Full wwPDB X-ray Structure Validation Report ⓘ

Sep 16, 2023 – 08:22 PM EDT

PDB ID	:	4WS9
Title	:	Crystal structure of sMAT N159G from Sulfolobus solfataricus
Authors	:	Wang, F.; Brady, E.L.; Singh, S.; Clinger, J.A.; Huber, T.D.; Thorson, J.S.; Phillips Jr., G.N.
Deposited on	:	2014-10-26
Resolution	:	2.80 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

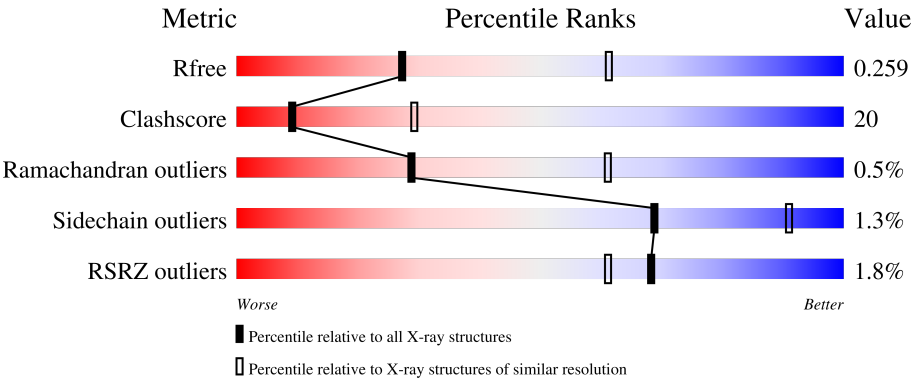
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	413	59% 35% • 5%
1	B	413	57% 37% • 5%
1	C	413	64% 30% • 5%
1	D	413	55% 39% • 5%
1	E	413	55% 39% 5%

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Mol	Chain	Length	Quality of chain
1	F	413	2% 57% 37% • 5%
1	G	413	2% 66% 27% • 5%
1	H	413	3% 54% 38% • 5%
1	I	413	2% 65% 29% • 5%
1	J	413	2% 59% 35% 5%
1	K	413	% 62% 32% • 5%
1	L	413	2% 57% 37% • 5%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PO4	A	502	-	-	X	-
2	PO4	D	502	-	-	-	X
2	PO4	G	501	-	-	X	-
2	PO4	I	502	-	-	-	X
2	PO4	L	501	-	-	X	-

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 37566 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 S-adenosylmethionine synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	391	Total	C	N	O	S	0	0	0
			3043	1928	523	585	7			
1	B	392	Total	C	N	O	S	0	0	0
			3046	1930	524	586	6			
1	C	391	Total	C	N	O	S	0	0	0
			3043	1928	523	585	7			
1	D	392	Total	C	N	O	S	0	0	0
			3046	1930	524	586	6			
1	E	391	Total	C	N	O	S	0	0	0
			3043	1928	523	585	7			
1	F	392	Total	C	N	O	S	0	0	0
			3046	1930	524	586	6			
1	G	391	Total	C	N	O	S	0	0	0
			3043	1928	523	585	7			
1	H	392	Total	C	N	O	S	0	0	0
			3046	1930	524	586	6			
1	I	391	Total	C	N	O	S	0	0	0
			3043	1928	523	585	7			
1	J	392	Total	C	N	O	S	0	0	0
			3046	1930	524	586	6			
1	K	391	Total	C	N	O	S	0	0	0
			3043	1928	523	585	7			
1	L	392	Total	C	N	O	S	0	0	0
			3046	1930	524	586	6			

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	GLY	-	expression tag	UNP Q980S9
A	-7	SER	-	expression tag	UNP Q980S9
A	-6	HIS	-	expression tag	UNP Q980S9
A	-5	MET	-	expression tag	UNP Q980S9
A	-4	PHE	-	expression tag	UNP Q980S9

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLU	-	expression tag	UNP Q980S9
A	-2	GLU	-	expression tag	UNP Q980S9
A	-1	PRO	-	expression tag	UNP Q980S9
A	0	ILE	-	expression tag	UNP Q980S9
A	159	GLY	ASN	conflict	UNP Q980S9
B	-8	GLY	-	expression tag	UNP Q980S9
B	-7	SER	-	expression tag	UNP Q980S9
B	-6	HIS	-	expression tag	UNP Q980S9
B	-5	MET	-	expression tag	UNP Q980S9
B	-4	PHE	-	expression tag	UNP Q980S9
B	-3	GLU	-	expression tag	UNP Q980S9
B	-2	GLU	-	expression tag	UNP Q980S9
B	-1	PRO	-	expression tag	UNP Q980S9
B	0	ILE	-	expression tag	UNP Q980S9
B	159	GLY	ASN	conflict	UNP Q980S9
C	-8	GLY	-	expression tag	UNP Q980S9
C	-7	SER	-	expression tag	UNP Q980S9
C	-6	HIS	-	expression tag	UNP Q980S9
C	-5	MET	-	expression tag	UNP Q980S9
C	-4	PHE	-	expression tag	UNP Q980S9
C	-3	GLU	-	expression tag	UNP Q980S9
C	-2	GLU	-	expression tag	UNP Q980S9
C	-1	PRO	-	expression tag	UNP Q980S9
C	0	ILE	-	expression tag	UNP Q980S9
C	159	GLY	ASN	conflict	UNP Q980S9
D	-8	GLY	-	expression tag	UNP Q980S9
D	-7	SER	-	expression tag	UNP Q980S9
D	-6	HIS	-	expression tag	UNP Q980S9
D	-5	MET	-	expression tag	UNP Q980S9
D	-4	PHE	-	expression tag	UNP Q980S9
D	-3	GLU	-	expression tag	UNP Q980S9
D	-2	GLU	-	expression tag	UNP Q980S9
D	-1	PRO	-	expression tag	UNP Q980S9
D	0	ILE	-	expression tag	UNP Q980S9
D	159	GLY	ASN	conflict	UNP Q980S9
E	-8	GLY	-	expression tag	UNP Q980S9
E	-7	SER	-	expression tag	UNP Q980S9
E	-6	HIS	-	expression tag	UNP Q980S9
E	-5	MET	-	expression tag	UNP Q980S9
E	-4	PHE	-	expression tag	UNP Q980S9
E	-3	GLU	-	expression tag	UNP Q980S9
E	-2	GLU	-	expression tag	UNP Q980S9

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-1	PRO	-	expression tag	UNP Q980S9
E	0	ILE	-	expression tag	UNP Q980S9
E	159	GLY	ASN	conflict	UNP Q980S9
F	-8	GLY	-	expression tag	UNP Q980S9
F	-7	SER	-	expression tag	UNP Q980S9
F	-6	HIS	-	expression tag	UNP Q980S9
F	-5	MET	-	expression tag	UNP Q980S9
F	-4	PHE	-	expression tag	UNP Q980S9
F	-3	GLU	-	expression tag	UNP Q980S9
F	-2	GLU	-	expression tag	UNP Q980S9
F	-1	PRO	-	expression tag	UNP Q980S9
F	0	ILE	-	expression tag	UNP Q980S9
F	159	GLY	ASN	conflict	UNP Q980S9
G	-8	GLY	-	expression tag	UNP Q980S9
G	-7	SER	-	expression tag	UNP Q980S9
G	-6	HIS	-	expression tag	UNP Q980S9
G	-5	MET	-	expression tag	UNP Q980S9
G	-4	PHE	-	expression tag	UNP Q980S9
G	-3	GLU	-	expression tag	UNP Q980S9
G	-2	GLU	-	expression tag	UNP Q980S9
G	-1	PRO	-	expression tag	UNP Q980S9
G	0	ILE	-	expression tag	UNP Q980S9
G	159	GLY	ASN	conflict	UNP Q980S9
H	-8	GLY	-	expression tag	UNP Q980S9
H	-7	SER	-	expression tag	UNP Q980S9
H	-6	HIS	-	expression tag	UNP Q980S9
H	-5	MET	-	expression tag	UNP Q980S9
H	-4	PHE	-	expression tag	UNP Q980S9
H	-3	GLU	-	expression tag	UNP Q980S9
H	-2	GLU	-	expression tag	UNP Q980S9
H	-1	PRO	-	expression tag	UNP Q980S9
H	0	ILE	-	expression tag	UNP Q980S9
H	159	GLY	ASN	conflict	UNP Q980S9
I	-8	GLY	-	expression tag	UNP Q980S9
I	-7	SER	-	expression tag	UNP Q980S9
I	-6	HIS	-	expression tag	UNP Q980S9
I	-5	MET	-	expression tag	UNP Q980S9
I	-4	PHE	-	expression tag	UNP Q980S9
I	-3	GLU	-	expression tag	UNP Q980S9
I	-2	GLU	-	expression tag	UNP Q980S9
I	-1	PRO	-	expression tag	UNP Q980S9
I	0	ILE	-	expression tag	UNP Q980S9

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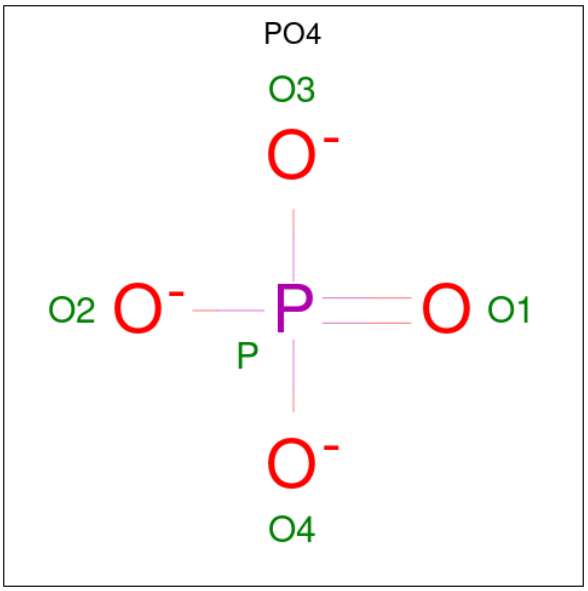
Chain	Residue	Modelled	Actual	Comment	Reference
I	159	GLY	ASN	conflict	UNP Q980S9
J	-8	GLY	-	expression tag	UNP Q980S9
J	-7	SER	-	expression tag	UNP Q980S9
J	-6	HIS	-	expression tag	UNP Q980S9
J	-5	MET	-	expression tag	UNP Q980S9
J	-4	PHE	-	expression tag	UNP Q980S9
J	-3	GLU	-	expression tag	UNP Q980S9
J	-2	GLU	-	expression tag	UNP Q980S9
J	-1	PRO	-	expression tag	UNP Q980S9
J	0	ILE	-	expression tag	UNP Q980S9
J	159	GLY	ASN	conflict	UNP Q980S9
K	-8	GLY	-	expression tag	UNP Q980S9
K	-7	SER	-	expression tag	UNP Q980S9
K	-6	HIS	-	expression tag	UNP Q980S9
K	-5	MET	-	expression tag	UNP Q980S9
K	-4	PHE	-	expression tag	UNP Q980S9
K	-3	GLU	-	expression tag	UNP Q980S9
K	-2	GLU	-	expression tag	UNP Q980S9
K	-1	PRO	-	expression tag	UNP Q980S9
K	0	ILE	-	expression tag	UNP Q980S9
K	159	GLY	ASN	conflict	UNP Q980S9
L	-8	GLY	-	expression tag	UNP Q980S9
L	-7	SER	-	expression tag	UNP Q980S9
L	-6	HIS	-	expression tag	UNP Q980S9
L	-5	MET	-	expression tag	UNP Q980S9
L	-4	PHE	-	expression tag	UNP Q980S9
L	-3	GLU	-	expression tag	UNP Q980S9
L	-2	GLU	-	expression tag	UNP Q980S9
L	-1	PRO	-	expression tag	UNP Q980S9
L	0	ILE	-	expression tag	UNP Q980S9
L	159	GLY	ASN	conflict	UNP Q980S9

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O P 5 4 1	0	0
2	A	1	Total O P 5 4 1	0	0
2	B	1	Total O P 5 4 1	0	0
2	C	1	Total O P 5 4 1	0	0
2	D	1	Total O P 5 4 1	0	0
2	D	1	Total O P 5 4 1	0	0
2	E	1	Total O P 5 4 1	0	0
2	E	1	Total O P 5 4 1	0	0
2	F	1	Total O P 5 4 1	0	0
2	G	1	Total O P 5 4 1	0	0
2	G	1	Total O P 5 4 1	0	0
2	H	1	Total O P 5 4 1	0	0
2	I	1	Total O P 5 4 1	0	0
2	I	1	Total O P 5 4 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	J	1	Total O P 5 4 1	0	0
2	K	1	Total O P 5 4 1	0	0
2	K	1	Total O P 5 4 1	0	0
2	L	1	Total O P 5 4 1	0	0

- Molecule 3 is water.

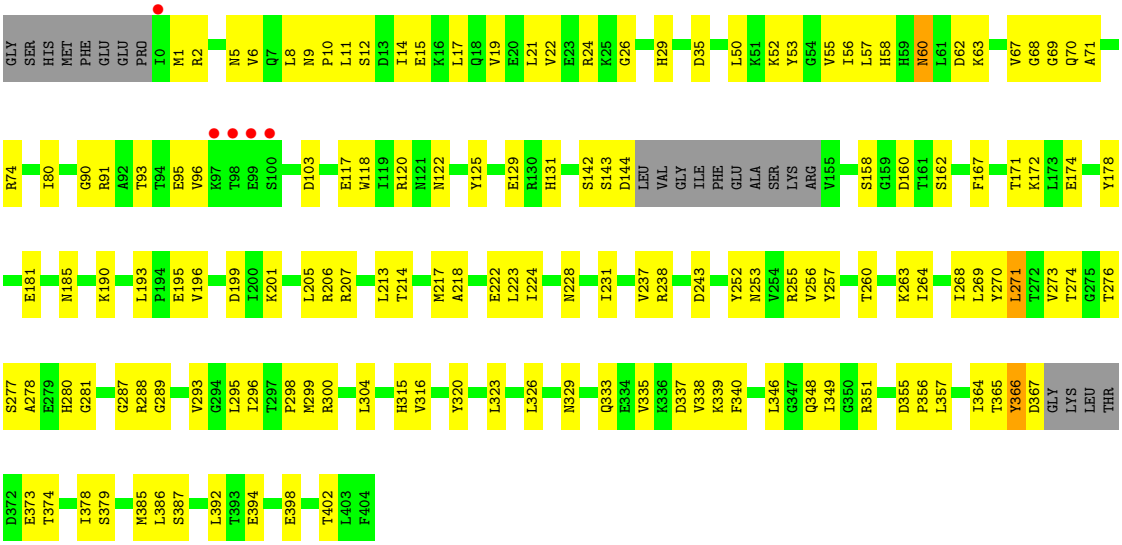
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	111	Total O 111 111	0	0
3	B	96	Total O 96 96	0	0
3	C	84	Total O 84 84	0	0
3	D	82	Total O 82 82	0	0
3	E	123	Total O 123 123	0	0
3	F	110	Total O 110 110	0	0
3	G	45	Total O 45 45	0	0
3	H	74	Total O 74 74	0	0
3	I	31	Total O 31 31	0	0
3	J	43	Total O 43 43	0	0
3	K	72	Total O 72 72	0	0
3	L	71	Total O 71 71	0	0

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.

