ILE:CD1	5:L:747:LEU:HD21	1.69	1.21
2:H:912:ASP:CB	2:H:913:VAL:HG13	1.70	1.21
5:L:372:MET:C	5:L:374:GLY:HA3	1.59	1.20
5:L:68:GLN:O	5:L:69:MET:HG2	1.04	1.20
5:L:493:TRP:CZ2	5:L:609:HIS:NE2	2.08	1.20
5:K:408:MET:SD	5:K:691:ILE:HG22	1.80	1.20
5:L:244:ASN:CB	5:L:245:PRO:HD2	1.70	1.20
3:I:78:LEU:HB2	5:K:746:MET:N	1.54	1.19
5:L:148:ARG:HH12	5:L:709:GLN:CB	1.56	1.19
5:L:538:MET:HG2	5:L:542:GLU:CD	1.62	1.19
5:L:62:THR:HA	5:L:68:GLN:OE1	1.39	1.18
5:L:54:MET:SD	5:L:81:LEU:CD1	2.32	1.18

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:852:LEU:O	5:L:852:LEU:HD12	1.43	1.18
5:K:72:GLU:O	5:K:73:GLU:CG	1.90	1.17
5:K:72:GLU:O	5:K:73:GLU:HG2	1.02	1.17
5:L:720:MET:HB3	5:L:730:GLN:OE1	1.37	1.17
5:L:494:LEU:CD2	5:L:523:LEU:CD2	2.21	1.17
5:K:580:MET:HB2	5:K:610:VAL:CG1	1.75	1.17
5:K:69:MET:HE3	5:K:83:TYR:CB	1.74	1.17
2:C:912:ASP:CB	2:C:913:VAL:HG13	1.72	1.16
5:K:372:MET:H	5:K:375:GLU:CG	1.56	1.16
5:K:70:GLN:HE21	5:K:86:THR:HB	1.07	1.16
5:L:219:MET:HA	5:L:225:LEU:CD1	1.73	1.16
5:L:70:GLN:HB3	5:L:71:VAL:CB	1.75	1.16
5:K:376:MET:O	5:K:377:ILE:CG1	1.94	1.16
5:K:843:MET:SD	5:K:850:ASN:HB3	1.85	1.16
5:L:494:LEU:CD1	5:L:523:LEU:CD2	2.24	1.15
3:I:78:LEU:HD12	5:K:746:MET:SD	1.85	1.15
5:L:69:MET:HB2	5:L:86:THR:O	1.45	1.15
5:L:123:MET:HG2	5:L:865:LEU:CB	1.74	1.15
5:L:353:ALA:HA	5:L:356:VAL:HG23	1.23	1.15
5:L:843:MET:HG2	5:L:850:ASN:HD22	1.11	1.15
6:M:15:DG:N1	7:N:1:A:H2	1.35	1.15
5:L:220:LEU:HA	5:L:225:LEU:N	1.59	1.14
5:L:376:MET:HG3	5:L:410:ARG:HD2	1.29	1.14
2:C:912:ASP:HB2	2:C:913:VAL:CG1	1.77	1.14
5:L:68:GLN:O	5:L:69:MET:CG	1.93	1.14
6:M:15:DG:N2	7:N:1:A:C2	2.15	1.14
3:D:78:LEU:HB3	5:L:746:MET:HB2	1.29	1.14
5:L:219:MET:CA	5:L:225:LEU:HD12	1.77	1.14
5:L:434:HIS:CD2	5:L:436:ILE:CD1	2.25	1.14
5:L:70:GLN:CB	5:L:71:VAL:HB	1.76	1.13
5:L:843:MET:HG2	5:L:850:ASN:ND2	1.62	1.13
2:H:912:ASP:HB2	2:H:913:VAL:CG1	1.78	1.12
5:L:407:LEU:HG	5:L:688:LEU:HD13	1.20	1.12
5:K:123:MET:CG	5:K:865:LEU:HD13	1.79	1.12
5:K:408:MET:HA	5:K:688:LEU:CD1	1.80	1.12
5:L:184:THR:HG22	5:L:312:LEU:HD23	1.16	1.12
5:L:581:PHE:HD2	5:L:582:ASP:OD1	1.31	1.11
5:L:175:LEU:HD22	5:L:187:ALA:HB1	1.25	1.11
5:K:720:MET:CE	5:K:738:ILE:HD13	1.80	1.11
3:D:814:CYS:SG	3:D:898:CYS:CB	2.39	1.11
5:K:408:MET:CE	5:K:691:ILE:HG22	1.81	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:184:THR:HG22	5:L:312:LEU:HD21	1.12	1.10
5:L:376:MET:CG	5:L:410:ARG:HD2	1.81	1.10
5:K:61:ILE:HB	5:K:69:MET:HE2	1.25	1.10
5:L:123:MET:CG	5:L:865:LEU:CB	2.30	1.10
5:L:74:VAL:CG1	5:L:81:LEU:CD1	2.30	1.10
5:K:371:ASN:ND2	5:K:375:GLU:HG3	1.67	1.10
5:K:726:ILE:HG23	5:K:747:LEU:HD22	1.29	1.10
5:K:578:MET:SD	5:K:608:ILE:CG1	2.40	1.09
5:K:69:MET:HG2	5:K:97:LEU:HD22	1.14	1.09
5:L:123:MET:H	5:L:865:LEU:HD22	1.03	1.09
3:I:78:LEU:CB	5:K:746:MET:HA	1.82	1.09
5:L:468:LEU:CA	5:L:617:ALA:HB3	1.80	1.09
5:K:408:MET:HE1	5:K:691:ILE:CG2	1.82	1.09
5:L:494:LEU:HD11	5:L:523:LEU:CD1	1.82	1.09
5:L:60:THR:HA	5:L:70:GLN:HB2	1.24	1.09
6:M:3:DG:H2''	6:M:4:DA:H5'	1.29	1.09
3:D:77:ARG:HD2	5:L:747:LEU:HB2	1.11	1.09
5:K:408:MET:CE	5:K:691:ILE:CG2	2.29	1.09
5:L:407:LEU:CG	5:L:688:LEU:HD13	1.82	1.09
5:L:468:LEU:HA	5:L:617:ALA:HB2	1.09	1.09
3:I:814:CYS:SG	3:I:898:CYS:CB	2.39	1.08
5:K:322:GLU:CG	5:K:324:HIS:CD2	2.35	1.08
3:D:77:ARG:HE	5:L:747:LEU:HB3	1.07	1.08
5:K:371:ASN:HD22	5:K:375:GLU:HG3	0.92	1.08
5:L:737:MET:HA	5:L:738:ILE:CB	1.74	1.08
5:K:408:MET:HA	5:K:688:LEU:HD12	1.09	1.08
5:L:726:ILE:O	5:L:746:MET:HG2	1.47	1.08
5:L:911:ASP:OD1	5:L:947:MET:HE3	1.51	1.08
3:D:77:ARG:CD	5:L:747:LEU:CB	2.32	1.08
5:K:408:MET:CA	5:K:688:LEU:HD12	1.84	1.08
5:L:468:LEU:HG	5:L:617:ALA:HB1	1.36	1.08
5:K:720:MET:CB	5:K:730:GLN:OE1	2.02	1.07
5:L:148:ARG:HH12	5:L:709:GLN:HB3	0.94	1.07
5:L:219:MET:HA	5:L:225:LEU:HD12	1.08	1.07
5:L:219:MET:HE3	5:L:253:ILE:HG21	1.35	1.07
5:L:728:ILE:HD11	5:L:747:LEU:HD21	1.12	1.07
5:K:322:GLU:CG	5:K:324:HIS:HD2	1.66	1.07
5:K:406:MET:HG2	5:K:410:ARG:HE	1.19	1.07
3:I:78:LEU:HB3	5:K:746:MET:HA	1.14	1.07
5:K:358:MET:HG3	5:K:365:LEU:HD22	1.29	1.07
5:K:578:MET:HB3	5:K:607:GLN:O	1.52	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:K:466:ASP:H	5:K:467:MET:HB3	1.13	1.06
5:K:746:MET:HB3	5:K:747:LEU:HB2	1.37	1.06
5:K:372:MET:H	5:K:375:GLU:HG2	1.20	1.06
5:L:737:MET:HB3	5:L:738:ILE:HG21	1.30	1.06
5:K:69:MET:HE3	5:K:83:TYR:HB3	1.07	1.06
5:K:123:MET:CG	5:K:865:LEU:CD1	2.34	1.06
5:K:61:ILE:HD11	5:K:83:TYR:CZ	1.91	1.06
5:K:843:MET:HE2	5:K:850:ASN:CG	1.76	1.06
5:K:322:GLU:HG2	5:K:324:HIS:HD2	1.19	1.05
5:K:580:MET:HB2	5:K:610:VAL:HG12	1.37	1.05
5:K:61:ILE:HB	5:K:69:MET:HB2	1.37	1.05
3:D:77:ARG:HD2	5:L:747:LEU:CB	1.86	1.05
5:K:406:MET:HG3	5:K:410:ARG:CZ	1.86	1.05
5:L:494:LEU:HD11	5:L:523:LEU:HD11	1.29	1.05
5:K:407:LEU:HD11	5:K:408:MET:HE3	1.08	1.05
5:K:727:GLY:CA	5:K:745:HIS:O	2.05	1.05
5:L:139:GLN:HG3	5:L:142:MET:CE	1.87	1.05
5:K:69:MET:SD	5:K:97:LEU:HB3	1.96	1.04
5:L:494:LEU:HD21	5:L:523:LEU:HD22	1.06	1.04
5:K:214:GLN:HG2	5:K:218:GLU:OE2	1.53	1.04
5:K:52:ARG:HG3	5:K:54:MET:CE	1.86	1.04
5:K:467:MET:CE	5:K:654:LEU:HB3	1.87	1.04
5:L:219:MET:CE	5:L:253:ILE:HG21	1.87	1.04
5:L:581:PHE:CD2	5:L:582:ASP:OD1	2.11	1.04
5:K:720:MET:SD	5:K:730:GLN:NE2	2.31	1.03
5:K:322:GLU:HG3	5:K:324:HIS:CD2	1.94	1.03
5:K:407:LEU:HG	5:K:408:MET:HG2	1.40	1.03
5:L:728:ILE:HD11	5:L:747:LEU:CD2	1.87	1.03
5:K:407:LEU:CD1	5:K:408:MET:CE	2.36	1.03
5:L:435:THR:HG21	5:L:437:LYS:HZ1	1.19	1.03
5:L:720:MET:HA	5:L:720:MET:HE3	1.35	1.03
5:L:577:HIS:NE2	5:L:607:GLN:OE1	1.92	1.03
5:L:74:VAL:HG13	5:L:81:LEU:CD1	1.89	1.03
5:L:580:MET:N	5:L:609:HIS:O	1.92	1.03
5:L:433:LEU:HD12	5:L:632:PHE:CG	1.93	1.03
5:K:843:MET:CE	5:K:850:ASN:CG	2.27	1.02
5:K:407:LEU:CD1	5:K:408:MET:HE2	1.89	1.02
5:K:52:ARG:CG	5:K:54:MET:SD	2.47	1.02
5:L:737:MET:CA	5:L:738:ILE:CB	2.33	1.02
5:K:188:GLY:HA3	5:K:223:PHE:CZ	1.94	1.02
5:L:69:MET:HG3	5:L:88:LEU:HB2	1.39	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:K:743:SER:O	5:K:746:MET:O	1.77	1.02
3:I:78:LEU:HB2	5:K:746:MET:H	0.89	1.02
5:K:406:MET:HG3	5:K:410:ARG:NH2	1.74	1.02
5:K:61:ILE:CB	5:K:69:MET:HE2	1.88	1.02
5:K:123:MET:H	5:K:865:LEU:CD1	1.72	1.02
5:L:353:ALA:CA	5:L:356:VAL:HG23	1.88	1.02
5:K:70:GLN:NE2	5:K:86:THR:CB	2.22	1.02
5:L:184:THR:CG2	5:L:312:LEU:HD23	1.85	1.02
5:L:123:MET:H	5:L:865:LEU:CD2	1.72	1.01
5:K:843:MET:HA	5:K:850:ASN:HD22	1.19	1.01
5:L:62:THR:CA	5:L:68:GLN:OE1	2.08	1.01
5:L:726:ILE:O	5:L:746:MET:HG3	1.54	1.01
5:K:377:ILE:O	5:K:379:GLU:HB3	1.59	1.01
5:L:720:MET:CE	5:L:720:MET:HA	1.90	1.01
5:K:727:GLY:HA2	5:K:745:HIS:O	1.60	1.01
5:K:123:MET:H	5:K:865:LEU:HD13	1.25	1.01
5:L:123:MET:HB3	5:L:865:LEU:HD13	1.39	1.01
5:K:408:MET:HE1	5:K:691:ILE:HG21	1.40	1.01
5:L:720:MET:HG3	5:L:730:GLN:NE2	1.75	1.01
5:K:355:ALA:HA	5:K:358:MET:HG2	1.40	1.01
5:K:69:MET:HG2	5:K:97:LEU:CD2	1.81	1.01
2:H:912:ASP:CB	2:H:913:VAL:CG1	2.37	1.01
5:L:468:LEU:CA	5:L:617:ALA:HB2	1.81	1.01
5:L:123:MET:N	5:L:865:LEU:HD22	1.75	1.00
5:K:468:LEU:HD23	5:K:469:TYR:CG	1.95	1.00
5:L:468:LEU:HA	5:L:617:ALA:HB3	1.02	1.00
5:L:74:VAL:HG13	5:L:81:LEU:HD11	1.06	1.00
5:K:70:GLN:NE2	5:K:86:THR:HB	1.76	1.00
5:L:219:MET:CG	5:L:227:PHE:CD1	2.40	1.00
5:L:352:VAL:O	5:L:356:VAL:HG23	1.61	0.99
5:L:727:GLY:HA2	5:L:745:HIS:O	1.62	0.99
3:I:78:LEU:CB	5:K:746:MET:H	1.74	0.99
5:L:61:ILE:CG2	5:L:70:GLN:NE2	2.23	0.99
3:I:396:ALA:HB2	5:K:733:ARG:HD2	1.39	0.99
5:L:494:LEU:HD22	5:L:523:LEU:CD2	1.91	0.99
5:L:720:MET:CE	5:L:723:PHE:CE2	2.07	0.99
3:I:396:ALA:CB	5:K:733:ARG:HH11	1.73	0.99
5:K:406:MET:HG2	5:K:410:ARG:NE	1.78	0.99
5:K:69:MET:CE	5:K:83:TYR:CB	2.41	0.99
5:L:356:VAL:O	5:L:358:MET:N	1.96	0.99
5:L:747:LEU:HD22	5:L:751:PHE:HE2	1.26	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:220:LEU:HA	5:L:225:LEU:H	1.23	0.98
5:K:720:MET:HA	5:K:723:PHE:CE2	1.98	0.98
5:L:185:ILE:HG13	5:L:222:ARG:NE	1.77	0.98
5:L:494:LEU:HD22	5:L:523:LEU:HD22	1.45	0.98
5:K:150:GLN:HG2	5:K:189:MET:SD	2.03	0.98
5:L:498:LEU:HD21	5:L:529:ILE:HG12	1.45	0.98
5:K:720:MET:HE3	5:K:738:ILE:HD13	1.46	0.98
6:M:15:DG:C2	7:N:1:A:C2	2.42	0.98
5:K:188:GLY:C	5:K:223:PHE:CE1	2.37	0.98
5:L:493:TRP:CZ2	5:L:609:HIS:CE1	2.51	0.98
5:L:720:MET:HE3	5:L:723:PHE:CZ	1.99	0.97
5:L:716:ILE:HD12	5:L:761:ILE:HD13	1.46	0.97
3:I:78:LEU:CB	5:K:746:MET:CA	2.41	0.97
5:L:494:LEU:HD13	5:L:523:LEU:HD21	0.97	0.97
5:K:407:LEU:HD11	5:K:408:MET:HE2	1.44	0.97
5:K:498:LEU:HD21	5:K:529:ILE:HG12	1.46	0.97
5:K:580:MET:CB	5:K:610:VAL:HG12	1.94	0.97
5:L:162:ALA:HB2	5:L:189:MET:HB3	1.43	0.97
5:L:175:LEU:HD22	5:L:187:ALA:CB	1.93	0.97
5:K:69:MET:HG3	5:K:97:LEU:HD22	0.97	0.97
5:K:843:MET:CE	5:K:850:ASN:ND2	2.29	0.96
5:L:720:MET:HA	5:L:723:PHE:CE2	2.00	0.96
3:I:78:LEU:CB	5:K:746:MET:N	2.27	0.96
5:L:219:MET:CE	5:L:253:ILE:CG2	2.44	0.96
5:L:435:THR:HG21	5:L:437:LYS:NZ	1.80	0.96
5:L:123:MET:HG2	5:L:865:LEU:HB2	0.98	0.96
2:C:912:ASP:CB	2:C:913:VAL:CG1	2.38	0.96
5:K:843:MET:SD	5:K:850:ASN:CB	2.54	0.96
5:L:376:MET:CB	5:L:410:ARG:HD2	1.95	0.96
5:L:184:THR:HG22	5:L:312:LEU:HD22	1.48	0.96
5:L:728:ILE:HG13	5:L:747:LEU:HD11	1.46	0.95
5:K:70:GLN:HB3	5:K:86:THR:CB	1.94	0.95
5:L:509:ILE:O	5:L:581:PHE:HB3	1.66	0.95
5:L:721:ASN:O	5:L:725:ILE:HD13	1.64	0.95
5:K:726:ILE:HG23	5:K:747:LEU:CD2	1.95	0.95
5:K:727:GLY:HA3	5:K:746:MET:HB2	1.47	0.95
5:L:123:MET:CB	5:L:865:LEU:HB2	1.96	0.95
5:K:185:ILE:HG13	5:K:222:ARG:HD3	1.47	0.95
3:I:396:ALA:CB	5:K:733:ARG:NH1	2.28	0.94
3:I:77:ARG:HB3	5:K:746:MET:O	1.66	0.94
5:L:359:LEU:H	5:L:359:LEU:HD23	1.32	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:K:143:PRO:HD2	5:K:148:ARG:NH2	1.82	0.94
5:K:70:GLN:HE21	5:K:86:THR:CB	1.77	0.94
3:I:396:ALA:HB1	5:K:733:ARG:NH1	1.82	0.94
5:L:433:LEU:HD12	5:L:632:PHE:CB	1.97	0.94
5:L:54:MET:SD	5:L:81:LEU:HD13	2.07	0.94
5:K:69:MET:SD	5:K:97:LEU:CB	2.55	0.94
5:K:162:ALA:HA	5:K:190:ILE:CD1	1.97	0.94
5:K:371:ASN:HD22	5:K:375:GLU:CG	1.78	0.94
5:K:123:MET:HG3	5:K:865:LEU:HD13	0.96	0.94
3:I:78:LEU:HB3	5:K:746:MET:CA	1.96	0.94
5:K:466:ASP:N	5:K:467:MET:HB3	1.82	0.94
5:K:580:MET:CB	5:K:610:VAL:CG1	2.45	0.94
5:L:842:ARG:O	5:L:843:MET:HG2	1.68	0.93
5:K:468:LEU:HD21	5:K:469:TYR:CE2	2.01	0.93
5:K:580:MET:HB2	5:K:610:VAL:HG13	1.49	0.93
5:K:818:LEU:O	5:K:843:MET:HB2	1.68	0.93
5:L:219:MET:CA	5:L:225:LEU:HB2	1.99	0.93
5:K:70:GLN:CB	5:K:86:THR:HB	1.99	0.93
2:C:912:ASP:HB2	2:C:913:VAL:HG13	0.93	0.93
5:L:433:LEU:HD23	5:L:434:HIS:N	1.82	0.93
5:L:61:ILE:HG23	5:L:70:GLN:HE22	1.24	0.93
2:H:912:ASP:HB2	2:H:913:VAL:HG13	0.93	0.93
5:L:220:LEU:O	5:L:224:ASN:CA	2.16	0.92
5:L:465:ARG:O	5:L:469:TYR:HD2	1.50	0.92
5:K:53:VAL:N	5:K:54:MET:HE2	1.83	0.92
5:L:185:ILE:HG13	5:L:222:ARG:NH1	1.84	0.92
5:L:74:VAL:HG11	5:L:81:LEU:HD11	1.52	0.92
5:K:188:GLY:HA3	5:K:223:PHE:CE2	2.04	0.92
5:K:578:MET:CB	5:K:607:GLN:O	2.17	0.92
5:K:69:MET:CE	5:K:83:TYR:HB3	1.98	0.92
5:K:70:GLN:HB3	5:K:86:THR:HB	1.52	0.92
5:L:353:ALA:HA	5:L:356:VAL:HG21	1.49	0.92
5:L:188:GLY:O	5:L:190:ILE:N	2.02	0.92
6:M:2:DC:H2'	6:M:3:DG:N7	1.85	0.92
5:K:222:ARG:HH11	5:K:222:ARG:HG3	1.35	0.91
5:L:376:MET:HG3	5:L:410:ARG:CD	2.00	0.91
5:K:578:MET:N	5:K:607:GLN:O	2.03	0.91
5:L:737:MET:HB2	5:L:760:THR:HA	1.51	0.91
5:K:373:LEU:O	5:K:376:MET:O	1.88	0.91
5:K:720:MET:HB3	5:K:730:GLN:CD	1.90	0.91
5:L:494:LEU:HD13	5:L:523:LEU:CD2	1.94	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:139:GLN:HG3	5:L:142:MET:HE1	1.51	0.91
5:K:468:LEU:CD2	5:K:469:TYR:CG	2.50	0.91
5:K:61:ILE:HD11	5:K:83:TYR:CE1	2.06	0.91
5:L:727:GLY:CA	5:L:746:MET:N	2.17	0.90
3:D:78:LEU:CB	5:L:746:MET:HB2	2.02	0.90
5:L:720:MET:CB	5:L:730:GLN:OE1	2.20	0.90
5:L:158:GLN:HG2	5:L:186:GLU:CG	2.01	0.90
5:L:466:ASP:O	5:L:468:LEU:N	2.03	0.90
5:K:863:ARG:HB3	5:K:961:ARG:HH21	1.34	0.90
5:K:185:ILE:HG13	5:K:222:ARG:CD	2.02	0.90
5:K:72:GLU:C	5:K:73:GLU:HG2	1.89	0.90
5:K:720:MET:HE1	5:K:738:ILE:HD13	1.52	0.89
5:K:72:GLU:HB2	5:K:84:ILE:O	1.70	0.89
5:L:60:THR:HA	5:L:70:GLN:CB	2.02	0.89
3:D:668:PHE:CE2	3:D:669:GLN:NE2	2.41	0.89
5:L:911:ASP:OD1	5:L:947:MET:CE	2.21	0.89
6:M:2:DC:H2'	6:M:3:DG:C8	2.08	0.89
6:M:15:DG:N2	7:N:1:A:N3	2.14	0.89
3:I:77:ARG:HB3	5:K:746:MET:C	1.93	0.89
5:K:406:MET:CG	5:K:410:ARG:NH2	2.36	0.89
5:K:466:ASP:HB3	5:K:467:MET:HB2	1.53	0.89
5:L:538:MET:HG2	5:L:542:GLU:OE1	1.72	0.89
5:L:842:ARG:O	5:L:843:MET:CG	2.21	0.88
3:I:78:LEU:HB2	5:K:746:MET:CA	2.03	0.88
5:K:318:GLN:O	5:K:319:LEU:HD23	1.72	0.88
5:K:406:MET:CG	5:K:410:ARG:CZ	2.50	0.88
5:K:406:MET:CG	5:K:410:ARG:NE	2.36	0.88
5:L:216:LEU:CA	5:L:219:MET:SD	2.60	0.88
5:L:219:MET:SD	5:L:227:PHE:CE1	2.66	0.88
5:K:378:GLY:HA2	5:K:379:GLU:CB	2.02	0.88
5:L:184:THR:CG2	5:L:312:LEU:HD21	1.91	0.88
5:K:123:MET:SD	5:K:124:ASP:N	2.46	0.88
5:K:467:MET:SD	5:K:654:LEU:O	2.32	0.88
5:K:372:MET:N	5:K:375:GLU:CG	2.36	0.88
5:K:54:MET:HA	5:K:83:TYR:OH	1.74	0.88
5:L:219:MET:HE1	5:L:253:ILE:HG23	1.53	0.87
5:L:494:LEU:O	5:L:498:LEU:CB	2.22	0.87
5:L:494:LEU:HD11	5:L:523:LEU:HD21	1.56	0.87
5:L:726:ILE:O	5:L:746:MET:O	1.91	0.87
5:L:942:ASN:O	5:L:946:VAL:HG23	1.72	0.87
5:K:321:MET:O	5:K:322:GLU:C	2.03	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:M:15:DG:N2	7:N:1:A:H2	1.62	0.87
3:D:78:LEU:HB2	5:L:746:MET:HA	1.55	0.87
5:K:372:MET:HA	5:K:375:GLU:HB2	1.57	0.87
5:K:737:MET:SD	5:K:771:ARG:NH1	2.48	0.87
5:L:219:MET:O	5:L:225:LEU:HG	1.75	0.87
5:L:54:MET:HA	5:L:83:TYR:OH	1.74	0.87
5:L:373:LEU:N	5:L:374:GLY:HA3	1.78	0.86
5:L:468:LEU:CB	5:L:617:ALA:CB	2.54	0.86
5:K:70:GLN:NE2	5:K:86:THR:CG2	2.39	0.86
5:K:19:LEU:HD13	5:K:102:LEU:HD23	1.56	0.86
5:K:818:LEU:O	5:K:843:MET:CB	2.22	0.86
5:L:219:MET:N	5:L:225:LEU:HD12	1.90	0.86
5:L:737:MET:CB	5:L:738:ILE:CB	2.53	0.86
5:K:727:GLY:HA3	5:K:745:HIS:O	1.73	0.86
5:K:223:PHE:O	5:K:225:LEU:HD12	1.75	0.86
5:K:535:HIS:HE1	5:K:538:MET:HG2	1.41	0.86
5:L:158:GLN:HG2	5:L:186:GLU:HG2	1.56	0.86
5:L:219:MET:HA	5:L:225:LEU:HB2	1.57	0.86
5:K:223:PHE:O	5:K:225:LEU:CD1	2.24	0.86
5:K:244:ASN:HB3	5:K:245:PRO:CD	2.05	0.86
3:I:396:ALA:HB2	5:K:733:ARG:HH11	1.41	0.85
5:K:863:ARG:HD2	5:K:961:ARG:HE	1.41	0.85
5:L:139:GLN:C	5:L:142:MET:HB2	1.96	0.85
5:K:122:ARG:O	5:K:125:ARG:HG2	1.76	0.85
5:K:214:GLN:O	5:K:218:GLU:HG3	1.75	0.85
5:K:70:GLN:NE2	5:K:86:THR:HG21	1.91	0.85
5:K:189:MET:N	5:K:223:PHE:CE1	2.45	0.85
5:L:535:HIS:CE1	5:L:538:MET:H	1.94	0.85
5:L:244:ASN:HB3	5:L:245:PRO:HD2	0.85	0.85
5:L:493:TRP:CH2	5:L:609:HIS:CE1	2.64	0.85
5:L:509:ILE:O	5:L:581:PHE:CB	2.25	0.85
5:L:578:MET:HB3	5:L:607:GLN:O	1.76	0.84
6:M:3:DG:H2"	6:M:4:DA:C5'	2.07	0.84
5:K:42:LEU:HG	5:K:242:ALA:HB1	1.59	0.84
5:L:495:MET:HE1	5:L:499:THR:HG22	1.59	0.84
5:L:583:LEU:HD11	5:L:622:VAL:HG22	1.60	0.84
5:K:214:GLN:CG	5:K:218:GLU:OE2	2.26	0.84
5:L:494:LEU:HD11	5:L:523:LEU:CD2	2.02	0.84
5:K:162:ALA:HA	5:K:190:ILE:HD11	1.57	0.84
5:K:369:GLU:O	5:K:373:LEU:HG	1.78	0.84
5:K:378:GLY:HA2	5:K:379:GLU:HB3	1.57	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:K:467:MET:HE2	5:K:654:LEU:HB3	1.58	0.84
5:K:188:GLY:CA	5:K:223:PHE:CZ	2.60	0.84
5:K:322:GLU:HG2	5:K:324:HIS:CD2	2.07	0.84
5:L:42:LEU:HG	5:L:242:ALA:HB1	1.59	0.84
5:K:843:MET:CA	5:K:850:ASN:HD22	1.90	0.84
5:K:61:ILE:HG13	5:K:69:MET:CE	2.07	0.83
5:L:185:ILE:HG23	5:L:222:ARG:HD3	1.58	0.83
5:L:358:MET:HE2	5:L:358:MET:HA	1.59	0.83
5:K:408:MET:SD	5:K:691:ILE:CG2	2.64	0.83
5:K:57:PRO:HA	5:K:71:VAL:HG11	1.61	0.83
5:K:61:ILE:CD1	5:K:83:TYR:CE1	2.60	0.83
3:I:501:VAL:HG12	3:I:502:PRO:HD2	1.59	0.83
5:L:139:GLN:CG	5:L:142:MET:CE	2.56	0.83
5:K:408:MET:SD	5:K:691:ILE:C	2.57	0.83
5:L:435:THR:CG2	5:L:437:LYS:NZ	2.40	0.83
5:L:577:HIS:O	5:L:578:MET:HB2	1.77	0.83
5:K:322:GLU:O	5:K:323:SER:OG	1.95	0.83
5:L:219:MET:HE1	5:L:253:ILE:CG2	2.09	0.83
5:K:374:GLY:O	5:K:378:GLY:C	2.16	0.83
5:K:843:MET:HA	5:K:850:ASN:ND2	1.94	0.83
5:K:355:ALA:CA	5:K:358:MET:HG2	2.08	0.83
5:K:69:MET:HG3	5:K:97:LEU:HD23	1.61	0.83
5:L:407:LEU:HG	5:L:688:LEU:CD1	2.07	0.83
5:K:52:ARG:C	5:K:54:MET:HE2	1.98	0.83
5:K:720:MET:SD	5:K:730:GLN:CD	2.56	0.83
5:L:182:GLY:O	5:L:186:GLU:HG3	1.79	0.83
5:L:535:HIS:CE1	5:L:538:MET:HB2	2.13	0.83
5:K:863:ARG:HD2	5:K:961:ARG:NE	1.94	0.82
5:L:494:LEU:HD21	5:L:523:LEU:CD2	1.99	0.82
5:L:538:MET:O	5:L:543:ARG:CZ	2.27	0.82
5:K:408:MET:SD	5:K:692:HIS:N	2.52	0.82
5:L:737:MET:HA	5:L:738:ILE:HB	0.87	0.82
5:K:322:GLU:HG3	5:K:324:HIS:NE2	1.93	0.82
5:K:818:LEU:HB2	5:K:843:MET:HB3	1.59	0.82
5:L:220:LEU:CA	5:L:225:LEU:H	1.92	0.82
3:D:501:VAL:HG12	3:D:502:PRO:HD2	1.60	0.82
5:K:726:ILE:CG2	5:K:747:LEU:HD22	2.10	0.82
5:K:61:ILE:CG1	5:K:69:MET:HE2	2.10	0.82
5:L:220:LEU:HD12	5:L:224:ASN:HA	1.62	0.82
5:L:538:MET:O	5:L:543:ARG:NH2	2.13	0.82
5:L:408:MET:HA	5:L:688:LEU:HD12	1.59	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:747:LEU:HD22	5:L:751:PHE:CE2	2.14	0.82
5:K:378:GLY:CA	5:K:379:GLU:CB	2.57	0.81
3:I:396:ALA:HB2	5:K:733:ARG:CD	2.08	0.81
5:K:69:MET:HG2	5:K:97:LEU:CG	2.10	0.81
5:L:468:LEU:CG	5:L:617:ALA:HB1	2.09	0.81
5:L:69:MET:CG	5:L:88:LEU:HB2	2.10	0.81
5:L:407:LEU:HD13	5:L:410:ARG:NH2	1.96	0.81
5:L:535:HIS:NE2	5:L:538:MET:HB2	1.95	0.81
3:D:814:CYS:CB	3:D:898:CYS:SG	2.69	0.80
5:K:70:GLN:HE22	5:K:86:THR:HG21	1.46	0.80
5:L:720:MET:HG3	5:L:730:GLN:HE22	1.42	0.80
7:P:1:A:H2'	7:P:2:U:C5	2.16	0.80
5:L:219:MET:HA	5:L:225:LEU:CG	2.09	0.80
5:L:219:MET:HA	5:L:225:LEU:CB	2.11	0.80
5:K:466:ASP:HB3	5:K:467:MET:CB	2.11	0.80
5:L:220:LEU:C	5:L:224:ASN:HA	2.01	0.80
5:L:54:MET:SD	5:L:81:LEU:HD12	2.22	0.80
5:K:186:GLU:O	5:K:190:ILE:HD13	1.80	0.80
5:K:364:LYS:HG2	5:K:391:SER:HB3	1.64	0.80
5:K:506:VAL:HG13	5:K:577:HIS:HB3	1.64	0.80
5:L:737:MET:CG	5:L:738:ILE:HG21	2.12	0.80
5:K:467:MET:HA	5:K:617:ALA:HB2	1.64	0.79
5:L:185:ILE:HD11	5:L:222:ARG:NH2	1.95	0.79
5:L:407:LEU:O	5:L:409:ASP:N	2.15	0.79
5:L:219:MET:SD	5:L:227:PHE:CG	2.76	0.79
5:K:378:GLY:HA2	5:K:380:GLN:H	1.48	0.79
5:K:377:ILE:HD12	5:K:410:ARG:HE	1.46	0.79
5:K:946:VAL:O	5:K:949:SER:N	2.16	0.79
5:L:59:ASP:O	5:L:70:GLN:HB2	1.83	0.79
5:K:185:ILE:HD12	5:K:185:ILE:H	1.48	0.79
5:L:356:VAL:HG12	5:L:358:MET:HE3	1.65	0.79
5:L:123:MET:HB2	5:L:961:ARG:NH2	1.98	0.79
5:L:818:LEU:O	5:L:843:MET:HB2	1.83	0.78
5:L:494:LEU:O	5:L:498:LEU:HB3	1.82	0.78
5:L:843:MET:CG	5:L:850:ASN:HD22	1.93	0.78
3:D:77:ARG:CD	5:L:747:LEU:HD12	2.11	0.78
3:I:814:CYS:CB	3:I:898:CYS:SG	2.70	0.78
5:K:467:MET:HE1	5:K:654:LEU:HD22	1.65	0.78
5:L:436:ILE:HG12	5:L:609:HIS:CE1	2.17	0.78
3:D:78:LEU:HB3	5:L:746:MET:CB	2.11	0.78
5:K:123:MET:CG	5:K:865:LEU:HD12	2.13	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:720:MET:HE1	5:L:723:PHE:HE2	1.44	0.78
5:K:185:ILE:HG13	5:K:222:ARG:NE	1.99	0.78
5:L:738:ILE:HG23	5:L:759:ILE:HG22	1.65	0.78
5:L:495:MET:CE	5:L:499:THR:CG2	2.62	0.77
5:L:148:ARG:NH1	5:L:709:GLN:CB	2.29	0.77
5:L:455:GLY:O	5:L:456:ALA:HB2	1.82	0.77
5:L:407:LEU:CD1	5:L:688:LEU:HD13	2.15	0.77
5:L:737:MET:HE3	5:L:761:ILE:HG22	1.66	0.77
5:L:434:HIS:CD2	5:L:609:HIS:ND1	2.53	0.77
5:L:468:LEU:HG	5:L:617:ALA:CB	2.12	0.77
5:L:122:ARG:HB3	5:L:124:ASP:OD1	1.84	0.77
5:L:175:LEU:CD2	5:L:187:ALA:HB1	2.09	0.77
3:D:78:LEU:CB	5:L:746:MET:CB	2.61	0.77
5:K:185:ILE:O	5:K:223:PHE:HZ	1.67	0.77
5:K:733:ARG:O	5:K:733:ARG:HD3	1.84	0.77
5:L:139:GLN:HG3	5:L:142:MET:HE3	1.67	0.77
5:K:244:ASN:HB3	5:K:245:PRO:HD3	1.65	0.77
5:K:69:MET:HG2	5:K:97:LEU:CB	2.14	0.77
5:K:726:ILE:CG2	5:K:747:LEU:CD2	2.63	0.76
5:K:747:LEU:HG	5:K:748:VAL:HG23	1.66	0.76
5:L:162:ALA:CB	5:L:189:MET:HB3	2.15	0.76
3:I:519:ASN:ND2	3:I:709:ARG:HB2	2.00	0.76
5:L:352:VAL:O	5:L:356:VAL:CG2	2.33	0.76
5:L:60:THR:CG2	5:L:69:MET:HA	2.16	0.76
5:L:494:LEU:O	5:L:498:LEU:HB2	1.84	0.76
5:L:737:MET:CE	5:L:761:ILE:CG2	2.63	0.76
5:K:369:GLU:CG	5:K:373:LEU:HD11	2.15	0.76
5:L:373:LEU:N	5:L:374:GLY:CA	2.48	0.76
3:D:77:ARG:NE	5:L:747:LEU:HB3	1.85	0.76
5:K:578:MET:CA	5:K:607:GLN:O	2.32	0.76
5:K:61:ILE:CG1	5:K:69:MET:CE	2.64	0.76
3:I:393:THR:OG1	5:K:733:ARG:HG3	1.86	0.76
5:K:722:LEU:HD11	5:K:726:ILE:HD11	1.66	0.76
5:K:19:LEU:HD13	5:K:102:LEU:CD2	2.16	0.76
5:K:151:ARG:HB3	5:K:222:ARG:HA	1.67	0.75
5:L:219:MET:C	5:L:225:LEU:HB2	2.06	0.75
5:K:123:MET:CB	5:K:865:LEU:CD1	2.64	0.75
5:K:377:ILE:HD12	5:K:406:MET:HG2	1.68	0.75
5:L:219:MET:CG	5:L:227:PHE:HE1	1.77	0.75
5:L:186:GLU:O	5:L:189:MET:CG	2.34	0.75
5:L:220:LEU:HD12	5:L:224:ASN:CA	2.17	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:42:LEU:CD1	5:L:242:ALA:HB2	2.16	0.75
5:L:372:MET:O	5:L:374:GLY:HA3	1.87	0.75
5:K:320:GLY:CA	5:K:321:MET:HB2	2.17	0.75
5:L:215:TRP:O	5:L:219:MET:HG3	1.87	0.75
5:K:494:LEU:O	5:K:498:LEU:HB3	1.87	0.75
5:K:61:ILE:HB	5:K:69:MET:CE	2.13	0.75
5:K:720:MET:HE3	5:K:738:ILE:CD1	2.16	0.75
5:L:498:LEU:HD21	5:L:529:ILE:CG1	2.16	0.75
5:K:407:LEU:HG	5:K:408:MET:N	2.02	0.75
5:L:185:ILE:CD1	5:L:222:ARG:CZ	2.64	0.75
5:L:374:GLY:O	5:L:376:MET:N	2.20	0.75
5:L:376:MET:HB2	5:L:410:ARG:HD2	1.67	0.75
5:K:863:ARG:CB	5:K:961:ARG:NH2	2.49	0.74
5:L:185:ILE:CG1	5:L:222:ARG:NE	2.43	0.74
5:K:377:ILE:CG2	5:K:410:ARG:HD2	2.17	0.74
5:K:61:ILE:CB	5:K:69:MET:CE	2.66	0.74
5:L:139:GLN:O	5:L:142:MET:N	2.20	0.74
5:L:158:GLN:CG	5:L:186:GLU:HG2	2.17	0.74
5:L:358:MET:HA	5:L:358:MET:CE	2.16	0.74
5:L:60:THR:CA	5:L:70:GLN:HB2	2.12	0.74
5:L:737:MET:CA	5:L:738:ILE:CG2	2.65	0.74
5:L:139:GLN:HG2	5:L:142:MET:SD	2.26	0.74
5:L:408:MET:HE1	5:L:691:ILE:HG22	1.68	0.74
5:K:372:MET:H	5:K:375:GLU:HG3	1.53	0.74
5:K:538:MET:O	5:K:539:SER:HB2	1.86	0.74
5:L:186:GLU:O	5:L:189:MET:HG2	1.87	0.74
5:L:407:LEU:HG	5:L:408:MET:H	1.53	0.74
5:K:498:LEU:HD21	5:K:529:ILE:CG1	2.17	0.74
5:L:468:LEU:HD22	5:L:469:TYR:CE2	2.22	0.74
5:K:377:ILE:HG13	5:K:378:GLY:H	1.51	0.74
5:L:139:GLN:O	5:L:142:MET:HB3	1.85	0.74
5:L:538:MET:CG	5:L:542:GLU:CD	2.50	0.74
5:K:407:LEU:HD12	5:K:408:MET:HE2	1.70	0.74
5:L:721:ASN:O	5:L:725:ILE:CD1	2.36	0.74
5:K:42:LEU:CD1	5:K:242:ALA:HB2	2.17	0.73
5:K:364:LYS:NZ	5:K:392:ASP:OD2	2.20	0.73
5:K:69:MET:CG	5:K:97:LEU:CB	2.67	0.73
3:I:85:CYS:SG	3:I:86:GLU:N	2.61	0.73
3:D:85:CYS:SG	3:D:86:GLU:N	2.61	0.73
5:L:175:LEU:CD2	5:L:187:ALA:CB	2.66	0.73
5:L:54:MET:SD	5:L:74:VAL:HG11	2.29	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:K:371:ASN:O	5:K:372:MET:HB2	1.88	0.73
5:K:377:ILE:HG13	5:K:378:GLY:N	2.03	0.73
5:L:578:MET:O	5:L:609:HIS:HB3	1.88	0.73
5:L:60:THR:HG23	5:L:69:MET:HA	1.70	0.73
5:K:358:MET:CG	5:K:365:LEU:HD22	2.15	0.73
5:L:495:MET:SD	5:L:527:GLU:HB3	2.29	0.73
5:K:863:ARG:CB	5:K:961:ARG:HH21	2.02	0.73
5:K:69:MET:SD	5:K:97:LEU:HB2	2.29	0.72
5:L:436:ILE:N	5:L:436:ILE:HD12	2.04	0.72
5:L:468:LEU:O	5:L:468:LEU:HD23	1.89	0.72
5:L:495:MET:O	5:L:499:THR:N	2.18	0.72
5:K:123:MET:N	5:K:865:LEU:CD1	2.52	0.72
5:K:143:PRO:HD2	5:K:148:ARG:HH22	1.52	0.72
5:K:123:MET:N	5:K:865:LEU:HD13	2.02	0.72
5:L:577:HIS:CE1	5:L:607:GLN:OE1	2.42	0.72
3:D:70:CYS:SG	3:D:72:CYS:N	2.63	0.72
