



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 30, 2023 – 06:08 PM JST

PDB ID : 4X8F  
Title : Vibrio cholerae O395 Ribokinase in apo form  
Authors : Paul, R.; Patra, M.D.; Sen, U.  
Deposited on : 2014-12-10  
Resolution : 3.40 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

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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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) : 1.13  
EDS : 2.36  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

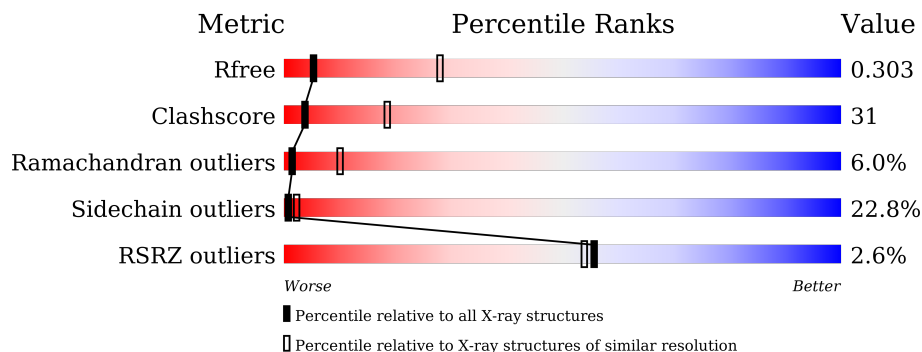
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.40 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

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

Mol	Chain	Length	Quality of chain
1	A	309	<div style="display: flex; align-items: center;"> <div style="width: 6%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 43%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 42%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 14%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey; margin-right: 5px;"></div> </div> <p style="font-size: small; margin-top: 5px;">6% 43% 42% 14% .</p>
1	B	309	<div style="display: flex; align-items: center;"> <div style="width: 4%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 36%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 45%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 17%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey; margin-right: 5px;"></div> </div> <p style="font-size: small; margin-top: 5px;">4% 36% 45% 17% ..</p>
1	C	309	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 40%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 44%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 14%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey; margin-right: 5px;"></div> </div> <p style="font-size: small; margin-top: 5px;">2% 40% 44% 14% ..</p>
1	D	309	<div style="display: flex; align-items: center;"> <div style="width: 0%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 40%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 44%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 14%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey; margin-right: 5px;"></div> </div> <p style="font-size: small; margin-top: 5px;">% 40% 44% 14% ..</p>
1	E	309	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 47%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 42%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 10%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey; margin-right: 5px;"></div> </div> <p style="font-size: small; margin-top: 5px;">2% 47% 42% 10% .</p>
1	F	309	<div style="display: flex; align-items: center;"> <div style="width: 0%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 36%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 50%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 12%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey; margin-right: 5px;"></div> </div> <p style="font-size: small; margin-top: 5px;">% 36% 50% 12% ..</p>

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Mol	Chain	Length	Quality of chain
1	G	309	<p>2% 32% 49% 17% ..</p>
1	H	309	<p>2% 36% 41% 20% ..</p>
1	I	309	<p>2% 42% 45% 11% .</p>
1	J	309	<p>2% 43% 44% 11% ..</p>
1	K	309	<p>2% 34% 48% 16% ..</p>
1	L	309	<p>2% 37% 51% 10% .</p>
1	M	309	<p>3% 46% 41% 12% .</p>
1	N	309	<p>3% 42% 43% 14% .</p>
1	O	309	<p>4% 39% 44% 15% .</p>
1	P	309	<p>8% 43% 44% 12% ..</p>

## 2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 36000 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 Ribokinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	306	2250	1408	391	441	10	0	0	0
1	B	306	2250	1408	391	441	10	0	0	0
1	C	306	2250	1408	391	441	10	0	0	0
1	D	306	2250	1408	391	441	10	0	0	0
1	E	306	2250	1408	391	441	10	0	0	0
1	F	306	2250	1408	391	441	10	0	0	0
1	G	306	2250	1408	391	441	10	0	0	0
1	H	306	2250	1408	391	441	10	0	0	0
1	I	306	2250	1408	391	441	10	0	0	0
1	J	306	2250	1408	391	441	10	0	0	0
1	K	306	2250	1408	391	441	10	0	0	0
1	L	306	2250	1408	391	441	10	0	0	0
1	M	306	2250	1408	391	441	10	0	0	0
1	N	306	2250	1408	391	441	10	0	0	0
1	O	306	2250	1408	391	441	10	0	0	0
1	P	306	2250	1408	391	441	10	0	0	0

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP A5F1B7
A	-1	SER	-	expression tag	UNP A5F1B7
A	0	HIS	-	expression tag	UNP A5F1B7
B	-2	GLY	-	expression tag	UNP A5F1B7
B	-1	SER	-	expression tag	UNP A5F1B7
B	0	HIS	-	expression tag	UNP A5F1B7
C	-2	GLY	-	expression tag	UNP A5F1B7
C	-1	SER	-	expression tag	UNP A5F1B7
C	0	HIS	-	expression tag	UNP A5F1B7
D	-2	GLY	-	expression tag	UNP A5F1B7
D	-1	SER	-	expression tag	UNP A5F1B7
D	0	HIS	-	expression tag	UNP A5F1B7
E	-2	GLY	-	expression tag	UNP A5F1B7
E	-1	SER	-	expression tag	UNP A5F1B7
E	0	HIS	-	expression tag	UNP A5F1B7
F	-2	GLY	-	expression tag	UNP A5F1B7
F	-1	SER	-	expression tag	UNP A5F1B7
F	0	HIS	-	expression tag	UNP A5F1B7
G	-2	GLY	-	expression tag	UNP A5F1B7
G	-1	SER	-	expression tag	UNP A5F1B7
G	0	HIS	-	expression tag	UNP A5F1B7
H	-2	GLY	-	expression tag	UNP A5F1B7
H	-1	SER	-	expression tag	UNP A5F1B7
H	0	HIS	-	expression tag	UNP A5F1B7
I	-2	GLY	-	expression tag	UNP A5F1B7
I	-1	SER	-	expression tag	UNP A5F1B7
I	0	HIS	-	expression tag	UNP A5F1B7
J	-2	GLY	-	expression tag	UNP A5F1B7
J	-1	SER	-	expression tag	UNP A5F1B7
J	0	HIS	-	expression tag	UNP A5F1B7
K	-2	GLY	-	expression tag	UNP A5F1B7
K	-1	SER	-	expression tag	UNP A5F1B7
K	0	HIS	-	expression tag	UNP A5F1B7
L	-2	GLY	-	expression tag	UNP A5F1B7
L	-1	SER	-	expression tag	UNP A5F1B7
L	0	HIS	-	expression tag	UNP A5F1B7
M	-2	GLY	-	expression tag	UNP A5F1B7
M	-1	SER	-	expression tag	UNP A5F1B7
M	0	HIS	-	expression tag	UNP A5F1B7
N	-2	GLY	-	expression tag	UNP A5F1B7
N	-1	SER	-	expression tag	UNP A5F1B7
N	0	HIS	-	expression tag	UNP A5F1B7

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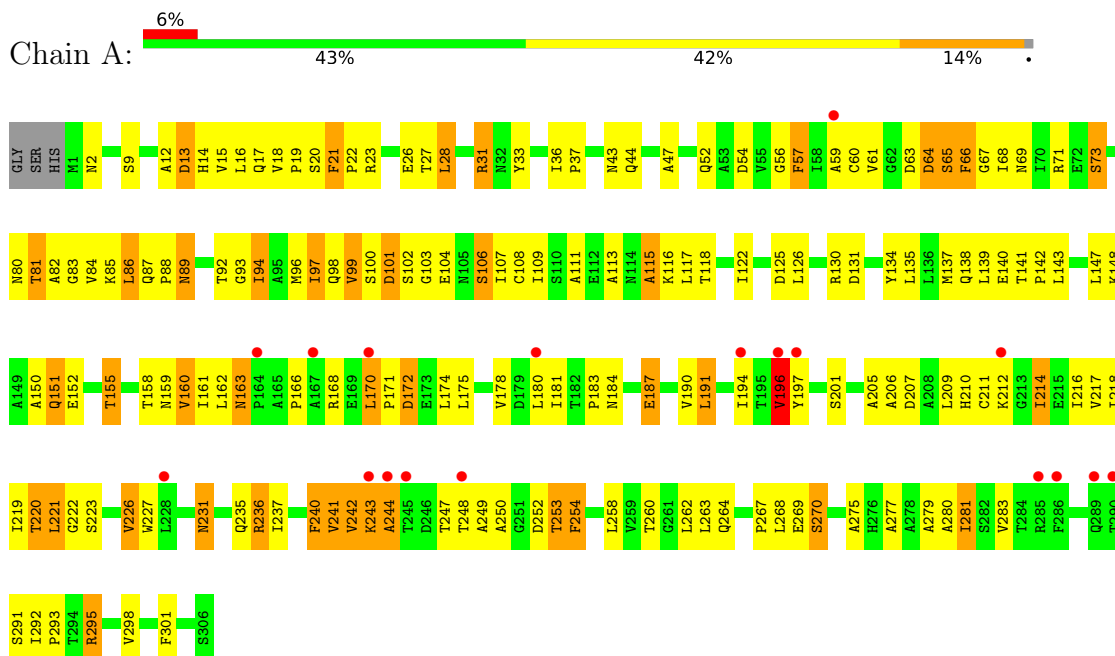
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<b>Chain</b>	<b>Residue</b>	<b>Modelled</b>	<b>Actual</b>	<b>Comment</b>	<b>Reference</b>
O	-2	GLY	-	expression tag	UNP A5F1B7
O	-1	SER	-	expression tag	UNP A5F1B7
O	0	HIS	-	expression tag	UNP A5F1B7
P	-2	GLY	-	expression tag	UNP A5F1B7
P	-1	SER	-	expression tag	UNP A5F1B7
P	0	HIS	-	expression tag	UNP A5F1B7

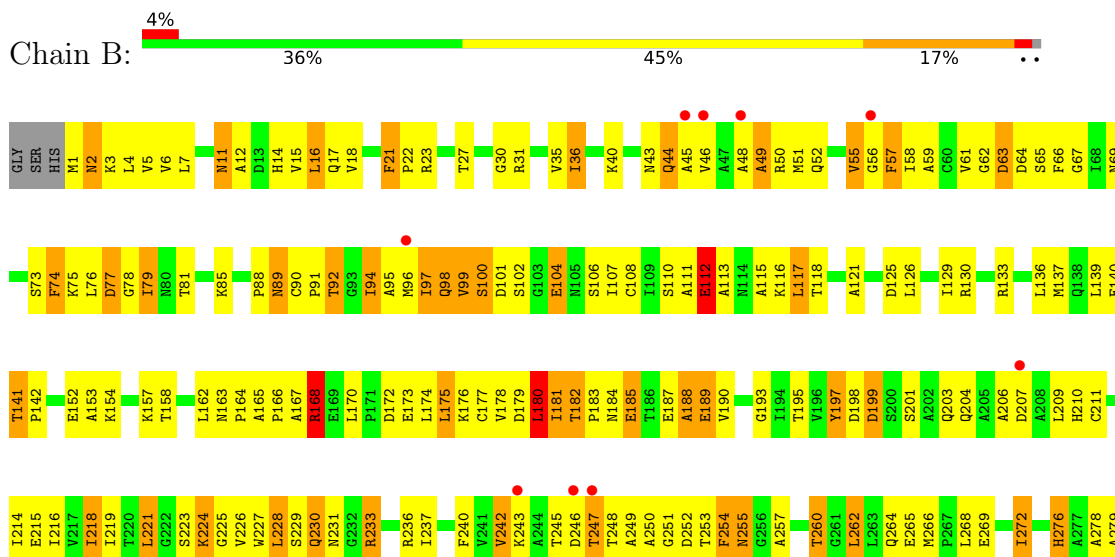
### 3 Residue-property plots [i](#)

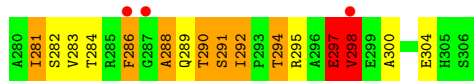
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: Ribokinase

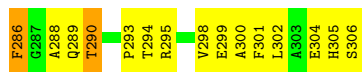
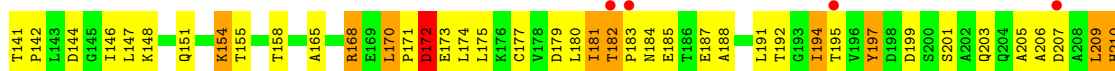
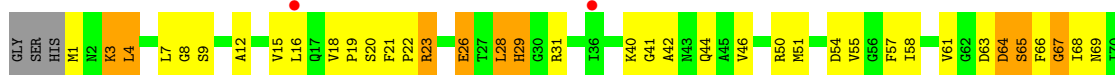


- Molecule 1: Ribokinase

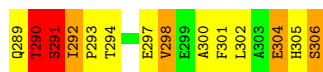




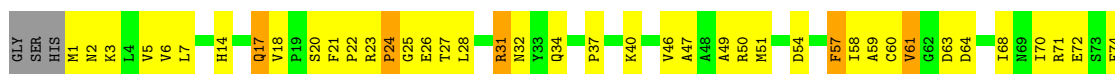
• Molecule 1: Ribokinase



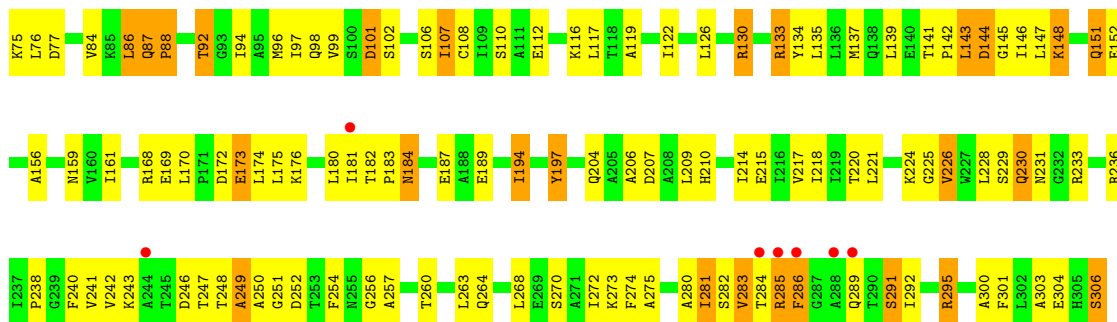
• Molecule 1: Ribokinase



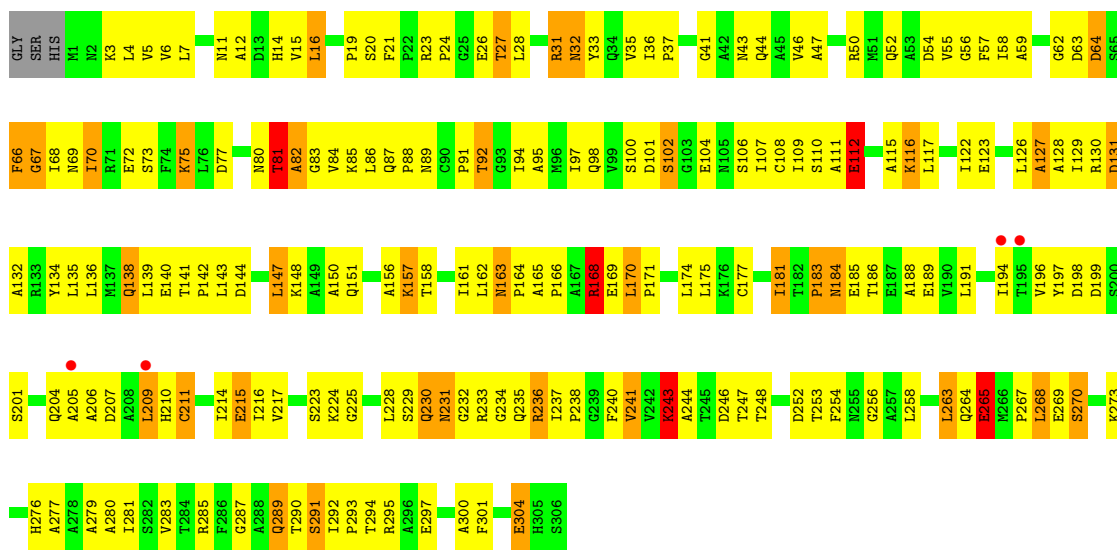
• Molecule 1: Ribokinase



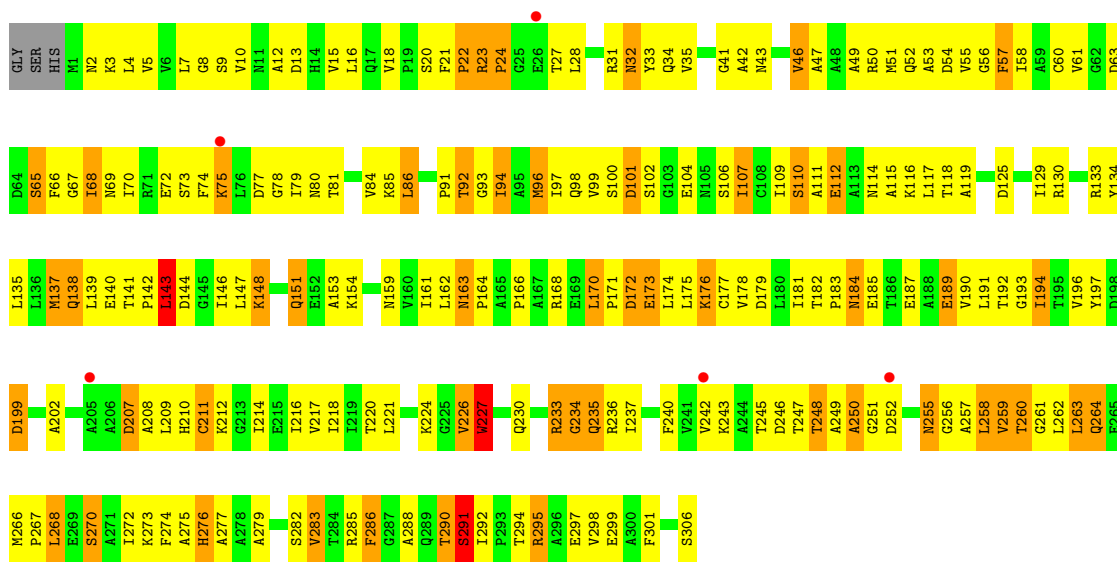




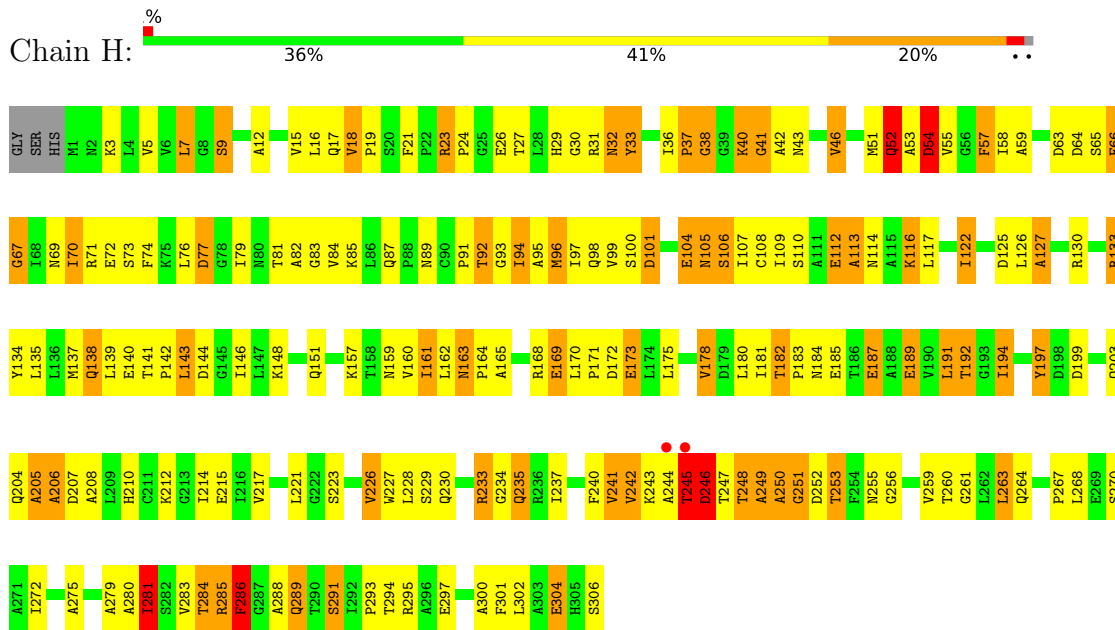
● Molecule 1: Ribokinase



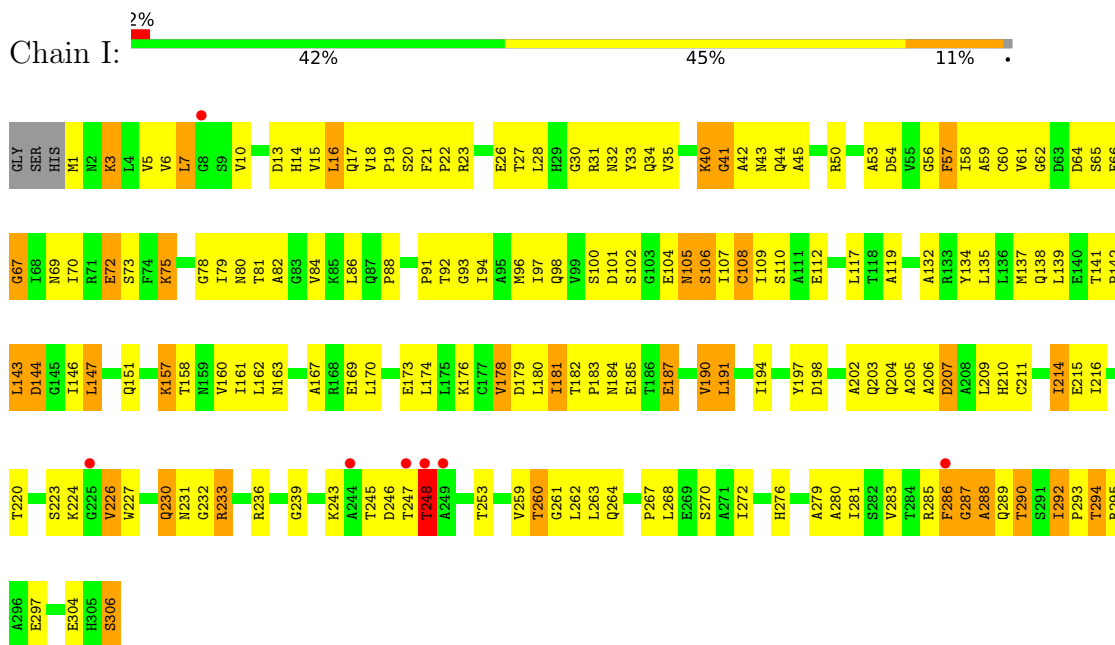
● Molecule 1: Ribokinase



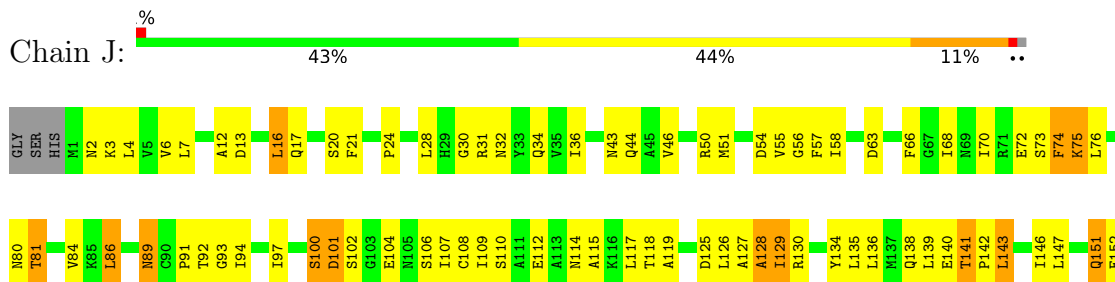
- Molecule 1: Ribokinase



- Molecule 1: Ribokinase

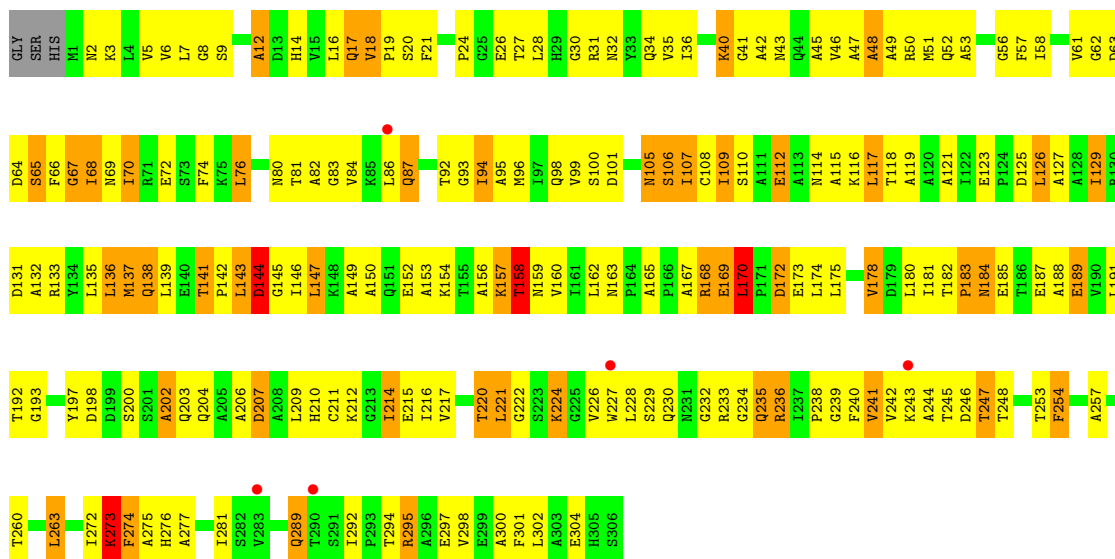


- Molecule 1: Ribokinase

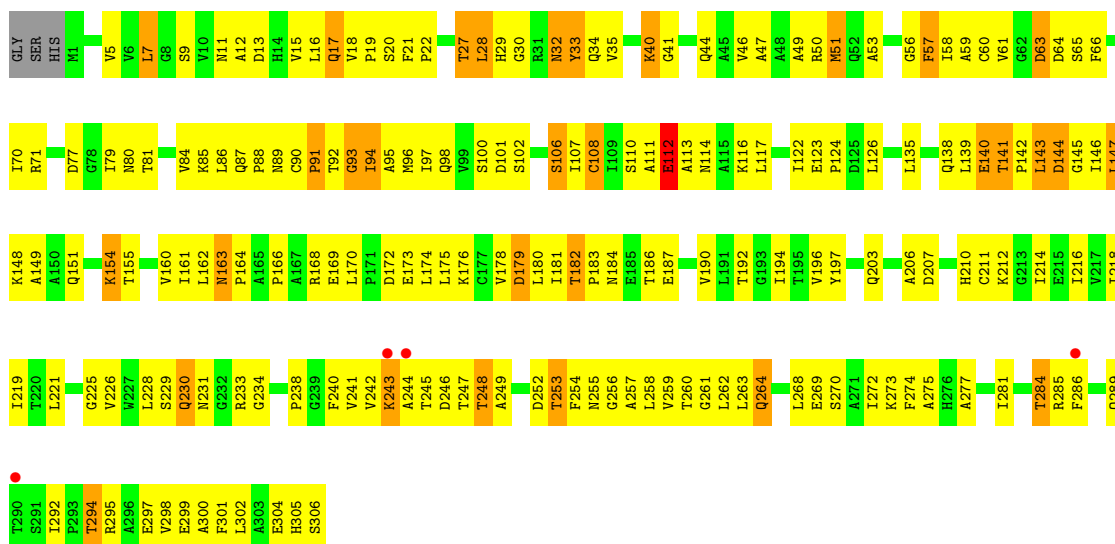




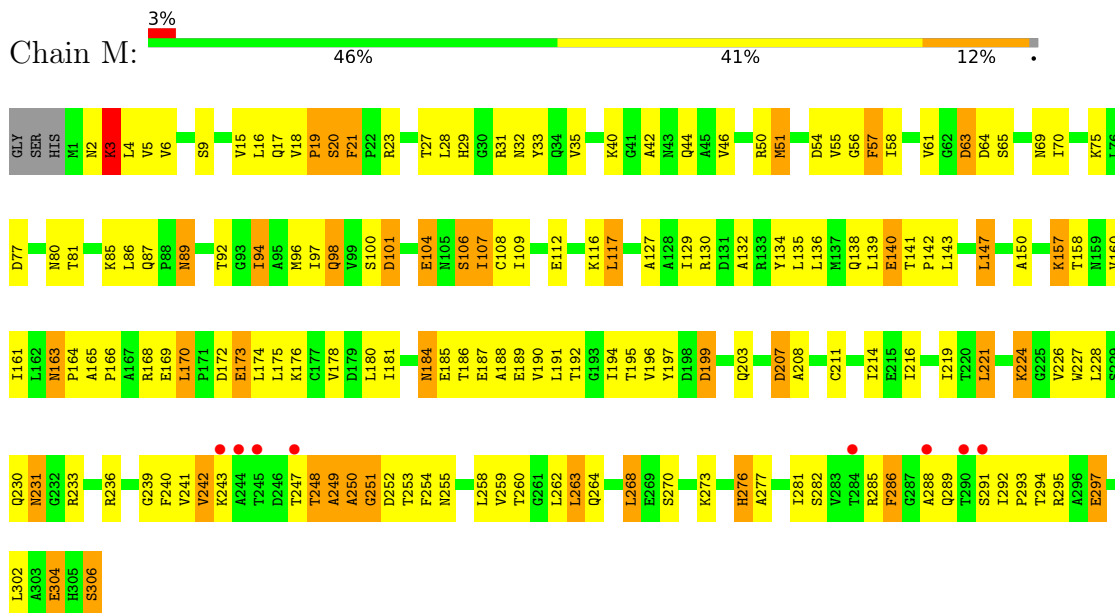
● Molecule 1: Ribokinase



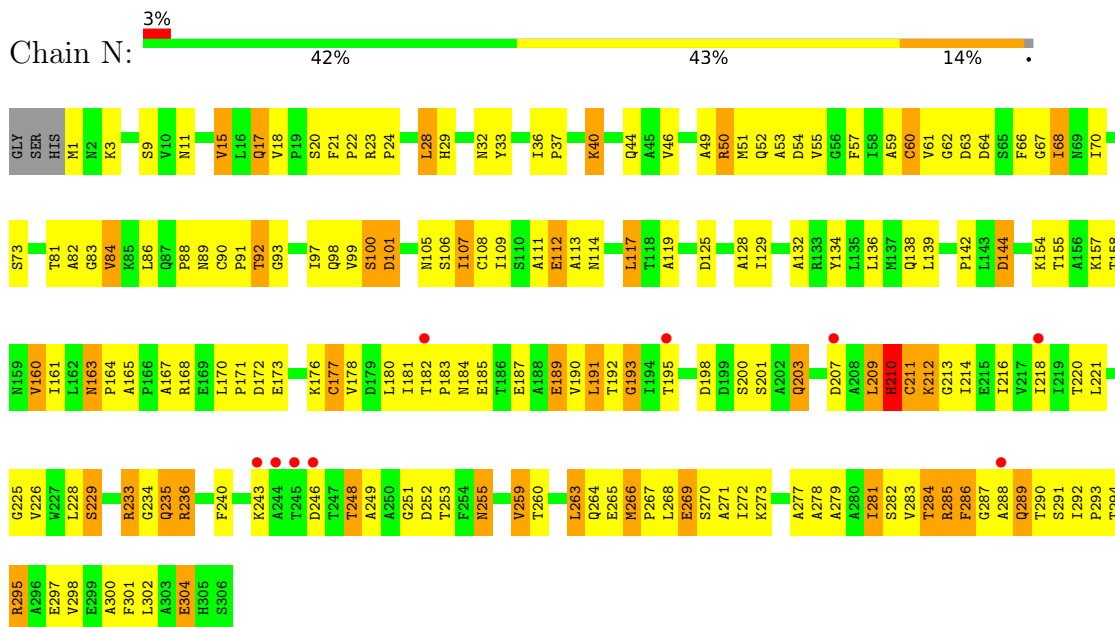
● Molecule 1: Ribokinase



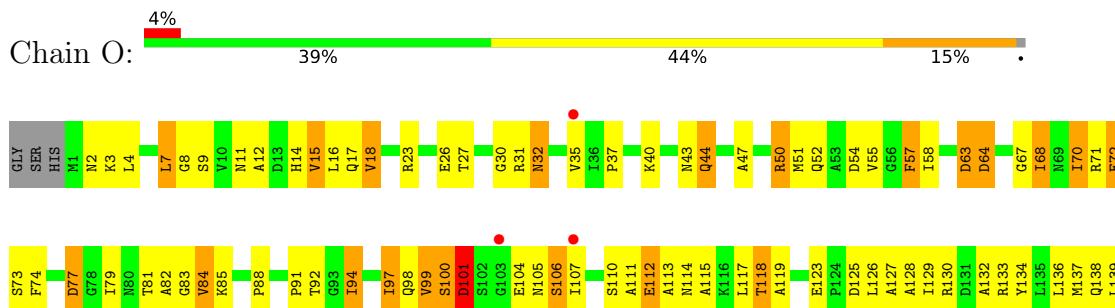
- Molecule 1: Ribokinase

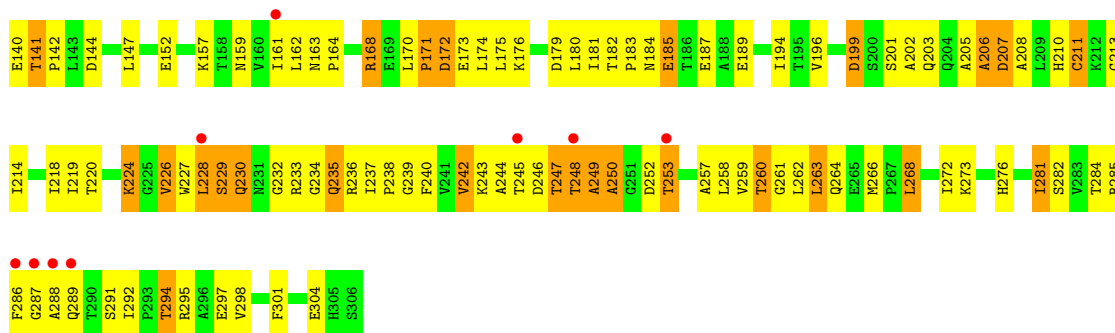


- Molecule 1: Ribokinase

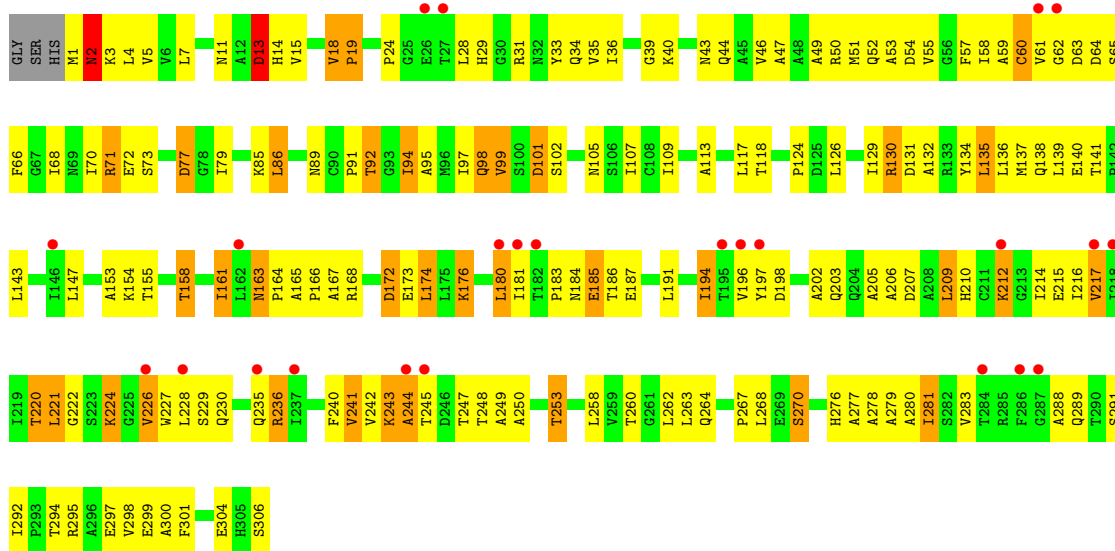
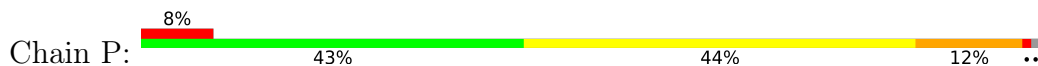


