



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 28, 2016 – 05:41 PM EDT

PDB ID : 4YG7  
Title : Structure of FL autorepression promoter complex  
Authors : Schumacher, M.A.  
Deposited on : 2015-02-25  
Resolution : 3.77 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  
Mogul : unknown  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20027107  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : rb-20027107

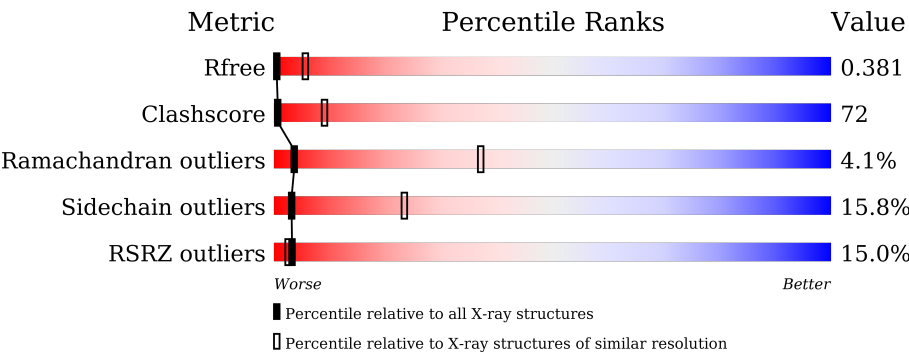
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.77 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.



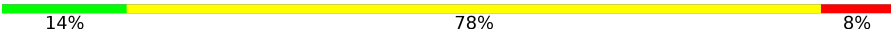
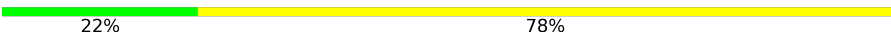
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	1273 (4.06-3.50)
Clashscore	102246	1412 (4.06-3.50)
Ramachandran outliers	100387	1351 (4.06-3.50)
Sidechain outliers	100360	1347 (4.06-3.50)
RSRZ outliers	91569	1281 (4.06-3.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	B	71	<div><div>10%</div><div>18%55%24%</div><div>18%</div></div>
1	C	71	<div><div>18%</div><div>18%69%13%</div><div>18%</div></div>
1	E	71	<div><div>10%</div><div>23%61%14%</div><div>23%</div></div>
1	G	71	<div><div>17%</div><div>24%61%15%</div><div>24%</div></div>
2	D	436	<div><div>20%</div><div>26%59%9%5%</div><div>26%</div></div>
2	K	436	<div><div>13%</div><div>20%59%16%6%</div><div>20%</div></div>

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Mol	Chain	Length	Quality of chain
3	R	50	 14% 78% 8%
4	T	50	 22% 78%

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10806 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 Antitoxin HipB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	69	Total	C	N	O	S	0	0	0
			550	349	92	106	3			
1	E	69	Total	C	N	O	S	0	0	0
			550	349	92	106	3			
1	C	71	Total	C	N	O	S	0	0	0
			565	358	95	109	3			
1	G	71	Total	C	N	O	S	0	0	0
			565	358	95	109	3			

- Molecule 2 is a protein called Serine/threonine-protein kinase HipA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	414	Total	C	N	O	S	0	0	0
			3275	2100	570	593	12			
2	K	412	Total	C	N	O	S	0	0	0
			3256	2087	568	589	12			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	309	GLN	ASP	conflict	UNP P23874
K	309	GLN	ASP	conflict	UNP P23874

- Molecule 3 is a DNA chain called DNA (50-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	R	50	Total	C	N	O	P	0	0	0
			1022	491	184	298	49			

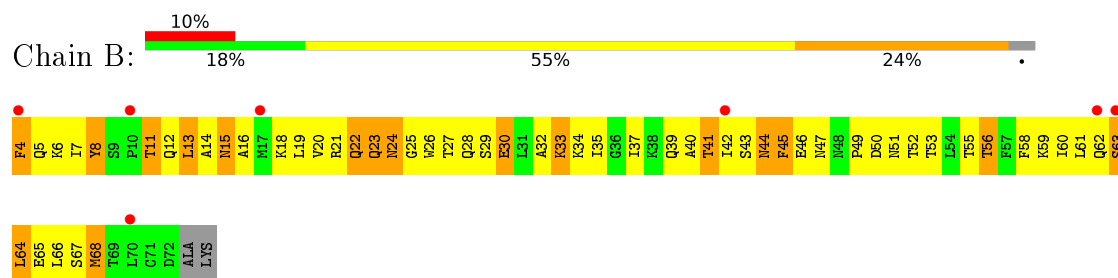
- Molecule 4 is a DNA chain called DNA (50-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	T	50	Total	C	N	O	P	0	0	0
			1023	491	184	299	49			

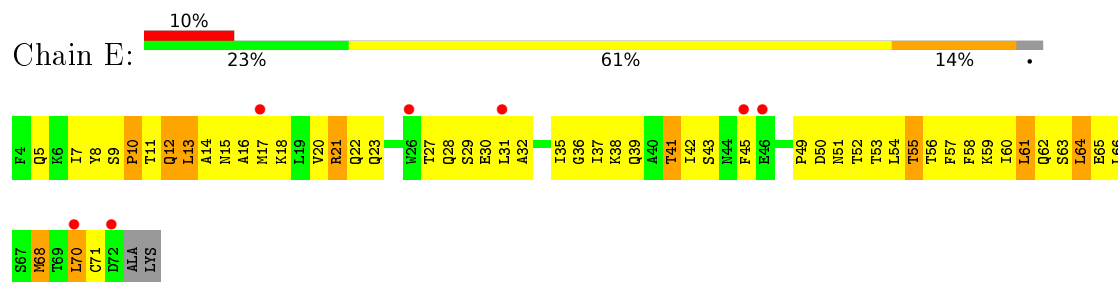
### 3 Residue-property plots

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

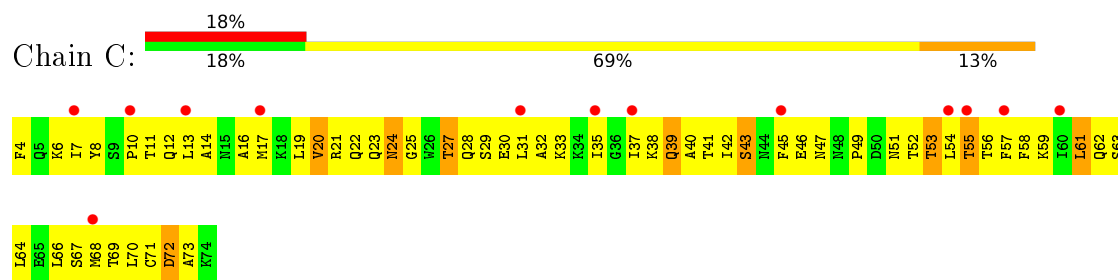
#### • Molecule 1: Antitoxin HipB



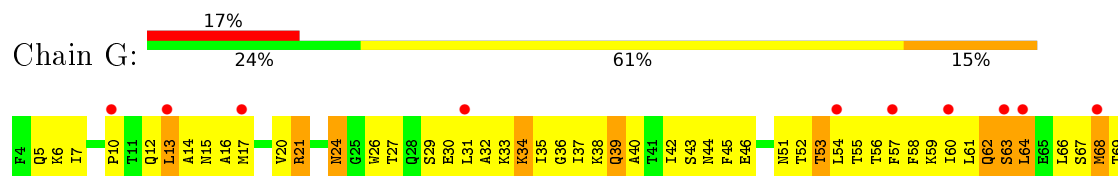
#### • Molecule 1: Antitoxin HipB

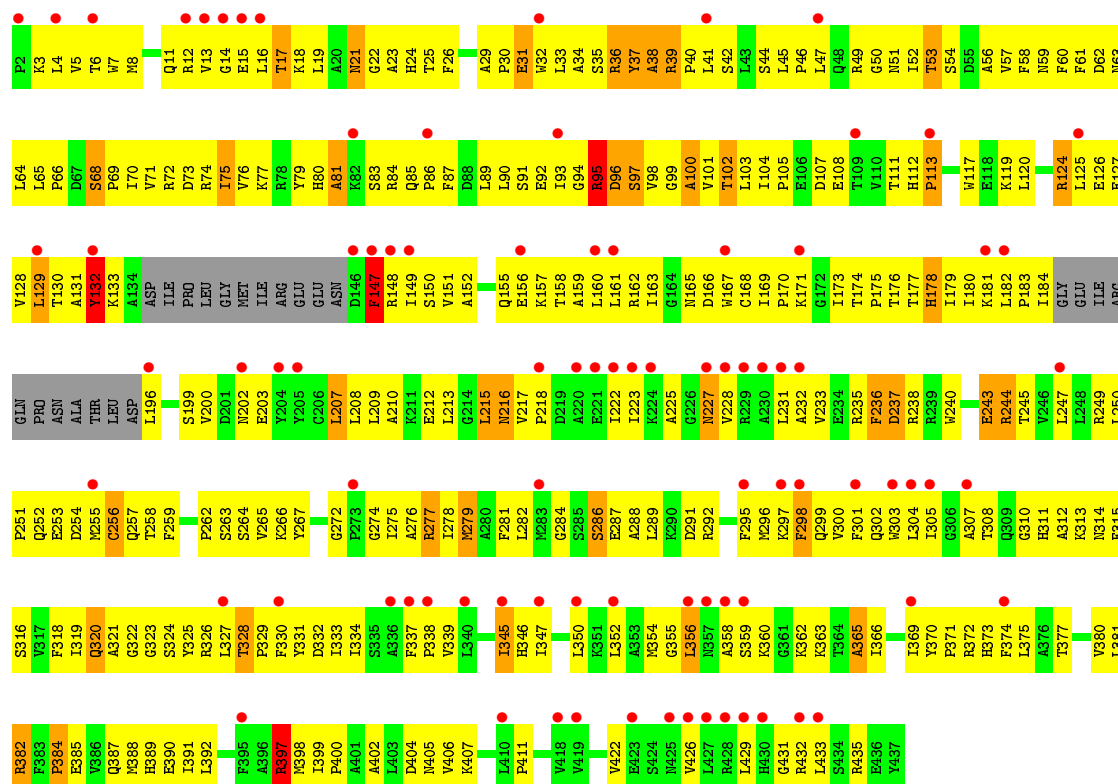


#### • Molecule 1: Antitoxin HipB

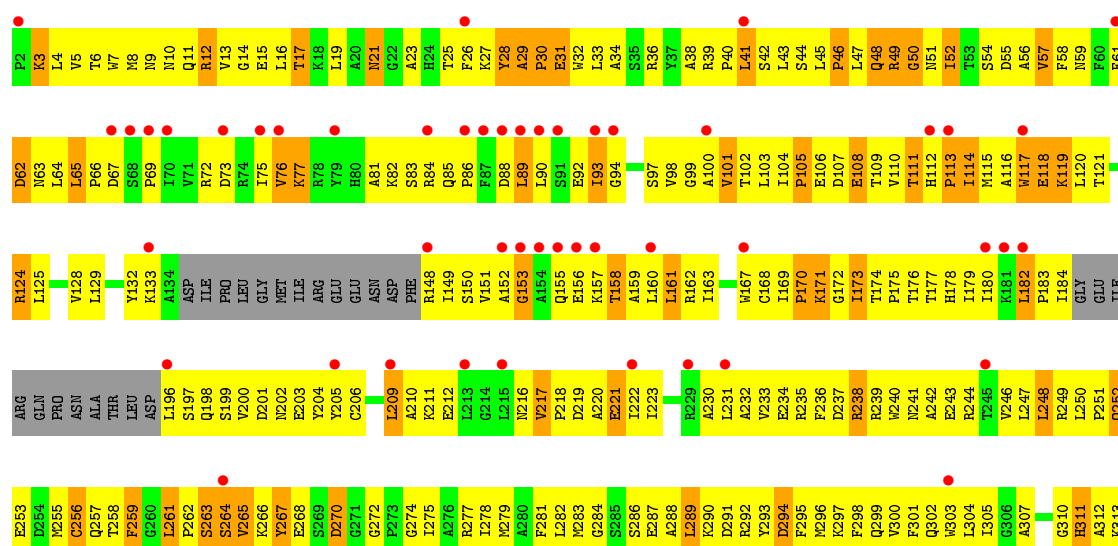


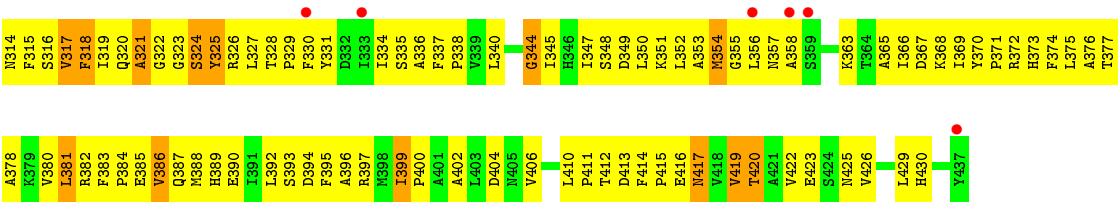
#### • Molecule 1: Antitoxin HipB



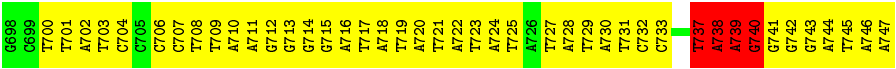
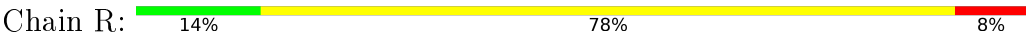


- Molecule 2: Serine/threonine-protein kinase HipA

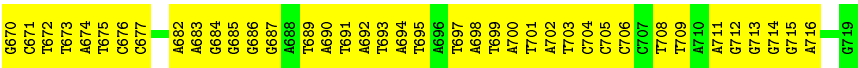
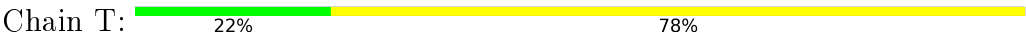




• Molecule 3: DNA (50-MER)



• Molecule 4: DNA (50-MER)





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	228.20 Å   228.20 Å   130.80 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	161.40 – 3.77 85.98 – 3.75	Depositor EDS
% Data completeness (in resolution range)	93.6 (161.40-3.77) 97.3 (85.98-3.75)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.64 (at 3.78 Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.384   ,   0.379 0.385   ,   0.381	Depositor DCC
$R_{free}$ test set	2894 reflections (8.38%)	DCC
Wilson B-factor (Å <sup>2</sup> )	157.6	Xtriage
Anisotropy	0.648	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 167.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.38$ , $\langle L^2 \rangle = 0.21$	Xtriage
Outliers	5 of 35034 reflections (0.014%)	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	10806	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	180.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.26% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	B	0.70	0/558	0.74	0/753
1	C	0.58	0/573	0.65	0/771
1	E	0.65	0/558	0.79	0/753
1	G	0.75	0/573	0.82	0/771
2	D	0.66	6/3348 (0.2%)	0.76	2/4535 (0.0%)
2	K	0.64	0/3328	0.76	0/4508
3	R	1.10	11/1146 (1.0%)	1.12	15/1767 (0.8%)
4	T	0.52	0/1147	0.73	0/1769
All	All	0.70	17/11231 (0.2%)	0.80	17/15627 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	D	0	2
3	R	0	4
All	All	0	6

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	R	738	DA	C5-C6	-13.42	1.28	1.41
2	D	147	PHE	CE1-CZ	12.80	1.61	1.37
3	R	738	DA	N9-C4	-11.10	1.31	1.37
3	R	739	DA	C5-C6	-11.03	1.31	1.41
3	R	738	DA	N1-C2	9.38	1.42	1.34
2	D	132	TYR	CD1-CE1	-7.74	1.27	1.39
3	R	739	DA	N9-C8	7.40	1.43	1.37
2	D	147	PHE	CE2-CZ	6.81	1.50	1.37
3	R	737	DT	C4-C5	6.47	1.50	1.45
3	R	739	DA	C2-N3	6.43	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	R	740	DG	C2-N3	6.41	1.37	1.32
3	R	738	DA	N3-C4	-6.11	1.31	1.34
3	R	738	DA	C6-N1	6.11	1.39	1.35
3	R	739	DA	C6-N1	5.77	1.39	1.35
2	D	132	TYR	CB-CG	-5.58	1.43	1.51
2	D	279	MET	CG-SD	-5.12	1.67	1.81
2	D	132	TYR	CD2-CE2	-5.09	1.31	1.39

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	R	738	DA	N1-C6-N6	11.69	125.61	118.60
3	R	739	DA	C5-C6-N6	-11.54	114.47	123.70
3	R	738	DA	C5-C6-N6	-9.85	115.82	123.70
3	R	739	DA	N1-C6-N6	8.52	123.71	118.60
3	R	739	DA	C5-C6-N1	8.10	121.75	117.70
3	R	740	DG	C1'-O4'-C4'	-7.94	102.16	110.10
2	D	129	LEU	CB-CA-C	-7.35	96.24	110.20
3	R	739	DA	C6-C5-N7	-6.52	127.74	132.30
3	R	738	DA	C6-C5-N7	-6.40	127.82	132.30
2	D	37	TYR	CB-CA-C	-6.37	97.66	110.40
3	R	738	DA	C2-N3-C4	-6.17	107.51	110.60
3	R	738	DA	O4'-C1'-C2'	6.06	110.75	105.90
3	R	739	DA	C4-C5-N7	6.02	113.71	110.70
3	R	738	DA	C6-N1-C2	-5.81	115.11	118.60
3	R	739	DA	C6-N1-C2	-5.67	115.20	118.60
3	R	738	DA	N3-C4-C5	5.57	130.70	126.80
3	R	740	DG	C2-N3-C4	-5.33	109.23	111.90

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	132	TYR	Sidechain
2	D	147	PHE	Sidechain
3	R	737	DT	Sidechain
3	R	738	DA	Sidechain
3	R	739	DA	Sidechain
3	R	740	DG	Sidechain

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	550	0	559	124	0
1	C	565	0	577	102	0
1	E	550	0	559	114	0
1	G	565	0	577	130	0
2	D	3275	0	3317	461	0
2	K	3256	0	3304	547	2
3	R	1022	0	568	86	0
4	T	1023	0	568	75	0
All	All	10806	0	10029	1505	2

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 72.