5:K:69:MET:HG2	5:K:97:LEU:HB2	1.70	0.72
5:K:69:MET:HE1	5:K:83:TYR:CG	2.24	0.72
5:L:727:GLY:HA3	5:L:746:MET:H	0.62	0.72
5:K:369:GLU:HG2	5:K:373:LEU:HD11	1.70	0.72
5:K:408:MET:HB3	5:K:688:LEU:HB2	1.70	0.72
5:K:61:ILE:HG13	5:K:69:MET:HE2	1.66	0.72
5:L:215:TRP:O	5:L:219:MET:SD	2.47	0.72
5:L:220:LEU:CA	5:L:225:LEU:N	2.47	0.72
5:K:403:LEU:HA	5:K:407:LEU:HB2	1.72	0.72
5:K:407:LEU:HG	5:K:408:MET:H	1.54	0.72
5:K:720:MET:CB	5:K:730:GLN:CD	2.53	0.72
5:L:139:GLN:O	5:L:142:MET:CA	2.37	0.72
3:D:1185:PRO:O	3:D:1186:TYR:HB2	1.89	0.72
3:I:78:LEU:HD12	5:K:746:MET:CE	2.20	0.72
5:L:217:VAL:HG12	5:L:218:GLU:HG3	1.71	0.72
5:L:123:MET:HB3	5:L:865:LEU:CD1	2.16	0.72
5:K:56:ASN:O	5:K:71:VAL:HG21	1.89	0.71
5:L:943:ARG:HG2	5:L:947:MET:SD	2.30	0.71
6:O:2:DC:H2"	6:O:3:DG:OP1	1.90	0.71
5:L:453:ILE:HD12	5:L:453:ILE:N	2.05	0.71
5:L:733:ARG:HD3	5:L:733:ARG:O	1.91	0.71
5:K:219:MET:CB	5:K:227:PHE:HE1	2.02	0.71
5:K:720:MET:HB2	5:K:730:GLN:OE1	1.90	0.71
5:K:737:MET:HE1	5:K:771:ARG:HH11	1.54	0.71
5:L:190:ILE:N	5:L:190:ILE:HD12	2.06	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:370:LEU:O	5:L:370:LEU:HD23	1.91	0.71
3:D:78:LEU:HG	5:L:746:MET:HB3	1.70	0.71
5:K:719:ALA:C	5:K:723:PHE:CE1	2.63	0.71
5:L:352:VAL:C	5:L:356:VAL:HG23	2.11	0.71
5:L:538:MET:HG2	5:L:542:GLU:CB	2.21	0.71
5:K:59:ASP:O	5:K:71:VAL:HG23	1.89	0.71
5:L:220:LEU:HA	5:L:224:ASN:C	2.09	0.71
5:L:727:GLY:CA	5:L:745:HIS:O	2.37	0.71
5:L:583:LEU:O	5:L:584:PRO:O	2.08	0.71
5:K:374:GLY:CA	5:K:378:GLY:O	2.39	0.71
5:L:408:MET:CA	5:L:688:LEU:HD12	2.21	0.71
5:L:720:MET:HE1	5:L:740:LEU:HD21	1.73	0.71
3:I:70:CYS:SG	3:I:72:CYS:N	2.64	0.71
5:K:185:ILE:HD12	5:K:185:ILE:N	2.04	0.71
5:K:52:ARG:CZ	5:K:54:MET:SD	2.79	0.71
5:K:219:MET:HG3	5:K:227:PHE:HE1	1.56	0.71
5:K:357:ALA:C	5:K:359:LEU:H	1.94	0.71
5:L:408:MET:CE	5:L:691:ILE:HG22	2.21	0.71
5:L:185:ILE:HD12	5:L:185:ILE:N	2.06	0.70
5:L:408:MET:H	5:L:688:LEU:CD1	2.04	0.70
3:D:43:THR:OG1	3:D:44:ILE:N	2.24	0.70
5:K:42:LEU:HG	5:K:242:ALA:CB	2.21	0.70
5:K:737:MET:CE	5:K:771:ARG:NH1	2.55	0.70
5:L:220:LEU:HA	5:L:224:ASN:HA	1.73	0.70
5:K:54:MET:HG2	5:K:81:LEU:HD12	1.74	0.70
5:K:798:SER:O	5:K:865:LEU:HD12	1.91	0.70
5:L:215:TRP:O	5:L:219:MET:CG	2.40	0.70
5:L:359:LEU:H	5:L:359:LEU:CD2	2.03	0.70
5:L:725:ILE:N	5:L:725:ILE:HD12	2.06	0.70
5:K:372:MET:N	5:K:375:GLU:HG2	2.02	0.70
5:K:376:MET:C	5:K:377:ILE:HG12	2.09	0.70
5:K:403:LEU:HB3	5:K:407:LEU:HD13	1.73	0.70
5:K:863:ARG:HE	5:K:961:ARG:CZ	2.05	0.70
2:C:790:ASP:O	2:C:792:GLY:N	2.25	0.70
5:L:42:LEU:HG	5:L:242:ALA:CB	2.22	0.70
3:I:70:CYS:SG	3:I:71:LEU:N	2.65	0.70
5:K:720:MET:CE	5:K:738:ILE:CD1	2.65	0.70
5:L:911:ASP:OD2	5:L:947:MET:HE1	1.91	0.70
3:I:519:ASN:HD21	3:I:710:ASP:H	1.40	0.69
5:L:444:TYR:CE1	5:L:470:PRO:HB2	2.26	0.69
5:L:535:HIS:CE1	5:L:538:MET:N	2.59	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:K:162:ALA:HA	5:K:190:ILE:HD12	1.70	0.69
5:K:453:ILE:N	5:K:453:ILE:HD12	2.06	0.69
3:I:43:THR:OG1	3:I:44:ILE:N	2.25	0.69
5:L:220:LEU:HA	5:L:224:ASN:CA	2.22	0.69
5:L:219:MET:HG2	5:L:227:PHE:HE1	0.83	0.69
5:L:494:LEU:CG	5:L:523:LEU:HD21	2.19	0.69
3:I:854:ALA:O	3:I:855:ASP:HB2	1.91	0.69
5:K:378:GLY:HA2	5:K:380:GLN:N	2.07	0.69
5:K:942:ASN:O	5:K:946:VAL:HG23	1.93	0.69
5:L:494:LEU:CG	5:L:523:LEU:CD2	2.70	0.69
5:L:852:LEU:O	5:L:852:LEU:CD1	2.32	0.69
5:L:219:MET:SD	5:L:227:PHE:HD1	2.07	0.69
5:L:727:GLY:CA	5:L:745:HIS:C	2.61	0.69
2:H:790:ASP:O	2:H:792:GLY:N	2.25	0.69
5:K:318:GLN:O	5:K:319:LEU:CD2	2.38	0.69
5:K:722:LEU:CD1	5:K:726:ILE:HD11	2.23	0.69
5:L:61:ILE:CG2	5:L:70:GLN:HE22	1.96	0.69
5:L:737:MET:CE	5:L:761:ILE:HG22	2.22	0.69
5:L:69:MET:CB	5:L:86:THR:O	2.34	0.69
5:K:53:VAL:CA	5:K:54:MET:HE2	2.22	0.69
5:K:69:MET:CE	5:K:83:TYR:CG	2.76	0.69
5:L:843:MET:HA	5:L:850:ASN:HB2	1.74	0.69
5:L:582:ASP:O	5:L:593:ARG:CZ	2.40	0.69
5:K:468:LEU:HD23	5:K:468:LEU:C	2.14	0.68
5:K:720:MET:HA	5:K:723:PHE:CZ	2.27	0.68
5:L:433:LEU:CD1	5:L:632:PHE:CG	2.76	0.68
5:L:720:MET:CG	5:L:730:GLN:NE2	2.54	0.68
5:K:320:GLY:HA2	5:K:321:MET:HB2	1.74	0.68
5:L:165:VAL:HB	5:L:190:ILE:HG12	1.75	0.68
5:L:436:ILE:HD13	5:L:610:VAL:O	1.94	0.68
3:D:1181:ASP:O	3:D:1183:SER:N	2.26	0.68
3:D:70:CYS:SG	3:D:71:LEU:N	2.66	0.68
3:I:620:PHE:CZ	3:I:624:ILE:HD11	2.28	0.68
5:K:746:MET:HB3	5:K:747:LEU:CB	2.21	0.68
5:L:218:GLU:OE1	5:L:222:ARG:HG3	1.94	0.68
3:D:77:ARG:HD3	5:L:747:LEU:HD12	1.76	0.68
5:L:123:MET:HG3	5:L:865:LEU:CB	2.23	0.68
5:K:408:MET:HG3	5:K:692:HIS:HB2	1.74	0.68
5:K:818:LEU:CB	5:K:843:MET:HB3	2.24	0.68
5:L:535:HIS:HE2	5:L:538:MET:HB2	1.58	0.68
5:L:728:ILE:HD12	5:L:747:LEU:HD21	1.69	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:77:ARG:HD2	5:L:747:LEU:CG	2.24	0.68
5:L:141:ARG:CG	5:L:141:ARG:O	2.42	0.68
5:L:737:MET:HE3	5:L:761:ILE:CG2	2.21	0.68
5:K:364:LYS:HE2	5:K:391:SER:HB2	1.75	0.68
5:K:733:ARG:C	5:K:733:ARG:HD3	2.13	0.68
3:I:396:ALA:HB2	5:K:733:ARG:NH1	2.04	0.68
5:L:162:ALA:HB2	5:L:189:MET:CB	2.23	0.68
5:L:494:LEU:HD11	5:L:523:LEU:CG	2.24	0.68
3:D:620:PHE:CZ	3:D:624:ILE:HD11	2.29	0.68
5:L:727:GLY:HA2	5:L:745:HIS:C	2.13	0.68
5:L:775:GLN:O	5:L:777:ILE:N	2.27	0.68
5:L:123:MET:HB3	5:L:865:LEU:HB2	1.74	0.68
5:K:406:MET:CG	5:K:410:ARG:HH21	2.07	0.67
5:L:455:GLY:O	5:L:456:ALA:CB	2.41	0.67
2:C:662:SER:OG	2:C:663:VAL:N	2.27	0.67
2:H:813:GLU:O	3:I:461:PHE:O	2.11	0.67
5:K:69:MET:HE1	5:K:83:TYR:CD1	2.29	0.67
5:L:448:ILE:HD13	5:L:467:MET:HA	1.76	0.67
3:I:773:PHE:O	3:I:776:THR:OG1	2.10	0.67
5:L:272:ALA:O	5:L:273:GLU:HG2	1.95	0.67
5:L:578:MET:CB	5:L:607:GLN:O	2.42	0.67
5:K:322:GLU:HG2	5:K:323:SER:H	1.60	0.67
5:K:727:GLY:CA	5:K:746:MET:HB2	2.23	0.67
5:L:843:MET:HA	5:L:850:ASN:HD22	1.58	0.67
2:H:524:ILE:HD11	2:H:712:SER:HB3	1.77	0.67
5:K:863:ARG:CD	5:K:961:ARG:NE	2.57	0.67
5:L:435:THR:C	5:L:436:ILE:HD12	2.13	0.67
5:L:469:TYR:O	5:L:473:ILE:HB	1.94	0.67
5:K:188:GLY:C	5:K:223:PHE:CZ	2.67	0.67
5:L:219:MET:C	5:L:225:LEU:H	1.98	0.67
3:I:396:ALA:HB1	5:K:733:ARG:HH11	1.42	0.67
5:K:360:LEU:HD12	5:K:360:LEU:N	2.10	0.67
5:K:408:MET:CE	5:K:691:ILE:HG21	2.08	0.67
2:H:662:SER:OG	2:H:663:VAL:N	2.27	0.67
5:L:453:ILE:H	5:L:453:ILE:HD12	1.58	0.67
5:K:736:ASN:HD22	5:K:765:ARG:NH2	1.93	0.66
5:L:185:ILE:HD12	5:L:185:ILE:H	1.60	0.66
5:L:185:ILE:HG12	5:L:222:ARG:CZ	2.23	0.66
5:L:583:LEU:HD11	5:L:622:VAL:CG2	2.25	0.66
5:L:61:ILE:HG23	5:L:70:GLN:CD	2.15	0.66
5:K:464:ALA:O	5:K:467:MET:HG3	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:716:ILE:HG13	5:L:761:ILE:HG21	1.76	0.66
3:D:88:CYS:SG	8:D:1501:ZN:ZN	1.83	0.66
5:K:406:MET:HB3	5:K:410:ARG:HG3	1.75	0.66
5:L:376:MET:HG3	5:L:410:ARG:CG	2.26	0.66
5:K:494:LEU:O	5:K:498:LEU:CB	2.43	0.66
3:D:773:PHE:O	3:D:776:THR:OG1	2.10	0.66
5:K:225:LEU:HD12	5:K:225:LEU:N	2.11	0.66
5:L:220:LEU:CA	5:L:224:ASN:HA	2.25	0.66
5:L:61:ILE:H	5:L:70:GLN:HG3	1.59	0.66
5:K:219:MET:CG	5:K:227:PHE:HE1	2.08	0.66
5:K:433:LEU:HD23	5:K:434:HIS:N	2.11	0.66
3:D:290:ILE:HB	2:H:352:ARG:O	1.96	0.65
5:K:371:ASN:O	5:K:372:MET:CB	2.44	0.65
5:L:244:ASN:CB	5:L:245:PRO:CD	2.36	0.65
5:L:448:ILE:HG21	5:L:467:MET:HG2	1.77	0.65
3:D:78:LEU:HD12	5:L:746:MET:CE	2.25	0.65
2:C:524:ILE:HD11	2:C:712:SER:HB3	1.78	0.65
3:I:501:VAL:HG12	3:I:502:PRO:CD	2.26	0.65
5:L:217:VAL:O	5:L:218:GLU:CG	2.44	0.65
5:L:219:MET:H	5:L:225:LEU:HD12	1.58	0.65
5:L:373:LEU:O	5:L:373:LEU:HD13	1.96	0.65
5:L:433:LEU:HD23	5:L:433:LEU:C	2.17	0.65
5:L:720:MET:CG	5:L:730:GLN:CD	2.65	0.65
7:P:1:A:H8	7:P:1:A:O5'	1.80	0.65
5:K:123:MET:H	5:K:865:LEU:HD11	1.57	0.65
5:K:151:ARG:NH1	5:K:221:ARG:O	2.28	0.65
5:L:376:MET:CB	5:L:410:ARG:CD	2.72	0.65
5:L:70:GLN:HB3	5:L:71:VAL:HB	0.83	0.65
5:L:54:MET:SD	5:L:81:LEU:HD11	2.31	0.65
5:K:123:MET:HB3	5:K:865:LEU:HD12	1.78	0.65
5:K:222:ARG:NH1	5:K:222:ARG:HG3	2.11	0.65
5:K:863:ARG:HB2	5:K:961:ARG:NH2	2.12	0.65
5:L:737:MET:CB	5:L:738:ILE:HB	2.22	0.65
5:K:775:GLN:O	5:K:777:ILE:N	2.28	0.65
5:L:465:ARG:O	5:L:469:TYR:CD2	2.42	0.65
5:L:493:TRP:CZ2	5:L:609:HIS:CD2	2.84	0.65
5:K:719:ALA:C	5:K:723:PHE:CZ	2.70	0.65
5:K:377:ILE:HG21	5:K:410:ARG:HD2	1.79	0.65
5:K:743:SER:HA	5:K:744:ASP:HB2	1.79	0.65
5:K:843:MET:SD	5:K:845:LEU:HD22	2.37	0.65
5:L:373:LEU:HD22	5:L:373:LEU:O	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:625:GLU:HG2	2:H:626:GLU:H	1.62	0.64
5:K:61:ILE:HG23	5:K:102:LEU:CD1	2.28	0.64
5:K:372:MET:N	5:K:375:GLU:HG3	2.07	0.64
5:L:494:LEU:CD1	5:L:523:LEU:HD11	2.17	0.64
5:L:842:ARG:O	5:L:850:ASN:ND2	2.30	0.64
5:K:69:MET:CE	5:K:83:TYR:HB2	2.26	0.64
5:K:722:LEU:CD1	5:K:726:ILE:CD1	2.75	0.64
5:L:538:MET:HG2	5:L:542:GLU:CG	2.26	0.64
2:C:625:GLU:HG2	2:C:626:GLU:H	1.62	0.64
5:L:219:MET:C	5:L:225:LEU:CB	2.66	0.64
5:K:52:ARG:CG	5:K:54:MET:CE	2.69	0.64
5:K:580:MET:HB3	5:K:610:VAL:HG12	1.79	0.64
5:K:722:LEU:C	5:K:722:LEU:HD13	2.17	0.64
5:L:495:MET:HE3	5:L:499:THR:CG2	2.26	0.64
5:L:582:ASP:HB2	5:L:593:ARG:HH22	1.60	0.64
5:L:737:MET:CG	5:L:738:ILE:CG2	2.70	0.64
5:L:818:LEU:HB2	5:L:843:MET:HB3	1.79	0.64
2:H:1065:LYS:NZ	7:N:8:C:O2'	2.30	0.64
3:I:393:THR:OG1	5:K:733:ARG:CG	2.45	0.64
5:K:467:MET:SD	5:K:654:LEU:C	2.76	0.64
5:K:863:ARG:NE	5:K:961:ARG:NE	2.46	0.64
5:L:436:ILE:CD1	5:L:609:HIS:CE1	2.81	0.64
5:K:466:ASP:CA	5:K:467:MET:HB3	2.27	0.64
5:L:719:ALA:O	5:L:723:PHE:CE1	2.50	0.64
5:L:158:GLN:HG2	5:L:186:GLU:CD	2.18	0.64
5:K:61:ILE:HD12	5:K:83:TYR:CD1	2.33	0.63
5:L:158:GLN:CD	5:L:186:GLU:HG2	2.19	0.63
5:L:377:ILE:HG22	5:L:377:ILE:O	1.98	0.63
5:L:535:HIS:CE1	5:L:538:MET:CB	2.80	0.63
5:L:123:MET:HG3	5:L:865:LEU:HD22	1.80	0.63
5:K:407:LEU:CG	5:K:408:MET:HG2	2.25	0.63
5:K:842:ARG:O	5:K:850:ASN:ND2	2.32	0.63
7:P:2:U:O5'	7:P:2:U:H6	1.81	0.63
5:K:123:MET:CB	5:K:865:LEU:HD12	2.28	0.63
5:K:578:MET:HB3	5:K:607:GLN:C	2.19	0.63
5:K:53:VAL:O	5:K:54:MET:HG3	1.98	0.63
1:B:44:ARG:CZ	3:D:538:ARG:HD2	2.29	0.63
3:D:501:VAL:HG12	3:D:502:PRO:CD	2.27	0.63
5:K:726:ILE:O	5:K:746:MET:CB	2.47	0.63
2:H:1273:MET:HA	2:H:1276:TRP:CD1	2.34	0.63
5:K:364:LYS:HG2	5:K:391:SER:CB	2.28	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:538:MET:CG	5:L:542:GLU:CB	2.77	0.63
3:I:1279:GLN:HB2	3:I:1282:TYR:HB2	1.81	0.63
5:L:357:ALA:HB1	5:L:362:GLY:N	2.13	0.63
2:C:1273:MET:HA	2:C:1276:TRP:CD1	2.34	0.62
7:P:2:U:H2'	7:P:3:C:C6	2.34	0.62
5:K:377:ILE:C	5:K:379:GLU:HB3	2.20	0.62
5:K:720:MET:SD	5:K:730:GLN:HG3	2.39	0.62
5:K:189:MET:N	5:K:223:PHE:CZ	2.68	0.62
5:K:219:MET:HG3	5:K:227:PHE:CE1	2.34	0.62
5:L:493:TRP:CE2	5:L:609:HIS:NE2	2.66	0.62
5:L:407:LEU:HG	5:L:408:MET:N	2.13	0.62
5:K:42:LEU:HD11	5:K:242:ALA:HB2	1.82	0.62
5:L:185:ILE:CG1	5:L:222:ARG:NH2	2.62	0.62
5:L:318:GLN:O	5:L:319:LEU:HD23	1.99	0.62
2:C:689:ALA:HA	2:C:1235:LEU:HA	1.81	0.62
5:L:218:GLU:OE2	5:L:221:ARG:HB3	2.00	0.62
5:K:185:ILE:CD1	5:K:185:ILE:H	2.12	0.62
5:K:357:ALA:O	5:K:359:LEU:N	2.32	0.62
5:K:222:ARG:CG	5:K:222:ARG:HH11	2.12	0.62
5:K:61:ILE:HD12	5:K:83:TYR:CE1	2.33	0.62
5:K:494:LEU:HD13	5:K:523:LEU:HD21	1.82	0.62
5:K:537:GLY:H	5:K:543:ARG:HH21	1.47	0.62
5:K:863:ARG:HB3	5:K:961:ARG:NH2	2.07	0.62
5:L:220:LEU:N	5:L:225:LEU:H	1.98	0.62
5:L:911:ASP:CG	5:L:947:MET:CE	2.67	0.62
3:D:77:ARG:CD	5:L:747:LEU:CD1	2.78	0.62
5:K:377:ILE:O	5:K:379:GLU:CB	2.43	0.62
5:L:42:LEU:HD11	5:L:242:ALA:HB2	1.82	0.62
5:L:538:MET:CE	5:L:542:GLU:OE1	2.48	0.62
5:K:123:MET:O	5:K:126:PHE:HB3	1.99	0.61
5:L:737:MET:HE1	5:L:761:ILE:CG2	2.30	0.61
5:K:405:SER:HB3	5:K:406:MET:SD	2.40	0.61
5:L:468:LEU:CB	5:L:617:ALA:HB1	2.30	0.61
5:L:725:ILE:HD12	5:L:725:ILE:H	1.63	0.61
2:H:689:ALA:HA	2:H:1235:LEU:HA	1.81	0.61
5:K:433:LEU:C	5:K:433:LEU:HD23	2.20	0.61
5:K:490:ARG:O	5:K:494:LEU:HG	2.00	0.61
5:K:52:ARG:C	5:K:54:MET:CE	2.68	0.61
2:H:841:ARG:CZ	3:I:257:GLY:HA2	2.30	0.61
5:K:403:LEU:CB	5:K:407:LEU:HD13	2.29	0.61
5:K:843:MET:HA	5:K:850:ASN:HB2	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:K:863:ARG:NE	5:K:961:ARG:CZ	2.64	0.61
5:L:270:CYS:O	5:L:272:ALA:N	2.32	0.61
5:L:433:LEU:HD12	5:L:632:PHE:HB2	1.83	0.61
5:L:468:LEU:HD22	5:L:469:TYR:CD2	2.36	0.61
5:L:578:MET:HG2	5:L:579:VAL:N	2.15	0.61
3:D:1279:GLN:HB2	3:D:1282:TYR:HB2	1.82	0.61
3:D:267:ASP:OD1	6:O:15:DG:O3'	2.17	0.61
2:H:912:ASP:CA	2:H:913:VAL:HG13	2.31	0.61
5:K:403:LEU:CA	5:K:407:LEU:HB2	2.30	0.61
5:K:61:ILE:HB	5:K:69:MET:CB	2.23	0.61
5:L:469:TYR:O	5:L:473:ILE:CG1	2.49	0.61
5:L:468:LEU:CG	5:L:617:ALA:CB	2.72	0.61
5:K:578:MET:SD	5:K:608:ILE:CD1	2.89	0.61
5:L:436:ILE:CG1	5:L:609:HIS:CE1	2.84	0.61
5:K:357:ALA:C	5:K:359:LEU:N	2.54	0.61
5:L:185:ILE:HD11	5:L:222:ARG:CZ	2.29	0.61
5:L:495:MET:HE3	5:L:499:THR:HG21	1.81	0.61
5:L:407:LEU:HA	5:L:410:ARG:HB3	1.82	0.61
5:L:123:MET:HG3	5:L:865:LEU:HB2	1.65	0.61
3:D:366:CYS:SG	3:D:367:GLY:N	2.74	0.61
3:I:366:CYS:SG	3:I:367:GLY:N	2.73	0.61
5:L:737:MET:CA	5:L:738:ILE:HG22	2.25	0.61
5:K:69:MET:CG	5:K:97:LEU:HB2	2.28	0.61
5:L:59:ASP:O	5:L:70:GLN:CB	2.48	0.61
3:I:393:THR:OG1	5:K:733:ARG:CD	2.49	0.60
5:K:322:GLU:HG2	5:K:323:SER:N	2.16	0.60
5:L:579:VAL:HA	5:L:609:HIS:HB3	1.83	0.60
5:K:185:ILE:O	5:K:189:MET:HG2	2.01	0.60
5:L:217:VAL:O	5:L:218:GLU:HG3	2.00	0.60
5:L:436:ILE:HD11	5:L:609:HIS:CE1	2.36	0.60
5:L:738:ILE:HG23	5:L:759:ILE:CG2	2.29	0.60
2:H:887:VAL:HB	2:H:913:VAL:HG21	1.84	0.60
5:K:219:MET:HB2	5:K:227:PHE:CE1	2.36	0.60
2:C:912:ASP:CB	2:C:913:VAL:HG12	2.30	0.60
2:H:850:ILE:HA	2:H:885:GLY:O	2.01	0.60
5:K:140:PHE:O	5:K:142:MET:HG3	2.00	0.60
2:C:850:ILE:HA	2:C:885:GLY:O	2.01	0.60
5:K:495:MET:O	5:K:499:THR:HG22	2.01	0.60
5:K:226:ARG:HH22	5:K:752:PRO:HB3	1.67	0.60
5:L:469:TYR:O	5:L:473:ILE:HG13	2.01	0.60
2:C:799:ASN:HA	2:C:1230:MET:O	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:644:MET:O	3:D:764:ARG:NH1	2.35	0.60
5:K:374:GLY:HA3	5:K:378:GLY:O	2.01	0.60
5:L:737:MET:CB	5:L:738:ILE:HG21	1.95	0.60
5:L:726:ILE:HG22	5:L:747:LEU:HD23	1.84	0.60
5:K:617:ALA:O	5:K:620:VAL:HG22	2.02	0.60
3:I:644:MET:O	3:I:764:ARG:NH1	2.35	0.60
5:L:62:THR:CB	5:L:68:GLN:OE1	2.50	0.60
3:D:584:PRO:O	3:D:586:GLY:N	2.35	0.60
5:L:617:ALA:O	5:L:620:VAL:HG22	2.02	0.60
3:I:925:GLU:HB3	3:I:926:PRO:HD3	1.83	0.59
5:K:737:MET:HE1	5:K:771:ARG:NH1	2.17	0.59
5:L:370:LEU:C	5:L:370:LEU:HD23	2.22	0.59
1:B:193:GLU:OE1	3:D:409:TRP:HB2	2.02	0.59
2:H:799:ASN:HA	2:H:1230:MET:O	2.01	0.59
5:K:453:ILE:H	5:K:453:ILE:HD12	1.67	0.59
5:K:719:ALA:O	5:K:723:PHE:CE1	2.55	0.59
5:K:70:GLN:HB2	5:K:86:THR:HB	1.82	0.59
2:C:1061:GLN:HB2	2:C:1062:PRO:CD	2.32	0.59
3:D:925:GLU:HB3	3:D:926:PRO:HD3	1.83	0.59
2:H:1061:GLN:HB2	2:H:1062:PRO:CD	2.32	0.59
5:K:433:LEU:HD12	5:K:632:PHE:CB	2.32	0.59
5:K:841:VAL:HG22	5:K:842:ARG:O	2.02	0.59
5:L:435:THR:CG2	5:L:437:LYS:HZ2	2.14	0.59
5:L:535:HIS:NE2	5:L:542:GLU:OE2	2.35	0.59
5:K:54:MET:HE3	5:K:54:MET:N	2.17	0.59
5:K:52:ARG:NH1	5:K:54:MET:SD	2.75	0.59
5:L:185:ILE:HG13	5:L:222:ARG:CD	2.32	0.59
5:L:185:ILE:CD1	5:L:222:ARG:NH2	2.64	0.59
5:L:720:MET:HA	5:L:723:PHE:CZ	2.37	0.59
3:D:532:GLU:HA	3:D:535:ARG:HD3	1.85	0.59
5:K:406:MET:O	5:K:407:LEU:HB3	2.03	0.59
5:K:578:MET:HB3	5:K:608:ILE:HA	1.83	0.59
5:K:580:MET:CB	5:K:610:VAL:HG13	2.24	0.59
5:L:185:ILE:HD11	5:L:222:ARG:HH22	1.68	0.59
5:L:510:CYS:HA	5:L:581:PHE:HB3	1.84	0.59
5:L:737:MET:HB3	5:L:738:ILE:HG22	0.59	0.59
5:K:57:PRO:HA	5:K:71:VAL:CG1	2.31	0.59
2:C:490:GLN:O	2:C:492:MET:N	2.36	0.59
3:D:1179:PRO:HD2	3:D:1183:SER:O	2.02	0.59
3:D:1323:ALA:HB1	3:D:1328:THR:HG22	1.85	0.59
3:I:584:PRO:O	3:I:586:GLY:N	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:K:185:ILE:CG1	5:K:222:ARG:HD3	2.27	0.59
5:K:407:LEU:CG	5:K:408:MET:H	2.14	0.59
5:K:843:MET:CE	5:K:850:ASN:CB	2.80	0.59
5:K:726:ILE:O	5:K:746:MET:HB2	2.02	0.59
5:K:433:LEU:HD12	5:K:632:PHE:CG	2.38	0.58
5:L:162:ALA:HA	5:L:190:ILE:CD1	2.32	0.58
5:K:124:ASP:OD1	5:K:125:ARG:N	2.35	0.58
5:K:726:ILE:O	5:K:747:LEU:HB2	2.02	0.58
5:L:371:ASN:N	5:L:371:ASN:HD22	1.99	0.58
2:C:1215:GLY:O	2:C:1217:THR:N	2.35	0.58
3:D:77:ARG:NE	5:L:747:LEU:CD1	2.66	0.58
2:H:490:GLN:O	2:H:492:MET:N	2.36	0.58
5:K:720:MET:CA	5:K:723:PHE:CZ	2.85	0.58
5:L:184:THR:OG1	5:L:185:ILE:HD12	2.03	0.58
5:L:577:HIS:O	5:L:578:MET:CB	2.40	0.58
5:L:736:ASN:HD22	5:L:736:ASN:N	1.99	0.58
2:H:1215:GLY:O	2:H:1217:THR:N	2.36	0.58
5:K:451:SER:O	5:K:455:GLY:N	2.37	0.58
5:L:219:MET:HE1	5:L:253:ILE:HD12	1.86	0.58
3:I:520:ALA:O	3:I:521:LYS:C	2.41	0.58
5:L:359:LEU:HD23	5:L:359:LEU:N	2.11	0.58
5:L:726:ILE:C	5:L:746:MET:HG2	2.22	0.58
5:L:123:MET:SD	5:L:961:ARG:NH2	2.77	0.58
5:K:467:MET:HE1	5:K:654:LEU:HB3	1.78	0.58
3:I:78:LEU:CD1	5:K:746:MET:SD	2.78	0.58
5:L:468:LEU:C	5:L:468:LEU:HD23	2.23	0.58
5:L:61:ILE:HG12	5:L:70:GLN:HE21	1.66	0.58
5:L:580:MET:CE	5:L:593:ARG:HD3	2.33	0.58
5:L:773:ASP:O	5:L:778:THR:HG21	2.04	0.58
3:I:1323:ALA:HB1	3:I:1328:THR:HG22	1.85	0.58
3:I:164:GLN:O	3:I:166:LEU:N	2.37	0.58
5:K:520:GLU:HG3	5:K:533:VAL:HG22	1.85	0.58
1:F:50:SER:O	1:F:51:MET:HB2	2.04	0.58
5:K:218:GLU:O	5:K:222:ARG:HB3	2.03	0.58
5:K:224:ASN:C	5:K:225:LEU:HD12	2.24	0.58
5:L:218:GLU:HG2	5:L:221:ARG:CA	2.34	0.58
5:L:277:LEU:HB3	5:L:309:VAL:HG12	1.86	0.58
5:L:727:GLY:HA3	5:L:746:MET:O	2.03	0.58
3:D:164:GLN:O	3:D:166:LEU:N	2.37	0.58
5:K:83:TYR:HB2	5:K:97:LEU:O	2.04	0.58
5:L:184:THR:CB	5:L:312:LEU:HD21	2.32	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:231:PHE:HB2	1:G:221:ALA:HB3	1.85	0.57
2:H:81:ASP:O	2:H:85:CYS:N	2.36	0.57
5:K:54:MET:HG2	5:K:81:LEU:CD1	2.34	0.57
5:L:185:ILE:CD1	5:L:222:ARG:NH1	2.67	0.57
5:L:444:TYR:CD1	5:L:470:PRO:HB2	2.38	0.57
5:L:720:MET:SD	5:L:730:GLN:CD	2.82	0.57
3:D:208:THR:HG22	3:I:196:GLN:HB3	1.86	0.57
5:L:141:ARG:O	5:L:141:ARG:HG3	2.04	0.57
5:K:185:ILE:HA	5:K:222:ARG:HD3	1.86	0.57
5:K:377:ILE:HB	5:K:410:ARG:HD2	1.85	0.57
5:L:469:TYR:O	5:L:473:ILE:CB	2.53	0.57
3:D:338:PHE:CZ	3:D:1323:ALA:HB3	2.39	0.57
3:D:78:LEU:HD12	5:L:746:MET:HE3	1.86	0.57
5:K:403:LEU:HB2	5:K:407:LEU:HD22	1.86	0.57
5:K:61:ILE:CD1	5:K:83:TYR:CD1	2.87	0.57
5:K:720:MET:N	5:K:723:PHE:CZ	2.73	0.57
5:K:720:MET:SD	5:K:730:GLN:CG	2.92	0.57
5:K:907:ARG:HH21	5:K:947:MET:CE	2.17	0.57
5:K:726:ILE:CG2	5:K:747:LEU:HD23	2.34	0.57
5:L:83:TYR:HB2	5:L:97:LEU:O	2.04	0.57
3:I:520:ALA:O	3:I:522:GLY:N	2.36	0.57
5:K:143:PRO:HD2	5:K:148:ARG:HH21	1.67	0.57
5:K:358:MET:HB3	5:K:365:LEU:HB2	1.87	0.57
5:L:520:GLU:HG3	5:L:533:VAL:HG22	1.85	0.57
3:D:78:LEU:CB	5:L:746:MET:HA	2.32	0.57
2:H:807:TRP:O	2:H:809:GLY:N	2.38	0.57
2:H:912:ASP:CB	2:H:913:VAL:HG12	2.31	0.57
5:K:355:ALA:HA	5:K:358:MET:CG	2.26	0.57
5:K:743:SER:CA	5:K:744:ASP:HB2	2.34	0.57
5:K:773:ASP:O	5:K:778:THR:HG21	2.04	0.57
5:L:316:PRO:O	5:L:318:GLN:N	2.37	0.57
5:L:453:ILE:H	5:L:453:ILE:CD1	2.17	0.57
2:C:807:TRP:O	2:C:809:GLY:N	2.38	0.57
3:I:1264:ALA:HB2	3:I:1280:VAL:HG22	1.86	0.57
5:K:219:MET:HB2	5:K:227:PHE:HE1	1.69	0.57
5:L:407:LEU:HD13	5:L:410:ARG:HH21	1.65	0.57
2:C:561:ILE:O	2:C:680:LEU:HD13	2.05	0.57
2:C:912:ASP:CA	2:C:913:VAL:HG13	2.35	0.57
5:K:277:LEU:HB3	5:K:309:VAL:HG12	1.86	0.57
5:K:70:GLN:O	5:K:85:GLY:HA2	2.04	0.57
5:K:185:ILE:HG13	5:K:222:ARG:CZ	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:K:341:GLN:O	5:K:343:VAL:N	2.38	0.56
5:K:538:MET:O	5:K:539:SER:CB	2.53	0.56
2:H:906:PHE:HA	5:K:540:ILE:HD13	1.86	0.56
3:I:338:PHE:CZ	3:I:1323:ALA:HB3	2.40	0.56
5:K:162:ALA:CA	5:K:190:ILE:HD11	2.31	0.56
5:K:335:ARG:NH1	5:K:928:ASN:OD1	2.38	0.56
5:L:185:ILE:CD1	5:L:185:ILE:H	2.18	0.56
5:L:720:MET:HG3	5:L:730:GLN:CD	2.24	0.56
5:K:407:LEU:CG	5:K:408:MET:N	2.68	0.56
5:L:219:MET:CE	5:L:253:ILE:HD12	2.36	0.56
5:L:335:ARG:NH1	5:L:928:ASN:OD1	2.38	0.56
2:C:81:ASP:O	2:C:85:CYS:N	2.37	0.56
2:C:887:VAL:HB	2:C:913:VAL:HG21	1.86	0.56
5:K:53:VAL:C	5:K:54:MET:HE2	2.26	0.56
5:L:580:MET:HE1	5:L:593:ARG:HD3	1.87	0.56
5:L:434:HIS:HB3	5:L:609:HIS:HA	1.85	0.56
5:L:123:MET:HG3	5:L:865:LEU:CD2	2.35	0.56
1:A:50:SER:O	1:A:51:MET:HB2	2.04	0.56
4:E:6:VAL:HG13	4:E:6:VAL:O	2.06	0.56
2:H:912:ASP:CA	2:H:913:VAL:CG1	2.84	0.56
5:L:341:GLN:O	5:L:343:VAL:N	2.38	0.56
4:J:6:VAL:HG13	4:J:6:VAL:O	2.06	0.56
5:K:225:LEU:HB3	5:K:251:LEU:CD1	2.36	0.56
5:K:720:MET:HE1	5:K:738:ILE:CD1	2.30	0.56
5:L:123:MET:O	5:L:123:MET:SD	2.64	0.56
5:L:174:LEU:HD12	5:L:328:LEU:HD21	1.87	0.56
3:I:854:ALA:O	3:I:855:ASP:CB	2.54	0.56
5:L:433:LEU:HD23	5:L:434:HIS:C	2.26	0.56
2:C:698:PRO:O	2:C:699:LEU:C	2.44	0.56
3:I:1181:ASP:O	3:I:1183:SER:N	2.38	0.56
5:K:463:ARG:O	5:K:466:ASP:HB2	2.06	0.56
5:K:60:THR:HB	5:K:69:MET:O	2.05	0.56
5:L:356:VAL:HG12	5:L:358:MET:CE	2.33	0.56
5:L:433:LEU:HD12	5:L:632:PHE:CD2	2.39	0.56
5:L:535:HIS:NE2	5:L:538:MET:CB	2.66	0.56
2:C:914:LYS:O	2:C:916:SER:N	2.38	0.56
3:D:1264:ALA:HB2	3:D:1280:VAL:HG22	1.87	0.56
5:K:217:VAL:O	5:K:221:ARG:N	2.39	0.56
5:K:466:ASP:CB	5:K:467:MET:CB	2.84	0.56
2:C:94:ALA:HB2	2:C:129:LEU:HD11	1.87	0.56
2:H:1126:ASP:HA	2:H:1129:ASN:HB3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:561:ILE:O	2:H:680:LEU:HD13	2.06	0.56
3:I:519:ASN:ND2	3:I:710:ASP:H	2.03	0.56
3:I:532:GLU:HA	3:I:535:ARG:HD3	1.86	0.56
2:C:637:ARG:O	2:C:638:SER:HB3	2.06	0.56
2:H:637:ARG:O	2:H:638:SER:HB3	2.06	0.56
2:C:907:GLY:HA3	5:L:539:SER:OG	2.07	0.56
5:L:540:ILE:HD12	5:L:540:ILE:H	1.70	0.56
3:D:270:ARG:O	3:D:273:ILE:N	2.39	0.55
5:K:535:HIS:CE1	5:K:538:MET:HG2	2.32	0.55
5:K:437:LYS:HG3	5:K:612:TYR:CE1	2.42	0.55
2:C:788:SER:O	2:C:795:ALA:N	2.36	0.55
2:H:698:PRO:O	2:H:699:LEU:C	2.43	0.55
2:H:94:ALA:HB2	2:H:129:LEU:HD11	1.87	0.55
5:K:174:LEU:HD12	5:K:328:LEU:HD21	1.87	0.55
5:K:405:SER:CB	5:K:406:MET:SD	2.94	0.55
5:K:539:SER:HB3	5:K:542:GLU:OE2	2.05	0.55
5:L:498:LEU:HD21	5:L:529:ILE:CD1	2.36	0.55
5:L:60:THR:HA	5:L:70:GLN:CG	2.36	0.55
5:L:761:ILE:HG12	5:L:761:ILE:O	2.06	0.55
1:G:44:ARG:CZ	3:I:538:ARG:HD2	2.36	0.55
5:K:59:ASP:C	5:K:71:VAL:HG23	2.26	0.55
5:L:61:ILE:HG12	5:L:70:GLN:NE2	2.21	0.55
5:K:376:MET:O	5:K:377:ILE:HG13	1.98	0.55
5:L:139:GLN:CG	5:L:142:MET:SD	2.94	0.55
5:L:69:MET:O	5:L:70:GLN:CG	2.54	0.55
3:I:270:ARG:O	3:I:273:ILE:N	2.39	0.55
5:K:377:ILE:CB	5:K:410:ARG:HD2	2.37	0.55
5:K:70:GLN:HB3	5:K:86:THR:OG1	2.07	0.55
5:L:583:LEU:CD1	5:L:622:VAL:CG2	2.84	0.55
5:K:316:PRO:O	5:K:318:GLN:N	2.38	0.55
5:K:123:MET:CB	5:K:865:LEU:HD13	2.30	0.55
5:L:123:MET:SD	5:L:123:MET:C	2.85	0.55
5:L:538:MET:CG	5:L:542:GLU:OE1	2.51	0.55
2:C:488:MET:HB2	2:C:489:PRO:HD3	1.89	0.55
2:C:698:PRO:HA	2:C:1231:TYR:CE1	2.41	0.55
3:D:212:THR:OG1	3:I:150:GLY:O	2.21	0.55
5:K:464:ALA:O	5:K:467:MET:CG	2.55	0.55
5:K:498:LEU:HD21	5:K:529:ILE:CD1	2.37	0.55
5:K:408:MET:CG	5:K:692:HIS:HB2	2.37	0.55
2:C:1126:ASP:HA	2:C:1129:ASN:HB3	1.87	0.55
3:D:268:LEU:HD13	3:D:306:LEU:HA	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:268:LEU:HD13	3:I:306:LEU:HA	1.89	0.55
5:L:376:MET:HG3	5:L:410:ARG:HH11	1.70	0.55
5:L:470:PRO:HD2	5:L:471:GLU:H	1.72	0.55
2:C:625:GLU:HG2	2:C:626:GLU:N	2.22	0.55
2:H:625:GLU:HG2	2:H:626:GLU:N	2.22	0.55
3:I:520:ALA:HB2	3:I:545:HIS:HB2	1.89	0.55
5:K:272:ALA:O	5:K:273:GLU:C	2.46	0.55