- Molecule 1: Ribokinase





● Molecule 1: Ribokinase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	129.22Å 130.85Å 145.69Å 110.52° 90.00° 119.59°	Depositor
Resolution (Å)	43.57 – 3.40 49.34 – 3.40	Depositor EDS
% Data completeness (in resolution range)	92.8 (43.57-3.40) 92.9 (49.34-3.40)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.15	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.13 (at 3.40Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, $R_{free}$	0.239 , 0.308 0.237 , 0.303	Depositor DCC
$R_{free}$ test set	4831 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	63.2	Xtrriage
Anisotropy	0.563	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 55.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.26$	Xtrriage
Estimated twinning fraction	0.277 for h,-h-k,-l	Xtrriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	36000	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	88.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.86% 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

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	0.48	0/2283	0.81	1/3105 (0.0%)
1	B	0.48	0/2283	0.81	0/3105
1	C	0.52	0/2283	0.86	1/3105 (0.0%)
1	D	0.56	0/2283	0.91	1/3105 (0.0%)
1	E	0.62	0/2283	0.91	0/3105
1	F	0.55	0/2283	0.83	1/3105 (0.0%)
1	G	0.64	1/2283 (0.0%)	0.93	1/3105 (0.0%)
1	H	0.64	0/2283	0.95	1/3105 (0.0%)
1	I	0.56	0/2283	0.83	0/3105
1	J	0.55	0/2283	0.85	1/3105 (0.0%)
1	K	0.57	0/2283	0.93	3/3105 (0.1%)
1	L	0.62	0/2283	0.85	0/3105
1	M	0.56	0/2283	0.84	0/3105
1	N	0.51	0/2283	0.80	0/3105
1	O	0.47	0/2283	0.80	1/3105 (0.0%)
1	P	0.43	0/2283	0.74	0/3105
All	All	0.55	1/36528 (0.0%)	0.86	11/49680 (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
1	D	0	1
1	G	0	1
1	J	0	1
1	K	0	2
1	N	0	1
All	All	0	6

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	227	TRP	CB-CG	-5.13	1.41	1.50

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	143	LEU	CA-CB-CG	8.59	135.05	115.30
1	A	93	GLY	N-CA-C	-7.56	94.21	113.10
1	J	170	LEU	CA-CB-CG	7.36	132.22	115.30
1	F	168	ARG	NE-CZ-NH1	-6.72	116.94	120.30
1	D	86	LEU	CA-CB-CG	6.60	130.47	115.30
1	H	245	THR	N-CA-C	-6.20	94.26	111.00
1	K	136	LEU	CA-CB-CG	6.06	129.23	115.30
1	K	221	LEU	CA-CB-CG	5.57	128.12	115.30
1	K	170	LEU	CA-CB-CG	5.52	127.99	115.30
1	C	23	ARG	N-CA-C	-5.34	96.58	111.00
1	O	228	LEU	CA-CB-CG	5.08	126.99	115.30

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	290	THR	Peptide
1	G	100	SER	Peptide
1	J	100	SER	Peptide
1	K	156	ALA	Peptide
1	K	157	LYS	Peptide
1	N	100	SER	Peptide

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2250	0	2273	147	0
1	B	2250	0	2273	184	0
1	C	2250	0	2273	125	0
1	D	2250	0	2273	165	0
1	E	2250	0	2273	133	0
1	F	2250	0	2273	145	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	2250	0	2273	165	0
1	H	2250	0	2273	203	0
1	I	2250	0	2273	123	0
1	J	2250	0	2273	123	0
1	K	2250	0	2273	170	0
1	L	2250	0	2273	167	0
1	M	2250	0	2273	119	0
1	N	2250	0	2273	126	0
1	O	2250	0	2273	134	0
1	P	2250	0	2273	132	0
All	All	36000	0	36368	2252	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 31.