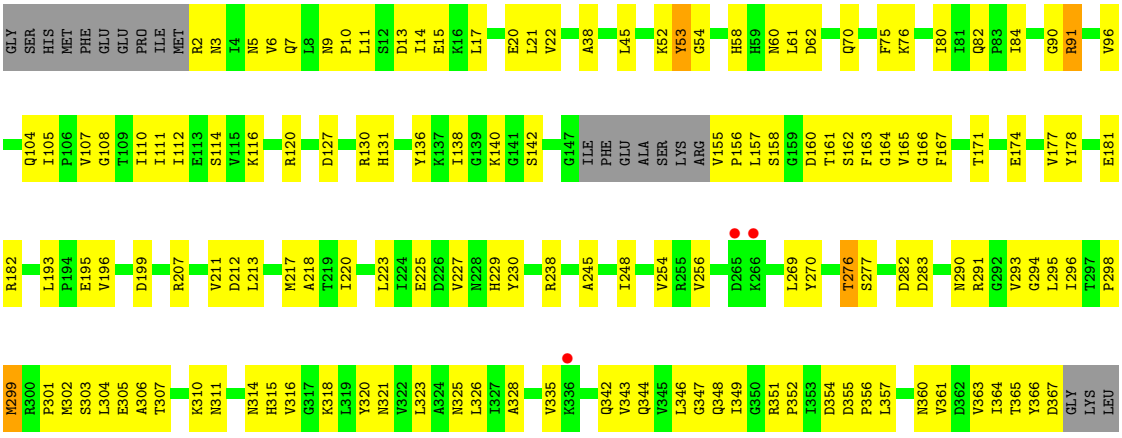
• Molecule 1: S-adenosylmethionine synthase

Chain A:



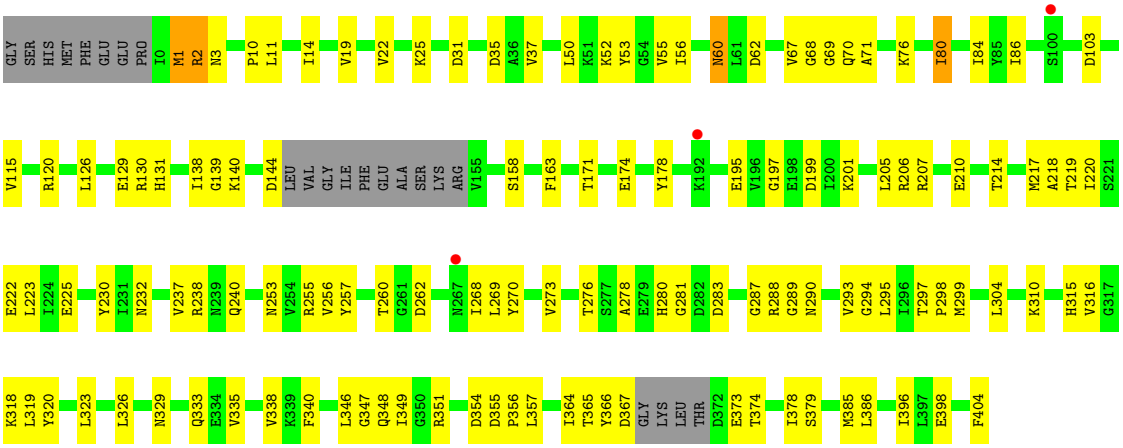
• Molecule 1: S-adenosylmethionine synthase

Chain B:



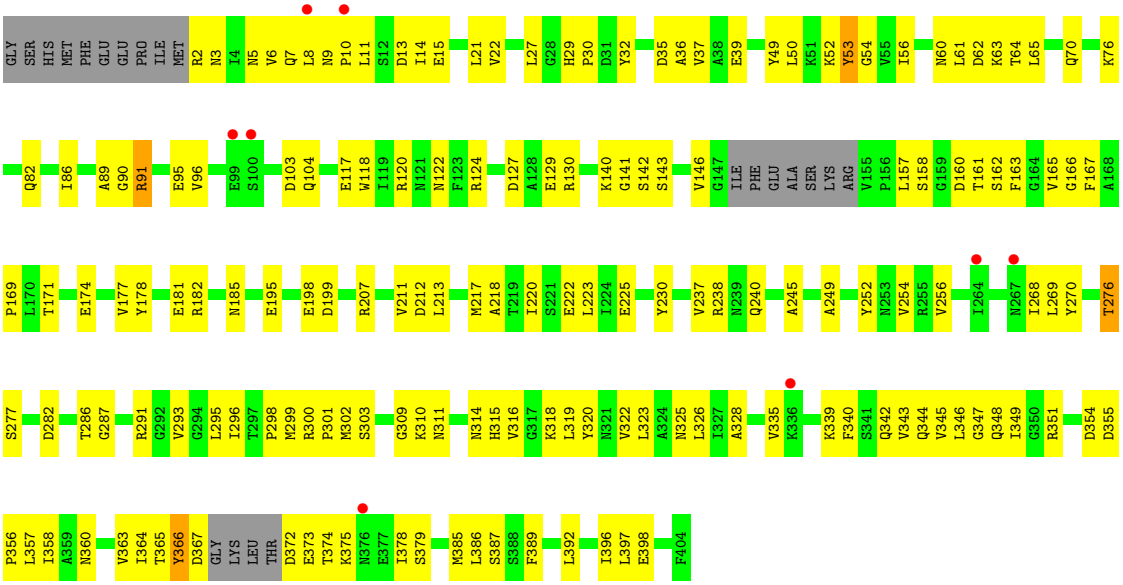
• Molecule 1: S-adenosylmethionine synthase

Chain C:



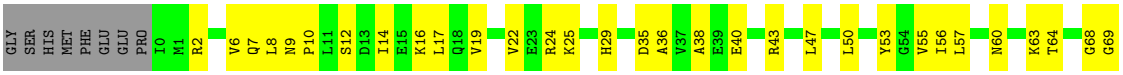
• Molecule 1: S-adenosylmethionine synthase

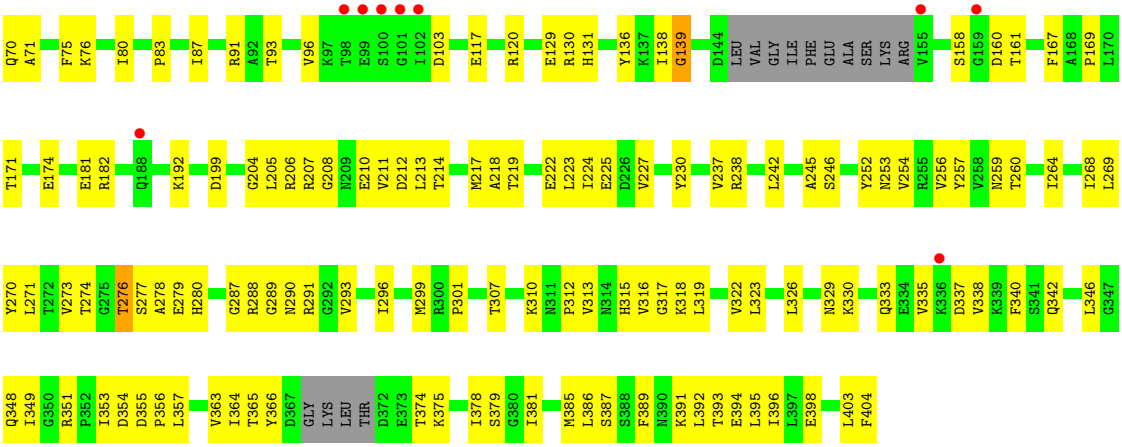
Chain D:



• Molecule 1: S-adenosylmethionine synthase

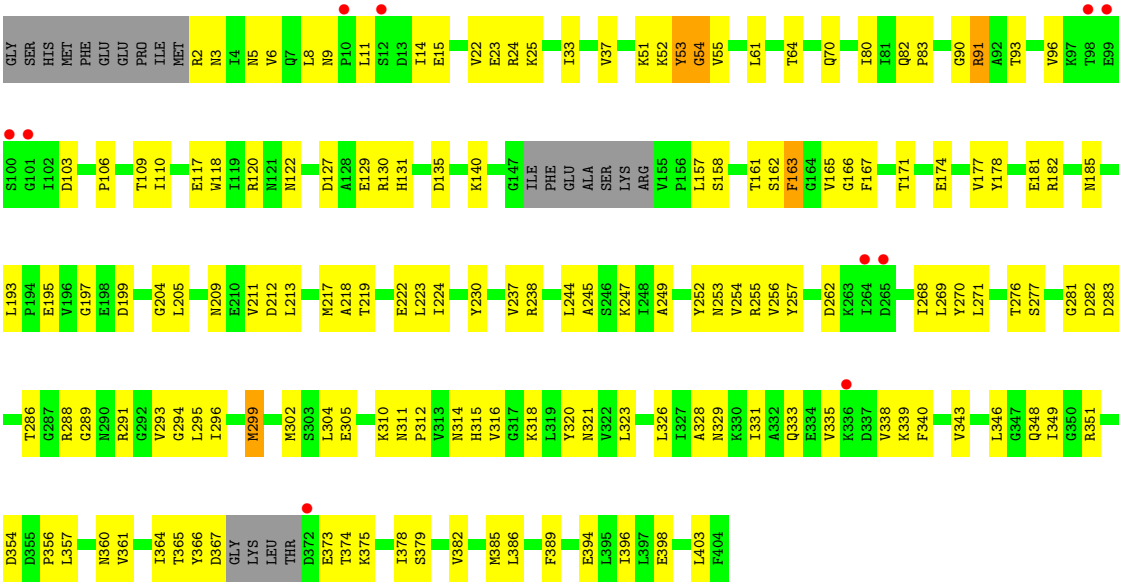
Chain E:





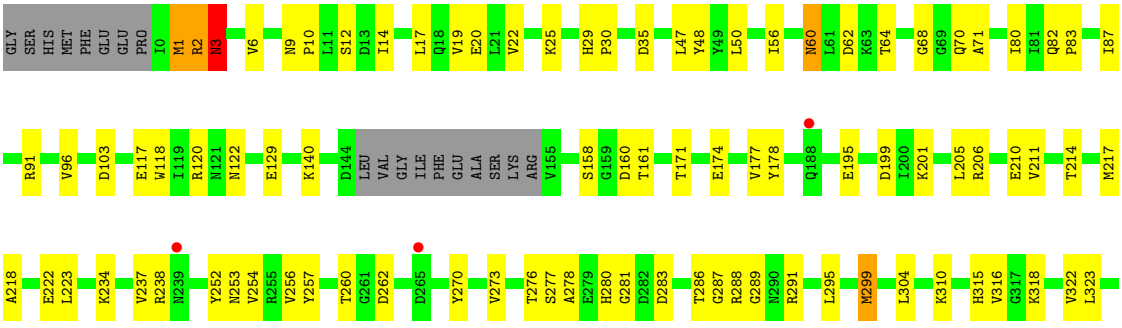
• Molecule 1: S-adenosylmethionine synthase

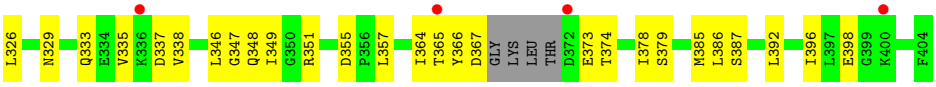
Chain F:



• Molecule 1: S-adenosylmethionine synthase

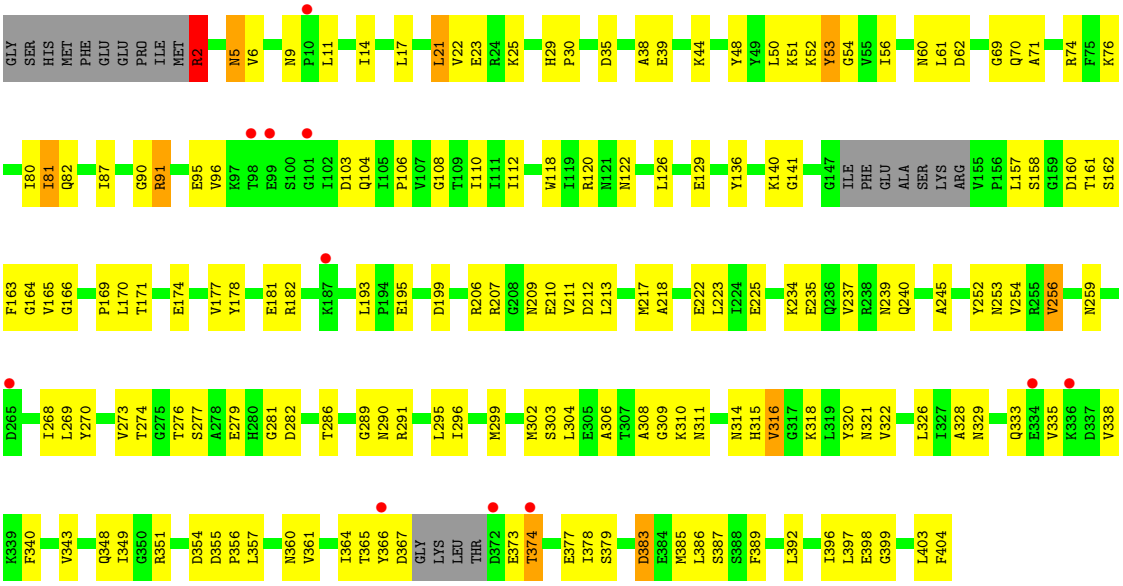
Chain G:





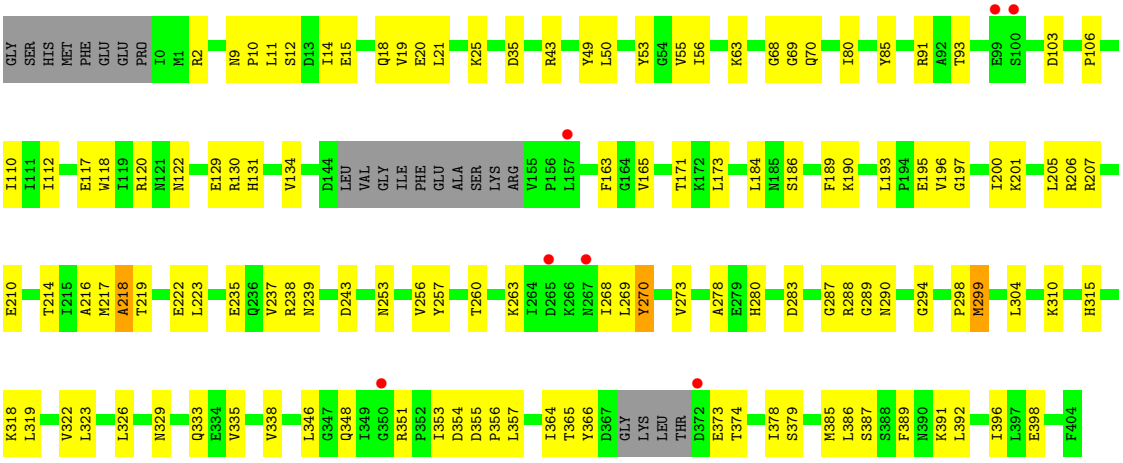
• Molecule 1: S-adenosylmethionine synthase

Chain H:



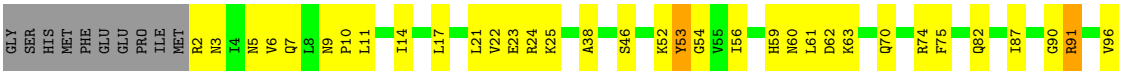
• Molecule 1: S-adenosylmethionine synthase

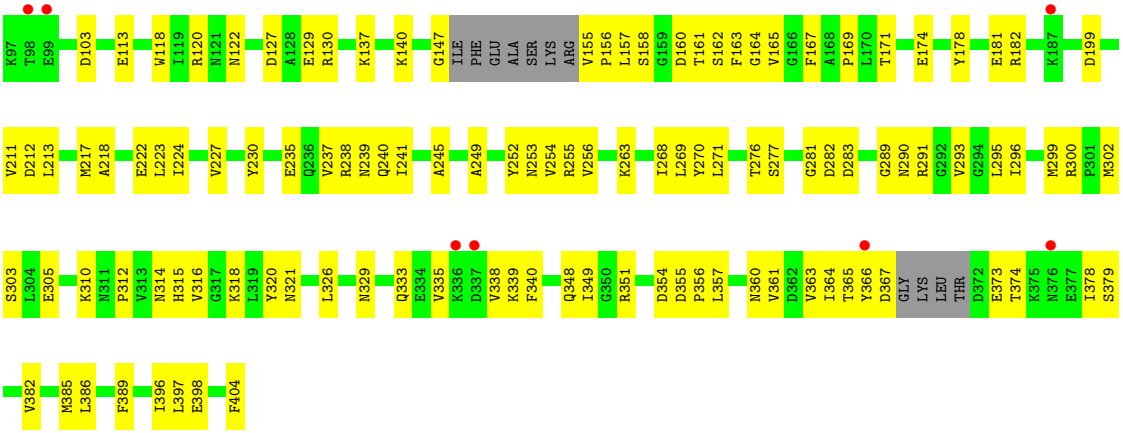
Chain I:



• Molecule 1: S-adenosylmethionine synthase

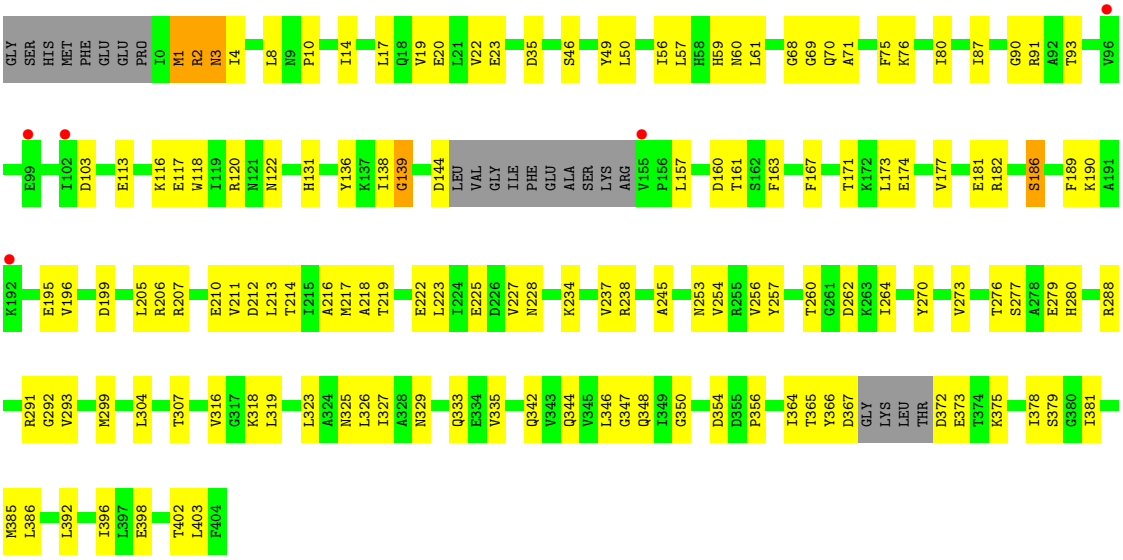
Chain J:





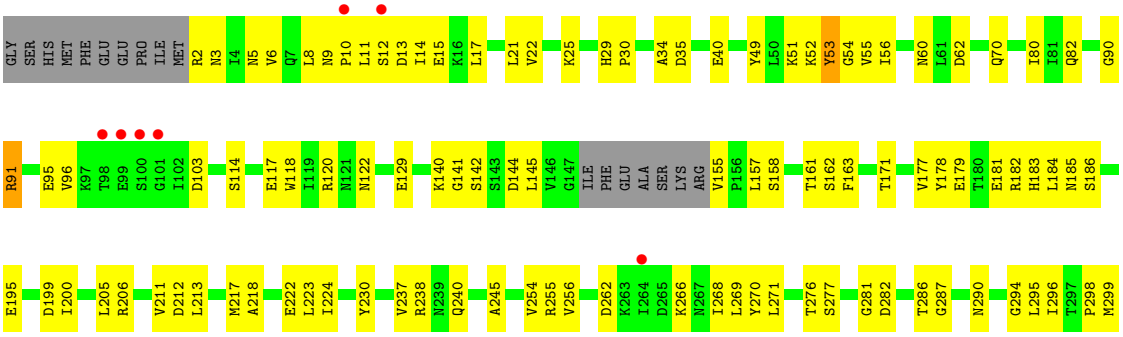
• Molecule 1: S-adenosylmethionine synthase

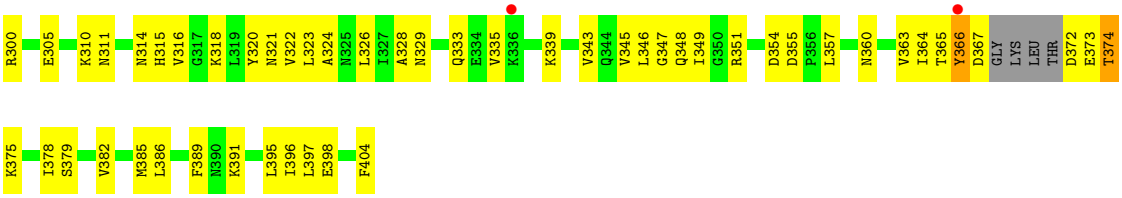
Chain K:



• Molecule 1: S-adenosylmethionine synthase

Chain L:




R300
E305
K310
N311
N314
H315
V316
G317
K318
L319
Y320
N321
V322
L323
A324
N325
L326
I327
A328
N329
Q333
E334
V335
K336
K339
V343
Q344
V345
L346
G347
Q348
I349
G350
R351
D354
D355
P356
L357
N360
V363
I364
T365
Y366
D367
GLY
LYS
LEU
THR
D372
E373
T374
K375
I378
S379
V382
M385
L386
F389
N390
K391
L395
I396
L397
E398
F404

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	74.72Å 289.20Å 174.69Å 90.00° 99.85° 90.00°	Depositor
Resolution (Å)	30.00 – 2.80 30.01 – 2.80	Depositor EDS
% Data completeness (in resolution range)	75.6 (30.00-2.80) 67.1 (30.01-2.80)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	0.16	Depositor
$< I/\sigma(I) >$ [1]	1.15 (at 2.80Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.221 , 0.256 0.226 , 0.259	Depositor DCC
R_{free} test set	1530 reflections (1.14%)	wwPDB-VP
Wilson B-factor (Å^2)	37.8	Xtriage
Anisotropy	1.226	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 42.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.031 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	37566	wwPDB-VP
Average B, all atoms (Å^2)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.52% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PO4

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	0.77	0/3086	0.83	2/4172 (0.0%)
1	B	0.73	0/3089	0.79	0/4177
1	C	0.71	0/3086	0.79	1/4172 (0.0%)
1	D	0.70	0/3089	0.80	0/4177
1	E	0.84	0/3086	0.83	2/4172 (0.0%)
1	F	0.75	0/3089	0.81	2/4177 (0.0%)
1	G	0.70	0/3086	0.77	0/4172
1	H	0.82	1/3089 (0.0%)	0.89	5/4177 (0.1%)
1	I	0.70	2/3086 (0.1%)	0.81	4/4172 (0.1%)
1	J	0.71	0/3089	0.79	1/4177 (0.0%)
1	K	0.73	0/3086	0.80	1/4172 (0.0%)
1	L	0.69	0/3089	0.77	0/4177
All	All	0.74	3/37050 (0.0%)	0.81	18/50094 (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	C	0	1
1	G	0	1
1	K	0	1
All	All	0	3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	270	TYR	CE2-CZ	-7.73	1.28	1.38
1	H	2	ARG	CZ-NH1	-7.60	1.23	1.33
1	I	218	ALA	CA-CB	-5.45	1.41	1.52

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	2	ARG	NE-CZ-NH2	11.29	125.94	120.30
1	I	270	TYR	CB-CG-CD2	-7.53	116.48	121.00
1	I	270	TYR	CD1-CE1-CZ	-7.14	113.37	119.80
1	H	2	ARG	CD-NE-CZ	6.43	132.60	123.60
1	I	218	ALA	N-CA-C	6.13	127.54	111.00
1	A	8	LEU	CA-CB-CG	6.04	129.18	115.30
1	F	257	TYR	CA-CB-CG	5.68	124.19	113.40
1	I	270	TYR	CB-CG-CD1	5.66	124.40	121.00
1	H	256	VAL	CG1-CB-CG2	-5.65	101.86	110.90
1	E	288	ARG	NE-CZ-NH1	-5.51	117.55	120.30
1	E	139	GLY	N-CA-C	-5.43	99.51	113.10
1	A	271	LEU	CA-CB-CG	5.40	127.73	115.30
1	H	81	ILE	CG1-CB-CG2	-5.35	99.62	111.40
1	F	8	LEU	CA-CB-CG	5.24	127.35	115.30
1	K	139	GLY	N-CA-C	-5.17	100.18	113.10
1	J	163	PHE	N-CA-CB	-5.14	101.35	110.60
1	H	21	LEU	CB-CG-CD1	-5.07	102.39	111.00
1	C	80	ILE	CG1-CB-CG2	-5.01	100.38	111.40

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	1	MET	Peptide
1	G	1	MET	Peptide
1	K	1	MET	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	3043	0	3119	149	0
1	B	3046	0	3119	140	0
1	C	3043	0	3119	114	0
1	D	3046	0	3119	158	0
1	E	3043	0	3119	147	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	3046	0	3119	154	0
1	G	3043	0	3119	96	0
1	H	3046	0	3119	146	0
1	I	3043	0	3119	102	0
1	J	3046	0	3119	124	0
1	K	3043	0	3119	111	0
1	L	3046	0	3119	144	0
2	A	10	0	0	3	0
2	B	5	0	0	0	0
2	C	5	0	0	1	0
2	D	10	0	0	1	0
2	E	10	0	0	0	0
2	F	5	0	0	1	0
2	G	10	0	0	2	0
2	H	5	0	0	0	0
2	I	10	0	0	0	0
2	J	5	0	0	1	0
2	K	10	0	0	0	0
2	L	5	0	0	2	0
3	A	111	0	0	45	0
3	B	96	0	0	36	0
3	C	84	0	0	24	0
3	D	82	0	0	36	0
3	E	123	0	0	33	0
3	F	110	0	0	35	0
3	G	45	0	0	9	0
3	H	74	0	0	29	0
3	I	31	0	0	6	0
3	J	43	0	0	13	0
3	K	72	0	0	22	0
3	L	71	0	0	28	0
All	All	37566	0	37428	1483	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 20.