All (1505) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:8:MET:HB3	2:K:32:TRP:CH2	1.71	1.26
2:K:242:ALA:HB3	2:K:243:GLU:OE2	1.37	1.22
2:D:263:SER:O	2:D:266:LYS:HG2	1.45	1.16
1:E:21:ARG:HH22	1:E:27:THR:C	1.50	1.13
2:D:274:GLY:O	2:D:278:ILE:HG12	1.48	1.12
2:D:76:VAL:HG13	2:D:81:ALA:HB3	1.23	1.11
2:K:11:GLN:HB2	2:K:32:TRP:HZ3	1.12	1.11
2:K:111:THR:HG22	2:K:114:ILE:HD11	1.28	1.10
2:K:3:LYS:HD3	2:K:17:THR:HG23	1.25	1.10
2:D:308:THR:HG21	2:D:350:LEU:HD22	1.19	1.10
2:K:12:ARG:HG2	2:K:29:ALA:HB1	1.13	1.09
3:R:724:DA:H2"	3:R:725:DT:H5'	1.23	1.08
1:E:70:LEU:HD23	1:E:70:LEU:H	1.14	1.07
2:D:266:LYS:HE3	2:D:313:LYS:HD3	1.37	1.06
4:T:675:DT:H2"	4:T:676:DC:H5'	1.32	1.05
2:K:65:LEU:HD13	2:K:89:LEU:HD13	1.39	1.04
1:B:28:GLN:HE22	1:B:43:SER:HA	1.15	1.04
2:K:11:GLN:HB2	2:K:32:TRP:CZ3	1.90	1.04
3:R:702:DA:H2"	3:R:703:DT:H5"	1.39	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:4:LEU:HD21	2:D:91:SER:HA	1.36	1.03
1:E:35:ILE:HD11	1:E:37:ILE:HG12	1.39	1.03
2:D:308:THR:HG21	2:D:350:LEU:CD2	1.88	1.02
2:K:26:PHE:HB3	2:K:52:ILE:HG13	1.38	1.02
1:B:28:GLN:HE21	1:B:42:ILE:HG22	1.20	1.01
3:R:719:DT:H2"	3:R:720:DA:H5"	1.43	1.00
2:D:129:LEU:CD1	2:D:228:VAL:HG11	1.92	0.99
1:B:18:LYS:HA	1:B:21:ARG:HG2	1.43	0.99
1:G:58:PHE:HA	1:G:61:LEU:HD12	1.00	0.99
2:D:308:THR:CG2	2:D:350:LEU:HD22	1.91	0.99
2:D:117:TRP:HA	2:D:171:LYS:HD3	1.42	0.98
2:D:124:ARG:HB3	2:D:124:ARG:HH11	1.28	0.98
2:D:320:GLN:HB2	2:D:324:SER:OG	1.63	0.98
1:C:54:LEU:HD22	1:G:13:LEU:HD11	1.45	0.97
1:G:58:PHE:CA	1:G:61:LEU:HD12	1.95	0.97
3:R:730:DA:H2"	3:R:731:DT:H5"	1.43	0.97
2:K:12:ARG:HG2	2:K:29:ALA:CB	1.94	0.97
2:D:63:ASN:HD22	2:D:257:GLN:HG2	1.25	0.96
1:G:58:PHE:HA	1:G:61:LEU:CD1	1.94	0.96
2:K:26:PHE:HB3	2:K:52:ILE:CG1	1.95	0.96
2:K:289:LEU:HD12	2:K:289:LEU:H	1.30	0.96
3:R:703:DT:H2"	3:R:704:DC:H5'	1.47	0.96
2:K:365:ALA:HB3	2:K:368:LYS:HB2	1.45	0.95
1:C:10:PRO:HA	1:G:58:PHE:HE1	1.26	0.95
2:K:128:VAL:O	2:K:132:TYR:CE1	2.19	0.95
2:K:12:ARG:HH11	2:K:12:ARG:HB2	1.31	0.95
2:K:365:ALA:O	2:K:369:ILE:HG12	1.65	0.95
1:E:64:LEU:O	1:E:66:LEU:HD13	1.67	0.95
4:T:683:DA:H5"	1:C:51:ASN:HB3	1.46	0.95
2:K:12:ARG:HB3	2:K:31:GLU:CG	1.97	0.94
2:K:8:MET:HB3	2:K:32:TRP:CZ3	2.02	0.94
2:D:75:ILE:HG21	2:D:89:LEU:HD23	1.49	0.94
1:G:64:LEU:HB2	1:G:66:LEU:HD13	1.50	0.94
2:D:126:GLU:HB2	2:D:225:ALA:O	1.68	0.94
1:B:4:PHE:HA	1:E:70:LEU:HD21	1.50	0.94
2:D:258:THR:HG21	2:D:281:PHE:CE2	2.03	0.93
1:C:10:PRO:HA	1:G:58:PHE:CE1	2.03	0.93
2:D:147:PHE:CZ	2:D:149:ILE:HD12	2.02	0.93
2:D:279:MET:HA	2:D:282:LEU:HD12	1.48	0.93
2:K:8:MET:CB	2:K:32:TRP:CH2	2.51	0.93
2:D:244:ARG:HH11	2:D:244:ARG:HG2	1.33	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:279:MET:HA	2:D:282:LEU:CD1	1.99	0.93
2:K:27:LYS:N	2:K:52:ILE:HD11	1.84	0.92
1:B:7:ILE:HG22	1:B:8:TYR:H	1.32	0.92
2:D:38:ALA:HB1	2:D:47:LEU:HD11	1.48	0.92
2:D:263:SER:HB2	2:D:266:LYS:NZ	1.84	0.92
1:G:64:LEU:HD13	1:G:66:LEU:HD22	1.51	0.92
2:D:16:LEU:HD22	2:D:61:PHE:CE2	2.04	0.91
2:D:258:THR:HG21	2:D:281:PHE:HE2	1.33	0.91
2:D:3:LYS:HG2	2:D:17:THR:HG23	1.52	0.91
3:R:719:DT:H3	4:T:700:DA:H2	1.19	0.91
2:K:5:VAL:HG13	2:K:15:GLU:HG3	1.52	0.90
1:B:12:GLN:O	1:B:15:ASN:ND2	2.03	0.90
1:E:21:ARG:NH2	1:E:27:THR:C	2.24	0.90
2:K:160:LEU:CD2	2:K:161:LEU:H	1.84	0.90
1:E:21:ARG:HH22	1:E:28:GLN:N	1.68	0.90
2:D:130:THR:HA	2:D:133:LYS:HD3	1.53	0.90
2:K:266:LYS:HB2	2:K:311:HIS:HB2	1.53	0.90
2:K:12:ARG:HD2	2:K:31:GLU:OE1	1.71	0.90
4:T:705:DC:H1'	4:T:706:DC:H5'	1.53	0.90
2:D:263:SER:HB2	2:D:266:LYS:HZ3	1.35	0.90
1:C:69:THR:HA	1:G:7:ILE:HD12	1.53	0.90
2:K:16:LEU:HD12	2:K:17:THR:H	1.35	0.89
2:D:4:LEU:HD13	2:D:103:LEU:HD13	1.52	0.89
1:E:8:TYR:H	1:E:12:GLN:NE2	1.71	0.89
2:K:128:VAL:O	2:K:132:TYR:HE1	1.55	0.89
2:D:69:PRO:HD2	2:D:70:ILE:HD12	1.54	0.88
2:K:151:VAL:HG12	2:K:157:LYS:HG3	1.55	0.88
1:E:21:ARG:HG3	1:E:22:GLN:N	1.85	0.88
1:B:21:ARG:HH21	1:B:28:GLN:N	1.70	0.88
2:K:299:GLN:HA	2:K:302:GLN:HE21	1.39	0.87
1:G:29:SER:HB2	1:G:39:GLN:HG3	1.57	0.87
2:D:345:ILE:H	2:D:345:ILE:HD12	1.38	0.87
2:D:76:VAL:CG1	2:D:81:ALA:HB3	2.05	0.87
2:D:254:ASP:HA	2:D:316:SER:HA	1.55	0.87
1:G:58:PHE:O	1:G:61:LEU:HB2	1.75	0.87
2:K:411:PRO:HG2	2:K:414:PHE:HB2	1.55	0.87
2:K:12:ARG:CD	2:K:31:GLU:OE1	2.23	0.87
1:B:28:GLN:NE2	1:B:42:ILE:HG22	1.90	0.87
2:K:120:LEU:HD11	2:K:169:ILE:HG13	1.55	0.87
2:K:256:CYS:HA	2:K:261:LEU:HD12	1.56	0.87
2:D:318:PHE:CE1	2:D:328:THR:HB	2.10	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:17:MET:HE3	1:G:61:LEU:HG	1.56	0.86
1:G:64:LEU:CD1	1:G:66:LEU:HD22	2.04	0.86
2:K:298:PHE:O	2:K:301:PHE:HB3	1.76	0.86
2:D:352:LEU:HG	2:D:366:ILE:HG12	1.55	0.86
2:D:279:MET:CE	2:D:295:PHE:HD2	1.88	0.86
2:D:382:ARG:HH11	2:D:382:ARG:HB2	1.40	0.86
2:D:71:VAL:O	2:D:75:ILE:HD12	1.74	0.86
2:D:278:ILE:O	2:D:282:LEU:HG	1.75	0.85
2:K:3:LYS:HG2	2:K:17:THR:HA	1.56	0.85
1:B:66:LEU:HD23	1:B:67:SER:H	1.40	0.85
2:K:161:LEU:HD13	2:K:176:THR:HA	1.57	0.85
2:K:371:PRO:HB3	2:K:392:LEU:HD11	1.58	0.85
2:K:238:ARG:HD3	2:K:249:ARG:HG2	1.59	0.84
2:K:65:LEU:HD12	2:K:72:ARG:NH1	1.92	0.84
2:K:12:ARG:HB3	2:K:31:GLU:HG3	1.59	0.84
1:B:35:ILE:HG23	1:B:63:SER:HB2	1.58	0.84
1:G:31:LEU:HD13	1:G:63:SER:HB2	1.58	0.84
3:R:723:DT:H1'	3:R:724:DA:H5''	1.56	0.84
1:B:61:LEU:HD13	1:B:67:SER:HA	1.57	0.83
2:K:350:LEU:O	2:K:366:ILE:HD13	1.78	0.83
3:R:730:DA:C2'	3:R:731:DT:H5''	2.08	0.83
1:C:7:ILE:HD13	1:G:69:THR:HA	1.59	0.83
2:D:72:ARG:HA	2:D:75:ILE:HD13	1.58	0.83
1:B:21:ARG:NH2	1:B:28:GLN:HG3	1.94	0.82
1:C:8:TYR:CE2	2:K:286:SER:HA	2.14	0.82
2:D:129:LEU:HD12	2:D:228:VAL:HG11	1.58	0.82
2:D:39:ARG:HD3	2:D:319:ILE:HG22	1.61	0.82
1:G:54:LEU:O	1:G:57:PHE:HB3	1.78	0.82
4:T:697:DT:H1'	4:T:698:DA:H5'	1.61	0.82
2:D:279:MET:HE1	2:D:296:MET:SD	2.19	0.82
2:K:317:VAL:HG11	2:K:325:TYR:HB2	1.58	0.82
1:B:12:GLN:HA	1:B:15:ASN:HD21	1.44	0.82
2:D:377:THR:O	2:D:380:VAL:HG22	1.78	0.82
1:E:8:TYR:H	1:E:12:GLN:HE22	1.27	0.82
2:K:13:VAL:HG11	2:K:41:LEU:HD11	1.61	0.82
2:K:7:TRP:HE1	2:K:12:ARG:NH1	1.78	0.82
2:K:325:TYR:CD1	2:K:325:TYR:N	2.47	0.82
2:D:16:LEU:HD13	2:D:61:PHE:CZ	2.14	0.82
2:K:340:LEU:HD23	2:K:345:ILE:O	1.79	0.82
1:E:21:ARG:NH2	1:E:28:GLN:N	2.27	0.81
1:B:44:ASN:HD22	1:B:45:PHE:N	1.79	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:62:GLN:NE2	2:D:288:ALA:HB3	1.95	0.81
2:K:97:SER:HB3	2:K:101:VAL:O	1.79	0.81
1:E:70:LEU:CD2	1:E:70:LEU:H	1.94	0.81
2:K:16:LEU:HD12	2:K:17:THR:N	1.95	0.81
2:D:179:ILE:HB	2:D:233:VAL:HB	1.62	0.80
1:B:51:ASN:O	4:T:711:DA:H5''	1.81	0.80
1:E:35:ILE:HG13	1:E:36:GLY:H	1.46	0.80
2:D:4:LEU:HB3	2:D:103:LEU:HD22	1.61	0.80
1:B:18:LYS:HA	1:B:21:ARG:CG	2.11	0.80
1:C:66:LEU:HB3	1:G:70:LEU:HD22	1.62	0.79
2:K:27:LYS:HG2	2:K:28:TYR:N	1.95	0.79
1:B:52:THR:O	1:E:54:LEU:HB2	1.81	0.79
1:G:62:GLN:HA	1:G:62:GLN:OE1	1.82	0.79
1:B:14:ALA:HB2	1:B:49:PRO:HG3	1.63	0.79
2:K:27:LYS:HG2	2:K:28:TYR:H	1.47	0.79
2:D:89:LEU:O	2:D:93:ILE:HG12	1.83	0.79
2:D:255:MET:HE2	2:D:278:ILE:HD13	1.64	0.79
2:K:203:GLU:HB3	2:K:231:LEU:HD21	1.63	0.78
2:K:13:VAL:C	2:K:29:ALA:HB3	2.04	0.78
4:T:683:DA:H1'	4:T:684:DG:H5'	1.64	0.78
2:D:63:ASN:ND2	2:D:257:GLN:HG2	1.97	0.78
1:C:10:PRO:HG3	1:G:58:PHE:HD1	1.46	0.78
2:K:203:GLU:HA	2:K:206:CYS:SG	2.23	0.78
2:K:296:MET:O	2:K:299:GLN:HB2	1.83	0.78
2:K:175:PRO:HG3	2:K:249:ARG:CZ	2.13	0.78
1:B:28:GLN:HE22	1:B:43:SER:CA	1.96	0.78
2:D:54:SER:O	2:D:57:VAL:HG23	1.84	0.78
2:D:208:LEU:HD22	2:D:406:VAL:HG13	1.66	0.78
2:D:262:PRO:HG2	2:D:264:SER:OG	1.82	0.77
2:K:93:ILE:H	2:K:93:ILE:HD13	1.47	0.77
2:K:200:VAL:HA	2:K:231:LEU:HD22	1.65	0.77
1:B:7:ILE:HG21	1:B:13:LEU:HD23	1.64	0.77
1:C:58:PHE:CE1	1:G:13:LEU:HD12	2.18	0.77
2:D:203:GLU:HG2	2:D:231:LEU:HD21	1.65	0.77
2:K:241:ASN:ND2	2:K:246:VAL:H	1.82	0.77
3:R:730:DA:H2''	3:R:731:DT:C5'	2.11	0.77
4:T:675:DT:C2'	4:T:676:DC:H5'	2.13	0.77
2:D:266:LYS:CE	2:D:313:LYS:HD3	2.13	0.77
2:K:125:LEU:HD11	2:K:167:TRP:HB2	1.67	0.77
1:B:7:ILE:HG22	1:B:8:TYR:N	1.99	0.76
1:G:20:VAL:O	1:G:24:ASN:OD1	2.02	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:740:DG:OP1	1:G:53:THR:N	2.18	0.76
1:B:35:ILE:HG21	1:B:59:LYS:O	1.85	0.76
1:E:53:THR:HB	1:E:56:THR:OG1	1.85	0.76
1:E:70:LEU:HD23	1:E:70:LEU:N	1.98	0.76
2:D:100:ALA:HB3	2:D:251:PRO:HG3	1.65	0.76
2:D:179:ILE:O	2:D:232:ALA:HA	1.85	0.76
1:E:35:ILE:HG13	1:E:36:GLY:N	2.00	0.76
1:B:8:TYR:O	1:E:58:PHE:CD2	2.38	0.76
1:C:10:PRO:CA	1:G:58:PHE:CE1	2.68	0.76
2:K:84:ARG:O	2:K:89:LEU:HD12	1.86	0.76
1:B:12:GLN:CA	1:B:15:ASN:HD21	1.99	0.76
3:R:713:DG:H2''	3:R:714:DG:H5'	1.68	0.76
2:D:23:ALA:N	2:K:23:ALA:HB2	2.01	0.75
2:D:65:LEU:HD11	2:D:90:LEU:HG	1.67	0.75
3:R:740:DG:OP1	1:G:52:THR:HA	1.85	0.75
2:D:103:LEU:O	2:D:104:ILE:HD13	1.85	0.75
2:K:242:ALA:CB	2:K:243:GLU:OE2	2.27	0.75
1:G:55:THR:HB	1:G:59:LYS:HE3	1.67	0.75
2:D:178:HIS:HD2	2:D:232:ALA:HB1	1.52	0.75
3:R:737:DT:H1'	3:R:738:DA:O5'	1.87	0.74
2:D:266:LYS:HE3	2:D:313:LYS:CD	2.15	0.74
1:G:54:LEU:HD22	1:G:57:PHE:HD2	1.51	0.74
2:K:300:VAL:HG22	2:K:374:PHE:CD2	2.21	0.74
1:C:69:THR:HA	1:G:7:ILE:CD1	2.18	0.74
1:C:53:THR:CG2	1:G:51:ASN:HA	2.16	0.74
2:D:49:ARG:H	1:E:22:GLN:NE2	1.85	0.74
2:K:266:LYS:HG3	2:K:267:TYR:HD1	1.52	0.74
2:K:221:GLU:O	2:K:232:ALA:HB3	1.87	0.74
2:K:356:LEU:HD23	2:K:356:LEU:H	1.53	0.74
2:D:356:LEU:HB2	2:D:363:LYS:O	1.87	0.74
1:C:10:PRO:CA	1:G:58:PHE:HE1	2.01	0.74
1:C:53:THR:HG21	1:G:51:ASN:HA	1.70	0.74
2:K:206:CYS:O	2:K:210:ALA:HB2	1.88	0.74
2:K:160:LEU:HD23	2:K:161:LEU:H	1.53	0.74
2:K:237:ASP:HA	2:K:250:LEU:HB2	1.68	0.74
4:T:684:DG:H2''	4:T:685:DG:OP2	1.88	0.73
1:B:21:ARG:HH21	1:B:28:GLN:H	1.32	0.73
2:K:377:THR:O	2:K:380:VAL:HG22	1.86	0.73
2:D:237:ASP:OD1	2:D:238:ARG:HG2	1.88	0.73
4:T:711:DA:H2''	4:T:712:DG:C8	2.24	0.73
1:E:21:ARG:HH22	1:E:27:THR:CA	2.02	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:116:ALA:O	2:K:171:LYS:HB2	1.88	0.73
2:K:209:LEU:HB2	2:K:406:VAL:HG21	1.70	0.73
2:D:279:MET:CE	2:D:296:MET:SD	2.77	0.73
2:D:279:MET:HE1	2:D:295:PHE:HD2	1.54	0.73
2:K:288:ALA:O	2:K:292:ARG:HG3	1.88	0.73
1:B:11:THR:O	1:B:15:ASN:OD1	2.07	0.73
1:C:28:GLN:HE21	1:C:42:ILE:HG22	1.54	0.73
2:D:256:CYS:SG	2:D:312:ALA:HB1	2.29	0.72
2:K:13:VAL:C	2:K:29:ALA:CB	2.57	0.72
2:D:286:SER:HA	1:E:8:TYR:CG	2.24	0.72
2:K:9:ASN:O	2:K:10:ASN:HB2	1.89	0.72
2:D:77:LYS:HB2	2:K:264:SER:HB3	1.72	0.72
1:E:14:ALA:HB2	1:E:49:PRO:HG3	1.72	0.72
2:D:99:GLY:O	2:D:101:VAL:HG23	1.90	0.72
1:C:10:PRO:HG3	1:G:58:PHE:CD1	2.24	0.72
1:B:68:MET:HE3	1:E:7:ILE:HB	1.72	0.72
2:K:279:MET:HE1	2:K:296:MET:SD	2.30	0.72
1:B:5:GLN:HG3	1:B:6:LYS:H	1.55	0.72
1:G:45:PHE:HD1	1:G:52:THR:HG1	1.38	0.72
1:G:64:LEU:HB2	1:G:66:LEU:CD1	2.20	0.72
1:C:68:MET:O	1:G:7:ILE:HB	1.90	0.72
1:B:16:ALA:O	1:B:19:LEU:HB3	1.89	0.72
2:K:13:VAL:O	2:K:29:ALA:N	2.23	0.72
2:K:28:TYR:HD1	2:K:48:GLN:O	1.72	0.71
1:B:7:ILE:O	1:B:8:TYR:CG	2.43	0.71
2:K:3:LYS:CD	2:K:17:THR:HG23	2.13	0.71
2:D:331:TYR:O	2:D:333:ILE:HD12	1.91	0.71
2:K:247:LEU:C	2:K:247:LEU:HD23	2.11	0.71
2:K:237:ASP:C	2:K:250:LEU:HG	2.11	0.71
3:R:702:DA:C2'	3:R:703:DT:H5''	2.17	0.71
4:T:715:DG:H1'	4:T:716:DA:H5'	1.71	0.71
2:D:295:PHE:O	2:D:299:GLN:HG2	1.91	0.71
2:K:161:LEU:HD12	2:K:177:THR:HG23	1.72	0.71
1:E:5:GLN:O	1:E:7:ILE:HD12	1.91	0.71
2:K:5:VAL:HG12	2:K:6:THR:N	2.06	0.71
1:E:7:ILE:HG23	1:E:12:GLN:HB3	1.73	0.70
2:D:126:GLU:CB	2:D:225:ALA:O	2.39	0.70
2:D:274:GLY:O	2:D:278:ILE:CG1	2.36	0.70
2:K:217:VAL:HG12	2:K:330:PHE:O	1.91	0.70
2:K:160:LEU:HD23	2:K:161:LEU:N	2.06	0.70
1:B:8:TYR:O	1:E:58:PHE:HD2	1.75	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:65:LEU:HD12	2:K:72:ARG:HH12	1.55	0.70
1:G:35:ILE:HG13	1:G:36:GLY:N	2.07	0.70
2:K:419:VAL:O	2:K:423:GLU:HB2	1.92	0.69
2:K:320:GLN:OE1	2:K:326:ARG:HD3	1.93	0.69
2:K:311:HIS:CE1	2:K:314:ASN:ND2	2.59	0.69
2:D:133:LYS:HA	2:D:156:GLU:HG2	1.72	0.69
2:K:289:LEU:HD12	2:K:289:LEU:N	2.05	0.69
2:K:241:ASN:HD21	2:K:246:VAL:H	1.40	0.69
3:R:724:DA:H2''	3:R:725:DT:C5'	2.12	0.69
2:D:263:SER:CB	2:D:266:LYS:NZ	2.56	0.69
2:D:291:ASP:OD1	2:D:327:LEU:HB3	1.92	0.69
2:K:162:ARG:HB2	2:K:167:TRP:CZ3	2.27	0.69
2:K:340:LEU:HD11	2:K:350:LEU:HD11	1.75	0.69
1:B:68:MET:CE	1:E:7:ILE:HB	2.22	0.69
2:K:237:ASP:O	2:K:250:LEU:N	2.18	0.69
1:G:37:ILE:HD12	1:G:38:LYS:O	1.92	0.69
1:B:62:GLN:CD	2:D:288:ALA:HB3	2.13	0.68
2:D:5:VAL:HG11	2:D:12:ARG:NH1	2.08	0.68
1:E:57:PHE:CE2	1:E:61:LEU:HD12	2.28	0.68
2:D:117:TRP:HB2	2:D:168:CYS:HB3	1.75	0.68
2:D:365:ALA:O	2:D:369:ILE:HG12	1.93	0.68
3:R:742:DG:H2''	3:R:743:DG:O5'	1.92	0.68
1:G:62:GLN:CA	1:G:62:GLN:OE1	2.42	0.68
1:E:45:PHE:CD1	1:E:49:PRO:HB3	2.27	0.68
2:K:33:LEU:HD12	2:K:34:ALA:N	2.08	0.68
1:C:13:LEU:HD11	1:C:57:PHE:CZ	2.28	0.68
2:K:108:GLU:O	2:K:110:VAL:HG23	1.94	0.68
2:K:380:VAL:HG23	2:K:381:LEU:HG	1.75	0.68
2:D:160:LEU:HD21	2:D:169:ILE:HG12	1.76	0.68
3:R:715:DG:N2	4:T:705:DC:H42	1.92	0.68
2:D:320:GLN:NE2	2:D:324:SER:HB2	2.09	0.67
2:D:7:TRP:HB2	2:D:102:THR:OG1	1.93	0.67
1:G:54:LEU:CD2	1:G:57:PHE:HD2	2.07	0.67
1:E:45:PHE:CD2	1:E:60:ILE:HD13	2.29	0.67