All (2252) 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)
1:H:31:ARG:NH2	1:H:101:ASP:OD1	1.89	1.06
1:K:94:ILE:HD12	1:K:95:ALA:H	1.18	1.04
1:L:51:MET:HB2	1:L:260:THR:HG21	1.43	1.00
1:H:243:LYS:HG3	1:K:101:ASP:HA	1.42	1.00
1:E:87:GLN:HG2	1:E:116:LYS:HG3	1.45	0.99
1:D:250:ALA:H	1:D:252:ASP:HB2	1.23	0.98
1:A:21:PHE:HD2	1:A:22:PRO:HD2	1.28	0.98
1:H:204:GLN:HE22	1:O:234:GLY:H	1.11	0.97
1:E:94:ILE:HG22	1:E:110:SER:H	1.29	0.97
1:G:209:LEU:HB3	1:G:214:ILE:HD11	1.46	0.97
1:M:224:LYS:HB2	1:M:236:ARG:HH12	1.28	0.96
1:H:285:ARG:NH2	1:H:297:GLU:OE2	1.99	0.95
1:E:130:ARG:NH1	1:E:152:GLU:OE1	2.00	0.94
1:E:50:ARG:HD2	1:E:292:ILE:HG22	1.50	0.94
1:H:264:GLN:OE1	1:H:295:ARG:NH1	2.03	0.92
1:B:181:ILE:HG23	1:B:183:PRO:HD3	1.52	0.91
1:G:181:ILE:HG23	1:G:183:PRO:HD3	1.53	0.90
1:N:212:LYS:O	1:N:214:ILE:N	2.04	0.90
1:C:3:LYS:HB2	1:C:54:ASP:HB3	1.52	0.90
1:G:285:ARG:HG2	1:G:291:SER:HA	1.51	0.90
1:P:14:HIS:ND1	1:P:33:TYR:OH	2.00	0.90
1:O:224:LYS:O	1:O:236:ARG:NH1	2.05	0.89
1:F:181:ILE:HG23	1:F:183:PRO:HD3	1.52	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:207:ASP:OD1	1:G:207:ASP:N	1.99	0.89
1:L:181:ILE:HG23	1:L:183:PRO:HD3	1.51	0.88
1:J:31:ARG:HH21	1:J:101:ASP:HB3	1.38	0.88
1:H:97:ILE:HG22	1:H:107:ILE:HA	1.52	0.87
1:H:51:MET:HB2	1:H:260:THR:HG21	1.57	0.87
1:B:154:LYS:NZ	1:B:177:CYS:O	2.08	0.86
1:G:251:GLY:O	1:G:255:ASN:ND2	2.08	0.86
1:L:97:ILE:HG12	1:L:107:ILE:HG23	1.56	0.86
1:O:285:ARG:HB2	1:O:291:SER:HB2	1.59	0.85
1:K:126:LEU:HA	1:K:129:ILE:HG13	1.60	0.84
1:C:209:LEU:O	1:C:211:CYS:N	2.09	0.84
1:M:249:ALA:O	1:M:251:GLY:N	2.11	0.84
1:A:138:GLN:HG3	1:A:163:ASN:HB3	1.58	0.83
1:E:60:CYS:SG	1:E:87:GLN:NE2	2.51	0.83
1:G:163:ASN:ND2	1:G:255:ASN:OD1	2.11	0.83
1:C:125:ASP:O	1:C:127:ALA:N	2.11	0.83
1:B:230:GLN:HG3	1:B:233:ARG:HG3	1.61	0.83
1:F:143:LEU:HG	1:F:168:ARG:HH12	1.41	0.83
1:J:128:ALA:O	1:J:130:ARG:N	2.11	0.82
1:D:3:LYS:HG2	1:D:54:ASP:HB2	1.60	0.82
1:K:12:ALA:O	1:K:94:ILE:HD13	1.77	0.82
1:D:126:LEU:O	1:D:128:ALA:N	2.13	0.82
1:K:52:GLN:HG3	1:K:295:ARG:HG3	1.61	0.82
1:C:74:PHE:HA	1:C:79:ILE:HD12	1.62	0.82
1:F:81:THR:O	1:F:83:GLY:N	2.12	0.81
1:L:207:ASP:OD1	1:M:233:ARG:N	2.13	0.81
1:H:38:GLY:HA2	1:H:289:GLN:HG3	1.62	0.81
1:L:143:LEU:O	1:L:146:ILE:N	2.14	0.81
1:E:285:ARG:HG3	1:E:291:SER:HA	1.61	0.81
1:O:81:THR:O	1:O:83:GLY:N	2.13	0.81
1:E:143:LEU:O	1:E:145:GLY:N	2.14	0.81
1:P:19:PRO:HD2	1:P:28:LEU:HD11	1.61	0.81
1:C:243:LYS:HD2	1:C:284:THR:HA	1.62	0.81
1:D:249:ALA:HB3	1:D:250:ALA:HB3	1.63	0.81
1:L:248:THR:OG1	1:L:249:ALA:N	2.14	0.81
1:L:143:LEU:O	1:L:145:GLY:N	2.14	0.80
1:C:154:LYS:HD2	1:C:177:CYS:SG	2.20	0.80
1:D:143:LEU:O	1:D:145:GLY:N	2.14	0.80
1:E:116:LYS:NZ	1:I:304:GLU:OE2	2.14	0.80
1:I:15:VAL:HG22	1:I:97:ILE:HB	1.62	0.80
1:K:95:ALA:HB2	1:K:109:ILE:HG23	1.61	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:143:LEU:HD12	1:K:168:ARG:HH21	1.46	0.80
1:D:13:ASP:HA	1:D:95:ALA:HB3	1.62	0.80
1:L:53:ALA:HB2	1:L:260:THR:HG23	1.64	0.79
1:H:240:PHE:HD1	1:H:301:PHE:HE2	1.29	0.79
1:K:273:LYS:O	1:K:276:HIS:N	2.15	0.79
1:I:43:ASN:OD1	1:I:289:GLN:NE2	2.16	0.79
1:N:281:ILE:O	1:N:284:THR:OG1	2.00	0.79
1:E:168:ARG:NH1	1:I:306:SER:O	2.16	0.78
1:O:110:SER:OG	1:O:112:GLU:OE2	2.01	0.78
1:O:8:GLY:HA2	1:O:141:THR:HG21	1.65	0.78
1:O:15:VAL:HG13	1:O:97:ILE:HB	1.65	0.78
1:A:21:PHE:CD2	1:A:22:PRO:HD2	2.18	0.78
1:B:140:GLU:HG3	1:B:166:PRO:HD3	1.64	0.78
1:D:87:GLN:HG2	1:D:116:LYS:HG3	1.65	0.78
1:K:167:ALA:HB2	1:K:187:GLU:HG2	1.65	0.78
1:A:2:ASN:ND2	1:A:54:ASP:OD1	2.17	0.78
1:D:22:PRO:HD3	1:D:28:LEU:HD21	1.66	0.78
1:L:240:PHE:HD1	1:L:301:PHE:HE2	1.33	0.77
1:H:294:THR:N	1:H:297:GLU:OE1	2.17	0.77
1:K:94:ILE:HD12	1:K:95:ALA:N	1.98	0.77
1:N:62:GLY:H	1:N:92:THR:HG23	1.49	0.77
1:H:306:SER:OG	1:L:143:LEU:N	2.17	0.77
1:G:286:PHE:O	1:G:290:THR:OG1	1.99	0.77
1:O:4:LEU:HB2	1:O:263:LEU:HD11	1.67	0.77
1:G:267:PRO:HD2	1:G:270:SER:HB2	1.66	0.77
1:K:198:ASP:OD1	1:K:200:SER:OG	2.03	0.77
1:A:249:ALA:O	1:A:253:THR:OG1	2.04	0.76
1:D:256:GLY:O	1:D:260:THR:OG1	2.02	0.76
1:L:97:ILE:HG23	1:L:107:ILE:HG12	1.67	0.76
1:P:14:HIS:HD1	1:P:33:TYR:HH	0.77	0.76
1:N:51:MET:HB2	1:N:260:THR:HG21	1.66	0.76
1:D:7:LEU:HD13	1:D:58:ILE:HG22	1.68	0.76
1:K:7:LEU:HB3	1:K:137:MET:HG2	1.67	0.76
1:B:4:LEU:HD23	1:B:55:VAL:HB	1.68	0.76
1:B:100:SER:OG	1:B:104:GLU:O	2.02	0.76
1:E:143:LEU:H	1:I:306:SER:HB2	1.51	0.76
1:P:132:ALA:O	1:P:158:THR:OG1	2.04	0.76
1:B:74:PHE:HB3	1:B:79:ILE:HD11	1.66	0.76
1:H:182:THR:O	1:H:182:THR:OG1	2.00	0.76
1:K:143:LEU:O	1:K:145:GLY:N	2.17	0.76
1:N:228:LEU:HD11	1:N:268:LEU:HD23	1.66	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:21:PHE:CE2	1:G:106:SER:HB3	2.20	0.76
1:C:230:GLN:O	1:C:232:GLY:N	2.19	0.76
1:M:248:THR:O	1:M:250:ALA:N	2.18	0.76
1:B:15:VAL:HG22	1:B:97:ILE:HD11	1.68	0.75
1:F:95:ALA:HB2	1:F:109:ILE:HD12	1.66	0.75
1:A:43:ASN:ND2	1:A:252:ASP:OD1	2.18	0.75
1:B:64:ASP:O	1:B:66:PHE:N	2.19	0.75
1:D:2:ASN:OD1	1:D:2:ASN:N	2.18	0.75
1:D:245:THR:OG1	1:D:283:VAL:O	2.04	0.75
1:I:91:PRO:HG2	1:I:112:GLU:HG3	1.67	0.75
1:G:65:SER:O	1:G:69:ASN:ND2	2.19	0.75
1:I:97:ILE:HG12	1:I:107:ILE:HG23	1.69	0.75
1:B:182:THR:OG1	1:B:255:ASN:OD1	2.04	0.75
1:D:281:ILE:HB	1:D:293:PRO:HG3	1.69	0.75
1:P:60:CYS:HB2	1:P:117:LEU:HD13	1.68	0.75
1:P:15:VAL:HG22	1:P:97:ILE:HB	1.68	0.75
1:C:283:VAL:HG23	1:C:284:THR:H	1.52	0.75
1:F:101:ASP:OD1	1:I:243:LYS:NZ	2.18	0.75
1:N:11:ASN:OD1	1:N:114:ASN:ND2	2.20	0.74
1:A:65:SER:O	1:A:69:ASN:ND2	2.16	0.74
1:K:147:LEU:HD22	1:K:174:LEU:HB2	1.68	0.74
1:G:226:VAL:HG12	1:G:227:TRP:H	1.52	0.74
1:J:207:ASP:HB3	1:K:232:GLY:HA3	1.70	0.74
1:K:94:ILE:CD1	1:K:95:ALA:H	2.00	0.74
1:K:203:GLN:HE22	1:K:232:GLY:HA2	1.53	0.74
1:P:36:ILE:HG21	1:P:288:ALA:HB3	1.69	0.74
1:C:44:GLN:NE2	1:C:252:ASP:OD1	2.17	0.74
1:H:122:ILE:HG22	1:H:125:ASP:HB2	1.70	0.73
1:D:239:GLY:HA2	1:D:276:HIS:CD2	2.22	0.73
1:H:15:VAL:HG22	1:H:97:ILE:HD11	1.70	0.73
1:J:81:THR:HG22	1:J:84:VAL:HB	1.70	0.73
1:K:239:GLY:HA2	1:K:276:HIS:CD2	2.23	0.73
1:A:181:ILE:HB	1:A:214:ILE:HG21	1.69	0.73
1:N:181:ILE:HG22	1:N:183:PRO:HD3	1.69	0.73
1:E:251:GLY:HA2	1:E:254:PHE:HB3	1.70	0.73
1:H:161:ILE:HG23	1:H:180:LEU:HB3	1.71	0.73
1:K:133:ARG:HE	1:K:158:THR:HG21	1.54	0.73
1:G:111:ALA:HA	1:G:114:ASN:HD22	1.53	0.73
1:H:285:ARG:HB3	1:H:291:SER:HB2	1.69	0.73
1:J:211:CYS:HA	1:K:233:ARG:HD3	1.71	0.73
1:N:64:ASP:OD2	1:N:92:THR:N	2.21	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:119:ALA:N	1:K:144:ASP:OD2	2.20	0.72
1:D:62:GLY:H	1:D:92:THR:HG22	1.53	0.72
1:L:294:THR:N	1:L:297:GLU:OE1	2.22	0.72
1:H:126:LEU:O	1:H:130:ARG:HG3	1.90	0.72
1:K:47:ALA:O	1:K:49:ALA:N	2.21	0.72
1:A:12:ALA:HB3	1:A:94:ILE:HG13	1.70	0.72
1:E:240:PHE:CD1	1:E:301:PHE:HE2	2.08	0.72
1:F:143:LEU:CG	1:F:168:ARG:HH12	2.02	0.72
1:F:267:PRO:HD2	1:F:270:SER:HB2	1.71	0.72
1:K:6:VAL:HG12	1:K:136:LEU:HB3	1.69	0.72
1:A:98:GLN:OE1	1:A:106:SER:OG	2.05	0.72
1:D:110:SER:OG	1:D:112:GLU:OE2	2.07	0.72
1:D:250:ALA:HA	1:D:252:ASP:N	2.05	0.72
1:L:246:ASP:O	1:L:248:THR:N	2.23	0.72
1:A:99:VAL:HG12	1:A:100:SER:H	1.55	0.72
1:D:130:ARG:NH1	1:D:152:GLU:OE1	2.22	0.72
1:B:18:VAL:H	1:B:99:VAL:HG12	1.55	0.71
1:A:244:ALA:HA	1:A:283:VAL:HB	1.72	0.71
1:I:17:GLN:OE1	1:I:32:ASN:ND2	2.22	0.71
1:J:63:ASP:OD2	1:J:89:ASN:N	2.21	0.71
1:J:140:GLU:HG3	1:J:166:PRO:HD3	1.71	0.71
1:N:134:TYR:HD1	1:N:161:ILE:HD11	1.55	0.71
1:I:50:ARG:HD2	1:I:292:ILE:HG22	1.73	0.71
1:O:206:ALA:O	1:O:208:ALA:N	2.23	0.71
1:L:169:GLU:HG2	1:L:190:VAL:HG12	1.71	0.71
1:B:85:LYS:NZ	1:B:121:ALA:O	2.16	0.71
1:A:19:PRO:HA	1:A:101:ASP:HB2	1.73	0.71
1:G:143:LEU:HD12	1:G:168:ARG:HH12	1.56	0.71
1:J:126:LEU:HD23	1:J:129:ILE:HD13	1.72	0.71
1:M:19:PRO:O	1:M:21:PHE:N	2.22	0.71
1:A:44:GLN:OE1	1:A:138:GLN:NE2	2.24	0.71
1:H:40:LYS:O	1:H:43:ASN:N	2.23	0.71
1:N:192:THR:OG1	1:N:193:GLY:N	2.20	0.71
1:M:101:ASP:HA	1:P:243:LYS:HD3	1.72	0.71
1:H:184:ASN:H	1:H:187:GLU:HB2	1.56	0.71
1:A:97:ILE:HD12	1:A:107:ILE:HG13	1.71	0.71
1:E:97:ILE:HG12	1:E:107:ILE:HD13	1.73	0.71
1:K:43:ASN:OD1	1:K:289:GLN:HG3	1.91	0.71
1:G:207:ASP:O	1:G:211:CYS:N	2.22	0.70
1:A:13:ASP:HB2	1:A:36:ILE:HG22	1.73	0.70
1:B:7:LEU:HB3	1:B:137:MET:HG2	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:61:VAL:HG23	1:D:86:LEU:HD23	1.74	0.70
1:E:184:ASN:ND2	1:E:187:GLU:H	1.89	0.70
1:H:181:ILE:HG12	1:H:183:PRO:HD3	1.72	0.70
1:A:220:THR:HA	1:A:226:VAL:HG23	1.74	0.70
1:K:143:LEU:HD12	1:K:168:ARG:NH2	2.06	0.70
1:L:182:THR:OG1	1:L:182:THR:O	2.08	0.70
1:G:147:LEU:HD11	1:G:151:GLN:HE21	1.57	0.70
1:J:187:GLU:O	1:J:189:GLU:N	2.24	0.70
1:B:61:VAL:HA	1:B:92:THR:HG23	1.73	0.70
1:G:174:LEU:O	1:G:176:LYS:N	2.25	0.70
1:O:183:PRO:HG2	1:O:219:ILE:HG12	1.74	0.70
1:A:126:LEU:HD13	1:A:152:GLU:HG2	1.74	0.70
1:C:221:LEU:HD11	1:C:227:TRP:HB2	1.73	0.70
1:I:147:LEU:HD12	1:I:151:GLN:HB3	1.74	0.70
1:E:224:LYS:O	1:E:236:ARG:NH1	2.24	0.69
1:H:70:ILE:O	1:H:73:SER:HB2	1.92	0.69
1:O:9:SER:OG	1:O:140:GLU:OE1	2.10	0.69
1:M:294:THR:OG1	1:M:297:GLU:OE2	2.09	0.69
1:P:181:ILE:HG23	1:P:183:PRO:HD3	1.74	0.69
1:B:207:ASP:OD1	1:I:203:GLN:NE2	2.25	0.69
1:H:245:THR:CG2	1:H:284:THR:HA	2.22	0.69
1:P:136:LEU:HD13	1:P:161:ILE:HG22	1.75	0.69
1:P:97:ILE:HG23	1:P:107:ILE:HG12	1.73	0.69
1:G:53:ALA:HB2	1:G:260:THR:HG23	1.75	0.69
1:H:245:THR:HG21	1:H:284:THR:HA	1.75	0.69
1:J:281:ILE:HB	1:J:293:PRO:HG3	1.72	0.69
1:B:51:MET:HA	1:B:295:ARG:HG3	1.75	0.69
1:H:40:LYS:O	1:H:42:ALA:N	2.24	0.69
1:I:110:SER:OG	1:I:112:GLU:OE2	2.09	0.69
1:L:41:GLY:HA2	1:L:138:GLN:HE22	1.57	0.69
1:A:61:VAL:O	1:A:87:GLN:HB2	1.93	0.69
1:K:300:ALA:O	1:K:304:GLU:HG3	1.92	0.69
1:N:209:LEU:O	1:N:211:CYS:N	2.20	0.69
1:B:184:ASN:N	1:B:187:GLU:OE2	2.26	0.69
1:I:224:LYS:O	1:I:236:ARG:NH1	2.25	0.69
1:K:126:LEU:HB2	1:K:152:GLU:HG2	1.74	0.69
1:N:181:ILE:HG13	1:N:214:ILE:HG21	1.72	0.69
1:O:126:LEU:HA	1:O:129:ILE:HD12	1.75	0.69
1:A:181:ILE:HG22	1:A:217:VAL:HA	1.74	0.69
1:C:134:TYR:HD2	1:C:263:LEU:HD23	1.57	0.69
1:D:181:ILE:HG13	1:D:214:ILE:HG21	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:300:ALA:O	1:P:304:GLU:HG3	1.94	0.69
1:B:91:PRO:HD2	1:B:112:GLU:HG2	1.75	0.68
1:F:194:ILE:HD13	1:F:204:GLN:HB3	1.76	0.68
1:G:295:ARG:C	1:G:295:ARG:HD3	2.14	0.68
1:H:306:SER:HB3	1:L:143:LEU:HG	1.74	0.68
1:K:18:VAL:HG21	1:K:98:GLN:HB3	1.75	0.68
1:L:172:ASP:O	1:L:174:LEU:N	2.26	0.68
1:M:100:SER:OG	1:M:104:GLU:O	2.09	0.68
1:M:170:LEU:HD23	1:M:174:LEU:HD23	1.76	0.68
1:N:264:GLN:OE1	1:N:295:ARG:NH2	2.27	0.68
1:B:231:ASN:HD22	1:I:232:GLY:HA3	1.55	0.68
1:H:81:THR:O	1:H:83:GLY:N	2.27	0.68
1:B:180:LEU:HG	1:B:216:ILE:HB	1.75	0.68
1:B:228:LEU:HD12	1:B:229:SER:N	2.09	0.68
1:M:249:ALA:C	1:M:251:GLY:H	1.96	0.68
1:P:44:GLN:OE1	1:P:138:GLN:NE2	2.24	0.68
1:H:279:ALA:O	1:H:283:VAL:N	2.25	0.68
1:K:6:VAL:HG21	1:K:45:ALA:HB2	1.76	0.68
1:L:40:LYS:NZ	1:L:252:ASP:OD1	2.26	0.68
1:A:117:LEU:O	1:A:142:PRO:HG2	1.93	0.68
1:C:72:GLU:HA	1:C:75:LYS:HG3	1.75	0.68
1:F:233:ARG:HD3	1:G:211:CYS:HB2	1.75	0.68
1:L:63:ASP:OD2	1:L:89:ASN:N	2.25	0.68
1:M:135:LEU:HD23	1:M:160:VAL:HG13	1.76	0.68
1:D:291:SER:OG	1:D:292:ILE:N	2.24	0.68
1:F:26:GLU:HG3	1:F:27:THR:N	2.09	0.68
1:J:249:ALA:HB2	1:J:288:ALA:HB1	1.76	0.68
1:M:251:GLY:O	1:M:255:ASN:ND2	2.26	0.68
1:P:228:LEU:HD11	1:P:268:LEU:HD21	1.76	0.68
1:C:182:THR:OG1	1:C:182:THR:O	2.10	0.68
1:F:241:VAL:HG13	1:I:19:PRO:HB3	1.75	0.68
1:H:230:GLN:O	1:H:233:ARG:HG3	1.94	0.68
1:H:250:ALA:HB1	1:H:283:VAL:HG12	1.74	0.68
1:K:14:HIS:H	1:K:94:ILE:HD11	1.59	0.68
1:P:77:ASP:HB3	1:P:79:ILE:HG13	1.76	0.68
1:G:51:MET:HB2	1:G:260:THR:HG21	1.77	0.67
1:A:140:GLU:HG3	1:A:166:PRO:HD3	1.76	0.67
1:B:245:THR:HG21	1:B:286:PHE:HD2	1.59	0.67
1:H:87:GLN:HG3	1:H:116:LYS:HG3	1.77	0.67
1:J:56:GLY:HA2	1:J:80:ASN:HB3	1.76	0.67
1:J:91:PRO:HG2	1:J:112:GLU:HG3	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:183:PRO:HG2	1:L:219:ILE:HG12	1.75	0.67
1:F:184:ASN:ND2	1:F:186:THR:H	1.93	0.67
1:C:147:LEU:O	1:C:151:GLN:HG3	1.94	0.67
1:C:171:PRO:O	1:C:173:GLU:N	2.28	0.67
1:F:83:GLY:O	1:F:85:LYS:NZ	2.27	0.67
1:I:230:GLN:O	1:I:233:ARG:HG3	1.94	0.67
1:B:110:SER:OG	1:B:112:GLU:OE2	2.09	0.67
1:F:228:LEU:HD21	1:F:268:LEU:HD21	1.76	0.67
1:M:187:GLU:O	1:M:191:LEU:HB2	1.94	0.67
1:D:143:LEU:HD21	1:D:168:ARG:NH1	2.09	0.67
1:H:110:SER:OG	1:H:112:GLU:OE2	2.12	0.67
1:L:163:ASN:HA	1:L:182:THR:HG23	1.77	0.67
1:H:74:PHE:HB3	1:H:79:ILE:HB	1.76	0.67
1:M:175:LEU:HD22	1:M:214:ILE:HD11	1.76	0.67
1:F:66:PHE:O	1:F:68:ILE:N	2.28	0.67
1:K:138:GLN:N	1:K:138:GLN:HE21	1.92	0.67
1:N:139:LEU:HD11	1:N:170:LEU:HD11	1.76	0.67
1:P:138:GLN:HG3	1:P:163:ASN:HB3	1.77	0.67
1:A:134:TYR:CD1	1:A:159:ASN:HB2	2.30	0.67
1:J:234:GLY:N	1:K:207:ASP:OD2	2.28	0.67
1:H:280:ALA:HA	1:H:283:VAL:HG22	1.77	0.66
1:J:86:LEU:H	1:J:86:LEU:HD12	1.59	0.66
1:K:133:ARG:NE	1:K:158:THR:HG21	2.10	0.66
1:M:216:ILE:HD13	1:M:268:LEU:HD21	1.77	0.66
1:D:20:SER:OG	1:D:21:PHE:N	2.22	0.66
1:H:221:LEU:HD12	1:H:227:TRP:H	1.58	0.66
1:K:3:LYS:HB3	1:K:263:LEU:HD21	1.76	0.66
1:L:207:ASP:HB3	1:M:233:ARG:HB3	1.76	0.66
1:A:27:THR:HG22	1:B:107:ILE:HB	1.75	0.66
1:F:229:SER:HA	1:F:234:GLY:HA2	1.77	0.66
1:G:189:GLU:O	1:G:193:GLY:N	2.28	0.66
1:L:225:GLY:HA3	1:L:238:PRO:HA	1.77	0.66
1:E:181:ILE:HG23	1:E:183:PRO:HD3	1.78	0.66
1:H:294:THR:OG1	1:H:297:GLU:HG3	1.95	0.66
1:L:50:ARG:HD2	1:L:292:ILE:HG22	1.77	0.66
1:L:253:THR:HG23	1:L:292:ILE:HG12	1.76	0.66
1:E:94:ILE:HG22	1:E:110:SER:N	2.07	0.66
1:E:246:ASP:HB2	1:E:283:VAL:HG23	1.77	0.66
1:C:15:VAL:HG22	1:C:97:ILE:HD12	1.78	0.66
1:H:279:ALA:O	1:H:283:VAL:HG13	1.95	0.66
1:J:21:PHE:HE2	1:J:106:SER:HB3	1.59	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:234:GLY:O	1:J:235:GLN:HB3	1.95	0.66
1:B:66:PHE:O	1:B:69:ASN:N	2.29	0.65
1:G:234:GLY:O	1:G:235:GLN:HB2	1.95	0.65
1:L:138:GLN:OE1	1:L:138:GLN:N	2.28	0.65
1:O:16:LEU:HD21	1:O:30:GLY:HA3	1.77	0.65
1:B:249:ALA:O	1:B:252:ASP:N	2.27	0.65
1:I:203:GLN:OE1	1:I:227:TRP:NE1	2.28	0.65
1:N:216:ILE:HG12	1:N:268:LEU:HD21	1.78	0.65
1:F:47:ALA:HB3	1:F:256:GLY:HA3	1.78	0.65
1:G:56:GLY:HA2	1:G:80:ASN:HB3	1.78	0.65
1:H:175:LEU:HB3	1:H:214:ILE:HD11	1.77	0.65
1:O:181:ILE:HG23	1:O:183:PRO:HD3	1.77	0.65
1:O:202:ALA:HB3	1:O:227:TRP:CZ3	2.32	0.65
1:A:66:PHE:O	1:A:68:ILE:N	2.29	0.65
1:C:104:GLU:HB2	1:D:25:GLY:H	1.60	0.65
1:F:91:PRO:HG2	1:F:112:GLU:HG2	1.78	0.65
1:F:101:ASP:OD1	1:I:243:LYS:HG3	1.97	0.65
1:G:110:SER:OG	1:G:112:GLU:HG2	1.96	0.65
1:H:281:ILE:O	1:H:285:ARG:HG3	1.96	0.65
1:F:232:GLY:C	1:G:207:ASP:HB3	2.17	0.65
1:J:207:ASP:O	1:J:210:HIS:HB2	1.97	0.65
1:M:189:GLU:HG2	1:M:195:THR:HA	1.77	0.65
1:N:249:ALA:O	1:N:252:ASP:N	2.27	0.65
1:A:15:VAL:HG13	1:A:97:ILE:HG12	1.78	0.65
1:K:209:LEU:HB3	1:K:214:ILE:HD11	1.79	0.65
1:L:91:PRO:HG2	1:L:112:GLU:HB3	1.78	0.65
1:D:248:THR:HG23	1:D:249:ALA:HA	1.79	0.65
1:H:42:ALA:O	1:H:46:VAL:HG22	1.96	0.65
1:I:117:LEU:O	1:I:142:PRO:HG2	1.97	0.65
1:B:139:LEU:HD13	1:B:168:ARG:HD2	1.79	0.65
1:I:167:ALA:HB1	1:I:190:VAL:HG21	1.78	0.65
1:J:171:PRO:HB2	1:J:173:GLU:HG3	1.79	0.65
1:L:47:ALA:HB3	1:L:256:GLY:HA3	1.79	0.65
1:L:184:ASN:H	1:L:187:GLU:HB2	1.61	0.65
1:A:181:ILE:HG21	1:A:209:LEU:HD13	1.78	0.64
1:G:261:GLY:O	1:G:263:LEU:N	2.29	0.64
1:L:15:VAL:O	1:L:34:GLN:N	2.28	0.64
1:D:126:LEU:O	1:D:129:ILE:N	2.30	0.64
1:E:64:ASP:OD1	1:E:92:THR:OG1	2.13	0.64
1:F:5:VAL:O	1:F:135:LEU:HD22	1.97	0.64
1:F:143:LEU:HG	1:F:168:ARG:NH1	2.11	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:243:LYS:CG	1:K:101:ASP:HA	2.22	0.64
1:H:250:ALA:O	1:H:253:THR:N	2.30	0.64
1:I:3:LYS:HB2	1:I:54:ASP:HB3	1.79	0.64
1:C:117:LEU:O	1:C:142:PRO:HG2	1.97	0.64
1:D:97:ILE:HG22	1:D:107:ILE:HD12	1.79	0.64
1:F:31:ARG:NH2	1:F:101:ASP:OD1	2.29	0.64
1:H:19:PRO:HB3	1:K:241:VAL:HG13	1.79	0.64
1:I:181:ILE:HG12	1:I:183:PRO:HD3	1.79	0.64
1:M:259:VAL:O	1:M:263:LEU:HB2	1.97	0.64
1:D:62:GLY:H	1:D:92:THR:CG2	2.10	0.64
1:K:180:LEU:HD12	1:K:216:ILE:HB	1.79	0.64
1:C:139:LEU:HD11	1:C:170:LEU:HD11	1.78	0.64
1:H:18:VAL:O	1:H:101:ASP:HB2	1.97	0.64
1:C:151:GLN:HA	1:C:154:LYS:HD3	1.78	0.64
1:G:134:TYR:HD1	1:G:161:ILE:HD11	1.62	0.64
1:G:216:ILE:HG21	1:G:268:LEU:HD21	1.79	0.64
1:C:281:ILE:HG23	1:C:293:PRO:HG3	1.78	0.64
1:O:57:PHE:HB2	1:O:79:ILE:HG21	1.78	0.64
1:A:183:PRO:HB3	1:A:187:GLU:HB3	1.80	0.64
1:M:127:ALA:HA	1:M:130:ARG:HH21	1.61	0.64
1:O:7:LEU:HD12	1:O:58:ILE:HG21	1.79	0.64
1:B:187:GLU:O	1:B:190:VAL:HG22	1.96	0.64
1:D:232:GLY:O	1:D:234:GLY:N	2.31	0.64
1:E:225:GLY:HA3	1:E:238:PRO:HA	1.80	0.64
1:L:240:PHE:CD1	1:L:301:PHE:HE2	2.15	0.64
1:D:100:SER:HA	1:D:101:ASP:HB3	1.81	0.63
1:C:194:ILE:HG13	1:C:205:ALA:HA	1.81	0.63
1:K:65:SER:O	1:K:69:ASN:ND2	2.31	0.63
1:B:126:LEU:HB3	1:B:152:GLU:HG2	1.80	0.63
1:C:230:GLN:O	1:C:233:ARG:N	2.18	0.63
1:N:172:ASP:O	1:N:176:LYS:HG3	1.99	0.63
1:N:295:ARG:HG2	1:N:295:ARG:HH11	1.63	0.63
1:B:88:PRO:O	1:B:89:ASN:ND2	2.31	0.63
1:C:106:SER:O	1:C:106:SER:OG	2.12	0.63
1:E:218:ILE:HG12	1:E:228:LEU:HD13	1.80	0.63
1:F:300:ALA:O	1:F:304:GLU:HG2	1.98	0.63
1:G:162:LEU:HD11	1:G:174:LEU:HD21	1.80	0.63
1:K:99:VAL:HA	1:K:105:ASN:HB3	1.80	0.63
1:K:204:GLN:HA	1:K:207:ASP:HB2	1.80	0.63
1:A:56:GLY:HA2	1:A:80:ASN:HB3	1.79	0.63
1:F:58:ILE:HD11	1:F:122:ILE:HG22	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:53:ALA:HB2	1:I:260:THR:HG23	1.79	0.63
1:O:171:PRO:HG2	1:O:174:LEU:HB3	1.81	0.63
1:B:99:VAL:HG13	1:B:101:ASP:HB2	1.80	0.63
1:E:184:ASN:C	1:E:184:ASN:HD22	2.01	0.63
1:H:112:GLU:O	1:H:114:ASN:N	2.32	0.63
1:P:63:ASP:OD2	1:P:89:ASN:N	2.29	0.63
1:P:294:THR:HG22	1:P:297:GLU:OE2	1.99	0.63
1:D:300:ALA:O	1:D:304:GLU:HG2	1.99	0.63
1:H:261:GLY:O	1:H:264:GLN:N	2.29	0.63
1:K:294:THR:O	1:K:298:VAL:HG23	1.99	0.63
1:C:64:ASP:N	1:C:64:ASP:OD2	2.32	0.63
1:J:240:PHE:CD2	1:J:301:PHE:HE2	2.16	0.63
1:M:248:THR:OG1	1:M:249:ALA:N	2.32	0.63
1:J:240:PHE:HE1	1:J:273:LYS:HE3	1.64	0.62
1:O:3:LYS:HD2	1:O:133:ARG:NH1	2.14	0.62
1:B:187:GLU:O	1:B:189:GLU:N	2.33	0.62
1:P:134:TYR:CD2	1:P:263:LEU:HD23	2.34	0.62
1:C:139:LEU:HD13	1:C:168:ARG:HG2	1.81	0.62
1:D:197:TYR:HD1	1:D:197:TYR:H	1.45	0.62
1:M:239:GLY:HA2	1:M:276:HIS:CD2	2.34	0.62
1:H:3:LYS:HB2	1:H:54:ASP:HB2	1.81	0.62
1:H:184:ASN:N	1:H:187:GLU:OE2	2.33	0.62
1:K:5:VAL:O	1:K:135:LEU:HA	1.99	0.62
1:B:182:THR:OG1	1:B:182:THR:O	2.18	0.62
1:D:294:THR:HG22	1:D:297:GLU:HG3	1.81	0.62
1:F:170:LEU:HD13	1:F:171:PRO:HD2	1.81	0.62
1:F:264:GLN:O	1:F:265:GLU:HB2	1.99	0.62
1:L:142:PRO:O	1:L:146:ILE:HG12	1.99	0.62
1:O:100:SER:OG	1:O:105:ASN:OD1	2.13	0.62
1:D:68:ILE:HG23	1:D:86:LEU:HD11	1.82	0.62
1:A:151:GLN:O	1:A:155:THR:OG1	2.17	0.62
1:C:4:LEU:HD21	1:C:55:VAL:HG23	1.80	0.62
1:C:224:LYS:HE3	1:C:236:ARG:NH2	2.15	0.62
1:F:126:LEU:HD21	1:F:148:LYS:HG3	1.82	0.62
1:G:98:GLN:NE2	1:G:106:SER:OG	2.33	0.62
1:N:53:ALA:HB2	1:N:260:THR:HG23	1.82	0.62
1:A:92:THR:O	1:A:113:ALA:N	2.33	0.62
1:A:126:LEU:O	1:A:130:ARG:HG3	2.00	0.62
1:D:61:VAL:CG2	1:D:86:LEU:HD23	2.29	0.62
1:E:148:LYS:HA	1:E:151:GLN:HG3	1.82	0.62
1:M:188:ALA:O	1:M:192:THR:N	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:44:GLN:NE2	1:N:252:ASP:OD1	2.30	0.62
1:B:221:LEU:HD21	1:B:227:TRP:HB2	1.82	0.62
1:H:243:LYS:HG3	1:K:101:ASP:CA	2.25	0.62
1:P:134:TYR:HD2	1:P:263:LEU:HD23	1.63	0.62
1:O:27:THR:HG22	1:P:107:ILE:HB	1.81	0.61
1:P:53:ALA:HB2	1:P:260:THR:HG23	1.80	0.61
1:G:119:ALA:HB1	1:G:148:LYS:HE2	1.82	0.61
1:H:139:LEU:HD11	1:H:170:LEU:HD11	1.81	0.61
1:M:97:ILE:HG23	1:M:107:ILE:HG23	1.83	0.61
1:N:198:ASP:OD1	1:N:201:SER:OG	2.13	0.61
1:B:300:ALA:O	1:B:304:GLU:HG2	2.01	0.61
1:F:37:PRO:O	1:F:289:GLN:HB2	2.00	0.61
1:G:3:LYS:HD3	1:G:133:ARG:HG3	1.82	0.61
1:N:171:PRO:HB2	1:N:173:GLU:OE1	2.00	0.61
1:E:14:HIS:CD2	1:E:94:ILE:HD11	2.35	0.61
1:H:117:LEU:O	1:H:142:PRO:HG2	1.99	0.61
1:L:95:ALA:HA	1:L:108:CYS:O	2.00	0.61
1:D:101:ASP:O	1:D:102:SER:OG	2.16	0.61
1:O:97:ILE:HD13	1:O:107:ILE:HG23	1.81	0.61
1:A:18:VAL:O	1:A:101:ASP:HB2	2.01	0.61
1:J:161:ILE:HD12	1:J:259:VAL:HG23	1.83	0.61
1:N:176:LYS:HG2	1:N:212:LYS:HB3	1.82	0.61
1:F:14:HIS:CE1	1:F:33:TYR:HH	2.17	0.61
1:O:37:PRO:O	1:O:289:GLN:NE2	2.33	0.61
1:B:74:PHE:HB3	1:B:79:ILE:CD1	2.30	0.61
1:C:16:LEU:HD11	1:D:110:SER:HB2	1.83	0.61
1:F:162:LEU:O	1:F:164:PRO:HD3	2.01	0.61
1:G:171:PRO:HB2	1:G:173:GLU:HG3	1.83	0.61
1:I:207:ASP:N	1:I:207:ASP:OD1	2.26	0.61
1:J:92:THR:HG22	1:J:93:GLY:H	1.66	0.61
1:O:264:GLN:OE1	1:O:295:ARG:NH2	2.34	0.61
1:B:175:LEU:HA	1:B:178:VAL:HG23	1.83	0.61
1:C:134:TYR:CD2	1:C:263:LEU:HD23	2.35	0.61
1:G:295:ARG:HD3	1:G:295:ARG:O	2.01	0.61
1:N:81:THR:O	1:N:83:GLY:N	2.34	0.61
1:N:259:VAL:O	1:N:263:LEU:HD23	2.00	0.61
1:E:230:GLN:O	1:E:233:ARG:HG3	2.01	0.60
1:L:16:LEU:HD12	1:L:33:TYR:HB2	1.81	0.60
1:A:216:ILE:HG21	1:A:268:LEU:HD11	1.83	0.60
1:G:50:ARG:O	1:G:295:ARG:HB2	2.00	0.60
1:N:154:LYS:HE2	1:N:177:CYS:HA	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:17:GLN:HA	1:B:99:VAL:CG1	2.31	0.60
1:D:139:LEU:C	1:D:166:PRO:HD2	2.21	0.60
1:F:64:ASP:OD1	1:F:64:ASP:N	2.34	0.60
1:G:43:ASN:ND2	1:G:252:ASP:OD2	2.27	0.60
1:I:43:ASN:HA	1:I:289:GLN:HE21	1.65	0.60
1:P:28:LEU:HD22	1:P:29:HIS:H	1.66	0.60
1:B:170:LEU:HD23	1:B:174:LEU:HD23	1.82	0.60
1:G:94:ILE:CG1	1:G:110:SER:HB2	2.32	0.60
1:K:228:LEU:HD22	1:K:272:ILE:HD12	1.84	0.60
1:O:227:TRP:HE1	1:O:234:GLY:HA3	1.66	0.60
1:B:43:ASN:HB3	1:B:252:ASP:HB3	1.83	0.60
1:H:249:ALA:O	1:H:251:GLY:N	2.33	0.60
1:B:253:THR:O	1:B:257:ALA:N	2.31	0.60
1:H:191:LEU:H	1:H:191:LEU:HD12	1.65	0.60
1:K:100:SER:HA	1:K:101:ASP:HB2	1.84	0.60
1:L:111:ALA:O	1:L:113:ALA:N	2.34	0.60
1:L:135:LEU:HD21	1:L:149:ALA:HB1	1.84	0.60
1:D:64:ASP:OD1	1:D:64:ASP:N	2.33	0.60
1:D:139:LEU:O	1:D:166:PRO:HD2	2.02	0.60
1:D:249:ALA:H	1:D:250:ALA:C	2.04	0.60
1:A:253:THR:HG23	1:A:292:ILE:HG12	1.84	0.60
1:D:241:VAL:O	1:D:242:VAL:HG22	2.01	0.60
1:E:50:ARG:HH11	1:E:50:ARG:HG3	1.67	0.60
1:E:175:LEU:HB3	1:E:214:ILE:HD11	1.82	0.60
1:M:147:LEU:HA	1:M:174:LEU:HD13	1.84	0.60
1:A:170:LEU:HD11	1:A:191:LEU:HD22	1.84	0.60
1:C:246:ASP:CG	1:C:286:PHE:HB2	2.22	0.60
1:N:134:TYR:CD1	1:N:161:ILE:HD11	2.37	0.60
1:P:298:VAL:O	1:P:301:PHE:HB3	2.02	0.60
1:C:184:ASN:H	1:C:187:GLU:HB2	1.67	0.59
1:G:189:GLU:OE1	1:G:190:VAL:HG23	2.02	0.59
1:C:249:ALA:HB1	1:C:288:ALA:HB2	1.83	0.59
1:G:255:ASN:ND2	1:G:255:ASN:H	1.99	0.59
1:K:110:SER:HB3	1:L:16:LEU:HD11	1.83	0.59
1:A:98:GLN:HE22	1:B:98:GLN:HE22	1.50	0.59
1:D:53:ALA:HB2	1:D:260:THR:HG22	1.83	0.59
1:F:131:ASP:N	1:F:131:ASP:OD1	2.33	0.59
1:K:229:SER:HA	1:K:234:GLY:HA2	1.83	0.59
1:C:181:ILE:HG23	1:C:183:PRO:HD3	1.83	0.59
1:C:264:GLN:O	1:C:265:GLU:HG2	2.02	0.59
1:E:7:LEU:HD12	1:E:58:ILE:HG21	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:207:ASP:OD2	1:M:208:ALA:N	2.35	0.59
1:D:13:ASP:HB3	1:D:97:ILE:HD11	1.83	0.59
1:E:50:ARG:HD2	1:E:292:ILE:CG2	2.29	0.59
1:F:134:TYR:HB2	1:F:263:LEU:HD21	1.84	0.59
1:I:14:HIS:ND1	1:I:35:VAL:HG22	2.16	0.59
1:N:269:GLU:O	1:N:273:LYS:HG2	2.02	0.59
1:O:207:ASP:HA	1:O:210:HIS:HB2	1.84	0.59
1:P:203:GLN:O	1:P:207:ASP:HB2	2.03	0.59
1:B:180:LEU:HD23	1:B:181:ILE:H	1.67	0.59
1:C:246:ASP:OD2	1:C:286:PHE:HB2	2.02	0.59
1:F:232:GLY:O	1:G:207:ASP:HB3	2.03	0.59
1:K:56:GLY:HA2	1:K:80:ASN:HB3	1.85	0.59
1:A:63:ASP:OD1	1:A:89:ASN:N	2.35	0.59
1:G:226:VAL:HG23	1:G:237:ILE:O	2.02	0.59
1:K:62:GLY:O	1:K:64:ASP:N	2.31	0.59
1:L:300:ALA:O	1:L:304:GLU:HG3	2.02	0.59
1:A:106:SER:OG	1:A:106:SER:O	2.19	0.59
1:A:295:ARG:HA	1:A:298:VAL:HG12	1.85	0.59
1:B:249:ALA:O	1:B:251:GLY:N	2.35	0.59
1:H:43:ASN:OD1	1:H:289:GLN:HG2	2.03	0.59
1:M:186:THR:O	1:M:190:VAL:HG23	2.02	0.59
1:A:172:ASP:C	1:A:174:LEU:H	2.06	0.59
1:C:12:ALA:HB2	1:C:66:PHE:CE2	2.37	0.59
1:C:95:ALA:HB2	1:C:109:ILE:HG23	1.83	0.59
1:N:279:ALA:HA	1:N:282:SER:OG	2.02	0.59
1:O:63:ASP:OD2	1:O:88:PRO:HA	2.02	0.59
1:B:203:GLN:HE22	1:I:204:GLN:HG3	1.68	0.59
1:F:4:LEU:HD23	1:F:55:VAL:HG12	1.84	0.59
1:G:267:PRO:HD2	1:G:270:SER:CB	2.32	0.59
1:H:37:PRO:O	1:H:289:GLN:NE2	2.35	0.59
1:I:220:THR:HA	1:I:226:VAL:HG23	1.84	0.59
1:K:230:GLN:O	1:K:233:ARG:HG3	2.02	0.59
1:D:68:ILE:HA	1:D:86:LEU:HD21	1.84	0.58
1:G:295:ARG:O	1:G:298:VAL:HG12	2.03	0.58
1:H:294:THR:H	1:H:297:GLU:CD	2.03	0.58
1:F:87:GLN:OE1	1:F:116:LYS:HB3	2.03	0.58
1:G:81:THR:HG22	1:G:84:VAL:HG21	1.85	0.58
1:J:196:VAL:HG13	1:J:202:ALA:HB2	1.84	0.58
1:K:64:ASP:O	1:K:68:ILE:HG12	2.03	0.58
1:L:210:HIS:CE1	1:L:231:ASN:H	2.21	0.58
1:C:136:LEU:HD22	1:C:259:VAL:HG11	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:145:GLY:O	1:K:149:ALA:N	2.33	0.58
1:L:240:PHE:HD1	1:L:301:PHE:CE2	2.17	0.58
1:A:226:VAL:HG12	1:A:237:ILE:HB	1.84	0.58
1:F:147:LEU:HD12	1:F:151:GLN:OE1	2.04	0.58
1:G:12:ALA:HB2	1:G:66:PHE:CE2	2.38	0.58
1:J:240:PHE:HD2	1:J:301:PHE:HE2	1.50	0.58
1:L:139:LEU:O	1:L:166:PRO:HD2	2.04	0.58
1:J:207:ASP:CB	1:K:232:GLY:HA3	2.33	0.58
1:K:47:ALA:C	1:K:49:ALA:H	2.07	0.58
1:L:162:LEU:O	1:L:164:PRO:HD3	2.03	0.58
1:B:17:GLN:HA	1:B:99:VAL:HG12	1.86	0.58
1:B:180:LEU:HA	1:B:216:ILE:O	2.04	0.58
1:B:286:PHE:O	1:B:290:THR:OG1	2.13	0.58
1:G:53:ALA:HB2	1:G:260:THR:CG2	2.33	0.58
1:H:171:PRO:HB2	1:H:173:GLU:HG2	1.86	0.58
1:M:306:SER:O	1:O:168:ARG:NH2	2.27	0.58
1:N:278:ALA:O	1:N:282:SER:N	2.36	0.58
1:P:224:LYS:O	1:P:236:ARG:NH1	2.36	0.58
1:G:3:LYS:H	1:G:54:ASP:HB3	1.67	0.58
1:G:117:LEU:O	1:G:142:PRO:HG2	2.04	0.58
1:J:58:ILE:HD11	1:J:125:ASP:HB3	1.86	0.58
1:N:210:HIS:C	1:N:212:LYS:H	2.07	0.58
1:N:267:PRO:HD2	1:N:270:SER:HB3	1.86	0.58
1:B:99:VAL:HG13	1:B:101:ASP:CB	2.34	0.58
1:B:229:SER:HA	1:B:233:ARG:O	2.03	0.58
1:B:297:GLU:O	1:B:300:ALA:N	2.37	0.58
1:H:281:ILE:HD11	1:H:301:PHE:HB2	1.86	0.58
1:N:68:ILE:HG23	1:N:86:LEU:HD11	1.86	0.58
1:A:31:ARG:HE	1:D:241:VAL:HG23	1.69	0.58
1:C:138:GLN:O	1:C:146:ILE:HD11	2.04	0.58
1:C:184:ASN:OD1	1:C:187:GLU:N	2.36	0.58
1:F:285:ARG:HB3	1:F:291:SER:HB3	1.86	0.58
1:F:304:GLU:HB2	1:J:115:ALA:HB1	1.85	0.58
1:G:67:GLY:HA2	1:G:70:ILE:HG22	1.85	0.58
1:I:43:ASN:HA	1:I:289:GLN:NE2	2.19	0.58
1:K:30:GLY:O	1:L:110:SER:OG	2.19	0.58
1:L:15:VAL:O	1:L:33:TYR:HA	2.03	0.58
1:C:65:SER:O	1:C:69:ASN:ND2	2.32	0.57
1:E:139:LEU:HD11	1:E:170:LEU:HD11	1.84	0.57
1:E:170:LEU:HD13	1:E:174:LEU:HD23	1.85	0.57
1:J:162:LEU:HD23	1:J:178:VAL:HG21	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:95:ALA:HA	1:K:108:CYS:O	2.04	0.57
1:L:12:ALA:HB2	1:L:66:PHE:CZ	2.39	0.57
1:M:51:MET:HB3	1:M:260:THR:HG21	1.83	0.57
1:P:184:ASN:ND2	1:P:187:GLU:OE2	2.37	0.57
1:A:14:HIS:ND1	1:A:33:TYR:OH	2.37	0.57
1:A:143:LEU:HD21	1:A:168:ARG:NH1	2.19	0.57
1:C:46:VAL:HG21	1:C:289:GLN:HG2	1.86	0.57
1:H:204:GLN:HE22	1:O:234:GLY:N	1.92	0.57
1:J:154:LYS:O	1:J:154:LYS:NZ	2.30	0.57
1:J:203:GLN:NE2	1:K:207:ASP:OD1	2.37	0.57
1:L:281:ILE:HD11	1:L:301:PHE:HB2	1.85	0.57
1:P:154:LYS:HG3	1:P:155:THR:N	2.19	0.57
1:B:198:ASP:OD1	1:B:201:SER:OG	2.21	0.57
1:C:108:CYS:SG	1:D:28:LEU:HD13	2.45	0.57
1:E:47:ALA:HB3	1:E:256:GLY:HA3	1.86	0.57
1:J:226:VAL:HG11	1:J:254:PHE:HE2	1.68	0.57
1:L:41:GLY:HA2	1:L:138:GLN:NE2	2.19	0.57
1:N:44:GLN:OE1	1:N:138:GLN:NE2	2.36	0.57
1:N:63:ASP:OD2	1:N:89:ASN:N	2.37	0.57
1:B:21:PHE:CZ	1:B:106:SER:HB3	2.39	0.57
1:D:170:LEU:HD12	1:D:191:LEU:HD21	1.85	0.57
1:G:162:LEU:O	1:G:164:PRO:HD3	2.05	0.57
1:M:251:GLY:HA2	1:M:254:PHE:HB3	1.86	0.57
1:A:227:TRP:CE3	1:A:236:ARG:HG3	2.39	0.57
1:E:220:THR:HA	1:E:226:VAL:HG23	1.86	0.57
1:K:183:PRO:O	1:K:220:THR:HG23	2.03	0.57
1:L:21:PHE:CD2	1:L:22:PRO:HD2	2.39	0.57
1:O:194:ILE:HD13	1:O:205:ALA:HA	1.85	0.57
1:P:2:ASN:ND2	1:P:4:LEU:H	2.03	0.57
1:D:281:ILE:O	1:D:285:ARG:HG2	2.05	0.57
1:E:3:LYS:HE2	1:E:263:LEU:HD11	1.86	0.57
1:E:71:ARG:O	1:E:75:LYS:HG3	2.04	0.57
1:G:135:LEU:HD21	1:G:137:MET:SD	2.44	0.57
1:I:294:THR:HB	1:I:297:GLU:H	1.68	0.57
1:J:216:ILE:HD13	1:J:268:LEU:HD21	1.86	0.57
1:O:248:THR:O	1:O:250:ALA:N	2.37	0.57
1:E:242:VAL:HG21	1:E:280:ALA:HA	1.87	0.57
1:G:72:GLU:O	1:G:75:LYS:HG3	2.05	0.57
1:G:208:ALA:O	1:G:212:LYS:HG3	2.04	0.57
1:O:31:ARG:HG2	1:O:32:ASN:N	2.19	0.57
1:P:249:ALA:O	1:P:253:THR:OG1	2.21	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:31:ARG:NH2	1:B:101:ASP:OD2	2.37	0.57
1:B:183:PRO:HB2	1:B:188:ALA:HB2	1.86	0.57
1:D:9:SER:OG	1:D:140:GLU:OE1	2.17	0.57
1:D:234:GLY:O	1:E:204:GLN:NE2	2.38	0.57
1:D:240:PHE:CD1	1:D:301:PHE:CE2	2.93	0.57
1:N:15:VAL:HG23	1:N:97:ILE:HB	1.86	0.57
1:N:291:SER:O	1:N:292:ILE:HG13	2.05	0.57
1:B:153:ALA:HB1	1:B:158:THR:HB	1.86	0.57
1:D:181:ILE:HG22	1:D:183:PRO:HD3	1.86	0.57
1:D:184:ASN:H	1:D:187:GLU:HB2	1.69	0.57
1:H:38:GLY:CA	1:H:289:GLN:HG3	2.35	0.57
1:I:44:GLN:OE1	1:I:138:GLN:NE2	2.36	0.57
1:J:73:SER:OG	1:J:74:PHE:N	2.38	0.57
1:N:97:ILE:HG12	1:N:107:ILE:HG22	1.85	0.57
1:B:117:LEU:HD23	1:B:141:THR:OG1	2.05	0.56
1:D:203:GLN:O	1:D:206:ALA:HB3	2.05	0.56
1:D:280:ALA:O	1:D:283:VAL:HG22	2.05	0.56
1:F:52:GLN:HB2	1:F:295:ARG:HH21	1.69	0.56
1:I:184:ASN:OD1	1:I:187:GLU:HG3	2.04	0.56
1:J:147:LEU:HD11	1:J:151:GLN:HE21	1.70	0.56
1:P:62:GLY:H	1:P:92:THR:HG23	1.70	0.56
1:C:22:PRO:HG3	1:C:98:GLN:NE2	2.21	0.56
1:D:61:VAL:HG23	1:D:86:LEU:HA	1.86	0.56
1:E:57:PHE:CE1	1:E:59:ALA:HB2	2.40	0.56
1:L:151:GLN:O	1:L:155:THR:HG23	2.06	0.56
1:M:285:ARG:HB2	1:M:291:SER:CB	2.34	0.56
1:N:9:SER:HB2	1:N:114:ASN:ND2	2.19	0.56
1:A:64:ASP:C	1:A:66:PHE:H	2.09	0.56
1:B:183:PRO:HG2	1:B:219:ILE:HG12	1.87	0.56
1:D:4:LEU:HB2	1:D:263:LEU:HD11	1.85	0.56
1:D:44:GLN:HG2	1:D:252:ASP:O	2.05	0.56
1:E:7:LEU:HD22	1:E:137:MET:SD	2.45	0.56
1:F:240:PHE:CD1	1:F:301:PHE:HE2	2.22	0.56
1:I:31:ARG:NH2	1:I:101:ASP:OD2	2.38	0.56
1:J:172:ASP:O	1:J:174:LEU:N	2.39	0.56
1:K:95:ALA:HA	1:K:109:ILE:HA	1.86	0.56
1:K:96:MET:HE2	1:L:98:GLN:HE21	1.70	0.56
1:K:115:ALA:HA	1:K:142:PRO:HD3	1.85	0.56
1:K:215:GLU:HB3	1:K:216:ILE:HG13	1.87	0.56
1:L:207:ASP:HA	1:L:210:HIS:CD2	2.40	0.56
1:L:230:GLN:O	1:L:233:ARG:HG3	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:251:GLY:O	1:N:255:ASN:HB2	2.05	0.56
1:P:278:ALA:HA	1:P:281:ILE:HD12	1.86	0.56
1:A:218:ILE:HG22	1:A:226:VAL:HG21	1.88	0.56
1:F:66:PHE:CE1	1:F:70:ILE:HG21	2.41	0.56
1:F:279:ALA:O	1:F:283:VAL:HG13	2.05	0.56
1:J:184:ASN:ND2	1:J:187:GLU:HG3	2.20	0.56
1:L:181:ILE:HD12	1:L:214:ILE:HD13	1.86	0.56
1:L:242:VAL:O	1:L:243:LYS:HB2	2.04	0.56
1:P:2:ASN:ND2	1:P:54:ASP:O	2.36	0.56
1:B:206:ALA:O	1:B:210:HIS:N	2.31	0.56
1:B:281:ILE:O	1:B:284:THR:HG22	2.05	0.56
1:E:5:VAL:O	1:E:135:LEU:HD12	2.06	0.56
1:F:174:LEU:O	1:F:177:CYS:N	2.29	0.56
1:I:139:LEU:HD11	1:I:170:LEU:HD11	1.88	0.56
1:M:224:LYS:O	1:M:236:ARG:NH1	2.39	0.56
1:P:4:LEU:HD23	1:P:55:VAL:HB	1.85	0.56
1:M:2:ASN:HD21	1:M:80:ASN:HD22	1.54	0.56
1:N:3:LYS:HG2	1:N:263:LEU:HD12	1.86	0.56
1:O:218:ILE:HD13	1:O:272:ILE:HD11	1.88	0.56
1:B:199:ASP:OD2	1:B:199:ASP:N	2.38	0.56
1:B:207:ASP:OD2	1:I:203:GLN:HG3	2.05	0.56
1:D:163:ASN:HD22	1:D:164:PRO:N	2.04	0.56
1:F:207:ASP:O	1:F:210:HIS:HB2	2.06	0.56
1:F:233:ARG:HA	1:G:207:ASP:HB2	1.88	0.56
1:G:230:GLN:O	1:G:233:ARG:HG3	2.06	0.56
1:K:72:GLU:O	1:K:76:LEU:HD22	2.06	0.56
1:A:178:VAL:HG23	1:A:214:ILE:HG23	1.86	0.56
1:B:14:HIS:CD2	1:B:94:ILE:HG23	2.41	0.56
1:B:246:ASP:OD1	1:B:247:THR:N	2.39	0.56
1:E:161:ILE:HD12	1:E:180:LEU:HD23	1.86	0.56
1:H:51:MET:HA	1:H:295:ARG:HB2	1.88	0.56
1:I:264:GLN:OE1	1:I:295:ARG:NH2	2.39	0.56
1:K:117:LEU:O	1:K:142:PRO:HG2	2.05	0.56
1:O:285:ARG:O	1:O:287:GLY:N	2.39	0.56
1:D:161:ILE:HG23	1:D:180:LEU:HD22	1.86	0.56
1:E:228:LEU:HD11	1:E:268:LEU:HD21	1.86	0.56
1:F:21:PHE:CE2	1:F:106:SER:HB2	2.41	0.56
1:G:56:GLY:CA	1:G:80:ASN:HB3	2.36	0.56
1:H:57:PHE:HB2	1:H:79:ILE:HG21	1.86	0.56
1:J:138:GLN:O	1:J:146:ILE:HD11	2.06	0.56
1:N:136:LEU:HD22	1:N:259:VAL:HG11	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:257:ALA:O	1:B:260:THR:N	2.39	0.56
1:H:94:ILE:HG12	1:H:95:ALA:N	2.21	0.56
1:K:192:THR:HG21	1:K:209:LEU:HD22	1.88	0.56
1:N:283:VAL:O	1:N:285:ARG:N	2.39	0.56
1:P:85:LYS:NZ	1:P:124:PRO:HG2	2.20	0.56
1:B:46:VAL:HG21	1:B:289:GLN:HE22	1.71	0.55
1:C:172:ASP:OD2	1:C:172:ASP:N	2.37	0.55
1:D:195:THR:O	1:D:201:SER:OG	2.17	0.55
1:A:220:THR:CA	1:A:226:VAL:HG23	2.36	0.55
1:D:184:ASN:OD1	1:D:187:GLU:HG3	2.05	0.55
1:D:259:VAL:O	1:D:263:LEU:HB2	2.05	0.55
1:K:12:ALA:HB2	1:K:66:PHE:CE1	2.41	0.55
1:L:139:LEU:HD11	1:L:170:LEU:HD11	1.86	0.55
1:A:249:ALA:HA	1:A:252:ASP:HB2	1.89	0.55
1:B:14:HIS:HD2	1:B:94:ILE:HG23	1.71	0.55
1:B:57:PHE:HD1	1:B:58:ILE:H	1.54	0.55
1:M:31:ARG:HH22	1:P:243:LYS:HG3	1.72	0.55
1:M:50:ARG:NE	1:M:77:ASP:OD1	2.35	0.55
1:C:224:LYS:HE3	1:C:236:ARG:HH21	1.71	0.55
1:D:99:VAL:O	1:D:101:ASP:HB3	2.06	0.55
1:G:61:VAL:HA	1:G:92:THR:HG23	1.88	0.55
1:L:56:GLY:HA2	1:L:80:ASN:HB3	1.88	0.55
1:N:111:ALA:O	1:N:114:ASN:N	2.39	0.55
1:O:44:GLN:HE21	1:O:44:GLN:N	2.04	0.55
1:O:236:ARG:HH12	1:O:238:PRO:HA	1.70	0.55
1:E:63:ASP:HB3	1:E:86:LEU:HD23	1.89	0.55
1:G:163:ASN:ND2	1:G:182:THR:OG1	2.38	0.55
1:G:257:ALA:O	1:G:259:VAL:N	2.39	0.55
1:J:267:PRO:HD2	1:J:270:SER:HB2	1.87	0.55
1:I:5:VAL:O	1:I:135:LEU:HD12	2.07	0.55
1:L:91:PRO:O	1:L:113:ALA:HB2	2.06	0.55
1:A:97:ILE:HD12	1:A:107:ILE:CG1	2.35	0.55
1:E:97:ILE:HG12	1:E:107:ILE:HG23	1.88	0.55
1:I:72:GLU:HG3	1:I:75:LYS:HE2	1.87	0.55
1:N:284:THR:HG22	1:N:285:ARG:HG2	1.89	0.55
1:C:71:ARG:HB2	1:C:84:VAL:HG11	1.88	0.55
1:P:5:VAL:O	1:P:135:LEU:HA	2.06	0.55
1:P:247:THR:HA	1:P:250:ALA:HB3	1.88	0.55
1:E:303:ALA:O	1:E:306:SER:OG	2.24	0.55
1:F:267:PRO:O	1:F:269:GLU:N	2.40	0.55
1:B:76:LEU:O	1:B:78:GLY:N	2.35	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:170:LEU:CD1	1:F:174:LEU:HD23	2.38	0.55
1:H:12:ALA:HB2	1:H:66:PHE:CE1	2.41	0.55
1:M:3:LYS:HG3	1:M:54:ASP:HB3	1.89	0.55
1:N:17:GLN:HG3	1:N:99:VAL:HG23	1.89	0.55
1:O:199:ASP:O	1:O:202:ALA:N	2.39	0.55
1:A:101:ASP:N	1:A:102:SER:HA	2.22	0.54
1:B:44:GLN:HB3	1:B:136:LEU:HD21	1.90	0.54
1:C:264:GLN:C	1:C:265:GLU:HG2	2.27	0.54
1:J:211:CYS:HA	1:K:233:ARG:HH11	1.72	0.54
1:N:300:ALA:O	1:N:304:GLU:HG2	2.06	0.54
1:P:147:LEU:HD13	1:P:174:LEU:HB2	1.89	0.54
1:P:180:LEU:HD11	1:P:216:ILE:HD12	1.89	0.54
1:A:61:VAL:HA	1:A:92:THR:HG23	1.89	0.54
1:B:228:LEU:HD12	1:B:229:SER:H	1.73	0.54
1:B:230:GLN:O	1:B:233:ARG:NE	2.39	0.54
1:E:46:VAL:HG12	1:E:292:ILE:HG12	1.89	0.54
1:E:189:GLU:HG2	1:E:194:ILE:O	2.07	0.54
1:H:226:VAL:HG12	1:H:237:ILE:O	2.06	0.54
1:J:210:HIS:CD2	1:J:231:ASN:HA	2.43	0.54
1:J:233:ARG:HD3	1:K:211:CYS:HA	1.90	0.54
1:L:64:ASP:OD1	1:L:92:THR:OG1	2.26	0.54
1:G:92:THR:HG22	1:G:93:GLY:H	1.72	0.54
1:L:170:LEU:HB2	1:L:175:LEU:HD11	1.89	0.54
1:P:221:LEU:HD11	1:P:227:TRP:HB2	1.89	0.54
1:H:113:ALA:O	1:H:116:LYS:HB2	2.07	0.54
1:L:57:PHE:HD1	1:L:58:ILE:H	1.55	0.54
1:C:58:ILE:HD12	1:C:125:ASP:OD1	2.08	0.54
1:H:38:GLY:HA2	1:H:289:GLN:CG	2.35	0.54
1:H:182:THR:HG21	1:H:255:ASN:OD1	2.07	0.54
1:H:243:LYS:HE2	1:K:101:ASP:HA	1.89	0.54
1:I:61:VAL:HG23	1:I:86:LEU:HD23	1.90	0.54
1:J:3:LYS:HB3	1:J:263:LEU:HD21	1.90	0.54
1:A:242:VAL:HG11	1:A:280:ALA:HB1	1.88	0.54
1:D:285:ARG:HB3	1:D:291:SER:CB	2.36	0.54
1:F:206:ALA:HA	1:F:217:VAL:HG11	1.89	0.54
1:F:225:GLY:HA3	1:F:238:PRO:HA	1.90	0.54
1:H:134:TYR:HB2	1:H:263:LEU:HD11	1.90	0.54
1:I:147:LEU:HD22	1:I:174:LEU:HB2	1.89	0.54
1:J:295:ARG:NH1	1:J:299:GLU:OE2	2.41	0.54
1:K:107:ILE:HB	1:L:27:THR:OG1	2.08	0.54
1:L:93:GLY:HA2	1:L:112:GLU:HB2	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:277:ALA:O	1:P:281:ILE:HG13	2.07	0.54
1:A:89:ASN:N	1:A:89:ASN:OD1	2.41	0.54
1:D:129:ILE:HD12	1:D:135:LEU:HD22	1.88	0.54
1:H:64:ASP:OD2	1:H:64:ASP:N	2.41	0.54
1:L:139:LEU:HD13	1:L:170:LEU:HD21	1.89	0.54
1:M:87:GLN:HG3	1:M:116:LYS:HG3	1.88	0.54
1:M:172:ASP:O	1:M:174:LEU:N	2.41	0.54
1:M:277:ALA:HB2	1:M:302:LEU:HD21	1.89	0.54
1:P:97:ILE:HG22	1:P:99:VAL:HG13	1.88	0.54
1:P:253:THR:HG23	1:P:292:ILE:HG12	1.90	0.54
1:A:183:PRO:O	1:A:219:ILE:HA	2.08	0.54
1:B:57:PHE:HD1	1:B:58:ILE:N	2.04	0.54
1:B:281:ILE:HD11	1:B:298:VAL:HG13	1.90	0.54
1:B:172:ASP:HA	1:B:175:LEU:HD12	1.89	0.54
1:B:249:ALA:HB1	1:B:252:ASP:HB2	1.89	0.54
1:C:206:ALA:O	1:C:209:LEU:HB2	2.08	0.54
1:D:240:PHE:CD1	1:D:301:PHE:HE2	2.25	0.54
1:H:228:LEU:HD11	1:H:268:LEU:HD21	1.90	0.54
1:H:279:ALA:C	1:H:283:VAL:HG13	2.28	0.54
1:J:202:ALA:O	1:J:206:ALA:N	2.30	0.54
1:J:245:THR:HB	1:J:283:VAL:O	2.07	0.54
1:O:4:LEU:HD23	1:O:55:VAL:HB	1.88	0.54
1:O:4:LEU:O	1:O:55:VAL:HA	2.08	0.54
1:P:60:CYS:HB3	1:P:113:ALA:O	2.07	0.54
1:A:98:GLN:HG2	1:B:96:MET:HE1	1.90	0.54
1:C:274:PHE:HA	1:C:302:LEU:HD11	1.89	0.54
1:E:59:ALA:HB3	1:E:84:VAL:HG22	1.90	0.54
1:J:97:ILE:HG13	1:J:107:ILE:HG23	1.90	0.54
1:N:98:GLN:HE21	1:N:106:SER:HB3	1.73	0.54
1:P:19:PRO:HG2	1:P:28:LEU:HD21	1.89	0.54
1:P:40:LYS:HE3	1:P:165:ALA:HB1	1.88	0.54
1:B:281:ILE:HD11	1:B:298:VAL:CG1	2.38	0.53
1:D:139:LEU:HD11	1:D:170:LEU:HD11	1.89	0.53
1:G:184:ASN:H	1:G:187:GLU:HB2	1.73	0.53
1:H:7:LEU:HD22	1:H:137:MET:SD	2.48	0.53
1:H:64:ASP:OD1	1:H:92:THR:OG1	2.25	0.53
1:L:21:PHE:HE2	1:L:106:SER:HB2	1.73	0.53
1:M:264:GLN:OE1	1:M:295:ARG:NH2	2.42	0.53
1:B:278:ALA:HA	1:B:281:ILE:HG13	1.90	0.53
1:M:18:VAL:HG21	1:M:98:GLN:HB3	1.90	0.53
1:E:247:THR:C	1:E:249:ALA:H	2.11	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:207:ASP:HA	1:F:210:HIS:CD2	2.43	0.53
1:G:21:PHE:HE2	1:G:106:SER:HB3	1.72	0.53
1:G:58:ILE:CD1	1:G:125:ASP:HB3	2.38	0.53
1:N:198:ASP:OD2	1:N:200:SER:OG	2.18	0.53
1:N:295:ARG:HG2	1:N:295:ARG:NH1	2.23	0.53
1:A:267:PRO:HB2	1:A:269:GLU:OE1	2.09	0.53
1:I:21:PHE:CG	1:I:22:PRO:HD2	2.42	0.53
1:I:132:ALA:O	1:I:158:THR:OG1	2.19	0.53
1:O:3:LYS:HE2	1:O:54:ASP:HB2	1.89	0.53
1:P:206:ALA:O	1:P:209:LEU:HB2	2.07	0.53
1:C:240:PHE:O	1:C:242:VAL:HG13	2.09	0.53
1:H:226:VAL:O	1:H:226:VAL:HG13	2.08	0.53
1:K:12:ALA:HB2	1:K:66:PHE:CZ	2.43	0.53
1:N:220:THR:HA	1:N:226:VAL:HA	1.89	0.53
1:A:181:ILE:HG21	1:A:209:LEU:CD1	2.37	0.53
1:B:189:GLU:O	1:B:193:GLY:N	2.40	0.53
1:B:257:ALA:O	1:B:260:THR:HG22	2.09	0.53
1:C:139:LEU:N	1:C:165:ALA:O	2.29	0.53
1:E:3:LYS:HB3	1:E:263:LEU:HD21	1.91	0.53
1:H:81:THR:HB	1:H:84:VAL:HG12	1.89	0.53
1:A:194:ILE:HG22	1:A:196:VAL:H	1.73	0.53
1:J:92:THR:HG22	1:J:93:GLY:N	2.23	0.53
1:N:17:GLN:NE2	1:N:32:ASN:OD1	2.42	0.53
1:O:37:PRO:HB2	1:O:289:GLN:HE22	1.74	0.53
1:B:288:ALA:O	1:B:291:SER:OG	2.23	0.53
1:E:181:ILE:C	1:E:183:PRO:HD3	2.29	0.53
1:G:49:ALA:HB1	1:G:77:ASP:O	2.09	0.53
1:H:243:LYS:NZ	1:H:244:ALA:HB3	2.24	0.53
1:I:44:GLN:HE22	1:I:138:GLN:HG2	1.74	0.53
1:K:53:ALA:HB2	1:K:260:THR:HG23	1.90	0.53
1:L:180:LEU:HD21	1:L:218:ILE:HD12	1.91	0.53
1:L:244:ALA:O	1:L:246:ASP:N	2.41	0.53
1:O:175:LEU:HB3	1:O:214:ILE:HD11	1.90	0.53
1:G:21:PHE:O	1:G:23:ARG:N	2.42	0.53
1:L:20:SER:OG	1:L:21:PHE:N	2.42	0.53
1:N:3:LYS:HE3	1:N:263:LEU:HD12	1.91	0.53
1:P:243:LYS:HE2	1:P:244:ALA:H	1.73	0.53
1:A:19:PRO:HA	1:A:101:ASP:CB	2.39	0.53
1:D:9:SER:HB3	1:D:140:GLU:HB3	1.90	0.53
1:D:197:TYR:CD1	1:D:197:TYR:N	2.77	0.53
1:H:180:LEU:HD23	1:H:181:ILE:N	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:139:LEU:HD13	1:G:168:ARG:HG2	1.91	0.52
1:G:294:THR:HB	1:G:297:GLU:HB2	1.90	0.52
1:J:188:ALA:HA	1:J:191:LEU:HG	1.89	0.52
1:J:209:LEU:HB3	1:J:214:ILE:HD12	1.90	0.52
1:M:18:VAL:CG2	1:M:98:GLN:HB3	2.39	0.52
1:N:139:LEU:N	1:N:165:ALA:O	2.37	0.52
1:N:233:ARG:O	1:N:235:GLN:N	2.41	0.52
1:B:2:ASN:O	1:B:3:LYS:HD3	2.09	0.52
1:J:73:SER:O	1:J:76:LEU:N	2.25	0.52
1:D:138:GLN:HA	1:D:163:ASN:HB3	1.91	0.52
1:I:280:ALA:HA	1:I:283:VAL:HG22	1.90	0.52
1:J:16:LEU:HD11	1:J:30:GLY:HA3	1.91	0.52
1:K:16:LEU:HD11	1:L:110:SER:HB2	1.90	0.52
1:N:266:MET:HB3	1:N:271:ALA:HB2	1.90	0.52
1:O:203:GLN:HB2	1:O:227:TRP:CZ2	2.44	0.52
1:A:66:PHE:C	1:A:68:ILE:H	2.12	0.52
1:B:15:VAL:HG21	1:B:36:ILE:HD11	1.92	0.52
1:H:70:ILE:HD13	1:H:74:PHE:CZ	2.45	0.52
1:J:226:VAL:HG11	1:J:254:PHE:CE2	2.44	0.52
1:L:51:MET:N	1:L:51:MET:SD	2.83	0.52
1:L:111:ALA:O	1:L:114:ASN:N	2.39	0.52
1:M:285:ARG:HB2	1:M:291:SER:HB3	1.90	0.52
1:N:81:THR:C	1:N:83:GLY:H	2.13	0.52
1:D:14:HIS:HB2	1:D:95:ALA:O	2.10	0.52
1:F:110:SER:OG	1:F:112:GLU:OE2	2.23	0.52
1:G:86:LEU:HD23	1:G:86:LEU:N	2.24	0.52
1:I:215:GLU:HG2	1:I:216:ILE:HG13	1.92	0.52
1:B:225:GLY:HA2	1:B:237:ILE:O	2.10	0.52
1:B:245:THR:N	1:B:283:VAL:O	2.42	0.52
1:E:31:ARG:HG3	1:E:32:ASN:H	1.73	0.52
1:E:126:LEU:HB3	1:E:152:GLU:HG2	1.90	0.52
1:G:111:ALA:HA	1:G:114:ASN:ND2	2.24	0.52
1:G:192:THR:HG23	1:G:194:ILE:HG13	1.90	0.52
1:H:248:THR:OG1	1:H:249:ALA:N	2.42	0.52
1:N:185:GLU:CD	1:N:221:LEU:HA	2.30	0.52
1:P:131:ASP:OD2	1:P:132:ALA:N	2.43	0.52
1:P:139:LEU:N	1:P:165:ALA:O	2.33	0.52
1:B:91:PRO:HD2	1:B:112:GLU:CG	2.39	0.52
1:B:117:LEU:O	1:B:142:PRO:HG2	2.09	0.52
1:D:163:ASN:HD22	1:D:164:PRO:CD	2.23	0.52
1:E:147:LEU:O	1:E:151:GLN:HG2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:173:GLU:O	1:E:176:LYS:HE3	2.10	0.52
1:F:58:ILE:HD11	1:F:122:ILE:CG2	2.39	0.52
1:N:184:ASN:H	1:N:187:GLU:HB2	1.75	0.52
1:P:14:HIS:CD2	1:P:94:ILE:HD11	2.44	0.52
1:C:203:GLN:O	1:C:207:ASP:HB2	2.09	0.52
1:E:63:ASP:OD2	1:E:88:PRO:HA	2.09	0.52
1:G:15:VAL:HG12	1:G:34:GLN:O	2.10	0.52
1:G:282:SER:O	1:G:285:ARG:HB2	2.10	0.52
1:H:294:THR:HG23	1:H:297:GLU:OE1	2.10	0.52
1:D:196:VAL:HA	1:D:201:SER:OG	2.10	0.52
1:E:130:ARG:O	1:E:130:ARG:HG2	2.10	0.52
1:G:23:ARG:HB2	1:G:24:PRO:HD2	1.91	0.52
1:H:15:VAL:O	1:H:33:TYR:HA	2.09	0.52
1:H:242:VAL:HG21	1:H:283:VAL:HG21	1.91	0.52
1:K:175:LEU:HD11	1:K:191:LEU:HD21	1.91	0.52
1:L:98:GLN:HB2	1:L:106:SER:HB3	1.92	0.52
1:N:40:LYS:HB3	1:N:138:GLN:HG2	1.91	0.52
1:A:172:ASP:O	1:A:174:LEU:N	2.36	0.51
1:B:74:PHE:O	1:B:76:LEU:N	2.42	0.51
1:B:218:ILE:HD13	1:B:272:ILE:HD11	1.92	0.51
1:C:154:LYS:HG2	1:C:155:THR:HG23	1.92	0.51
1:C:283:VAL:O	1:C:285:ARG:N	2.43	0.51
1:D:240:PHE:HD1	1:D:301:PHE:CE2	2.28	0.51
1:E:3:LYS:HB2	1:E:54:ASP:HB3	1.91	0.51
1:H:16:LEU:HD11	1:H:30:GLY:HA3	1.92	0.51
1:H:51:MET:C	1:H:52:GLN:HG2	2.30	0.51
1:H:92:THR:HG22	1:H:93:GLY:H	1.75	0.51
1:J:159:ASN:HA	1:J:179:ASP:OD2	2.10	0.51
1:A:15:VAL:HG22	1:A:97:ILE:CG2	2.41	0.51
1:C:183:PRO:O	1:C:220:THR:HG23	2.10	0.51
1:D:172:ASP:O	1:D:174:LEU:N	2.43	0.51
1:H:245:THR:HG23	1:H:283:VAL:O	2.10	0.51
1:I:215:GLU:HG3	1:I:231:ASN:OD1	2.10	0.51
1:M:46:VAL:HG13	1:M:292:ILE:HD13	1.92	0.51
1:M:56:GLY:HA2	1:M:80:ASN:HB3	1.92	0.51
1:B:17:GLN:HB2	1:B:31:ARG:HG2	1.92	0.51
1:F:4:LEU:HD23	1:F:55:VAL:CG1	2.41	0.51
1:H:91:PRO:HG2	1:H:112:GLU:HG3	1.92	0.51
1:J:21:PHE:CE2	1:J:106:SER:HB3	2.42	0.51
1:J:46:VAL:HG12	1:J:292:ILE:HD13	1.91	0.51
1:K:48:ALA:O	1:K:53:ALA:HB3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:110:SER:OG	1:K:112:GLU:OE2	2.27	0.51
1:L:9:SER:CB	1:L:140:GLU:HG2	2.40	0.51
1:A:21:PHE:CE1	1:A:104:GLU:HB2	2.46	0.51
1:C:42:ALA:O	1:C:46:VAL:HG22	2.10	0.51
1:D:49:ALA:HB1	1:D:77:ASP:O	2.09	0.51
1:D:126:LEU:C	1:D:128:ALA:H	2.08	0.51
1:E:228:LEU:HD22	1:E:272:ILE:CD1	2.41	0.51
1:F:126:LEU:HA	1:F:129:ILE:HD12	1.92	0.51
1:G:86:LEU:HD23	1:G:86:LEU:H	1.76	0.51
1:G:94:ILE:HG12	1:G:110:SER:HB2	1.92	0.51
1:G:115:ALA:HA	1:G:142:PRO:HD3	1.92	0.51
1:G:249:ALA:HA	1:G:252:ASP:HB2	1.93	0.51
1:I:57:PHE:HD1	1:I:58:ILE:H	1.58	0.51
1:J:72:GLU:O	1:J:75:LYS:HG3	2.11	0.51
1:K:87:GLN:HG3	1:K:116:LYS:HG3	1.91	0.51
1:P:172:ASP:O	1:P:174:LEU:N	2.43	0.51
1:C:46:VAL:HG21	1:C:289:GLN:CG	2.41	0.51
1:H:141:THR:HB	1:H:142:PRO:HD2	1.91	0.51
1:A:16:LEU:HD11	1:B:110:SER:HB2	1.92	0.51
1:I:281:ILE:HB	1:I:293:PRO:HG3	1.92	0.51
1:B:11:ASN:O	1:B:11:ASN:ND2	2.43	0.51
1:C:151:GLN:HA	1:C:154:LYS:HB3	1.93	0.51
1:E:210:HIS:CE1	1:E:215:GLU:O	2.64	0.51
1:F:26:GLU:HG3	1:F:27:THR:H	1.74	0.51
1:F:141:THR:HB	1:F:142:PRO:HD2	1.93	0.51
1:H:31:ARG:HH22	1:H:101:ASP:CG	2.09	0.51
1:I:3:LYS:HE2	1:I:263:LEU:HG	1.92	0.51
1:L:252:ASP:O	1:L:256:GLY:N	2.43	0.51
1:N:132:ALA:O	1:N:158:THR:OG1	2.17	0.51
1:A:194:ILE:HG13	1:A:205:ALA:HA	1.93	0.51
1:C:28:LEU:HD22	1:C:29:HIS:N	2.26	0.51
1:E:57:PHE:HD1	1:E:58:ILE:H	1.58	0.51
1:E:110:SER:OG	1:E:112:GLU:OE2	2.29	0.51
1:H:143:LEU:HG	1:H:168:ARG:NH1	2.26	0.51
1:K:96:MET:HE1	1:L:96:MET:HB3	1.92	0.51
1:L:294:THR:O	1:L:298:VAL:HG23	2.11	0.51
1:P:220:THR:HA	1:P:226:VAL:HG22	1.91	0.51
1:A:60:CYS:SG	1:A:116:LYS:HB2	2.50	0.51
1:D:221:LEU:O	1:D:224:LYS:HD3	2.11	0.51
1:D:285:ARG:HB3	1:D:291:SER:CA	2.41	0.51
1:F:235:GLN:HG2	1:F:235:GLN:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:142:PRO:O	1:H:146:ILE:HG13	2.11	0.51
1:H:162:LEU:O	1:H:164:PRO:HD3	2.11	0.51
1:H:207:ASP:O	1:H:210:HIS:HB2	2.11	0.51
1:I:57:PHE:CE1	1:I:59:ALA:HB2	2.46	0.51
1:N:119:ALA:N	1:N:144:ASP:OD1	2.29	0.51
1:A:96:MET:O	1:A:108:CYS:N	2.44	0.51
1:K:273:LYS:O	1:K:274:PHE:C	2.49	0.51
1:L:59:ALA:HB3	1:L:84:VAL:HG13	1.92	0.51
1:L:100:SER:O	1:L:102:SER:N	2.44	0.51
1:C:289:GLN:O	1:C:290:THR:OG1	2.27	0.50
1:E:284:THR:HG23	1:E:285:ARG:HE	1.75	0.50
1:I:173:GLU:HA	1:I:176:LYS:HD3	1.93	0.50
1:J:66:PHE:CZ	1:J:70:ILE:HD12	2.46	0.50
1:J:135:LEU:HD22	1:J:160:VAL:HG22	1.93	0.50
1:L:46:VAL:HG12	1:L:292:ILE:HD13	1.92	0.50
1:L:161:ILE:HD13	1:L:259:VAL:HG12	1.92	0.50
1:N:64:ASP:OD1	1:N:67:GLY:N	2.25	0.50
1:O:64:ASP:OD1	1:O:64:ASP:N	2.36	0.50
1:P:71:ARG:HH11	1:P:71:ARG:HB2	1.76	0.50
1:A:69:ASN:O	1:A:73:SER:HB2	2.11	0.50
1:G:4:LEU:O	1:G:55:VAL:HA	2.10	0.50
1:I:60:CYS:SG	1:I:117:LEU:HD13	2.51	0.50
1:P:53:ALA:HB2	1:P:260:THR:CG2	2.41	0.50
1:C:301:PHE:HA	1:C:304:GLU:HG3	1.92	0.50
1:F:81:THR:HG22	1:F:84:VAL:HG11	1.93	0.50
1:I:187:GLU:O	1:I:191:LEU:HD11	2.10	0.50
1:I:239:GLY:HA2	1:I:276:HIS:ND1	2.26	0.50
1:K:139:LEU:HD13	1:K:170:LEU:HD21	1.94	0.50
1:L:7:LEU:HD12	1:L:58:ILE:HG21	1.93	0.50
1:O:77:ASP:OD2	1:O:77:ASP:N	2.43	0.50
1:O:162:LEU:O	1:O:164:PRO:HD3	2.12	0.50
1:P:279:ALA:O	1:P:283:VAL:HG13	2.12	0.50
1:D:178:VAL:HG12	1:D:180:LEU:H	1.77	0.50
1:D:277:ALA:HB1	1:D:301:PHE:HD2	1.76	0.50
1:E:183:PRO:HA	1:E:187:GLU:OE1	2.11	0.50
1:F:240:PHE:HD1	1:F:301:PHE:HE2	1.59	0.50
1:P:66:PHE:CE1	1:P:70:ILE:HD12	2.46	0.50
1:A:16:LEU:CD1	1:B:110:SER:HB2	2.41	0.50
1:A:254:PHE:HA	1:A:275:ALA:HB1	1.94	0.50
1:B:180:LEU:HD21	1:B:218:ILE:HD11	1.94	0.50
1:B:215:GLU:HB3	1:B:216:ILE:HG13	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:61:VAL:HB	1:C:67:GLY:HA2	1.93	0.50
1:O:237:ILE:HG22	1:O:239:GLY:H	1.75	0.50
1:A:143:LEU:H	1:A:143:LEU:HD12	1.77	0.50
1:B:245:THR:HG21	1:B:286:PHE:CD2	2.43	0.50
1:D:94:ILE:O	1:D:109:ILE:HG13	2.11	0.50
1:D:282:SER:HA	1:D:285:ARG:HB2	1.94	0.50
1:F:139:LEU:HD13	1:F:168:ARG:HD2	1.92	0.50
1:H:240:PHE:HD1	1:H:301:PHE:CE2	2.18	0.50
1:H:243:LYS:HE2	1:K:101:ASP:H	1.77	0.50
1:N:97:ILE:HG23	1:N:107:ILE:HG23	1.93	0.50
1:O:127:ALA:HA	1:O:130:ARG:NH1	2.27	0.50
1:O:234:GLY:C	1:O:235:GLN:HG2	2.31	0.50
1:E:21:PHE:CD2	1:E:22:PRO:HD2	2.47	0.50
1:G:60:CYS:SG	1:G:117:LEU:HD13	2.52	0.50
1:H:133:ARG:O	1:H:159:ASN:N	2.42	0.50
1:H:267:PRO:HD2	1:H:270:SER:HB3	1.94	0.50
1:H:280:ALA:O	1:H:284:THR:HG22	2.12	0.50
1:K:50:ARG:NH1	1:K:292:ILE:HB	2.27	0.50
1:L:228:LEU:HD22	1:L:272:ILE:HD12	1.92	0.50
1:O:229:SER:HA	1:O:233:ARG:O	2.11	0.50
1:B:125:ASP:O	1:B:129:ILE:HG12	2.12	0.50
1:B:182:THR:HG21	1:B:255:ASN:HD21	1.77	0.50
1:G:63:ASP:O	1:G:68:ILE:HD11	2.12	0.50
1:K:226:VAL:HG11	1:K:272:ILE:HD13	1.93	0.50
1:L:218:ILE:CG2	1:L:226:VAL:HG21	2.41	0.50
1:A:162:LEU:HD23	1:A:181:ILE:HD11	1.94	0.50
1:E:240:PHE:O	1:E:242:VAL:HG12	2.12	0.50
1:G:261:GLY:C	1:G:263:LEU:H	2.15	0.50
1:H:53:ALA:O	1:H:55:VAL:N	2.45	0.50
1:K:81:THR:O	1:K:84:VAL:HG12	2.12	0.50
1:L:160:VAL:HG12	1:L:178:VAL:HA	1.94	0.50
1:O:57:PHE:HB2	1:O:79:ILE:CG2	2.41	0.50
1:B:12:ALA:HB2	1:B:66:PHE:CE1	2.47	0.49
1:E:181:ILE:HG21	1:E:209:LEU:HD13	1.94	0.49
1:F:189:GLU:HA	1:F:194:ILE:O	2.12	0.49
1:F:224:LYS:O	1:F:236:ARG:NH1	2.43	0.49
1:G:13:ASP:O	1:G:35:VAL:HA	2.11	0.49
1:H:164:PRO:HG3	1:H:181:ILE:HD11	1.93	0.49
1:H:246:ASP:OD1	1:H:286:PHE:HA	2.11	0.49
1:K:109:ILE:O	1:L:29:HIS:HA	2.12	0.49
1:L:141:THR:HB	1:L:142:PRO:HD2	1.92	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:40:LYS:NZ	1:M:165:ALA:HB3	2.26	0.49
1:O:18:VAL:H	1:O:99:VAL:HG12	1.77	0.49
1:B:167:ALA:HB2	1:B:187:GLU:HB3	1.94	0.49
1:E:184:ASN:HD22	1:E:187:GLU:H	1.57	0.49
1:J:170:LEU:HD12	1:J:174:LEU:HD23	1.94	0.49
1:K:257:ALA:O	1:K:260:THR:N	2.45	0.49
1:L:57:PHE:HD1	1:L:58:ILE:N	2.10	0.49
1:L:91:PRO:HG2	1:L:112:GLU:CB	2.41	0.49
1:L:243:LYS:HB3	1:L:244:ALA:HB2	1.95	0.49
1:O:40:LYS:HG3	1:O:140:GLU:OE2	2.12	0.49
1:A:247:THR:HA	1:A:250:ALA:HB2	1.93	0.49
1:B:117:LEU:HB3	1:B:141:THR:HG23	1.94	0.49
1:B:264:GLN:O	1:B:266:MET:N	2.45	0.49
1:F:110:SER:OG	1:F:111:ALA:N	2.44	0.49
1:H:26:GLU:HG3	1:H:27:THR:H	1.77	0.49
1:I:248:THR:HG21	1:I:288:ALA:HB1	1.95	0.49
1:L:113:ALA:O	1:L:116:LYS:HB2	2.12	0.49
1:N:63:ASP:OD2	1:N:88:PRO:HA	2.12	0.49
1:O:30:GLY:N	1:P:109:ILE:O	2.33	0.49
1:O:176:LYS:HA	1:O:213:GLY:HA3	1.93	0.49
1:P:164:PRO:HG2	1:P:183:PRO:HA	1.93	0.49
1:B:91:PRO:HG2	1:B:112:GLU:HG2	1.93	0.49
1:B:201:SER:HA	1:B:204:GLN:OE1	2.11	0.49
1:E:46:VAL:HG21	1:E:289:GLN:OE1	2.12	0.49
1:F:243:LYS:CD	1:F:244:ALA:H	2.26	0.49
1:H:138:GLN:NE2	1:H:138:GLN:H	2.10	0.49
1:J:46:VAL:O	1:J:50:ARG:HG2	2.13	0.49
1:K:230:GLN:OE1	1:K:233:ARG:NH2	2.43	0.49
1:L:57:PHE:HB2	1:L:79:ILE:HG21	1.92	0.49
1:N:167:ALA:HB1	1:N:190:VAL:HG21	1.94	0.49
1:A:143:LEU:HD21	1:A:168:ARG:HH11	1.77	0.49
1:B:6:VAL:HG11	1:B:45:ALA:HB2	1.95	0.49
1:B:294:THR:OG1	1:B:297:GLU:OE1	2.27	0.49
1:C:29:HIS:HA	1:D:109:ILE:O	2.12	0.49
1:C:51:MET:HG3	1:C:260:THR:HG21	1.94	0.49
1:C:118:THR:H	1:C:121:ALA:HB3	1.77	0.49
1:C:221:LEU:N	1:C:225:GLY:O	2.42	0.49
1:E:6:VAL:O	1:E:58:ILE:N	2.41	0.49
1:E:143:LEU:H	1:I:306:SER:CB	2.24	0.49
1:F:56:GLY:HA2	1:F:80:ASN:HB3	1.93	0.49
1:H:197:TYR:N	1:H:197:TYR:CD1	2.80	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:252:ASP:O	1:H:256:GLY:N	2.41	0.49
1:P:184:ASN:H	1:P:187:GLU:HB2	1.78	0.49