All (1483) 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:I:214:THR:HG21	1:J:161:THR:HG21	1.43	1.00
1:B:310:LYS:HB2	1:B:318:LYS:HD2	1.45	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:214:THR:HG21	1:H:161:THR:HG21	1.48	0.95
1:C:140:LYS:NZ	3:C:657:HOH:O	2.00	0.93
1:B:90:GLY:O	1:B:91:ARG:NH1	2.04	0.90
1:J:14:ILE:HD11	1:J:171:THR:HG21	1.55	0.89
1:K:318:LYS:HE2	1:K:396:ILE:HD13	1.55	0.88
1:K:71:ALA:H	1:K:280:HIS:HD2	1.21	0.87
1:A:214:THR:HG21	1:B:161:THR:HG21	1.56	0.87
1:D:90:GLY:O	1:D:91:ARG:NH1	2.07	0.87
1:A:26:GLY:HA2	3:A:640:HOH:O	1.74	0.87
1:J:90:GLY:O	1:J:91:ARG:NH1	2.08	0.86
1:L:158:SER:OG	1:L:348:GLN:O	1.94	0.84
1:L:90:GLY:O	1:L:91:ARG:NH1	2.11	0.84
1:F:14:ILE:HD11	1:F:171:THR:HG21	1.59	0.83
1:I:205:LEU:HD23	1:J:357:LEU:HD22	1.61	0.83
1:A:71:ALA:H	1:A:280:HIS:HD2	1.27	0.83
1:D:60:ASN:OD1	3:D:604:HOH:O	1.97	0.82
1:C:14:ILE:HD11	1:C:171:THR:HG21	1.61	0.82
1:K:189:PHE:HB3	3:K:670:HOH:O	1.78	0.82
1:J:326:LEU:HB3	1:J:385:MET:HE1	1.62	0.81
1:K:144:ASP:OD1	3:K:640:HOH:O	1.97	0.81
1:E:68:GLY:O	1:F:91:ARG:NH2	2.12	0.81
1:C:201:LYS:NZ	1:D:160:ASP:OD2	2.14	0.81
1:H:245:ALA:HB1	1:H:254:VAL:HG21	1.62	0.81
1:F:158:SER:OG	1:F:348:GLN:O	1.98	0.80
1:A:364:ILE:O	3:A:650:HOH:O	1.98	0.80
1:B:211:VAL:HB	1:B:254:VAL:HG12	1.63	0.80
1:L:60:ASN:OD1	3:L:603:HOH:O	1.99	0.80
1:D:335:VAL:HG21	1:D:378:ILE:HG22	1.64	0.80
1:D:372:ASP:N	3:D:638:HOH:O	2.13	0.80
1:K:50:LEU:HD13	1:K:56:ILE:HG13	1.64	0.79
1:E:214:THR:HG21	1:F:161:THR:HG21	1.63	0.79
1:K:234:LYS:NZ	1:K:262:ASP:OD2	2.14	0.79
1:F:90:GLY:O	1:F:91:ARG:NH1	2.15	0.79
1:A:117:GLU:OE1	1:A:120:ARG:NH1	2.15	0.79
1:J:158:SER:OG	1:J:348:GLN:O	2.00	0.78
1:A:14:ILE:HD11	1:A:171:THR:HG21	1.64	0.78
1:L:52:LYS:O	1:L:54:GLY:N	2.17	0.78
1:I:197:GLY:N	1:I:218:ALA:O	2.14	0.78
1:B:335:VAL:HG21	1:B:378:ILE:HG22	1.66	0.78
1:G:117:GLU:OE1	1:G:120:ARG:NH1	2.16	0.78
1:K:214:THR:HG21	1:L:161:THR:HG21	1.65	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:335:VAL:HG21	1:G:378:ILE:HG22	1.66	0.77
1:D:14:ILE:HD11	1:D:171:THR:HG21	1.65	0.77
1:G:60:ASN:ND2	3:G:626:HOH:O	2.17	0.77
1:L:14:ILE:HD11	1:L:171:THR:HG21	1.65	0.77
1:B:14:ILE:HD11	1:B:171:THR:HG21	1.65	0.77
1:I:273:VAL:O	3:I:615:HOH:O	2.03	0.77
1:K:205:LEU:HD23	1:L:357:LEU:HD22	1.66	0.77
1:K:398:GLU:N	1:K:398:GLU:OE1	2.18	0.77
1:L:213:LEU:HB3	1:L:256:VAL:HG12	1.67	0.77
1:L:40:GLU:O	3:L:667:HOH:O	2.02	0.76
1:J:245:ALA:HB1	1:J:254:VAL:HG21	1.67	0.76
1:H:304:LEU:O	3:H:669:HOH:O	2.02	0.76
1:C:214:THR:HG21	1:D:161:THR:HG21	1.68	0.76
1:L:290:ASN:ND2	1:L:404:PHE:O	2.14	0.76
1:H:326:LEU:HB3	1:H:385:MET:HE1	1.68	0.75
1:J:398:GLU:OE1	1:J:398:GLU:N	2.19	0.75
1:D:50:LEU:HD13	1:D:56:ILE:HG13	1.68	0.75
1:F:321:ASN:ND2	3:F:656:HOH:O	2.19	0.75
1:K:117:GLU:OE1	1:K:120:ARG:NH1	2.18	0.75
1:K:228:ASN:HB3	3:K:606:HOH:O	1.87	0.75
1:H:213:LEU:HB3	1:H:256:VAL:HG12	1.67	0.75
1:C:217:MET:HE3	1:C:237:VAL:HG11	1.68	0.75
1:C:71:ALA:H	1:C:280:HIS:HD2	1.32	0.75
1:H:30:PRO:HG3	3:H:664:HOH:O	1.86	0.75
1:H:178:TYR:HB2	1:H:295:LEU:HD21	1.68	0.75
1:J:53:TYR:CE1	1:J:96:VAL:HG21	2.22	0.75
1:J:60:ASN:ND2	3:J:621:HOH:O	2.19	0.74
1:H:335:VAL:HG21	1:H:378:ILE:HG22	1.68	0.74
1:A:335:VAL:HG21	1:A:378:ILE:HG22	1.67	0.74
1:A:367:ASP:O	3:A:649:HOH:O	2.04	0.74
1:B:155:VAL:HG23	3:B:641:HOH:O	1.86	0.74
1:H:310:LYS:HB2	1:H:318:LYS:HD2	1.69	0.74
1:E:335:VAL:HG21	1:E:378:ILE:HG22	1.70	0.74
1:L:9:ASN:O	3:L:663:HOH:O	2.06	0.73
1:A:60:ASN:ND2	1:A:62:ASP:OD1	2.21	0.73
1:C:197:GLY:N	1:C:218:ALA:O	2.15	0.73
1:I:351:ARG:NE	1:I:355:ASP:O	2.20	0.73
1:L:335:VAL:HG21	1:L:378:ILE:HG22	1.70	0.73
1:C:318:LYS:HE2	1:C:396:ILE:HD13	1.69	0.73
1:G:14:ILE:HD11	1:G:171:THR:HG21	1.71	0.73
1:A:300:ARG:NH2	3:A:652:HOH:O	2.22	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:502:PO4:O1	3:A:702:HOH:O	2.06	0.72
1:D:118:TRP:O	1:D:122:ASN:ND2	2.20	0.72
1:L:13:ASP:O	3:L:615:HOH:O	2.07	0.72
1:J:52:LYS:O	1:J:54:GLY:N	2.23	0.72
1:K:71:ALA:H	1:K:280:HIS:CD2	2.07	0.72
1:D:310:LYS:HB2	1:D:318:LYS:HD2	1.71	0.72
1:L:157:LEU:O	1:L:314:ASN:HB2	1.90	0.71
1:L:391:LYS:O	3:L:639:HOH:O	2.07	0.71
1:F:52:LYS:O	1:F:54:GLY:N	2.23	0.71
1:I:270:TYR:HD1	3:J:633:HOH:O	1.72	0.71
1:B:398:GLU:OE1	1:B:398:GLU:N	2.23	0.71
1:E:71:ALA:H	1:E:280:HIS:HD2	1.38	0.71
1:L:310:LYS:NZ	2:L:501:PO4:O3	2.23	0.71
1:K:61:LEU:N	3:K:662:HOH:O	2.22	0.71
1:E:398:GLU:OE1	1:E:398:GLU:N	2.23	0.71
1:D:143:SER:OG	3:D:669:HOH:O	2.09	0.71
1:G:71:ALA:H	1:G:280:HIS:HD2	1.39	0.71
1:K:113:GLU:OE1	3:K:661:HOH:O	2.09	0.71
1:L:372:ASP:N	1:L:375:LYS:HZ3	1.89	0.71
1:H:273:VAL:O	3:H:628:HOH:O	2.08	0.70
1:C:374:THR:HG21	3:C:632:HOH:O	1.91	0.70
1:K:14:ILE:HD11	1:K:171:THR:HG21	1.73	0.70
1:L:211:VAL:HB	1:L:254:VAL:HG12	1.72	0.70
1:A:144:ASP:OD2	3:A:638:HOH:O	2.10	0.70
1:E:287:GLY:O	3:E:650:HOH:O	2.08	0.70
1:H:14:ILE:HD11	1:H:171:THR:HG21	1.74	0.70
1:G:205:LEU:HD23	1:H:357:LEU:HD22	1.73	0.70
1:F:318:LYS:HE2	1:F:396:ILE:HD13	1.74	0.70
1:B:158:SER:OG	1:B:348:GLN:O	2.10	0.70
1:G:337:ASP:O	1:G:365:THR:OG1	2.09	0.70
1:B:321:ASN:ND2	3:B:632:HOH:O	2.23	0.70
1:E:211:VAL:HB	1:E:254:VAL:HG12	1.73	0.70
1:A:398:GLU:N	1:A:398:GLU:OE1	2.24	0.69
1:E:10:PRO:HA	1:E:364:ILE:HD11	1.74	0.69
1:F:398:GLU:N	1:F:398:GLU:OE1	2.24	0.69
1:H:290:ASN:ND2	1:H:404:PHE:O	2.24	0.69
1:A:238:ARG:HB2	1:A:256:VAL:HG23	1.74	0.69
1:C:255:ARG:NH1	3:C:623:HOH:O	2.25	0.69
1:E:204:GLY:O	3:E:721:HOH:O	2.09	0.69
1:F:211:VAL:HB	1:F:254:VAL:HG12	1.74	0.69
1:I:49:TYR:OH	1:I:93:THR:O	2.09	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:217:MET:HE3	1:I:237:VAL:HG11	1.74	0.69
1:J:178:TYR:HB2	1:J:295:LEU:HD21	1.73	0.69
1:F:135:ASP:OD1	3:F:700:HOH:O	2.09	0.69
1:J:310:LYS:HE2	1:J:315:HIS:CE1	2.27	0.69
1:G:365:THR:HG23	1:G:367:ASP:HB2	1.72	0.69
1:H:351:ARG:NE	1:H:355:ASP:O	2.26	0.69
1:F:348:GLN:N	3:F:687:HOH:O	2.24	0.69
1:B:107:VAL:HA	3:B:691:HOH:O	1.92	0.69
1:D:310:LYS:HE2	1:D:315:HIS:CE1	2.27	0.69
1:F:230:TYR:OH	1:F:262:ASP:OD2	2.09	0.69
1:F:310:LYS:HB2	1:F:318:LYS:HD2	1.73	0.69
1:H:306:ALA:O	1:H:310:LYS:NZ	2.20	0.69
1:A:346:LEU:HD11	1:B:21:LEU:HD11	1.74	0.69
1:F:24:ARG:HH21	1:F:182:ARG:HH11	1.40	0.69
1:H:310:LYS:HE2	1:H:315:HIS:CE1	2.28	0.68
1:H:60:ASN:ND2	3:H:603:HOH:O	2.02	0.68
2:A:502:PO4:O3	3:A:664:HOH:O	2.09	0.68
1:H:211:VAL:HB	1:H:254:VAL:HG12	1.75	0.68
1:I:326:LEU:HB3	1:I:385:MET:HE1	1.75	0.68
1:C:323:LEU:HD21	1:C:386:LEU:HD11	1.74	0.68
1:G:118:TRP:O	1:G:122:ASN:ND2	2.24	0.68
1:F:52:LYS:NZ	3:F:697:HOH:O	2.27	0.68
1:F:385:MET:HB2	3:F:705:HOH:O	1.92	0.68
1:F:351:ARG:HD3	3:F:687:HOH:O	1.93	0.68
1:K:325:ASN:HB3	3:K:655:HOH:O	1.93	0.68
1:B:293:VAL:O	3:B:695:HOH:O	2.12	0.68
1:C:35:ASP:OD1	1:C:287:GLY:N	2.25	0.67
1:D:344:GLN:O	3:D:662:HOH:O	2.12	0.67
1:E:14:ILE:HD11	1:E:171:THR:HG21	1.76	0.67
1:F:245:ALA:HB1	1:F:254:VAL:HG21	1.76	0.67
1:F:293:VAL:O	3:F:701:HOH:O	2.13	0.67
1:L:326:LEU:HB3	1:L:385:MET:HE1	1.76	0.67
1:L:398:GLU:OE1	1:L:398:GLU:N	2.28	0.67
1:K:10:PRO:HA	1:K:364:ILE:HD11	1.75	0.67
1:E:318:LYS:HE2	1:E:396:ILE:HD13	1.75	0.67
1:H:398:GLU:N	1:H:398:GLU:OE1	2.26	0.67
1:C:144:ASP:OD2	3:C:645:HOH:O	2.13	0.67
1:K:35:ASP:OD2	3:K:629:HOH:O	2.11	0.67
1:E:224:ILE:HG13	3:E:712:HOH:O	1.93	0.67
1:J:113:GLU:OE1	3:J:626:HOH:O	2.12	0.67
1:A:71:ALA:H	1:A:280:HIS:CD2	2.10	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:398:GLU:N	1:I:398:GLU:OE1	2.27	0.67
1:L:311:ASN:HB3	1:L:315:HIS:HB2	1.77	0.67
1:C:207:ARG:HE	1:D:5:ASN:HD22	1.42	0.67
2:C:501:PO4:O2	3:C:637:HOH:O	2.11	0.67
1:C:335:VAL:HG21	1:C:378:ILE:HG22	1.77	0.67
1:E:312:PRO:O	1:E:393:THR:OG1	2.06	0.67
1:F:311:ASN:ND2	1:F:314:ASN:OD1	2.28	0.67
1:G:398:GLU:OE1	1:G:398:GLU:N	2.28	0.67
1:K:372:ASP:N	1:K:375:LYS:HZ3	1.93	0.67
1:C:398:GLU:N	1:C:398:GLU:OE1	2.28	0.66
1:E:219:THR:OG1	1:E:270:TYR:O	2.12	0.66
1:F:335:VAL:HG21	1:F:378:ILE:HG22	1.78	0.66
1:C:71:ALA:H	1:C:280:HIS:CD2	2.14	0.66
1:K:68:GLY:O	1:L:91:ARG:NH2	2.28	0.66
1:L:245:ALA:HB1	1:L:254:VAL:HG21	1.76	0.66
1:D:53:TYR:CE1	1:D:96:VAL:HG21	2.30	0.66
1:K:323:LEU:HB2	1:K:392:LEU:HD21	1.76	0.66
1:F:310:LYS:HE2	1:F:315:HIS:CE1	2.31	0.66
1:J:213:LEU:HB3	1:J:256:VAL:HG12	1.78	0.66
1:K:372:ASP:N	3:K:648:HOH:O	2.29	0.66
1:B:13:ASP:O	3:B:616:HOH:O	2.13	0.66
1:I:263:LYS:HB2	1:I:268:ILE:HD11	1.78	0.66
1:J:162:SER:OG	1:J:316:VAL:HG12	1.96	0.66
1:F:311:ASN:O	3:F:663:HOH:O	2.14	0.65
1:I:50:LEU:HD13	1:I:56:ILE:HG13	1.78	0.65
1:I:120:ARG:NH2	1:I:129:GLU:OE2	2.29	0.65
1:L:35:ASP:OD2	3:L:625:HOH:O	2.14	0.65
1:L:310:LYS:HB2	1:L:318:LYS:HD2	1.78	0.65
1:K:207:ARG:HE	1:L:5:ASN:HD22	1.45	0.65
1:B:385:MET:HB2	3:B:640:HOH:O	1.95	0.65
1:C:367:ASP:O	3:C:613:HOH:O	2.14	0.65
1:D:22:VAL:HG11	1:D:174:GLU:HA	1.77	0.65
1:G:17:LEU:O	1:G:206:ARG:NH2	2.22	0.65
1:C:223:LEU:HB2	3:C:646:HOH:O	1.95	0.65
1:K:373:GLU:N	3:K:648:HOH:O	2.30	0.65
1:E:24:ARG:NH1	3:E:681:HOH:O	2.29	0.65
1:C:293:VAL:O	3:C:676:HOH:O	2.15	0.65
1:K:120:ARG:NH2	3:K:663:HOH:O	2.30	0.65
1:B:352:PRO:HB3	3:B:641:HOH:O	1.97	0.65
1:G:2:ARG:O	1:G:3:ASN:HB2	1.95	0.65
1:B:245:ALA:HB1	1:B:254:VAL:HG21	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:161:THR:HG22	1:J:349:ILE:H	1.61	0.64
1:A:60:ASN:C	1:A:60:ASN:HD22	2.00	0.64
1:B:382:VAL:O	3:B:640:HOH:O	2.13	0.64
1:A:178:TYR:HB2	1:A:295:LEU:HD21	1.79	0.64
1:F:70:GLN:HB2	1:F:82:GLN:HB3	1.79	0.64
1:I:2:ARG:HH12	1:I:387:SER:HB3	1.62	0.64
1:L:35:ASP:OD1	1:L:287:GLY:N	2.30	0.64
1:E:120:ARG:NH2	1:E:129:GLU:OE2	2.31	0.64
1:C:326:LEU:HB3	1:C:385:MET:HE1	1.80	0.64
1:G:273:VAL:O	3:G:615:HOH:O	2.15	0.64
1:F:213:LEU:HB3	1:F:256:VAL:HG12	1.78	0.64
1:G:2:ARG:HH12	1:G:387:SER:HB3	1.62	0.64
2:G:501:PO4:O3	3:G:635:HOH:O	2.15	0.64
1:G:318:LYS:HE2	1:G:396:ILE:HD13	1.78	0.64
1:G:29:HIS:NE2	2:G:501:PO4:O1	2.30	0.63
1:H:378:ILE:HG13	1:H:379:SER:N	2.13	0.63
1:J:253:ASN:OD1	1:J:255:ARG:NH2	2.31	0.63
1:A:68:GLY:O	1:B:91:ARG:NH2	2.30	0.63
1:D:10:PRO:HA	1:D:364:ILE:HD11	1.80	0.63
1:L:305:GLU:HB3	3:L:666:HOH:O	1.98	0.63
1:A:207:ARG:HE	1:B:5:ASN:HD22	1.46	0.63
1:D:161:THR:HG22	1:D:349:ILE:H	1.63	0.63
1:C:163:PHE:O	3:C:668:HOH:O	2.15	0.63
1:F:277:SER:O	1:F:282:ASP:HB2	1.98	0.63
1:H:53:TYR:CE1	1:H:96:VAL:HG21	2.34	0.63
1:H:162:SER:OG	1:H:316:VAL:HG12	1.99	0.63
1:A:253:ASN:HB2	3:A:671:HOH:O	1.99	0.63