1:B:62:GLN:C	1:B:64:LEU:H	1.98	0.67
2:D:255:MET:CE	2:D:278:ILE:HA	2.23	0.67
2:D:422:VAL:O	2:D:426:VAL:HG23	1.94	0.67
1:B:4:PHE:HA	1:E:70:LEU:CD2	2.24	0.67
2:K:388:MET:CE	2:K:392:LEU:HB2	2.25	0.67
1:B:7:ILE:O	1:B:8:TYR:CD1	2.47	0.67
1:E:65:GLU:O	1:E:66:LEU:HD12	1.93	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:35:ILE:HG13	1:G:36:GLY:H	1.58	0.67
1:B:12:GLN:C	1:B:15:ASN:HD21	1.97	0.67
2:D:99:GLY:O	2:D:101:VAL:N	2.22	0.67
1:E:49:PRO:HA	1:E:52:THR:OG1	1.94	0.67
1:B:21:ARG:HD3	1:B:46:GLU:OE2	1.94	0.67
2:K:237:ASP:O	2:K:238:ARG:HG2	1.94	0.67
2:K:238:ARG:N	2:K:250:LEU:HG	2.09	0.67
4:T:683:DA:C2'	4:T:684:DG:H5'	2.25	0.66
2:D:126:GLU:OE1	2:D:227:ASN:ND2	2.27	0.66
2:K:394:ASP:O	2:K:397:ARG:HG3	1.94	0.66
2:D:75:ILE:CG2	2:D:89:LEU:HD23	2.24	0.66
2:D:244:ARG:NH1	2:D:244:ARG:HG2	2.05	0.66
2:D:68:SER:OG	2:D:70:ILE:HD13	1.94	0.66
1:G:64:LEU:HD13	1:G:66:LEU:CD2	2.23	0.66
2:K:14:GLY:N	2:K:29:ALA:HB2	2.11	0.66
1:C:8:TYR:CD2	2:K:286:SER:HA	2.30	0.66
2:K:358:ALA:HB2	2:K:363:LYS:H	1.60	0.66
2:D:238:ARG:NH2	2:D:249:ARG:HD3	2.11	0.66
1:B:41:THR:HG22	1:B:42:ILE:N	2.11	0.66
2:K:397:ARG:O	2:K:400:PRO:HD2	1.95	0.66
3:R:737:DT:H2"	3:R:738:DA:OP2	1.95	0.66
2:D:388:MET:HE3	2:D:391:ILE:HD12	1.77	0.66
2:K:304:LEU:O	2:K:429:LEU:HD12	1.95	0.66
2:D:70:ILE:H	2:D:70:ILE:HD12	1.61	0.66
2:D:209:LEU:HG	2:D:213:LEU:HD11	1.77	0.66
2:D:253:GLU:OE1	2:D:258:THR:HA	1.96	0.66
2:K:292:ARG:HH11	2:K:292:ARG:HG2	1.60	0.66
3:R:715:DG:H1'	3:R:716:DA:H5'	1.78	0.66
2:K:352:LEU:HD22	2:K:354:MET:O	1.96	0.65
1:E:57:PHE:HE2	1:E:61:LEU:HD12	1.62	0.65
2:K:290:LYS:HE2	2:K:294:ASP:OD2	1.97	0.65
2:D:305:ILE:HD11	2:D:307:ALA:HB2	1.77	0.65
1:E:60:ILE:O	1:E:64:LEU:HG	1.97	0.65
1:G:54:LEU:CD2	1:G:57:PHE:CD2	2.79	0.65
2:D:98:VAL:HG12	2:D:252:GLN:NE2	2.11	0.65
2:K:106:GLU:HG2	2:K:106:GLU:O	1.96	0.65
2:K:128:VAL:O	2:K:132:TYR:CD1	2.49	0.65
2:D:100:ALA:CB	2:D:251:PRO:HG3	2.25	0.65
2:K:284:GLY:O	2:K:325:TYR:CZ	2.49	0.65
2:K:300:VAL:HG22	2:K:374:PHE:CE2	2.31	0.65
2:K:7:TRP:CD1	2:K:12:ARG:HA	2.31	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:289:LEU:CD1	2:K:289:LEU:H	2.03	0.65
2:K:314:ASN:HA	2:K:331:TYR:CE1	2.32	0.65
2:K:217:VAL:HG12	2:K:218:PRO:HD2	1.78	0.65
1:C:57:PHE:O	1:C:61:LEU:HB2	1.96	0.65
1:B:24:ASN:HB3	1:B:26:TRP:CE3	2.32	0.64
1:B:44:ASN:ND2	1:B:45:PHE:N	2.45	0.64
2:D:16:LEU:HD22	2:D:61:PHE:HE2	1.58	0.64
2:D:8:MET:SD	2:D:251:PRO:HG2	2.36	0.64
2:K:54:SER:O	2:K:57:VAL:CG2	2.46	0.64
2:K:5:VAL:HG12	2:K:6:THR:H	1.61	0.64
2:D:124:ARG:O	2:D:128:VAL:HG23	1.97	0.64
2:D:279:MET:SD	2:D:295:PHE:CD2	2.90	0.64
2:D:284:GLY:CA	1:E:9:SER:HB2	2.28	0.64
2:K:6:THR:O	2:K:13:VAL:HB	1.98	0.64
4:T:683:DA:H2''	4:T:684:DG:H5'	1.79	0.64
2:K:8:MET:HG2	2:K:32:TRP:CH2	2.32	0.64
2:D:72:ARG:O	2:D:75:ILE:HB	1.97	0.64
2:K:8:MET:CG	2:K:32:TRP:CH2	2.80	0.64
2:K:258:THR:HB	2:K:259:PHE:CE1	2.32	0.64
1:B:42:ILE:HD11	1:B:60:ILE:HG12	1.80	0.64
2:D:147:PHE:CE1	2:D:149:ILE:HD12	2.31	0.64
2:D:40:PRO:HB3	2:D:46:PRO:HA	1.80	0.64
1:E:10:PRO:O	1:E:13:LEU:HB2	1.97	0.64
1:E:27:THR:OG1	1:E:30:GLU:HG2	1.97	0.64
2:K:169:ILE:HG23	2:K:170:PRO:HD2	1.78	0.64
4:T:683:DA:C1'	4:T:684:DG:H5'	2.28	0.64
1:C:12:GLN:HE22	2:K:324:SER:HA	1.62	0.64
2:D:18:LYS:HE2	2:D:22:GLY:HA2	1.80	0.64
2:D:132:TYR:OH	2:D:147:PHE:CD1	2.51	0.64
2:D:175:PRO:HG3	2:D:249:ARG:CZ	2.28	0.64
1:E:28:GLN:O	1:E:42:ILE:HG21	1.98	0.64
2:D:159:ALA:HA	2:D:180:ILE:HD12	1.80	0.64
2:K:372:ARG:HA	2:K:375:LEU:CD1	2.28	0.64
4:T:703:DT:H2''	4:T:704:DC:H5'	1.80	0.64
2:K:262:PRO:O	2:K:265:VAL:HG22	1.98	0.64
2:K:399:ILE:HG22	2:K:400:PRO:CD	2.27	0.64
2:D:327:LEU:HD21	2:D:330:PHE:CZ	2.33	0.63
2:D:117:TRP:CA	2:D:171:LYS:HD3	2.22	0.63
2:K:241:ASN:OD1	2:K:243:GLU:HG2	1.98	0.63
2:K:375:LEU:O	2:K:378:ALA:HB3	1.98	0.63
2:K:3:LYS:HB2	2:K:3:LYS:NZ	2.13	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:54:LEU:HD22	1:G:13:LEU:CD1	2.25	0.63
2:D:132:TYR:O	2:D:156:GLU:OE2	2.17	0.63
2:K:340:LEU:HD22	2:K:347:ILE:HA	1.80	0.63
4:T:686:DG:H2''	4:T:687:DG:O5'	1.98	0.63
2:D:210:ALA:HB3	2:D:217:VAL:HG21	1.81	0.63
1:G:17:MET:O	1:G:20:VAL:HB	1.98	0.63
2:K:41:LEU:HD22	2:K:41:LEU:H	1.62	0.63
2:D:181:LYS:C	2:D:182:LEU:HD22	2.19	0.63
2:D:65:LEU:HD13	2:D:89:LEU:HB2	1.80	0.63
2:K:274:GLY:O	2:K:278:ILE:CG1	2.47	0.63
3:R:742:DG:OP1	2:K:382:ARG:HD3	1.99	0.63
2:D:388:MET:O	2:D:392:LEU:HG	1.98	0.63
2:D:337:PHE:HD1	2:D:422:VAL:HA	1.64	0.63
2:D:76:VAL:HA	2:D:81:ALA:CB	2.28	0.63
1:E:29:SER:HA	1:E:39:GLN:HG2	1.78	0.63
1:E:53:THR:O	1:E:56:THR:HB	1.99	0.63
2:K:11:GLN:CB	2:K:32:TRP:CZ3	2.77	0.63
2:K:82:LYS:HD2	2:K:88:ASP:OD1	1.99	0.63
2:D:279:MET:CE	2:D:295:PHE:CD2	2.76	0.62
2:K:12:ARG:HH11	2:K:12:ARG:CB	2.08	0.62
2:K:63:ASN:HB2	2:K:257:GLN:HE21	1.65	0.62
2:D:147:PHE:CE1	2:D:149:ILE:HG13	2.34	0.62
2:D:79:TYR:HB3	2:D:92:GLU:OE2	1.99	0.62
2:K:103:LEU:O	2:K:104:ILE:HG12	1.98	0.62
2:D:337:PHE:N	2:D:338:PRO:CD	2.62	0.62
1:E:21:ARG:CG	1:E:22:GLN:N	2.61	0.62
2:K:220:ALA:HB1	2:K:232:ALA:O	2.00	0.62
2:D:130:THR:HA	2:D:133:LYS:CD	2.28	0.62
1:C:61:LEU:HD11	1:G:70:LEU:CD2	2.29	0.62
1:C:61:LEU:HD11	1:G:70:LEU:HD21	1.81	0.62
2:D:65:LEU:HD22	2:D:93:ILE:HD11	1.82	0.62
1:B:21:ARG:NH2	1:B:28:GLN:H	1.97	0.62
2:K:15:GLU:N	2:K:15:GLU:OE2	2.28	0.62
2:K:237:ASP:CB	2:K:252:GLN:HG2	2.30	0.62
4:T:713:DG:H3'	4:T:713:DG:OP1	2.00	0.62
1:B:30:GLU:O	1:B:33:LYS:HB2	2.00	0.62
1:B:28:GLN:NE2	1:B:43:SER:HA	2.01	0.62
1:C:20:VAL:O	1:C:24:ASN:HB2	1.99	0.62
2:D:382:ARG:NH1	2:D:382:ARG:HB2	2.15	0.62
2:K:301:PHE:CE1	2:K:305:ILE:HG21	2.34	0.62
2:K:295:PHE:HE1	2:K:315:PHE:CE1	2.18	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:399:ILE:HG22	2:K:400:PRO:HD3	1.82	0.62
1:B:53:THR:HG22	4:T:712:DG:OP1	2.00	0.61
2:D:45:LEU:HD21	2:D:57:VAL:HA	1.81	0.61
1:G:32:ALA:HA	1:G:35:ILE:HD11	1.82	0.61
2:K:120:LEU:HD21	2:K:169:ILE:HG13	1.82	0.61
2:K:7:TRP:HD1	2:K:12:ARG:HA	1.65	0.61
2:D:202:ASN:HD22	2:D:338:PRO:HG2	1.65	0.61
2:D:76:VAL:HG11	2:K:262:PRO:HG3	1.81	0.61
2:K:40:PRO:HD3	2:K:47:LEU:HG	1.80	0.61
2:D:65:LEU:HD21	2:D:90:LEU:CD2	2.31	0.61
1:G:42:ILE:O	1:G:45:PHE:HB3	2.01	0.61
2:K:390:GLU:O	2:K:393:SER:HB3	2.00	0.61
2:D:126:GLU:O	2:D:126:GLU:HG2	2.01	0.61
2:D:331:TYR:C	2:D:333:ILE:HD12	2.21	0.61
1:G:5:GLN:CD	1:G:5:GLN:H	2.03	0.61
2:D:279:MET:SD	2:D:295:PHE:CE2	2.93	0.61
3:R:730:DA:C1'	3:R:731:DT:H5''	2.31	0.61
1:B:61:LEU:HB3	1:B:66:LEU:O	2.01	0.61
2:D:79:TYR:O	2:D:92:GLU:OE1	2.19	0.61
2:K:253:GLU:HG2	2:K:319:ILE:HD11	1.82	0.61
2:D:21:ASN:O	2:K:23:ALA:HA	2.01	0.61
2:D:244:ARG:CG	2:D:244:ARG:HH11	2.10	0.61
2:D:76:VAL:HG13	2:D:81:ALA:CB	2.15	0.61
1:C:70:LEU:HD22	1:G:66:LEU:HD23	1.82	0.61
2:K:237:ASP:C	2:K:250:LEU:H	2.03	0.61
2:D:200:VAL:HG13	2:D:231:LEU:HB2	1.83	0.60
2:D:83:SER:OG	2:D:85:GLN:HB2	2.00	0.60
2:K:161:LEU:CD1	2:K:177:THR:HG23	2.30	0.60
3:R:723:DT:C1'	3:R:724:DA:H5''	2.30	0.60
2:D:147:PHE:CZ	2:D:149:ILE:CD1	2.83	0.60
2:D:63:ASN:HB3	2:D:313:LYS:NZ	2.17	0.60
2:D:66:PRO:HA	2:D:152:ALA:HA	1.83	0.60
2:K:14:GLY:CA	2:K:29:ALA:H	2.13	0.60
2:K:304:LEU:HD23	2:K:429:LEU:HB3	1.82	0.60
3:R:724:DA:C2'	3:R:725:DT:H5'	2.16	0.60
3:R:730:DA:H1'	3:R:731:DT:H5''	1.82	0.60
2:D:151:VAL:HG12	2:D:157:LYS:HE3	1.84	0.60
2:D:284:GLY:HA2	1:E:8:TYR:O	2.02	0.60
2:D:124:ARG:HA	2:D:127:GLU:HB3	1.82	0.60
2:D:147:PHE:CE1	2:D:149:ILE:CG1	2.85	0.60
2:D:161:LEU:HD12	2:D:177:THR:HG23	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:316:SER:O	2:D:328:THR:HG23	2.02	0.60
1:G:61:LEU:HA	1:G:64:LEU:HD12	1.84	0.60
2:K:240:TRP:CE2	2:K:247:LEU:HD12	2.36	0.60
2:K:42:SER:O	2:K:45:LEU:N	2.28	0.60
2:K:52:ILE:HD13	2:K:52:ILE:N	2.16	0.60
4:T:701:DT:H72	4:T:702:DA:H62	1.66	0.60
1:C:28:GLN:NE2	1:C:42:ILE:HG22	2.17	0.60
2:D:311:HIS:H	2:D:314:ASN:ND2	2.00	0.60
2:K:202:ASN:ND2	2:K:338:PRO:HG2	2.17	0.60
2:K:99:GLY:HA2	2:K:252:GLN:HG3	1.83	0.60
2:D:169:ILE:HG23	2:D:170:PRO:HD2	1.84	0.60
1:G:31:LEU:CD2	1:G:34:LYS:HD2	2.32	0.60
3:R:701:DT:C2	3:R:702:DA:C5	2.89	0.60
2:D:98:VAL:HG12	2:D:252:GLN:HE22	1.66	0.60
2:K:149:ILE:HD11	2:K:170:PRO:HG3	1.84	0.60
2:K:202:ASN:O	2:K:206:CYS:SG	2.57	0.60
1:C:21:ARG:HH22	1:C:28:GLN:H	1.49	0.60
2:D:74:ARG:NH1	2:D:156:GLU:OE2	2.34	0.60
2:K:305:ILE:HG13	2:K:307:ALA:H	1.67	0.60
2:K:180:ILE:HG23	2:K:223:ILE:CD1	2.31	0.59
1:G:58:PHE:O	1:G:61:LEU:N	2.35	0.59
2:K:162:ARG:HD3	2:K:167:TRP:CH2	2.37	0.59
2:D:318:PHE:O	2:D:319:ILE:HD13	2.02	0.59
2:D:61:PHE:HA	2:D:64:LEU:CD1	2.32	0.59
2:D:65:LEU:HD21	2:D:90:LEU:HD23	1.84	0.59
2:D:85:GLN:O	2:D:89:LEU:HD12	2.02	0.59
2:K:160:LEU:HD22	2:K:161:LEU:H	1.67	0.59
2:K:324:SER:C	2:K:325:TYR:HD1	2.05	0.59
3:R:719:DT:C2'	3:R:720:DA:H5''	2.28	0.59
2:K:151:VAL:HB	2:K:157:LYS:O	2.02	0.59
2:D:298:PHE:HZ	2:D:333:ILE:HG12	1.67	0.59
2:K:175:PRO:HG3	2:K:249:ARG:NH2	2.17	0.59
2:K:284:GLY:O	2:K:325:TYR:CE2	2.56	0.59
1:C:22:GLN:HB3	2:K:49:ARG:HG3	1.84	0.59
2:D:369:ILE:CG2	2:D:374:PHE:HE1	2.14	0.59
2:D:95:ARG:NH2	2:D:104:ILE:CD1	2.66	0.59
2:K:357:ASN:ND2	2:K:380:VAL:HG11	2.17	0.59
2:K:350:LEU:C	2:K:366:ILE:HD13	2.21	0.59
2:K:335:SER:O	2:K:338:PRO:HD2	2.03	0.59
2:K:55:ASP:C	2:K:57:VAL:N	2.53	0.59
2:K:12:ARG:NH1	2:K:12:ARG:HB2	2.12	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:265:VAL:O	2:K:272:GLY:HA3	2.03	0.59
2:K:12:ARG:CG	2:K:29:ALA:HB1	2.08	0.59
2:K:258:THR:HB	2:K:259:PHE:CD1	2.38	0.59
3:R:738:DA:H4'	3:R:739:DA:H5'	1.83	0.59
2:D:119:LYS:HD3	2:D:166:ASP:OD1	2.03	0.59
2:D:132:TYR:OH	2:D:147:PHE:CG	2.56	0.59
1:G:13:LEU:HD23	1:G:13:LEU:C	2.23	0.59
2:D:38:ALA:HB1	2:D:47:LEU:CD1	2.27	0.58
2:K:268:GLU:OE1	2:K:355:GLY:N	2.35	0.58
2:K:372:ARG:HA	2:K:375:LEU:HD12	1.83	0.58
2:D:75:ILE:HG22	2:D:76:VAL:N	2.18	0.58
2:K:108:GLU:O	2:K:110:VAL:N	2.34	0.58
2:K:41:LEU:CD2	2:K:41:LEU:H	2.15	0.58
3:R:701:DT:C2	3:R:702:DA:N7	2.71	0.58
3:R:743:DG:N2	4:T:677:DC:N3	2.51	0.58
2:D:6:THR:HA	2:D:102:THR:O	2.02	0.58
2:D:147:PHE:HD1	2:D:147:PHE:O	1.86	0.58
2:D:40:PRO:CB	2:D:46:PRO:HA	2.34	0.58
2:K:357:ASN:HB2	2:K:377:THR:HG23	1.85	0.58
3:R:743:DG:H1	4:T:677:DC:H42	1.50	0.58
4:T:691:DT:H2''	4:T:692:DA:O5'	2.03	0.58
1:C:45:PHE:CE1	1:C:49:PRO:HB3	2.38	0.58
2:K:370:TYR:O	2:K:373:HIS:HB2	2.04	0.58
2:D:8:MET:O	2:D:11:GLN:HB2	2.02	0.58
2:K:118:GLU:C	2:K:168:CYS:HB3	2.23	0.58
2:K:202:ASN:OD1	2:K:334:ILE:HG13	2.04	0.58
1:B:18:LYS:CA	1:B:21:ARG:HG2	2.27	0.58
4:T:683:DA:C5'	1:C:51:ASN:HB3	2.26	0.58
2:K:274:GLY:O	2:K:278:ILE:HG12	2.04	0.58
2:K:300:VAL:HG13	2:K:374:PHE:CE2	2.39	0.58
4:T:697:DT:H2''	4:T:698:DA:O5'	2.04	0.58
2:D:124:ARG:CB	2:D:124:ARG:HH11	2.10	0.57
2:D:21:ASN:CB	2:K:23:ALA:HB1	2.34	0.57
2:D:284:GLY:HA2	1:E:9:SER:HB2	1.84	0.57
2:K:160:LEU:CD2	2:K:161:LEU:N	2.61	0.57
2:K:182:LEU:HD22	2:K:182:LEU:H	1.69	0.57
2:K:310:GLY:H	2:K:353:ALA:HB2	1.68	0.57
2:K:357:ASN:CB	2:K:377:THR:HG23	2.34	0.57
2:K:155:GLN:HG2	2:K:184:ILE:HG23	1.86	0.57
2:D:202:ASN:OD1	2:D:334:ILE:HG13	2.04	0.57
1:C:68:MET:HA	1:G:70:LEU:HA	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:328:THR:HB	2:K:329:PRO:CD	2.35	0.57
1:C:21:ARG:HG2	1:C:31:LEU:HD11	1.87	0.57
2:D:12:ARG:HB3	2:D:31:GLU:OE1	2.04	0.57
2:D:130:THR:CA	2:D:133:LYS:HD3	2.30	0.57
2:K:115:MET:HB3	2:K:117:TRP:CH2	2.39	0.57
2:K:67:ASP:O	2:K:69:PRO:HD3	2.04	0.57
2:D:129:LEU:CD1	2:D:228:VAL:CG1	2.77	0.57
2:D:397:ARG:CZ	2:D:398:MET:HG3	2.34	0.57
2:D:41:LEU:CD1	2:D:41:LEU:H	2.18	0.57
2:K:120:LEU:HD22	2:K:124:ARG:NH1	2.19	0.57
1:B:52:THR:HG23	4:T:712:DG:OP2	2.05	0.57
1:B:15:ASN:HD22	1:B:16:ALA:H	1.51	0.57
2:D:24:HIS:NE2	2:D:87:PHE:HB2	2.20	0.57
2:K:410:LEU:HD22	2:K:414:PHE:CD2	2.40	0.57
2:K:55:ASP:O	2:K:59:ASN:ND2	2.37	0.57
2:K:86:PRO:O	2:K:90:LEU:HD12	2.05	0.57
1:B:32:ALA:CB	1:B:37:ILE:HG13	2.34	0.57
1:B:41:THR:O	1:B:45:PHE:HB3	2.04	0.57
2:K:39:ARG:NH2	2:K:321:ALA:HB2	2.20	0.57
2:K:367:ASP:O	2:K:370:TYR:HE1	1.87	0.57
1:E:58:PHE:O	1:E:62:GLN:HG3	2.05	0.57
2:K:13:VAL:HA	2:K:32:TRP:HB2	1.87	0.57
2:K:8:MET:HB3	2:K:32:TRP:HH2	1.55	0.57
1:B:24:ASN:OD1	1:B:26:TRP:HZ3	1.88	0.56
2:K:13:VAL:CA	2:K:29:ALA:HB3	2.33	0.56
2:K:26:PHE:C	2:K:52:ILE:HD11	2.24	0.56
2:K:301:PHE:O	2:K:305:ILE:HG12	2.05	0.56
1:C:22:GLN:HE22	2:K:49:ARG:H	1.53	0.56
1:B:68:MET:SD	1:B:68:MET:C	2.83	0.56
1:C:58:PHE:HA	1:C:61:LEU:HB2	1.87	0.56
2:D:256:CYS:SG	2:D:312:ALA:CB	2.93	0.56
3:R:740:DG:P	1:G:52:THR:HA	2.46	0.56
3:R:740:DG:C6	3:R:741:DG:N7	2.73	0.56
2:D:237:ASP:O	2:D:250:LEU:HD12	2.05	0.56
1:B:49:PRO:O	1:E:54:LEU:HD13	2.04	0.56
2:D:318:PHE:CD1	2:D:328:THR:HG22	2.40	0.56
2:K:406:VAL:O	2:K:410:LEU:HG	2.04	0.56
2:K:54:SER:O	2:K:57:VAL:HG23	2.05	0.56
2:K:7:TRP:HA	2:K:11:GLN:O	2.05	0.56
2:K:98:VAL:HG23	2:K:150:SER:HB3	1.88	0.56
3:R:738:DA:O4'	3:R:738:DA:N3	2.32	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:130:THR:O	2:D:133:LYS:HG2	2.06	0.56
2:D:404:ASP:HA	2:D:407:LYS:HB3	1.87	0.56
1:E:7:ILE:HG23	1:E:12:GLN:CB	2.36	0.56
2:K:148:ARG:C	2:K:149:ILE:HG13	2.25	0.56
2:K:39:ARG:NH1	2:K:320:GLN:HA	2.21	0.56