1:A:148:LYS:HE3	1:A:152:GLU:HB2	1.94	0.49
1:B:126:LEU:O	1:B:130:ARG:HG3	2.12	0.49
1:B:201:SER:HA	1:B:204:GLN:HG3	1.94	0.49
1:D:147:LEU:O	1:D:151:GLN:HG3	2.12	0.49
1:E:240:PHE:HD1	1:E:301:PHE:HE2	1.58	0.49
1:F:223:SER:HA	1:F:243:LYS:HB3	1.93	0.49
1:H:221:LEU:CD1	1:H:227:TRP:H	2.25	0.49
1:H:306:SER:CB	1:L:143:LEU:H	2.24	0.49
1:I:16:LEU:HD21	1:I:30:GLY:HA3	1.94	0.49
1:I:161:ILE:HG23	1:I:180:LEU:HD22	1.94	0.49
1:I:210:HIS:CE1	1:I:215:GLU:O	2.65	0.49
1:N:253:THR:HB	1:N:282:SER:OG	2.13	0.49
1:O:81:THR:O	1:O:84:VAL:N	2.40	0.49
1:O:268:LEU:HD12	1:O:272:ILE:HG13	1.94	0.49
1:P:172:ASP:OD2	1:P:172:ASP:N	2.28	0.49
1:A:138:GLN:HA	1:A:163:ASN:O	2.11	0.49
1:A:231:ASN:OD1	1:A:231:ASN:N	2.44	0.49
1:D:7:LEU:HD13	1:D:58:ILE:CG2	2.40	0.49
1:D:89:ASN:O	1:D:89:ASN:ND2	2.46	0.49
1:E:134:TYR:CD1	1:E:159:ASN:HB2	2.47	0.49
1:E:172:ASP:OD1	1:E:172:ASP:N	2.46	0.49
1:J:229:SER:HA	1:J:233:ARG:O	2.11	0.49
1:K:135:LEU:HD21	1:K:137:MET:SD	2.52	0.49
1:M:40:LYS:HZ2	1:M:165:ALA:HB3	1.77	0.49
1:O:207:ASP:O	1:O:211:CYS:HB2	2.13	0.49
1:A:97:ILE:HA	1:A:107:ILE:HA	1.94	0.49
1:A:139:LEU:HD13	1:A:168:ARG:HG2	1.95	0.49
1:D:161:ILE:HD13	1:D:259:VAL:HG22	1.94	0.49
1:G:96:MET:HG2	1:H:96:MET:HE3	1.95	0.49
1:H:284:THR:HG23	1:H:285:ARG:H	1.77	0.49
1:J:101:ASP:N	1:J:102:SER:HA	2.28	0.49
1:M:6:VAL:HG13	1:M:136:LEU:HB3	1.94	0.49
1:N:18:VAL:O	1:N:101:ASP:HB2	2.13	0.49
1:N:168:ARG:HH22	1:P:306:SER:C	2.16	0.49
1:O:232:GLY:O	1:O:234:GLY:N	2.46	0.49
1:A:267:PRO:HD2	1:A:270:SER:HB2	1.95	0.49
1:G:33:TYR:CD1	1:H:94:ILE:HD12	2.47	0.49
1:H:7:LEU:HD12	1:H:58:ILE:HG21	1.94	0.49
1:K:93:GLY:HA2	1:K:112:GLU:H	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:219:ILE:HB	1:M:227:TRP:HB3	1.94	0.49
1:M:243:LYS:HB2	1:P:31:ARG:NE	2.27	0.49
1:N:129:ILE:H	1:N:129:ILE:HD12	1.77	0.49
1:P:47:ALA:HA	1:P:292:ILE:HG21	1.94	0.49
1:A:61:VAL:HG23	1:A:86:LEU:HD23	1.94	0.49
1:A:196:VAL:HG12	1:A:201:SER:O	2.13	0.49
1:E:300:ALA:O	1:E:304:GLU:HG3	2.13	0.49
1:G:187:GLU:O	1:G:191:LEU:HB2	2.13	0.49
1:G:240:PHE:CD1	1:G:301:PHE:HE2	2.30	0.49
1:H:17:GLN:OE1	1:H:32:ASN:ND2	2.46	0.49
1:J:181:ILE:HG23	1:J:183:PRO:HD3	1.94	0.49
1:A:68:ILE:HG13	1:A:69:ASN:N	2.27	0.48
1:A:243:LYS:HB2	1:D:31:ARG:HH12	1.77	0.48
1:A:279:ALA:O	1:A:283:VAL:HG13	2.12	0.48
1:C:227:TRP:CH2	1:C:234:GLY:HA3	2.47	0.48
1:F:230:GLN:HB2	1:F:233:ARG:HG3	1.95	0.48
1:M:17:GLN:HB2	1:M:31:ARG:HG2	1.95	0.48
1:N:62:GLY:H	1:N:92:THR:CG2	2.23	0.48
1:A:99:VAL:HG12	1:A:100:SER:N	2.25	0.48
1:D:151:GLN:O	1:D:155:THR:OG1	2.26	0.48
1:F:230:GLN:NE2	1:F:235:GLN:HE22	2.12	0.48
1:G:140:GLU:HG3	1:G:166:PRO:HD3	1.93	0.48
1:G:282:SER:O	1:G:291:SER:OG	2.31	0.48
1:K:126:LEU:CB	1:K:152:GLU:HG2	2.43	0.48
1:L:13:ASP:O	1:L:35:VAL:HA	2.13	0.48
1:M:64:ASP:CG	1:M:92:THR:HG1	2.17	0.48
1:M:100:SER:HA	1:M:101:ASP:HB2	1.94	0.48
1:N:37:PRO:O	1:N:289:GLN:HB2	2.12	0.48
1:P:207:ASP:HA	1:P:210:HIS:HD2	1.78	0.48
1:H:37:PRO:O	1:H:289:GLN:HG3	2.13	0.48
1:H:59:ALA:HB3	1:H:84:VAL:HG23	1.94	0.48
1:H:250:ALA:O	1:H:252:ASP:N	2.46	0.48
1:J:257:ALA:O	1:J:260:THR:HB	2.12	0.48
1:O:104:GLU:HB2	1:P:24:PRO:HB2	1.95	0.48
1:O:133:ARG:O	1:O:134:TYR:HD1	1.96	0.48
1:B:91:PRO:CD	1:B:112:GLU:HG2	2.44	0.48
1:E:215:GLU:HG3	1:E:231:ASN:ND2	2.29	0.48
1:H:70:ILE:HD13	1:H:74:PHE:CE1	2.48	0.48
1:H:250:ALA:C	1:H:252:ASP:H	2.17	0.48
1:M:63:ASP:OD1	1:M:63:ASP:N	2.39	0.48
1:N:235:GLN:HG3	1:N:236:ARG:N	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:59:ALA:HA	1:P:117:LEU:HD21	1.94	0.48
1:A:258:LEU:O	1:A:262:LEU:HG	2.14	0.48
1:B:218:ILE:HA	1:B:227:TRP:O	2.14	0.48
1:B:264:GLN:CD	1:B:295:ARG:HH22	2.16	0.48
1:C:104:GLU:CB	1:D:25:GLY:H	2.27	0.48
1:C:109:ILE:HD12	1:D:29:HIS:HE1	1.77	0.48
1:D:94:ILE:HG22	1:D:110:SER:H	1.77	0.48
1:D:100:SER:CA	1:D:101:ASP:HB3	2.43	0.48
1:F:12:ALA:HB2	1:F:66:PHE:CZ	2.48	0.48
1:G:138:GLN:HA	1:G:163:ASN:O	2.14	0.48
1:H:26:GLU:HG3	1:H:27:THR:N	2.28	0.48
1:H:127:ALA:HA	1:H:130:ARG:NH2	2.28	0.48
1:I:279:ALA:O	1:I:283:VAL:HG13	2.12	0.48
1:J:43:ASN:OD1	1:J:289:GLN:HG3	2.14	0.48
1:K:41:GLY:N	1:K:138:GLN:OE1	2.46	0.48
1:K:143:LEU:O	1:K:146:ILE:N	2.45	0.48
1:L:49:ALA:HB1	1:L:77:ASP:O	2.14	0.48
1:L:257:ALA:O	1:L:260:THR:N	2.47	0.48
1:M:40:LYS:HZ3	1:M:138:GLN:HB3	1.77	0.48
1:P:11:ASN:HB2	1:P:39:GLY:N	2.28	0.48
1:B:94:ILE:HG22	1:B:95:ALA:N	2.28	0.48
1:B:172:ASP:O	1:B:174:LEU:N	2.46	0.48
1:C:22:PRO:HG3	1:C:98:GLN:HE22	1.78	0.48
1:D:17:GLN:HG3	1:D:31:ARG:HG2	1.95	0.48
1:G:258:LEU:HB2	1:G:275:ALA:HB2	1.96	0.48
1:H:245:THR:OG1	1:H:284:THR:O	2.31	0.48
1:I:157:LYS:O	1:I:158:THR:OG1	2.30	0.48
1:I:262:LEU:HD21	1:I:268:LEU:HD12	1.95	0.48
1:I:287:GLY:O	1:I:290:THR:N	2.44	0.48
1:M:166:PRO:O	1:M:168:ARG:HG2	2.14	0.48
1:P:194:ILE:HD12	1:P:205:ALA:HA	1.96	0.48
1:B:197:TYR:CD1	1:B:197:TYR:N	2.80	0.48
1:D:280:ALA:HA	1:D:283:VAL:HG22	1.95	0.48
1:F:304:GLU:HB3	1:J:115:ALA:O	2.14	0.48
1:I:57:PHE:HD1	1:I:58:ILE:N	2.12	0.48
1:M:117:LEU:O	1:M:142:PRO:HG2	2.14	0.48
1:P:13:ASP:HB3	1:P:97:ILE:HD11	1.94	0.48
1:P:240:PHE:O	1:P:242:VAL:N	2.43	0.48
1:I:198:ASP:O	1:I:202:ALA:N	2.46	0.48
1:M:61:VAL:HA	1:M:92:THR:HG23	1.96	0.48
1:N:294:THR:H	1:N:297:GLU:HG2	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:52:GLN:HG3	1:P:295:ARG:HB2	1.95	0.48
1:C:51:MET:HB2	1:C:295:ARG:HD3	1.94	0.48
1:C:270:SER:O	1:C:273:LYS:N	2.39	0.48
1:G:27:THR:HA	1:H:107:ILE:O	2.14	0.48
1:G:147:LEU:HD11	1:G:151:GLN:NE2	2.28	0.48
1:K:99:VAL:HG23	1:K:105:ASN:ND2	2.29	0.48
1:P:209:LEU:HA	1:P:212:LYS:HD3	1.94	0.48
1:B:184:ASN:HB3	1:B:187:GLU:CD	2.33	0.48
1:D:184:ASN:OD1	1:D:187:GLU:N	2.46	0.48
1:F:15:VAL:HG22	1:F:97:ILE:HB	1.95	0.48
1:G:58:ILE:HD13	1:G:125:ASP:HB3	1.95	0.48
1:I:6:VAL:HG21	1:I:45:ALA:HB2	1.95	0.48
1:I:14:HIS:ND1	1:I:33:TYR:OH	2.47	0.48
1:I:141:THR:HB	1:I:142:PRO:HD2	1.96	0.48
1:J:285:ARG:HB2	1:J:291:SER:HB3	1.96	0.48
1:L:81:THR:HA	1:L:84:VAL:HG23	1.95	0.48
1:L:284:THR:HG23	1:L:285:ARG:HG3	1.95	0.48
1:M:180:LEU:HG	1:M:216:ILE:HB	1.96	0.48
1:N:20:SER:HB3	1:N:28:LEU:HD21	1.95	0.48
1:N:160:VAL:HB	1:N:178:VAL:HA	1.96	0.48
1:C:71:ARG:O	1:C:75:LYS:HG3	2.14	0.47
1:E:98:GLN:HB2	1:E:106:SER:HB3	1.96	0.47
1:E:197:TYR:N	1:E:197:TYR:CD1	2.82	0.47
1:G:199:ASP:HB3	1:G:227:TRP:HZ3	1.78	0.47
1:I:101:ASP:HA	1:I:102:SER:HA	1.47	0.47
1:J:31:ARG:NH2	1:J:101:ASP:O	2.47	0.47
1:J:228:LEU:HD13	1:J:272:ILE:HD11	1.96	0.47
1:L:91:PRO:HG2	1:L:112:GLU:CG	2.44	0.47
1:L:258:LEU:O	1:L:262:LEU:HG	2.14	0.47
1:M:101:ASP:N	1:M:101:ASP:OD1	2.47	0.47
1:M:109:ILE:O	1:N:29:HIS:HA	2.14	0.47
1:E:183:PRO:O	1:E:220:THR:N	2.41	0.47
1:G:47:ALA:HA	1:G:292:ILE:HG23	1.95	0.47
1:M:44:GLN:HG2	1:M:252:ASP:O	2.14	0.47
1:O:58:ILE:HD11	1:O:125:ASP:HB3	1.96	0.47
1:P:28:LEU:HD22	1:P:29:HIS:N	2.29	0.47
1:P:39:GLY:O	1:P:43:ASN:ND2	2.38	0.47
1:A:207:ASP:O	1:A:211:CYS:N	2.39	0.47
1:B:141:THR:HG23	1:B:142:PRO:HD2	1.96	0.47
1:E:17:GLN:H	1:E:17:GLN:HG2	1.48	0.47
1:E:68:ILE:H	1:E:68:ILE:HD12	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:70:ILE:HG13	1:E:74:PHE:CE1	2.49	0.47
1:E:210:HIS:NE2	1:E:229:SER:O	2.47	0.47
1:F:117:LEU:O	1:F:142:PRO:HG2	2.13	0.47
1:H:41:GLY:N	1:H:138:GLN:OE1	2.40	0.47
1:H:81:THR:HB	1:H:84:VAL:CG1	2.44	0.47
1:H:228:LEU:HD12	1:H:229:SER:H	1.79	0.47
1:K:40:LYS:NZ	1:K:165:ALA:HB1	2.29	0.47
1:K:202:ALA:HB1	1:K:227:TRP:CD1	2.48	0.47
1:O:196:VAL:HG13	1:O:202:ALA:CB	2.44	0.47
1:C:170:LEU:HD12	1:C:174:LEU:HD23	1.97	0.47
1:F:294:THR:OG1	1:F:297:GLU:HG3	2.14	0.47
1:G:137:MET:HE3	1:G:146:ILE:HG23	1.96	0.47
1:H:280:ALA:O	1:H:283:VAL:HG22	2.14	0.47
1:I:96:MET:HE3	1:I:96:MET:HB3	1.49	0.47
1:J:2:ASN:HB3	1:J:54:ASP:O	2.13	0.47
1:L:184:ASN:OD1	1:L:187:GLU:N	2.37	0.47
1:L:192:THR:HB	1:L:194:ILE:HD13	1.96	0.47
1:N:212:LYS:O	1:N:214:ILE:HG13	2.14	0.47
1:O:7:LEU:HA	1:O:58:ILE:HB	1.95	0.47
1:O:14:HIS:HD2	1:O:94:ILE:HG23	1.79	0.47
1:A:135:LEU:HD23	1:A:160:VAL:HB	1.95	0.47
1:D:228:LEU:HD22	1:D:272:ILE:HD12	1.96	0.47
1:G:129:ILE:HG23	1:G:135:LEU:HD13	1.97	0.47
1:H:204:GLN:O	1:H:207:ASP:HB2	2.14	0.47
1:H:302:LEU:HD23	1:H:302:LEU:HA	1.66	0.47
1:I:64:ASP:OD2	1:I:92:THR:OG1	2.33	0.47
1:J:4:LEU:O	1:J:55:VAL:HA	2.15	0.47
1:M:226:VAL:HG12	1:M:227:TRP:N	2.28	0.47
1:O:184:ASN:H	1:O:187:GLU:HB3	1.79	0.47
1:O:257:ALA:O	1:O:261:GLY:N	2.41	0.47
1:F:59:ALA:HA	1:F:117:LEU:CD1	2.45	0.47
1:N:60:CYS:HB2	1:N:117:LEU:HD23	1.95	0.47
1:P:85:LYS:HZ1	1:P:124:PRO:HG2	1.79	0.47
1:A:33:TYR:CZ	1:B:94:ILE:HD12	2.50	0.47
1:A:181:ILE:HG23	1:A:183:PRO:CD	2.45	0.47
1:B:4:LEU:O	1:B:56:GLY:N	2.43	0.47
1:B:62:GLY:HA3	1:B:90:CYS:O	2.15	0.47
1:B:110:SER:OG	1:B:111:ALA:N	2.47	0.47
1:D:14:HIS:HD2	1:D:94:ILE:HG13	1.80	0.47
1:D:37:PRO:HB3	1:D:70:ILE:HD11	1.97	0.47
1:D:40:LYS:HB2	1:D:140:GLU:OE1	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:247:THR:HG22	1:D:248:THR:H	1.79	0.47
1:D:290:THR:HB	1:D:291:SER:H	1.63	0.47
1:F:15:VAL:HG22	1:F:97:ILE:HD12	1.97	0.47
1:F:229:SER:O	1:F:231:ASN:N	2.47	0.47
1:G:248:THR:C	1:G:250:ALA:H	2.17	0.47
1:H:228:LEU:HD22	1:H:272:ILE:HD12	1.95	0.47
1:I:206:ALA:O	1:I:209:LEU:HB2	2.15	0.47
1:K:5:VAL:HG12	1:K:135:LEU:HD12	1.97	0.47
1:K:150:ALA:O	1:K:153:ALA:HB3	2.14	0.47
1:L:9:SER:OG	1:L:140:GLU:HG2	2.15	0.47
1:L:264:GLN:H	1:L:264:GLN:HG2	1.55	0.47
1:M:240:PHE:O	1:M:242:VAL:N	2.48	0.47
1:P:196:VAL:HG12	1:P:202:ALA:HA	1.96	0.47
1:P:249:ALA:HB1	1:P:292:ILE:HD11	1.96	0.47
1:C:185:GLU:HG2	1:C:221:LEU:HD23	1.97	0.47
1:F:72:GLU:OE1	1:F:75:LYS:HD2	2.15	0.47
1:J:3:LYS:H	1:J:54:ASP:HB3	1.80	0.47
1:J:126:LEU:O	1:J:130:ARG:HG3	2.15	0.47
1:L:57:PHE:HB2	1:L:79:ILE:CG2	2.44	0.47
1:L:61:VAL:HG23	1:L:86:LEU:HD23	1.96	0.47
1:L:147:LEU:HD21	1:L:174:LEU:HB2	1.96	0.47
1:L:207:ASP:HA	1:L:210:HIS:HD2	1.79	0.47
1:O:27:THR:CG2	1:P:107:ILE:HB	2.45	0.47
1:P:167:ALA:HA	1:P:187:GLU:HG2	1.96	0.47
1:B:221:LEU:HD12	1:B:225:GLY:C	2.34	0.47
1:D:145:GLY:O	1:D:149:ALA:N	2.39	0.47
1:D:228:LEU:HD22	1:D:272:ILE:CD1	2.44	0.47
1:G:192:THR:O	1:G:194:ILE:HG12	2.14	0.47
1:J:12:ALA:HB2	1:J:66:PHE:CZ	2.50	0.47
1:K:61:VAL:O	1:K:86:LEU:HA	2.15	0.47
1:M:89:ASN:N	1:M:89:ASN:OD1	2.48	0.47
1:N:61:VAL:HG23	1:N:86:LEU:HD23	1.97	0.47
1:O:281:ILE:HA	1:O:284:THR:HG22	1.96	0.47
1:A:116:LYS:O	1:A:118:THR:N	2.48	0.47
1:A:161:ILE:HG23	1:A:180:LEU:HD22	1.97	0.47
1:F:175:LEU:HD22	1:F:214:ILE:HD11	1.96	0.47
1:F:198:ASP:OD2	1:F:201:SER:OG	2.23	0.47
1:F:267:PRO:O	1:F:270:SER:N	2.31	0.47
1:H:241:VAL:HG22	1:K:19:PRO:HG2	1.97	0.47
1:J:190:VAL:HB	1:J:191:LEU:HD23	1.96	0.47
1:K:19:PRO:HA	1:K:101:ASP:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:58:ILE:HA	1:K:83:GLY:O	2.15	0.47
1:M:134:TYR:HD1	1:M:161:ILE:HD11	1.80	0.47
1:M:199:ASP:OD1	1:M:199:ASP:N	2.30	0.47
1:O:138:GLN:HA	1:O:163:ASN:O	2.15	0.47
1:O:249:ALA:HB2	1:O:288:ALA:HB1	1.96	0.47
1:P:7:LEU:HA	1:P:58:ILE:O	2.15	0.47
1:P:140:GLU:HB2	1:P:166:PRO:HD3	1.96	0.47
1:D:250:ALA:HA	1:D:252:ASP:H	1.76	0.46
1:E:51:MET:HB2	1:E:260:THR:HG21	1.97	0.46
1:H:228:LEU:HD12	1:H:229:SER:N	2.30	0.46
1:L:19:PRO:HD2	1:L:28:LEU:HD13	1.98	0.46
1:L:182:THR:HG21	1:L:255:ASN:OD1	2.15	0.46
1:N:228:LEU:O	1:N:229:SER:HB2	2.15	0.46
1:P:129:ILE:O	1:P:158:THR:HG21	2.15	0.46
1:A:103:GLY:O	1:A:104:GLU:HG2	2.15	0.46
1:D:61:VAL:O	1:D:87:GLN:N	2.37	0.46
1:D:204:GLN:O	1:D:207:ASP:HB3	2.15	0.46
1:E:7:LEU:O	1:E:7:LEU:HD23	2.14	0.46
1:E:241:VAL:O	1:E:241:VAL:HG12	2.16	0.46
1:F:287:GLY:HA3	1:F:290:THR:OG1	2.14	0.46
1:I:57:PHE:HB2	1:I:79:ILE:CG2	2.45	0.46
1:J:274:PHE:CE1	1:J:298:VAL:HG11	2.50	0.46
1:K:274:PHE:HZ	1:K:295:ARG:HE	1.61	0.46
1:O:17:GLN:O	1:O:31:ARG:N	2.46	0.46
1:O:207:ASP:O	1:O:211:CYS:N	2.45	0.46
1:A:130:ARG:O	1:A:158:THR:OG1	2.32	0.46
1:A:243:LYS:HE2	1:D:31:ARG:HH22	1.80	0.46
1:F:59:ALA:HB3	1:F:84:VAL:HG23	1.97	0.46
1:F:157:LYS:O	1:F:158:THR:OG1	2.32	0.46
1:G:172:ASP:CG	1:G:212:LYS:HD3	2.35	0.46
1:I:134:TYR:HD1	1:I:161:ILE:HD11	1.80	0.46
1:L:18:VAL:HB	1:L:28:LEU:HD12	1.98	0.46
1:O:244:ALA:HA	1:O:284:THR:HA	1.96	0.46
1:A:171:PRO:O	1:A:175:LEU:HD13	2.15	0.46
1:B:175:LEU:HB3	1:B:214:ILE:HD11	1.97	0.46
1:C:99:VAL:HG23	1:C:105:ASN:OD1	2.16	0.46
1:F:147:LEU:HD21	1:F:174:LEU:HB2	1.96	0.46
1:H:65:SER:O	1:H:69:ASN:ND2	2.47	0.46
1:H:74:PHE:N	1:H:74:PHE:CD1	2.80	0.46
1:I:7:LEU:HD22	1:I:137:MET:SD	2.55	0.46
1:I:226:VAL:HG11	1:I:272:ILE:HG21	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:139:LEU:HD13	1:J:168:ARG:HG2	1.98	0.46
1:C:93:GLY:HA2	1:C:112:GLU:HB2	1.97	0.46
1:C:278:ALA:HA	1:C:281:ILE:HG22	1.97	0.46
1:C:294:THR:O	1:C:298:VAL:HG23	2.16	0.46
1:D:240:PHE:HD1	1:D:301:PHE:HE2	1.62	0.46
1:D:253:THR:O	1:D:257:ALA:N	2.42	0.46
1:E:27:THR:HG23	1:F:107:ILE:O	2.16	0.46
1:G:15:VAL:HG23	1:G:97:ILE:HB	1.98	0.46
1:G:209:LEU:O	1:G:214:ILE:HG12	2.15	0.46
1:H:138:GLN:H	1:H:138:GLN:CD	2.19	0.46
1:P:49:ALA:HB2	1:P:55:VAL:HG11	1.96	0.46
1:P:64:ASP:N	1:P:64:ASP:OD1	2.49	0.46
1:C:151:GLN:CA	1:C:154:LYS:HD3	2.43	0.46
1:C:154:LYS:HG2	1:C:155:THR:N	2.29	0.46
1:C:240:PHE:CE2	1:C:301:PHE:HE2	2.32	0.46
1:E:72:GLU:OE1	1:E:75:LYS:HD2	2.14	0.46
1:F:224:LYS:HB3	1:F:236:ARG:HH12	1.80	0.46
1:H:185:GLU:CD	1:H:221:LEU:HD23	2.35	0.46
1:I:207:ASP:O	1:I:210:HIS:HB2	2.15	0.46
1:K:51:MET:HA	1:K:295:ARG:HG2	1.98	0.46
1:K:51:MET:O	1:K:260:THR:HG21	2.16	0.46
1:K:182:THR:O	1:K:182:THR:OG1	2.30	0.46
1:N:218:ILE:HD13	1:N:272:ILE:HD11	1.98	0.46
1:N:298:VAL:O	1:N:301:PHE:HB3	2.16	0.46
1:P:258:LEU:O	1:P:262:LEU:HG	2.16	0.46
1:C:220:THR:HA	1:C:226:VAL:HA	1.97	0.46
1:E:142:PRO:O	1:E:146:ILE:HG13	2.16	0.46
1:F:4:LEU:O	1:F:55:VAL:HA	2.15	0.46
1:H:66:PHE:O	1:H:69:ASN:N	2.49	0.46
1:H:243:LYS:HZ2	1:H:244:ALA:HB3	1.81	0.46
1:I:81:THR:HG22	1:I:84:VAL:HG21	1.98	0.46
1:I:210:HIS:HE1	1:I:215:GLU:O	1.99	0.46
1:M:185:GLU:O	1:M:189:GLU:HG3	2.16	0.46
1:P:7:LEU:HD22	1:P:137:MET:SD	2.55	0.46
1:P:143:LEU:HD21	1:P:168:ARG:NH1	2.30	0.46
1:D:153:ALA:O	1:D:156:ALA:N	2.36	0.46
1:F:81:THR:HB	1:F:82:ALA:H	1.62	0.46
1:G:47:ALA:HB2	1:G:292:ILE:HG12	1.98	0.46
1:H:37:PRO:HB2	1:H:289:GLN:HE21	1.81	0.46
1:H:228:LEU:HD22	1:H:272:ILE:CD1	2.46	0.46
1:J:117:LEU:HD23	1:J:141:THR:HG21	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:11:ASN:OD1	1:L:12:ALA:N	2.48	0.46
1:M:42:ALA:O	1:M:46:VAL:HG12	2.15	0.46
1:A:216:ILE:CG2	1:A:268:LEU:HD11	2.46	0.46
1:E:206:ALA:HA	1:E:217:VAL:HG11	1.98	0.46
1:E:228:LEU:HD22	1:E:272:ILE:HD12	1.98	0.46
1:G:261:GLY:O	1:G:264:GLN:N	2.49	0.46
1:H:250:ALA:C	1:H:252:ASP:N	2.69	0.46
1:K:61:VAL:HG23	1:K:86:LEU:CD2	2.46	0.46
1:K:138:GLN:N	1:K:138:GLN:NE2	2.60	0.46
1:M:132:ALA:O	1:M:158:THR:OG1	2.16	0.46
1:H:19:PRO:HA	1:H:101:ASP:CB	2.46	0.46
1:H:97:ILE:H	1:H:97:ILE:HG13	1.59	0.46
1:H:280:ALA:HA	1:H:283:VAL:CG2	2.45	0.46
1:I:22:PRO:HG3	1:I:98:GLN:NE2	2.31	0.46
1:K:184:ASN:ND2	1:K:187:GLU:OE2	2.49	0.46
1:K:236:ARG:NH2	1:K:238:PRO:HA	2.31	0.46
1:N:233:ARG:O	1:N:233:ARG:HG2	2.16	0.46
1:D:286:PHE:HD2	1:D:286:PHE:O	1.99	0.45
1:E:3:LYS:O	1:E:133:ARG:N	2.45	0.45
1:F:277:ALA:O	1:F:280:ALA:N	2.49	0.45
1:G:274:PHE:HE1	1:G:298:VAL:HG11	1.81	0.45
1:I:261:GLY:O	1:I:264:GLN:N	2.49	0.45
1:J:13:ASP:HB3	1:J:97:ILE:HD12	1.98	0.45
1:J:207:ASP:CG	1:K:232:GLY:HA3	2.36	0.45
1:K:139:LEU:CD1	1:K:170:LEU:HD21	2.46	0.45
1:K:277:ALA:HB2	1:K:302:LEU:HD21	1.98	0.45
1:N:189:GLU:OE1	1:N:195:THR:HG23	2.15	0.45
1:N:203:GLN:HE21	1:N:203:GLN:HB2	1.59	0.45
1:O:3:LYS:H	1:O:54:ASP:HB3	1.80	0.45
1:O:72:GLU:C	1:O:74:PHE:H	2.19	0.45
1:B:57:PHE:CE1	1:B:59:ALA:HB2	2.51	0.45
1:C:277:ALA:O	1:C:281:ILE:HG22	2.15	0.45
1:E:130:ARG:HB2	1:E:156:ALA:CB	2.47	0.45
1:G:8:GLY:HA3	1:G:41:GLY:HA3	1.99	0.45
1:H:21:PHE:O	1:H:23:ARG:N	2.49	0.45
1:K:61:VAL:HG23	1:K:86:LEU:HD22	1.98	0.45
1:L:179:ASP:N	1:L:179:ASP:OD1	2.48	0.45
1:O:247:THR:O	1:O:248:THR:HG23	2.17	0.45
1:P:51:MET:HE1	1:P:298:VAL:HG21	1.99	0.45
1:A:64:ASP:C	1:A:66:PHE:N	2.70	0.45
1:C:4:LEU:CD2	1:C:55:VAL:HG23	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:99:VAL:HA	1:D:105:ASN:CG	2.37	0.45
1:F:122:ILE:O	1:F:126:LEU:N	2.49	0.45
1:G:259:VAL:O	1:G:263:LEU:HB2	2.17	0.45
1:H:300:ALA:O	1:H:304:GLU:HG3	2.16	0.45
1:J:240:PHE:CE1	1:J:273:LYS:HE3	2.49	0.45
1:J:260:THR:O	1:J:264:GLN:HB2	2.17	0.45
1:M:65:SER:O	1:M:69:ASN:ND2	2.47	0.45
1:P:126:LEU:O	1:P:130:ARG:HG2	2.15	0.45
1:P:243:LYS:H	1:P:283:VAL:HG21	1.82	0.45
1:B:66:PHE:HA	1:B:69:ASN:HB2	1.99	0.45
1:D:139:LEU:HD13	1:D:168:ARG:HG2	1.99	0.45
1:E:61:VAL:HG23	1:E:92:THR:HG23	1.97	0.45
1:E:251:GLY:HA2	1:E:254:PHE:CB	2.42	0.45
1:G:234:GLY:O	1:G:235:GLN:CB	2.64	0.45
1:H:163:ASN:O	1:H:165:ALA:N	2.48	0.45
1:F:267:PRO:HD2	1:F:270:SER:CB	2.43	0.45
1:I:20:SER:OG	1:I:21:PHE:N	2.48	0.45
1:I:40:LYS:O	1:I:42:ALA:N	2.49	0.45
1:J:134:TYR:OH	1:J:262:LEU:HB3	2.16	0.45
1:K:105:ASN:OD1	1:K:105:ASN:N	2.50	0.45
1:K:137:MET:C	1:K:138:GLN:HE21	2.20	0.45
1:O:26:GLU:HG3	1:O:27:THR:N	2.32	0.45
1:O:236:ARG:HH12	1:O:238:PRO:CA	2.29	0.45
1:E:249:ALA:O	1:E:252:ASP:HB2	2.15	0.45
1:E:281:ILE:O	1:E:284:THR:HG22	2.15	0.45
1:H:99:VAL:HG12	1:H:105:ASN:HB3	1.99	0.45
1:H:135:LEU:HD21	1:H:137:MET:SD	2.57	0.45
1:H:163:ASN:C	1:H:163:ASN:HD22	2.20	0.45
1:H:197:TYR:N	1:H:197:TYR:HD1	2.14	0.45
1:I:137:MET:O	1:I:162:LEU:HD12	2.17	0.45
1:J:212:LYS:O	1:J:214:ILE:HG13	2.15	0.45
1:K:64:ASP:HB3	1:K:67:GLY:H	1.82	0.45
1:K:189:GLU:O	1:K:193:GLY:N	2.42	0.45
1:L:221:LEU:HD12	1:L:226:VAL:HA	1.99	0.45
1:M:31:ARG:HH22	1:P:243:LYS:NZ	2.15	0.45
1:M:249:ALA:O	1:M:252:ASP:N	2.49	0.45
1:N:3:LYS:CB	1:N:54:ASP:HB3	2.47	0.45
1:O:104:GLU:HB2	1:P:24:PRO:CB	2.46	0.45
1:P:240:PHE:N	1:P:242:VAL:HG13	2.32	0.45
1:A:184:ASN:H	1:A:187:GLU:HB2	1.81	0.45
1:B:262:LEU:HD21	1:B:268:LEU:HD12	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:276:HIS:HA	1:B:279:ALA:HB3	1.97	0.45
1:E:87:GLN:HA	1:E:88:PRO:HD3	1.79	0.45
1:F:87:GLN:HA	1:F:88:PRO:HD3	1.74	0.45
1:H:97:ILE:HD12	1:H:97:ILE:O	2.16	0.45
1:I:281:ILE:O	1:I:285:ARG:HB2	2.17	0.45
1:L:100:SER:O	1:L:100:SER:OG	2.25	0.45
1:L:154:LYS:HE3	1:L:154:LYS:HB3	1.85	0.45
1:O:273:LYS:HA	1:O:276:HIS:HB2	1.99	0.45
1:P:163:ASN:HD22	1:P:164:PRO:HD2	1.82	0.45
1:P:198:ASP:OD1	1:P:198:ASP:N	2.50	0.45
1:B:172:ASP:HA	1:B:175:LEU:CD1	2.47	0.45
1:C:58:ILE:HA	1:C:83:GLY:O	2.16	0.45
1:G:274:PHE:O	1:G:277:ALA:HB3	2.17	0.45
1:H:18:VAL:HG23	1:H:100:SER:HA	1.98	0.45
1:K:20:SER:OG	1:K:28:LEU:HD21	2.16	0.45
1:M:108:CYS:C	1:M:109:ILE:HD12	2.36	0.45
1:M:138:GLN:O	1:M:139:LEU:HD23	2.17	0.45
1:M:294:THR:H	1:M:297:GLU:HG3	1.82	0.45
1:O:7:LEU:HD22	1:O:137:MET:SD	2.57	0.45
1:O:31:ARG:HG2	1:O:32:ASN:HB2	1.99	0.45
1:P:281:ILE:HD12	1:P:298:VAL:HG22	1.98	0.45
1:A:181:ILE:HG23	1:A:183:PRO:HD2	1.98	0.45
1:C:228:LEU:HD12	1:C:229:SER:H	1.82	0.45
1:D:19:PRO:O	1:D:102:SER:OG	2.33	0.45
1:D:178:VAL:HG11	1:D:181:ILE:HG12	1.99	0.45
1:E:182:THR:N	1:E:183:PRO:HD3	2.31	0.45
1:G:10:VAL:HG22	1:G:42:ALA:HB2	1.97	0.45
1:H:192:THR:HB	1:H:194:ILE:HG12	1.99	0.45
1:H:235:GLN:NE2	1:H:237:ILE:HD11	2.31	0.45
1:L:60:CYS:SG	1:L:117:LEU:HD13	2.57	0.45
1:L:186:THR:OG1	1:L:187:GLU:N	2.50	0.45
1:M:64:ASP:N	1:M:64:ASP:OD1	2.49	0.45
1:N:66:PHE:CE1	1:N:70:ILE:HD12	2.52	0.45
1:N:216:ILE:CG1	1:N:268:LEU:HD21	2.46	0.45
1:N:255:ASN:O	1:N:259:VAL:HG12	2.17	0.45
1:O:44:GLN:HE21	1:O:44:GLN:H	1.65	0.45
1:B:61:VAL:HG12	1:B:92:THR:HG21	1.98	0.45
1:D:197:TYR:HD1	1:D:197:TYR:N	2.12	0.45
1:G:249:ALA:CA	1:G:252:ASP:HB2	2.47	0.45
1:I:18:VAL:HG11	1:I:98:GLN:HB3	1.98	0.45
1:J:126:LEU:HD22	1:J:152:GLU:HG2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:178:VAL:HG12	1:J:214:ILE:HG23	1.99	0.45
1:N:21:PHE:CD2	1:N:22:PRO:HD2	2.52	0.45
1:O:47:ALA:HB2	1:O:253:THR:HA	1.99	0.45
1:B:97:ILE:HG23	1:B:107:ILE:HG23	1.99	0.44
1:D:226:VAL:HG12	1:D:276:HIS:NE2	2.32	0.44
1:E:264:GLN:OE1	1:E:295:ARG:NH2	2.50	0.44
1:F:62:GLY:HA3	1:F:91:PRO:C	2.36	0.44
1:F:175:LEU:HB3	1:F:214:ILE:HD11	2.00	0.44
1:H:71:ARG:NE	1:H:72:GLU:OE2	2.49	0.44
1:J:191:LEU:HD23	1:J:191:LEU:N	2.33	0.44
1:J:227:TRP:CZ2	1:J:234:GLY:HA3	2.52	0.44
1:O:50:ARG:HG3	1:O:292:ILE:HG22	1.99	0.44
1:O:273:LYS:O	1:O:276:HIS:HB2	2.17	0.44
1:P:99:VAL:HG12	1:P:105:ASN:CG	2.38	0.44
1:P:217:VAL:HG13	1:P:229:SER:HB3	1.98	0.44
1:P:281:ILE:CD1	1:P:298:VAL:HG22	2.48	0.44
1:A:122:ILE:O	1:A:125:ASP:HB2	2.18	0.44
1:B:79:ILE:HD11	1:B:81:THR:HG22	1.98	0.44
1:B:218:ILE:HG22	1:B:226:VAL:HG12	1.99	0.44
1:D:64:ASP:OD1	1:D:92:THR:HG23	2.17	0.44
1:D:164:PRO:HG2	1:D:183:PRO:HB3	1.99	0.44
1:F:66:PHE:CD1	1:F:67:GLY:N	2.86	0.44
1:I:18:VAL:HG22	1:I:100:SER:HA	1.97	0.44
1:K:184:ASN:OD1	1:K:185:GLU:N	2.49	0.44
1:L:122:ILE:C	1:L:124:PRO:HD2	2.37	0.44
1:N:125:ASP:O	1:N:128:ALA:N	2.48	0.44
1:P:153:ALA:HA	1:P:158:THR:HG22	1.99	0.44
1:D:16:LEU:O	1:D:98:GLN:HA	2.17	0.44
1:D:281:ILE:HD11	1:D:298:VAL:HA	1.98	0.44
1:E:184:ASN:HD21	1:E:187:GLU:HG3	1.82	0.44
1:F:199:ASP:OD1	1:F:236:ARG:HG3	2.17	0.44
1:G:267:PRO:CD	1:G:270:SER:HB2	2.43	0.44
1:H:5:VAL:O	1:H:135:LEU:HD12	2.17	0.44
1:L:7:LEU:HD12	1:L:58:ILE:CG2	2.47	0.44
1:L:143:LEU:HA	1:L:146:ILE:HB	1.98	0.44
1:M:18:VAL:HB	1:M:28:LEU:HD21	1.98	0.44
1:M:40:LYS:NZ	1:M:138:GLN:HB3	2.33	0.44
1:N:46:VAL:O	1:N:50:ARG:HB2	2.17	0.44
1:N:99:VAL:HG12	1:N:105:ASN:CG	2.38	0.44
1:N:178:VAL:HG13	1:N:214:ILE:HG23	1.99	0.44
1:P:185:GLU:OE2	1:P:221:LEU:HA	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:LEU:HB3	1:A:181:ILE:HD12	1.99	0.44
1:B:59:ALA:HA	1:B:117:LEU:HD21	2.00	0.44
1:B:264:GLN:OE1	1:B:295:ARG:NH2	2.51	0.44
1:C:305:HIS:O	1:C:306:SER:OG	2.27	0.44
1:D:240:PHE:CE1	1:D:301:PHE:CE2	3.06	0.44
1:G:139:LEU:O	1:G:166:PRO:HD2	2.18	0.44
1:H:40:LYS:HE3	1:H:165:ALA:C	2.37	0.44
1:H:306:SER:O	1:L:168:ARG:NH1	2.50	0.44
1:I:13:ASP:O	1:I:35:VAL:HA	2.17	0.44
1:I:93:GLY:HA2	1:I:112:GLU:HB2	1.99	0.44
1:I:119:ALA:N	1:I:144:ASP:OD1	2.39	0.44
1:I:292:ILE:HA	1:I:293:PRO:HD3	1.67	0.44
1:K:240:PHE:O	1:K:242:VAL:N	2.51	0.44
1:M:106:SER:C	1:M:107:ILE:HG13	2.36	0.44
1:P:18:VAL:HB	1:P:28:LEU:HD11	1.98	0.44
1:P:280:ALA:HA	1:P:283:VAL:HG22	2.00	0.44
1:B:43:ASN:O	1:B:45:ALA:N	2.50	0.44
1:D:3:LYS:HG2	1:D:3:LYS:H	1.55	0.44
1:E:254:PHE:CD1	1:E:275:ALA:HB1	2.53	0.44
1:H:203:GLN:HG2	1:O:207:ASP:OD2	2.17	0.44
1:I:10:VAL:HG11	1:I:70:ILE:HG21	1.99	0.44
1:I:22:PRO:HG3	1:I:98:GLN:HE22	1.83	0.44
1:K:58:ILE:HD11	1:K:125:ASP:HB3	1.98	0.44
1:K:273:LYS:O	1:K:275:ALA:N	2.50	0.44
1:L:229:SER:HA	1:L:234:GLY:HA2	1.98	0.44
1:M:173:GLU:O	1:M:176:LYS:HG2	2.17	0.44
1:M:258:LEU:O	1:M:262:LEU:HG	2.18	0.44
1:A:207:ASP:HA	1:A:210:HIS:HB2	2.00	0.44
1:F:3:LYS:HE3	1:F:54:ASP:HB2	2.00	0.44
1:F:7:LEU:HA	1:F:58:ILE:HG23	2.00	0.44
1:F:15:VAL:CG2	1:F:97:ILE:HD12	2.48	0.44
1:G:50:ARG:C	1:G:52:GLN:H	2.19	0.44
1:H:77:ASP:N	1:H:77:ASP:OD1	2.51	0.44
1:J:254:PHE:CD1	1:J:275:ALA:HB1	2.51	0.44
1:L:18:VAL:O	1:L:100:SER:HA	2.17	0.44
1:L:21:PHE:HE2	1:L:106:SER:CB	2.31	0.44
1:L:87:GLN:HB3	1:L:90:CYS:CB	2.47	0.44
1:N:117:LEU:O	1:N:142:PRO:HG2	2.17	0.44
1:N:170:LEU:HD12	1:N:191:LEU:HD21	1.98	0.44
1:O:115:ALA:HA	1:O:142:PRO:HD3	1.99	0.44
1:O:258:LEU:O	1:O:262:LEU:HG	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:5:VAL:HG11	1:P:129:ILE:HD13	1.99	0.44
1:A:31:ARG:HE	1:D:241:VAL:CG2	2.30	0.44
1:A:206:ALA:O	1:A:209:LEU:HB2	2.18	0.44
1:B:164:PRO:HG2	1:B:183:PRO:HB3	1.99	0.44
1:C:63:ASP:OD2	1:C:88:PRO:HA	2.18	0.44
1:C:218:ILE:HG23	1:C:226:VAL:HG13	1.99	0.44
1:E:184:ASN:HA	1:E:220:THR:O	2.18	0.44
1:F:41:GLY:N	1:F:138:GLN:OE1	2.50	0.44
1:F:43:ASN:OD1	1:F:289:GLN:HG2	2.18	0.44
1:F:100:SER:HB3	1:F:104:GLU:O	2.17	0.44
1:F:150:ALA:HB1	1:F:177:CYS:HB2	1.99	0.44
1:F:285:ARG:HH22	1:F:293:PRO:HB3	1.83	0.44
1:G:52:GLN:HG2	1:G:295:ARG:HG2	2.00	0.44
1:I:21:PHE:CZ	1:J:24:PRO:HA	2.53	0.44
1:J:181:ILE:HG22	1:J:217:VAL:HG22	1.99	0.44
1:K:169:GLU:H	1:K:169:GLU:CD	2.21	0.44
1:K:235:GLN:HB3	1:K:236:ARG:H	1.49	0.44
1:L:147:LEU:CD2	1:L:174:LEU:HB2	2.47	0.44
1:N:51:MET:CB	1:N:260:THR:HG21	2.42	0.44
1:N:67:GLY:O	1:N:70:ILE:HG22	2.17	0.44
1:O:117:LEU:O	1:O:142:PRO:HG2	2.18	0.44
1:O:161:ILE:HD12	1:O:259:VAL:HG23	1.99	0.44
1:P:61:VAL:HG23	1:P:86:LEU:HB3	1.98	0.44
1:A:57:PHE:CE1	1:A:59:ALA:HB2	2.53	0.44
1:B:249:ALA:CA	1:B:252:ASP:HB2	2.48	0.44
1:C:46:VAL:O	1:C:50:ARG:HB2	2.18	0.44
1:D:99:VAL:HG13	1:D:105:ASN:HD21	1.83	0.44
1:F:138:GLN:HG3	1:F:163:ASN:HB3	1.99	0.44
1:G:134:TYR:CD1	1:G:161:ILE:HD11	2.48	0.44
1:I:66:PHE:O	1:I:69:ASN:N	2.51	0.44
1:I:143:LEU:O	1:I:146:ILE:HB	2.18	0.44
1:J:93:GLY:HA3	1:J:114:ASN:HD21	1.83	0.44
1:K:162:LEU:HB3	1:K:178:VAL:HG11	2.00	0.44
1:K:240:PHE:CE2	1:K:301:PHE:HE2	2.35	0.44
1:L:123:GLU:HA	1:L:126:LEU:HG	1.99	0.44
1:P:209:LEU:HA	1:P:209:LEU:HD22	1.77	0.44
1:A:81:THR:HA	1:A:84:VAL:HG23	2.00	0.44
1:B:40:LYS:HA	1:B:252:ASP:OD1	2.18	0.44
1:B:50:ARG:HD2	1:B:292:ILE:HG22	2.00	0.44
1:C:203:GLN:HA	1:C:203:GLN:OE1	2.18	0.44
1:D:71:ARG:O	1:D:81:THR:HG21	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:139:LEU:O	1:F:166:PRO:HD2	2.18	0.44
1:H:205:ALA:O	1:H:208:ALA:N	2.51	0.44
1:H:285:ARG:NH2	1:H:293:PRO:HB3	2.33	0.44
1:H:306:SER:HB3	1:L:168:ARG:HH12	1.83	0.44
1:I:104:GLU:HG3	1:I:105:ASN:H	1.82	0.44
1:J:117:LEU:O	1:J:142:PRO:HG2	2.17	0.44
1:J:228:LEU:HD22	1:J:272:ILE:HD12	1.99	0.44
1:K:8:GLY:HA2	1:K:141:THR:HG21	1.99	0.44
1:K:110:SER:O	1:K:112:GLU:N	2.50	0.44
1:K:172:ASP:OD2	1:K:172:ASP:N	2.51	0.44
1:L:170:LEU:HB3	1:L:174:LEU:HD23	2.00	0.44
1:L:216:ILE:HG21	1:L:268:LEU:HD21	2.00	0.44
1:M:15:VAL:O	1:M:33:TYR:HA	2.18	0.44
1:O:128:ALA:O	1:O:132:ALA:HB2	2.16	0.44
1:O:228:LEU:HD11	1:O:230:GLN:OE1	2.18	0.44
1:B:165:ALA:HB2	1:B:187:GLU:OE1	2.18	0.43
1:C:117:LEU:HD12	1:C:117:LEU:HA	1.77	0.43
1:E:147:LEU:HD12	1:E:151:GLN:HE21	1.83	0.43
1:E:228:LEU:HD12	1:E:229:SER:H	1.83	0.43
1:F:44:GLN:HG2	1:F:252:ASP:O	2.18	0.43
1:F:101:ASP:HA	1:F:102:SER:HA	1.80	0.43
1:G:91:PRO:HD2	1:G:112:GLU:HB3	1.99	0.43
1:J:50:ARG:HB2	1:J:51:MET:HE3	2.00	0.43
1:K:240:PHE:CD2	1:K:301:PHE:HE2	2.36	0.43
1:K:254:PHE:C	1:K:254:PHE:CD2	2.91	0.43
1:M:304:GLU:H	1:M:304:GLU:HG2	1.47	0.43
1:N:112:GLU:OE1	1:N:112:GLU:HA	2.18	0.43
1:P:138:GLN:HA	1:P:163:ASN:O	2.18	0.43
1:A:56:GLY:CA	1:A:80:ASN:HB3	2.48	0.43
1:A:172:ASP:OD1	1:A:212:LYS:HD3	2.18	0.43
1:B:7:LEU:HD22	1:B:137:MET:SD	2.58	0.43
1:D:50:ARG:NE	1:D:77:ASP:OD1	2.51	0.43
1:D:289:GLN:HA	1:D:292:ILE:HD12	2.00	0.43
1:I:40:LYS:O	1:I:43:ASN:N	2.51	0.43
1:J:249:ALA:O	1:J:252:ASP:HB2	2.18	0.43
1:K:129:ILE:HG21	1:K:153:ALA:HB2	1.99	0.43
1:L:170:LEU:HD13	1:L:174:LEU:HD23	2.00	0.43
1:L:254:PHE:CD1	1:L:275:ALA:HB1	2.53	0.43
1:M:243:LYS:HB2	1:P:31:ARG:CD	2.47	0.43
1:O:199:ASP:HA	1:O:227:TRP:HZ3	1.82	0.43
1:P:216:ILE:HG12	1:P:230:GLN:HA	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:LEU:O	1:A:223:SER:N	2.52	0.43
1:A:240:PHE:CE2	1:A:301:PHE:HE2	2.36	0.43
1:A:254:PHE:C	1:A:254:PHE:CD2	2.92	0.43
1:D:126:LEU:HD23	1:D:126:LEU:HA	1.76	0.43
1:D:180:LEU:HA	1:D:216:ILE:O	2.18	0.43
1:F:66:PHE:HD1	1:F:67:GLY:N	2.17	0.43
1:F:148:LYS:HD3	1:F:148:LYS:HA	1.77	0.43
1:G:196:VAL:HG13	1:G:202:ALA:HB2	1.99	0.43
1:J:281:ILE:O	1:J:285:ARG:HG3	2.18	0.43
1:K:298:VAL:O	1:K:301:PHE:HB3	2.17	0.43
1:L:5:VAL:O	1:L:135:LEU:HA	2.18	0.43
1:M:31:ARG:HH22	1:P:243:LYS:HZ2	1.65	0.43
1:M:33:TYR:HB3	1:N:112:GLU:OE2	2.18	0.43
1:M:282:SER:HB2	1:M:293:PRO:HD3	2.00	0.43
1:N:111:ALA:O	1:N:113:ALA:N	2.52	0.43
1:B:79:ILE:HG13	1:B:79:ILE:O	2.16	0.43
1:B:216:ILE:HG21	1:B:268:LEU:CD2	2.48	0.43
1:C:21:PHE:CD2	1:C:22:PRO:HD2	2.52	0.43
1:C:210:HIS:HA	1:C:214:ILE:O	2.19	0.43
1:F:101:ASP:CG	1:I:243:LYS:HG3	2.39	0.43
1:G:8:GLY:C	1:G:41:GLY:HA3	2.38	0.43
1:H:126:LEU:HD11	1:H:148:LYS:HZ1	1.83	0.43
1:H:203:GLN:OE1	1:H:227:TRP:NE1	2.45	0.43
1:I:64:ASP:OD2	1:I:64:ASP:N	2.48	0.43
1:J:135:LEU:HD13	1:J:153:ALA:HB2	2.00	0.43
1:J:162:LEU:O	1:J:164:PRO:HD3	2.19	0.43
1:J:197:TYR:CD1	1:J:197:TYR:N	2.86	0.43
1:K:106:SER:C	1:K:107:ILE:HG13	2.39	0.43
1:L:87:GLN:HB3	1:L:90:CYS:HB3	2.01	0.43
1:N:221:LEU:N	1:N:225:GLY:O	2.38	0.43
1:O:118:THR:OG1	1:O:119:ALA:N	2.49	0.43
1:O:139:LEU:HD11	1:O:170:LEU:HD11	1.99	0.43
1:D:15:VAL:HG22	1:D:97:ILE:HG13	1.99	0.43
1:E:206:ALA:CB	1:E:217:VAL:HG11	2.48	0.43
1:G:2:ASN:HA	1:G:54:ASP:OD2	2.18	0.43
1:I:26:GLU:CD	1:I:27:THR:H	2.22	0.43
1:K:96:MET:HE2	1:L:98:GLN:HG2	2.01	0.43
1:L:17:GLN:HG3	1:L:32:ASN:HB2	2.00	0.43
1:L:248:THR:HG1	1:L:249:ALA:H	1.57	0.43
1:L:274:PHE:CZ	1:L:295:ARG:NE	2.87	0.43
1:M:19:PRO:HG3	1:P:241:VAL:HG23	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:243:LYS:HB2	1:P:31:ARG:HD2	1.99	0.43
1:O:3:LYS:HE2	1:O:54:ASP:CB	2.48	0.43
1:O:81:THR:O	1:O:84:VAL:HG23	2.18	0.43
1:P:97:ILE:HD12	1:P:97:ILE:N	2.34	0.43
1:A:19:PRO:HD2	1:A:28:LEU:CD2	2.49	0.43
1:A:196:VAL:HA	1:A:201:SER:HB2	2.00	0.43
1:B:179:ASP:O	1:B:180:LEU:HB2	2.18	0.43
1:D:57:PHE:HB3	1:D:84:VAL:HG23	2.00	0.43
1:D:304:GLU:HB2	1:D:305:HIS:HD1	1.83	0.43
1:E:170:LEU:HD13	1:E:174:LEU:CD2	2.49	0.43
1:F:254:PHE:CE2	1:F:258:LEU:HD22	2.53	0.43
1:G:272:ILE:O	1:G:276:HIS:HB2	2.19	0.43
1:H:37:PRO:HA	1:H:66:PHE:HZ	1.84	0.43
1:H:191:LEU:HD12	1:H:191:LEU:N	2.33	0.43
1:H:275:ALA:O	1:H:279:ALA:N	2.36	0.43
1:K:212:LYS:N	1:K:212:LYS:HD2	2.33	0.43
1:L:260:THR:O	1:L:264:GLN:HG2	2.18	0.43
1:M:5:VAL:O	1:M:135:LEU:HA	2.18	0.43
1:P:101:ASP:HA	1:P:102:SER:HA	1.56	0.43
1:B:57:PHE:CD1	1:B:58:ILE:N	2.85	0.43
1:C:28:LEU:O	1:D:108:CYS:HA	2.19	0.43
1:C:79:ILE:O	1:C:80:ASN:C	2.57	0.43
1:C:180:LEU:HD23	1:C:181:ILE:N	2.33	0.43
1:C:203:GLN:HB2	1:C:227:TRP:CH2	2.54	0.43
1:G:170:LEU:CD1	1:G:174:LEU:HD23	2.48	0.43
1:G:207:ASP:O	1:G:210:HIS:HB2	2.18	0.43
1:G:240:PHE:CE1	1:G:301:PHE:HE2	2.37	0.43
1:H:63:ASP:OD2	1:H:89:ASN:N	2.32	0.43
1:H:105:ASN:N	1:H:105:ASN:OD1	2.52	0.43
1:H:126:LEU:HD11	1:H:148:LYS:NZ	2.34	0.43
1:I:181:ILE:HG12	1:I:182:THR:N	2.31	0.43
1:K:243:LYS:HG2	1:K:244:ALA:N	2.34	0.43
1:L:16:LEU:HD21	1:L:30:GLY:HA3	2.00	0.43
1:L:184:ASN:ND2	1:L:187:GLU:OE2	2.52	0.43
1:M:40:LYS:HB3	1:M:40:LYS:HE2	1.58	0.43
1:M:185:GLU:H	1:M:185:GLU:HG3	1.38	0.43
1:P:91:PRO:O	1:P:113:ALA:HB2	2.19	0.43
1:B:15:VAL:HA	1:B:97:ILE:CD1	2.48	0.43
1:B:98:GLN:HE21	1:B:98:GLN:HB2	1.66	0.43
1:C:132:ALA:O	1:C:158:THR:OG1	2.24	0.43
1:D:9:SER:CB	1:D:140:GLU:HB3	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:22:PRO:CD	1:D:28:LEU:HD21	2.42	0.43
1:D:199:ASP:HB3	1:D:227:TRP:HZ3	1.83	0.43
1:F:3:LYS:NZ	1:F:264:GLN:HE22	2.17	0.43
1:G:61:VAL:CA	1:G:92:THR:HG23	2.48	0.43
1:G:292:ILE:O	1:G:292:ILE:HG22	2.19	0.43
1:I:21:PHE:CD1	1:I:22:PRO:HD2	2.54	0.43
1:J:44:GLN:OE1	1:J:136:LEU:HD21	2.18	0.43
1:J:51:MET:CB	1:J:260:THR:HG21	2.48	0.43
1:K:181:ILE:HG12	1:K:183:PRO:HD3	1.99	0.43
1:L:47:ALA:O	1:L:50:ARG:N	2.51	0.43
1:L:212:LYS:HA	1:L:212:LYS:HD3	1.88	0.43
1:M:143:LEU:HD13	1:M:168:ARG:HH22	1.84	0.43
1:M:170:LEU:CD2	1:M:174:LEU:HD23	2.47	0.43
1:B:245:THR:CG2	1:B:286:PHE:HD2	2.28	0.43
1:B:262:LEU:HD23	1:B:262:LEU:H	1.82	0.43
1:E:87:GLN:HG2	1:E:116:LYS:CG	2.32	0.43
1:E:119:ALA:HB2	1:E:144:ASP:O	2.19	0.43
1:F:198:ASP:OD2	1:F:198:ASP:N	2.50	0.43
1:G:22:PRO:HA	1:G:28:LEU:HD11	2.01	0.43
1:I:56:GLY:HA2	1:I:80:ASN:HB3	2.01	0.43
1:J:13:ASP:HB3	1:J:97:ILE:CD1	2.49	0.43
1:J:215:GLU:HG3	1:J:231:ASN:HB2	2.01	0.43
1:K:137:MET:HE3	1:K:146:ILE:HG23	2.00	0.43
1:N:59:ALA:HB3	1:N:84:VAL:HG12	2.01	0.43
1:N:98:GLN:HE21	1:N:98:GLN:HB2	1.68	0.43
1:N:277:ALA:O	1:N:281:ILE:HG13	2.19	0.43
1:O:130:ARG:HD3	1:O:152:GLU:OE1	2.19	0.43
1:O:230:GLN:HE21	1:O:230:GLN:HB3	1.46	0.43
1:A:12:ALA:HB3	1:A:94:ILE:CG1	2.45	0.43
1:A:15:VAL:HG22	1:A:97:ILE:HG21	1.99	0.43
1:E:20:SER:OG	1:E:21:PHE:N	2.52	0.43
1:F:115:ALA:HA	1:F:142:PRO:HD3	2.00	0.43
1:G:261:GLY:C	1:G:263:LEU:N	2.73	0.43
1:G:291:SER:HB3	1:G:292:ILE:H	1.61	0.43
1:H:210:HIS:CE1	1:H:217:VAL:HG23	2.53	0.43
1:H:210:HIS:CE1	1:H:215:GLU:O	2.72	0.43
1:I:142:PRO:O	1:I:146:ILE:HG13	2.19	0.43
1:J:172:ASP:C	1:J:174:LEU:H	2.22	0.43
1:K:202:ALA:HB1	1:K:227:TRP:CG	2.53	0.43
1:K:224:LYS:HE2	1:K:224:LYS:HB3	1.66	0.43
1:K:239:GLY:HA2	1:K:276:HIS:HD2	1.78	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:43:ASN:CB	1:O:252:ASP:HB3	2.48	0.43
1:B:168:ARG:HD3	1:B:170:LEU:HD12	2.01	0.42
1:C:95:ALA:HA	1:C:108:CYS:O	2.18	0.42
1:D:137:MET:CE	1:D:146:ILE:HG23	2.48	0.42
1:E:99:VAL:O	1:E:101:ASP:HB2	2.19	0.42
1:F:211:CYS:HA	1:G:233:ARG:HD3	2.01	0.42
1:F:215:GLU:OE1	1:F:216:ILE:HD11	2.18	0.42
1:H:16:LEU:HD21	1:H:30:GLY:HA3	2.01	0.42
1:H:169:GLU:C	1:H:170:LEU:HD23	2.39	0.42
1:H:175:LEU:O	1:H:178:VAL:HG23	2.19	0.42
1:I:62:GLY:O	1:I:67:GLY:HA3	2.18	0.42
1:K:254:PHE:C	1:K:254:PHE:HD2	2.22	0.42
1:N:154:LYS:HG3	1:N:177:CYS:SG	2.59	0.42
1:N:286:PHE:O	1:N:291:SER:HB3	2.19	0.42
1:O:17:GLN:NE2	1:O:31:ARG:HH21	2.17	0.42
1:P:154:LYS:HE2	1:P:176:LYS:HE3	2.01	0.42
1:A:240:PHE:H	1:A:240:PHE:HD1	1.66	0.42
1:B:17:GLN:O	1:B:31:ARG:N	2.51	0.42
1:B:240:PHE:HB3	1:B:242:VAL:CG2	2.48	0.42
1:C:115:ALA:HA	1:C:142:PRO:HD3	2.01	0.42
1:H:57:PHE:HD1	1:H:58:ILE:H	1.67	0.42
1:H:97:ILE:HG22	1:H:106:SER:O	2.19	0.42
1:J:274:PHE:O	1:J:277:ALA:HB3	2.19	0.42
1:L:94:ILE:HG23	1:L:95:ALA:N	2.34	0.42
1:L:218:ILE:HG22	1:L:226:VAL:HG21	2.01	0.42
1:M:75:LYS:HE3	1:M:81:THR:OG1	2.19	0.42
1:O:202:ALA:O	1:O:205:ALA:HB3	2.18	0.42
1:O:294:THR:O	1:O:298:VAL:HG22	2.19	0.42
1:E:7:LEU:HA	1:E:58:ILE:O	2.19	0.42
1:E:181:ILE:HG23	1:E:183:PRO:CD	2.47	0.42
1:K:69:ASN:O	1:K:72:GLU:HB2	2.19	0.42
1:K:206:ALA:HA	1:K:217:VAL:HG11	2.01	0.42
1:L:160:VAL:N	1:L:179:ASP:OD2	2.45	0.42
1:M:19:PRO:HA	1:M:101:ASP:O	2.19	0.42
1:N:66:PHE:HE1	1:N:70:ILE:HD12	1.84	0.42
1:O:17:GLN:HB3	1:O:31:ARG:NH2	2.35	0.42
1:P:136:LEU:HA	1:P:161:ILE:O	2.20	0.42
1:A:100:SER:HB3	1:A:104:GLU:O	2.19	0.42
1:B:99:VAL:HG22	1:B:101:ASP:HB2	2.01	0.42
1:B:294:THR:O	1:B:298:VAL:HG22	2.20	0.42
1:C:87:GLN:HB3	1:C:90:CYS:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:139:LEU:HD12	1:D:164:PRO:O	2.19	0.42
1:E:274:PHE:HZ	1:E:295:ARG:HE	1.67	0.42
1:F:14:HIS:ND1	1:F:35:VAL:HG22	2.35	0.42
1:F:184:ASN:O	1:F:188:ALA:N	2.31	0.42
1:G:96:MET:CG	1:H:96:MET:HE3	2.50	0.42
1:H:97:ILE:CG2	1:H:107:ILE:HA	2.38	0.42
1:H:240:PHE:CD1	1:H:301:PHE:HE2	2.21	0.42
1:L:274:PHE:HZ	1:L:295:ARG:NE	2.17	0.42
1:M:18:VAL:O	1:M:101:ASP:HB2	2.19	0.42
1:M:28:LEU:O	1:N:108:CYS:HA	2.19	0.42
1:O:172:ASP:O	1:O:174:LEU:N	2.53	0.42
1:P:14:HIS:N	1:P:95:ALA:O	2.46	0.42
1:A:43:ASN:O	1:A:47:ALA:N	2.45	0.42
1:A:210:HIS:ND1	1:A:214:ILE:O	2.33	0.42
1:B:139:LEU:HD21	1:B:162:LEU:HD11	2.01	0.42
1:B:207:ASP:HA	1:B:210:HIS:HB2	2.01	0.42
1:C:95:ALA:CB	1:C:109:ILE:HG23	2.48	0.42
1:D:119:ALA:HA	1:D:145:GLY:HA2	2.00	0.42
1:D:206:ALA:O	1:D:209:LEU:HB2	2.19	0.42
1:G:75:LYS:C	1:G:78:GLY:H	2.23	0.42
1:G:171:PRO:O	1:G:173:GLU:N	2.41	0.42
1:H:189:GLU:HA	1:H:194:ILE:O	2.20	0.42
1:H:205:ALA:O	1:H:206:ALA:C	2.57	0.42
1:I:209:LEU:HB3	1:I:214:ILE:HD12	2.00	0.42
1:K:17:GLN:HG3	1:K:99:VAL:HG13	2.01	0.42
1:K:114:ASN:O	1:K:116:LYS:N	2.53	0.42
1:K:123:GLU:HA	1:K:126:LEU:HD21	2.00	0.42
1:L:175:LEU:HD12	1:L:175:LEU:N	2.35	0.42
1:O:63:ASP:O	1:O:68:ILE:HD11	2.19	0.42
1:O:137:MET:O	1:O:162:LEU:HD12	2.19	0.42
1:O:240:PHE:CG	1:O:301:PHE:HE2	2.36	0.42
1:B:221:LEU:HD21	1:B:227:TRP:CB	2.48	0.42
1:C:194:ILE:HG22	1:C:195:THR:H	1.83	0.42
1:E:141:THR:HB	1:E:142:PRO:HD2	2.00	0.42
1:E:283:VAL:O	1:E:283:VAL:HG22	2.20	0.42
1:G:129:ILE:HD13	1:G:135:LEU:HD11	2.00	0.42
1:K:133:ARG:HA	1:K:158:THR:HB	2.01	0.42
1:K:175:LEU:HD23	1:K:175:LEU:HA	1.81	0.42
1:K:191:LEU:O	1:K:191:LEU:HD23	2.19	0.42
1:L:139:LEU:CD1	1:L:170:LEU:HD21	2.48	0.42
1:M:94:ILE:HD12	1:N:33:TYR:CE1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:3:LYS:HB2	1:N:54:ASP:HB3	2.00	0.42
1:O:248:THR:HG22	1:O:288:ALA:HB2	2.02	0.42
1:P:294:THR:CG2	1:P:297:GLU:HG2	2.50	0.42
1:A:116:LYS:O	1:A:118:THR:HG22	2.19	0.42
1:A:162:LEU:HB3	1:A:181:ILE:CD1	2.49	0.42
1:A:227:TRP:CZ3	1:A:236:ARG:HG3	2.54	0.42
1:D:118:THR:HB	1:D:144:ASP:OD1	2.20	0.42
1:E:49:ALA:HB1	1:E:77:ASP:O	2.20	0.42
1:F:127:ALA:O	1:F:130:ARG:HB2	2.19	0.42
1:G:147:LEU:CD1	1:G:151:GLN:HE21	2.29	0.42
1:H:9:SER:OG	1:H:140:GLU:HB3	2.20	0.42
1:H:95:ALA:HA	1:H:109:ILE:HA	2.01	0.42
1:I:3:LYS:HD3	1:I:54:ASP:HB3	2.01	0.42
1:K:26:GLU:HG3	1:K:27:THR:H	1.84	0.42
1:M:29:HIS:ND1	1:N:109:ILE:HB	2.35	0.42
1:N:163:ASN:HD22	1:N:164:PRO:HD2	1.85	0.42
1:O:170:LEU:HD23	1:O:170:LEU:HA	1.86	0.42
1:P:94:ILE:O	1:P:109:ILE:HG23	2.19	0.42
1:A:240:PHE:O	1:A:242:VAL:N	2.52	0.42
1:A:281:ILE:HB	1:A:293:PRO:HG3	2.02	0.42
1:B:233:ARG:CZ	1:I:211:CYS:HB2	2.49	0.42
1:C:197:TYR:HE1	1:C:201:SER:HB3	1.85	0.42
1:C:239:GLY:HA2	1:C:276:HIS:CE1	2.55	0.42
1:D:184:ASN:O	1:D:186:THR:N	2.53	0.42
1:E:46:VAL:HG13	1:E:50:ARG:NH1	2.34	0.42
1:F:138:GLN:CG	1:F:163:ASN:HB3	2.50	0.42
1:F:235:GLN:O	1:F:237:ILE:HG13	2.20	0.42
1:G:7:LEU:HA	1:G:58:ILE:O	2.20	0.42
1:G:12:ALA:HB2	1:G:66:PHE:CZ	2.55	0.42
1:J:73:SER:O	1:J:75:LYS:N	2.52	0.42
1:J:127:ALA:HA	1:J:130:ARG:NH2	2.34	0.42
1:K:26:GLU:HG3	1:K:27:THR:N	2.34	0.42
1:O:236:ARG:HH22	1:O:238:PRO:HB3	1.85	0.42
1:P:51:MET:CE	1:P:298:VAL:HG21	2.49	0.42
1:C:236:ARG:HG3	1:C:237:ILE:N	2.33	0.42
1:G:151:GLN:C	1:G:153:ALA:H	2.23	0.42
1:G:279:ALA:O	1:G:283:VAL:HG13	2.20	0.42
1:H:148:LYS:O	1:H:151:GLN:HG2	2.20	0.42
1:I:160:VAL:HG12	1:I:178:VAL:HG13	2.01	0.42
1:K:21:PHE:CZ	1:K:106:SER:HB2	2.55	0.42
1:M:9:SER:HB3	1:M:140:GLU:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:203:GLN:HB2	1:M:227:TRP:CZ2	2.54	0.42
1:O:43:ASN:HB3	1:O:252:ASP:HB3	2.00	0.42
1:P:86:LEU:H	1:P:86:LEU:HD12	1.85	0.42
1:A:96:MET:SD	1:B:16:LEU:HD22	2.60	0.42
1:A:131:ASP:N	1:A:131:ASP:OD2	2.53	0.42
1:A:277:ALA:O	1:A:281:ILE:HG13	2.20	0.42
1:B:4:LEU:HD12	1:B:5:VAL:H	1.84	0.42
1:D:2:ASN:HD22	1:D:55:VAL:C	2.22	0.42
1:D:184:ASN:C	1:D:186:THR:H	2.24	0.42
1:G:199:ASP:HA	1:G:227:TRP:CZ3	2.55	0.42
1:I:181:ILE:CD1	1:I:209:LEU:HD13	2.50	0.42
1:L:57:PHE:CD1	1:L:58:ILE:N	2.87	0.42
1:L:139:LEU:HD23	1:L:139:LEU:HA	1.55	0.42
1:L:218:ILE:HG23	1:L:226:VAL:HG21	2.02	0.42
1:P:46:VAL:O	1:P:50:ARG:HB2	2.20	0.42
1:A:63:ASP:OD2	1:A:88:PRO:HA	2.20	0.41
1:A:148:LYS:HA	1:A:148:LYS:HD2	1.79	0.41
1:A:269:GLU:CD	1:A:269:GLU:H	2.23	0.41
1:B:254:PHE:C	1:B:254:PHE:CD2	2.93	0.41
1:C:8:GLY:HA2	1:C:141:THR:HG21	2.02	0.41
1:F:263:LEU:HD13	1:F:263:LEU:HA	1.81	0.41
1:G:68:ILE:H	1:G:68:ILE:HG12	1.67	0.41
1:H:205:ALA:O	1:H:207:ASP:N	2.53	0.41
1:I:41:GLY:HA2	1:I:138:GLN:HE22	1.85	0.41
1:I:57:PHE:CD1	1:I:58:ILE:N	2.88	0.41
1:J:6:VAL:HG13	1:J:136:LEU:HD23	2.01	0.41
1:J:143:LEU:HG	1:J:168:ARG:CZ	2.50	0.41
1:K:143:LEU:HB3	1:K:144:ASP:H	1.73	0.41
1:L:44:GLN:NE2	1:L:163:ASN:OD1	2.48	0.41
1:L:116:LYS:HA	1:L:116:LYS:HD3	1.90	0.41
1:L:299:GLU:HA	1:L:302:LEU:HD12	2.02	0.41
1:M:40:LYS:NZ	1:M:165:ALA:O	2.53	0.41
1:M:129:ILE:HD12	1:M:135:LEU:HD13	2.02	0.41
1:M:174:LEU:O	1:M:178:VAL:HG23	2.20	0.41
1:P:267:PRO:HD2	1:P:270:SER:HB3	2.02	0.41
1:A:109:ILE:O	1:B:30:GLY:N	2.53	0.41
1:A:122:ILE:H	1:A:122:ILE:HG13	1.73	0.41
1:E:197:TYR:N	1:E:197:TYR:HD1	2.18	0.41
1:F:163:ASN:C	1:F:165:ALA:H	2.24	0.41
1:F:183:PRO:HB2	1:F:184:ASN:H	1.73	0.41
1:F:304:GLU:HG2	1:F:304:GLU:H	1.70	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:16:LEU:HD11	1:H:110:SER:HB2	2.00	0.41
1:G:72:GLU:C	1:G:74:PHE:H	2.23	0.41
1:G:285:ARG:HB3	1:G:286:PHE:H	1.63	0.41
1:J:264:GLN:HB2	1:J:264:GLN:HE21	1.51	0.41
1:K:24:PRO:O	1:K:26:GLU:N	2.50	0.41
1:K:125:ASP:C	1:K:127:ALA:N	2.72	0.41
1:M:19:PRO:HB2	1:M:20:SER:H	1.68	0.41
1:M:57:PHE:HD1	1:M:58:ILE:H	1.68	0.41
1:O:14:HIS:ND1	1:O:35:VAL:HG22	2.35	0.41
1:O:218:ILE:HG23	1:O:226:VAL:HG13	2.03	0.41
1:O:285:ARG:HB2	1:O:291:SER:CB	2.39	0.41
1:P:7:LEU:HB3	1:P:137:MET:HG2	2.02	0.41
1:A:81:THR:HG22	1:A:84:VAL:HG21	2.02	0.41
1:B:115:ALA:O	1:D:304:GLU:HB3	2.20	0.41
1:B:181:ILE:HG21	1:B:209:LEU:HD13	2.03	0.41
1:D:51:MET:HB2	1:D:260:THR:HG21	2.01	0.41
1:E:184:ASN:ND2	1:E:187:GLU:HG3	2.34	0.41
1:F:75:LYS:H	1:F:75:LYS:HG3	1.59	0.41
1:G:46:VAL:HG13	1:G:292:ILE:HG21	2.01	0.41
1:G:47:ALA:HB3	1:G:256:GLY:HA3	2.01	0.41
1:G:143:LEU:CD1	1:G:168:ARG:HH12	2.29	0.41
1:I:75:LYS:HB3	1:I:75:LYS:HE3	1.83	0.41
1:I:108:CYS:SG	1:J:28:LEU:HB2	2.60	0.41
1:L:261:GLY:O	1:L:264:GLN:N	2.50	0.41
1:N:50:ARG:C	1:N:52:GLN:H	2.22	0.41
1:B:74:PHE:O	1:B:77:ASP:N	2.54	0.41
1:C:4:LEU:HD23	1:C:55:VAL:HA	2.01	0.41
1:C:175:LEU:HD23	1:C:175:LEU:HA	1.78	0.41
1:D:71:ARG:HB2	1:D:84:VAL:HG11	2.01	0.41
1:E:51:MET:CB	1:E:260:THR:HG21	2.51	0.41
1:F:228:LEU:HD11	1:F:268:LEU:HD21	2.02	0.41
1:G:97:ILE:HG23	1:G:107:ILE:CD1	2.50	0.41
1:H:7:LEU:O	1:H:7:LEU:HD23	2.21	0.41
1:H:285:ARG:HH21	1:H:293:PRO:HB3	1.84	0.41
1:I:194:ILE:HD13	1:I:205:ALA:HA	2.02	0.41
1:J:183:PRO:HG2	1:J:219:ILE:HD12	2.03	0.41
1:M:4:LEU:HD23	1:M:55:VAL:HB	2.02	0.41
1:N:49:ALA:HB2	1:N:55:VAL:HG11	2.02	0.41
1:N:294:THR:H	1:N:297:GLU:CG	2.34	0.41
1:O:11:ASN:HB3	1:O:12:ALA:H	1.62	0.41
1:O:68:ILE:C	1:O:70:ILE:H	2.24	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:91:PRO:O	1:O:113:ALA:HB2	2.20	0.41
1:A:113:ALA:O	1:A:115:ALA:N	2.51	0.41
1:A:254:PHE:C	1:A:254:PHE:HD2	2.24	0.41
1:E:26:GLU:OE1	1:E:26:GLU:HA	2.20	0.41
1:E:63:ASP:O	1:E:68:ILE:HD11	2.20	0.41
1:E:247:THR:HA	1:E:250:ALA:HB2	2.02	0.41
1:F:16:LEU:HA	1:F:32:ASN:O	2.20	0.41
1:G:9:SER:N	1:G:41:GLY:HA3	2.35	0.41
1:G:93:GLY:HA3	1:G:114:ASN:HD21	1.86	0.41
1:G:181:ILE:HG22	1:G:217:VAL:HA	2.03	0.41
1:G:184:ASN:CG	1:G:185:GLU:N	2.74	0.41
1:G:236:ARG:O	1:G:237:ILE:HG13	2.20	0.41
1:H:117:LEU:HD12	1:H:117:LEU:HA	1.81	0.41
1:I:187:GLU:HG3	1:I:187:GLU:H	1.63	0.41
1:I:267:PRO:O	1:I:270:SER:OG	2.34	0.41
1:K:42:ALA:HB1	1:K:74:PHE:HZ	1.85	0.41
1:O:239:GLY:HA2	1:O:276:HIS:CD2	2.54	0.41
1:P:180:LEU:HG	1:P:216:ILE:HB	2.01	0.41
1:A:36:ILE:HA	1:A:37:PRO:HD3	1.83	0.41
1:B:233:ARG:H	1:B:233:ARG:HG2	1.40	0.41
1:B:245:THR:HB	1:B:283:VAL:O	2.20	0.41
1:C:131:ASP:OD1	1:C:131:ASP:N	2.49	0.41
1:C:233:ARG:HG3	1:C:233:ARG:O	2.21	0.41
1:C:299:GLU:O	1:C:300:ALA:C	2.59	0.41
1:D:48:ALA:O	1:D:260:THR:HG21	2.21	0.41
1:D:199:ASP:HB3	1:D:227:TRP:CZ3	2.55	0.41
1:D:277:ALA:HB2	1:D:302:LEU:HD21	2.03	0.41
1:E:37:PRO:HB2	1:E:289:GLN:HG3	2.02	0.41
1:E:181:ILE:HG12	1:E:183:PRO:HG3	2.03	0.41
1:G:208:ALA:O	1:G:212:LYS:CG	2.68	0.41
1:H:100:SER:HB3	1:H:104:GLU:O	2.20	0.41
1:J:129:ILE:HG23	1:J:135:LEU:CD1	2.50	0.41
1:J:236:ARG:HG3	1:J:237:ILE:N	2.34	0.41
1:K:87:GLN:HE21	1:K:116:LYS:HB3	1.86	0.41
1:N:91:PRO:O	1:N:112:GLU:HB3	2.19	0.41
1:N:302:LEU:HD23	1:N:302:LEU:HA	1.71	0.41
1:B:16:LEU:HD21	1:B:98:GLN:HG3	2.02	0.41
1:C:3:LYS:HB3	1:C:263:LEU:HD11	2.02	0.41
1:E:240:PHE:CE1	1:E:301:PHE:HE2	2.39	0.41
1:F:6:VAL:HG22	1:F:136:LEU:HB3	2.03	0.41
1:F:66:PHE:O	1:F:69:ASN:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:7:LEU:HD22	1:G:137:MET:HG2	2.02	0.41
1:I:161:ILE:HD13	1:I:259:VAL:HG22	2.02	0.41
1:K:42:ALA:O	1:K:46:VAL:HG12	2.21	0.41
1:K:143:LEU:HB2	1:K:168:ARG:HH22	1.85	0.41
1:N:287:GLY:HA2	1:N:291:SER:OG	2.21	0.41
1:O:159:ASN:HA	1:O:179:ASP:OD2	2.21	0.41
1:O:226:VAL:HG11	1:O:272:ILE:HD13	2.02	0.41
1:A:241:VAL:HG13	1:D:19:PRO:HG3	2.01	0.41
1:B:49:ALA:HB2	1:B:55:VAL:HG11	2.02	0.41
1:B:96:MET:HE2	1:B:96:MET:HB2	1.71	0.41
1:C:87:GLN:HA	1:C:88:PRO:HD3	1.92	0.41
1:D:137:MET:HE3	1:D:146:ILE:HG23	2.02	0.41
1:E:96:MET:CE	1:F:98:GLN:HE21	2.33	0.41
1:G:13:ASP:HB3	1:G:97:ILE:HD12	2.02	0.41
1:G:199:ASP:HB3	1:G:227:TRP:CZ3	2.55	0.41
1:G:236:ARG:CG	1:G:237:ILE:N	2.83	0.41
1:H:36:ILE:O	1:H:38:GLY:N	2.53	0.41
1:H:210:HIS:HE1	1:H:229:SER:O	2.03	0.41
1:J:197:TYR:HD1	1:J:197:TYR:H	1.68	0.41
1:K:80:ASN:HD21	1:K:82:ALA:HB3	1.85	0.41
1:L:172:ASP:C	1:L:174:LEU:H	2.24	0.41
1:N:93:GLY:HA2	1:N:112:GLU:HB2	2.02	0.41
1:N:292:ILE:HA	1:N:293:PRO:HD3	1.85	0.41
1:B:63:ASP:OD2	1:B:88:PRO:HA	2.20	0.41
1:B:168:ARG:HH22	1:D:306:SER:C	2.24	0.41
1:D:215:GLU:HG3	1:D:231:ASN:OD1	2.21	0.41
1:D:243:LYS:NZ	1:D:245:THR:HG23	2.36	0.41
1:F:50:ARG:NH1	1:F:292:ILE:O	2.54	0.41
1:F:185:GLU:HG2	1:F:196:VAL:HB	2.03	0.41
1:G:50:ARG:NE	1:G:77:ASP:OD1	2.51	0.41
1:H:40:LYS:HB3	1:H:138:GLN:HG2	2.03	0.41
1:H:169:GLU:O	1:H:170:LEU:HD23	2.21	0.41
1:H:229:SER:HA	1:H:234:GLY:HA2	2.03	0.41
1:I:97:ILE:HA	1:I:106:SER:O	2.20	0.41
1:I:117:LEU:HA	1:I:117:LEU:HD12	1.73	0.41
1:J:204:GLN:HG3	1:K:203:GLN:HG2	2.03	0.41
1:K:109:ILE:N	1:L:28:LEU:O	2.46	0.41
1:L:32:ASN:O	1:L:33:TYR:O	2.39	0.41
1:L:57:PHE:CE1	1:L:59:ALA:HB2	2.55	0.41
1:L:175:LEU:HD12	1:L:175:LEU:H	1.85	0.41
1:L:203:GLN:O	1:L:206:ALA:HB3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:139:LEU:CD1	1:M:170:LEU:HD11	2.51	0.41
1:M:141:THR:HB	1:M:142:PRO:HD2	2.03	0.41
1:M:185:GLU:HB3	1:M:196:VAL:HB	2.02	0.41
1:M:221:LEU:O	1:M:224:LYS:HG2	2.20	0.41
1:O:92:THR:O	1:O:94:ILE:HD12	2.21	0.41
1:O:94:ILE:HD13	1:P:33:TYR:CD2	2.56	0.41
1:O:98:GLN:OE1	1:O:106:SER:OG	2.37	0.41
1:O:99:VAL:HG13	1:O:101:ASP:HB2	2.03	0.41
1:O:185:GLU:H	1:O:185:GLU:HG3	1.51	0.41
1:P:13:ASP:HB3	1:P:97:ILE:CD1	2.50	0.41
1:B:43:ASN:C	1:B:45:ALA:H	2.24	0.41
1:B:139:LEU:HA	1:B:139:LEU:HD23	1.82	0.41
1:B:180:LEU:HD21	1:B:218:ILE:CD1	2.51	0.41
1:B:185:GLU:H	1:B:185:GLU:HG3	1.34	0.41
1:E:204:GLN:HA	1:E:207:ASP:OD2	2.21	0.41
1:G:227:TRP:CD2	1:G:235:GLN:O	2.74	0.41
1:H:267:PRO:O	1:H:270:SER:HB3	2.21	0.41
1:J:236:ARG:HH12	1:J:238:PRO:HB3	1.85	0.41
1:M:163:ASN:HD22	1:M:164:PRO:HD2	1.86	0.41
1:O:51:MET:HG3	1:O:260:THR:HG21	2.03	0.41
1:A:64:ASP:O	1:A:66:PHE:N	2.55	0.40
1:B:50:ARG:HH11	1:B:292:ILE:CG2	2.34	0.40
1:D:218:ILE:HG12	1:D:228:LEU:HD13	2.03	0.40
1:F:5:VAL:HG21	1:F:128:ALA:HB1	2.02	0.40
1:F:205:ALA:O	1:F:209:LEU:HD12	2.21	0.40
1:G:207:ASP:HA	1:G:210:HIS:HB2	2.03	0.40
1:H:160:VAL:O	1:H:160:VAL:HG12	2.21	0.40
1:H:245:THR:O	1:H:246:ASP:C	2.59	0.40
1:J:168:ARG:HG3	1:J:169:GLU:O	2.21	0.40
1:K:66:PHE:CZ	1:K:70:ILE:HG13	2.56	0.40
1:K:188:ALA:O	1:K:192:THR:OG1	2.21	0.40
1:L:21:PHE:CE2	1:L:106:SER:HB2	2.54	0.40
1:L:274:PHE:O	1:L:277:ALA:HB3	2.21	0.40
1:M:116:LYS:HA	1:M:116:LYS:HD3	1.95	0.40
1:M:161:ILE:N	1:M:161:ILE:HD12	2.36	0.40
1:M:184:ASN:ND2	1:M:186:THR:H	2.18	0.40
1:N:64:ASP:OD1	1:N:66:PHE:HB3	2.21	0.40
1:N:187:GLU:HA	1:N:190:VAL:HG22	2.03	0.40
1:O:40:LYS:N	1:O:140:GLU:OE1	2.54	0.40
1:O:111:ALA:O	1:O:114:ASN:N	2.54	0.40
1:B:216:ILE:HG21	1:B:268:LEU:HD21	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3:LYS:HD3	1:C:3:LYS:HA	1.55	0.40
1:C:188:ALA:O	1:C:192:THR:HG23	2.22	0.40
1:C:197:TYR:HD1	1:C:197:TYR:H	1.68	0.40
1:C:254:PHE:C	1:C:254:PHE:CD2	2.94	0.40
1:D:304:GLU:HG2	1:D:304:GLU:H	1.52	0.40
1:E:24:PRO:O	1:E:26:GLU:N	2.54	0.40
1:E:151:GLN:HG2	1:E:151:GLN:H	1.63	0.40
1:F:92:THR:O	1:F:94:ILE:HG23	2.21	0.40
1:G:181:ILE:HG22	1:G:217:VAL:HG22	2.02	0.40
1:G:192:THR:O	1:G:192:THR:OG1	2.38	0.40
1:H:204:GLN:NE2	1:H:207:ASP:OD2	2.55	0.40
1:J:93:GLY:HA3	1:J:114:ASN:ND2	2.37	0.40
1:K:16:LEU:HD21	1:K:30:GLY:HA3	2.03	0.40
1:K:118:THR:H	1:K:121:ALA:HB3	1.86	0.40
1:L:194:ILE:N	1:L:194:ILE:HD12	2.36	0.40
1:N:81:THR:C	1:N:83:GLY:N	2.73	0.40
1:B:262:LEU:HD23	1:B:262:LEU:N	2.36	0.40
1:C:76:LEU:HD22	1:C:76:LEU:HA	1.78	0.40
1:D:14:HIS:CD2	1:D:94:ILE:HG13	2.57	0.40
1:D:21:PHE:HE2	1:D:106:SER:HG	1.66	0.40
1:F:11:ASN:HB3	1:F:12:ALA:H	1.59	0.40
1:G:258:LEU:HB2	1:G:275:ALA:CB	2.51	0.40
1:H:19:PRO:HD3	1:H:29:HIS:O	2.22	0.40
1:H:66:PHE:HB3	1:H:67:GLY:H	1.69	0.40
1:L:305:HIS:O	1:L:306:SER:OG	2.29	0.40
1:M:178:VAL:O	1:M:214:ILE:HG23	2.21	0.40
1:P:7:LEU:O	1:P:137:MET:HA	2.21	0.40
1:A:18:VAL:HG21	1:A:98:GLN:HB3	2.03	0.40
1:A:137:MET:HE1	1:A:150:ALA:HB2	2.02	0.40
1:B:3:LYS:HE2	1:B:133:ARG:HG3	2.02	0.40
1:B:17:GLN:HB3	1:B:31:ARG:CZ	2.51	0.40
1:C:95:ALA:HA	1:C:109:ILE:HA	2.02	0.40
1:D:172:ASP:C	1:D:174:LEU:N	2.73	0.40
1:E:257:ALA:HB3	1:E:275:ALA:HA	2.04	0.40
1:F:3:LYS:CE	1:F:54:ASP:HB2	2.51	0.40
1:F:11:ASN:O	1:F:12:ALA:HB2	2.21	0.40
1:F:231:ASN:HB2	1:F:233:ARG:HE	1.86	0.40
1:G:57:PHE:HD1	1:G:58:ILE:H	1.70	0.40
1:M:100:SER:HA	1:M:101:ASP:CB	2.52	0.40
1:M:178:VAL:HB	1:M:214:ILE:HG12	2.02	0.40
1:N:98:GLN:NE2	1:N:106:SER:HB3	2.35	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:126:LEU:O	1:O:129:ILE:HB	2.21	0.40
1:A:135:LEU:N	1:A:159:ASN:O	2.54	0.40
1:A:206:ALA:O	1:A:209:LEU:N	2.55	0.40
1:B:40:LYS:HD2	1:B:140:GLU:HG3	2.04	0.40
1:B:112:GLU:HB3	1:B:113:ALA:H	1.79	0.40
1:B:187:GLU:O	1:B:190:VAL:N	2.51	0.40
1:E:110:SER:HB2	1:F:16:LEU:HD13	2.03	0.40
1:I:5:VAL:O	1:I:135:LEU:HA	2.22	0.40
1:J:51:MET:HB2	1:J:260:THR:HG21	2.03	0.40
1:J:197:TYR:N	1:J:197:TYR:HD1	2.19	0.40
1:K:135:LEU:HD23	1:K:160:VAL:HG22	2.03	0.40
1:L:13:ASP:OD1	1:L:95:ALA:HB3	2.22	0.40
1:O:44:GLN:HB3	1:O:136:LEU:HD21	2.03	0.40
1:O:50:ARG:HG3	1:O:292:ILE:CG2	2.50	0.40
1:P:18:VAL:HG11	1:P:98:GLN:HB2	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	304/309 (98%)	242 (80%)	46 (15%)	16 (5%)	2	13
1	B	304/309 (98%)	228 (75%)	50 (16%)	26 (9%)	1	5
1	C	304/309 (98%)	236 (78%)	46 (15%)	22 (7%)	1	7
1	D	304/309 (98%)	251 (83%)	33 (11%)	20 (7%)	1	8
1	E	304/309 (98%)	261 (86%)	34 (11%)	9 (3%)	4	23
1	F	304/309 (98%)	239 (79%)	46 (15%)	19 (6%)	1	9
1	G	304/309 (98%)	236 (78%)	50 (16%)	18 (6%)	1	11
1	H	304/309 (98%)	238 (78%)	38 (12%)	28 (9%)	1	4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	I	304/309 (98%)	264 (87%)	27 (9%)	13 (4%)	2	17
1	J	304/309 (98%)	244 (80%)	46 (15%)	14 (5%)	2	15
1	K	304/309 (98%)	238 (78%)	39 (13%)	27 (9%)	1	5
1	L	304/309 (98%)	259 (85%)	30 (10%)	15 (5%)	2	14
1	M	304/309 (98%)	253 (83%)	31 (10%)	20 (7%)	1	8
1	N	304/309 (98%)	262 (86%)	27 (9%)	15 (5%)	2	14
1	O	304/309 (98%)	245 (81%)	40 (13%)	19 (6%)	1	9
1	P	304/309 (98%)	259 (85%)	36 (12%)	9 (3%)	4	23
All	All	4864/4944 (98%)	3955 (81%)	619 (13%)	290 (6%)	1	10