1:C:80:ILE:HG13	1:C:131:HIS:CD2	2.34	0.63
1:C:69:GLY:O	1:C:70:GLN:HG3	1.99	0.63
1:E:205:LEU:HD23	1:F:357:LEU:HD22	1.79	0.63
1:G:326:LEU:HB3	1:G:385:MET:HE1	1.80	0.63
1:E:91:ARG:HH21	1:F:281:GLY:C	2.02	0.62
1:E:329:ASN:O	1:E:333:GLN:HG3	2.00	0.62
1:F:161:THR:HG22	1:F:349:ILE:H	1.63	0.62
1:K:327:ILE:HG12	3:K:666:HOH:O	1.99	0.62
1:D:86:ILE:HG23	3:D:651:HOH:O	2.00	0.62
1:D:245:ALA:HB1	1:D:254:VAL:HG21	1.81	0.62
1:K:19:VAL:HG21	1:L:360:ASN:ND2	2.15	0.62
1:G:288:ARG:NH2	1:H:62:ASP:O	2.32	0.62
1:D:35:ASP:OD1	1:D:287:GLY:N	2.26	0.62
1:J:277:SER:O	1:J:282:ASP:HB2	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:205:LEU:HD23	1:B:357:LEU:HD22	1.82	0.62
1:E:378:ILE:HG13	1:E:379:SER:N	2.15	0.62
1:B:157:LEU:O	1:B:314:ASN:HB2	2.00	0.62
1:D:351:ARG:NE	1:D:355:ASP:O	2.30	0.62
1:H:51:LYS:NZ	3:H:649:HOH:O	2.31	0.62
1:A:238:ARG:HB2	1:A:256:VAL:CG2	2.30	0.62
1:C:378:ILE:HG13	1:C:379:SER:N	2.15	0.62
1:D:222:GLU:HB2	1:D:223:LEU:HD12	1.81	0.62
1:F:118:TRP:O	1:F:122:ASN:ND2	2.27	0.62
1:J:60:ASN:ND2	3:J:639:HOH:O	2.32	0.62
1:K:186:SER:N	3:K:670:HOH:O	2.33	0.62
1:H:274:THR:O	3:H:616:HOH:O	2.16	0.62
1:K:22:VAL:HG11	1:K:174:GLU:HA	1.81	0.62
1:D:365:THR:HG23	1:D:367:ASP:HB2	1.82	0.61
1:J:155:VAL:N	3:J:634:HOH:O	2.31	0.61
1:K:253:ASN:ND2	3:K:601:HOH:O	2.21	0.61
1:L:178:TYR:HB2	1:L:295:LEU:HD21	1.82	0.61
1:L:373:GLU:HG2	1:L:374:THR:H	1.64	0.61
1:F:346:LEU:HG	3:F:651:HOH:O	2.00	0.61
1:J:63:LYS:NZ	3:J:643:HOH:O	2.33	0.61
1:K:2:ARG:O	1:K:3:ASN:HB2	1.99	0.61
1:E:91:ARG:N	3:E:706:HOH:O	2.32	0.61
1:K:335:VAL:HG21	1:K:378:ILE:HG22	1.81	0.61
1:I:288:ARG:NH2	1:J:62:ASP:O	2.32	0.61
1:J:22:VAL:HG11	1:J:174:GLU:HA	1.83	0.61
1:G:373:GLU:HG2	1:G:374:THR:H	1.66	0.61
1:L:277:SER:O	1:L:282:ASP:HB2	2.01	0.61
1:D:311:ASN:HB3	1:D:315:HIS:HB2	1.83	0.61
1:E:199:ASP:HB2	1:E:276:THR:HA	1.81	0.61
1:L:40:GLU:HG3	3:L:667:HOH:O	2.01	0.61
1:E:207:ARG:HE	1:F:5:ASN:HD22	1.47	0.61
1:A:19:VAL:HG21	1:B:360:ASN:ND2	2.15	0.61
1:E:69:GLY:O	1:E:70:GLN:HG3	2.00	0.61
1:F:311:ASN:HB3	1:F:315:HIS:HB2	1.82	0.61
1:L:354:ASP:HA	1:L:389:PHE:HE2	1.65	0.61
1:J:217:MET:HE3	1:J:237:VAL:HG11	1.83	0.61
1:B:310:LYS:HE2	1:B:315:HIS:CE1	2.36	0.60
1:D:398:GLU:N	1:D:398:GLU:OE1	2.34	0.60
1:D:211:VAL:HB	1:D:254:VAL:HG12	1.84	0.60
1:K:326:LEU:HB3	1:K:385:MET:HE1	1.83	0.60
1:L:300:ARG:NH1	3:L:636:HOH:O	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:378:ILE:HG13	1:F:379:SER:N	2.16	0.60
1:J:238:ARG:HB2	1:J:256:VAL:HG23	1.83	0.60
1:K:181:GLU:OE1	1:K:182:ARG:HD2	2.02	0.60
1:A:120:ARG:NH2	1:A:129:GLU:OE2	2.33	0.60
1:D:326:LEU:HB3	1:D:385:MET:HE1	1.84	0.60
1:L:118:TRP:O	1:L:122:ASN:ND2	2.33	0.60
1:B:110:ILE:HB	3:B:691:HOH:O	2.01	0.60
1:K:23:GLU:OE2	3:K:660:HOH:O	2.17	0.60
1:A:273:VAL:O	3:A:683:HOH:O	2.17	0.60
1:F:224:ILE:HG21	1:F:271:LEU:HD21	1.83	0.60
1:H:6:VAL:HG11	1:H:378:ILE:HD11	1.84	0.60
1:L:310:LYS:HE2	1:L:315:HIS:CE1	2.37	0.60
1:B:76:LYS:HG3	1:B:225:GLU:HA	1.84	0.60
1:I:348:GLN:NE2	1:J:212:ASP:OD2	2.34	0.60
1:K:19:VAL:HG21	1:L:360:ASN:HD21	1.67	0.60
1:C:232:ASN:HB2	3:C:604:HOH:O	2.02	0.60
1:E:57:LEU:HD22	1:E:93:THR:HG21	1.83	0.60
1:F:339:LYS:HB3	1:F:364:ILE:HG22	1.83	0.60
1:B:70:GLN:HB2	1:B:82:GLN:HB3	1.84	0.59
1:J:378:ILE:HG13	1:J:379:SER:N	2.14	0.59
1:B:277:SER:O	1:B:282:ASP:HB2	2.02	0.59
1:C:50:LEU:HD13	1:C:56:ILE:HG13	1.83	0.59
1:F:109:THR:N	3:F:704:HOH:O	2.34	0.59
1:A:402:THR:HG22	3:A:645:HOH:O	2.02	0.59
1:E:71:ALA:H	1:E:280:HIS:CD2	2.18	0.59
1:F:204:GLY:O	3:F:703:HOH:O	2.17	0.59
1:K:323:LEU:HD21	1:K:386:LEU:HD11	1.82	0.59
1:C:288:ARG:HG3	3:C:671:HOH:O	2.01	0.59
1:D:2:ARG:N	3:D:612:HOH:O	2.35	0.59
1:K:199:ASP:HB2	1:K:276:THR:HA	1.84	0.59
1:H:9:ASN:OD1	1:H:11:LEU:HD13	2.03	0.59
1:L:53:TYR:CE1	1:L:96:VAL:HG21	2.38	0.59
1:B:178:TYR:HB2	1:B:295:LEU:HD21	1.84	0.59
1:E:218:ALA:HA	1:E:270:TYR:CD2	2.38	0.59
1:F:53:TYR:CE1	1:F:96:VAL:HG21	2.37	0.59
1:A:195:GLU:N	1:A:195:GLU:OE1	2.34	0.59
1:B:112:ILE:HG21	3:C:638:HOH:O	2.01	0.59
1:D:160:ASP:HB3	3:D:640:HOH:O	2.02	0.59
1:H:218:ALA:HA	1:H:270:TYR:HD2	1.68	0.59
1:I:117:GLU:OE1	1:I:120:ARG:NH1	2.34	0.59
1:B:218:ALA:HA	1:B:270:TYR:HD2	1.66	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:19:VAL:HG21	1:D:360:ASN:ND2	2.18	0.59
1:D:277:SER:O	1:D:282:ASP:HB2	2.03	0.59
1:E:117:GLU:OE1	1:E:120:ARG:NH1	2.35	0.59
1:F:338:VAL:HB	3:F:695:HOH:O	2.02	0.59
1:G:348:GLN:NE2	1:H:212:ASP:OD2	2.36	0.59
1:I:354:ASP:HA	1:I:389:PHE:HE2	1.66	0.59
1:A:349:ILE:HD12	3:A:706:HOH:O	2.01	0.58
1:C:220:ILE:HB	3:C:646:HOH:O	2.03	0.58
1:I:207:ARG:HE	1:J:5:ASN:HD22	1.50	0.58
1:L:311:ASN:ND2	1:L:314:ASN:OD1	2.36	0.58
1:C:218:ALA:HA	1:C:270:TYR:CE2	2.38	0.58
1:E:9:ASN:O	1:E:12:SER:HB3	2.04	0.58
1:E:398:GLU:HB2	3:E:715:HOH:O	2.04	0.58
1:I:35:ASP:OD1	1:I:287:GLY:N	2.30	0.58
1:I:318:LYS:HE2	1:I:396:ILE:HD13	1.84	0.58
1:B:22:VAL:HG11	1:B:174:GLU:HA	1.84	0.58
1:A:24:ARG:NE	3:A:640:HOH:O	2.36	0.58
1:A:52:LYS:NZ	3:A:698:HOH:O	2.36	0.58
1:B:52:LYS:O	1:B:54:GLY:N	2.35	0.58
1:D:178:TYR:HB2	1:D:295:LEU:HD21	1.84	0.58
1:G:50:LEU:HD13	1:G:56:ILE:HG13	1.84	0.58
1:H:308:ALA:HA	3:H:631:HOH:O	2.02	0.58
1:H:237:VAL:O	1:H:240:GLN:HB2	2.04	0.58
1:K:211:VAL:HB	1:K:254:VAL:HG12	1.84	0.58
1:K:238:ARG:HB2	1:K:256:VAL:CG2	2.34	0.58
1:A:199:ASP:HB2	1:A:276:THR:HA	1.85	0.58
1:D:117:GLU:OE1	1:D:120:ARG:NH1	2.36	0.58
1:E:40:GLU:HB2	3:E:718:HOH:O	2.03	0.58
1:J:373:GLU:HG2	1:J:374:THR:H	1.69	0.57
1:A:118:TRP:O	1:A:122:ASN:ND2	2.29	0.57
1:A:196:VAL:HB	3:A:701:HOH:O	2.03	0.57
1:A:222:GLU:HB2	1:A:223:LEU:HD12	1.86	0.57
1:C:158:SER:O	1:C:349:ILE:HA	2.04	0.57
1:C:288:ARG:NH2	1:D:62:ASP:O	2.36	0.57
1:B:326:LEU:HB3	1:B:385:MET:HE1	1.86	0.57
1:E:386:LEU:HA	3:E:677:HOH:O	2.05	0.57
1:J:312:PRO:HB2	3:J:628:HOH:O	2.04	0.57
1:A:14:ILE:N	3:A:648:HOH:O	2.26	0.57
1:A:243:ASP:HB3	3:A:668:HOH:O	2.05	0.57
1:B:294:GLY:HA3	3:B:695:HOH:O	2.03	0.57
1:B:400:LYS:HE3	3:B:620:HOH:O	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:326:LEU:HB3	1:F:385:MET:HE1	1.87	0.57
1:A:315:HIS:HB3	3:A:695:HOH:O	2.03	0.57
1:B:161:THR:HG22	1:B:349:ILE:H	1.69	0.57
1:F:22:VAL:HG11	1:F:174:GLU:HA	1.86	0.57
1:I:218:ALA:HA	1:I:270:TYR:HE2	1.67	0.57
1:L:218:ALA:HA	1:L:270:TYR:HD2	1.70	0.57
1:A:9:ASN:O	1:A:12:SER:HB3	2.03	0.57
1:B:344:GLN:HA	3:B:650:HOH:O	2.02	0.57
1:D:36:ALA:HB3	3:D:646:HOH:O	2.04	0.57
1:J:238:ARG:HB2	1:J:256:VAL:CG2	2.34	0.57
1:J:181:GLU:OE1	1:J:182:ARG:HD2	2.05	0.57
1:E:326:LEU:HB3	1:E:385:MET:HE1	1.87	0.57
1:D:37:VAL:HG13	3:D:646:HOH:O	2.05	0.56
1:I:19:VAL:HG21	1:J:360:ASN:ND2	2.19	0.56
1:I:217:MET:CE	1:I:237:VAL:HG11	2.34	0.56
1:B:108:GLY:O	1:B:112:ILE:HG12	2.04	0.56
1:F:162:SER:OG	1:F:316:VAL:HG12	2.05	0.56
1:D:157:LEU:O	1:D:314:ASN:HB2	2.05	0.56
1:E:22:VAL:HG11	1:E:174:GLU:HA	1.86	0.56
1:F:222:GLU:HG3	3:F:635:HOH:O	2.04	0.56
1:F:331:ILE:HG23	3:F:666:HOH:O	2.05	0.56
1:I:25:LYS:NZ	2:J:501:PO4:O2	2.38	0.56
1:L:95:GLU:HB2	1:L:140:LYS:NZ	2.20	0.56
1:C:195:GLU:HA	3:C:646:HOH:O	2.05	0.56
1:D:8:LEU:HD11	1:D:365:THR:HG22	1.88	0.56
1:D:65:LEU:O	3:D:651:HOH:O	2.16	0.56
1:E:351:ARG:NE	1:E:355:ASP:O	2.37	0.56
1:I:197:GLY:HA3	1:I:218:ALA:HB3	1.87	0.56
1:B:199:ASP:HB2	1:B:276:THR:HA	1.87	0.56
1:C:217:MET:CE	1:C:237:VAL:HG11	2.36	0.56
1:C:351:ARG:NH2	3:C:602:HOH:O	2.38	0.56
1:H:316:VAL:HG13	1:H:320:TYR:CD2	2.41	0.56
1:A:288:ARG:NE	3:A:690:HOH:O	2.39	0.56
1:D:167:PHE:CZ	1:D:293:VAL:HG11	2.40	0.56
1:H:103:ASP:O	3:H:658:HOH:O	2.18	0.56
1:H:39:GLU:OE1	1:H:318:LYS:NZ	2.33	0.56
1:I:130:ARG:HB2	3:I:630:HOH:O	2.05	0.56
1:J:9:ASN:OD1	1:J:11:LEU:HD13	2.06	0.56
1:C:11:LEU:HD23	1:D:11:LEU:HG	1.88	0.56
1:E:213:LEU:HD23	1:E:256:VAL:HG12	1.88	0.56
1:F:294:GLY:HA3	3:F:701:HOH:O	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:80:ILE:HG13	1:K:131:HIS:CD2	2.41	0.56
1:K:381:ILE:HG22	3:K:666:HOH:O	2.06	0.56
1:C:25:LYS:HD2	1:C:289:GLY:HA2	1.87	0.56
1:C:199:ASP:HB2	1:C:276:THR:HA	1.87	0.56
1:C:374:THR:HA	3:C:644:HOH:O	2.05	0.56
1:D:2:ARG:NH2	1:D:387:SER:HB3	2.21	0.56
1:H:118:TRP:O	1:H:122:ASN:ND2	2.30	0.56
1:J:120:ARG:NH2	3:J:629:HOH:O	2.10	0.56
1:A:24:ARG:CZ	3:A:640:HOH:O	2.54	0.55
1:C:219:THR:OG1	1:C:270:TYR:O	2.22	0.55
1:C:348:GLN:NE2	1:D:212:ASP:OD2	2.35	0.55
1:E:212:ASP:OD2	1:F:357:LEU:HD21	2.06	0.55
1:I:323:LEU:HB2	1:I:392:LEU:HD21	1.86	0.55
1:A:70:GLN:OE1	1:B:140:LYS:N	2.24	0.55
1:E:19:VAL:HG21	1:F:360:ASN:ND2	2.21	0.55
1:E:374:THR:HA	3:E:678:HOH:O	2.06	0.55
1:G:35:ASP:OD1	1:G:287:GLY:N	2.32	0.55
1:G:91:ARG:HH21	1:H:281:GLY:C	2.10	0.55
1:B:373:GLU:HG2	1:B:374:THR:H	1.71	0.55
1:G:234:LYS:NZ	1:G:262:ASP:OD2	2.33	0.55
1:H:310:LYS:HA	3:H:633:HOH:O	2.06	0.55
1:L:316:VAL:HG13	1:L:320:TYR:CD2	2.41	0.55
1:D:52:LYS:O	1:D:54:GLY:N	2.40	0.55
1:I:335:VAL:HG21	1:I:378:ILE:HG22	1.87	0.55
1:K:219:THR:OG1	1:K:270:TYR:O	2.24	0.55
1:A:144:ASP:HB3	3:A:661:HOH:O	2.05	0.55
1:C:37:VAL:HB	1:C:115:VAL:HG22	1.88	0.55
1:E:6:VAL:HB	1:E:375:LYS:HE3	1.88	0.55
1:G:346:LEU:HD11	1:H:21:LEU:HD11	1.89	0.55
1:A:373:GLU:HG2	1:A:374:THR:H	1.71	0.55
1:B:9:ASN:OD1	1:B:11:LEU:HD13	2.07	0.55
1:C:310:LYS:HE2	1:C:315:HIS:NE2	2.22	0.55
1:E:257:TYR:HB3	1:E:260:THR:CG2	2.37	0.55
1:F:6:VAL:CG1	1:F:378:ILE:HD11	2.37	0.55
1:F:53:TYR:O	1:F:55:VAL:HG22	2.07	0.55
1:F:316:VAL:HG21	3:F:706:HOH:O	2.07	0.55
1:I:80:ILE:HG13	1:I:131:HIS:CD2	2.41	0.55
1:A:10:PRO:HA	1:A:364:ILE:HD11	1.87	0.55
1:A:74:ARG:HD3	3:A:609:HOH:O	2.06	0.55
1:A:217:MET:HE3	1:A:237:VAL:HG11	1.89	0.55
1:B:379:SER:HB2	3:B:687:HOH:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:178:TYR:HB2	1:C:295:LEU:HD21	1.89	0.55
1:H:140:LYS:O	3:H:637:HOH:O	2.18	0.55
1:J:310:LYS:HB2	1:J:318:LYS:HD2	1.89	0.55
1:L:324:ALA:N	3:L:657:HOH:O	2.39	0.55
1:B:213:LEU:HB3	1:B:256:VAL:HG12	1.89	0.55
1:I:304:LEU:HD12	1:J:296:ILE:HG23	1.88	0.55
1:D:103:ASP:OD1	1:D:103:ASP:N	2.39	0.55
1:D:181:GLU:OE2	1:D:185:ASN:ND2	2.39	0.55
1:D:301:PRO:HA	3:D:636:HOH:O	2.07	0.55
1:E:138:ILE:HG22	1:E:139:GLY:O	2.07	0.55
1:F:354:ASP:HA	1:F:389:PHE:HE2	1.72	0.55
1:H:209:ASN:O	1:H:253:ASN:N	2.30	0.55
1:I:14:ILE:HD11	1:I:171:THR:HG21	1.88	0.55
1:K:238:ARG:HB2	1:K:256:VAL:HG23	1.89	0.55
1:L:181:GLU:OE1	1:L:182:ARG:HD2	2.07	0.55
1:C:288:ARG:NH1	2:D:501:PO4:O1	2.38	0.54