2:K:337:PHE:HB3	2:K:422:VAL:HA	1.88	0.56
2:D:203:GLU:HG2	2:D:231:LEU:CD2	2.34	0.56
2:K:162:ARG:HD3	2:K:167:TRP:CZ2	2.40	0.56
4:T:714:DG:H2''	4:T:715:DG:O5'	2.04	0.56
1:B:52:THR:HG22	1:B:53:THR:N	2.20	0.56
1:G:13:LEU:HD23	1:G:14:ALA:N	2.21	0.56
2:K:104:ILE:HG23	2:K:105:PRO:HD2	1.88	0.56
2:K:197:SER:O	2:K:198:GLN:HG3	2.06	0.56
2:D:126:GLU:CG	2:D:225:ALA:O	2.54	0.56
2:D:244:ARG:CG	2:D:244:ARG:NH1	2.68	0.56
2:D:36:ARG:HD3	2:D:36:ARG:H	1.69	0.56
1:G:55:THR:OG1	1:G:56:THR:N	2.37	0.56
2:K:395:PHE:O	2:K:396:ALA:C	2.44	0.56
1:B:66:LEU:HD23	1:B:67:SER:N	2.15	0.56
2:K:77:LYS:HE2	2:K:77:LYS:O	2.06	0.56
3:R:746:DA:H2''	3:R:747:DA:O5'	2.05	0.56
1:B:12:GLN:C	1:B:15:ASN:ND2	2.58	0.56
2:K:40:PRO:CA	2:K:47:LEU:HD21	2.36	0.56
2:K:54:SER:O	2:K:57:VAL:HG21	2.06	0.56
2:D:21:ASN:CG	2:K:23:ALA:HB1	2.26	0.56
2:K:113:PRO:O	2:K:115:MET:N	2.39	0.56
2:D:311:HIS:CD2	2:D:314:ASN:HD21	2.24	0.55
2:D:18:LYS:CE	2:D:22:GLY:HA2	2.35	0.55
1:G:61:LEU:HA	1:G:64:LEU:CD1	2.36	0.55
2:K:352:LEU:O	2:K:353:ALA:C	2.44	0.55
1:B:14:ALA:CB	1:B:49:PRO:HG3	2.36	0.55
2:D:237:ASP:C	2:D:250:LEU:HD12	2.27	0.55
1:C:53:THR:HG21	1:G:51:ASN:CA	2.35	0.55
1:C:54:LEU:HD12	1:G:52:THR:HB	1.88	0.55
1:G:58:PHE:O	1:G:61:LEU:CB	2.53	0.55
2:K:313:LYS:CG	2:K:313:LYS:O	2.55	0.55
2:K:41:LEU:HD22	2:K:41:LEU:N	2.22	0.55
2:D:263:SER:CB	2:D:266:LYS:HZ3	2.10	0.55
2:K:158:THR:HG22	2:K:182:LEU:HD21	1.87	0.55
2:K:217:VAL:CB	2:K:218:PRO:HD2	2.35	0.55
2:K:350:LEU:H	2:K:351:LYS:HE3	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:76:VAL:HG21	2:K:84:ARG:HG2	1.89	0.55
1:B:32:ALA:HB1	1:B:37:ILE:HG13	1.88	0.55
1:C:17:MET:HE2	1:C:64:LEU:HD12	1.88	0.55
1:C:11:THR:HA	1:C:49:PRO:HG3	1.87	0.55
2:D:253:GLU:OE2	2:D:258:THR:N	2.40	0.55
2:D:384:PRO:HG2	2:D:387:GLN:HE21	1.72	0.55
2:K:107:ASP:O	2:K:108:GLU:HB2	2.05	0.55
2:K:240:TRP:CZ3	2:K:247:LEU:HB2	2.41	0.55
2:K:28:TYR:HE2	2:K:41:LEU:HD21	1.72	0.55
2:D:179:ILE:HG12	2:D:235:ARG:HG2	1.89	0.55
2:K:287:GLU:HB2	2:K:291:ASP:OD1	2.07	0.55
2:K:4:LEU:O	2:K:15:GLU:HB3	2.06	0.55
2:K:383:PHE:HE2	2:K:388:MET:HB2	1.72	0.55
2:K:151:VAL:HG13	2:K:179:ILE:HD12	1.89	0.55
2:K:220:ALA:CB	2:K:233:VAL:HA	2.37	0.55
2:K:290:LYS:HD3	2:K:290:LYS:C	2.27	0.55
2:D:126:GLU:HG3	2:D:225:ALA:O	2.06	0.55
1:G:31:LEU:HD22	1:G:34:LYS:HD2	1.89	0.55
1:C:53:THR:HG22	1:G:51:ASN:HA	1.88	0.55
2:K:196:LEU:HD12	2:K:334:ILE:HD11	1.87	0.55
1:B:7:ILE:CG2	1:B:8:TYR:H	2.15	0.55
1:E:31:LEU:O	1:E:35:ILE:HG12	2.07	0.55
1:E:32:ALA:HB1	1:E:37:ILE:O	2.06	0.55
1:G:38:LYS:HG2	1:G:39:GLN:H	1.71	0.55
2:K:222:ILE:HG22	2:K:223:ILE:N	2.22	0.55
3:R:743:DG:H1	4:T:677:DC:N4	2.05	0.55
1:B:33:LYS:O	2:D:384:PRO:HG3	2.07	0.54
2:K:240:TRP:CE3	2:K:247:LEU:HB2	2.42	0.54
2:D:167:TRP:CZ2	2:D:223:ILE:HD13	2.42	0.54
2:D:64:LEU:HD12	2:D:90:LEU:HD11	1.89	0.54
1:B:40:ALA:O	1:B:43:SER:HB3	2.08	0.54
1:B:41:THR:CG2	1:B:42:ILE:N	2.70	0.54
1:E:7:ILE:CG2	1:E:12:GLN:HB3	2.35	0.54
3:R:740:DG:OP1	1:G:52:THR:CA	2.54	0.54
2:K:120:LEU:HD11	2:K:169:ILE:CG1	2.34	0.54
2:K:200:VAL:HG13	2:K:231:LEU:HD13	1.90	0.54
2:D:149:ILE:HD13	2:D:159:ALA:O	2.08	0.54
2:D:236:PHE:CE2	2:D:329:PRO:HB2	2.42	0.54
2:D:253:GLU:OE2	2:D:257:GLN:HB3	2.07	0.54
2:K:169:ILE:CG2	2:K:170:PRO:HD2	2.36	0.54
2:D:320:GLN:HG3	2:D:324:SER:O	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:17:MET:HE2	1:E:64:LEU:HD12	1.89	0.54
2:K:352:LEU:HD13	2:K:356:LEU:HD22	1.88	0.54
2:K:356:LEU:N	2:K:356:LEU:HD23	2.22	0.54
1:C:32:ALA:HB1	1:C:37:ILE:HG13	1.90	0.54
2:D:52:ILE:HG22	2:D:53:THR:H	1.73	0.54
1:G:30:GLU:HA	1:G:33:LYS:CD	2.38	0.54
2:K:120:LEU:HG	2:K:168:CYS:HA	1.88	0.54
2:K:66:PRO:HG3	2:K:152:ALA:HB2	1.88	0.54
2:D:76:VAL:HA	2:D:81:ALA:HB2	1.88	0.54
2:K:358:ALA:CB	2:K:363:LYS:H	2.21	0.54
3:R:728:DA:H2"	3:R:729:DT:H72	1.90	0.54
2:D:304:LEU:HD23	2:D:429:LEU:HB2	1.89	0.54
1:G:57:PHE:O	1:G:60:ILE:HB	2.08	0.54
2:K:235:ARG:NH1	2:K:238:ARG:CZ	2.71	0.54
2:D:162:ARG:NH1	2:D:165:ASN:HA	2.23	0.54
2:K:200:VAL:CG1	2:K:231:LEU:HD13	2.38	0.54
2:K:8:MET:CG	2:K:32:TRP:HH2	2.20	0.54
1:C:39:GLN:HA	1:C:42:ILE:CG1	2.38	0.54
2:K:99:GLY:HA2	2:K:252:GLN:CG	2.38	0.54
3:R:701:DT:H2"	3:R:702:DA:OP2	2.08	0.54
2:D:129:LEU:HD11	2:D:228:VAL:HG11	1.84	0.53
1:G:60:ILE:O	1:G:63:SER:OG	2.16	0.53
2:K:26:PHE:CE1	2:K:61:PHE:HZ	2.26	0.53
2:D:128:VAL:O	2:D:131:ALA:HB3	2.07	0.53
2:D:147:PHE:CE1	2:D:149:ILE:CD1	2.91	0.53
2:D:30:PRO:HA	2:D:33:LEU:HD12	1.89	0.53
2:D:387:GLN:O	2:D:391:ILE:HG13	2.07	0.53
2:K:300:VAL:HG12	2:K:303:TRP:HE3	1.72	0.53
2:K:411:PRO:CG	2:K:414:PHE:HB2	2.32	0.53
1:C:28:GLN:HE22	1:C:43:SER:HA	1.73	0.53
2:K:199:SER:O	2:K:202:ASN:HB3	2.08	0.53
2:K:177:THR:O	2:K:235:ARG:HG3	2.09	0.53
2:K:28:TYR:O	2:K:30:PRO:N	2.41	0.53
4:T:712:DG:H2"	4:T:713:DG:OP2	2.09	0.53
2:D:147:PHE:CD1	2:D:147:PHE:O	2.62	0.53
2:D:4:LEU:CD2	2:D:91:SER:HA	2.24	0.53
2:K:211:LYS:HB2	2:K:217:VAL:HG23	1.90	0.53
2:K:180:ILE:HG23	2:K:223:ILE:HD11	1.90	0.53
2:K:5:VAL:HG13	2:K:15:GLU:CG	2.32	0.53
1:B:37:ILE:HD12	1:B:41:THR:CG2	2.39	0.53
1:C:13:LEU:C	1:C:13:LEU:HD23	2.29	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:415:PRO:HB2	2:K:417:ASN:ND2	2.24	0.53
1:C:20:VAL:CG1	1:C:64:LEU:HD22	2.39	0.53
1:C:67:SER:O	1:G:71:CYS:N	2.42	0.53
2:D:284:GLY:HA3	1:E:9:SER:HB2	1.91	0.53
2:D:352:LEU:HG	2:D:366:ILE:CG1	2.33	0.53
1:G:42:ILE:HD13	1:G:60:ILE:HG12	1.91	0.53
2:K:286:SER:OG	2:K:326:ARG:HB3	2.09	0.53
2:K:393:SER:O	2:K:396:ALA:HB3	2.09	0.53
2:K:399:ILE:HG22	2:K:400:PRO:N	2.23	0.53
2:K:75:ILE:N	2:K:75:ILE:HD12	2.24	0.53
1:B:66:LEU:HD23	1:E:71:CYS:O	2.09	0.53
2:D:21:ASN:HB2	2:K:23:ALA:HB1	1.91	0.53
2:D:21:ASN:HD22	2:D:22:GLY:N	2.06	0.53
2:D:311:HIS:H	2:D:314:ASN:HD22	1.57	0.53
2:D:286:SER:HA	1:E:8:TYR:CD2	2.43	0.53
2:K:328:THR:HB	2:K:329:PRO:HD2	1.90	0.53
2:K:55:ASP:O	2:K:57:VAL:N	2.41	0.53
1:C:14:ALA:HB2	1:C:49:PRO:HB3	1.90	0.53
2:D:210:ALA:HA	2:D:215:LEU:HD12	1.91	0.53
2:K:266:LYS:HG3	2:K:267:TYR:CD1	2.39	0.53
3:R:739:DA:H5"	1:G:51:ASN:HB3	1.91	0.53
1:B:27:THR:OG1	3:R:700:DT:H3'	2.09	0.52
1:C:29:SER:O	1:C:33:LYS:HG3	2.10	0.52
2:D:129:LEU:HD13	2:D:228:VAL:HG21	1.91	0.52
2:D:184:ILE:H	2:D:199:SER:HB3	1.74	0.52
2:K:40:PRO:HB2	2:K:45:LEU:O	2.09	0.52
1:B:60:ILE:O	1:B:64:LEU:HB2	2.09	0.52
1:C:35:ILE:HD13	1:C:59:LYS:O	2.09	0.52
2:D:52:ILE:HG22	2:D:53:THR:N	2.24	0.52
2:K:256:CYS:C	2:K:258:THR:H	2.13	0.52
2:D:279:MET:HE3	2:D:282:LEU:CD1	2.39	0.52
2:D:278:ILE:HG22	2:D:282:LEU:HD21	1.92	0.52
2:K:162:ARG:N	2:K:177:THR:OG1	2.40	0.52
2:K:279:MET:HE2	2:K:296:MET:CE	2.40	0.52
1:B:29:SER:OG	3:R:700:DT:H2'	2.09	0.52
2:D:292:ARG:O	2:D:296:MET:HG2	2.08	0.52
1:G:21:ARG:HB3	1:G:26:TRP:HE3	1.74	0.52
2:K:151:VAL:HG21	2:K:159:ALA:N	2.24	0.52
2:K:303:TRP:CE3	2:K:304:LEU:HG	2.43	0.52
3:R:742:DG:H2"	3:R:743:DG:C5'	2.39	0.52
2:D:318:PHE:C	2:D:319:ILE:HD13	2.30	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:153:GLY:N	2:K:157:LYS:HE2	2.25	0.52
2:K:247:LEU:O	2:K:247:LEU:HD23	2.10	0.52
2:K:3:LYS:HZ3	2:K:3:LYS:HB2	1.72	0.52
2:K:337:PHE:CE1	2:K:425:ASN:HB2	2.45	0.52
4:T:708:DT:H2''	4:T:709:DT:C5	2.45	0.52
1:B:20:VAL:HA	1:B:23:GLN:HG2	1.91	0.52
2:D:160:LEU:HD22	2:D:168:CYS:O	2.10	0.52
1:E:57:PHE:HA	1:E:60:ILE:HD12	1.92	0.52
2:D:209:LEU:HG	2:D:213:LEU:CD1	2.39	0.52
2:D:59:ASN:O	2:D:62:ASP:N	2.43	0.52
1:G:31:LEU:O	1:G:35:ILE:HG12	2.10	0.52
2:K:148:ARG:O	2:K:149:ILE:HG13	2.09	0.52
1:B:21:ARG:NH2	1:B:28:GLN:N	2.50	0.52
1:C:19:LEU:O	1:C:23:GLN:HB2	2.10	0.52
1:C:57:PHE:CE1	1:C:61:LEU:HD23	2.44	0.52
2:K:321:ALA:C	2:K:323:GLY:H	2.13	0.52
1:C:13:LEU:HD23	1:C:17:MET:HG3	1.92	0.52
2:D:333:ILE:H	2:D:333:ILE:HD12	1.73	0.52
1:G:16:ALA:O	1:G:20:VAL:HG23	2.10	0.52
1:G:45:PHE:HD1	1:G:52:THR:OG1	1.91	0.52
1:C:10:PRO:N	1:G:58:PHE:CE1	2.77	0.52
2:K:241:ASN:O	2:K:244:ARG:NH1	2.43	0.52
2:K:299:GLN:NE2	2:K:302:GLN:HE22	2.08	0.52
2:K:311:HIS:CE1	2:K:314:ASN:HD21	2.27	0.52
2:K:205:TYR:HE1	2:K:410:LEU:HD11	1.73	0.52
2:K:42:SER:O	2:K:43:LEU:C	2.48	0.52
3:R:731:DT:H2''	3:R:732:DC:H5'	1.91	0.52
4:T:713:DG:H2''	4:T:714:DG:OP2	2.10	0.52
2:D:251:PRO:O	2:D:319:ILE:HG12	2.11	0.52
1:G:27:THR:H	1:G:30:GLU:HG2	1.74	0.52
2:K:116:ALA:HB1	2:K:171:LYS:HD3	1.92	0.52
2:K:261:LEU:HB3	2:K:265:VAL:HG21	1.92	0.52
2:K:58:PHE:O	2:K:59:ASN:C	2.46	0.52
1:G:38:LYS:CG	1:G:39:GLN:H	2.23	0.51
2:K:279:MET:CE	2:K:296:MET:SD	2.99	0.51
2:K:54:SER:OG	2:K:55:ASP:N	2.42	0.51
2:D:300:VAL:HG22	2:D:374:PHE:CD2	2.44	0.51
1:E:61:LEU:HD21	1:E:66:LEU:HB3	1.91	0.51
1:G:14:ALA:HB2	1:G:45:PHE:CZ	2.44	0.51
2:K:217:VAL:CG1	2:K:218:PRO:HD2	2.39	0.51
2:K:50:GLY:O	2:K:52:ILE:HD13	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:301:PHE:C	2:D:303:TRP:H	2.13	0.51
2:K:118:GLU:O	2:K:168:CYS:HB3	2.10	0.51
2:K:247:LEU:CD2	2:K:247:LEU:C	2.78	0.51
3:R:745:DT:H2"	3:R:746:DA:N7	2.26	0.51
1:B:53:THR:HG23	1:B:55:THR:HG22	1.93	0.51
2:K:307:ALA:HA	2:K:335:SER:HA	1.91	0.51
2:K:55:ASP:C	2:K:57:VAL:H	2.14	0.51
2:D:399:ILE:HB	2:D:400:PRO:HD3	1.92	0.51
1:C:10:PRO:CG	1:G:58:PHE:CD1	2.92	0.51
2:K:388:MET:HE2	2:K:392:LEU:HB2	1.92	0.51
3:R:715:DG:N2	4:T:705:DC:N4	2.59	0.51
2:D:222:ILE:HG22	2:D:222:ILE:O	2.10	0.51
2:D:304:LEU:HD11	2:D:433:LEU:HD11	1.93	0.51
3:R:710:DA:H4'	3:R:711:DA:H5'	1.93	0.51
1:B:7:ILE:C	1:B:8:TYR:CD1	2.84	0.51
2:D:358:ALA:HB2	2:D:363:LYS:HB2	1.93	0.51
1:C:38:LYS:HE2	1:C:40:ALA:HB2	1.93	0.51
1:E:23:GLN:NE2	1:E:23:GLN:HA	2.25	0.51
1:E:38:LYS:CD	3:R:713:DG:H2'	2.41	0.51
1:G:14:ALA:O	1:G:15:ASN:C	2.49	0.51
1:B:35:ILE:CG2	1:B:63:SER:HB2	2.33	0.51
2:D:279:MET:HE2	2:D:296:MET:SD	2.51	0.51
2:K:170:PRO:O	2:K:171:LYS:HG3	2.11	0.51
2:K:311:HIS:ND1	2:K:314:ASN:ND2	2.59	0.51
2:K:324:SER:C	2:K:325:TYR:CD1	2.83	0.51
4:T:672:DT:H2"	4:T:673:DT:OP2	2.09	0.51
2:K:7:TRP:NE1	2:K:12:ARG:NH1	2.54	0.51
2:K:17:THR:HB	2:K:25:THR:OG1	2.11	0.51
2:K:295:PHE:CE1	2:K:315:PHE:CE1	2.99	0.51
3:R:714:DG:H2"	3:R:715:DG:O5'	2.11	0.51
3:R:740:DG:C6	3:R:741:DG:C5	2.99	0.51
1:C:21:ARG:HH22	1:C:28:GLN:N	2.10	0.50
2:D:208:LEU:HD22	2:D:406:VAL:CG1	2.39	0.50
2:D:372:ARG:HA	2:D:375:LEU:HD12	1.92	0.50
2:D:304:LEU:O	2:D:426:VAL:HG13	2.11	0.50
2:K:402:ALA:O	2:K:406:VAL:HG23	2.11	0.50
2:D:208:LEU:HD22	2:D:406:VAL:HG22	1.93	0.50
2:D:337:PHE:CD1	2:D:422:VAL:HA	2.45	0.50
2:D:5:VAL:HG22	2:D:15:GLU:HG2	1.92	0.50
2:K:3:LYS:CG	2:K:17:THR:HA	2.35	0.50
2:K:209:LEU:O	2:K:212:GLU:HB3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:T:715:DG:H2"	4:T:716:DA:O5'	2.10	0.50
2:D:311:HIS:CE1	2:D:313:LYS:HB2	2.46	0.50
2:K:118:GLU:CA	2:K:171:LYS:HZ2	2.24	0.50
2:D:265:VAL:O	2:D:272:GLY:HA3	2.10	0.50
2:D:275:ILE:O	2:D:279:MET:HG2	2.12	0.50
2:D:132:TYR:OH	2:D:147:PHE:CE1	2.64	0.50
1:B:58:PHE:CZ	1:E:13:LEU:HD12	2.46	0.50
2:K:222:ILE:HG22	2:K:223:ILE:H	1.76	0.50
2:K:6:THR:OG1	2:K:103:LEU:CD2	2.60	0.50
3:R:706:DC:H2"	3:R:707:DC:O5'	2.11	0.50
1:B:62:GLN:OE1	2:D:289:LEU:N	2.35	0.50
2:D:178:HIS:CD2	2:D:232:ALA:HB1	2.41	0.50
1:E:8:TYR:N	1:E:12:GLN:NE2	2.52	0.50
1:E:39:GLN:O	1:E:42:ILE:HB	2.11	0.50
2:K:266:LYS:HD2	2:K:311:HIS:CD2	2.47	0.50
2:K:83:SER:H	2:K:88:ASP:HB3	1.75	0.50
1:C:21:ARG:NH2	1:C:27:THR:HA	2.27	0.50
2:D:180:ILE:HA	2:D:231:LEU:O	2.12	0.50
2:K:76:VAL:HG21	2:K:84:ARG:CG	2.42	0.50
1:E:51:ASN:O	3:R:711:DA:H5"	2.11	0.50
1:C:28:GLN:NE2	1:C:46:GLU:HG3	2.26	0.50
2:D:49:ARG:HB2	1:E:22:GLN:HE21	1.76	0.50
2:K:120:LEU:CD1	2:K:169:ILE:HG13	2.36	0.50
1:G:32:ALA:HB1	1:G:37:ILE:O	2.11	0.50
2:K:32:TRP:HE1	2:K:39:ARG:H	1.60	0.50
2:D:151:VAL:CG1	2:D:157:LYS:HE3	2.41	0.49
2:D:363:LYS:HD2	2:D:373:HIS:HE1	1.77	0.49
2:K:292:ARG:NH1	2:K:292:ARG:HG2	2.25	0.49
1:B:27:THR:HG23	1:B:30:GLU:HG3	1.93	0.49
2:K:290:LYS:HD3	2:K:290:LYS:O	2.13	0.49
1:C:7:ILE:HB	1:G:68:MET:O	2.11	0.49
2:D:257:GLN:O	2:D:258:THR:C	2.50	0.49
2:D:263:SER:O	2:D:266:LYS:CG	2.37	0.49
2:D:399:ILE:HD12	2:D:399:ILE:N	2.27	0.49
2:K:349:ASP:O	2:K:350:LEU:HG	2.12	0.49
4:T:685:DG:H2"	4:T:686:DG:H5'	1.93	0.49
2:D:181:LYS:HB2	2:D:231:LEU:HD23	1.94	0.49
2:D:318:PHE:CE1	2:D:328:THR:CB	2.91	0.49
1:B:12:GLN:HA	1:B:15:ASN:ND2	2.23	0.49
1:B:56:THR:O	1:B:60:ILE:HG13	2.12	0.49
1:B:58:PHE:CE1	1:E:13:LEU:HD12	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:5:GLN:N	1:G:5:GLN:OE1	2.37	0.49
2:D:218:PRO:HD3	2:D:236:PHE:HE2	1.78	0.49
2:D:76:VAL:HA	2:D:81:ALA:HB3	1.93	0.49
2:K:85:GLN:O	2:K:89:LEU:HB2	2.12	0.49
2:K:8:MET:CB	2:K:32:TRP:HH2	2.18	0.49
2:D:256:CYS:SG	2:D:312:ALA:C	2.91	0.49
2:D:75:ILE:HG21	2:D:89:LEU:CD2	2.33	0.49
1:E:8:TYR:N	1:E:12:GLN:HE22	2.05	0.49
1:C:22:GLN:HE22	2:K:49:ARG:N	2.11	0.49
3:R:728:DA:H2"	3:R:729:DT:C7	2.42	0.49
2:D:369:ILE:HG21	2:D:374:PHE:HE1	1.77	0.49
2:D:56:ALA:HA	2:D:59:ASN:HB2	1.95	0.49
1:E:45:PHE:CE2	1:E:60:ILE:HD13	2.47	0.49
1:C:10:PRO:CD	1:G:58:PHE:CD1	2.96	0.49
2:K:119:LYS:HA	2:K:168:CYS:SG	2.52	0.49
2:K:422:VAL:O	2:K:426:VAL:HG23	2.13	0.49
2:K:56:ALA:HA	2:K:59:ASN:ND2	2.28	0.49
2:D:95:ARG:NH2	2:D:104:ILE:HD12	2.27	0.49
2:D:107:ASP:O	2:D:108:GLU:HG3	2.13	0.49
2:D:132:TYR:CZ	2:D:147:PHE:CZ	3.01	0.49