All (290) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	64	ASP
1	A	67	GLY
1	A	82	ALA
1	A	172	ASP
1	A	196	VAL
1	A	222	GLY
1	A	240	PHE
1	A	244	ALA
1	B	65	SER
1	B	75	LYS
1	B	102	SER
1	B	112	GLU
1	B	157	LYS
1	B	173	GLU
1	B	188	ALA
1	B	250	ALA
1	B	265	GLU
1	B	288	ALA
1	B	297	GLU
1	C	77	ASP
1	C	126	LEU
1	C	172	ASP
1	C	209	LEU
1	C	210	HIS
1	C	231	ASN
1	C	247	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C	284	THR
1	D	112	GLU
1	D	127	ALA
1	D	143	LEU
1	D	167	ALA
1	D	173	GLU
1	D	242	VAL
1	E	143	LEU
1	E	144	ASP
1	F	66	PHE
1	F	67	GLY
1	F	82	ALA
1	F	112	GLU
1	F	127	ALA
1	F	132	ALA
1	F	230	GLN
1	F	265	GLU
1	F	268	LEU
1	G	175	LEU
1	G	176	LYS
1	G	235	GLN
1	G	258	LEU
1	H	40	LYS
1	H	41	GLY
1	H	82	ALA
1	H	113	ALA
1	H	206	ALA
1	H	226	VAL
1	H	246	ASP
1	H	248	THR
1	H	285	ARG
1	H	286	PHE
1	H	288	ALA
1	H	291	SER
1	I	288	ALA
1	I	292	ILE
1	J	32	ASN
1	J	74	PHE
1	J	119	ALA
1	J	128	ALA
1	J	173	GLU
1	J	188	ALA