1:D:373:GLU:HG2	1:D:374:THR:H	1.72	0.54
1:G:257:TYR:HB3	1:G:260:THR:CG2	2.37	0.54
1:D:344:GLN:HG3	3:D:619:HOH:O	2.07	0.54
1:F:83:PRO:O	3:F:614:HOH:O	2.19	0.54
1:F:157:LEU:O	1:F:314:ASN:HB2	2.07	0.54
1:G:218:ALA:HA	1:G:270:TYR:HD2	1.72	0.54
1:G:323:LEU:HD12	1:G:385:MET:HE2	1.89	0.54
1:L:238:ARG:HG3	3:L:640:HOH:O	2.07	0.54
1:L:270:TYR:OH	1:L:277:SER:HB3	2.07	0.54
1:L:378:ILE:HG13	1:L:379:SER:N	2.21	0.54
1:H:48:TYR:CZ	1:H:52:LYS:HD2	2.42	0.54
1:J:270:TYR:OH	1:J:277:SER:HB3	2.06	0.54
1:E:338:VAL:HB	3:E:664:HOH:O	2.07	0.54
1:H:169:PRO:HD2	1:H:340:PHE:HD1	1.72	0.54
1:K:46:SER:OG	1:K:59:HIS:NE2	2.40	0.54
1:A:35:ASP:OD1	1:A:287:GLY:N	2.32	0.54
1:H:218:ALA:HA	1:H:270:TYR:CD2	2.42	0.54
1:A:6:VAL:CG1	1:A:378:ILE:HD11	2.36	0.54
1:B:328:ALA:HB2	1:B:343:VAL:HG23	1.90	0.54
1:G:71:ALA:H	1:G:280:HIS:CD2	2.22	0.54
1:H:315:HIS:N	3:H:640:HOH:O	2.35	0.54
1:I:184:LEU:O	1:I:190:LYS:NZ	2.41	0.54
1:F:218:ALA:HA	1:F:270:TYR:HD2	1.73	0.54
1:F:382:VAL:O	3:F:705:HOH:O	2.18	0.54
1:I:378:ILE:HG13	1:I:379:SER:N	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:70:GLN:HB2	1:D:82:GLN:HB3	1.88	0.54
1:E:50:LEU:N	3:E:674:HOH:O	2.41	0.54
1:F:219:THR:OG1	1:F:270:TYR:O	2.26	0.54
1:G:19:VAL:HG21	1:H:360:ASN:ND2	2.22	0.54
1:I:346:LEU:CD1	1:J:21:LEU:HD11	2.38	0.54
1:L:179:GLU:O	3:L:658:HOH:O	2.17	0.54
1:B:378:ILE:HG13	1:B:379:SER:N	2.22	0.54
1:G:210:GLU:HG2	1:G:253:ASN:HB3	1.89	0.54
1:H:158:SER:HB3	1:H:348:GLN:O	2.08	0.54
1:J:335:VAL:HG21	1:J:378:ILE:HG22	1.88	0.54
1:L:345:VAL:HG21	3:L:657:HOH:O	2.08	0.54
1:B:2:ARG:NH2	1:B:387:SER:HB3	2.23	0.54
1:B:45:LEU:HD13	3:B:691:HOH:O	2.08	0.54
1:C:68:GLY:O	1:D:91:ARG:NH2	2.40	0.54
1:D:2:ARG:HG3	1:D:3:ASN:H	1.73	0.54
1:D:373:GLU:N	3:D:638:HOH:O	2.38	0.54
1:I:289:GLY:N	3:I:625:HOH:O	2.40	0.54
1:C:70:GLN:HG2	1:C:280:HIS:CD2	2.44	0.53
1:C:294:GLY:HA3	3:C:676:HOH:O	2.07	0.53
1:D:158:SER:HB3	1:D:348:GLN:O	2.08	0.53
1:F:195:GLU:OE1	1:F:195:GLU:N	2.39	0.53
1:H:222:GLU:HG3	3:H:628:HOH:O	2.07	0.53
1:A:329:ASN:O	1:A:333:GLN:HG3	2.08	0.53
1:B:6:VAL:CG1	1:B:378:ILE:HD11	2.38	0.53
1:E:217:MET:HE3	1:E:237:VAL:HG11	1.90	0.53
1:F:2:ARG:N	3:F:682:HOH:O	2.40	0.53
1:J:147:GLY:O	3:J:631:HOH:O	2.18	0.53
1:J:354:ASP:HA	1:J:389:PHE:HE2	1.74	0.53
1:B:207:ARG:HD3	3:B:602:HOH:O	2.08	0.53
1:B:365:THR:C	1:B:367:ASP:H	2.12	0.53
1:C:70:GLN:OE1	1:D:140:LYS:N	2.34	0.53
1:D:311:ASN:N	3:D:604:HOH:O	2.22	0.53
1:D:318:LYS:HE2	1:D:396:ILE:HD13	1.90	0.53
1:I:103:ASP:OD1	1:I:103:ASP:N	2.36	0.53
1:L:316:VAL:HB	3:L:656:HOH:O	2.08	0.53
1:A:357:LEU:O	1:A:357:LEU:HD23	2.08	0.53
1:B:165:VAL:HG22	3:B:650:HOH:O	2.08	0.53
1:C:205:LEU:HD23	1:D:357:LEU:HD22	1.90	0.53
1:C:273:VAL:HB	3:C:682:HOH:O	2.08	0.53
1:J:74:ARG:HD3	3:J:603:HOH:O	2.08	0.53
1:J:318:LYS:HE2	1:J:396:ILE:HD13	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:228:ASN:ND2	1:E:264:ILE:HG12	2.24	0.53
1:A:228:ASN:CG	1:E:264:ILE:HG21	2.29	0.53
1:A:337:ASP:O	3:A:707:HOH:O	2.18	0.53
1:E:256:VAL:HG11	3:E:661:HOH:O	2.09	0.53
1:F:302:MET:N	3:F:641:HOH:O	2.34	0.53
1:K:195:GLU:OE1	1:K:195:GLU:N	2.39	0.53
1:L:218:ALA:HA	1:L:270:TYR:CD2	2.44	0.53
1:H:277:SER:O	1:H:282:ASP:HB2	2.08	0.53
1:K:22:VAL:HB	1:K:177:VAL:HG21	1.90	0.53
1:K:70:GLN:HA	1:K:280:HIS:CD2	2.44	0.53
1:F:9:ASN:OD1	1:F:11:LEU:HD13	2.08	0.53
1:I:373:GLU:HG2	1:I:374:THR:H	1.74	0.53
1:K:378:ILE:HG13	1:K:379:SER:N	2.23	0.53
1:L:300:ARG:HG2	3:L:636:HOH:O	2.08	0.53
1:A:268:ILE:C	1:A:269:LEU:HD12	2.29	0.53
1:H:5:ASN:C	1:H:5:ASN:HD22	2.12	0.53
1:I:207:ARG:NE	1:J:5:ASN:HD22	2.06	0.53
1:J:199:ASP:HB2	1:J:276:THR:HA	1.91	0.53
1:L:14:ILE:HB	1:L:17:LEU:HD12	1.91	0.53
1:L:144:ASP:OD1	1:L:145:LEU:HD12	2.09	0.53
1:L:161:THR:HG22	1:L:349:ILE:H	1.73	0.53
1:F:238:ARG:HB2	1:F:256:VAL:CG2	2.38	0.53
1:K:196:VAL:HB	3:K:642:HOH:O	2.09	0.53
1:A:263:LYS:HB2	1:A:268:ILE:CG1	2.39	0.52
1:I:329:ASN:O	1:I:333:GLN:HG3	2.09	0.52
1:L:230:TYR:OH	1:L:262:ASP:OD2	2.22	0.52
1:A:218:ALA:HA	1:A:270:TYR:HD2	1.74	0.52
1:C:31:ASP:HB3	3:C:628:HOH:O	2.09	0.52
1:D:169:PRO:HD2	1:D:340:PHE:HD1	1.74	0.52
1:D:375:LYS:HG3	3:D:638:HOH:O	2.08	0.52
1:L:282:ASP:N	3:L:632:HOH:O	2.41	0.52
1:A:271:LEU:HG	3:A:655:HOH:O	2.09	0.52
1:A:340:PHE:N	3:A:650:HOH:O	2.42	0.52
1:B:53:TYR:CE1	1:B:96:VAL:HG21	2.43	0.52
1:C:120:ARG:NH2	1:C:129:GLU:OE2	2.42	0.52
1:E:222:GLU:HG3	3:E:663:HOH:O	2.09	0.52
1:F:328:ALA:HB2	1:F:343:VAL:HG23	1.90	0.52
1:G:323:LEU:HD21	1:G:386:LEU:HD11	1.91	0.52
1:J:211:VAL:HB	1:J:254:VAL:HG12	1.91	0.52
1:K:118:TRP:O	1:K:122:ASN:ND2	2.37	0.52
1:B:22:VAL:HB	1:B:177:VAL:HG21	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:207:ARG:NE	1:D:5:ASN:HD22	2.07	0.52
1:F:6:VAL:HG11	1:F:378:ILE:HD11	1.92	0.52
1:F:299:MET:HB2	3:F:648:HOH:O	2.09	0.52
1:L:9:ASN:OD1	1:L:11:LEU:HD13	2.09	0.52
1:G:346:LEU:HD23	1:G:347:GLY:N	2.25	0.52
1:H:140:LYS:N	3:H:637:HOH:O	2.42	0.52
1:J:10:PRO:HA	1:J:364:ILE:HD11	1.91	0.52
1:J:120:ARG:NH2	1:J:129:GLU:OE2	2.43	0.52
1:J:217:MET:O	1:J:270:TYR:HD2	1.93	0.52
1:D:162:SER:OG	1:D:316:VAL:HG12	2.09	0.52
1:D:316:VAL:HG13	1:D:320:TYR:CD2	2.44	0.52
1:J:14:ILE:HB	1:J:17:LEU:HD12	1.91	0.52
1:D:222:GLU:HG3	3:D:634:HOH:O	2.10	0.52
1:G:222:GLU:HG3	3:G:615:HOH:O	2.09	0.52
1:I:238:ARG:HB2	1:I:256:VAL:HG23	1.92	0.52
1:E:136:TYR:HD2	1:E:138:ILE:HG12	1.75	0.52
1:E:296:ILE:HG21	3:F:658:HOH:O	2.10	0.52
1:F:218:ALA:HA	1:F:270:TYR:CD2	2.45	0.52
1:K:103:ASP:OD1	1:K:103:ASP:N	2.34	0.52
1:L:181:GLU:OE2	1:L:185:ASN:ND2	2.38	0.52
1:L:222:GLU:HB2	1:L:223:LEU:HD12	1.92	0.52
1:C:2:ARG:O	1:C:3:ASN:HB2	2.10	0.52
1:F:163:PHE:CD1	1:F:163:PHE:C	2.83	0.52
1:G:288:ARG:HG3	3:G:644:HOH:O	2.10	0.52
1:K:346:LEU:HD23	1:K:347:GLY:N	2.25	0.52
1:C:68:GLY:HA2	1:C:278:ALA:O	2.10	0.51
1:C:86:ILE:N	3:C:642:HOH:O	2.23	0.51
1:G:329:ASN:O	1:G:333:GLN:HG3	2.08	0.51
1:J:24:ARG:HH21	1:J:182:ARG:HH11	1.56	0.51
1:K:75:PHE:CZ	1:K:227:VAL:HG22	2.45	0.51
1:K:304:LEU:HD12	1:L:296:ILE:HG12	1.92	0.51
1:A:2:ARG:HH12	1:A:387:SER:HB3	1.75	0.51
1:A:323:LEU:HB2	1:A:392:LEU:HD21	1.92	0.51
1:E:316:VAL:HG21	3:E:639:HOH:O	2.10	0.51
1:E:337:ASP:O	1:E:365:THR:OG1	2.19	0.51
1:F:199:ASP:HB2	1:F:276:THR:HA	1.90	0.51
1:I:323:LEU:HD21	1:I:386:LEU:HD11	1.91	0.51
1:K:91:ARG:HH21	1:L:281:GLY:C	2.13	0.51
1:L:15:GLU:HG3	1:L:171:THR:HB	1.92	0.51
1:A:238:ARG:NH2	3:A:653:HOH:O	2.29	0.51
1:D:9:ASN:OD1	1:D:11:LEU:HD13	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:237:VAL:O	1:D:240:GLN:HB2	2.11	0.51
1:F:382:VAL:O	1:F:386:LEU:HD13	2.10	0.51
1:H:81:ILE:HD13	3:H:627:HOH:O	2.11	0.51
1:L:14:ILE:CD1	1:L:171:THR:HG21	2.40	0.51
1:D:56:ILE:HD11	1:D:397:LEU:HD11	1.92	0.51
1:F:127:ASP:OD1	1:F:130:ARG:HG3	2.10	0.51
1:F:238:ARG:HB2	1:F:256:VAL:HG23	1.92	0.51
1:G:199:ASP:OD2	1:G:277:SER:OG	2.22	0.51
1:I:270:TYR:O	1:I:270:TYR:CD2	2.63	0.51
1:A:29:HIS:NE2	2:A:501:PO4:O2	2.42	0.51
1:C:373:GLU:HG2	1:C:374:THR:H	1.76	0.51
1:J:291:ARG:HG3	1:J:302:MET:HG2	1.92	0.51
1:L:2:ARG:HG3	1:L:3:ASN:H	1.74	0.51
1:B:161:THR:HG23	1:B:349:ILE:HG22	1.92	0.51
1:C:354:ASP:C	1:C:356:PRO:HD3	2.31	0.51
1:E:8:LEU:HD11	1:E:365:THR:HG22	1.92	0.51
1:I:70:GLN:HG2	1:I:280:HIS:CE1	2.45	0.51
1:I:222:GLU:HG3	3:I:615:HOH:O	2.09	0.51
1:B:195:GLU:OE1	1:B:195:GLU:N	2.40	0.51
1:B:218:ALA:HA	1:B:270:TYR:CD2	2.45	0.51
1:E:342:GLN:HG3	3:E:625:HOH:O	2.11	0.51
1:E:354:ASP:HB2	1:E:386:LEU:O	2.11	0.51
1:B:20:GLU:HA	1:B:299:MET:SD	2.50	0.51
1:D:320:TYR:HE2	1:D:347:GLY:HA3	1.75	0.51
1:H:6:VAL:CG1	1:H:378:ILE:HD11	2.40	0.51
1:A:300:ARG:HB3	3:A:689:HOH:O	2.10	0.51
1:A:378:ILE:HG13	1:A:379:SER:N	2.25	0.51
1:D:207:ARG:HD3	3:D:601:HOH:O	2.11	0.51
1:E:25:LYS:HD2	1:E:289:GLY:HA2	1.92	0.51
1:G:373:GLU:HG2	1:G:374:THR:N	2.26	0.51
1:H:182:ARG:NH1	3:H:605:HOH:O	2.43	0.51
1:A:289:GLY:N	3:A:704:HOH:O	2.43	0.51
1:B:60:ASN:ND2	3:B:661:HOH:O	2.35	0.51
1:D:339:LYS:HG3	1:D:366:TYR:CE1	2.46	0.51
1:E:138:ILE:HD12	3:E:706:HOH:O	2.11	0.51
1:H:373:GLU:HG2	1:H:374:THR:H	1.76	0.51
1:K:19:VAL:HG11	1:L:360:ASN:HD22	1.74	0.51
1:I:219:THR:OG1	1:I:270:TYR:O	2.29	0.50
1:L:12:SER:HB3	3:L:663:HOH:O	2.11	0.50
1:D:124:ARG:NE	1:D:198:GLU:OE2	2.40	0.50
1:F:197:GLY:N	1:F:218:ALA:O	2.34	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:318:LYS:HE2	1:L:396:ILE:HD13	1.92	0.50
1:A:50:LEU:HD13	1:A:56:ILE:HG13	1.93	0.50
1:A:199:ASP:OD2	1:A:277:SER:OG	2.21	0.50
3:A:694:HOH:O	1:B:90:GLY:N	2.40	0.50
1:A:14:ILE:CD1	1:A:171:THR:HG21	2.40	0.50
1:B:6:VAL:HG11	1:B:378:ILE:HD11	1.92	0.50
1:E:53:TYR:CE1	1:E:96:VAL:HG21	2.47	0.50
1:G:22:VAL:HB	1:G:177:VAL:HG21	1.94	0.50
1:H:52:LYS:O	1:H:54:GLY:N	2.42	0.50
1:I:91:ARG:HH21	1:J:281:GLY:C	2.14	0.50
1:L:162:SER:OG	1:L:316:VAL:HG12	2.11	0.50
1:A:69:GLY:O	1:A:70:GLN:HG3	2.12	0.50
1:A:348:GLN:NE2	1:B:212:ASP:OD2	2.35	0.50
1:F:163:PHE:HB2	1:F:346:LEU:HD13	1.93	0.50
1:J:354:ASP:HB2	1:J:386:LEU:O	2.12	0.50
1:B:160:ASP:HB3	3:B:693:HOH:O	2.10	0.50
1:E:16:LYS:HD3	3:E:620:HOH:O	2.12	0.50
1:E:76:LYS:HG3	1:E:225:GLU:HA	1.94	0.50
1:H:289:GLY:N	3:H:626:HOH:O	2.43	0.50
1:K:218:ALA:HA	1:K:270:TYR:CD2	2.46	0.50
1:L:163:PHE:HB3	1:L:346:LEU:HD13	1.94	0.50
1:E:36:ALA:O	3:E:718:HOH:O	2.20	0.50
1:H:354:ASP:HA	1:H:389:PHE:HE2	1.77	0.50
1:K:76:LYS:HG3	1:K:225:GLU:HA	1.94	0.50
1:B:14:ILE:CD1	1:B:171:THR:HG21	2.38	0.50
1:D:60:ASN:HA	3:D:604:HOH:O	2.11	0.50
1:F:323:LEU:O	1:F:326:LEU:N	2.45	0.50
1:G:199:ASP:HB2	1:G:276:THR:HA	1.94	0.50
1:J:354:ASP:HA	1:J:389:PHE:CE2	2.47	0.50
1:K:22:VAL:HG21	1:K:174:GLU:HG2	1.93	0.50
1:K:217:MET:HE3	1:K:237:VAL:HG11	1.93	0.50
1:E:55:VAL:O	3:E:674:HOH:O	2.17	0.50
1:E:268:ILE:C	1:E:269:LEU:HD12	2.32	0.50
1:F:80:ILE:HG13	1:F:131:HIS:CD2	2.47	0.50
1:F:373:GLU:HG2	1:F:374:THR:H	1.76	0.50
1:G:218:ALA:HA	1:G:270:TYR:CD2	2.47	0.50
1:H:50:LEU:HD13	1:H:56:ILE:HG13	1.93	0.50
1:H:103:ASP:OD1	1:H:103:ASP:N	2.45	0.50
1:J:2:ARG:HG3	1:J:3:ASN:H	1.77	0.50
1:A:269:LEU:HB3	3:A:655:HOH:O	2.12	0.49
1:C:238:ARG:HB2	1:C:256:VAL:CG2	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:90:GLY:N	3:D:644:HOH:O	2.38	0.49
1:E:103:ASP:OD1	1:E:103:ASP:N	2.42	0.49
1:I:10:PRO:HA	1:I:364:ILE:HD11	1.94	0.49
1:J:157:LEU:O	1:J:314:ASN:HB2	2.12	0.49
1:J:290:ASN:ND2	1:J:404:PHE:O	2.30	0.49
1:C:60:ASN:ND2	1:C:62:ASP:OD1	2.43	0.49
1:E:353:ILE:HD12	1:E:389:PHE:CE1	2.46	0.49