5:L:434:HIS:HD2	5:L:436:ILE:HD11	0.55	0.55
5:L:435:THR:HG22	5:L:437:LYS:NZ	2.22	0.55
2:H:488:MET:HB2	2:H:489:PRO:HD3	1.89	0.54
5:K:189:MET:N	5:K:223:PHE:HE1	2.01	0.54
5:K:377:ILE:C	5:K:379:GLU:CB	2.75	0.54
5:K:407:LEU:CD1	5:K:408:MET:HE3	2.04	0.54
5:K:843:MET:SD	5:K:850:ASN:ND2	2.80	0.54
1:B:153:VAL:O	1:B:158:ARG:NH1	2.40	0.54
1:G:153:VAL:O	1:G:158:ARG:NH1	2.40	0.54
5:K:431:ARG:NH2	5:K:635:THR:HG23	2.22	0.54
5:K:226:ARG:NH2	5:K:752:PRO:HB3	2.21	0.54
5:L:434:HIS:CD2	5:L:609:HIS:CE1	2.95	0.54
6:M:2:DC:C2'	6:M:3:DG:C8	2.86	0.54
5:K:466:ASP:CA	5:K:467:MET:CB	2.85	0.54
5:L:431:ARG:NH2	5:L:635:THR:HG23	2.23	0.54
5:L:493:TRP:HZ2	5:L:609:HIS:NE2	1.91	0.54
2:H:788:SER:O	2:H:795:ALA:N	2.36	0.54
5:L:198:GLY:O	5:L:200:ALA:N	2.37	0.54
5:L:216:LEU:O	5:L:219:MET:HB2	2.08	0.54
5:K:125:ARG:HG3	5:K:794:GLY:HA2	1.89	0.54
5:L:357:ALA:O	5:L:358:MET:HB2	2.07	0.54
5:L:493:TRP:HZ2	5:L:609:HIS:CD2	2.26	0.54
5:L:538:MET:HB3	5:L:542:GLU:OE2	2.08	0.54
5:L:437:LYS:HG3	5:L:612:TYR:CE1	2.41	0.54
3:D:1248:ILE:O	3:D:1249:ASN:C	2.46	0.54
2:H:914:LYS:O	2:H:916:SER:N	2.41	0.54
5:K:189:MET:CA	5:K:223:PHE:HE1	2.21	0.54
5:L:276:LEU:HA	5:L:308:GLY:O	2.08	0.54
5:L:736:ASN:O	5:L:760:THR:CB	2.56	0.54
3:D:1178:THR:HG22	3:D:1184:ASP:O	2.08	0.54
5:K:242:ALA:O	5:K:243:TYR:HB2	2.08	0.54
5:K:369:GLU:HG3	5:K:373:LEU:HD11	1.90	0.54
5:K:722:LEU:HD13	5:K:726:ILE:CD1	2.37	0.54
5:K:198:GLY:O	5:K:200:ALA:N	2.37	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:K:467:MET:CE	5:K:654:LEU:CB	2.75	0.53
5:K:52:ARG:NH1	5:K:54:MET:CG	2.71	0.53
5:L:123:MET:HB2	5:L:961:ARG:CZ	2.38	0.53
5:L:139:GLN:CA	5:L:142:MET:HB2	2.38	0.53
5:L:358:MET:CA	5:L:358:MET:CE	2.86	0.53
2:C:553:THR:O	2:C:554:HIS:C	2.46	0.53
5:K:188:GLY:O	5:K:192:HIS:N	2.32	0.53
5:K:453:ILE:O	5:K:453:ILE:HG22	2.08	0.53
5:K:467:MET:SD	5:K:654:LEU:HB3	2.48	0.53
5:K:533:VAL:HG12	5:K:535:HIS:HD2	1.72	0.53
5:L:242:ALA:O	5:L:243:TYR:HB2	2.08	0.53
5:L:725:ILE:H	5:L:725:ILE:CD1	2.20	0.53
2:C:1132:LEU:O	2:C:1135:GLN:N	2.40	0.53
5:K:720:MET:HG2	5:K:723:PHE:HZ	1.74	0.53
5:L:69:MET:O	5:L:70:GLN:HG3	2.07	0.53
5:L:747:LEU:CD2	5:L:751:PHE:HE2	2.10	0.53
3:D:363:LEU:HA	3:D:450:HIS:NE2	2.24	0.53
5:L:194:GLN:HG3	5:L:200:ALA:HB3	1.89	0.53
5:L:358:MET:HB2	5:L:360:LEU:CD2	2.38	0.53
2:C:1073:LYS:NZ	7:P:9:A:OP1	2.34	0.53
2:C:811:ASN:HB3	2:C:815:SER:O	2.08	0.53
2:C:912:ASP:CA	2:C:913:VAL:CG1	2.87	0.53
5:K:372:MET:H	5:K:375:GLU:CB	2.19	0.53
3:I:77:ARG:HB3	5:K:747:LEU:N	2.23	0.53
2:H:698:PRO:HA	2:H:1231:TYR:CE1	2.44	0.53
5:K:128:LEU:HD21	5:K:721:ASN:ND2	2.23	0.53
5:L:218:GLU:HG2	5:L:221:ARG:N	2.24	0.53
5:L:495:MET:HE1	5:L:499:THR:CG2	2.24	0.53
5:L:509:ILE:O	5:L:581:PHE:HB2	2.06	0.53
2:C:1061:GLN:HB2	2:C:1062:PRO:HD2	1.91	0.53
2:H:559:CYS:HB2	2:H:662:SER:HB2	1.91	0.53
5:L:436:ILE:HG22	5:L:438:LEU:HD22	1.90	0.53
5:K:364:LYS:NZ	5:K:392:ASP:CG	2.62	0.53
2:C:1072:ASN:OD1	2:C:1072:ASN:N	2.41	0.53
3:I:393:THR:OG1	5:K:733:ARG:HD2	2.09	0.53
5:L:352:VAL:O	5:L:356:VAL:N	2.42	0.53
5:L:407:LEU:CG	5:L:408:MET:H	2.20	0.53
5:L:123:MET:CB	5:L:865:LEU:HD13	2.25	0.53
5:L:843:MET:CE	5:L:894:GLN:O	2.57	0.53
3:D:334:LYS:HA	3:D:339:ARG:NE	2.24	0.52
5:K:61:ILE:HD11	5:K:83:TYR:CE2	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:376:MET:HB2	5:L:410:ARG:CD	2.37	0.52
5:L:538:MET:CG	5:L:542:GLU:HB2	2.38	0.52
5:L:74:VAL:HG13	5:L:81:LEU:CG	2.39	0.52
6:M:2:DC:O5'	6:M:2:DC:H6	1.92	0.52
1:B:159:ILE:HG22	1:B:159:ILE:O	2.10	0.52
2:H:553:THR:O	2:H:554:HIS:C	2.47	0.52
3:I:363:LEU:HA	3:I:450:HIS:NE2	2.24	0.52
5:K:219:MET:CB	5:K:227:PHE:CE1	2.88	0.52
5:K:378:GLY:CA	5:K:379:GLU:HB2	2.36	0.52
5:L:736:ASN:O	5:L:760:THR:HB	2.09	0.52
3:D:290:ILE:HD13	2:H:353:VAL:HA	1.90	0.52
2:H:811:ASN:HB3	2:H:815:SER:O	2.09	0.52
5:K:189:MET:HA	5:K:223:PHE:HE1	1.75	0.52
5:K:454:MET:CE	5:K:457:ARG:NH2	2.72	0.52
2:C:61:SER:HB3	2:C:479:LEU:HD13	1.91	0.52
3:I:334:LYS:HA	3:I:339:ARG:NE	2.24	0.52
5:K:726:ILE:O	5:K:746:MET:HB3	2.09	0.52
5:L:353:ALA:N	5:L:356:VAL:HG23	2.23	0.52
5:L:61:ILE:N	5:L:70:GLN:HG3	2.23	0.52
5:L:620:VAL:HG21	5:L:654:LEU:HD23	1.91	0.52
5:L:408:MET:N	5:L:688:LEU:HD12	2.24	0.52
5:L:716:ILE:CD1	5:L:761:ILE:HG21	2.39	0.52
2:H:1061:GLN:HB2	2:H:1062:PRO:HD2	1.91	0.52
3:I:1248:ILE:O	3:I:1249:ASN:C	2.48	0.52
2:C:516:ASP:HA	2:C:761:GLN:HE22	1.74	0.52
1:G:159:ILE:O	1:G:159:ILE:HG22	2.10	0.52
3:I:140:TYR:O	3:I:141:PHE:HB2	2.09	0.52
4:J:20:VAL:O	4:J:24:ALA:N	2.35	0.52
5:L:189:MET:CB	5:L:190:ILE:HD12	2.39	0.52
3:D:814:CYS:CB	3:D:895:CYS:SG	2.98	0.52
2:H:61:SER:HB3	2:H:479:LEU:HD13	1.91	0.52
3:D:112:ALA:HA	3:D:238:ILE:HG23	1.92	0.52
3:I:112:ALA:HA	3:I:238:ILE:HG23	1.92	0.52
5:K:748:VAL:HG13	5:K:749:PRO:HD2	1.92	0.52
5:L:218:GLU:HA	5:L:219:MET:C	2.29	0.52
5:L:408:MET:H	5:L:688:LEU:HD13	1.75	0.52
5:L:843:MET:CG	5:L:850:ASN:ND2	2.54	0.52
5:K:225:LEU:CD1	5:K:225:LEU:N	2.73	0.52
5:K:244:ASN:CB	5:K:245:PRO:CD	2.86	0.52
5:K:276:LEU:HA	5:K:308:GLY:O	2.08	0.52
5:K:539:SER:O	5:K:543:ARG:HG3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:K:620:VAL:HG21	5:K:654:LEU:HD23	1.91	0.52
5:L:511:ALA:HB2	5:L:582:ASP:OD2	2.09	0.52
5:L:716:ILE:CG1	5:L:761:ILE:HG21	2.40	0.52
5:L:738:ILE:CG2	5:L:759:ILE:CG2	2.88	0.52
2:C:674:ASP:N	2:C:674:ASP:OD1	2.43	0.52
5:L:538:MET:CB	5:L:542:GLU:OE2	2.58	0.52
5:L:433:LEU:CD1	5:L:632:PHE:CD2	2.93	0.51
5:L:737:MET:HE1	5:L:761:ILE:HB	1.92	0.51
2:C:144:VAL:HG11	2:C:527:LYS:HG2	1.91	0.51
2:H:822:VAL:O	2:H:825:GLU:O	2.28	0.51
5:K:195:LEU:HD11	5:K:225:LEU:CD2	2.39	0.51
5:K:360:LEU:N	5:K:360:LEU:CD1	2.73	0.51
5:K:745:HIS:O	5:K:746:MET:HB2	2.10	0.51
2:C:822:VAL:O	2:C:825:GLU:O	2.28	0.51
3:D:140:TYR:O	3:D:141:PHE:HB2	2.10	0.51
5:K:495:MET:O	5:K:499:THR:N	2.36	0.51
5:K:54:MET:CE	5:K:54:MET:N	2.73	0.51
5:K:75:LYS:HB2	5:K:82:THR:HB	1.92	0.51
5:L:205:ILE:HB	5:L:253:ILE:HG22	1.91	0.51
2:C:559:CYS:HB2	2:C:662:SER:HB2	1.92	0.51
5:L:408:MET:H	5:L:688:LEU:HD12	1.76	0.51
5:L:406:MET:O	5:L:410:ARG:HB2	2.11	0.51
5:L:436:ILE:N	5:L:436:ILE:CD1	2.73	0.51
2:C:907:GLY:CA	5:L:539:SER:OG	2.59	0.51
2:C:436:ARG:HG2	2:C:436:ARG:HH11	1.74	0.51
1:F:159:ILE:O	1:F:159:ILE:HG22	2.11	0.51
2:H:820:GLU:HB2	2:H:1081:PRO:HA	1.93	0.51
5:K:620:VAL:HG21	5:K:654:LEU:CD2	2.41	0.51
5:L:216:LEU:O	5:L:219:MET:CB	2.59	0.51
5:L:582:ASP:O	5:L:593:ARG:NH2	2.43	0.51
5:L:843:MET:CA	5:L:850:ASN:HD22	2.21	0.51
2:H:436:ARG:HH11	2:H:436:ARG:HG2	1.74	0.51
2:H:144:VAL:HG11	2:H:527:LYS:HG2	1.91	0.51
5:K:396:ALA:O	5:K:398:SER:N	2.43	0.51
5:K:408:MET:O	5:K:411:HIS:HB2	2.11	0.51
5:K:843:MET:HE1	5:K:850:ASN:CG	2.26	0.51
5:K:123:MET:HB3	5:K:865:LEU:CD1	2.36	0.51
5:L:620:VAL:HG21	5:L:654:LEU:CD2	2.41	0.51
5:L:68:GLN:O	5:L:69:MET:CB	2.58	0.51
5:L:737:MET:CB	5:L:760:THR:HA	2.34	0.51
3:D:369:PRO:O	3:D:372:MET:N	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:K:372:MET:O	5:K:376:MET:HG2	2.10	0.51
5:K:453:ILE:N	5:K:453:ILE:CD1	2.73	0.51
5:K:52:ARG:NH1	5:K:54:MET:HG3	2.26	0.51
5:K:52:ARG:HG2	5:K:54:MET:SD	2.46	0.51
5:K:61:ILE:CG1	5:K:69:MET:HE1	2.38	0.51
5:L:407:LEU:CD1	5:L:688:LEU:CD1	2.88	0.51
5:L:510:CYS:HA	5:L:581:PHE:CD2	2.46	0.51
5:K:205:ILE:HB	5:K:253:ILE:HG22	1.91	0.51
5:L:219:MET:CB	5:L:225:LEU:HB2	2.41	0.51
5:L:746:MET:O	5:L:747:LEU:HD23	2.11	0.51
5:L:716:ILE:CD1	5:L:761:ILE:HD13	2.28	0.51
2:C:149:LEU:HD23	2:C:150:HIS:N	2.26	0.51
3:D:436:ALA:HB3	3:D:485:MET:HA	1.93	0.51
5:K:453:ILE:H	5:K:453:ILE:CD1	2.23	0.51
5:K:470:PRO:HA	5:K:473:ILE:HB	1.92	0.51
5:K:844:LEU:H	5:K:850:ASN:HB2	1.74	0.51
5:L:122:ARG:CB	5:L:124:ASP:OD1	2.55	0.51
5:L:75:LYS:HB2	5:L:82:THR:HB	1.92	0.51
1:A:159:ILE:O	1:A:159:ILE:HG22	2.10	0.51
2:H:516:ASP:HA	2:H:761:GLN:HE22	1.75	0.51
2:H:577:VAL:HG23	2:H:661:VAL:O	2.11	0.51
5:K:194:GLN:HG3	5:K:200:ALA:HB3	1.92	0.51
5:K:372:MET:CA	5:K:375:GLU:HB2	2.36	0.51
5:L:218:GLU:HG2	5:L:221:ARG:H	1.76	0.51
5:L:577:HIS:CD2	5:L:607:GLN:OE1	2.63	0.51
5:L:719:ALA:O	5:L:723:PHE:CZ	2.64	0.51
1:F:131:CYS:SG	1:F:132:HIS:N	2.84	0.50
5:K:194:GLN:CG	5:K:200:ALA:HB3	2.40	0.50
5:L:372:MET:HA	5:L:375:GLU:HG2	1.91	0.50
5:L:433:LEU:HD23	5:L:434:HIS:CA	2.41	0.50
6:O:15:DG:O6	7:P:1:A:H2	1.93	0.50
2:C:820:GLU:HB2	2:C:1081:PRO:HA	1.92	0.50
2:C:135:THR:HG22	2:C:144:VAL:HG22	1.93	0.50
2:H:149:LEU:HD23	2:H:150:HIS:N	2.25	0.50
5:K:722:LEU:HD11	5:K:726:ILE:CD1	2.39	0.50
5:L:219:MET:O	5:L:225:LEU:CG	2.56	0.50
2:C:842:ASP:HB2	2:C:1047:LEU:HG	1.93	0.50
3:I:814:CYS:CB	3:I:895:CYS:SG	2.99	0.50
5:K:722:LEU:O	5:K:722:LEU:HD13	2.10	0.50
5:K:843:MET:SD	5:K:850:ASN:CG	2.88	0.50
5:L:219:MET:C	5:L:225:LEU:CG	2.80	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:322:GLU:HA	5:L:324:HIS:CD2	2.46	0.50
2:H:842:ASP:HB2	2:H:1047:LEU:HG	1.94	0.50
2:H:135:THR:HG22	2:H:144:VAL:HG22	1.94	0.50
2:C:577:VAL:HG23	2:C:661:VAL:O	2.11	0.50
1:G:193:GLU:OE1	3:I:409:TRP:HB2	2.11	0.50
3:I:791:ALA:HB2	6:M:5:DC:C5	2.47	0.50
5:L:435:THR:HG22	5:L:437:LYS:HZ2	1.76	0.50
5:L:538:MET:HG2	5:L:542:GLU:HB2	1.91	0.50
5:L:721:ASN:C	5:L:725:ILE:HD13	2.31	0.50
5:K:743:SER:HB2	5:K:744:ASP:HB2	1.93	0.50
5:K:812:GLY:O	5:K:813:THR:C	2.49	0.50
5:L:218:GLU:HG2	5:L:221:ARG:CB	2.42	0.50
5:L:561:LEU:HD13	5:L:562:CYS:N	2.27	0.50
5:L:578:MET:O	5:L:609:HIS:CB	2.57	0.50
5:L:725:ILE:N	5:L:725:ILE:CD1	2.73	0.50
2:C:496:LYS:HB3	2:C:497:PRO:HD3	1.94	0.50
2:H:674:ASP:OD1	2:H:674:ASP:N	2.44	0.50
5:K:123:MET:HB3	5:K:798:SER:O	2.12	0.50
5:K:546:ALA:O	5:K:550:PHE:N	2.39	0.50
5:L:818:LEU:O	5:L:843:MET:CB	2.57	0.50
2:C:359:ARG:NE	2:C:363:LEU:HD11	2.27	0.50
5:L:139:GLN:CG	5:L:142:MET:HE3	2.33	0.50
3:D:78:LEU:CG	5:L:746:MET:CB	2.89	0.50
2:C:798:GLN:O	2:C:1231:TYR:HA	2.12	0.50
3:D:814:CYS:HB3	3:D:895:CYS:SG	2.51	0.50
2:H:704:MET:O	2:H:708:VAL:HG23	2.12	0.50
5:K:151:ARG:HB2	5:K:221:ARG:O	2.12	0.50
5:K:374:GLY:O	5:K:378:GLY:N	2.44	0.50
5:L:128:LEU:CD2	5:L:721:ASN:O	2.60	0.50
2:C:194:LEU:O	2:C:206:ALA:HB2	2.11	0.49
2:C:704:MET:O	2:C:708:VAL:HG23	2.12	0.49
3:I:436:ALA:HB3	3:I:485:MET:HA	1.94	0.49
5:K:318:GLN:O	5:K:319:LEU:CG	2.59	0.49
5:K:466:ASP:CB	5:K:467:MET:HB3	2.42	0.49
5:K:123:MET:HG3	5:K:865:LEU:HB2	1.94	0.49
5:K:491:VAL:HA	5:K:494:LEU:HD12	1.93	0.49
5:K:719:ALA:HB1	5:K:723:PHE:HE1	1.77	0.49
1:G:131:CYS:SG	1:G:132:HIS:N	2.85	0.49
2:H:359:ARG:NE	2:H:363:LEU:HD11	2.27	0.49
3:I:814:CYS:HB3	3:I:895:CYS:SG	2.52	0.49
5:L:219:MET:CE	5:L:227:PHE:CE1	2.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:80:HIS:CE1	5:L:54:MET:CE	2.95	0.49
2:H:798:GLN:O	2:H:1231:TYR:HA	2.12	0.49
2:H:194:LEU:O	2:H:206:ALA:HB2	2.11	0.49
5:K:19:LEU:CD1	5:K:102:LEU:CD2	2.88	0.49
5:K:321:MET:O	5:K:323:SER:N	2.45	0.49
5:K:410:ARG:HG2	5:K:927:VAL:HG13	1.95	0.49
5:L:448:ILE:HG23	5:L:467:MET:HG3	1.93	0.49
5:K:341:GLN:O	5:K:342:PHE:C	2.51	0.49
5:K:467:MET:O	5:K:467:MET:HE3	2.12	0.49
5:L:580:MET:HE2	5:L:583:LEU:HD23	1.93	0.49
1:A:131:CYS:SG	1:A:132:HIS:N	2.85	0.49
2:C:475:VAL:HG12	2:C:479:LEU:HD12	1.95	0.49
2:H:672:GLU:O	3:I:767:LEU:HD13	2.11	0.49
5:K:190:ILE:N	5:K:190:ILE:HD12	2.28	0.49
5:K:374:GLY:C	5:K:378:GLY:O	2.50	0.49
5:K:433:LEU:HD12	5:K:632:PHE:HB2	1.95	0.49
3:I:392:THR:HB	5:K:733:ARG:NH2	2.28	0.49
5:K:843:MET:HA	5:K:850:ASN:CB	2.40	0.49
5:L:720:MET:CA	5:L:720:MET:HE2	2.42	0.49
5:L:812:GLY:O	5:L:813:THR:C	2.50	0.49
5:L:911:ASP:OD2	5:L:947:MET:CE	2.58	0.49
3:D:78:LEU:HB2	5:L:746:MET:CA	2.34	0.49
5:L:405:SER:O	5:L:406:MET:C	2.48	0.49
2:H:1072:ASN:N	2:H:1072:ASN:OD1	2.41	0.49
3:I:369:PRO:O	3:I:372:MET:N	2.45	0.49
3:I:506:VAL:HG13	3:I:628:GLY:HA3	1.95	0.49
5:K:356:VAL:O	5:K:359:LEU:N	2.43	0.49
5:K:561:LEU:HD13	5:K:562:CYS:N	2.27	0.49
5:L:436:ILE:HG22	5:L:438:LEU:CD2	2.42	0.49
5:L:433:LEU:HA	5:L:608:ILE:HB	1.94	0.49
2:C:1065:LYS:NZ	7:P:8:C:O2'	2.46	0.49
2:C:692:THR:HG21	2:C:798:GLN:OE1	2.12	0.49
3:D:270:ARG:O	3:D:271:ARG:C	2.51	0.49
3:I:270:ARG:O	3:I:271:ARG:C	2.51	0.49
3:I:848:VAL:HG13	3:I:850:LYS:HG2	1.95	0.49
5:K:408:MET:SD	5:K:691:ILE:CB	3.01	0.49
5:K:748:VAL:HG12	5:K:749:PRO:N	2.26	0.49
5:L:243:TYR:O	5:L:244:ASN:HB2	2.13	0.49
2:H:1132:LEU:O	2:H:1135:GLN:N	2.39	0.49
2:H:1255:THR:O	2:H:1257:GLN:N	2.46	0.49
2:H:1336:ASN:HB2	3:I:29:MET:SD	2.53	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:30:MET:HG2	4:J:35:LYS:HB3	1.95	0.49
5:K:143:PRO:CD	5:K:148:ARG:HH22	2.23	0.49
5:K:377:ILE:HB	5:K:410:ARG:CD	2.42	0.49
5:L:720:MET:CE	5:L:720:MET:CA	2.66	0.49
2:H:1185:PRO:O	2:H:1186:VAL:C	2.51	0.48
3:I:51:PRO:HB2	3:I:57:PHE:C	2.33	0.48
5:K:144:TYR:CG	5:K:706:ILE:HD11	2.48	0.48
5:K:190:ILE:N	5:K:190:ILE:CD1	2.76	0.48
5:K:843:MET:CE	5:K:850:ASN:HB3	2.39	0.48
5:L:184:THR:HA	5:L:312:LEU:HD21	1.94	0.48
2:H:692:THR:HG21	2:H:798:GLN:OE1	2.13	0.48
5:K:192:HIS:HB2	5:K:223:PHE:HD1	1.78	0.48
5:K:539:SER:O	5:K:543:ARG:CZ	2.61	0.48
5:K:467:MET:HE1	5:K:654:LEU:CB	2.41	0.48
5:L:190:ILE:N	5:L:190:ILE:CD1	2.73	0.48
2:C:700:VAL:HG21	2:C:1114:GLU:HG3	1.95	0.48
3:D:488:ASN:OD1	4:E:16:ARG:NE	2.46	0.48
3:D:87:LYS:HD2	5:L:78:ASN:HA	1.94	0.48
2:H:496:LYS:HB3	2:H:497:PRO:HD3	1.94	0.48
5:K:195:LEU:HD11	5:K:225:LEU:HD23	1.95	0.48
5:K:454:MET:HE3	5:K:457:ARG:NH2	2.28	0.48
5:L:217:VAL:C	5:L:218:GLU:HG3	2.33	0.48
5:L:546:ALA:O	5:L:550:PHE:N	2.38	0.48
5:L:578:MET:CG	5:L:579:VAL:N	2.76	0.48
5:L:736:ASN:O	5:L:737:MET:HB2	2.13	0.48
1:B:131:CYS:SG	1:B:132:HIS:N	2.86	0.48
4:E:30:MET:HG2	4:E:35:LYS:HB3	1.95	0.48
2:H:1120:ALA:HB1	2:H:1198:LEU:CD2	2.44	0.48
5:K:495:MET:O	5:K:499:THR:CB	2.61	0.48
2:C:185:ASP:HB2	2:C:197:ARG:HB2	1.96	0.48
2:C:676:ALA:O	2:C:677:ASN:C	2.51	0.48
5:K:946:VAL:C	5:K:948:GLU:N	2.65	0.48
5:K:946:VAL:C	5:K:949:SER:H	2.14	0.48
5:K:815:LEU:O	5:K:962:LEU:HB3	2.13	0.48
5:L:578:MET:N	5:L:607:GLN:O	2.47	0.48
5:L:785:ARG:O	5:L:789:ASP:N	2.46	0.48
2:C:813:GLU:O	3:D:461:PHE:O	2.30	0.48
2:H:1269:ARG:HA	3:I:346:ARG:HA	1.95	0.48
2:H:475:VAL:HG12	2:H:479:LEU:HD12	1.94	0.48
5:L:737:MET:CE	5:L:761:ILE:HG21	2.41	0.48
2:C:1120:ALA:HB1	2:C:1198:LEU:CD2	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1255:THR:O	2:C:1257:GLN:N	2.47	0.48
2:H:1329:GLU:O	2:H:1333:LEU:HB2	2.14	0.48
5:K:121:ASP:HB2	5:K:125:ARG:HD2	1.95	0.48
5:L:188:GLY:O	5:L:191:LEU:N	2.43	0.48
5:L:341:GLN:O	5:L:342:PHE:C	2.51	0.48
5:L:342:PHE:O	5:L:345:GLU:N	2.47	0.48
5:L:535:HIS:HE1	5:L:538:MET:N	2.09	0.48
5:L:738:ILE:CG2	5:L:759:ILE:HG22	2.39	0.48
2:C:193:ASN:OD1	2:C:194:LEU:N	2.47	0.48
2:C:458:GLU:O	2:C:461:GLU:HB3	2.13	0.48
2:H:676:ALA:O	2:H:677:ASN:C	2.50	0.48
5:K:369:GLU:HG2	5:K:373:LEU:CD1	2.42	0.48
5:K:450:VAL:HA	5:K:453:ILE:HD13	1.96	0.48
5:K:826:ALA:HB3	5:K:832:LEU:HD13	1.95	0.48
5:L:665:ASP:O	5:L:669:ASN:N	2.47	0.48
5:L:715:LEU:HB3	5:L:761:ILE:HD11	1.95	0.48
5:L:826:ALA:HB3	5:L:832:LEU:HD13	1.94	0.48
2:C:114:VAL:O	2:C:115:LYS:C	2.52	0.48
3:D:51:PRO:HB2	3:D:57:PHE:C	2.34	0.48
3:I:77:ARG:HD2	5:K:746:MET:O	2.14	0.48
5:K:488:ASP:C	5:K:488:ASP:OD1	2.52	0.48
5:K:719:ALA:HB1	5:K:723:PHE:CE1	2.49	0.48
3:D:365:GLN:HA	3:D:438:GLU:O	2.14	0.48
1:F:66:HIS:CE1	1:F:69:SER:HB3	2.49	0.48
2:H:458:GLU:O	2:H:461:GLU:HB3	2.13	0.48
5:K:217:VAL:O	5:K:220:LEU:N	2.47	0.48
5:K:356:VAL:O	5:K:357:ALA:C	2.52	0.48
5:K:539:SER:OG	5:K:540:ILE:N	2.47	0.48
5:K:796:THR:HG22	5:K:960:LEU:HB2	1.96	0.48
5:L:538:MET:HE2	5:L:542:GLU:OE1	2.13	0.48
6:M:3:DG:C2'	6:M:4:DA:C5'	2.86	0.48
2:H:21:VAL:HG21	2:H:592:ARG:NH1	2.28	0.47
5:K:373:LEU:O	5:K:377:ILE:HG12	2.13	0.47
5:K:907:ARG:NH2	5:K:947:MET:CE	2.77	0.47
5:L:189:MET:HB2	5:L:190:ILE:HD12	1.96	0.47
5:L:353:ALA:CA	5:L:356:VAL:CG2	2.55	0.47
2:C:1329:GLU:O	2:C:1333:LEU:HB2	2.14	0.47
3:D:78:LEU:CB	5:L:746:MET:CA	2.91	0.47
2:H:1215:GLY:O	2:H:1216:ARG:C	2.52	0.47
2:H:700:VAL:HG21	2:H:1114:GLU:HG3	1.96	0.47
5:K:358:MET:HA	5:K:362:GLY:HA3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:K:362:GLY:O	5:K:363:ASN:HB2	2.14	0.47
5:K:372:MET:O	5:K:376:MET:CG	2.62	0.47
5:K:495:MET:O	5:K:499:THR:CG2	2.61	0.47
5:K:495:MET:O	5:K:499:THR:HB	2.14	0.47
5:L:436:ILE:HD11	5:L:609:HIS:ND1	2.28	0.47
5:L:63:SER:H	5:L:68:GLN:HB3	1.79	0.47
1:A:67:GLU:O	1:A:78:ILE:HB	2.14	0.47
2:H:193:ASN:OD1	2:H:194:LEU:N	2.47	0.47
3:I:136:GLU:HA	3:I:139:LEU:HD22	1.96	0.47
5:K:123:MET:N	5:K:865:LEU:HD11	2.25	0.47
5:K:243:TYR:O	5:K:244:ASN:HB2	2.14	0.47
5:K:843:MET:SD	5:K:845:LEU:CD2	3.01	0.47
2:H:114:VAL:O	2:H:115:LYS:C	2.53	0.47
2:H:912:ASP:HB3	2:H:913:VAL:CG1	2.37	0.47
3:I:365:GLN:HA	3:I:438:GLU:O	2.13	0.47
5:K:374:GLY:O	5:K:378:GLY:CA	2.63	0.47
5:K:907:ARG:NH2	5:K:947:MET:HE2	2.28	0.47
5:K:907:ARG:HH21	5:K:947:MET:HE3	1.78	0.47
2:C:832:HIS:CG	2:C:1058:ARG:HE	2.33	0.47
3:D:136:GLU:HA	3:D:139:LEU:HD22	1.96	0.47
3:D:814:CYS:SG	3:D:898:CYS:HB3	2.48	0.47
5:K:467:MET:HE1	5:K:654:LEU:CD2	2.40	0.47
5:L:220:LEU:HD12	5:L:224:ASN:CB	2.44	0.47
5:L:422:ARG:HG3	5:L:428:PHE:CZ	2.49	0.47
5:L:720:MET:CG	5:L:730:GLN:OE1	2.63	0.47
1:F:67:GLU:O	1:F:78:ILE:HB	2.14	0.47
5:K:342:PHE:O	5:K:345:GLU:N	2.47	0.47
5:K:422:ARG:HG3	5:K:428:PHE:CZ	2.49	0.47
5:L:61:ILE:O	5:L:68:GLN:HB2	2.14	0.47
5:L:818:LEU:HB2	5:L:843:MET:CB	2.44	0.47
2:H:206:ALA:HB3	2:H:350:THR:HG21	1.97	0.47
5:K:397:GLN:O	5:K:401:GLN:NE2	2.48	0.47
5:K:433:LEU:HD21	5:K:435:THR:HG23	1.96	0.47
5:L:186:GLU:O	5:L:189:MET:HB2	2.15	0.47
5:L:448:ILE:CG2	5:L:467:MET:CG	2.93	0.47
2:C:21:VAL:HG21	2:C:592:ARG:NH1	2.29	0.47
3:D:814:CYS:HB3	3:D:895:CYS:CB	2.45	0.47
3:I:1256:ILE:O	3:I:1259:GLN:N	2.48	0.47
5:K:506:VAL:HG12	5:K:579:VAL:HG23	1.97	0.47
5:L:187:ALA:O	5:L:188:GLY:C	2.52	0.47
5:L:186:GLU:O	5:L:189:MET:CB	2.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:583:LEU:CD1	5:L:622:VAL:HG23	2.44	0.47
5:L:636:CYS:SG	5:L:639:GLY:N	2.88	0.47
3:D:78:LEU:CG	5:L:746:MET:HB3	2.43	0.47
5:L:815:LEU:O	5:L:962:LEU:HB3	2.15	0.47
1:B:67:GLU:O	1:B:78:ILE:HB	2.14	0.47
3:D:334:LYS:HG2	3:D:339:ARG:HD2	1.97	0.47
3:D:506:VAL:HG13	3:D:628:GLY:HA3	1.95	0.47
3:D:80:HIS:HB3	3:D:83:VAL:CG2	2.45	0.47
3:I:895:CYS:O	3:I:896:ALA:HB3	2.15	0.47
5:K:665:ASP:O	5:K:669:ASN:N	2.47	0.47
5:L:184:THR:HG23	5:L:312:LEU:HD23	1.88	0.47
5:L:488:ASP:OD1	5:L:488:ASP:C	2.52	0.47
2:C:1215:GLY:O	2:C:1216:ARG:C	2.52	0.47
2:C:206:ALA:HB3	2:C:350:THR:HG21	1.97	0.47
3:I:1259:GLN:HA	3:I:1262:ARG:HG2	1.97	0.47
3:I:292:VAL:O	3:I:295:GLU:N	2.38	0.47
5:K:128:LEU:HD21	5:K:721:ASN:CG	2.35	0.47
5:K:151:ARG:HD2	5:K:221:ARG:O	2.15	0.47
5:K:364:LYS:HZ1	5:K:392:ASP:CG	2.17	0.47
5:K:736:ASN:HD22	5:K:765:ARG:CZ	2.27	0.47
5:L:796:THR:HG22	5:L:960:LEU:HB2	1.96	0.47
2:C:18:ARG:NH1	2:C:621:SER:O	2.47	0.46
2:C:6:THR:O	2:C:6:THR:HG22	2.15	0.46
5:K:123:MET:SD	5:K:123:MET:C	2.94	0.46
5:K:375:GLU:OE1	5:K:375:GLU:HA	2.15	0.46
5:K:493:TRP:C	5:K:495:MET:H	2.18	0.46
5:K:408:MET:C	5:K:688:LEU:HD12	2.34	0.46
5:K:69:MET:SD	5:K:97:LEU:O	2.74	0.46
5:K:70:GLN:HB3	5:K:86:THR:N	2.30	0.46
5:K:74:VAL:HG12	5:K:81:LEU:HD22	1.96	0.46
5:K:785:ARG:O	5:K:789:ASP:N	2.45	0.46
2:C:1329:GLU:O	2:C:1333:LEU:N	2.48	0.46
3:D:78:LEU:HG	5:L:746:MET:CB	2.40	0.46
2:H:551:HIS:O	2:H:553:THR:N	2.48	0.46
3:I:1266:ILE:HG21	3:I:1300:ALA:HB1	1.97	0.46
3:I:334:LYS:HG2	3:I:339:ARG:HD2	1.97	0.46
5:K:123:MET:HG2	5:K:799:SER:HG	1.80	0.46
2:C:906:PHE:HA	5:L:540:ILE:HD13	1.96	0.46
5:L:843:MET:HA	5:L:850:ASN:ND2	2.27	0.46
2:C:634:VAL:N	2:C:645:PHE:O	2.44	0.46
2:H:185:ASP:HB2	2:H:197:ARG:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:165:TYR:OH	3:I:178:ALA:HB3	2.15	0.46
3:I:80:HIS:HB3	3:I:83:VAL:CG2	2.45	0.46
5:K:222:ARG:CG	5:K:222:ARG:NH1	2.73	0.46
5:K:342:PHE:O	5:K:343:VAL:C	2.53	0.46
5:L:123:MET:HB3	5:L:865:LEU:CB	2.42	0.46
5:L:185:ILE:HG12	5:L:222:ARG:NE	2.28	0.46
5:L:407:LEU:HD11	5:L:688:LEU:HD13	1.93	0.46
3:D:77:ARG:CD	5:L:747:LEU:CG	2.87	0.46
5:K:636:CYS:SG	5:K:639:GLY:N	2.88	0.46
5:L:311:LEU:HD21	5:L:331:LEU:HD21	1.98	0.46
1:A:66:HIS:CE1	1:A:69:SER:HB3	2.51	0.46
3:D:165:TYR:OH	3:D:178:ALA:HB3	2.15	0.46
5:K:102:LEU:HG	5:K:103:ASP:N	2.31	0.46
5:L:149:GLY:H	5:L:777:ILE:HD11	1.79	0.46
5:L:220:LEU:O	5:L:224:ASN:N	2.48	0.46
5:L:939:ILE:HA	5:L:942:ASN:HB3	1.98	0.46
2:C:1185:PRO:O	2:C:1186:VAL:C	2.53	0.46
3:D:1266:ILE:HG21	3:D:1300:ALA:HB1	1.97	0.46
5:K:192:HIS:HB2	5:K:223:PHE:CD1	2.50	0.46
5:K:405:SER:C	5:K:406:MET:SD	2.94	0.46
5:K:561:LEU:HD11	5:K:565:ILE:HD11	1.97	0.46
5:L:244:ASN:HB3	5:L:245:PRO:HD3	1.78	0.46
5:L:454:MET:HG3	5:L:454:MET:O	2.16	0.46
5:L:74:VAL:HG11	5:L:81:LEU:CD1	2.26	0.46
5:K:378:GLY:N	5:K:379:GLU:HB2	2.30	0.46
5:L:342:PHE:O	5:L:343:VAL:C	2.53	0.46
5:L:375:GLU:HA	5:L:375:GLU:OE1	2.16	0.46
3:D:474:LEU:HD21	4:E:31:GLN:OE1	2.16	0.46
2:H:832:HIS:CG	2:H:1058:ARG:HE	2.34	0.46
2:H:1112:ILE:HG22	2:H:1116:HIS:CD2	2.51	0.46
2:H:1156:ARG:O	2:H:1158:LYS:N	2.49	0.46
2:H:6:THR:HG22	2:H:6:THR:O	2.15	0.46
5:K:378:GLY:CA	5:K:379:GLU:HB3	2.31	0.46
5:K:533:VAL:CG1	5:K:535:HIS:HD2	2.29	0.46
5:K:509:ILE:HG23	5:K:561:LEU:HD12	1.97	0.46
5:K:939:ILE:HA	5:K:942:ASN:HB3	1.98	0.46
5:L:407:LEU:CG	5:L:408:MET:N	2.78	0.46
5:L:407:LEU:HD21	5:L:688:LEU:HD22	1.98	0.46
5:L:561:LEU:HD11	5:L:565:ILE:HD11	1.97	0.46
2:C:170:VAL:O	2:C:170:VAL:HG13	2.16	0.46
5:K:270:CYS:O	5:K:272:ALA:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:K:404:VAL:HG23	5:K:405:SER:N	2.31	0.46
5:K:468:LEU:HD23	5:K:469:TYR:N	2.30	0.46
5:L:522:VAL:O	5:L:526:ARG:N	2.49	0.46
3:D:80:HIS:HE1	5:L:54:MET:CE	2.28	0.46
1:A:67:GLU:HA	1:A:78:ILE:HG21	1.98	0.45
2:C:14:ASP:HA	2:C:1183:ALA:HB3	1.98	0.45
2:C:551:HIS:O	2:C:553:THR:N	2.48	0.45
3:D:77:ARG:O	5:L:744:ASP:O	2.32	0.45
1:G:67:GLU:O	1:G:78:ILE:HB	2.15	0.45
2:H:90:VAL:O	2:H:140:GLY:N	2.49	0.45
3:I:519:ASN:HD21	3:I:710:ASP:N	2.11	0.45
5:K:315:THR:H	5:K:316:PRO:HD3	1.81	0.45
5:L:732:ASP:O	5:L:738:ILE:HA	2.16	0.45
5:L:801:ILE:O	5:L:803:LEU:N	2.48	0.45
3:D:1256:ILE:O	3:D:1259:GLN:N	2.49	0.45
3:D:86:GLU:N	3:D:86:GLU:CD	2.70	0.45
1:F:67:GLU:HA	1:F:78:ILE:HG21	1.98	0.45
2:H:213:LEU:HD21	2:H:390:PHE:CZ	2.50	0.45
5:K:843:MET:HE2	5:K:850:ASN:HD21	1.64	0.45
5:L:326:ALA:O	5:L:330:LEU:HD13	2.16	0.45
5:L:509:ILE:HG23	5:L:561:LEU:HD12	1.97	0.45
5:L:928:ASN:N	5:L:929:PRO:CD	2.79	0.45
2:C:1072:ASN:ND2	2:C:1111:GLN:OE1	2.49	0.45
2:C:1274:GLU:N	2:C:1274:GLU:OE1	2.50	0.45
2:H:14:ASP:HA	2:H:1183:ALA:HB3	1.99	0.45
5:K:320:GLY:CA	5:K:321:MET:CB	2.84	0.45
5:L:448:ILE:CG2	5:L:467:MET:HG2	2.44	0.45
5:L:580:MET:HB3	5:L:610:VAL:HB	1.98	0.45
2:C:1156:ARG:O	2:C:1158:LYS:N	2.50	0.45
2:C:213:LEU:HD21	2:C:390:PHE:CZ	2.51	0.45
3:D:895:CYS:O	3:D:896:ALA:HB3	2.16	0.45
3:I:392:THR:O	3:I:392:THR:HG22	2.16	0.45
3:I:814:CYS:HB3	3:I:895:CYS:CB	2.45	0.45
5:K:326:ALA:O	5:K:330:LEU:HD13	2.16	0.45
5:K:368:ASP:O	5:K:371:ASN:O	2.34	0.45
5:K:125:ARG:HG3	5:K:794:GLY:CA	2.46	0.45
5:K:907:ARG:HH21	5:K:947:MET:HE2	1.81	0.45
5:L:122:ARG:C	5:L:124:ASP:H	2.19	0.45
5:L:321:MET:O	5:L:322:GLU:HG3	2.16	0.45
5:L:722:LEU:O	5:L:726:ILE:HG13	2.16	0.45