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	J	292	ILE
1	K	2	ASN
1	K	12	ALA
1	K	48	ALA
1	K	63	ASP
1	K	112	GLU
1	K	131	ASP
1	K	132	ALA
1	K	144	ASP
1	K	157	LYS
1	K	235	GLN
1	K	245	THR
1	K	274	PHE
1	L	33	TYR
1	L	93	GLY
1	L	101	ASP
1	L	112	GLU
1	L	144	ASP
1	L	173	GLU
1	L	245	THR
1	L	247	THR
1	L	248	THR
1	M	3	LYS
1	M	19	PRO
1	M	20	SER
1	M	21	PHE
1	M	112	GLU
1	M	249	ALA
1	M	250	ALA
1	N	82	ALA
1	N	112	GLU
1	N	213	GLY
1	N	248	THR
1	N	284	THR
1	N	288	ALA
1	O	82	ALA
1	O	112	GLU
1	O	199	ASP
1	O	206	ALA
1	O	249	ALA
1	O	281	ILE
1	O	286	PHE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	P	13	ASP
1	P	19	PRO
1	P	173	GLU
1	A	111	ALA
1	B	52	GLN
1	B	180	LEU
1	B	298	VAL
1	C	80	ASN
1	C	112	GLU
1	C	194	ILE
1	C	283	VAL
1	D	66	PHE
1	D	102	SER
1	D	144	ASP
1	D	185	GLU
1	D	233	ARG
1	D	251	GLY
1	D	252	ASP
1	D	288	ALA
1	D	291	SER
1	E	2	ASN
1	E	25	GLY
1	E	249	ALA
1	F	19	PRO
1	F	156	ALA
1	F	231	ASN
1	G	24	PRO
1	G	32	ASN
1	G	112	GLU
1	G	172	ASP
1	G	234	GLY
1	G	250	ALA
1	G	262	LEU
1	G	288	ALA
1	G	291	SER
1	H	33	TYR
1	H	54	ASP
1	H	205	ALA
1	H	250	ALA
1	H	251	GLY
1	I	82	ALA
1	I	190	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	I	248	THR
1	I	287	GLY
1	J	101	ASP
1	J	129	ILE
1	J	210	HIS
1	J	213	GLY
1	J	235	GLN
1	K	32	ASN
1	K	143	LEU
1	K	158	THR
1	K	159	ASN
1	K	173	GLU
1	K	222	GLY
1	L	143	LEU
1	L	241	VAL
1	L	286	PHE
1	M	32	ASN
1	M	157	LYS
1	M	173	GLU
1	M	248	THR
1	N	209	LEU
1	N	229	SER
1	N	234	GLY
1	O	2	ASN
1	O	171	PRO
1	O	173	GLU
1	O	247	THR
1	O	250	ALA
1	P	222	GLY
1	P	241	VAL
1	P	248	THR
1	A	65	SER
1	A	83	GLY
1	A	248	THR
1	B	44	GLN
1	B	48	ALA
1	B	49	ALA
1	B	74	PHE
1	B	77	ASP
1	B	223	SER
1	C	20	SER
1	C	26	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C	41	GLY
1	D	119	ALA
1	E	40	LYS
1	E	248	THR
1	E	286	PHE
1	F	32	ASN
1	F	63	ASP
1	F	81	THR
1	F	243	LYS
1	G	227	TRP
1	G	248	THR
1	H	32	ASN
1	H	52	GLN
1	H	67	GLY
1	H	138	GLN
1	H	249	ALA
1	I	40	LYS
1	I	157	LYS
1	I	247	THR
1	J	187	GLU
1	K	202	ALA
1	K	210	HIS
1	K	236	ARG
1	K	247	THR
1	K	273	LYS
1	M	150	ALA
1	M	247	THR
1	M	286	PHE
1	M	288	ALA
1	M	289	GLN
1	N	40	LYS
1	N	211	CYS
1	O	242	VAL
1	P	244	ALA
1	A	99	VAL
1	A	115	ALA
1	C	40	LYS
1	C	290	THR
1	D	248	THR
1	D	283	VAL
1	F	157	LYS
1	F	183	PRO