1:F:51:LYS:HE2	3:F:696:HOH:O	2.12	0.49
1:F:217:MET:HE3	1:F:237:VAL:HG11	1.94	0.49
1:F:316:VAL:HG13	1:F:320:TYR:CD2	2.47	0.49
1:G:210:GLU:HA	1:G:253:ASN:HB3	1.93	0.49
1:K:348:GLN:NE2	1:L:212:ASP:OD2	2.45	0.49
1:A:24:ARG:NH2	3:A:685:HOH:O	2.34	0.49
1:C:257:TYR:HB3	1:C:260:THR:CG2	2.42	0.49
1:G:348:GLN:HB2	1:G:357:LEU:HD12	1.94	0.49
1:H:311:ASN:N	3:H:603:HOH:O	2.29	0.49
1:I:195:GLU:OE1	1:I:195:GLU:N	2.43	0.49
1:A:181:GLU:OE2	1:A:185:ASN:ND2	2.45	0.49
1:A:257:TYR:HD2	1:B:348:GLN:HE22	1.58	0.49
1:C:130:ARG:HD3	3:C:651:HOH:O	2.11	0.49
1:D:181:GLU:OE1	1:D:182:ARG:HD2	2.11	0.49
1:F:24:ARG:HH21	1:F:182:ARG:NH1	2.08	0.49
1:L:238:ARG:HB2	1:L:256:VAL:HG23	1.94	0.49
1:A:158:SER:O	1:A:349:ILE:HA	2.13	0.49
1:A:373:GLU:HG2	1:A:374:THR:N	2.27	0.49
1:B:356:PRO:HG2	1:B:386:LEU:HD21	1.95	0.49
1:D:310:LYS:HB2	1:D:318:LYS:HB2	1.93	0.49
1:E:323:LEU:HB2	1:E:392:LEU:HD21	1.94	0.49
1:E:335:VAL:O	1:E:338:VAL:HG22	2.12	0.49
1:F:14:ILE:CD1	1:F:171:THR:HG21	2.39	0.49
1:A:57:LEU:HD22	1:A:93:THR:HG21	1.95	0.49
1:B:218:ALA:HB2	1:B:270:TYR:HE2	1.78	0.49
1:D:6:VAL:CG1	1:D:378:ILE:HD11	2.43	0.49
1:D:61:LEU:O	3:D:641:HOH:O	2.20	0.49
1:E:25:LYS:HD3	1:E:29:HIS:CE1	2.48	0.49
1:E:273:VAL:N	1:E:279:GLU:OE2	2.31	0.49
1:I:335:VAL:O	1:I:338:VAL:HG22	2.13	0.49
1:D:143:SER:O	1:D:146:VAL:HG12	2.13	0.49
1:E:158:SER:O	1:E:349:ILE:HA	2.12	0.49
1:L:310:LYS:HB2	1:L:318:LYS:HB2	1.95	0.49
1:A:351:ARG:NE	1:A:355:ASP:O	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:291:ARG:HG3	1:B:302:MET:HG2	1.94	0.49
1:B:354:ASP:HA	1:B:389:PHE:HE2	1.78	0.49
1:C:103:ASP:OD1	1:C:103:ASP:N	2.41	0.49
1:K:365:THR:HG23	1:K:367:ASP:HB2	1.95	0.49
1:B:75:PHE:CZ	1:B:227:VAL:HG22	2.48	0.49
1:C:10:PRO:HA	1:C:364:ILE:HD11	1.95	0.49
1:C:320:TYR:OH	3:C:630:HOH:O	2.18	0.49
1:J:237:VAL:O	1:J:240:GLN:HB2	2.13	0.49
1:K:167:PHE:CZ	1:K:293:VAL:HG21	2.48	0.49
1:A:228:ASN:HD21	1:E:264:ILE:HG12	1.78	0.48
1:B:162:SER:OG	1:B:316:VAL:HG12	2.13	0.48
1:C:346:LEU:HD23	1:C:347:GLY:N	2.28	0.48
1:E:274:THR:N	1:E:279:GLU:OE1	2.41	0.48
1:I:118:TRP:O	1:I:122:ASN:ND2	2.32	0.48
1:K:190:LYS:HD3	3:K:642:HOH:O	2.12	0.48
1:K:213:LEU:HD23	1:K:256:VAL:HG12	1.94	0.48
1:A:213:LEU:HB3	1:A:256:VAL:HG12	1.95	0.48
1:B:165:VAL:HG23	1:B:303:SER:HB2	1.95	0.48
1:C:218:ALA:HA	1:C:270:TYR:CD2	2.47	0.48
1:D:320:TYR:HE2	1:D:347:GLY:CA	2.26	0.48
1:D:328:ALA:HB2	1:D:343:VAL:HG23	1.95	0.48
1:E:169:PRO:O	3:E:673:HOH:O	2.20	0.48
1:H:70:GLN:HB2	1:H:82:GLN:HB3	1.94	0.48
1:H:120:ARG:NH2	3:H:634:HOH:O	2.25	0.48
1:L:268:ILE:C	1:L:269:LEU:HD12	2.34	0.48
1:A:338:VAL:HB	3:A:650:HOH:O	2.13	0.48
1:E:2:ARG:HH12	1:E:387:SER:HB3	1.78	0.48
1:F:2:ARG:HG3	1:F:3:ASN:H	1.78	0.48
1:A:326:LEU:HB3	1:A:385:MET:HE1	1.96	0.48
1:D:27:LEU:O	3:D:678:HOH:O	2.20	0.48
1:D:249:ALA:O	1:D:252:TYR:HB2	2.14	0.48
1:E:207:ARG:NH2	1:F:5:ASN:HB2	2.27	0.48
1:H:2:ARG:NH1	1:H:387:SER:HB3	2.28	0.48
1:K:223:LEU:HD12	1:K:223:LEU:N	2.28	0.48
1:L:195:GLU:OE1	1:L:195:GLU:N	2.39	0.48
1:E:206:ARG:HD2	1:E:252:TYR:CZ	2.48	0.48
1:F:253:ASN:OD1	1:F:255:ARG:NH2	2.45	0.48
1:H:39:GLU:HA	1:H:309:GLY:HA2	1.95	0.48
1:I:243:ASP:HB3	3:I:604:HOH:O	2.13	0.48
1:L:354:ASP:HA	1:L:389:PHE:CE2	2.46	0.48
1:A:190:LYS:HD3	3:A:701:HOH:O	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:138:ILE:HG22	1:C:139:GLY:O	2.14	0.48
1:E:68:GLY:HA2	1:E:278:ALA:O	2.13	0.48
1:L:70:GLN:HB2	1:L:82:GLN:HB3	1.96	0.48
1:E:63:LYS:HE2	1:F:283:ASP:HB2	1.95	0.48
1:E:242:LEU:HG	3:E:661:HOH:O	2.13	0.48
1:G:6:VAL:CG1	1:G:378:ILE:HD11	2.44	0.48
1:I:20:GLU:HA	1:I:299:MET:SD	2.54	0.48
1:I:193:LEU:HD23	1:I:193:LEU:HA	1.70	0.48
1:I:373:GLU:HG2	1:I:374:THR:N	2.29	0.48
1:L:15:GLU:CG	1:L:171:THR:HB	2.44	0.48
1:L:171:THR:HG23	1:L:300:ARG:HH21	1.78	0.48
1:L:329:ASN:O	1:L:333:GLN:HG3	2.14	0.48
1:E:280:HIS:CE1	1:F:140:LYS:O	2.67	0.48
1:F:103:ASP:OD1	1:F:103:ASP:N	2.44	0.48
1:H:157:LEU:O	1:H:314:ASN:HB2	2.14	0.48
1:H:291:ARG:HG3	1:H:302:MET:HG2	1.96	0.48
1:I:280:HIS:CE1	1:J:140:LYS:O	2.67	0.48
1:A:71:ALA:N	1:A:280:HIS:HD2	2.05	0.48
1:A:320:TYR:OH	3:A:679:HOH:O	2.18	0.48
1:B:7:GLN:O	1:B:363:VAL:HG12	2.13	0.48
1:D:13:ASP:HA	3:D:676:HOH:O	2.13	0.48
1:D:230:TYR:CD2	1:D:269:LEU:HD23	2.49	0.48
1:D:301:PRO:HD2	3:D:635:HOH:O	2.12	0.48
1:E:238:ARG:NH2	3:E:717:HOH:O	2.46	0.48
1:F:163:PHE:HE1	1:F:165:VAL:HG22	1.79	0.48
1:F:244:LEU:HA	1:F:247:LYS:HD3	1.94	0.48
1:F:310:LYS:HA	3:F:667:HOH:O	2.13	0.48
1:H:235:GLU:O	1:H:239:ASN:ND2	2.47	0.48
1:A:263:LYS:HB2	1:A:268:ILE:HG12	1.96	0.47
1:A:323:LEU:HD21	1:A:386:LEU:HD11	1.96	0.47
1:D:220:ILE:HB	3:D:677:HOH:O	2.14	0.47
1:F:15:GLU:HG3	1:F:171:THR:HB	1.96	0.47
1:F:167:PHE:CZ	1:F:293:VAL:HG11	2.48	0.47
1:G:158:SER:O	1:G:349:ILE:HA	2.13	0.47
1:I:310:LYS:HE2	1:I:315:HIS:NE2	2.29	0.47
1:K:116:LYS:HB3	3:K:663:HOH:O	2.14	0.47
1:B:58:HIS:ND1	3:B:676:HOH:O	2.35	0.47
1:B:342:GLN:O	3:B:612:HOH:O	2.20	0.47
1:C:329:ASN:O	1:C:333:GLN:HG3	2.15	0.47
1:D:323:LEU:HB2	1:D:392:LEU:HD21	1.95	0.47
1:G:96:VAL:HG11	3:G:616:HOH:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:339:LYS:HG3	1:A:366:TYR:HE1	1.79	0.47
1:B:320:TYR:HE2	1:B:347:GLY:HA3	1.80	0.47
1:C:346:LEU:HD11	1:D:21:LEU:HD11	1.97	0.47
1:E:242:LEU:N	3:E:661:HOH:O	2.47	0.47
1:E:301:PRO:O	3:E:713:HOH:O	2.20	0.47
1:J:365:THR:C	1:J:367:ASP:H	2.18	0.47
1:K:160:ASP:OD1	1:K:161:THR:N	2.47	0.47
1:K:307:THR:OG1	1:K:403:LEU:HB3	2.14	0.47
1:L:382:VAL:O	1:L:386:LEU:HD13	2.14	0.47
1:C:195:GLU:OE1	1:C:195:GLU:N	2.46	0.47
1:D:142:SER:N	3:D:672:HOH:O	2.23	0.47
1:D:163:PHE:CZ	1:D:165:VAL:HG22	2.49	0.47
1:G:335:VAL:O	1:G:338:VAL:HG22	2.14	0.47
1:I:290:ASN:HB3	1:I:294:GLY:C	2.35	0.47
1:A:224:ILE:HD12	3:A:703:HOH:O	2.14	0.47
1:I:318:LYS:O	1:I:322:VAL:HG23	2.14	0.47
1:F:193:LEU:HA	1:F:193:LEU:HD23	1.71	0.47
3:F:704:HOH:O	1:G:83:PRO:HD3	2.14	0.47
1:L:6:VAL:CG1	1:L:378:ILE:HD11	2.45	0.47
1:L:224:ILE:HG21	1:L:271:LEU:HD21	1.97	0.47
1:L:321:ASN:ND2	3:L:623:HOH:O	2.48	0.47
1:A:255:ARG:HH21	1:E:246:SER:CB	2.27	0.47
1:A:385:MET:HE3	1:A:385:MET:HB3	1.60	0.47
1:B:111:ILE:O	1:B:114:SER:OG	2.21	0.47
1:B:296:ILE:HG22	1:B:298:PRO:HD3	1.95	0.47
1:D:378:ILE:HG13	1:D:379:SER:N	2.30	0.47
1:E:14:ILE:HB	1:E:17:LEU:HD12	1.96	0.47
1:E:230:TYR:HD1	3:E:712:HOH:O	1.98	0.47
1:G:238:ARG:HB2	1:G:256:VAL:CG2	2.44	0.47
1:H:108:GLY:O	1:H:112:ILE:HG12	2.14	0.47
1:J:127:ASP:OD1	1:J:130:ARG:HG3	2.14	0.47
1:A:6:VAL:HG11	1:A:378:ILE:HD11	1.97	0.47
1:E:167:PHE:CZ	1:E:293:VAL:HG21	2.50	0.47
1:E:381:ILE:HD12	3:E:671:HOH:O	2.15	0.47
1:G:201:LYS:NZ	1:H:160:ASP:OD2	2.43	0.47
1:L:305:GLU:HG2	2:L:501:PO4:O2	2.15	0.47
1:A:60:ASN:ND2	1:A:60:ASN:C	2.68	0.47
1:E:22:VAL:HG21	1:E:174:GLU:HG2	1.97	0.47
1:B:305:GLU:HB2	3:B:632:HOH:O	2.14	0.47
1:D:14:ILE:CD1	1:D:171:THR:HG21	2.38	0.47
1:G:178:TYR:HB2	1:G:295:LEU:HD21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:5:ASN:HD22	1:H:6:VAL:N	2.13	0.47
1:K:14:ILE:CD1	1:K:171:THR:HG21	2.43	0.47
1:L:161:THR:HG23	1:L:349:ILE:HG22	1.97	0.47
1:A:304:LEU:HD12	1:B:296:ILE:HG12	1.97	0.46
1:D:161:THR:HG23	1:D:349:ILE:HG22	1.97	0.46
1:D:270:TYR:OH	1:D:277:SER:HB3	2.15	0.46
1:F:117:GLU:OE1	1:F:120:ARG:NH1	2.47	0.46
1:F:403:LEU:HD22	3:F:662:HOH:O	2.14	0.46
1:G:195:GLU:OE1	1:G:195:GLU:N	2.40	0.46
1:H:354:ASP:HB2	1:H:386:LEU:O	2.15	0.46
1:I:91:ARG:HG3	3:J:617:HOH:O	2.15	0.46
1:J:75:PHE:CZ	1:J:227:VAL:HG22	2.50	0.46
1:J:356:PRO:HG2	1:J:386:LEU:HD21	1.97	0.46
1:B:316:VAL:HG13	1:B:320:TYR:CD2	2.49	0.46
1:D:373:GLU:HG2	1:D:374:THR:N	2.30	0.46
1:E:213:LEU:HB3	1:E:256:VAL:HG12	1.97	0.46
1:E:395:LEU:HA	1:E:398:GLU:OE2	2.16	0.46
1:H:161:THR:HG22	1:H:349:ILE:H	1.79	0.46
1:H:206:ARG:HD2	1:H:252:TYR:CZ	2.50	0.46
1:L:218:ALA:HB2	1:L:270:TYR:HE2	1.81	0.46
1:L:373:GLU:OE2	3:L:630:HOH:O	2.20	0.46
1:A:70:GLN:HG2	1:A:280:HIS:CD2	2.49	0.46
1:D:89:ALA:HB1	3:D:644:HOH:O	2.15	0.46
1:F:181:GLU:OE1	1:F:182:ARG:NH1	2.49	0.46
1:G:346:LEU:CD1	1:H:21:LEU:HD11	2.45	0.46
1:H:335:VAL:O	1:H:338:VAL:HG22	2.15	0.46
1:J:118:TRP:O	1:J:122:ASN:ND2	2.37	0.46
1:L:351:ARG:NE	1:L:355:ASP:O	2.43	0.46
1:A:339:LYS:N	3:A:650:HOH:O	2.48	0.46
1:C:222:GLU:HB2	1:C:223:LEU:HD12	1.97	0.46
1:E:91:ARG:HG3	3:E:680:HOH:O	2.15	0.46
1:H:392:LEU:O	1:H:396:ILE:HG13	2.15	0.46
1:J:373:GLU:HG2	1:J:374:THR:N	2.31	0.46
1:A:21:LEU:O	1:A:298:PRO:HD2	2.16	0.46
1:G:2:ARG:NH1	1:G:387:SER:HB3	2.29	0.46
1:H:14:ILE:CD1	1:H:171:THR:HG21	2.43	0.46
1:H:379:SER:O	1:H:383:ASP:HB2	2.16	0.46
1:J:230:TYR:CD2	1:J:269:LEU:HD23	2.51	0.46
1:L:56:ILE:HD11	1:L:397:LEU:HD11	1.97	0.46
1:A:58:HIS:HD2	3:A:647:HOH:O	1.97	0.46
1:A:162:SER:OG	1:A:316:VAL:HG23	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:LEU:HA	1:A:193:LEU:HD23	1.74	0.46
1:A:218:ALA:HA	1:A:270:TYR:CD2	2.51	0.46
1:B:165:VAL:HG12	1:B:166:GLY:N	2.31	0.46
1:B:248:ILE:HG22	3:B:685:HOH:O	2.16	0.46
1:D:217:MET:O	1:D:270:TYR:HD2	1.98	0.46
1:F:338:VAL:HG11	3:F:666:HOH:O	2.14	0.46
1:G:222:GLU:HB2	1:G:223:LEU:HD12	1.96	0.46
1:J:70:GLN:HB2	1:J:82:GLN:HB3	1.97	0.46
1:H:95:GLU:HB2	1:H:140:LYS:NZ	2.30	0.46
1:I:53:TYR:O	1:I:55:VAL:HG22	2.15	0.46
1:J:316:VAL:HG13	1:J:320:TYR:CD2	2.49	0.46
1:J:351:ARG:NE	1:J:355:ASP:O	2.43	0.46
1:A:14:ILE:HB	1:A:17:LEU:HD12	1.98	0.46
1:C:365:THR:HG23	1:C:367:ASP:HB2	1.98	0.46
1:D:268:ILE:C	1:D:269:LEU:HD12	2.36	0.46
1:E:19:VAL:HG21	1:F:360:ASN:HD21	1.81	0.46
1:E:307:THR:OG1	1:E:403:LEU:HB3	2.16	0.46
1:F:181:GLU:OE2	1:F:185:ASN:ND2	2.38	0.46
1:F:291:ARG:HG3	1:F:302:MET:HG2	1.97	0.46
1:H:340:PHE:O	1:H:364:ILE:N	2.48	0.46
1:C:340:PHE:HB2	1:C:364:ILE:HB	1.98	0.46
1:F:205:LEU:O	1:F:211:VAL:HA	2.16	0.46
1:H:365:THR:C	1:H:367:ASP:H	2.19	0.46
1:J:235:GLU:O	1:J:239:ASN:ND2	2.47	0.46
1:K:223:LEU:HD13	3:K:669:HOH:O	2.15	0.46
1:L:114:SER:HB2	3:L:667:HOH:O	2.15	0.46
1:A:58:HIS:CE1	3:A:646:HOH:O	2.68	0.46
1:B:301:PRO:HD2	3:B:671:HOH:O	2.15	0.46
1:H:268:ILE:C	1:H:269:LEU:HD12	2.36	0.46
1:H:403:LEU:HD13	3:H:631:HOH:O	2.16	0.46
1:I:310:LYS:O	1:I:318:LYS:NZ	2.41	0.46
1:L:373:GLU:HG2	1:L:374:THR:N	2.29	0.46
1:E:70:GLN:HA	1:E:280:HIS:CD2	2.50	0.45
1:E:223:LEU:N	1:E:223:LEU:HD12	2.31	0.45
1:E:310:LYS:HE2	1:E:315:HIS:NE2	2.30	0.45
1:I:20:GLU:OE1	1:I:206:ARG:NE	2.45	0.45
1:I:68:GLY:HA2	1:I:278:ALA:O	2.16	0.45