2:C:1112:ILE:HG22	2:C:1116:HIS:CD2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:514:PHE:CD1	2:C:760:ASN:HB3	2.52	0.45
3:I:139:LEU:HD23	3:I:140:TYR:N	2.31	0.45
5:L:165:VAL:HG13	5:L:168:ARG:HD2	1.98	0.45
2:C:557:ARG:NE	2:C:608:ALA:HB2	2.32	0.45
2:C:90:VAL:O	2:C:140:GLY:N	2.48	0.45
3:D:307:LEU:O	3:D:328:ALA:HB2	2.16	0.45
3:D:350:SER:HA	3:D:468:VAL:O	2.17	0.45
2:H:1072:ASN:ND2	2:H:1111:GLN:OE1	2.49	0.45
2:H:488:MET:CB	2:H:489:PRO:HD3	2.46	0.45
2:H:12:ARG:NH1	2:H:698:PRO:O	2.50	0.45
3:I:77:ARG:HD2	5:K:743:SER:O	2.16	0.45
4:J:10:VAL:HG22	4:J:19:LEU:HD22	1.99	0.45
3:I:77:ARG:CD	5:K:743:SER:O	2.65	0.45
5:L:746:MET:O	5:L:747:LEU:HG	2.17	0.45
2:C:488:MET:CB	2:C:489:PRO:HD3	2.46	0.45
2:C:692:THR:OG1	2:C:693:LEU:N	2.48	0.45
3:D:363:LEU:HA	3:D:450:HIS:CE1	2.52	0.45
2:H:1274:GLU:OE1	2:H:1274:GLU:N	2.50	0.45
2:H:170:VAL:O	2:H:170:VAL:HG13	2.17	0.45
2:H:634:VAL:N	2:H:645:PHE:O	2.44	0.45
5:K:522:VAL:O	5:K:526:ARG:N	2.49	0.45
5:K:52:ARG:CG	5:K:54:MET:HE1	2.44	0.45
5:L:162:ALA:HA	5:L:190:ILE:HD11	1.98	0.45
5:L:315:THR:H	5:L:316:PRO:HD3	1.81	0.45
5:L:807:LYS:HB3	5:L:808:ALA:HA	1.99	0.45
2:C:624:ASP:O	2:C:625:GLU:HB3	2.17	0.45
3:D:1144:LEU:HD13	3:D:1237:VAL:HG22	1.98	0.45
3:D:1259:GLN:HA	3:D:1262:ARG:HG2	1.97	0.45
3:D:57:PHE:CE1	3:D:252:LEU:HD12	2.52	0.45
4:E:10:VAL:HG22	4:E:19:LEU:HD22	1.99	0.45
1:G:67:GLU:HA	1:G:78:ILE:HG21	1.99	0.45
2:H:1329:GLU:O	2:H:1333:LEU:N	2.49	0.45
3:I:1144:LEU:HD13	3:I:1237:VAL:HG22	1.98	0.45
3:I:372:MET:HG2	3:I:376:LEU:HD11	1.99	0.45
3:I:77:ARG:CB	5:K:747:LEU:N	2.80	0.45
5:L:720:MET:HE1	5:L:723:PHE:CE2	2.29	0.45
5:L:817:GLU:HA	5:L:844:LEU:HD23	1.97	0.45
3:D:1145:PHE:HB3	3:D:1309:ILE:HD11	1.99	0.45
2:H:557:ARG:NE	2:H:608:ALA:HB2	2.32	0.45
3:I:57:PHE:CE1	3:I:252:LEU:HD12	2.51	0.45
5:K:397:GLN:HB3	5:K:400:ARG:HB2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:124:ASP:O	5:L:125:ARG:HB3	2.17	0.45
5:L:371:ASN:N	5:L:371:ASN:ND2	2.65	0.45
5:L:468:LEU:C	5:L:468:LEU:CD2	2.86	0.45
3:D:139:LEU:HD23	3:D:140:TYR:N	2.32	0.45
2:H:464:PHE:O	2:H:468:LEU:HG	2.16	0.45
5:K:433:LEU:CD2	5:K:433:LEU:C	2.86	0.45
5:K:722:LEU:CD1	5:K:726:ILE:HD12	2.45	0.45
5:K:720:MET:HE1	5:K:738:ILE:HG21	1.99	0.45
5:L:374:GLY:C	5:L:376:MET:N	2.71	0.45
5:L:911:ASP:CG	5:L:947:MET:HE3	2.25	0.45
5:K:222:ARG:HD2	5:K:223:PHE:CE2	2.53	0.44
5:K:408:MET:HB3	5:K:688:LEU:CB	2.45	0.44
5:K:467:MET:HE2	5:K:654:LEU:HD13	1.99	0.44
5:K:578:MET:HE2	5:K:580:MET:SD	2.58	0.44
2:C:94:ALA:CB	2:C:129:LEU:HD11	2.47	0.44
3:I:363:LEU:HA	3:I:450:HIS:CE1	2.52	0.44
4:J:63:ILE:O	4:J:63:ILE:HG22	2.18	0.44
5:K:219:MET:O	5:K:225:LEU:N	2.32	0.44
5:K:311:LEU:HD21	5:K:331:LEU:HD21	1.98	0.44
5:K:721:ASN:O	5:K:725:ILE:HD13	2.17	0.44
5:L:204:LEU:HD22	5:L:269:LEU:HD22	1.99	0.44
5:L:769:LEU:HD13	5:L:771:ARG:CZ	2.47	0.44
2:C:12:ARG:NH1	2:C:698:PRO:O	2.50	0.44
2:H:30:ILE:HG23	2:H:581:THR:OG1	2.18	0.44
2:H:624:ASP:O	2:H:625:GLU:HB3	2.17	0.44
5:K:353:ALA:O	5:K:356:VAL:HB	2.17	0.44
5:K:580:MET:HG2	5:K:608:ILE:HG23	2.00	0.44
5:L:185:ILE:CG1	5:L:222:ARG:NH1	2.57	0.44
5:L:246:PHE:CD2	5:L:246:PHE:O	2.70	0.44
6:O:2:DC:O5'	6:O:2:DC:C6	2.71	0.44
2:C:464:PHE:O	2:C:468:LEU:HG	2.17	0.44
3:D:372:MET:HG2	3:D:376:LEU:HD11	2.00	0.44
3:D:364:HIS:O	3:D:438:GLU:N	2.51	0.44
1:F:162:GLU:OE2	1:F:166:ARG:NH2	2.51	0.44
2:H:94:ALA:CB	2:H:129:LEU:HD11	2.47	0.44
5:K:165:VAL:HG13	5:K:168:ARG:HD2	1.98	0.44
5:K:466:ASP:HB3	5:K:467:MET:HB3	1.94	0.44
5:K:464:ALA:HB2	5:K:651:ILE:HD11	2.00	0.44
5:L:372:MET:O	5:L:373:LEU:HB3	2.17	0.44
2:C:558:VAL:HG13	2:C:573:ASN:HB3	2.00	0.44
2:H:591:TYR:CE2	2:H:616:ILE:HD13	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:887:VAL:HB	2:H:913:VAL:CG2	2.46	0.44
3:I:1145:PHE:HB3	3:I:1309:ILE:HD11	1.99	0.44
3:I:890:THR:O	3:I:891:ASP:C	2.56	0.44
5:L:370:LEU:C	5:L:370:LEU:CD2	2.86	0.44
7:N:2:U:O5'	7:N:2:U:C6	2.70	0.44
6:O:15:DG:O6	7:P:1:A:C2	2.70	0.44
2:C:812:PHE:CE2	3:D:451:PRO:O	2.70	0.44
2:C:887:VAL:HB	2:C:913:VAL:CG2	2.47	0.44
2:H:803:ALA:HB3	2:H:1097:VAL:HA	2.00	0.44
2:H:786:GLY:N	2:H:789:THR:OG1	2.46	0.44
3:I:350:SER:HA	3:I:468:VAL:O	2.16	0.44
5:K:733:ARG:CD	5:K:733:ARG:C	2.86	0.44
5:L:407:LEU:O	5:L:408:MET:HB2	2.18	0.44
6:M:2:DC:H4'	6:M:3:DG:OP1	2.18	0.44
1:B:67:GLU:HA	1:B:78:ILE:HG21	1.99	0.44
2:C:1330:ILE:HG22	2:C:1335:ILE:HB	2.00	0.44
2:C:519:ASN:ND2	2:C:689:ALA:O	2.51	0.44
3:D:746:LEU:HA	3:D:758:PRO:HB3	2.00	0.44
3:D:475:GLU:OE2	4:E:24:ALA:HB1	2.18	0.44
4:E:63:ILE:O	4:E:63:ILE:HG22	2.17	0.44
2:H:811:ASN:HA	2:H:815:SER:HB2	2.00	0.44
5:K:314:ALA:O	5:K:315:THR:CB	2.66	0.44
5:K:688:LEU:O	5:K:692:HIS:N	2.48	0.44
5:L:538:MET:HG3	5:L:542:GLU:CB	2.46	0.44
5:L:735:ASP:C	5:L:737:MET:H	2.19	0.44
5:L:737:MET:HE1	5:L:761:ILE:HG21	1.98	0.44
2:C:661:VAL:HG12	2:C:662:SER:N	2.33	0.44
2:H:166:SER:OG	2:H:167:SER:N	2.51	0.44
2:H:454:ARG:HD3	2:H:462:ASN:ND2	2.33	0.44
2:H:18:ARG:NH1	2:H:621:SER:O	2.47	0.44
3:I:368:LEU:HD23	3:I:369:PRO:HD2	2.00	0.44
5:K:222:ARG:HD2	5:K:223:PHE:HE2	1.83	0.44
5:K:408:MET:HE1	5:K:691:ILE:CB	2.45	0.44
5:K:580:MET:N	5:K:609:HIS:O	2.34	0.44
5:K:61:ILE:HG23	5:K:102:LEU:HD13	1.98	0.44
5:L:255:SER:O	5:L:258:PHE:HB3	2.18	0.44
5:L:376:MET:CG	5:L:410:ARG:CD	2.70	0.44
5:L:495:MET:O	5:L:498:LEU:N	2.50	0.44
5:L:535:HIS:CD2	5:L:542:GLU:OE2	2.71	0.44
5:L:540:ILE:N	5:L:540:ILE:HD12	2.33	0.44
7:N:2:U:O5'	7:N:2:U:H6	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:668:ILE:HB	2:H:671:LEU:HD13	2.00	0.44
3:I:145:VAL:CG1	3:I:184:ALA:HB1	2.48	0.44
3:I:307:LEU:O	3:I:328:ALA:HB2	2.16	0.44
3:I:59:ALA:CB	3:I:71:LEU:HD21	2.48	0.44
5:K:122:ARG:HB3	5:K:124:ASP:OD1	2.18	0.44
5:K:373:LEU:O	5:K:376:MET:HB2	2.18	0.44
5:K:70:GLN:HB3	5:K:86:THR:CA	2.46	0.44
5:K:769:LEU:HD13	5:K:771:ARG:CZ	2.47	0.44
5:L:139:GLN:CG	5:L:142:MET:HE1	2.31	0.44
5:L:175:LEU:O	5:L:313:THR:N	2.51	0.44
5:L:155:ILE:CG2	5:L:600:ILE:HG21	2.48	0.44
3:D:356:THR:HG22	3:D:357:VAL:N	2.34	0.43
2:H:1066:MET:HA	2:H:1233:LEU:O	2.18	0.43
2:H:131:THR:OG1	2:H:135:THR:N	2.50	0.43
2:H:672:GLU:HB3	3:I:767:LEU:H	1.82	0.43
5:K:467:MET:HE3	5:K:617:ALA:HB1	1.99	0.43
5:L:185:ILE:CD1	5:L:185:ILE:N	2.73	0.43
5:L:219:MET:HB3	5:L:227:PHE:HD1	1.83	0.43
5:L:219:MET:CA	5:L:225:LEU:CG	2.90	0.43
5:L:60:THR:HG23	5:L:69:MET:CA	2.45	0.43
2:C:666:SER:HA	2:C:1186:VAL:HG22	2.00	0.43
3:D:504:GLN:O	3:D:507:VAL:HB	2.18	0.43
3:D:842:ARG:NH1	3:D:884:SER:OG	2.51	0.43
1:G:91:ARG:HB2	1:G:122:GLU:O	2.18	0.43
2:H:36:GLN:O	2:H:40:GLU:HB2	2.18	0.43
2:H:964:LEU:O	2:H:968:GLU:HB2	2.18	0.43
3:I:504:GLN:O	3:I:507:VAL:HB	2.18	0.43
5:K:123:MET:HG2	5:K:799:SER:OG	2.18	0.43
5:K:494:LEU:O	5:K:498:LEU:HB2	2.16	0.43
5:K:818:LEU:O	5:K:843:MET:CG	2.65	0.43
5:L:218:GLU:HB3	5:L:222:ARG:HB2	2.00	0.43
5:L:523:LEU:O	5:L:524:ARG:C	2.57	0.43
5:L:748:VAL:HG13	5:L:749:PRO:HD2	2.01	0.43
5:L:810:PRO:O	5:L:811:VAL:C	2.56	0.43
2:C:454:ARG:HD3	2:C:462:ASN:ND2	2.33	0.43
2:C:93:SER:OG	2:C:94:ALA:N	2.51	0.43
2:H:1330:ILE:HG22	2:H:1335:ILE:HB	2.00	0.43
2:H:395:TYR:CE2	2:H:420:LEU:HG	2.54	0.43
2:H:638:SER:O	2:H:639:LYS:C	2.57	0.43
3:I:86:GLU:CD	3:I:86:GLU:N	2.72	0.43
5:K:255:SER:O	5:K:258:PHE:HB3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:K:352:VAL:O	5:K:356:VAL:N	2.50	0.43
5:K:365:LEU:HD12	5:K:366:SER:H	1.82	0.43
5:K:408:MET:HB3	5:K:688:LEU:O	2.18	0.43
5:K:540:ILE:HD12	5:K:540:ILE:N	2.33	0.43
5:K:722:LEU:CD1	5:K:722:LEU:C	2.85	0.43
3:D:77:ARG:HB3	5:L:747:LEU:N	2.34	0.43
2:C:433:ILE:O	2:C:434:ASP:C	2.57	0.43
2:C:591:TYR:CE2	2:C:616:ILE:HD13	2.54	0.43
2:C:964:LEU:HD12	2:C:1025:PHE:CE2	2.53	0.43
3:D:292:VAL:O	3:D:295:GLU:N	2.39	0.43
2:H:692:THR:OG1	2:H:693:LEU:N	2.48	0.43
2:H:789:THR:HA	2:H:793:GLU:O	2.18	0.43
3:I:746:LEU:HA	3:I:758:PRO:HB3	2.00	0.43
5:K:123:MET:CG	5:K:865:LEU:HB2	2.48	0.43
5:L:142:MET:CG	5:L:143:PRO:CD	2.96	0.43
3:D:80:HIS:HE1	5:L:54:MET:HE3	1.83	0.43
2:C:131:THR:OG1	2:C:135:THR:N	2.50	0.43
3:D:615:LYS:N	3:D:616:PRO:CD	2.82	0.43
3:D:77:ARG:C	5:L:744:ASP:O	2.57	0.43
2:H:509:SER:OG	2:H:510:GLN:N	2.52	0.43
2:H:514:PHE:CD1	2:H:760:ASN:HB3	2.53	0.43
2:H:661:VAL:HG12	2:H:662:SER:N	2.34	0.43
5:K:155:ILE:CG2	5:K:600:ILE:HG21	2.48	0.43
5:K:536:GLU:OE1	5:K:536:GLU:HA	2.19	0.43
5:K:53:VAL:C	5:K:54:MET:CE	2.86	0.43
3:I:78:LEU:HB3	5:K:746:MET:SD	2.59	0.43
5:K:807:LYS:HB3	5:K:808:ALA:HA	2.00	0.43
3:D:77:ARG:HB3	5:L:747:LEU:H	1.83	0.43
5:L:810:PRO:O	5:L:812:GLY:N	2.52	0.43
2:C:395:TYR:CE2	2:C:420:LEU:HG	2.54	0.43
2:C:660:VAL:HG23	2:C:661:VAL:HG23	2.00	0.43
2:H:455:SER:O	2:H:456:VAL:C	2.57	0.43
2:H:519:ASN:ND2	2:H:689:ALA:O	2.52	0.43
2:H:964:LEU:HD12	2:H:1025:PHE:CE2	2.53	0.43
3:I:356:THR:HG22	3:I:357:VAL:N	2.34	0.43
3:I:364:HIS:O	3:I:438:GLU:N	2.51	0.43
3:I:842:ARG:NH1	3:I:884:SER:OG	2.52	0.43
5:K:578:MET:CE	5:K:580:MET:SD	3.07	0.43
5:K:801:ILE:O	5:K:803:LEU:N	2.50	0.43
5:K:810:PRO:O	5:K:811:VAL:C	2.56	0.43
3:D:1262:ARG:O	3:D:1263:LYS:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:67:ASP:O	3:D:68:TYR:C	2.56	0.43
2:H:937:ASP:HA	2:H:1039:GLY:HA2	2.01	0.43
3:I:776:THR:O	3:I:780:ARG:HB2	2.18	0.43
5:K:928:ASN:N	5:K:929:PRO:CD	2.81	0.43
3:D:145:VAL:CG1	3:D:184:ALA:HB1	2.48	0.43
3:I:80:HIS:HB3	3:I:83:VAL:HB	2.01	0.43
5:K:175:LEU:O	5:K:313:THR:N	2.52	0.43
5:K:438:LEU:HD22	5:K:438:LEU:N	2.34	0.43
5:K:612:TYR:CD2	5:K:619:SER:HA	2.54	0.43
5:L:184:THR:HG21	5:L:215:TRP:CZ2	2.53	0.43
5:L:219:MET:C	5:L:225:LEU:HG	2.34	0.43
5:L:407:LEU:C	5:L:409:ASP:N	2.72	0.43
6:M:2:DC:H2"	6:M:3:DG:OP1	2.18	0.43
1:B:33:ARG:HD2	1:B:197:ASP:HB3	2.01	0.43
2:C:1066:MET:HA	2:C:1233:LEU:O	2.19	0.43
2:C:803:ALA:HB3	2:C:1097:VAL:HA	1.99	0.43
3:D:80:HIS:HB3	3:D:83:VAL:HB	2.01	0.43
2:H:93:SER:OG	2:H:94:ALA:N	2.51	0.43
3:I:1262:ARG:O	3:I:1263:LYS:HB2	2.19	0.43
5:K:147:LEU:HD22	5:K:189:MET:HE2	1.99	0.43
5:K:409:ASP:C	5:K:411:HIS:H	2.22	0.43
5:K:493:TRP:C	5:K:495:MET:N	2.72	0.43
5:K:61:ILE:HD12	5:K:69:MET:HE1	2.01	0.43
5:K:720:MET:CG	5:K:730:GLN:NE2	2.82	0.43
2:C:36:GLN:O	2:C:40:GLU:HB2	2.18	0.43
2:C:30:ILE:HG23	2:C:581:THR:OG1	2.19	0.43
2:C:937:ASP:HA	2:C:1039:GLY:HA2	2.01	0.43
2:C:964:LEU:O	2:C:968:GLU:HB2	2.19	0.43
3:D:616:PRO:O	3:D:620:PHE:HB3	2.19	0.43
3:D:801:VAL:HG22	3:D:920:ALA:HB3	2.00	0.43
2:H:839:VAL:HG11	2:H:841:ARG:NH2	2.34	0.43
3:I:353:SER:OG	3:I:354:VAL:N	2.52	0.43
3:I:615:LYS:N	3:I:616:PRO:CD	2.82	0.43
3:I:519:ASN:HD22	3:I:709:ARG:HB2	1.80	0.43
3:I:801:VAL:HG22	3:I:920:ALA:HB3	2.00	0.43
5:K:194:GLN:NE2	5:K:194:GLN:O	2.52	0.43
5:K:219:MET:O	5:K:224:ASN:N	2.51	0.43
5:K:204:LEU:HD22	5:K:269:LEU:HD22	2.00	0.43
5:K:810:PRO:O	5:K:812:GLY:N	2.52	0.43
5:L:184:THR:CA	5:L:312:LEU:HD21	2.49	0.43
5:L:538:MET:HG3	5:L:542:GLU:HB3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:736:ASN:ND2	5:L:736:ASN:N	2.66	0.43
3:D:84:ILE:HB	5:L:73:GLU:HB2	2.01	0.43
5:L:818:LEU:C	5:L:843:MET:HB2	2.38	0.43
2:C:1138:VAL:HG13	2:C:1141:LEU:HD23	2.00	0.42
3:D:59:ALA:CB	3:D:71:LEU:HD21	2.49	0.42
5:K:179:VAL:HG12	5:K:180:GLY:N	2.34	0.42
5:K:72:GLU:O	5:K:73:GLU:CB	2.63	0.42
5:L:314:ALA:O	5:L:315:THR:CB	2.66	0.42
5:L:374:GLY:O	5:L:375:GLU:HB2	2.19	0.42
5:L:716:ILE:HD11	5:L:761:ILE:CG2	2.48	0.42
1:A:162:GLU:OE2	1:A:166:ARG:NH2	2.52	0.42
3:D:1347:LEU:O	3:D:1351:VAL:HG23	2.19	0.42
3:D:127:LEU:HD13	3:D:223:LEU:HD12	2.02	0.42
3:D:57:PHE:CD1	3:D:252:LEU:HD12	2.54	0.42
3:D:368:LEU:HD23	3:D:369:PRO:HD2	2.00	0.42
3:I:57:PHE:CD1	3:I:252:LEU:HD12	2.54	0.42
5:K:272:ALA:O	5:K:274:TRP:N	2.52	0.42
5:K:69:MET:HE2	5:K:69:MET:HB2	1.86	0.42
5:K:722:LEU:O	5:K:726:ILE:HG13	2.20	0.42
5:K:844:LEU:O	5:K:850:ASN:HA	2.18	0.42
5:K:863:ARG:CD	5:K:961:ARG:CZ	2.97	0.42
5:L:538:MET:CG	5:L:542:GLU:HB3	2.49	0.42
5:L:434:HIS:N	5:L:608:ILE:O	2.52	0.42
5:L:737:MET:HE1	5:L:761:ILE:CB	2.49	0.42
2:C:912:ASP:HB3	2:C:913:VAL:CG1	2.40	0.42
3:D:67:ASP:O	3:D:69:GLU:N	2.52	0.42
5:K:523:LEU:O	5:K:524:ARG:C	2.58	0.42
5:L:735:ASP:C	5:L:737:MET:N	2.73	0.42
1:A:207:THR:OG1	1:A:208:ASN:N	2.52	0.42
1:B:91:ARG:HB2	1:B:122:GLU:O	2.18	0.42
2:C:1118:GLY:C	2:C:1229:TYR:HB2	2.40	0.42
2:C:389:PHE:HB2	2:C:390:PHE:CD2	2.54	0.42
2:C:509:SER:OG	2:C:510:GLN:N	2.52	0.42
2:C:577:VAL:HG21	2:C:658:GLN:HG2	2.02	0.42
2:C:878:THR:HG22	2:C:879:GLY:N	2.34	0.42
3:D:161:THR:O	3:D:163:GLU:N	2.52	0.42
3:D:353:SER:OG	3:D:354:VAL:N	2.52	0.42
3:D:369:PRO:O	3:D:370:LYS:C	2.58	0.42
3:I:127:LEU:HD13	3:I:223:LEU:HD12	2.01	0.42
5:K:223:PHE:O	5:K:225:LEU:HD11	2.15	0.42
3:I:79:LYS:HB2	5:K:747:LEU:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1227:VAL:HG12	2:C:1228:GLY:N	2.34	0.42
2:C:176:ILE:HD11	2:C:428:VAL:HG11	2.02	0.42
2:H:1138:VAL:HG13	2:H:1141:LEU:HD23	2.01	0.42
3:I:616:PRO:O	3:I:620:PHE:HB3	2.19	0.42
5:K:506:VAL:CG1	5:K:579:VAL:HG23	2.50	0.42
5:L:438:LEU:HD22	5:L:438:LEU:N	2.33	0.42
5:L:612:TYR:CD2	5:L:619:SER:HA	2.54	0.42
5:L:720:MET:O	5:L:724:ASP:HB2	2.19	0.42
3:I:161:THR:O	3:I:163:GLU:N	2.52	0.42
4:J:39:VAL:O	4:J:40:PRO:C	2.58	0.42
5:K:139:GLN:O	5:K:142:MET:N	2.52	0.42
5:L:165:VAL:HG21	5:L:173:VAL:HG11	2.01	0.42
5:L:219:MET:CE	5:L:227:PHE:CD1	2.99	0.42
5:L:42:LEU:CG	5:L:242:ALA:CB	2.97	0.42
6:M:2:DC:C6	6:M:2:DC:O5'	2.71	0.42
2:C:568:ASN:HA	2:C:571:LEU:HD12	2.01	0.42
2:C:789:THR:HA	2:C:793:GLU:O	2.20	0.42
2:C:811:ASN:HA	2:C:815:SER:HB2	2.01	0.42
3:D:580:TRP:CZ3	3:D:583:VAL:HG11	2.55	0.42
4:E:20:VAL:O	4:E:24:ALA:N	2.36	0.42
3:I:67:ASP:O	3:I:68:TYR:C	2.57	0.42
5:K:321:MET:O	5:K:322:GLU:O	2.37	0.42
5:K:378:GLY:N	5:K:379:GLU:CB	2.83	0.42
5:K:726:ILE:HG22	5:K:726:ILE:O	2.20	0.42
2:C:1088:ASP:N	2:C:1091:GLY:O	2.52	0.42
2:C:1149:TYR:HB3	2:C:1159:VAL:HG21	2.02	0.42
2:C:795:ALA:HA	2:C:1231:TYR:OH	2.20	0.42
3:I:66:LYS:NZ	3:I:70:CYS:O	2.49	0.42
5:K:818:LEU:CA	5:K:843:MET:HB3	2.50	0.42
5:L:444:TYR:HE1	5:L:470:PRO:HB2	1.80	0.42
5:L:578:MET:HB3	5:L:608:ILE:HA	2.02	0.42
2:C:668:ILE:HB	2:C:671:LEU:HD13	2.00	0.42
3:D:35:PHE:O	3:D:61:ILE:HG23	2.20	0.42
3:D:77:ARG:HB2	5:L:747:LEU:O	2.20	0.42
2:H:1118:GLY:C	2:H:1229:TYR:HB2	2.40	0.42
3:I:35:PHE:O	3:I:61:ILE:HG23	2.20	0.42
5:K:245:PRO:O	5:K:246:PHE:C	2.58	0.42
5:K:318:GLN:O	5:K:319:LEU:HG	2.19	0.42
5:K:371:ASN:HA	5:K:375:GLU:CG	2.50	0.42
5:K:578:MET:HE3	5:K:594:ILE:HG12	2.01	0.42
5:K:843:MET:CE	5:K:894:GLN:HG3	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:218:GLU:N	5:L:219:MET:HB2	2.35	0.42
2:C:1131:MET:O	2:C:1133:LYS:N	2.53	0.42
2:H:666:SER:HA	2:H:1186:VAL:HG22	2.00	0.42
3:I:1347:LEU:O	3:I:1351:VAL:HG23	2.19	0.42
3:I:786:THR:HA	3:I:789:LYS:HB2	2.02	0.42
5:K:150:GLN:NE2	5:K:189:MET:HE3	2.35	0.42
5:K:223:PHE:C	5:K:225:LEU:CD1	2.86	0.42
5:L:372:MET:HG2	5:L:375:GLU:OE2	2.19	0.42
2:C:782:VAL:HG11	2:C:792:GLY:N	2.35	0.41
2:H:1227:VAL:HG12	2:H:1228:GLY:N	2.35	0.41
2:H:795:ALA:HA	2:H:1231:TYR:OH	2.20	0.41
2:H:878:THR:HG22	2:H:879:GLY:N	2.34	0.41
3:I:369:PRO:O	3:I:370:LYS:C	2.58	0.41
2:H:812:PHE:O	3:I:504:GLN:NE2	2.52	0.41
5:K:165:VAL:HG21	5:K:173:VAL:HG11	2.02	0.41
5:K:629:LEU:O	5:K:630:ASP:C	2.59	0.41
5:K:640:ARG:C	5:K:642:ILE:H	2.23	0.41
5:L:356:VAL:C	5:L:358:MET:N	2.70	0.41
5:L:540:ILE:CD1	5:L:540:ILE:H	2.32	0.41
5:L:887:ILE:O	5:L:887:ILE:HG22	2.21	0.41
2:C:455:SER:O	2:C:456:VAL:C	2.58	0.41
3:D:890:THR:O	3:D:891:ASP:C	2.58	0.41
2:H:1088:ASP:N	2:H:1091:GLY:O	2.54	0.41
2:H:429:MET:HA	2:H:432:LEU:HB3	2.02	0.41
2:H:433:ILE:O	2:H:434:ASP:C	2.57	0.41
2:H:519:ASN:HB2	2:H:520:PRO:HD2	2.03	0.41
2:H:660:VAL:HG23	2:H:661:VAL:HG23	2.01	0.41
2:H:782:VAL:HG11	2:H:792:GLY:N	2.35	0.41
5:K:355:ALA:C	5:K:358:MET:HG2	2.38	0.41
5:K:467:MET:CA	5:K:617:ALA:HB2	2.41	0.41
5:L:436:ILE:HG22	5:L:437:LYS:N	2.34	0.41
5:L:736:ASN:OD1	5:L:765:ARG:HG2	2.20	0.41
7:N:7:U:H2'	7:N:8:C:C6	2.55	0.41
2:C:839:VAL:HG11	2:C:841:ARG:NH2	2.35	0.41
2:C:912:ASP:HB3	2:C:913:VAL:HG12	2.02	0.41
4:E:39:VAL:O	4:E:40:PRO:C	2.58	0.41
1:F:11:PRO:HB3	1:F:31:LEU:HG	2.01	0.41
1:F:207:THR:OG1	1:F:208:ASN:N	2.53	0.41
2:H:15:PHE:CE2	2:H:1182:ILE:HG23	2.55	0.41
3:I:67:ASP:O	3:I:69:GLU:N	2.53	0.41
5:K:677:LEU:HA	5:K:680:GLN:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:179:VAL:HG12	5:L:180:GLY:N	2.34	0.41
5:L:220:LEU:O	5:L:224:ASN:OD1	2.38	0.41
5:L:371:ASN:O	5:L:372:MET:HB2	2.19	0.41
5:L:410:ARG:O	5:L:410:ARG:HG2	2.20	0.41
5:L:433:LEU:CD2	5:L:433:LEU:C	2.86	0.41
5:L:640:ARG:C	5:L:642:ILE:H	2.24	0.41
2:C:1254:VAL:HG13	2:C:1255:THR:H	1.85	0.41
2:C:429:MET:HA	2:C:432:LEU:HB3	2.02	0.41
2:C:847:PRO:HB3	2:C:1047:LEU:HD11	2.03	0.41
2:H:389:PHE:HB2	2:H:390:PHE:CD2	2.55	0.41
2:H:558:VAL:HG13	2:H:573:ASN:HB3	2.01	0.41
2:H:1269:ARG:HE	3:I:344:GLY:HA2	1.85	0.41
5:K:422:ARG:HG3	5:K:428:PHE:CE2	2.56	0.41
5:K:52:ARG:HG3	5:K:54:MET:HE2	1.91	0.41
5:K:887:ILE:O	5:K:887:ILE:HG22	2.21	0.41
5:L:122:ARG:HA	5:L:865:LEU:HD21	2.03	0.41
5:L:299:ILE:O	5:L:300:GLU:C	2.58	0.41
2:C:15:PHE:CE2	2:C:1182:ILE:HG23	2.55	0.41
3:D:1284:ARG:HA	3:D:1287:ILE:HG22	2.02	0.41
2:H:577:VAL:HG21	2:H:658:GLN:HG2	2.01	0.41
5:K:421:THR:O	5:K:425:VAL:HG12	2.21	0.41
5:K:491:VAL:HA	5:K:494:LEU:CD1	2.51	0.41
5:L:436:ILE:HG12	5:L:609:HIS:HE1	1.77	0.41
5:L:155:ILE:HG21	5:L:600:ILE:HG21	2.02	0.41
5:L:90:THR:O	5:L:91:GLU:HB2	2.21	0.41
2:C:638:SER:O	2:C:639:LYS:C	2.58	0.41
3:D:1184:ASP:OD1	3:D:1185:PRO:HD3	2.20	0.41
2:H:847:PRO:HB3	2:H:1047:LEU:HD11	2.03	0.41
5:K:225:LEU:HB3	5:K:251:LEU:HD11	2.03	0.41
5:K:468:LEU:HD23	5:K:469:TYR:CB	2.49	0.41
5:L:190:ILE:H	5:L:190:ILE:HD12	1.82	0.41
1:B:11:PRO:HB3	1:B:31:LEU:HG	2.02	0.41
3:D:41:PRO:HB3	3:D:273:ILE:CG2	2.51	0.41
3:D:776:THR:O	3:D:780:ARG:HB2	2.20	0.41
2:H:176:ILE:HD11	2:H:428:VAL:HG11	2.02	0.41
3:I:139:LEU:C	3:I:139:LEU:HD23	2.41	0.41
1:F:167:PRO:HB3	5:K:528:GLY:CA	2.51	0.41
5:K:623:ARG:HG2	5:K:627:GLU:HB2	2.03	0.41
5:K:844:LEU:N	5:K:850:ASN:HB2	2.35	0.41
5:L:122:ARG:C	5:L:124:ASP:N	2.74	0.41
5:L:183:LYS:O	5:L:187:ALA:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:737:MET:SD	5:L:738:ILE:HG21	2.59	0.41
5:L:842:ARG:O	5:L:843:MET:HG3	2.11	0.41
2:C:928:VAL:HG12	2:C:929:ILE:N	2.36	0.41
3:D:755:ILE:HD12	3:D:755:ILE:H	1.85	0.41
1:G:11:PRO:HB3	1:G:31:LEU:HG	2.02	0.41
2:H:1254:VAL:HG13	2:H:1255:THR:H	1.86	0.41
3:I:580:TRP:CZ3	3:I:583:VAL:HG11	2.56	0.41
5:K:231:ASP:OD1	5:K:231:ASP:N	2.54	0.41
5:L:422:ARG:HG3	5:L:428:PHE:CE2	2.56	0.41
5:L:748:VAL:CG1	5:L:749:PRO:HD2	2.51	0.41
2:C:1325:VAL:HG22	3:D:249:LEU:HD22	2.03	0.41
2:H:518:ASN:N	2:H:761:GLN:OE1	2.54	0.41
2:H:947:GLU:O	2:H:951:MET:HG2	2.21	0.41
3:I:755:ILE:HD12	3:I:755:ILE:H	1.86	0.41
5:K:58:GLY:H	5:K:71:VAL:HB	1.86	0.41
5:K:721:ASN:OD1	5:K:725:ILE:HD13	2.21	0.41
5:L:142:MET:CG	5:L:143:PRO:HD2	2.51	0.41
5:L:614:GLU:O	5:L:615:LYS:HB2	2.21	0.41
5:L:407:LEU:HD11	5:L:688:LEU:CD1	2.49	0.41
1:A:11:PRO:HB3	1:A:31:LEU:HG	2.02	0.41
2:C:947:GLU:O	2:C:951:MET:HG2	2.21	0.41
2:H:1047:LEU:HB3	2:H:1048:LYS:HG3	2.03	0.41
3:I:41:PRO:HB3	3:I:273:ILE:CG2	2.51	0.41
3:I:42:GLU:O	3:I:56:LEU:N	2.54	0.41
2:H:1281:TYR:CD2	3:I:484:MET:HG2	2.55	0.41
5:L:148:ARG:NH2	5:L:706:ILE:HG13	2.36	0.41
5:L:219:MET:CB	5:L:227:PHE:CD1	3.01	0.41
5:L:231:ASP:N	5:L:231:ASP:OD1	2.54	0.41
5:L:688:LEU:O	5:L:692:HIS:N	2.49	0.41
3:D:78:LEU:CG	5:L:746:MET:HB2	2.50	0.41
5:L:74:VAL:HG12	5:L:81:LEU:CD1	2.40	0.41
5:L:123:MET:N	5:L:865:LEU:CD2	2.55	0.41
3:D:475:GLU:HG3	4:E:24:ALA:CB	2.50	0.41
3:D:84:ILE:HB	5:L:73:GLU:CB	2.51	0.41
2:H:1121:ALA:C	2:H:1123:GLY:H	2.24	0.41
3:I:701:LEU:HG	3:I:701:LEU:O	2.22	0.41
5:K:173:VAL:HG23	5:K:175:LEU:HD11	2.03	0.41
5:K:726:ILE:C	5:K:746:MET:HB2	2.41	0.41
5:L:139:GLN:HA	5:L:142:MET:HB2	2.02	0.41
5:L:536:GLU:HA	5:L:536:GLU:OE1	2.21	0.41
2:C:786:GLY:N	2:C:789:THR:OG1	2.46	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1184:ASP:N	3:D:1184:ASP:OD1	2.47	0.40
3:D:139:LEU:HD23	3:D:139:LEU:C	2.41	0.40
3:D:775:SER:O	3:D:776:THR:C	2.58	0.40
2:H:445:ILE:O	2:H:451:ARG:HD3	2.22	0.40
3:I:1284:ARG:HA	3:I:1287:ILE:HG22	2.02	0.40
5:K:225:LEU:HB3	5:K:251:LEU:HD13	2.03	0.40
5:K:720:MET:HG2	5:K:723:PHE:CZ	2.54	0.40
5:L:62:THR:HG21	5:L:107:VAL:HG23	2.03	0.40
5:L:468:LEU:HD22	5:L:469:TYR:CZ	2.54	0.40
5:L:629:LEU:O	5:L:630:ASP:C	2.59	0.40
5:L:677:LEU:HA	5:L:680:GLN:HB3	2.02	0.40
6:M:7:DG:O6	6:M:8:DA:N6	2.53	0.40
3:D:372:MET:O	3:D:376:LEU:HG	2.22	0.40
3:D:42:GLU:O	3:D:56:LEU:N	2.54	0.40
3:D:786:THR:HA	3:D:789:LYS:HB2	2.03	0.40
2:H:1149:TYR:HB3	2:H:1159:VAL:HG21	2.02	0.40
2:H:866:ASP:O	2:H:867:GLU:HG3	2.21	0.40
5:K:322:GLU:O	5:K:323:SER:CB	2.70	0.40
5:L:769:LEU:HD13	5:L:771:ARG:NH2	2.36	0.40
1:A:150:ARG:NH1	1:B:6:THR:OG1	2.53	0.40
2:C:124:MET:HA	2:C:498:ILE:HD13	2.03	0.40
3:D:45:ASN:O	3:D:47:ARG:N	2.54	0.40
3:D:814:CYS:SG	3:D:814:CYS:O	2.79	0.40
1:G:33:ARG:HD2	1:G:197:ASP:HB3	2.02	0.40
5:K:743:SER:CB	5:K:744:ASP:HB2	2.51	0.40
5:L:173:VAL:HG23	5:L:175:LEU:HD11	2.02	0.40
5:L:404:VAL:HB	5:L:408:MET:SD	2.61	0.40
2:C:1047:LEU:HB3	2:C:1048:LYS:HG3	2.03	0.40
2:C:502:VAL:HG12	2:C:503:LYS:N	2.37	0.40
2:C:518:ASN:N	2:C:761:GLN:OE1	2.55	0.40
3:D:305:ALA:HB1	3:D:316:ILE:HD11	2.03	0.40
2:H:1199:LEU:HB3	2:H:1204:LEU:O	2.22	0.40
2:H:61:SER:CB	2:H:479:LEU:HD13	2.51	0.40
2:H:709:ALA:HB3	2:H:792:GLY:O	2.21	0.40
5:K:299:ILE:O	5:K:302:LEU:HB2	2.21	0.40
5:K:314:ALA:O	5:K:315:THR:OG1	2.33	0.40
5:K:720:MET:CA	5:K:723:PHE:CE2	2.86	0.40
5:K:745:HIS:O	5:K:746:MET:CB	2.69	0.40
5:L:421:THR:O	5:L:425:VAL:HG12	2.21	0.40
5:L:623:ARG:HG2	5:L:627:GLU:HB2	2.03	0.40
2:C:1199:LEU:HB3	2:C:1204:LEU:O	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:503:LYS:O	2:C:507:GLY:N	2.55	0.40
2:C:519:ASN:HB2	2:C:520:PRO:HD2	2.04	0.40
2:C:709:ALA:HB3	2:C:792:GLY:O	2.22	0.40
2:C:866:ASP:O	2:C:867:GLU:HG3	2.21	0.40
2:H:1120:ALA:HB1	2:H:1198:LEU:HD22	2.02	0.40
2:H:1131:MET:O	2:H:1133:LYS:N	2.54	0.40
2:H:928:VAL:HG12	2:H:929:ILE:N	2.37	0.40
3:I:1265:THR:HG21	3:I:1275:LEU:HG	2.03	0.40
3:I:305:ALA:HB1	3:I:316:ILE:HD11	2.03	0.40
3:I:372:MET:O	3:I:376:LEU:HG	2.20	0.40
5:K:19:LEU:CD1	5:K:102:LEU:HD23	2.39	0.40
5:K:614:GLU:O	5:K:615:LYS:HB2	2.21	0.40
5:L:141:ARG:O	5:L:141:ARG:HG2	2.19	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	225/329 (68%)	202 (90%)	19 (8%)	4 (2%)	10	50
1	B	225/329 (68%)	205 (91%)	20 (9%)	0	100	100
1	F	225/329 (68%)	202 (90%)	19 (8%)	4 (2%)	10	50
1	G	225/329 (68%)	205 (91%)	19 (8%)	1 (0%)	38	77
2	C	1171/1342 (87%)	894 (76%)	211 (18%)	66 (6%)	2	25
2	H	1165/1342 (87%)	889 (76%)	206 (18%)	70 (6%)	2	23
3	D	1143/1416 (81%)	867 (76%)	235 (21%)	41 (4%)	4	35
3	I	1156/1416 (82%)	869 (75%)	240 (21%)	47 (4%)	3	31
4	E	73/90 (81%)	59 (81%)	8 (11%)	6 (8%)	1	16
4	J	73/90 (81%)	59 (81%)	8 (11%)	6 (8%)	1	16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	K	959/974 (98%)	689 (72%)	201 (21%)	69 (7%)	1	20
5	L	959/974 (98%)	694 (72%)	200 (21%)	65 (7%)	1	21
All	All	7599/8960 (85%)	5834 (77%)	1386 (18%)	379 (5%)	2	28