2:D:162:ARG:CZ	2:D:165:ASN:HA	2.43	0.49
2:K:13:VAL:HG22	2:K:32:TRP:CD2	2.48	0.49
1:B:19:LEU:O	1:B:23:GLN:HB3	2.13	0.49
1:C:58:PHE:CZ	1:G:13:LEU:HD12	2.47	0.49
2:D:76:VAL:HG11	2:K:262:PRO:CG	2.42	0.49
1:C:53:THR:CG2	1:G:51:ASN:CA	2.89	0.49
1:C:10:PRO:CG	1:G:58:PHE:HD1	2.18	0.49
2:K:65:LEU:CD1	2:K:89:LEU:HD13	2.28	0.49
1:C:55:THR:HG22	1:G:10:PRO:HG2	1.95	0.48
2:K:205:TYR:CE1	2:K:410:LEU:HD11	2.48	0.48
2:K:233:VAL:HG12	2:K:234:GLU:N	2.28	0.48
2:K:39:ARG:HH12	2:K:320:GLN:HA	1.78	0.48
2:K:317:VAL:CG1	2:K:325:TYR:HB2	2.35	0.48
2:K:345:ILE:HD12	2:K:345:ILE:N	2.28	0.48
2:K:371:PRO:O	2:K:375:LEU:HG	2.12	0.48
2:K:251:PRO:HB3	2:K:319:ILE:HB	1.95	0.48
2:K:12:ARG:HD3	2:K:31:GLU:OE1	2.09	0.48
2:K:5:VAL:HA	2:K:15:GLU:HG3	1.95	0.48
1:E:38:LYS:HD3	3:R:713:DG:H2'	1.94	0.48
4:T:714:DG:H2"	4:T:715:DG:C5'	2.43	0.48
2:K:247:LEU:O	2:K:247:LEU:CD2	2.61	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:415:PRO:O	2:K:419:VAL:HG23	2.13	0.48
4:T:682:DA:C2	4:T:683:DA:N1	2.81	0.48
4:T:684:DG:OP1	1:C:52:THR:HG23	2.13	0.48
1:C:58:PHE:HA	1:C:61:LEU:CB	2.43	0.48
2:D:287:GLU:O	2:D:291:ASP:OD2	2.31	0.48
2:D:297:LYS:HA	2:D:391:ILE:HG21	1.96	0.48
2:D:44:SER:OG	2:D:45:LEU:HD12	2.13	0.48
2:D:40:PRO:HB2	2:D:45:LEU:O	2.13	0.48
2:K:336:ALA:HB3	2:K:350:LEU:HD21	1.95	0.48
2:K:357:ASN:HD22	2:K:380:VAL:HG11	1.78	0.48
1:E:45:PHE:O	1:E:49:PRO:HB3	2.13	0.48
2:K:318:PHE:HD1	2:K:326:ARG:NH1	2.11	0.48
2:K:344:GLY:C	2:K:345:ILE:HD12	2.34	0.48
2:K:275:ILE:CD1	2:K:354:MET:HB2	2.43	0.48
1:C:73:ALA:HB2	1:G:66:LEU:O	2.13	0.48
2:D:30:PRO:O	2:D:33:LEU:HB2	2.14	0.48
2:D:316:SER:C	2:D:328:THR:HG23	2.33	0.48
2:D:333:ILE:N	2:D:333:ILE:HD12	2.29	0.48
1:B:14:ALA:HB1	1:B:46:GLU:O	2.13	0.48
2:K:30:PRO:O	2:K:34:ALA:HB2	2.12	0.48
2:K:76:VAL:HA	2:K:81:ALA:H	1.78	0.48
4:T:697:DT:H2''	4:T:698:DA:H8	1.78	0.48
4:T:714:DG:H8	4:T:714:DG:H5'	1.79	0.48
1:C:7:ILE:CD1	1:G:69:THR:HA	2.39	0.48
2:K:237:ASP:HB2	2:K:250:LEU:O	2.13	0.48
2:K:62:ASP:O	2:K:65:LEU:HG	2.14	0.48
1:C:39:GLN:HA	1:C:42:ILE:HG12	1.95	0.48
2:D:147:PHE:HE1	2:D:149:ILE:HB	1.79	0.48
1:E:16:ALA:O	1:E:17:MET:C	2.50	0.48
1:E:58:PHE:O	1:E:59:LYS:C	2.53	0.48
2:K:249:ARG:NH1	2:K:249:ARG:HG3	2.28	0.48
2:K:249:ARG:HH11	2:K:249:ARG:HG3	1.79	0.48
2:K:385:GLU:HG2	2:K:389:HIS:CD2	2.48	0.48
1:B:27:THR:OG1	1:B:28:GLN:N	2.46	0.48
1:B:7:ILE:N	1:B:7:ILE:HD13	2.29	0.48
2:D:181:LYS:HD2	2:D:231:LEU:HD23	1.95	0.48
2:D:291:ASP:HA	2:D:327:LEU:HD23	1.95	0.48
2:D:382:ARG:HH11	2:D:382:ARG:CB	2.19	0.48
2:D:25:THR:C	2:D:57:VAL:HG11	2.35	0.48
3:R:740:DG:O6	3:R:741:DG:O6	2.32	0.48
2:D:21:ASN:O	2:K:23:ALA:CA	2.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:431:GLY:C	2:D:435:ARG:HH21	2.17	0.47
2:K:298:PHE:O	2:K:302:GLN:HG3	2.14	0.47
2:K:5:VAL:CG1	2:K:6:THR:N	2.76	0.47
1:B:27:THR:HG22	1:B:30:GLU:OE1	2.14	0.47
1:B:53:THR:CG2	1:B:55:THR:HG22	2.44	0.47
1:C:64:LEU:O	1:C:66:LEU:CD2	2.62	0.47
1:C:64:LEU:O	1:C:66:LEU:HD22	2.15	0.47
2:D:147:PHE:C	2:D:147:PHE:CD1	2.86	0.47
2:D:231:LEU:HG	2:D:232:ALA:N	2.29	0.47
2:D:278:ILE:HG21	2:D:295:PHE:CZ	2.49	0.47
2:D:347:ILE:HD12	2:D:350:LEU:HD12	1.95	0.47
2:D:41:LEU:HB3	2:D:60:PHE:CE2	2.49	0.47
1:E:13:LEU:HD21	1:E:57:PHE:HE1	1.79	0.47
2:K:310:GLY:N	2:K:353:ALA:HB2	2.29	0.47
3:R:746:DA:H1'	3:R:747:DA:H5'	1.94	0.47
3:R:715:DG:H22	4:T:705:DC:N4	2.12	0.47
1:B:44:ASN:C	1:B:44:ASN:ND2	2.68	0.47
4:T:713:DG:H3'	4:T:713:DG:P	2.53	0.47
1:C:20:VAL:HG21	1:C:64:LEU:HD13	1.95	0.47
2:D:266:LYS:CE	2:D:313:LYS:CD	2.85	0.47
1:E:14:ALA:O	1:E:15:ASN:C	2.53	0.47
1:C:58:PHE:HE1	1:G:13:LEU:HD12	1.74	0.47
1:G:14:ALA:O	1:G:16:ALA:N	2.48	0.47
2:K:26:PHE:HB3	2:K:52:ILE:CD1	2.44	0.47
4:T:674:DA:C2	4:T:675:DT:C4	3.02	0.47
3:R:715:DG:O6	4:T:704:DC:N4	2.47	0.47
1:B:62:GLN:C	1:B:64:LEU:N	2.65	0.47
1:C:35:ILE:HG13	1:C:37:ILE:HG12	1.95	0.47
2:D:212:GLU:O	2:D:212:GLU:HG3	2.15	0.47
2:D:26:PHE:O	2:D:51:ASN:HA	2.14	0.47
2:D:71:VAL:C	2:D:75:ILE:HD12	2.35	0.47
2:D:65:LEU:CD1	2:D:89:LEU:HB2	2.45	0.47
1:C:61:LEU:CD1	1:G:70:LEU:HD21	2.43	0.47
2:D:303:TRP:CE3	2:D:304:LEU:HG	2.49	0.47
1:E:53:THR:HB	1:E:56:THR:CB	2.43	0.47
1:E:61:LEU:CD2	1:E:66:LEU:HB3	2.44	0.47
2:K:12:ARG:O	2:K:32:TRP:HB2	2.15	0.47
2:K:5:VAL:CG1	2:K:15:GLU:HG3	2.36	0.47
2:K:12:ARG:HD2	2:K:31:GLU:CD	2.32	0.47
3:R:714:DG:H1'	3:R:715:DG:H5'	1.96	0.47
3:R:739:DA:H5''	1:G:51:ASN:CB	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:T:674:DA:H2"	4:T:675:DT:H5"	1.95	0.47
2:D:363:LYS:HD2	2:D:373:HIS:CE1	2.49	0.47
2:K:162:ARG:H	2:K:177:THR:HG1	1.60	0.47
1:G:62:GLN:O	2:K:289:LEU:HD21	2.15	0.47
1:C:20:VAL:HG11	1:C:64:LEU:HB3	1.96	0.47
2:D:151:VAL:CG2	2:D:158:THR:HA	2.45	0.47
2:D:314:ASN:HA	2:D:331:TYR:CE1	2.49	0.47
1:B:27:THR:OG1	3:R:701:DT:OP2	2.33	0.47
1:C:28:GLN:HE22	1:C:43:SER:CA	2.28	0.47
1:C:62:GLN:C	1:C:64:LEU:H	2.17	0.47
2:D:19:LEU:HB2	2:D:21:ASN:HD21	1.80	0.47
2:D:327:LEU:HD21	2:D:330:PHE:HZ	1.79	0.47
2:D:23:ALA:CA	2:K:23:ALA:HB2	2.45	0.47
2:K:295:PHE:HE1	2:K:315:PHE:CZ	2.33	0.47
2:K:75:ILE:H	2:K:75:ILE:HD12	1.80	0.47
2:K:92:GLU:HB3	2:K:148:ARG:HH12	1.80	0.47
1:B:52:THR:HG23	4:T:712:DG:P	2.54	0.47
1:C:16:ALA:HA	1:C:19:LEU:CD1	2.45	0.47
2:D:126:GLU:O	2:D:130:THR:CG2	2.63	0.47
2:D:95:ARG:HH21	2:D:104:ILE:CD1	2.27	0.47
2:K:132:TYR:O	2:K:133:LYS:HG2	2.15	0.47
2:K:369:ILE:HG22	2:K:374:PHE:CE1	2.49	0.47
1:B:58:PHE:O	1:B:61:LEU:N	2.48	0.47
2:D:16:LEU:HD13	2:D:61:PHE:CE2	2.50	0.47
2:K:161:LEU:CD1	2:K:177:THR:H	2.28	0.47
2:K:157:LYS:HA	2:K:182:LEU:CD2	2.45	0.47
2:K:223:ILE:HG13	2:K:230:ALA:HB3	1.97	0.47
4:T:713:DG:C4	4:T:714:DG:N7	2.83	0.47
2:D:298:PHE:CZ	2:D:333:ILE:HG12	2.50	0.46
2:K:220:ALA:HB2	2:K:233:VAL:HA	1.96	0.46
1:B:44:ASN:HD22	1:B:45:PHE:CA	2.28	0.46
2:D:61:PHE:HA	2:D:64:LEU:HD11	1.97	0.46
2:K:67:ASP:OD2	2:K:263:SER:HB2	2.14	0.46
2:K:40:PRO:HA	2:K:47:LEU:HD21	1.95	0.46
2:K:416:GLU:O	2:K:420:THR:OG1	2.33	0.46
4:T:670:DG:H2"	4:T:671:DC:C6	2.50	0.46
1:B:42:ILE:O	1:B:45:PHE:HD2	1.98	0.46
1:B:55:THR:O	1:B:59:LYS:NZ	2.48	0.46
2:D:157:LYS:HD3	2:D:181:LYS:HG2	1.98	0.46
2:D:167:TRP:CZ2	2:D:223:ILE:HG21	2.51	0.46
1:G:14:ALA:C	1:G:16:ALA:N	2.68	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:30:GLU:HA	1:G:33:LYS:HD2	1.96	0.46
2:K:300:VAL:HG13	2:K:374:PHE:CZ	2.49	0.46
1:B:15:ASN:HD22	1:B:16:ALA:N	2.12	0.46
2:D:174:THR:HA	2:D:175:PRO:HD3	1.76	0.46
2:D:276:ALA:O	2:D:277:ARG:C	2.53	0.46
2:K:120:LEU:HD12	2:K:125:LEU:HD12	1.97	0.46
2:K:236:PHE:CE1	2:K:328:THR:HG21	2.51	0.46
2:K:56:ALA:CA	2:K:59:ASN:HD22	2.28	0.46
2:D:126:GLU:O	2:D:130:THR:HG23	2.15	0.46
2:D:196:LEU:HD13	2:D:339:VAL:CG2	2.46	0.46
1:E:16:ALA:O	1:E:20:VAL:HG23	2.15	0.46
1:G:59:LYS:O	1:G:60:ILE:C	2.54	0.46
1:G:72:ASP:OD1	1:G:72:ASP:N	2.49	0.46
2:K:170:PRO:O	2:K:171:LYS:CG	2.63	0.46
2:D:76:VAL:HB	2:K:264:SER:OG	2.15	0.46
2:K:253:GLU:CG	2:K:319:ILE:HD11	2.45	0.46
2:K:82:LYS:HB2	2:K:88:ASP:OD1	2.16	0.46
3:R:733:DC:H42	4:T:687:DG:H1	1.62	0.46
1:C:28:GLN:HE22	1:C:43:SER:N	2.14	0.46
2:D:323:GLY:O	1:E:12:GLN:OE1	2.34	0.46
2:D:49:ARG:H	1:E:22:GLN:HE22	1.61	0.46
2:D:61:PHE:HA	2:D:64:LEU:HG	1.98	0.46
2:K:118:GLU:O	2:K:120:LEU:N	2.49	0.46
2:K:167:TRP:C	2:K:168:CYS:SG	2.93	0.46
2:K:4:LEU:CD2	2:K:105:PRO:HG3	2.45	0.46
1:B:21:ARG:CZ	1:B:28:GLN:HG3	2.46	0.46
2:K:274:GLY:O	2:K:278:ILE:HG13	2.16	0.46
2:K:279:MET:CE	2:K:296:MET:CE	2.94	0.46
2:K:386:VAL:HG13	2:K:387:GLN:H	1.81	0.46
4:T:697:DT:H2''	4:T:698:DA:C8	2.51	0.46
2:D:279:MET:N	2:D:279:MET:SD	2.87	0.46
2:D:202:ASN:HD22	2:D:338:PRO:CG	2.27	0.46
2:D:370:TYR:HB2	2:D:372:ARG:HG2	1.98	0.46
2:D:76:VAL:CB	2:D:81:ALA:HB3	2.46	0.46
2:K:177:THR:C	2:K:235:ARG:HG3	2.36	0.46
4:T:683:DA:H1'	4:T:684:DG:C5'	2.42	0.46
2:D:296:MET:O	2:D:299:GLN:N	2.49	0.45
1:E:68:MET:HB2	1:E:68:MET:HE3	1.83	0.45
2:K:377:THR:C	2:K:380:VAL:HG22	2.37	0.45
3:R:707:DC:H2''	3:R:708:DT:H72	1.98	0.45
4:T:694:DA:H2''	4:T:695:DT:H5'	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:39:GLN:HA	1:C:42:ILE:HG13	1.97	0.45
1:E:7:ILE:HG23	1:E:12:GLN:NE2	2.31	0.45
1:G:38:LYS:HE3	1:G:40:ALA:HB3	1.98	0.45
2:K:4:LEU:HA	2:K:105:PRO:HA	1.98	0.45
2:K:337:PHE:HA	2:K:340:LEU:HD12	1.98	0.45
2:K:8:MET:HG2	2:K:32:TRP:CZ2	2.51	0.45
4:T:692:DA:H2"	4:T:693:DT:C6	2.51	0.45
2:D:11:GLN:HA	2:D:11:GLN:OE1	2.16	0.45
2:K:237:ASP:HB3	2:K:252:GLN:HG2	1.97	0.45
3:R:728:DA:C2'	3:R:729:DT:H72	2.46	0.45
3:R:727:DT:O2	4:T:692:DA:N1	2.49	0.45
2:D:160:LEU:HB2	2:D:180:ILE:HD11	1.98	0.45
2:D:255:MET:HE1	2:D:278:ILE:HA	1.96	0.45
2:D:279:MET:HA	2:D:282:LEU:CG	2.46	0.45
2:D:304:LEU:HD11	2:D:433:LEU:CD1	2.47	0.45
2:D:41:LEU:CD1	2:D:41:LEU:N	2.79	0.45
1:E:29:SER:HA	1:E:39:GLN:CG	2.46	0.45
2:K:5:VAL:HA	2:K:15:GLU:CG	2.46	0.45
2:K:12:ARG:C	2:K:29:ALA:HB3	2.36	0.45
2:D:7:TRP:HA	2:D:13:VAL:HG23	1.99	0.45
2:D:207:LEU:HD21	2:D:218:PRO:O	2.17	0.45
2:D:314:ASN:HA	2:D:331:TYR:HE1	1.81	0.45
2:D:337:PHE:N	2:D:338:PRO:HD3	2.32	0.45
2:D:5:VAL:HG13	2:D:14:GLY:O	2.16	0.45
2:K:313:LYS:HG2	2:K:313:LYS:O	2.16	0.45
2:K:366:ILE:HG22	2:K:367:ASP:N	2.31	0.45
2:K:377:THR:O	2:K:380:VAL:CG2	2.61	0.45
3:R:741:DG:C5	3:R:742:DG:N7	2.85	0.45
1:B:24:ASN:HA	1:B:24:ASN:HD22	1.51	0.45
2:D:196:LEU:HD13	2:D:339:VAL:HG23	1.97	0.45
2:D:37:TYR:O	2:D:38:ALA:O	2.34	0.45
1:E:55:THR:O	1:E:56:THR:C	2.54	0.45
1:E:54:LEU:CD2	1:E:58:PHE:HE1	2.30	0.45
2:K:112:HIS:O	2:K:114:ILE:N	2.49	0.45
2:K:295:PHE:O	2:K:296:MET:C	2.55	0.45
2:K:64:LEU:HD12	2:K:90:LEU:HD13	1.99	0.45
2:K:9:ASN:O	2:K:10:ASN:CB	2.61	0.45
1:C:71:CYS:N	1:G:67:SER:O	2.49	0.45
2:D:21:ASN:ND2	2:D:21:ASN:N	2.63	0.45
2:D:275:ILE:HG13	2:D:354:MET:HB3	1.98	0.45
2:D:384:PRO:HB2	2:D:387:GLN:HG3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:388:MET:CE	2:D:391:ILE:HD12	2.46	0.45
1:E:13:LEU:HD21	1:E:57:PHE:CE1	2.52	0.45
2:D:322:GLY:HA3	1:E:5:GLN:HB3	1.97	0.45
2:K:5:VAL:HG23	2:K:105:PRO:O	2.17	0.45
1:B:44:ASN:O	1:B:45:PHE:C	2.54	0.45
1:B:8:TYR:C	1:E:58:PHE:CD2	2.90	0.45
1:G:55:THR:O	1:G:59:LYS:HG3	2.17	0.45
1:G:64:LEU:HG	1:G:64:LEU:H	1.59	0.45
2:K:202:ASN:ND2	2:K:334:ILE:HG13	2.32	0.45
2:K:337:PHE:HB2	2:K:422:VAL:HG22	1.99	0.45
2:K:93:ILE:HD13	2:K:93:ILE:N	2.24	0.45
2:D:40:PRO:HG3	2:D:46:PRO:HA	1.98	0.45
2:K:67:ASP:OD2	2:K:263:SER:O	2.33	0.45
2:K:236:PHE:HE1	2:K:328:THR:HG21	1.81	0.45
2:K:27:LYS:CA	2:K:52:ILE:HD11	2.44	0.45
2:K:76:VAL:HA	2:K:81:ALA:HB3	1.97	0.45
2:K:7:TRP:HE1	2:K:12:ARG:HH12	1.58	0.45
1:E:43:SER:OG	4:T:702:DA:OP2	2.28	0.45
2:D:120:LEU:HD22	2:D:124:ARG:HB3	1.98	0.45
2:D:243:GLU:O	2:D:245:THR:HG23	2.17	0.45
2:D:24:HIS:O	2:D:57:VAL:HB	2.17	0.45
2:D:302:GLN:HE22	2:D:315:PHE:HZ	1.65	0.45
2:D:305:ILE:CD1	2:D:307:ALA:HB2	2.45	0.45
2:D:286:SER:OG	2:D:325:TYR:O	2.33	0.45
2:D:97:SER:O	2:D:98:VAL:C	2.55	0.45
1:E:61:LEU:HD22	1:E:66:LEU:C	2.36	0.45
2:K:56:ALA:O	2:K:59:ASN:HB2	2.17	0.45
3:R:712:DG:C5	3:R:713:DG:N7	2.85	0.45
2:D:160:LEU:HA	2:D:160:LEU:HD23	1.86	0.44
2:D:355:GLY:HA3	2:D:362:LYS:NZ	2.32	0.44
2:D:75:ILE:O	2:D:76:VAL:C	2.53	0.44
2:K:161:LEU:CD1	2:K:177:THR:N	2.80	0.44
2:K:202:ASN:CG	2:K:334:ILE:HG13	2.37	0.44
2:K:251:PRO:CB	2:K:319:ILE:HB	2.47	0.44
2:K:40:PRO:N	2:K:47:LEU:HD21	2.32	0.44
3:R:712:DG:H1'	3:R:713:DG:H5'	1.98	0.44
1:B:18:LYS:O	1:B:19:LEU:C	2.54	0.44
1:B:27:THR:CG2	1:B:30:GLU:HG3	2.47	0.44
1:C:53:THR:CG2	1:G:51:ASN:C	2.86	0.44
2:D:16:LEU:HB2	2:D:26:PHE:CE1	2.51	0.44
2:D:278:ILE:HG22	2:D:282:LEU:HD11	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:50:GLY:O	2:D:51:ASN:C	2.55	0.44
1:E:28:GLN:HE21	1:E:42:ILE:HG22	1.82	0.44
1:E:17:MET:CE	1:E:64:LEU:HD12	2.46	0.44
1:G:42:ILE:CD1	1:G:60:ILE:HG12	2.47	0.44
2:K:352:LEU:HD23	2:K:353:ALA:N	2.32	0.44
2:K:415:PRO:HB2	2:K:417:ASN:HD21	1.82	0.44
1:C:67:SER:O	1:G:70:LEU:HD23	2.17	0.44
2:D:161:LEU:HD12	2:D:177:THR:CG2	2.48	0.44
2:K:292:ARG:O	2:K:295:PHE:HB3	2.17	0.44
2:K:256:CYS:CA	2:K:261:LEU:HD12	2.37	0.44
2:K:44:SER:O	2:K:46:PRO:CD	2.66	0.44
2:K:83:SER:H	2:K:88:ASP:CB	2.31	0.44
3:R:737:DT:C1'	3:R:738:DA:O5'	2.63	0.44
2:D:315:PHE:N	2:D:315:PHE:CD1	2.85	0.44
2:D:371:PRO:O	2:D:372:ARG:C	2.56	0.44
1:E:27:THR:HG23	1:E:30:GLU:OE1	2.17	0.44
2:K:161:LEU:CD1	2:K:176:THR:HA	2.40	0.44
2:K:239:ARG:HG2	2:K:240:TRP:N	2.29	0.44
2:K:39:ARG:NH1	2:K:319:ILE:O	2.44	0.44
2:K:399:ILE:CG2	2:K:400:PRO:N	2.80	0.44
2:K:40:PRO:HB3	2:K:47:LEU:CD2	2.48	0.44
2:K:40:PRO:CD	2:K:47:LEU:HG	2.46	0.44
3:R:717:DT:H2"	3:R:718:DA:C8	2.51	0.44
2:D:112:HIS:HB3	2:D:113:PRO:HD2	2.00	0.44
2:D:301:PHE:C	2:D:303:TRP:N	2.71	0.44
2:D:45:LEU:N	2:D:45:LEU:HD12	2.32	0.44
2:K:124:ARG:O	2:K:125:LEU:C	2.55	0.44
4:T:700:DA:H3'	4:T:700:DA:P	2.58	0.44
1:C:27:THR:OG1	1:C:28:GLN:N	2.51	0.44
1:C:59:LYS:O	1:C:63:SER:HB3	2.18	0.44
2:D:63:ASN:HB3	2:D:313:LYS:HZ3	1.81	0.44
2:D:44:SER:CB	2:D:45:LEU:HD12	2.47	0.44
2:D:71:VAL:HG12	2:D:75:ILE:CD1	2.48	0.44
2:K:12:ARG:HB3	2:K:31:GLU:CD	2.37	0.44
2:K:243:GLU:H	2:K:243:GLU:HG2	1.28	0.44
2:K:255:MET:HG2	2:K:315:PHE:HB2	2.00	0.44
2:K:321:ALA:O	2:K:323:GLY:N	2.51	0.44