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	H	127	ALA
1	J	291	SER
1	K	183	PRO
1	M	231	ASN
1	M	251	GLY
1	N	157	LYS
1	O	101	ASP
1	O	282	SER
1	P	235	GLN
1	B	67	GLY
1	B	168	ARG
1	C	19	PRO
1	C	106	SER
1	C	131	ASP
1	D	292	ILE
1	E	283	VAL
1	H	66	PHE
1	H	157	LYS
1	K	40	LYS
1	K	67	GLY
1	L	196	VAL
1	N	101	ASP
1	N	193	GLY
1	N	210	HIS
1	O	32	ASN
1	O	100	SER
1	O	157	LYS
1	P	2	ASN
1	B	22	PRO
1	B	224	LYS
1	F	241	VAL
1	G	101	ASP
1	I	286	PHE
1	L	243	LYS
1	C	67	GLY
1	C	78	GLY
1	G	22	PRO
1	K	241	VAL
1	M	242	VAL
1	O	67	GLY
1	H	37	PRO
1	H	281	ILE

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Mol	Chain	Res	Type
1	I	41	GLY
1	A	241	VAL
1	G	226	VAL
1	I	67	GLY
1	I	78	GLY
1	L	91	PRO
1	B	181	ILE
1	A	242	VAL
1	B	292	ILE
1	D	67	GLY
1	H	38	GLY
1	M	241	VAL