All (379) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	51	MET
2	C	43	PRO
2	C	63	SER
2	C	115	LYS
2	C	216	THR
2	C	488	MET
2	C	491	ASP
2	C	577	VAL
2	C	791	LEU
2	C	808	ASN
2	C	915	ASP
2	C	1216	ARG
2	C	1223	ARG
3	D	53	ARG
3	D	141	PHE
3	D	162	GLU
3	D	165	TYR
3	D	256	ASP
3	D	585	LYS
3	D	670	SER
3	D	706	VAL
3	D	834	PRO
3	D	891	ASP
3	D	1182	GLY
3	D	1186	TYR
4	E	44	ASP
1	F	51	MET
2	H	43	PRO
2	H	63	SER
2	H	115	LYS
2	H	216	THR
2	H	488	MET
2	H	491	ASP
2	H	577	VAL

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Mol	Chain	Res	Type
2	H	791	LEU
2	H	808	ASN
2	H	915	ASP
2	H	1216	ARG
2	H	1223	ARG
3	I	46	TYR
3	I	53	ARG
3	I	141	PHE
3	I	162	GLU
3	I	165	TYR
3	I	256	ASP
3	I	585	LYS
3	I	670	SER
3	I	706	VAL
3	I	834	PRO
3	I	855	ASP
3	I	891	ASP
3	I	1182	GLY
3	I	1185	PRO
4	J	44	ASP
5	K	92	GLU
5	K	199	ALA
5	K	244	ASN
5	K	273	GLU
5	K	315	THR
5	K	317	GLU
5	K	342	PHE
5	K	513	ALA
5	K	554	ASP
5	K	776	PHE
5	K	811	VAL
5	L	92	GLU
5	L	125	ARG
5	L	189	MET
5	L	199	ALA
5	L	244	ASN
5	L	315	THR
5	L	317	GLU
5	L	342	PHE
5	L	357	ALA
5	L	382	ILE
5	L	456	ALA