2:K:395:PHE:HB3	2:K:399:ILE:HD13	1.99	0.44
2:K:82:LYS:HB2	2:K:88:ASP:CG	2.38	0.44
2:K:86:PRO:O	2:K:90:LEU:HB2	2.18	0.44
3:R:728:DA:C1'	3:R:729:DT:H72	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:713:DG:O6	4:T:706:DC:N3	2.50	0.44
2:D:156:GLU:O	2:D:182:LEU:HD23	2.18	0.44
2:D:75:ILE:CB	2:D:89:LEU:HD23	2.47	0.44
2:K:248:LEU:HG	2:K:248:LEU:H	1.43	0.44
2:K:28:TYR:HE1	2:K:48:GLN:H	1.64	0.44
2:D:402:ALA:HA	2:D:405:ASN:HD22	1.82	0.44
2:D:38:ALA:CB	2:D:47:LEU:HD11	2.34	0.44
2:K:289:LEU:CD1	2:K:289:LEU:N	2.75	0.44
2:K:93:ILE:H	2:K:93:ILE:CD1	2.23	0.44
1:B:18:LYS:HG2	1:B:22:GLN:HG3	2.00	0.43
2:D:50:GLY:O	2:D:52:ILE:HD13	2.18	0.43
1:E:16:ALA:C	1:E:18:LYS:N	2.66	0.43
1:E:45:PHE:HD1	1:E:49:PRO:HB3	1.78	0.43
1:G:37:ILE:HD11	1:G:42:ILE:HG12	2.00	0.43
2:K:241:ASN:HD22	2:K:246:VAL:HB	1.82	0.43
4:T:693:DT:H2"	4:T:694:DA:O5'	2.18	0.43
2:D:95:ARG:HB2	2:D:148:ARG:HB3	2.00	0.43
2:D:243:GLU:C	2:D:245:THR:H	2.20	0.43
1:B:34:LYS:HA	2:D:384:PRO:HG2	1.99	0.43
2:D:429:LEU:HD23	2:D:432:ARG:NH1	2.33	0.43
2:K:196:LEU:HD22	2:K:196:LEU:N	2.33	0.43
2:K:350:LEU:O	2:K:351:LYS:HD3	2.18	0.43
2:D:119:LYS:HD3	2:D:166:ASP:CG	2.38	0.43
2:D:130:THR:HA	2:D:133:LYS:CG	2.49	0.43
2:D:291:ASP:OD1	2:D:327:LEU:N	2.38	0.43
2:D:63:ASN:HB2	2:D:257:GLN:NE2	2.33	0.43
1:E:45:PHE:O	1:E:49:PRO:HD3	2.18	0.43
2:K:129:LEU:HA	2:K:132:TYR:CD1	2.53	0.43
2:K:162:ARG:HD3	2:K:167:TRP:CZ3	2.53	0.43
2:K:161:LEU:HD12	2:K:177:THR:H	1.83	0.43
2:K:220:ALA:HB1	2:K:233:VAL:HA	2.01	0.43
2:K:290:LYS:CE	2:K:294:ASP:OD2	2.66	0.43
2:K:314:ASN:HA	2:K:331:TYR:HE1	1.82	0.43
1:B:18:LYS:C	1:B:20:VAL:N	2.69	0.43
2:D:291:ASP:HB3	2:D:327:LEU:CB	2.48	0.43
2:D:384:PRO:HG2	2:D:387:GLN:NE2	2.32	0.43
2:K:120:LEU:HB2	2:K:125:LEU:HD12	2.00	0.43
2:K:205:TYR:HE2	2:K:209:LEU:HD22	1.83	0.43
2:K:259:PHE:CD1	2:K:259:PHE:N	2.86	0.43
2:K:279:MET:SD	2:K:295:PHE:HD2	2.41	0.43
2:K:255:MET:HG2	2:K:315:PHE:CB	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:744:DA:C2	4:T:676:DC:N3	2.87	0.43
4:T:699:DT:H1'	4:T:700:DA:O5'	2.18	0.43
2:D:66:PRO:HG3	2:D:151:VAL:O	2.19	0.43
1:G:12:GLN:HA	1:G:15:ASN:HB2	2.00	0.43
1:G:29:SER:CB	1:G:39:GLN:HG3	2.39	0.43
2:K:116:ALA:CB	2:K:171:LYS:HD3	2.47	0.43
2:K:121:THR:O	2:K:125:LEU:HB2	2.18	0.43
2:K:204:TYR:CD2	2:K:222:ILE:HD11	2.54	0.43
3:R:707:DC:C2'	3:R:708:DT:H72	2.49	0.43
1:B:52:THR:HG22	1:B:53:THR:H	1.82	0.43
2:D:133:LYS:CA	2:D:156:GLU:HG2	2.45	0.43
2:D:70:ILE:O	2:D:74:ARG:HG3	2.18	0.43
1:G:43:SER:O	1:G:46:GLU:N	2.51	0.43
2:K:13:VAL:HG11	2:K:41:LEU:CD1	2.42	0.43
2:K:173:ILE:HG13	2:K:173:ILE:H	1.61	0.43
2:K:235:ARG:NH1	2:K:238:ARG:NH2	2.67	0.43
2:K:316:SER:OG	2:K:331:TYR:OH	2.34	0.43
2:K:83:SER:HB3	2:K:88:ASP:OD2	2.18	0.43
4:T:699:DT:H2''	4:T:700:DA:O5'	2.19	0.43
1:B:37:ILE:HD12	1:B:41:THR:HG22	2.01	0.43
2:D:45:LEU:HD11	2:D:56:ALA:HB1	2.00	0.43
1:G:33:LYS:C	1:G:35:ILE:H	2.22	0.43
2:K:297:LYS:O	2:K:298:PHE:C	2.55	0.43
4:T:684:DG:OP2	1:C:41:THR:HG23	2.18	0.43
2:D:177:THR:OG1	2:D:178:HIS:N	2.52	0.43
2:D:301:PHE:HE1	2:D:305:ILE:HG21	1.84	0.43
2:D:39:ARG:HD3	2:D:319:ILE:CG2	2.42	0.43
2:D:16:LEU:CD2	2:D:61:PHE:CE2	2.89	0.43
1:C:67:SER:C	1:G:70:LEU:HD23	2.38	0.43
2:K:113:PRO:C	2:K:115:MET:N	2.72	0.43
2:K:387:GLN:O	2:K:388:MET:C	2.55	0.43
2:K:62:ASP:OD2	2:K:86:PRO:HG2	2.18	0.43
3:R:716:DA:H2''	3:R:717:DT:OP2	2.18	0.43
1:B:18:LYS:CG	1:B:21:ARG:HH11	2.32	0.43
2:D:39:ARG:HH21	2:D:321:ALA:HB2	1.82	0.43
1:E:20:VAL:O	1:E:21:ARG:C	2.55	0.43
2:K:231:LEU:HA	2:K:231:LEU:HD12	1.82	0.43
2:D:26:PHE:O	2:D:52:ILE:HG12	2.19	0.43
2:D:266:LYS:HZ2	2:D:313:LYS:HD2	1.83	0.43
2:D:356:LEU:HD13	2:D:369:ILE:HD12	2.00	0.43
1:E:28:GLN:HB2	4:T:701:DT:OP2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:28:GLN:HG2	1:E:42:ILE:CG2	2.49	0.43
2:K:239:ARG:O	2:K:248:LEU:HD12	2.19	0.43
3:R:729:DT:H2"	1:C:43:SER:OG	2.19	0.42
2:D:380:VAL:HG23	2:D:381:LEU:N	2.34	0.42
2:D:71:VAL:O	2:D:74:ARG:HB2	2.18	0.42
1:G:24:ASN:OD1	1:G:24:ASN:N	2.52	0.42
2:K:90:LEU:O	2:K:94:GLY:HA3	2.19	0.42
3:R:729:DT:H2"	3:R:730:DA:OP2	2.19	0.42
2:D:44:SER:C	2:D:45:LEU:HD12	2.40	0.42
2:K:110:VAL:HG11	2:K:112:HIS:CE1	2.55	0.42
2:K:197:SER:C	2:K:198:GLN:HG3	2.39	0.42
2:K:255:MET:HA	2:K:258:THR:OG1	2.19	0.42
2:K:29:ALA:O	2:K:31:GLU:N	2.52	0.42
1:B:37:ILE:HD12	1:B:41:THR:HG21	2.00	0.42
1:B:7:ILE:C	1:B:8:TYR:CG	2.93	0.42
1:C:6:LYS:NZ	1:C:72:ASP:H	2.17	0.42
2:D:176:THR:O	2:D:247:LEU:HD21	2.19	0.42
2:K:235:ARG:HH12	2:K:238:ARG:NH2	2.18	0.42
2:K:275:ILE:HG22	2:K:275:ILE:O	2.19	0.42
2:K:281:PHE:C	2:K:283:MET:N	2.71	0.42
2:K:337:PHE:HD1	2:K:422:VAL:HG13	1.84	0.42
2:K:28:TYR:HE1	2:K:47:LEU:HA	1.84	0.42
1:E:41:THR:HG22	3:R:712:DG:OP2	2.20	0.42
1:B:28:GLN:HG2	1:B:42:ILE:HG22	2.01	0.42
1:C:70:LEU:C	1:C:71:CYS:SG	2.98	0.42
2:D:254:ASP:O	2:D:257:GLN:HB2	2.19	0.42
2:D:287:GLU:OE1	2:D:326:ARG:CZ	2.66	0.42
2:D:32:TRP:C	2:D:32:TRP:CD1	2.93	0.42
2:D:41:LEU:N	2:D:41:LEU:HD12	2.34	0.42
1:E:38:LYS:HD3	3:R:713:DG:C8	2.55	0.42
2:K:240:TRP:CZ2	2:K:247:LEU:HD12	2.54	0.42
2:K:279:MET:HG3	2:K:381:LEU:HD22	2.01	0.42
2:K:67:ASP:CG	2:K:263:SER:HB2	2.40	0.42
2:K:75:ILE:HG22	2:K:75:ILE:O	2.18	0.42
1:E:49:PRO:O	1:E:52:THR:OG1	2.37	0.42
2:K:27:LYS:HA	2:K:50:GLY:O	2.19	0.42
1:B:45:PHE:O	1:B:49:PRO:HB3	2.19	0.42
1:C:43:SER:O	1:C:47:ASN:ND2	2.52	0.42
1:C:62:GLN:C	1:C:64:LEU:N	2.72	0.42
2:D:93:ILE:HD12	2:D:150:SER:OG	2.19	0.42
2:D:355:GLY:HA3	2:D:362:LYS:HZ3	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:4:LEU:O	2:D:16:LEU:HB3	2.18	0.42
2:D:80:HIS:O	2:D:81:ALA:O	2.38	0.42
1:G:29:SER:HA	1:G:39:GLN:HB2	2.00	0.42
2:D:24:HIS:ND1	2:K:21:ASN:O	2.53	0.42
2:K:371:PRO:O	2:K:372:ARG:C	2.57	0.42
2:K:376:ALA:C	2:K:378:ALA:N	2.71	0.42
2:D:291:ASP:HB3	2:D:327:LEU:HB3	2.02	0.42
1:E:52:THR:HG22	1:E:53:THR:N	2.33	0.42
2:K:32:TRP:O	2:K:38:ALA:HB2	2.20	0.42
2:K:366:ILE:HD12	2:K:366:ILE:N	2.35	0.42
1:B:21:ARG:HG3	1:B:22:GLN:N	2.35	0.42
1:C:21:ARG:NH2	1:C:28:GLN:N	2.68	0.42
2:D:125:LEU:C	2:D:225:ALA:HB1	2.40	0.42
2:D:228:VAL:O	2:D:228:VAL:HG13	2.19	0.42
2:D:254:ASP:HB3	2:D:316:SER:OG	2.20	0.42
2:D:362:LYS:HB3	2:D:362:LYS:HE2	1.93	0.42
1:E:61:LEU:HD22	1:E:66:LEU:O	2.19	0.42
1:C:73:ALA:HB2	1:G:66:LEU:C	2.40	0.42
2:K:178:HIS:HB3	2:K:179:ILE:H	1.63	0.42
2:K:98:VAL:HG12	2:K:252:GLN:OE1	2.18	0.42
3:R:713:DG:H1'	3:R:714:DG:H5''	2.00	0.42
2:D:155:GLN:HB3	2:D:156:GLU:H	1.50	0.42
2:D:29:ALA:HA	2:D:30:PRO:HD3	1.81	0.42
2:D:39:ARG:CD	2:D:319:ILE:HG22	2.41	0.42
2:D:83:SER:HG	2:D:85:GLN:HB2	1.82	0.42
1:E:23:GLN:HA	1:E:23:GLN:HE21	1.85	0.42
1:E:32:ALA:HB2	1:E:42:ILE:HG13	2.01	0.42
1:G:61:LEU:O	1:G:64:LEU:N	2.53	0.42
2:K:340:LEU:CD1	2:K:350:LEU:HD11	2.47	0.42
2:K:373:HIS:O	2:K:374:PHE:C	2.58	0.42
2:K:374:PHE:HD1	2:K:374:PHE:H	1.68	0.42
2:D:103:LEU:HD23	2:D:103:LEU:HA	1.88	0.42
2:D:151:VAL:HG21	2:D:158:THR:HA	2.02	0.42
2:D:161:LEU:HD21	2:D:163:ILE:HD11	2.02	0.42
2:D:253:GLU:CD	2:D:258:THR:HA	2.40	0.42
2:D:65:LEU:HD13	2:D:89:LEU:CB	2.48	0.42
2:D:65:LEU:CD2	2:D:93:ILE:HD11	2.50	0.42
2:K:111:THR:HG22	2:K:114:ILE:CD1	2.21	0.42
4:T:713:DG:H1'	4:T:714:DG:H8	1.85	0.42
2:D:236:PHE:N	2:D:236:PHE:CD1	2.85	0.41
2:D:93:ILE:HG13	2:D:93:ILE:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:56:THR:O	1:E:57:PHE:C	2.58	0.41
1:E:54:LEU:O	1:E:57:PHE:HB3	2.20	0.41
1:G:6:LYS:HE3	1:G:71:CYS:HB3	2.02	0.41
2:K:327:LEU:CD2	2:K:328:THR:O	2.68	0.41
2:K:376:ALA:O	2:K:380:VAL:HG13	2.20	0.41
2:K:51:ASN:C	2:K:52:ILE:HD13	2.41	0.41
2:K:6:THR:OG1	2:K:103:LEU:HD21	2.19	0.41
2:K:64:LEU:HD12	2:K:90:LEU:CD1	2.50	0.41
3:R:715:DG:H1	4:T:704:DC:N4	2.18	0.41
3:R:721:DT:C2	3:R:722:DA:N7	2.88	0.41
2:D:182:LEU:HD22	2:D:182:LEU:N	2.35	0.41
2:D:236:PHE:CZ	2:D:331:TYR:HD2	2.39	0.41
2:D:356:LEU:CB	2:D:363:LYS:O	2.62	0.41
2:D:377:THR:O	2:D:380:VAL:N	2.53	0.41
2:D:47:LEU:N	2:D:47:LEU:HD23	2.34	0.41
2:K:299:GLN:NE2	2:K:302:GLN:NE2	2.69	0.41
2:K:28:TYR:OH	2:K:46:PRO:O	2.26	0.41
3:R:708:DT:H2'	3:R:709:DT:H71	2.01	0.41
2:D:37:TYR:O	2:D:38:ALA:C	2.59	0.41
2:D:397:ARG:NE	2:D:398:MET:HG3	2.35	0.41
2:D:44:SER:HB3	2:D:258:THR:O	2.20	0.41
2:D:5:VAL:HG12	2:D:7:TRP:NE1	2.34	0.41
1:G:43:SER:O	1:G:44:ASN:C	2.58	0.41
2:K:120:LEU:HD21	2:K:169:ILE:CG1	2.49	0.41
2:K:298:PHE:O	2:K:301:PHE:CB	2.60	0.41
3:R:728:DA:O4'	4:T:692:DA:H2	2.04	0.41
2:D:7:TRP:CZ2	2:D:12:ARG:NH1	2.88	0.41
1:E:28:GLN:NE2	1:E:43:SER:HA	2.35	0.41
1:G:58:PHE:O	1:G:59:LYS:C	2.57	0.41
2:K:394:ASP:O	2:K:395:PHE:C	2.59	0.41
4:T:682:DA:N3	4:T:683:DA:C6	2.89	0.41
4:T:689:DT:H2''	4:T:690:DA:OP2	2.20	0.41
1:B:28:GLN:HG2	1:B:42:ILE:CG2	2.50	0.41
1:B:58:PHE:O	1:B:59:LYS:C	2.57	0.41
1:B:7:ILE:HG12	1:E:68:MET:O	2.20	0.41
2:D:237:ASP:HB2	2:D:238:ARG:HH12	1.86	0.41
2:D:279:MET:SD	2:D:282:LEU:HD11	2.61	0.41
2:D:58:PHE:CE1	2:D:86:PRO:HG2	2.55	0.41
1:G:39:GLN:HE21	1:G:39:GLN:HB3	1.61	0.41
2:K:206:CYS:O	2:K:210:ALA:CB	2.61	0.41
2:K:39:ARG:HG3	2:K:39:ARG:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:385:GLU:HG2	2:D:389:HIS:NE2	2.36	0.41
2:D:42:SER:HB3	2:D:44:SER:OG	2.21	0.41
1:G:31:LEU:HD22	1:G:63:SER:CB	2.51	0.41
2:K:149:ILE:HG21	2:K:159:ALA:HB3	2.02	0.41
2:K:171:LYS:O	2:K:174:THR:CB	2.68	0.41
2:K:149:ILE:HG21	2:K:176:THR:HG21	2.03	0.41
2:K:19:LEU:HD12	2:K:23:ALA:O	2.21	0.41
2:K:265:VAL:HA	2:K:270:ASP:HB2	2.02	0.41
2:K:310:GLY:C	2:K:353:ALA:HB1	2.41	0.41
3:R:707:DC:H2''	3:R:708:DT:C7	2.51	0.41
4:T:689:DT:H1'	4:T:690:DA:C8	2.56	0.41
1:B:64:LEU:C	1:B:66:LEU:N	2.73	0.41
2:D:240:TRP:CD1	2:D:247:LEU:HD13	2.56	0.41
2:D:96:ASP:HB3	2:D:149:ILE:HA	2.02	0.41
2:D:96:ASP:OD1	2:D:96:ASP:C	2.58	0.41
1:E:70:LEU:N	1:E:70:LEU:CD2	2.67	0.41
2:K:385:GLU:HG2	2:K:389:HIS:NE2	2.36	0.41
2:K:393:SER:O	2:K:394:ASP:C	2.58	0.41
1:B:18:LYS:O	1:B:20:VAL:N	2.54	0.41
2:D:183:PRO:HA	2:D:199:SER:OG	2.21	0.41
2:D:209:LEU:HD12	2:D:212:GLU:HB3	2.03	0.41
2:D:179:ILE:CG1	2:D:235:ARG:HG2	2.50	0.41
2:D:253:GLU:OE2	2:D:257:GLN:CB	2.68	0.41
2:D:300:VAL:HA	2:D:374:PHE:HE2	1.85	0.41
2:D:40:PRO:CG	2:D:46:PRO:HA	2.50	0.41
2:D:65:LEU:CD1	2:D:90:LEU:HG	2.42	0.41
1:E:28:GLN:HG2	1:E:42:ILE:HG22	2.03	0.41
1:G:68:MET:HE3	1:G:68:MET:HB2	1.84	0.41
2:K:108:GLU:HG2	2:K:110:VAL:HG23	2.03	0.41
2:K:241:ASN:C	2:K:241:ASN:OD1	2.59	0.41
2:K:293:TYR:O	2:K:295:PHE:N	2.54	0.41
1:B:11:THR:O	1:B:15:ASN:CG	2.59	0.41
2:K:365:ALA:HB3	2:K:368:LYS:CB	2.32	0.41
2:K:28:TYR:CE1	2:K:47:LEU:HA	2.55	0.41
2:K:5:VAL:O	2:K:103:LEU:HD23	2.21	0.41
4:T:701:DT:H2''	4:T:702:DA:OP2	2.19	0.41
4:T:705:DC:H2''	4:T:706:DC:O5'	2.21	0.41
2:D:237:ASP:O	2:D:250:LEU:N	2.54	0.41
1:E:49:PRO:CA	1:E:52:THR:OG1	2.65	0.41
1:C:7:ILE:HB	1:G:68:MET:HG3	2.03	0.41
2:D:216:ASN:C	2:D:216:ASN:HD22	2.25	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:300:VAL:HA	2:D:374:PHE:CE2	2.56	0.41
2:K:300:VAL:CG1	2:K:303:TRP:HE3	2.34	0.41
1:C:39:GLN:HG2	1:C:39:GLN:O	2.20	0.40
2:D:255:MET:O	2:D:256:CYS:C	2.58	0.40
2:D:56:ALA:C	2:D:58:PHE:N	2.74	0.40
1:G:33:LYS:C	1:G:35:ILE:N	2.74	0.40
1:G:54:LEU:HA	1:G:57:PHE:HB3	2.03	0.40
1:G:62:GLN:OE1	1:G:62:GLN:N	2.53	0.40
2:K:157:LYS:HA	2:K:182:LEU:HD22	2.03	0.40
2:K:347:ILE:HG23	2:K:348:SER:N	2.36	0.40
2:D:132:TYR:CZ	2:D:147:PHE:CE1	3.09	0.40
2:D:44:SER:N	2:D:258:THR:O	2.54	0.40
2:D:90:LEU:O	2:D:91:SER:C	2.60	0.40
1:E:17:MET:HE2	1:E:64:LEU:CD1	2.51	0.40
1:E:32:ALA:HB1	1:E:38:LYS:C	2.42	0.40
1:E:63:SER:C	1:E:65:GLU:H	2.25	0.40
2:K:310:GLY:O	2:K:353:ALA:HB1	2.21	0.40
2:K:413:ASP:O	2:K:414:PHE:C	2.60	0.40
2:K:40:PRO:HB3	2:K:47:LEU:HD23	2.02	0.40
4:T:674:DA:H2''	4:T:675:DT:C5'	2.51	0.40
1:B:22:GLN:O	1:B:25:GLY:N	2.35	0.40
1:B:45:PHE:CD2	1:B:46:GLU:N	2.89	0.40
1:B:47:ASN:HD22	1:B:47:ASN:H	1.68	0.40
1:C:68:MET:O	1:G:7:ILE:CB	2.65	0.40
2:D:225:ALA:O	2:D:228:VAL:HG12	2.21	0.40
1:E:14:ALA:C	1:E:16:ALA:N	2.71	0.40
2:K:28:TYR:O	2:K:29:ALA:C	2.59	0.40
2:K:275:ILE:HD11	2:K:354:MET:HB2	2.04	0.40
4:T:672:DT:H3'	1:G:27:THR:HB	2.03	0.40
4:T:705:DC:C1'	4:T:706:DC:H5'	2.38	0.40
1:B:58:PHE:C	1:B:60:ILE:N	2.74	0.40
1:C:17:MET:HE2	1:C:64:LEU:CD1	2.48	0.40
1:C:21:ARG:O	1:C:25:GLY:N	2.55	0.40
2:D:178:HIS:HA	2:D:233:VAL:O	2.21	0.40
2:D:238:ARG:CZ	2:D:249:ARG:HD3	2.51	0.40
2:D:24:HIS:H	2:K:21:ASN:HB2	1.85	0.40
1:G:56:THR:O	1:G:60:ILE:HG13	2.22	0.40
2:K:102:THR:HG22	2:K:103:LEU:N	2.37	0.40
2:K:217:VAL:HB	2:K:218:PRO:HD2	2.02	0.40
2:K:266:LYS:HA	2:K:312:ALA:HB3	2.04	0.40
2:K:327:LEU:HD23	2:K:328:THR:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:376:ALA:C	2:K:378:ALA:H	2.25	0.40
2:K:55:ASP:O	2:K:56:ALA:C	2.58	0.40
1:B:16:ALA:O	1:B:20:VAL:HG23	2.22	0.40
2:D:18:LYS:HA	2:D:23:ALA:O	2.21	0.40
2:D:94:GLY:HA3	2:D:103:LEU:O	2.20	0.40
2:K:30:PRO:HA	2:K:33:LEU:HG	2.02	0.40
2:K:337:PHE:N	2:K:338:PRO:CD	2.84	0.40
2:K:5:VAL:HA	2:K:15:GLU:CB	2.51	0.40
3:R:723:DT:C2'	3:R:724:DA:H5''	2.51	0.40
3:R:724:DA:N1	4:T:695:DT:O2	2.54	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:111:THR:OG1	2:K:111:THR:OG1[7_555]	1.71	0.49
2:K:36:ARG:NH2	2:K:163:ILE:O[7_555]	1.82	0.38