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	237/239 (99%)	186 (78%)	51 (22%)	1 3
1	B	237/239 (99%)	171 (72%)	66 (28%)	0 1
1	C	237/239 (99%)	180 (76%)	57 (24%)	0 2
1	D	237/239 (99%)	185 (78%)	52 (22%)	1 3
1	E	237/239 (99%)	194 (82%)	43 (18%)	1 6
1	F	237/239 (99%)	181 (76%)	56 (24%)	1 2
1	G	237/239 (99%)	160 (68%)	77 (32%)	0 1
1	H	237/239 (99%)	178 (75%)	59 (25%)	0 2
1	I	237/239 (99%)	192 (81%)	45 (19%)	1 4
1	J	237/239 (99%)	185 (78%)	52 (22%)	1 3
1	K	237/239 (99%)	183 (77%)	54 (23%)	1 2
1	L	237/239 (99%)	197 (83%)	40 (17%)	2 8
1	M	237/239 (99%)	188 (79%)	49 (21%)	1 3
1	N	237/239 (99%)	186 (78%)	51 (22%)	1 3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	O	237/239 (99%)	181 (76%)	56 (24%)	1	2
1	P	237/239 (99%)	180 (76%)	57 (24%)	0	2
All	All	3792/3824 (99%)	2927 (77%)	865 (23%)	1	2

All (865) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	SER
1	A	13	ASP
1	A	17	GLN
1	A	20	SER
1	A	21	PHE
1	A	23	ARG
1	A	26	GLU
1	A	28	LEU
1	A	31	ARG
1	A	52	GLN
1	A	57	PHE
1	A	66	PHE
1	A	71	ARG
1	A	73	SER
1	A	81	THR
1	A	85	LYS
1	A	86	LEU
1	A	89	ASN
1	A	94	ILE
1	A	97	ILE
1	A	101	ASP
1	A	106	SER
1	A	141	THR
1	A	147	LEU
1	A	151	GLN
1	A	155	THR
1	A	160	VAL
1	A	163	ASN
1	A	170	LEU
1	A	187	GLU
1	A	190	VAL
1	A	191	LEU
1	A	196	VAL
1	A	197	TYR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	214	ILE
1	A	220	THR
1	A	221	LEU
1	A	226	VAL
1	A	231	ASN
1	A	235	GLN
1	A	236	ARG
1	A	243	LYS
1	A	253	THR
1	A	254	PHE
1	A	260	THR
1	A	263	LEU
1	A	264	GLN
1	A	270	SER
1	A	281	ILE
1	A	291	SER
1	A	295	ARG
1	B	1	MET
1	B	2	ASN
1	B	11	ASN
1	B	16	LEU
1	B	21	PHE
1	B	23	ARG
1	B	27	THR
1	B	35	VAL
1	B	36	ILE
1	B	55	VAL
1	B	57	PHE
1	B	63	ASP
1	B	73	SER
1	B	79	ILE
1	B	89	ASN
1	B	92	THR
1	B	94	ILE
1	B	97	ILE
1	B	98	GLN
1	B	99	VAL
1	B	100	SER
1	B	104	GLU
1	B	108	CYS
1	B	112	GLU
1	B	116	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	117	LEU
1	B	118	THR
1	B	141	THR
1	B	163	ASN
1	B	168	ARG
1	B	175	LEU
1	B	176	LYS
1	B	180	LEU
1	B	182	THR
1	B	185	GLU
1	B	189	GLU
1	B	195	THR
1	B	197	TYR
1	B	199	ASP
1	B	211	CYS
1	B	218	ILE
1	B	221	LEU
1	B	224	LYS
1	B	228	LEU
1	B	230	GLN
1	B	233	ARG
1	B	236	ARG
1	B	242	VAL
1	B	243	LYS
1	B	247	THR
1	B	248	THR
1	B	254	PHE
1	B	255	ASN
1	B	260	THR
1	B	262	LEU
1	B	269	GLU
1	B	272	ILE
1	B	276	HIS
1	B	281	ILE
1	B	282	SER
1	B	286	PHE
1	B	290	THR
1	B	291	SER
1	B	294	THR
1	B	297	GLU
1	B	298	VAL
1	C	1	MET

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C	3	LYS
1	C	4	LEU
1	C	7	LEU
1	C	9	SER
1	C	18	VAL
1	C	23	ARG
1	C	26	GLU
1	C	28	LEU
1	C	29	HIS
1	C	31	ARG
1	C	57	PHE
1	C	64	ASP
1	C	65	SER
1	C	68	ILE
1	C	71	ARG
1	C	73	SER
1	C	76	LEU
1	C	84	VAL
1	C	85	LYS
1	C	94	ILE
1	C	96	MET
1	C	97	ILE
1	C	98	GLN
1	C	102	SER
1	C	106	SER
1	C	107	ILE
1	C	108	CYS
1	C	109	ILE
1	C	118	THR
1	C	144	ASP
1	C	148	LYS
1	C	154	LYS
1	C	168	ARG
1	C	170	LEU
1	C	172	ASP
1	C	179	ASP
1	C	181	ILE
1	C	182	THR
1	C	191	LEU
1	C	197	TYR
1	C	199	ASP
1	C	220	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C	221	LEU
1	C	224	LYS
1	C	226	VAL
1	C	236	ARG
1	C	238	PRO
1	C	240	PHE
1	C	243	LYS
1	C	246	ASP
1	C	248	THR
1	C	253	THR
1	C	263	LEU
1	C	265	GLU
1	C	285	ARG
1	C	286	PHE
1	D	1	MET
1	D	2	ASN
1	D	3	LYS
1	D	17	GLN
1	D	20	SER
1	D	28	LEU
1	D	31	ARG
1	D	36	ILE
1	D	55	VAL
1	D	57	PHE
1	D	63	ASP
1	D	64	ASP
1	D	68	ILE
1	D	72	GLU
1	D	73	SER
1	D	89	ASN
1	D	94	ILE
1	D	97	ILE
1	D	100	SER
1	D	106	SER
1	D	112	GLU
1	D	133	ARG
1	D	157	LYS
1	D	163	ASN
1	D	176	LYS
1	D	182	THR
1	D	186	THR
1	D	197	TYR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	D	198	ASP
1	D	200	SER
1	D	203	GLN
1	D	204	GLN
1	D	211	CYS
1	D	214	ILE
1	D	220	THR
1	D	221	LEU
1	D	224	LYS
1	D	226	VAL
1	D	241	VAL
1	D	245	THR
1	D	248	THR
1	D	260	THR
1	D	263	LEU
1	D	270	SER
1	D	273	LYS
1	D	276	HIS
1	D	286	PHE
1	D	290	THR
1	D	291	SER
1	D	298	VAL
1	D	304	GLU
1	D	306	SER
1	E	1	MET
1	E	17	GLN
1	E	18	VAL
1	E	23	ARG
1	E	24	PRO
1	E	28	LEU
1	E	31	ARG
1	E	34	GLN
1	E	57	PHE
1	E	61	VAL
1	E	76	LEU
1	E	86	LEU
1	E	87	GLN
1	E	88	PRO
1	E	92	THR
1	E	101	ASP
1	E	102	SER
1	E	107	ILE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	E	108	CYS
1	E	117	LEU
1	E	122	ILE
1	E	130	ARG
1	E	133	ARG
1	E	148	LYS
1	E	151	GLN
1	E	169	GLU
1	E	173	GLU
1	E	184	ASN
1	E	194	ILE
1	E	197	TYR
1	E	221	LEU
1	E	226	VAL
1	E	230	GLN
1	E	243	LYS
1	E	270	SER
1	E	273	LYS
1	E	281	ILE
1	E	282	SER
1	E	285	ARG
1	E	286	PHE
1	E	291	SER
1	E	295	ARG
1	E	306	SER
1	F	16	LEU
1	F	20	SER
1	F	23	ARG
1	F	24	PRO
1	F	27	THR
1	F	28	LEU
1	F	31	ARG
1	F	36	ILE
1	F	46	VAL
1	F	57	PHE
1	F	64	ASP
1	F	70	ILE
1	F	73	SER
1	F	75	LYS
1	F	77	ASP
1	F	81	THR
1	F	86	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	F	89	ASN
1	F	92	THR
1	F	102	SER
1	F	108	CYS
1	F	112	GLU
1	F	116	LYS
1	F	123	GLU
1	F	131	ASP
1	F	138	GLN
1	F	140	GLU
1	F	144	ASP
1	F	147	LEU
1	F	161	ILE
1	F	163	ASN
1	F	168	ARG
1	F	169	GLU
1	F	170	LEU
1	F	181	ILE
1	F	184	ASN
1	F	191	LEU
1	F	197	TYR
1	F	209	LEU
1	F	211	CYS
1	F	215	GLU
1	F	236	ARG
1	F	243	LYS
1	F	246	ASP
1	F	247	THR
1	F	248	THR
1	F	253	THR
1	F	263	LEU
1	F	265	GLU
1	F	270	SER
1	F	273	LYS
1	F	276	HIS
1	F	281	ILE
1	F	289	GLN
1	F	291	SER
1	F	304	GLU
1	G	5	VAL
1	G	18	VAL
1	G	20	SER

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	G	23	ARG
1	G	31	ARG
1	G	32	ASN
1	G	46	VAL
1	G	57	PHE
1	G	65	SER
1	G	68	ILE
1	G	73	SER
1	G	75	LYS
1	G	79	ILE
1	G	85	LYS
1	G	86	LEU
1	G	92	THR
1	G	94	ILE
1	G	96	MET
1	G	99	VAL
1	G	101	ASP
1	G	102	SER
1	G	104	GLU
1	G	107	ILE
1	G	109	ILE
1	G	110	SER
1	G	116	LYS
1	G	118	THR
1	G	130	ARG
1	G	137	MET
1	G	138	GLN
1	G	141	THR
1	G	143	LEU
1	G	144	ASP
1	G	148	LYS
1	G	151	GLN
1	G	154	LYS
1	G	159	ASN
1	G	163	ASN
1	G	170	LEU
1	G	173	GLU
1	G	177	CYS
1	G	178	VAL
1	G	179	ASP
1	G	184	ASN
1	G	189	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	G	194	ILE
1	G	197	TYR
1	G	199	ASP
1	G	207	ASP
1	G	211	CYS
1	G	218	ILE
1	G	220	THR
1	G	221	LEU
1	G	224	LYS
1	G	233	ARG
1	G	242	VAL
1	G	243	LYS
1	G	245	THR
1	G	246	ASP
1	G	247	THR
1	G	255	ASN
1	G	259	VAL
1	G	260	THR
1	G	263	LEU
1	G	264	GLN
1	G	266	MET
1	G	268	LEU
1	G	270	SER
1	G	273	LYS
1	G	276	HIS
1	G	283	VAL
1	G	286	PHE
1	G	290	THR
1	G	291	SER
1	G	295	ARG
1	G	299	GLU
1	G	306	SER
1	H	7	LEU
1	H	9	SER
1	H	18	VAL
1	H	23	ARG
1	H	24	PRO
1	H	46	VAL
1	H	52	GLN
1	H	54	ASP
1	H	57	PHE
1	H	70	ILE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	H	76	LEU
1	H	77	ASP
1	H	85	LYS
1	H	92	THR
1	H	94	ILE
1	H	96	MET
1	H	98	GLN
1	H	101	ASP
1	H	104	GLU
1	H	105	ASN
1	H	106	SER
1	H	108	CYS
1	H	112	GLU
1	H	116	LYS
1	H	122	ILE
1	H	133	ARG
1	H	143	LEU
1	H	144	ASP
1	H	161	ILE
1	H	163	ASN
1	H	169	GLU
1	H	172	ASP
1	H	173	GLU
1	H	178	VAL
1	H	182	THR
1	H	187	GLU
1	H	189	GLU
1	H	191	LEU
1	H	192	THR
1	H	194	ILE
1	H	197	TYR
1	H	199	ASP
1	H	212	LYS
1	H	223	SER
1	H	233	ARG
1	H	235	GLN
1	H	241	VAL
1	H	242	VAL
1	H	245	THR
1	H	246	ASP
1	H	247	THR
1	H	253	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	H	259	VAL
1	H	263	LEU
1	H	281	ILE
1	H	284	THR
1	H	286	PHE
1	H	289	GLN
1	H	304	GLU
1	I	1	MET
1	I	3	LYS
1	I	7	LEU
1	I	16	LEU
1	I	23	ARG
1	I	28	LEU
1	I	34	GLN
1	I	57	PHE
1	I	65	SER
1	I	72	GLU
1	I	73	SER
1	I	75	LYS
1	I	88	PRO
1	I	94	ILE
1	I	105	ASN
1	I	106	SER
1	I	108	CYS
1	I	109	ILE
1	I	143	LEU
1	I	144	ASP
1	I	147	LEU
1	I	163	ASN
1	I	169	GLU
1	I	178	VAL
1	I	179	ASP
1	I	181	ILE
1	I	185	GLU
1	I	187	GLU
1	I	191	LEU
1	I	197	TYR
1	I	207	ASP
1	I	214	ILE
1	I	223	SER
1	I	226	VAL
1	I	230	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	I	233	ARG
1	I	245	THR
1	I	246	ASP
1	I	248	THR
1	I	253	THR
1	I	260	THR
1	I	286	PHE
1	I	290	THR
1	I	294	THR
1	I	306	SER
1	J	7	LEU
1	J	16	LEU
1	J	17	GLN
1	J	20	SER
1	J	34	GLN
1	J	36	ILE
1	J	57	PHE
1	J	68	ILE
1	J	75	LYS
1	J	81	THR
1	J	86	LEU
1	J	89	ASN
1	J	94	ILE
1	J	100	SER
1	J	104	GLU
1	J	108	CYS
1	J	109	ILE
1	J	110	SER
1	J	118	THR
1	J	141	THR
1	J	143	LEU
1	J	151	GLN
1	J	154	LYS
1	J	159	ASN
1	J	162	LEU
1	J	163	ASN
1	J	168	ARG
1	J	170	LEU
1	J	173	GLU
1	J	181	ILE
1	J	191	LEU
1	J	194	ILE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	J	197	TYR
1	J	212	LYS
1	J	220	THR
1	J	233	ARG
1	J	235	GLN
1	J	236	ARG
1	J	243	LYS
1	J	246	ASP
1	J	248	THR
1	J	254	PHE
1	J	263	LEU
1	J	264	GLN
1	J	268	LEU
1	J	270	SER
1	J	273	LYS
1	J	284	THR
1	J	286	PHE
1	J	289	GLN
1	J	292	ILE
1	J	304	GLU
1	K	9	SER
1	K	17	GLN
1	K	18	VAL
1	K	31	ARG
1	K	34	GLN
1	K	35	VAL
1	K	36	ILE
1	K	57	PHE
1	K	65	SER
1	K	68	ILE
1	K	70	ILE
1	K	76	LEU
1	K	87	GLN
1	K	92	THR
1	K	94	ILE
1	K	105	ASN
1	K	106	SER
1	K	107	ILE
1	K	109	ILE
1	K	117	LEU
1	K	126	LEU
1	K	129	ILE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	K	137	MET
1	K	138	GLN
1	K	141	THR
1	K	144	ASP
1	K	147	LEU
1	K	154	LYS
1	K	158	THR
1	K	163	ASN
1	K	168	ARG
1	K	169	GLU
1	K	170	LEU
1	K	172	ASP
1	K	178	VAL
1	K	184	ASN
1	K	189	GLU
1	K	197	TYR
1	K	207	ASP
1	K	214	ILE
1	K	220	THR
1	K	221	LEU
1	K	224	LYS
1	K	246	ASP
1	K	247	THR
1	K	248	THR
1	K	253	THR
1	K	254	PHE
1	K	263	LEU
1	K	273	LYS
1	K	281	ILE
1	K	289	GLN
1	K	295	ARG
1	K	297	GLU
1	L	7	LEU
1	L	17	GLN
1	L	27	THR
1	L	28	LEU
1	L	32	ASN
1	L	40	LYS
1	L	51	MET
1	L	57	PHE
1	L	63	ASP
1	L	65	SER

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	L	70	ILE
1	L	71	ARG
1	L	85	LYS
1	L	88	PRO
1	L	94	ILE
1	L	106	SER
1	L	108	CYS
1	L	112	GLU
1	L	140	GLU
1	L	141	THR
1	L	144	ASP
1	L	147	LEU
1	L	148	LYS
1	L	154	LYS
1	L	163	ASN
1	L	176	LYS
1	L	179	ASP
1	L	182	THR
1	L	197	TYR
1	L	211	CYS
1	L	230	GLN
1	L	253	THR
1	L	263	LEU
1	L	264	GLN
1	L	269	GLU
1	L	270	SER
1	L	273	LYS
1	L	284	THR
1	L	289	GLN
1	L	294	THR
1	M	3	LYS
1	M	16	LEU
1	M	23	ARG
1	M	27	THR
1	M	35	VAL
1	M	51	MET
1	M	57	PHE
1	M	63	ASP
1	M	70	ILE
1	M	85	LYS
1	M	86	LEU
1	M	89	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	M	94	ILE
1	M	96	MET
1	M	98	GLN
1	M	101	ASP
1	M	104	GLU
1	M	106	SER
1	M	107	ILE
1	M	117	LEU
1	M	140	GLU
1	M	147	LEU
1	M	157	LYS
1	M	163	ASN
1	M	169	GLU
1	M	170	LEU
1	M	181	ILE
1	M	184	ASN
1	M	194	ILE
1	M	197	TYR
1	M	199	ASP
1	M	207	ASP
1	M	211	CYS
1	M	221	LEU
1	M	224	LYS
1	M	228	LEU
1	M	230	GLN
1	M	231	ASN
1	M	253	THR
1	M	263	LEU
1	M	268	LEU
1	M	270	SER
1	M	273	LYS
1	M	276	HIS
1	M	281	ILE
1	M	286	PHE
1	M	297	GLU
1	M	304	GLU
1	M	306	SER
1	N	1	MET
1	N	15	VAL
1	N	17	GLN
1	N	23	ARG
1	N	24	PRO

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	N	28	LEU
1	N	36	ILE
1	N	50	ARG
1	N	57	PHE
1	N	60	CYS
1	N	68	ILE
1	N	73	SER
1	N	84	VAL
1	N	90	CYS
1	N	92	THR
1	N	100	SER
1	N	107	ILE
1	N	117	LEU
1	N	144	ASP
1	N	155	THR
1	N	160	VAL
1	N	163	ASN
1	N	177	CYS
1	N	180	LEU
1	N	182	THR
1	N	189	GLU
1	N	191	LEU
1	N	203	GLN
1	N	207	ASP
1	N	210	HIS
1	N	212	LYS
1	N	233	ARG
1	N	235	GLN
1	N	236	ARG
1	N	240	PHE
1	N	243	LYS
1	N	246	ASP
1	N	248	THR
1	N	255	ASN
1	N	259	VAL
1	N	263	LEU
1	N	265	GLU
1	N	266	MET
1	N	269	GLU
1	N	281	ILE
1	N	285	ARG
1	N	286	PHE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	N	289	GLN
1	N	290	THR
1	N	295	ARG
1	N	304	GLU
1	O	7	LEU
1	O	15	VAL
1	O	18	VAL
1	O	23	ARG
1	O	44	GLN
1	O	50	ARG
1	O	52	GLN
1	O	57	PHE
1	O	63	ASP
1	O	64	ASP
1	O	68	ILE
1	O	70	ILE
1	O	71	ARG
1	O	72	GLU
1	O	73	SER
1	O	77	ASP
1	O	84	VAL
1	O	85	LYS
1	O	94	ILE
1	O	97	ILE
1	O	99	VAL
1	O	101	ASP
1	O	106	SER
1	O	118	THR
1	O	123	GLU
1	O	141	THR
1	O	144	ASP
1	O	147	LEU
1	O	168	ARG
1	O	172	ASP
1	O	180	LEU
1	O	182	THR
1	O	185	GLU
1	O	189	GLU
1	O	201	SER
1	O	207	ASP
1	O	211	CYS
1	O	220	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	O	224	LYS
1	O	226	VAL
1	O	229	SER
1	O	230	GLN
1	O	235	GLN
1	O	242	VAL
1	O	243	LYS
1	O	245	THR
1	O	246	ASP
1	O	248	THR
1	O	253	THR
1	O	260	THR
1	O	263	LEU
1	O	266	MET
1	O	268	LEU
1	O	294	THR
1	O	297	GLU
1	O	304	GLU
1	P	1	MET
1	P	2	ASN
1	P	3	LYS
1	P	13	ASP
1	P	18	VAL
1	P	34	GLN
1	P	35	VAL
1	P	57	PHE
1	P	60	CYS
1	P	65	SER
1	P	68	ILE
1	P	71	ARG
1	P	72	GLU
1	P	73	SER
1	P	77	ASP
1	P	86	LEU
1	P	92	THR
1	P	94	ILE
1	P	98	GLN
1	P	99	VAL
1	P	101	ASP
1	P	118	THR
1	P	130	ARG
1	P	135	LEU

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Mol	Chain	Res	Type
1	P	141	THR
1	P	158	THR
1	P	161	ILE
1	P	163	ASN
1	P	172	ASP
1	P	174	LEU
1	P	176	LYS
1	P	180	LEU
1	P	185	GLU
1	P	186	THR
1	P	191	LEU
1	P	194	ILE
1	P	197	TYR
1	P	209	LEU
1	P	212	LYS
1	P	214	ILE
1	P	215	GLU
1	P	217	VAL
1	P	220	THR
1	P	221	LEU
1	P	224	LYS
1	P	226	VAL
1	P	236	ARG
1	P	243	LYS
1	P	245	THR
1	P	253	THR
1	P	264	GLN
1	P	270	SER
1	P	276	HIS
1	P	281	ILE
1	P	289	GLN
1	P	291	SER
1	P	299	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (82) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	GLN
1	A	87	GLN
1	A	98	GLN
1	B	11	ASN
1	B	44	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	89	ASN
1	B	163	ASN
1	B	203	GLN
1	B	230	GLN
1	B	231	ASN
1	B	289	GLN
1	D	17	GLN
1	D	29	HIS
1	D	163	ASN
1	D	204	GLN
1	E	87	GLN
1	E	151	GLN
1	E	159	ASN
1	E	184	ASN
1	E	231	ASN
1	E	305	HIS
1	F	98	GLN
1	F	184	ASN
1	F	230	GLN
1	F	264	GLN
1	G	52	GLN
1	G	69	ASN
1	G	98	GLN
1	G	114	ASN
1	G	138	GLN
1	G	151	GLN
1	G	163	ASN
1	G	264	GLN
1	G	305	HIS
1	H	17	GLN
1	H	32	ASN
1	H	204	GLN
1	I	43	ASN
1	I	98	GLN
1	I	151	GLN
1	I	289	GLN
1	J	17	GLN
1	J	32	ASN
1	J	114	ASN
1	J	151	GLN
1	J	163	ASN
1	J	235	GLN

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Mol	Chain	Res	Type
1	J	264	GLN
1	J	305	HIS
1	K	69	ASN
1	K	151	GLN
1	K	203	GLN
1	K	289	GLN
1	L	43	ASN
1	L	98	GLN
1	L	151	GLN
1	L	235	GLN
1	L	289	GLN
1	M	80	ASN
1	M	163	ASN
1	M	184	ASN
1	M	276	HIS
1	N	17	GLN
1	N	32	ASN
1	N	163	ASN
1	N	203	GLN
1	O	34	GLN
1	O	44	GLN
1	O	69	ASN
1	O	98	GLN
1	O	114	ASN
1	O	151	GLN
1	O	163	ASN
1	O	230	GLN
1	O	276	HIS
1	O	289	GLN
1	P	17	GLN
1	P	34	GLN
1	P	69	ASN
1	P	98	GLN
1	P	163	ASN
1	P	276	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



## 6 Fit of model and data [i](#)

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

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	306/309 (99%)	0.24	18 (5%) 22 23	61, 108, 179, 294	0
1	B	306/309 (99%)	0.16	12 (3%) 39 38	67, 98, 149, 239	0
1	C	306/309 (99%)	0.04	7 (2%) 60 59	42, 83, 141, 201	0
1	D	306/309 (99%)	-0.07	3 (0%) 82 81	34, 76, 134, 179	0
1	E	306/309 (99%)	-0.07	7 (2%) 60 59	38, 62, 112, 182	0
1	F	306/309 (99%)	-0.05	4 (1%) 77 76	46, 81, 140, 173	0
1	G	306/309 (99%)	-0.04	5 (1%) 72 70	40, 79, 131, 162	0
1	H	306/309 (99%)	-0.09	2 (0%) 87 87	36, 69, 125, 214	0
1	I	306/309 (99%)	-0.01	7 (2%) 60 59	43, 76, 125, 199	0
1	J	306/309 (99%)	-0.03	2 (0%) 87 87	43, 80, 130, 202	0
1	K	306/309 (99%)	-0.08	5 (1%) 72 70	47, 83, 140, 172	0
1	L	306/309 (99%)	-0.05	4 (1%) 77 76	36, 63, 112, 186	0
1	M	306/309 (99%)	0.07	8 (2%) 56 54	42, 73, 142, 206	0
1	N	306/309 (99%)	0.05	9 (2%) 51 50	44, 82, 146, 189	0
1	O	306/309 (99%)	0.15	12 (3%) 39 38	59, 96, 163, 215	0
1	P	306/309 (99%)	0.27	24 (7%) 13 14	61, 107, 170, 202	0
All	All	4896/4944 (99%)	0.03	129 (2%) 56 54	34, 82, 146, 294	0

All (129) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	245	THR	11.6
1	M	288	ALA	9.4
1	L	243	LYS	7.3
1	O	286	PHE	6.9
1	A	244	ALA	6.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	P	217	VAL	5.6
1	C	207	ASP	5.0
1	N	288	ALA	5.0
1	O	248	THR	4.9
1	M	290	THR	4.8
1	L	286	PHE	4.5
1	F	195	THR	4.4
1	P	195	THR	4.4
1	I	286	PHE	4.2
1	M	243	LYS	4.0
1	P	228	LEU	4.0
1	P	226	VAL	3.9
1	M	284	THR	3.8
1	A	164	PRO	3.8
1	B	207	ASP	3.7
1	B	247	THR	3.7
1	I	248	THR	3.7
1	C	183	PRO	3.6
1	N	207	ASP	3.5
1	P	245	THR	3.5
1	J	243	LYS	3.4
1	N	245	THR	3.4
1	P	146	ILE	3.4
1	B	46	VAL	3.4
1	C	243	LYS	3.4
1	A	286	PHE	3.3
1	K	283	VAL	3.3
1	B	298	VAL	3.3
1	P	197	TYR	3.3
1	N	244	ALA	3.2
1	E	286	PHE	3.2
1	B	45	ALA	3.1
1	A	289	GLN	3.1
1	E	288	ALA	3.1
1	D	22	PRO	3.1
1	P	287	GLY	3.0
1	P	180	LEU	3.0
1	A	290	THR	3.0
1	A	228	LEU	3.0
1	M	245	THR	3.0
1	O	289	GLN	3.0
1	B	286	PHE	2.9

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	I	244	ALA	2.9
1	O	288	ALA	2.9
1	M	244	ALA	2.9
1	P	244	ALA	2.9
1	B	56	GLY	2.9
1	G	205	ALA	2.9
1	E	285	ARG	2.9
1	A	170	LEU	2.9
1	I	225	GLY	2.8
1	A	167	ALA	2.8
1	L	244	ALA	2.8
1	D	161	ILE	2.8
1	P	212	LYS	2.7
1	B	287	GLY	2.7
1	C	36	ILE	2.7
1	O	245	THR	2.7
1	E	181	ILE	2.7
1	I	8	GLY	2.7
1	N	243	LYS	2.7
1	I	247	THR	2.7
1	B	243	LYS	2.7
1	A	196	VAL	2.7
1	P	286	PHE	2.6
1	P	27	THR	2.6
1	A	243	LYS	2.6
1	N	246	ASP	2.6
1	N	218	ILE	2.6
1	P	26	GLU	2.6
1	J	244	ALA	2.5
1	A	248	THR	2.5
1	P	284	THR	2.5
1	P	162	LEU	2.5
1	C	182	THR	2.5
1	A	285	ARG	2.5
1	I	249	ALA	2.5
1	B	96	MET	2.5
1	K	243	LYS	2.4
1	D	62	GLY	2.4
1	A	180	LEU	2.4
1	H	245	THR	2.4
1	H	244	ALA	2.4
1	E	244	ALA	2.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	M	247	THR	2.4
1	G	242	VAL	2.3
1	F	205	ALA	2.3
1	F	194	ILE	2.3
1	G	26	GLU	2.3
1	A	212	LYS	2.3
1	P	182	THR	2.3
1	O	228	LEU	2.3
1	N	182	THR	2.3
1	P	218	ILE	2.3
1	C	195	THR	2.2
1	K	86	LEU	2.2
1	M	291	SER	2.2
1	O	253	THR	2.2
1	G	75	LYS	2.2
1	P	235	GLN	2.2
1	E	289	GLN	2.2
1	P	181	ILE	2.2
1	P	237	ILE	2.2
1	O	161	ILE	2.2
1	E	284	THR	2.1
1	A	59	ALA	2.1
1	A	194	ILE	2.1
1	O	103	GLY	2.1
1	B	48	ALA	2.1
1	K	227	TRP	2.1
1	K	290	THR	2.1
1	O	107	ILE	2.1
1	G	252	ASP	2.1
1	P	62	GLY	2.1
1	O	35	VAL	2.1
1	P	61	VAL	2.1
1	P	196	VAL	2.1
1	F	209	LEU	2.0
1	O	287	GLY	2.0
1	B	246	ASP	2.0
1	A	197	TYR	2.0
1	L	290	THR	2.0
1	N	195	THR	2.0
1	C	16	LEU	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.