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Mol	Chain	Res	Type
5	L	513	ALA
5	L	554	ASP
5	L	584	PRO
5	L	611	PRO
5	L	738	ILE
5	L	776	PHE
5	L	811	VAL
2	C	456	VAL
2	C	502	VAL
2	C	552	PRO
2	C	677	ASN
2	C	692	THR
2	C	730	SER
2	C	844	LYS
2	C	926	GLY
2	C	1156	ARG
2	C	1157	GLN
2	C	1162	SER
2	C	1254	VAL
2	C	1297	ASP
3	D	68	TYR
3	D	79	LYS
3	D	155	GLU
3	D	711	GLY
3	D	1309	ILE
3	D	1311	LYS
2	H	456	VAL
2	H	502	VAL
2	H	552	PRO
2	H	677	ASN
2	H	692	THR
2	H	730	SER
2	H	844	LYS
2	H	926	GLY
2	H	1156	ARG
2	H	1157	GLN
2	H	1162	SER
2	H	1254	VAL
2	H	1297	ASP
3	I	68	TYR
3	I	79	LYS
3	I	155	GLU

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Mol	Chain	Res	Type
3	I	521	LYS
3	I	711	GLY
3	I	1183	SER
3	I	1309	ILE
3	I	1311	LYS
5	K	10	ILE
5	K	66	GLY
5	K	73	GLU
5	K	246	PHE
5	K	271	GLU
5	K	313	THR
5	K	316	PRO
5	K	323	SER
5	K	358	MET
5	K	379	GLU
5	K	397	GLN
5	K	478	GLU
5	K	511	ALA
5	K	584	PRO
5	K	595	GLY
5	K	813	THR
5	L	10	ILE
5	L	66	GLY
5	L	69	MET
5	L	313	THR
5	L	316	PRO
5	L	381	ASP
5	L	470	PRO
5	L	474	TYR
5	L	478	GLU
5	L	511	ALA
5	L	595	GLY
2	C	26	TYR
2	C	77	GLU
2	C	165	HIS
2	C	613	ASN
2	C	638	SER
2	C	912	ASP
2	C	1047	LEU
2	C	1103	VAL
2	C	1132	LEU
2	C	1153	ALA