## 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	B	67/71 (94%)	46 (69%)	19 (28%)	2 (3%)	5	46
1	C	69/71 (97%)	60 (87%)	9 (13%)	0	100	100
1	E	67/71 (94%)	52 (78%)	12 (18%)	3 (4%)	3	34
1	G	69/71 (97%)	49 (71%)	20 (29%)	0	100	100
2	D	408/436 (94%)	310 (76%)	83 (20%)	15 (4%)	4	40
2	K	406/436 (93%)	285 (70%)	96 (24%)	25 (6%)	2	27
All	All	1086/1156 (94%)	802 (74%)	239 (22%)	45 (4%)	3	37

All (45) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	38	ALA
2	D	81	ALA
2	D	95	ARG
2	D	100	ALA
2	D	105	PRO
2	K	100	ALA
2	K	105	PRO
2	K	108	GLU
2	K	119	LYS
1	B	8	TYR
2	D	243	GLU
2	D	365	ALA
2	K	46	PRO
2	K	50	GLY
2	K	57	VAL
2	K	114	ILE
2	K	170	PRO
2	K	109	THR
2	K	113	PRO
1	B	63	SER
2	D	113	PRO
2	D	173	ILE
2	K	30	PRO
2	K	321	ALA
2	D	397	ARG
1	E	10	PRO
1	E	50	ASP
1	E	64	LEU
2	K	153	GLY
2	K	267	TYR
2	K	384	PRO
2	D	34	ALA
2	D	310	GLY
2	K	171	LYS
2	K	173	ILE
2	K	412	THR
2	D	384	PRO
2	D	411	PRO
2	K	172	GLY
2	K	322	GLY
2	D	75	ILE
2	K	344	GLY