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Mol	Chain	Res	Type
2	C	1237	HIS
2	C	1238	LEU
2	C	1256	GLN
3	D	77	ARG
3	D	131	PRO
3	D	270	ARG
3	D	679	TYR
3	D	1150	PRO
4	E	43	ASN
2	H	26	TYR
2	H	77	GLU
2	H	165	HIS
2	H	912	ASP
2	H	1047	LEU
2	H	1103	VAL
2	H	1132	LEU
2	H	1153	ALA
2	H	1237	HIS
2	H	1238	LEU
2	H	1256	GLN
3	I	77	ARG
3	I	131	PRO
3	I	270	ARG
3	I	679	TYR
3	I	857	LEU
3	I	1150	PRO
4	J	43	ASN
5	K	241	ASP
5	K	272	ALA
5	K	372	MET
5	K	467	MET
5	K	474	TYR
5	K	539	SER
5	K	585	PHE
5	K	721	ASN
5	L	241	ASP
5	L	585	PHE
5	L	732	ASP
5	L	802	SER
5	L	813	THR
5	L	843	MET
2	C	27	LEU

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Mol	Chain	Res	Type
2	C	88	ARG
2	C	698	PRO
2	C	866	ASP
2	C	939	VAL
2	C	1131	MET
2	C	1155	VAL
2	C	1317	PRO
3	D	46	TYR
3	D	47	ARG
3	D	286	ALA
3	D	1275	LEU
4	E	35	LYS
2	H	27	LEU
2	H	88	ARG
2	H	613	ASN
2	H	638	SER
2	H	866	ASP
2	H	939	VAL
2	H	1131	MET
2	H	1155	VAL
2	H	1317	PRO
3	I	47	ARG
3	I	286	ALA
3	I	1275	LEU
4	J	35	LYS
5	K	3	PHE
5	K	65	ASP
5	K	142	MET
5	K	177	ASP
5	K	261	ARG
5	K	322	GLU
5	K	343	VAL
5	K	394	GLU
5	K	458	LYS
5	K	604	HIS
5	K	630	ASP
5	K	657	PRO
5	K	659	GLN
5	K	662	GLY
5	K	732	ASP
5	K	744	ASP
5	K	763	PHE

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Mol	Chain	Res	Type
5	K	802	SER
5	K	812	GLY
5	K	823	GLU
5	L	3	PHE
5	L	65	ASP
5	L	177	ASP
5	L	261	ARG
5	L	343	VAL
5	L	358	MET
5	L	458	LYS
5	L	604	HIS
5	L	630	ASP
5	L	657	PRO
5	L	659	GLN
5	L	763	PHE
5	L	812	GLY
5	L	823	GLU
1	A	165	GLU
1	A	214	GLU
2	C	214	ASN
2	C	436	ARG
2	C	487	LEU
2	C	1313	HIS
3	D	86	GLU
3	D	174	ASP
3	D	546	ALA
3	D	593	ASN
3	D	776	THR
4	E	40	PRO
4	E	41	GLU
1	F	165	GLU
1	F	214	GLU
2	H	214	ASN
2	H	436	ARG
2	H	487	LEU
2	H	698	PRO
2	H	910	ALA
2	H	1313	HIS
3	I	86	GLU
3	I	174	ASP
3	I	546	ALA
3	I	593	ASN

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Mol	Chain	Res	Type
3	I	776	THR
3	I	851	PRO
3	I	1184	ASP
4	J	40	PRO
4	J	41	GLU
5	K	27	ALA
5	K	318	GLN
5	K	341	GLN
5	K	485	TRP
5	K	641	THR
5	K	746	MET
5	K	810	PRO
5	K	869	ASN
5	L	27	ALA
5	L	341	GLN
5	L	393	SER
5	L	394	GLU
5	L	485	TRP
5	L	641	THR
5	L	662	GLY
5	L	737	MET
5	L	810	PRO
5	L	869	ASN
2	C	489	PRO
2	C	910	ALA
2	C	1122	LYS
2	C	1186	VAL
2	C	1215	GLY
2	C	1318	GLY
3	D	122	SER
3	D	313	GLY
3	D	879	ALA
1	F	179	PRO
1	G	214	GLU
2	H	108	GLU
2	H	352	ARG
2	H	451	ARG
2	H	489	PRO
2	H	498	ILE
2	H	1122	LYS
2	H	1186	VAL
2	H	1215	GLY

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Mol	Chain	Res	Type
2	H	1318	GLY
3	I	122	SER
3	I	313	GLY
3	I	879	ALA
3	I	1179	PRO
5	K	46	SER
5	K	111	PRO
5	K	522	VAL
5	K	873	GLY
5	L	46	SER
5	L	522	VAL
5	L	873	GLY
1	A	179	PRO
2	C	498	ILE
5	L	111	PRO
2	C	134	GLY
2	C	1185	PRO
2	C	1205	PRO
2	C	1334	GLY
3	D	671	GLY
3	D	1191	PRO
2	H	134	GLY
2	H	1205	PRO
2	H	1334	GLY
3	I	586	GLY
3	I	671	GLY
3	I	1191	PRO
5	K	110	LYS
5	L	110	LYS
2	C	178	PRO
3	D	233	LYS
2	H	1185	PRO
3	I	233	LYS
2	C	79	VAL
2	C	153	PRO
2	C	168	GLY
2	C	669	PRO
3	D	586	GLY
3	D	616	PRO
4	E	4	VAL
2	H	79	VAL
2	H	153	PRO

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Mol	Chain	Res	Type
2	H	168	GLY
2	H	178	PRO
2	H	669	PRO
5	K	245	PRO
3	D	92	VAL
2	H	355	PRO
3	I	92	VAL
4	J	4	VAL
5	L	727	GLY

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	195/286 (68%)	191 (98%)	4 (2%)	59	81
1	B	195/286 (68%)	188 (96%)	7 (4%)	40	69
1	F	195/286 (68%)	191 (98%)	4 (2%)	59	81
1	G	195/286 (68%)	188 (96%)	7 (4%)	40	69
2	C	1016/1157 (88%)	937 (92%)	79 (8%)	15	48
2	H	1011/1157 (87%)	934 (92%)	77 (8%)	15	49
3	D	962/1177 (82%)	879 (91%)	83 (9%)	12	44
3	I	971/1177 (82%)	889 (92%)	82 (8%)	13	45
4	E	65/74 (88%)	62 (95%)	3 (5%)	31	64
4	J	65/74 (88%)	62 (95%)	3 (5%)	31	64
5	K	822/835 (98%)	724 (88%)	98 (12%)	6	29
5	L	822/835 (98%)	732 (89%)	90 (11%)	7	33
All	All	6514/7630 (85%)	5977 (92%)	537 (8%)	13	46

All (537) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	GLU

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Mol	Chain	Res	Type
1	A	91	ARG
1	A	186	ASN
1	A	231	PHE
1	B	29	GLU
1	B	66	HIS
1	B	101	THR
1	B	134	THR
1	B	135	ASP
1	B	186	ASN
1	B	231	PHE
2	C	26	TYR
2	C	62	TYR
2	C	132	ASP
2	C	158	ASP
2	C	161	LYS
2	C	179	TYR
2	C	188	PHE
2	C	192	ASP
2	C	350	THR
2	C	365	GLU
2	C	379	GLU
2	C	396	ASP
2	C	397	LEU
2	C	403	MET
2	C	423	ASP
2	C	436	ARG
2	C	437	ASN
2	C	441	GLU
2	C	451	ARG
2	C	472	GLU
2	C	514	PHE
2	C	523	GLU
2	C	528	ARG
2	C	539	THR
2	C	541	GLU
2	C	545	PHE
2	C	554	HIS
2	C	574	SER
2	C	581	THR
2	C	628	HIS
2	C	632	ASP
2	C	643	SER

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Mol	Chain	Res	Type
2	C	657	THR
2	C	674	ASP
2	C	696	ASP
2	C	699	LEU
2	C	702	THR
2	C	714	VAL
2	C	725	GLN
2	C	728	ASP
2	C	733	VAL
2	C	737	ASN
2	C	748	ILE
2	C	749	ASP
2	C	757	THR
2	C	789	THR
2	C	799	ASN
2	C	811	ASN
2	C	834	GLN
2	C	835	GLU
2	C	840	SER
2	C	894	GLN
2	C	903	ARG
2	C	912	ASP
2	C	922	ASN
2	C	933	VAL
2	C	944	ARG
2	C	947	GLU
2	C	948	ILE
2	C	964	LEU
2	C	971	LEU
2	C	972	PHE
2	C	1020	GLU
2	C	1034	ARG
2	C	1058	ARG
2	C	1072	ASN
2	C	1082	ILE
2	C	1087	TYR
2	C	1096	ILE
2	C	1098	LEU
2	C	1156	ARG
2	C	1184	THR
2	C	1188	ASP
2	C	1231	TYR

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Mol	Chain	Res	Type
2	C	1244	HIS
2	C	1276	TRP
2	C	1306	LYS
2	C	1319	MET
2	C	1333	LEU
3	D	21	LYS
3	D	42	GLU
3	D	45	ASN
3	D	54	ASP
3	D	58	CYS
3	D	67	ASP
3	D	70	CYS
3	D	86	GLU
3	D	88	CYS
3	D	93	THR
3	D	139	LEU
3	D	156	ARG
3	D	157	GLN
3	D	159	ILE
3	D	169	LEU
3	D	171	GLU
3	D	199	GLU
3	D	208	THR
3	D	212	THR
3	D	223	LEU
3	D	229	GLN
3	D	250	ARG
3	D	252	LEU
3	D	285	LEU
3	D	290	ILE
3	D	294	ASN
3	D	300	GLN
3	D	316	ILE
3	D	329	ASP
3	D	330	MET
3	D	338	PHE
3	D	342	LEU
3	D	345	LYS
3	D	368	LEU
3	D	393	THR
3	D	416	ILE
3	D	438	GLU

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Mol	Chain	Res	Type
3	D	440	VAL
3	D	450	HIS
3	D	454	CYS
3	D	460	ASP
3	D	503	SER
3	D	515	ARG
3	D	534	GLU
3	D	572	THR
3	D	615	LYS
3	D	649	LYS
3	D	672	LEU
3	D	680	ASN
3	D	690	ASN
3	D	699	ASP
3	D	700	ASN
3	D	701	LEU
3	D	736	GLN
3	D	744	ARG
3	D	746	LEU
3	D	783	LEU
3	D	792	ASN
3	D	812	ASP
3	D	846	GLU
3	D	847	ASP
3	D	860	ARG
3	D	884	SER
3	D	889	ASP
3	D	891	ASP
3	D	898	CYS
3	D	1144	LEU
3	D	1155	ILE
3	D	1192	LYS
3	D	1198	VAL
3	D	1199	PHE
3	D	1231	ARG
3	D	1246	VAL
3	D	1262	ARG
3	D	1282	TYR
3	D	1290	ARG
3	D	1298	VAL
3	D	1305	ASP
3	D	1318	SER

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Mol	Chain	Res	Type
3	D	1330	ARG
3	D	1348	LYS
3	D	1366	HIS
3	D	1369	ARG
4	E	44	ASP
4	E	67	ARG
4	E	70	GLN
1	F	29	GLU
1	F	91	ARG
1	F	186	ASN
1	F	231	PHE
1	G	29	GLU
1	G	66	HIS
1	G	101	THR
1	G	134	THR
1	G	135	ASP
1	G	186	ASN
1	G	231	PHE
2	H	26	TYR
2	H	62	TYR
2	H	132	ASP
2	H	158	ASP
2	H	161	LYS
2	H	179	TYR
2	H	188	PHE
2	H	192	ASP
2	H	350	THR
2	H	365	GLU
2	H	379	GLU
2	H	396	ASP
2	H	397	LEU
2	H	403	MET
2	H	405	PHE
2	H	423	ASP
2	H	436	ARG
2	H	437	ASN
2	H	441	GLU
2	H	451	ARG
2	H	472	GLU
2	H	514	PHE
2	H	523	GLU
2	H	528	ARG

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Mol	Chain	Res	Type
2	H	539	THR
2	H	541	GLU
2	H	545	PHE
2	H	554	HIS
2	H	574	SER
2	H	581	THR
2	H	628	HIS
2	H	632	ASP
2	H	643	SER
2	H	657	THR
2	H	674	ASP
2	H	696	ASP
2	H	699	LEU
2	H	702	THR
2	H	725	GLN
2	H	728	ASP
2	H	733	VAL
2	H	748	ILE
2	H	749	ASP
2	H	757	THR
2	H	789	THR
2	H	799	ASN
2	H	811	ASN
2	H	834	GLN
2	H	840	SER
2	H	894	GLN
2	H	903	ARG
2	H	912	ASP
2	H	922	ASN
2	H	933	VAL
2	H	944	ARG
2	H	947	GLU
2	H	948	ILE
2	H	964	LEU
2	H	971	LEU
2	H	972	PHE
2	H	1020	GLU
2	H	1034	ARG
2	H	1058	ARG
2	H	1072	ASN
2	H	1082	ILE
2	H	1087	TYR

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Mol	Chain	Res	Type
2	H	1096	ILE
2	H	1098	LEU
2	H	1156	ARG
2	H	1184	THR
2	H	1188	ASP
2	H	1231	TYR
2	H	1244	HIS
2	H	1276	TRP
2	H	1306	LYS
2	H	1319	MET
2	H	1333	LEU
3	I	21	LYS
3	I	42	GLU
3	I	45	ASN
3	I	54	ASP
3	I	58	CYS
3	I	67	ASP
3	I	70	CYS
3	I	86	GLU
3	I	88	CYS
3	I	93	THR
3	I	139	LEU
3	I	156	ARG
3	I	157	GLN
3	I	159	ILE
3	I	169	LEU
3	I	171	GLU
3	I	199	GLU
3	I	208	THR
3	I	212	THR
3	I	223	LEU
3	I	229	GLN
3	I	250	ARG
3	I	252	LEU
3	I	285	LEU
3	I	290	ILE
3	I	294	ASN
3	I	300	GLN
3	I	316	ILE
3	I	329	ASP
3	I	330	MET
3	I	335	GLN

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Mol	Chain	Res	Type
3	I	338	PHE
3	I	342	LEU
3	I	345	LYS
3	I	368	LEU
3	I	393	THR
3	I	416	ILE
3	I	438	GLU
3	I	440	VAL
3	I	450	HIS
3	I	454	CYS
3	I	460	ASP
3	I	503	SER
3	I	515	ARG
3	I	534	GLU
3	I	572	THR
3	I	615	LYS
3	I	620	PHE
3	I	649	LYS
3	I	672	LEU
3	I	680	ASN
3	I	690	ASN
3	I	700	ASN
3	I	701	LEU
3	I	736	GLN
3	I	744	ARG
3	I	746	LEU
3	I	783	LEU
3	I	792	ASN
3	I	812	ASP
3	I	846	GLU
3	I	860	ARG
3	I	884	SER
3	I	889	ASP
3	I	898	CYS
3	I	1144	LEU
3	I	1155	ILE
3	I	1192	LYS
3	I	1198	VAL
3	I	1199	PHE
3	I	1231	ARG
3	I	1246	VAL
3	I	1262	ARG

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Mol	Chain	Res	Type
3	I	1282	TYR
3	I	1290	ARG
3	I	1298	VAL
3	I	1305	ASP
3	I	1318	SER
3	I	1330	ARG
3	I	1348	LYS
3	I	1366	HIS
3	I	1369	ARG
4	J	44	ASP
4	J	67	ARG
4	J	70	GLN
5	K	13	THR
5	K	19	LEU
5	K	42	LEU
5	K	54	MET
5	K	61	ILE
5	K	65	ASP
5	K	67	TRP
5	K	90	THR
5	K	108	PHE
5	K	113	ASP
5	K	114	ARG
5	K	115	LEU
5	K	123	MET
5	K	153	SER
5	K	155	ILE
5	K	174	LEU
5	K	178	GLU
5	K	183	LYS
5	K	191	LEU
5	K	193	GLN
5	K	196	LEU
5	K	216	LEU
5	K	232	ASP
5	K	246	PHE
5	K	253	ILE
5	K	254	CYS
5	K	256	LEU
5	K	260	ARG
5	K	273	GLU
5	K	275	ASP

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Mol	Chain	Res	Type
5	K	285	LEU
5	K	288	SER
5	K	301	GLN
5	K	311	LEU
5	K	313	THR
5	K	327	ARG
5	K	343	VAL
5	K	366	SER
5	K	370	LEU
5	K	371	ASN
5	K	386	LEU
5	K	400	ARG
5	K	401	GLN
5	K	402	GLU
5	K	408	MET
5	K	422	ARG
5	K	435	THR
5	K	440	LEU
5	K	443	GLN
5	K	445	GLN
5	K	476	GLU
5	K	488	ASP
5	K	504	GLN
5	K	512	LYS
5	K	515	THR
5	K	518	GLN
5	K	533	VAL
5	K	553	GLU
5	K	562	CYS
5	K	577	HIS
5	K	613	LEU
5	K	630	ASP
5	K	635	THR
5	K	641	THR
5	K	644	ASP
5	K	660	THR
5	K	665	ASP
5	K	675	GLU
5	K	688	LEU
5	K	706	ILE
5	K	710	ASP
5	K	723	PHE

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Mol	Chain	Res	Type
5	K	729	ASN
5	K	741	THR
5	K	744	ASP
5	K	759	ILE
5	K	760	THR
5	K	762	THR
5	K	769	LEU
5	K	775	GLN
5	K	779	TRP
5	K	788	LEU
5	K	814	LEU
5	K	831	GLN
5	K	843	MET
5	K	845	LEU
5	K	847	LYS
5	K	858	PHE
5	K	862	ASN
5	K	868	VAL
5	K	872	THR
5	K	877	VAL
5	K	881	GLN
5	K	912	GLU
5	K	931	ILE
5	K	932	ARG
5	K	960	LEU
5	K	962	LEU
5	L	13	THR
5	L	19	LEU
5	L	42	LEU
5	L	65	ASP
5	L	67	TRP
5	L	90	THR
5	L	108	PHE
5	L	113	ASP
5	L	114	ARG
5	L	115	LEU
5	L	123	MET
5	L	141	ARG
5	L	153	SER
5	L	155	ILE
5	L	174	LEU
5	L	178	GLU

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Mol	Chain	Res	Type
5	L	191	LEU
5	L	193	GLN
5	L	196	LEU
5	L	216	LEU
5	L	232	ASP
5	L	253	ILE
5	L	254	CYS
5	L	256	LEU
5	L	260	ARG
5	L	273	GLU
5	L	275	ASP
5	L	285	LEU
5	L	288	SER
5	L	301	GLN
5	L	311	LEU
5	L	313	THR
5	L	327	ARG
5	L	343	VAL
5	L	360	LEU
5	L	366	SER
5	L	386	LEU
5	L	400	ARG
5	L	401	GLN
5	L	402	GLU
5	L	422	ARG
5	L	440	LEU
5	L	443	GLN
5	L	445	GLN
5	L	476	GLU
5	L	488	ASP
5	L	504	GLN
5	L	512	LYS
5	L	515	THR
5	L	518	GLN
5	L	533	VAL
5	L	553	GLU
5	L	562	CYS
5	L	577	HIS
5	L	613	LEU
5	L	630	ASP
5	L	635	THR
5	L	641	THR

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Mol	Chain	Res	Type
5	L	644	ASP
5	L	660	THR
5	L	665	ASP
5	L	675	GLU
5	L	688	LEU
5	L	706	ILE
5	L	710	ASP
5	L	729	ASN
5	L	741	THR
5	L	759	ILE
5	L	760	THR
5	L	762	THR
5	L	769	LEU
5	L	775	GLN
5	L	779	TRP
5	L	788	LEU
5	L	814	LEU
5	L	831	GLN
5	L	845	LEU
5	L	847	LYS
5	L	858	PHE
5	L	862	ASN
5	L	868	VAL
5	L	872	THR
5	L	877	VAL
5	L	881	GLN
5	L	912	GLU
5	L	931	ILE
5	L	932	ARG
5	L	947	MET
5	L	960	LEU
5	L	962	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (62) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	HIS
1	A	186	ASN
1	B	186	ASN
2	C	60	GLN
2	C	673	HIS
2	C	737	ASN

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Mol	Chain	Res	Type
2	C	766	ASN
2	C	832	HIS
2	C	1116	HIS
2	C	1264	GLN
3	D	80	HIS
3	D	113	HIS
3	D	419	HIS
3	D	690	ASN
3	D	875	ASN
4	E	70	GLN
1	F	41	ASN
1	F	66	HIS
1	F	186	ASN
1	G	186	ASN
2	H	60	GLN
2	H	673	HIS
2	H	766	ASN
2	H	832	HIS
2	H	1116	HIS
2	H	1264	GLN
3	I	113	HIS
3	I	200	GLN
3	I	419	HIS
3	I	519	ASN
3	I	690	ASN
3	I	875	ASN
4	J	70	GLN
5	K	70	GLN
5	K	150	GLN
5	K	194	GLN
5	K	239	GLN
5	K	244	ASN
5	K	324	HIS
5	K	371	ASN
5	K	401	GLN
5	K	518	GLN
5	K	535	HIS
5	K	577	HIS
5	K	729	ASN
5	K	736	ASN
5	K	831	GLN
5	K	850	ASN

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Mol	Chain	Res	Type
5	K	851	ASN
5	L	239	GLN
5	L	244	ASN
5	L	324	HIS
5	L	371	ASN
5	L	434	HIS
5	L	518	GLN
5	L	521	GLN
5	L	535	HIS
5	L	729	ASN
5	L	736	ASN
5	L	831	GLN
5	L	850	ASN
5	L	851	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
7	N	8/9 (88%)	3 (37%)	0
7	P	8/9 (88%)	1 (12%)	0
All	All	16/18 (88%)	4 (25%)	0

All (4) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
7	N	2	U
7	N	6	C
7	N	7	U
7	P	7	U

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 carbohydrates 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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	227/329 (68%)	-0.50	0 <span>100</span> <span>100</span>	178, 268, 367, 400	0
1	B	227/329 (68%)	-0.05	14 (6%) <span>21</span> <span>19</span>	237, 380, 491, 539	0
1	F	227/329 (68%)	-0.49	0 <span>100</span> <span>100</span>	192, 268, 357, 401	0
1	G	227/329 (68%)	-0.20	1 (0%) <span>92</span> <span>88</span>	256, 379, 484, 537	0
2	C	1179/1342 (87%)	-0.58	15 (1%) <span>77</span> <span>70</span>	126, 241, 378, 510	0
2	H	1173/1342 (87%)	-0.57	6 (0%) <span>90</span> <span>86</span>	143, 251, 375, 532	0
3	D	1149/1416 (81%)	-0.40	29 (2%) <span>58</span> <span>50</span>	181, 301, 441, 641	0
3	I	1160/1416 (81%)	-0.38	32 (2%) <span>53</span> <span>46</span>	175, 282, 433, 662	0
4	E	75/90 (83%)	0.14	2 (2%) <span>55</span> <span>47</span>	285, 343, 385, 397	0
4	J	75/90 (83%)	0.10	3 (4%) <span>39</span> <span>32</span>	329, 349, 365, 376	0
5	K	961/974 (98%)	-0.35	25 (2%) <span>56</span> <span>49</span>	178, 278, 461, 664	0
5	L	961/974 (98%)	-0.35	26 (2%) <span>55</span> <span>47</span>	169, 269, 469, 638	0
6	M	15/15 (100%)	0.51	2 (13%) <span>4</span> <span>6</span>	321, 353, 461, 465	0
6	O	15/15 (100%)	0.45	2 (13%) <span>4</span> <span>6</span>	331, 351, 543, 550	0
7	N	9/9 (100%)	-0.01	0 <span>100</span> <span>100</span>	258, 268, 381, 391	0
7	P	9/9 (100%)	-0.04	0 <span>100</span> <span>100</span>	236, 245, 375, 395	0
All	All	7689/9008 (85%)	-0.41	157 (2%) <span>65</span> <span>58</span>	126, 279, 441, 664	0

All (157) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	L	65	ASP	15.6
5	K	6	GLY	8.5
5	L	64	HIS	8.1
5	K	5	LEU	6.4
5	K	25	VAL	6.2

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Mol	Chain	Res	Type	RSRZ
2	H	1263	ALA	6.0
5	L	871	HIS	5.9
5	K	871	HIS	5.9
5	L	72	GLU	5.6
5	L	813	THR	5.6
1	B	134	THR	5.5
3	I	1295	ASN	5.4
3	I	853	THR	5.4
3	I	1212	ASP	5.2
1	B	168	ILE	5.1
3	D	1212	ASP	4.9
1	B	136	GLU	4.9
3	I	1205	GLU	4.9
3	D	1189	MET	4.8
3	D	207	GLU	4.7
3	D	1191	PRO	4.6
3	I	1376	GLY	4.3
5	L	90	THR	4.3
5	L	61	ILE	4.3
5	L	105	LYS	4.2
5	K	72	GLU	4.2
2	C	974	ARG	4.1
3	D	174	ASP	4.1
5	K	64	HIS	4.0
3	I	1297	LYS	4.0
5	K	808	ALA	3.9
3	D	1188	GLU	3.9
4	E	76	GLU	3.8
5	K	48	SER	3.7
3	D	12	THR	3.7
1	B	70	THR	3.7
5	K	53	VAL	3.7
3	I	1213	GLY	3.7
3	D	1200	GLU	3.6
3	I	207	GLU	3.5
1	B	137	ASN	3.5
3	D	1187	GLU	3.4
3	I	1200	GLU	3.3
5	L	68	GLN	3.3
3	I	1199	PHE	3.3
5	K	105	LYS	3.3
2	H	212	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
5	L	872	THR	3.2
3	I	1207	GLY	3.1
3	I	1291	GLU	3.1
2	H	1020	GLU	3.1
2	C	1263	ALA	3.1
3	D	715	LYS	3.0
1	B	105	SER	3.0
6	M	15	DG	3.0
5	L	118	GLY	3.0
5	K	4	THR	3.0
2	C	108	GLU	3.0
3	D	1161	GLY	3.0
3	D	1180	VAL	3.0
1	B	122	GLU	2.9
5	L	104	SER	2.9
5	L	69	MET	2.9
1	G	168	ILE	2.9
1	B	106	GLY	2.9
3	D	831	VAL	2.8
2	C	910	ALA	2.8
4	J	33	GLY	2.7
5	K	38	GLY	2.7
3	I	1171	GLY	2.7
5	L	15	SER	2.7
3	I	1296	GLY	2.7
2	C	363	LEU	2.7
3	I	79	LYS	2.7
3	I	1167	LYS	2.7
3	D	1376	GLY	2.7
5	K	24	ALA	2.7
2	C	1262	LYS	2.7
5	K	26	ASP	2.7
1	B	167	PRO	2.7
5	L	71	VAL	2.6
3	I	855	ASP	2.6
3	I	1189	MET	2.6
4	J	50	ALA	2.6
5	K	7	GLN	2.6
3	I	1191	PRO	2.6
3	D	1206	ARG	2.6
3	D	1213	GLY	2.5
5	L	66	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
5	K	104	SER	2.5
1	B	163	GLU	2.5
3	I	854	ALA	2.5
5	K	39	GLU	2.5
5	L	70	GLN	2.5
2	C	207	THR	2.5
2	C	915	ASP	2.5
5	L	48	SER	2.5
5	K	811	VAL	2.5
2	H	747	GLY	2.5
6	M	3	DG	2.5
3	D	1299	GLY	2.4
5	L	271	GLU	2.4
2	H	118	LYS	2.4
3	I	174	ASP	2.4
3	I	14	THR	2.4
3	D	1190	ILE	2.4
3	D	206	ASN	2.4
5	K	103	ASP	2.4
3	I	1188	GLU	2.4
5	K	54	MET	2.3
3	D	830	ASP	2.3
3	D	1205	GLU	2.3
3	I	13	LYS	2.3
3	I	1375	ALA	2.3
3	I	1272	SER	2.3
3	I	284	ASP	2.3
5	L	91	GLU	2.3
6	O	2	DC	2.2
3	D	1155	ILE	2.2
2	C	1013	GLN	2.2
3	D	1149	ARG	2.2
2	C	747	GLY	2.2
5	L	811	VAL	2.2
6	O	1	DA	2.2
5	K	37	THR	2.2
5	L	959	ALA	2.2
3	D	1181	ASP	2.2
5	K	40	ASN	2.2
1	B	135	ASP	2.2
2	C	373	GLY	2.2
1	B	99	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
3	I	852	GLY	2.1
3	I	856	ILE	2.1
3	D	1305	ASP	2.1
5	K	408	MET	2.1
4	J	32	VAL	2.1
2	H	654	ASP	2.1
2	C	970	GLY	2.1
2	C	1014	LEU	2.1
5	L	38	GLY	2.1
1	B	54	CYS	2.1
3	D	1224	ARG	2.1
3	I	1305	ASP	2.1
2	C	372	PRO	2.1
5	K	52	ARG	2.1
4	E	43	ASN	2.1
3	D	1199	PHE	2.1
3	D	149	GLY	2.0
1	B	138	ALA	2.0
5	L	40	ASN	2.0
5	L	47	ASP	2.0
3	I	551	ARG	2.0
5	K	8	ARG	2.0
5	L	961	ARG	2.0
3	I	810	THR	2.0
2	C	1019	ASP	2.0
3	D	202	ARG	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
8	ZN	D	1502	1/1	0.98	0.20	-0.01	84,84,84,84	0
8	ZN	D	1501	1/1	0.90	0.17	-0.50	106,106,106,106	0
8	ZN	I	1501	1/1	0.76	0.13	-0.89	131,131,131,131	0
8	ZN	I	1502	1/1	0.96	0.10	-1.48	117,117,117,117	0
9	MG	I	1503	1/1	0.86	0.11	-	52,52,52,52	0
9	MG	D	1503	1/1	0.80	0.24	-	10,10,10,10	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.