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Mol	Chain	Res	Type
2	K	29	ALA
2	K	183	PRO
2	K	419	VAL

### 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	B	63/64 (98%)	45 (71%)	18 (29%)	0	4
1	C	64/64 (100%)	52 (81%)	12 (19%)	2	14
1	E	63/64 (98%)	54 (86%)	9 (14%)	4	28
1	G	64/64 (100%)	52 (81%)	12 (19%)	2	14
2	D	352/371 (95%)	311 (88%)	41 (12%)	7	36
2	K	350/371 (94%)	291 (83%)	59 (17%)	2	19
All	All	956/998 (96%)	805 (84%)	151 (16%)	3	23

All (151) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	4	PHE
1	B	11	THR
1	B	13	LEU
1	B	15	ASN
1	B	22	GLN
1	B	23	GLN
1	B	24	ASN
1	B	30	GLU
1	B	33	LYS
1	B	39	GLN
1	B	41	THR
1	B	44	ASN
1	B	45	PHE
1	B	50	ASP
1	B	56	THR

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Mol	Chain	Res	Type
1	B	64	LEU
1	B	65	GLU
1	B	68	MET
2	D	17	THR
2	D	21	ASN
2	D	31	GLU
2	D	35	SER
2	D	36	ARG
2	D	39	ARG
2	D	53	THR
2	D	68	SER
2	D	73	ASP
2	D	84	ARG
2	D	95	ARG
2	D	96	ASP
2	D	97	SER
2	D	102	THR
2	D	111	THR
2	D	124	ARG
2	D	178	HIS
2	D	207	LEU
2	D	215	LEU
2	D	216	ASN
2	D	227	ASN
2	D	236	PHE
2	D	237	ASP
2	D	244	ARG
2	D	256	CYS
2	D	259	PHE
2	D	267	TYR
2	D	277	ARG
2	D	286	SER
2	D	298	PHE
2	D	320	GLN
2	D	328	THR
2	D	332	ASP
2	D	345	ILE
2	D	346	HIS
2	D	356	LEU
2	D	359	SER
2	D	360	LYS
2	D	382	ARG

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Mol	Chain	Res	Type
2	D	390	GLU
2	D	397	ARG
1	E	11	THR
1	E	12	GLN
1	E	13	LEU
1	E	21	ARG
1	E	41	THR
1	E	55	THR
1	E	61	LEU
1	E	68	MET
1	E	70	LEU
1	C	4	PHE
1	C	20	VAL
1	C	24	ASN
1	C	27	THR
1	C	30	GLU
1	C	39	GLN
1	C	43	SER
1	C	53	THR
1	C	55	THR
1	C	56	THR
1	C	61	LEU
1	C	72	ASP
1	G	13	LEU
1	G	21	ARG
1	G	24	ASN
1	G	34	LYS
1	G	39	GLN
1	G	53	THR
1	G	62	GLN
1	G	63	SER
1	G	64	LEU
1	G	68	MET
1	G	71	CYS
1	G	74	LYS
2	K	3	LYS
2	K	12	ARG
2	K	17	THR
2	K	21	ASN
2	K	28	TYR
2	K	31	GLU
2	K	41	LEU

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Mol	Chain	Res	Type
2	K	48	GLN
2	K	49	ARG
2	K	52	ILE
2	K	62	ASP
2	K	65	LEU
2	K	73	ASP
2	K	76	VAL
2	K	77	LYS
2	K	89	LEU
2	K	93	ILE
2	K	101	VAL
2	K	111	THR
2	K	117	TRP
2	K	118	GLU
2	K	124	ARG
2	K	156	GLU
2	K	158	THR
2	K	161	LEU
2	K	182	LEU
2	K	201	ASP
2	K	209	LEU
2	K	216	ASN
2	K	217	VAL
2	K	219	ASP
2	K	221	GLU
2	K	238	ARG
2	K	248	LEU
2	K	252	GLN
2	K	256	CYS
2	K	259	PHE
2	K	261	LEU
2	K	263	SER
2	K	264	SER
2	K	265	VAL
2	K	270	ASP
2	K	277	ARG
2	K	282	LEU
2	K	289	LEU
2	K	294	ASP
2	K	311	HIS
2	K	317	VAL
2	K	318	PHE

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Mol	Chain	Res	Type
2	K	324	SER
2	K	325	TYR
2	K	354	MET
2	K	381	LEU
2	K	386	VAL
2	K	399	ILE
2	K	404	ASP
2	K	417	ASN
2	K	420	THR
2	K	430	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	12	GLN
1	B	15	ASN
1	B	22	GLN
1	B	23	GLN
1	B	24	ASN
1	B	28	GLN
1	B	44	ASN
1	B	47	ASN
2	D	10	ASN
2	D	21	ASN
2	D	48	GLN
2	D	59	ASN
2	D	63	ASN
2	D	178	HIS
2	D	216	ASN
2	D	252	GLN
2	D	314	ASN
2	D	373	HIS
2	D	387	GLN
2	D	405	ASN
1	E	12	GLN
1	E	15	ASN
1	E	22	GLN
1	E	23	GLN
1	E	39	GLN
1	C	12	GLN
1	C	22	GLN
1	C	28	GLN

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Mol	Chain	Res	Type
1	C	39	GLN
1	C	44	ASN
1	C	51	ASN
1	G	12	GLN
1	G	15	ASN
1	G	22	GLN
1	G	39	GLN
2	K	59	ASN
2	K	85	GLN
2	K	112	HIS
2	K	216	ASN
2	K	252	GLN
2	K	257	GLN
2	K	299	GLN
2	K	302	GLN
2	K	311	HIS
2	K	314	ASN
2	K	346	HIS
2	K	357	ASN
2	K	387	GLN
2	K	425	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.



## 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	B	69/71 (97%)	0.65	7 (10%) 9 6	103, 167, 204, 211	0
1	C	71/71 (100%)	0.81	13 (18%) 2 1	132, 163, 195, 201	0
1	E	69/71 (97%)	0.62	7 (10%) 9 6	126, 151, 195, 206	0
1	G	71/71 (100%)	0.73	12 (16%) 2 2	60, 150, 183, 239	0
2	D	414/436 (94%)	0.89	87 (21%) 1 1	102, 194, 238, 254	0
2	K	412/436 (94%)	0.73	55 (13%) 4 4	103, 164, 230, 243	0
3	R	50/50 (100%)	-0.67	0 100 100	50, 198, 255, 261	0
4	T	50/50 (100%)	-0.79	0 100 100	128, 213, 260, 262	0
All	All	1206/1256 (96%)	0.66	181 (15%) 3 2	50, 174, 236, 262	0

All (181) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	K	89	LEU	10.4
2	K	90	LEU	10.2
2	K	154	ALA	9.6
2	D	224	LYS	9.4
2	K	156	GLU	8.7
2	D	230	ALA	7.7
2	K	87	PHE	7.5
2	K	75	ILE	7.4
2	K	91	SER	7.3
1	G	68	MET	6.8
2	K	155	GLN	6.7
1	C	54	LEU	6.6
2	K	69	PRO	6.3
2	K	73	ASP	6.3
2	D	273	PRO	5.7
2	D	429	LEU	5.5

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Mol	Chain	Res	Type	RSRZ
2	D	125	LEU	5.5
2	D	395	PHE	5.4
2	D	228	VAL	5.4
2	D	345	ILE	5.4
1	B	63	SER	5.3
2	K	264	SER	5.2
2	K	70	ILE	5.0
2	D	223	ILE	5.0
2	K	153	GLY	4.8
2	D	336	ALA	4.7
2	D	146	ASP	4.7
2	D	204	TYR	4.7
2	K	86	PRO	4.6
2	K	113	PRO	4.6
1	G	74	LYS	4.6
2	K	2	PRO	4.4
2	K	358	ALA	4.4
2	D	303	TRP	4.3
2	D	227	ASN	4.3
2	D	231	LEU	4.3
2	D	347	ILE	4.3
2	K	76	VAL	4.2
2	D	338	PRO	4.1
2	K	67	ASP	4.1
2	D	222	ILE	4.1
1	E	72	ASP	4.1
2	D	221	GLU	4.0
1	C	37	ILE	4.0
1	G	17	MET	3.9
2	D	427	LEU	3.8
2	K	84	ARG	3.8
2	D	41	LEU	3.8
2	K	330	PHE	3.8
1	C	60	ILE	3.8
2	D	330	PHE	3.8
2	D	304	LEU	3.7
2	K	359	SER	3.7
2	D	129	LEU	3.6
2	D	13	VAL	3.5
2	D	220	ALA	3.5
2	D	430	HIS	3.5
2	K	213	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
2	K	181	LYS	3.4
2	D	161	LEU	3.4
2	D	356	LEU	3.4
2	K	79	TYR	3.4
2	D	4	LEU	3.4
2	D	305	ILE	3.3
2	K	182	LEU	3.3
2	D	148	ARG	3.3
2	D	298	PHE	3.2
2	K	205	TYR	3.2
2	K	303	TRP	3.2
2	D	369	ILE	3.2
2	K	180	ILE	3.2
2	D	205	TYR	3.1
2	K	88	ASP	3.1
2	K	26	PHE	3.1
2	D	113	PRO	3.0
2	D	410	LEU	3.0
2	D	147	PHE	3.0
1	E	46	GLU	3.0
2	D	32	TRP	3.0
2	K	437	TYR	3.0
2	K	93	ILE	3.0
2	D	426	VAL	3.0
2	D	418	VAL	2.9
2	D	16	LEU	2.9
1	G	73	ALA	2.9
2	D	301	PHE	2.9
1	C	57	PHE	2.9
2	K	196	LEU	2.9
2	D	132	TYR	2.9
1	G	57	PHE	2.8
1	E	26	TRP	2.8
1	C	68	MET	2.8
2	D	247	LEU	2.8
1	B	70	LEU	2.7
2	D	229	ARG	2.7
2	D	297	LYS	2.7
1	C	17	MET	2.7
2	D	350	LEU	2.7
2	D	232	ALA	2.7
2	D	218	PRO	2.7

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Mol	Chain	Res	Type	RSRZ
2	D	86	PRO	2.7
1	E	45	PHE	2.7
2	D	82	LYS	2.7
2	D	357	ASN	2.6
2	D	337	PHE	2.6
2	D	428	ARG	2.6
1	B	4	PHE	2.6
1	G	60	ILE	2.6
2	D	14	GLY	2.6
2	D	255	MET	2.6
2	K	133	LYS	2.6
2	D	182	LEU	2.6
2	D	374	PHE	2.6
2	K	152	ALA	2.5
2	D	167	TRP	2.5
2	K	229	ARG	2.5
2	K	160	LEU	2.5
2	D	196	LEU	2.5
2	K	117	TRP	2.5
1	C	45	PHE	2.5
1	B	62	GLN	2.5
2	K	112	HIS	2.4
2	D	156	GLU	2.4
2	K	231	LEU	2.4
1	E	17	MET	2.4
2	K	333	ILE	2.3
2	K	215	LEU	2.3
2	D	2	PRO	2.3
2	D	340	LEU	2.3
1	E	31	LEU	2.3
2	D	327	LEU	2.3
2	K	100	ALA	2.3
2	K	148	ARG	2.3
2	D	6	THR	2.3
1	G	54	LEU	2.3
2	D	425	ASN	2.3
2	K	222	ILE	2.3
2	D	93	ILE	2.3
1	C	7	ILE	2.3
2	D	181	LYS	2.3
2	D	12	ARG	2.3
2	D	307	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
2	D	358	ALA	2.2
2	D	419	VAL	2.2
2	D	47	LEU	2.2
2	K	61	PHE	2.2
1	B	10	PRO	2.2
1	C	31	LEU	2.2
2	D	160	LEU	2.2
2	D	109	THR	2.2
2	D	423	GLU	2.2
2	K	167	TRP	2.2
2	D	149	ILE	2.2
2	D	359	SER	2.2
2	D	433	LEU	2.2
2	K	356	LEU	2.2
1	E	70	LEU	2.1
2	K	68	SER	2.1
2	D	432	ARG	2.1
2	D	295	PHE	2.1
2	K	157	LYS	2.1
1	G	31	LEU	2.1
2	K	41	LEU	2.1
1	C	35	ILE	2.1
1	G	64	LEU	2.1
1	B	42	ILE	2.1
1	G	10	PRO	2.1
2	D	283	MET	2.1
1	C	13	LEU	2.1
2	K	209	LEU	2.1
1	C	55	THR	2.0
2	K	245	THR	2.0
2	D	202	ASN	2.0
1	C	10	PRO	2.0
1	G	63	SER	2.0
1	G	13	LEU	2.0
2	D	171	LYS	2.0
2	D	352	LEU	2.0
1	B	17	MET	2.0
2	D	15	GLU	2.0
2	K	94	GLY	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](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.