1:L:34:ALA:C	1:L:286:THR:HG22	2.36	0.45
1:L:328:ALA:HB2	1:L:343:VAL:HG23	1.98	0.45
1:B:116:LYS:HB3	3:B:654:HOH:O	2.16	0.45
1:C:238:ARG:HB2	1:C:256:VAL:HG23	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:304:LEU:HD23	1:C:304:LEU:HA	1.69	0.45
1:C:326:LEU:CB	1:C:385:MET:HE1	2.46	0.45
1:D:143:SER:HA	1:D:146:VAL:HG12	1.99	0.45
1:D:291:ARG:HG3	1:D:302:MET:HG2	1.96	0.45
1:E:181:GLU:OE1	1:E:182:ARG:HD2	2.16	0.45
1:E:238:ARG:HB2	1:E:256:VAL:CG2	2.46	0.45
1:F:310:LYS:HB2	1:F:318:LYS:HB2	1.98	0.45
1:G:14:ILE:HB	1:G:17:LEU:HD12	1.98	0.45
1:J:14:ILE:CD1	1:J:171:THR:HG21	2.36	0.45
1:A:17:LEU:O	1:A:206:ARG:NH2	2.39	0.45
1:E:8:LEU:HD12	1:E:363:VAL:HG13	1.97	0.45
1:E:346:LEU:HA	1:E:346:LEU:HD23	1.71	0.45
1:F:61:LEU:HD23	1:F:90:GLY:HA3	1.99	0.45
1:J:339:LYS:HB3	1:J:364:ILE:HG22	1.97	0.45
1:K:8:LEU:HD11	1:K:365:THR:HG22	1.99	0.45
1:L:199:ASP:HB2	1:L:276:THR:HA	1.97	0.45
1:L:212:ASP:OD1	1:L:255:ARG:HD2	2.17	0.45
1:L:296:ILE:HG22	1:L:298:PRO:HD3	1.97	0.45
1:B:323:LEU:HB2	1:B:392:LEU:HD21	1.98	0.45
1:D:15:GLU:HG3	1:D:171:THR:HB	1.98	0.45
1:D:345:VAL:HG22	3:D:662:HOH:O	2.15	0.45
1:E:291:ARG:HA	1:E:291:ARG:NE	2.32	0.45
1:G:238:ARG:HB2	1:G:256:VAL:HG23	1.99	0.45
1:G:304:LEU:HD12	1:H:296:ILE:HG23	1.98	0.45
1:I:21:LEU:O	1:I:298:PRO:HD2	2.16	0.45
1:I:63:LYS:HE2	1:J:283:ASP:HB2	1.98	0.45
1:I:283:ASP:OD2	1:J:90:GLY:HA2	2.16	0.45
1:J:56:ILE:HD11	1:J:397:LEU:HD11	1.99	0.45
1:K:4:ILE:HG21	1:K:379:SER:HB2	1.99	0.45
1:K:49:TYR:OH	1:K:93:THR:O	2.22	0.45
1:A:288:ARG:NH2	1:B:62:ASP:O	2.49	0.45
1:B:70:GLN:NE2	3:C:657:HOH:O	2.50	0.45
1:C:230:TYR:OH	1:C:262:ASP:OD2	2.25	0.45
1:D:120:ARG:NH2	1:D:129:GLU:OE2	2.50	0.45
1:D:356:PRO:HG2	1:D:386:LEU:HD21	1.97	0.45
1:K:20:GLU:HG2	1:K:173:LEU:HD23	1.99	0.45
1:K:319:LEU:HD23	1:K:319:LEU:HA	1.80	0.45
1:K:385:MET:HE3	1:K:385:MET:HB3	1.61	0.45
1:L:305:GLU:HB2	3:L:623:HOH:O	2.15	0.45
1:B:220:ILE:HB	1:B:223:LEU:HD13	1.98	0.45
1:B:360:ASN:OD1	1:B:361:VAL:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:207:ARG:NE	1:F:5:ASN:HD22	2.14	0.45
1:E:316:VAL:HG23	1:E:317:GLY:N	2.31	0.45
1:F:357:LEU:HB2	3:F:651:HOH:O	2.16	0.45
1:I:385:MET:HE3	1:I:385:MET:HB3	1.78	0.45
1:L:238:ARG:HB2	1:L:256:VAL:CG2	2.46	0.45
1:B:10:PRO:HA	1:B:364:ILE:HD11	1.98	0.45
1:C:346:LEU:CD1	1:D:21:LEU:HD11	2.47	0.45
1:E:210:GLU:HG2	1:E:253:ASN:HB3	1.98	0.45
1:E:217:MET:HB3	1:E:217:MET:HE2	1.78	0.45
1:G:68:GLY:HA2	1:G:278:ALA:O	2.17	0.45
1:H:112:ILE:HD11	1:H:136:TYR:HD1	1.82	0.45
1:H:120:ARG:NH2	1:H:129:GLU:OE2	2.49	0.45
1:H:207:ARG:O	1:H:210:GLU:HB2	2.17	0.45
1:H:322:VAL:O	1:H:326:LEU:HD13	2.17	0.45
1:J:164:GLY:HA2	1:J:321:ASN:ND2	2.32	0.45
1:K:273:VAL:H	1:K:279:GLU:CD	2.19	0.45
1:A:160:ASP:HA	3:A:706:HOH:O	2.16	0.45
1:A:201:LYS:HE3	3:B:636:HOH:O	2.16	0.45
1:B:320:TYR:HE2	1:B:347:GLY:CA	2.30	0.45
1:C:197:GLY:HA3	1:C:218:ALA:HB3	1.99	0.45
1:H:35:ASP:HA	1:H:286:THR:HG22	1.99	0.45
1:A:172:LYS:NZ	3:A:696:HOH:O	2.36	0.45
1:B:157:LEU:N	1:B:157:LEU:HD12	2.32	0.45
1:B:344:GLN:HG3	3:B:612:HOH:O	2.17	0.45
1:B:398:GLU:HB2	3:B:620:HOH:O	2.17	0.45
1:E:70:GLN:HG2	1:E:280:HIS:CD2	2.52	0.45
1:F:217:MET:CE	1:F:237:VAL:HG11	2.47	0.45
1:G:64:THR:HB	1:G:286:THR:HG23	1.99	0.45
1:H:195:GLU:OE1	1:H:195:GLU:N	2.45	0.45
1:J:268:ILE:C	1:J:269:LEU:HD12	2.38	0.45
1:B:112:ILE:HD11	1:B:136:TYR:HD1	1.82	0.45
1:C:290:ASN:HB2	1:C:404:PHE:O	2.17	0.45
1:G:281:GLY:CA	1:H:91:ARG:HE	2.30	0.45
1:H:181:GLU:OE1	1:H:182:ARG:HD2	2.17	0.45
1:A:298:PRO:O	1:B:301:PRO:HB3	2.17	0.44
1:B:104:GLN:HA	3:B:659:HOH:O	2.17	0.44
1:C:14:ILE:CD1	1:C:171:THR:HG21	2.39	0.44
1:F:329:ASN:O	1:F:333:GLN:HG3	2.17	0.44
1:G:14:ILE:CD1	1:G:171:THR:HG21	2.45	0.44
1:G:70:GLN:HB2	1:G:82:GLN:HB3	1.99	0.44
1:H:22:VAL:HG11	1:H:174:GLU:HA	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:399:GLY:HA2	3:H:674:HOH:O	2.16	0.44
1:I:190:LYS:HE3	1:I:196:VAL:O	2.17	0.44
1:J:169:PRO:HD2	1:J:340:PHE:HD1	1.82	0.44
1:J:321:ASN:ND2	3:J:619:HOH:O	2.50	0.44
1:B:351:ARG:NE	1:B:355:ASP:O	2.43	0.44
1:E:25:LYS:NZ	2:F:501:PO4:O2	2.46	0.44
1:H:38:ALA:HB1	1:H:61:LEU:O	2.17	0.44
1:I:374:THR:HG21	3:I:629:HOH:O	2.16	0.44
1:K:199:ASP:OD2	1:K:277:SER:OG	2.33	0.44
1:L:117:GLU:OE1	1:L:120:ARG:NH1	2.49	0.44
1:L:217:MET:HE2	1:L:217:MET:HB3	1.72	0.44
1:A:217:MET:CE	1:A:237:VAL:HG11	2.48	0.44
1:B:167:PHE:HB3	1:B:342:GLN:HB2	1.98	0.44
1:C:60:ASN:ND2	1:C:60:ASN:O	2.45	0.44
1:C:283:ASP:O	1:D:63:LYS:HE2	2.17	0.44
1:D:161:THR:CG2	1:D:349:ILE:H	2.30	0.44
1:E:326:LEU:CB	1:E:385:MET:HE1	2.47	0.44
1:I:15:GLU:HG3	1:I:171:THR:HB	2.00	0.44
1:J:6:VAL:CG1	1:J:378:ILE:HD11	2.48	0.44
1:J:162:SER:HB2	1:J:305:GLU:OE1	2.17	0.44
1:K:207:ARG:NH2	1:L:5:ASN:HB2	2.32	0.44
1:L:224:ILE:HG23	3:L:662:HOH:O	2.16	0.44
1:L:365:THR:C	1:L:367:ASP:H	2.21	0.44
1:A:339:LYS:HG3	1:A:366:TYR:CE1	2.52	0.44
1:B:311:ASN:HB3	1:B:315:HIS:HB2	1.98	0.44
1:E:330:LYS:HD3	1:E:381:ILE:HG23	1.98	0.44
1:J:249:ALA:O	1:J:252:TYR:HB2	2.17	0.44
1:K:157:LEU:HD21	1:K:350:GLY:HA2	1.98	0.44
1:A:231:ILE:HD11	1:A:264:ILE:HD11	1.99	0.44
1:D:95:GLU:HG2	1:D:104:GLN:OE1	2.17	0.44
1:D:217:MET:HE3	1:D:237:VAL:HG11	1.98	0.44
1:D:342:GLN:O	3:D:619:HOH:O	2.21	0.44
1:F:335:VAL:O	1:F:338:VAL:HG22	2.16	0.44
1:J:365:THR:O	1:J:367:ASP:N	2.39	0.44
1:D:199:ASP:HB2	1:D:276:THR:HA	1.98	0.44
1:E:83:PRO:O	3:E:622:HOH:O	2.21	0.44
1:F:93:THR:HA	3:F:684:HOH:O	2.17	0.44
1:F:178:TYR:HB2	1:F:295:LEU:HD21	1.99	0.44
1:A:22:VAL:HG11	1:A:174:GLU:HA	2.00	0.44
1:A:67:VAL:HG13	3:A:694:HOH:O	2.18	0.44
1:F:165:VAL:HG12	1:F:166:GLY:N	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:181:GLU:OE1	1:F:182:ARG:HD2	2.17	0.44
1:G:103:ASP:OD1	1:G:103:ASP:N	2.39	0.44
1:H:69:GLY:HA3	3:H:659:HOH:O	2.18	0.44
1:H:91:ARG:HG2	1:H:141:GLY:HA2	2.00	0.44
1:H:126:LEU:HD13	1:H:274:THR:HB	1.99	0.44
1:A:335:VAL:O	1:A:338:VAL:HG22	2.18	0.44
1:B:136:TYR:HD2	1:B:138:ILE:HG12	1.82	0.44
1:H:385:MET:HE3	1:H:385:MET:HB3	1.87	0.44
1:I:43:ARG:NH1	1:I:398:GLU:HA	2.33	0.44
1:I:69:GLY:O	1:I:70:GLN:HG3	2.17	0.44
1:A:5:ASN:N	3:A:663:HOH:O	2.50	0.44
1:D:91:ARG:HG2	1:D:141:GLY:HA2	2.00	0.44
1:G:318:LYS:O	1:G:322:VAL:HG23	2.18	0.44
1:G:351:ARG:HD3	1:G:355:ASP:O	2.17	0.44
1:H:14:ILE:HB	1:H:17:LEU:HD12	2.00	0.44
1:H:161:THR:HG22	1:H:348:GLN:HA	1.99	0.44
1:H:206:ARG:HD2	1:H:252:TYR:OH	2.18	0.44
1:I:270:TYR:O	1:I:270:TYR:HD2	2.01	0.44
1:L:103:ASP:OD1	1:L:103:ASP:N	2.46	0.44
1:L:142:SER:HB3	1:L:145:LEU:HD13	2.00	0.44
1:A:63:LYS:HE2	1:B:283:ASP:HB2	2.00	0.43
1:B:38:ALA:HB1	1:B:61:LEU:O	2.18	0.43
1:H:222:GLU:HB2	1:H:223:LEU:HD12	2.00	0.43
1:I:18:GLN:HB3	1:I:19:VAL:HG23	2.00	0.43
1:L:53:TYR:CZ	1:L:96:VAL:HG21	2.53	0.43
1:B:84:ILE:HA	3:B:696:HOH:O	2.17	0.43
1:B:110:ILE:HD12	3:B:691:HOH:O	2.17	0.43
1:B:325:ASN:HB2	3:B:627:HOH:O	2.17	0.43
1:D:195:GLU:HA	3:D:677:HOH:O	2.18	0.43
1:D:245:ALA:CB	1:D:254:VAL:HG21	2.47	0.43
1:G:25:LYS:HD2	1:G:289:GLY:HA2	2.00	0.43
1:H:44:LYS:HE3	3:H:636:HOH:O	2.18	0.43
1:H:76:LYS:HG3	1:H:225:GLU:HA	1.99	0.43
1:J:7:GLN:O	1:J:363:VAL:HG12	2.19	0.43
1:L:385:MET:HE3	1:L:385:MET:HB3	1.82	0.43
1:L:395:LEU:HA	1:L:398:GLU:OE2	2.18	0.43
1:B:307:THR:OG1	1:B:403:LEU:HB3	2.17	0.43
1:D:50:LEU:HD13	1:D:56:ILE:CG1	2.46	0.43
1:D:300:ARG:HG3	3:D:654:HOH:O	2.18	0.43
1:E:35:ASP:OD1	1:E:287:GLY:N	2.32	0.43
1:G:323:LEU:HB2	1:G:392:LEU:HD21	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:311:ASN:HB2	3:H:603:HOH:O	2.18	0.43
1:I:348:GLN:HB2	1:I:357:LEU:HD12	2.00	0.43
1:J:217:MET:CE	1:J:237:VAL:HG11	2.48	0.43
1:J:360:ASN:OD1	1:J:361:VAL:N	2.51	0.43
1:K:257:TYR:HB3	1:K:260:THR:CG2	2.48	0.43
1:B:373:GLU:HG2	1:B:374:THR:N	2.34	0.43
1:C:67:VAL:HG13	3:D:644:HOH:O	2.18	0.43
1:D:217:MET:O	1:D:270:TYR:CD2	2.71	0.43
1:E:315:HIS:O	1:E:319:LEU:HG	2.18	0.43
1:E:385:MET:HE3	1:E:385:MET:HB3	1.72	0.43
1:F:212:ASP:OD1	1:F:255:ARG:HD2	2.18	0.43
1:F:312:PRO:HB2	3:F:657:HOH:O	2.18	0.43
1:G:217:MET:HB3	1:G:217:MET:HE2	1.89	0.43
1:I:357:LEU:O	1:I:357:LEU:HD23	2.18	0.43
1:J:241:ILE:O	1:J:245:ALA:N	2.43	0.43
1:A:11:LEU:HD23	1:B:11:LEU:HG	2.01	0.43
1:A:296:ILE:HG12	1:B:304:LEU:HD12	2.00	0.43
1:B:193:LEU:HB3	1:B:196:VAL:HG23	2.00	0.43
1:B:290:ASN:ND2	1:B:404:PHE:O	2.35	0.43
1:C:19:VAL:HG21	1:D:360:ASN:HD21	1.80	0.43
1:C:268:ILE:C	1:C:269:LEU:HD12	2.38	0.43
1:C:355:ASP:N	1:C:356:PRO:HD3	2.33	0.43
1:E:56:ILE:HD12	1:E:313:VAL:HG23	2.00	0.43
1:F:22:VAL:HB	1:F:177:VAL:HG21	2.00	0.43
1:F:120:ARG:NH2	1:F:129:GLU:OE2	2.52	0.43
1:G:47:LEU:HD23	1:G:47:LEU:HA	1.74	0.43
1:H:29:HIS:HA	1:H:30:PRO:HD2	1.82	0.43
1:I:163:PHE:CZ	1:I:165:VAL:HG22	2.53	0.43
1:I:391:LYS:HD2	1:I:391:LYS:HA	1.78	0.43
1:J:165:VAL:HG23	1:J:303:SER:HB2	2.00	0.43
1:C:205:LEU:HD12	1:C:206:ARG:N	2.33	0.43
1:C:210:GLU:HG2	1:C:253:ASN:HB3	2.00	0.43
1:E:160:ASP:OD1	1:E:161:THR:N	2.50	0.43
1:F:304:LEU:HB2	3:F:658:HOH:O	2.18	0.43
1:J:340:PHE:O	1:J:364:ILE:N	2.49	0.43
1:K:375:LYS:HG3	3:K:648:HOH:O	2.18	0.43
1:A:281:GLY:H	1:B:91:ARG:HE	1.65	0.43
1:D:6:VAL:HG11	1:D:378:ILE:HD11	1.99	0.43
1:F:25:LYS:HD2	1:F:289:GLY:HA2	2.01	0.43
1:G:10:PRO:HA	1:G:364:ILE:HD11	2.01	0.43
1:G:48:TYR:OH	3:G:617:HOH:O	2.14	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:81:ILE:HD12	1:H:81:ILE:HG23	1.80	0.43
1:I:319:LEU:HD23	1:I:319:LEU:HA	1.88	0.43
1:J:23:GLU:HB3	1:J:296:ILE:HB	2.01	0.43
1:J:167:PHE:CZ	1:J:293:VAL:HG11	2.54	0.43
1:J:213:LEU:HD23	1:J:256:VAL:HG12	2.01	0.43
1:K:60:ASN:O	1:K:90:GLY:HA3	2.19	0.43
1:L:120:ARG:NH2	1:L:129:GLU:OE2	2.52	0.43
1:A:70:GLN:HA	1:A:280:HIS:CD2	2.53	0.43
1:A:207:ARG:NH2	1:B:5:ASN:HB2	2.34	0.43
1:C:373:GLU:HG2	1:C:374:THR:N	2.32	0.43
1:E:47:LEU:HA	1:E:47:LEU:HD23	1.78	0.43
1:G:120:ARG:NH2	1:G:129:GLU:OE2	2.52	0.43
1:H:104:GLN:HA	3:H:658:HOH:O	2.18	0.43
1:J:338:VAL:HA	1:J:365:THR:HG22	2.01	0.43
1:K:216:ALA:HB2	3:L:635:HOH:O	2.17	0.43
1:A:80:ILE:HG13	1:A:131:HIS:CD2	2.54	0.43
1:B:15:GLU:HG3	1:B:171:THR:HB	2.01	0.43
1:C:283:ASP:OD2	1:D:90:GLY:HA2	2.19	0.43
1:E:75:PHE:CZ	1:E:227:VAL:HG22	2.53	0.43
1:E:257:TYR:CD2	1:F:348:GLN:NE2	2.85	0.43
1:E:271:LEU:HD23	3:E:712:HOH:O	2.17	0.43
1:E:315:HIS:NE2	3:E:676:HOH:O	2.19	0.43
1:G:310:LYS:HE2	1:G:315:HIS:NE2	2.33	0.43
1:H:163:PHE:CE1	1:H:165:VAL:HG22	2.54	0.43
1:I:20:GLU:HG2	1:I:173:LEU:HD23	2.00	0.43
1:K:227:VAL:HG12	1:K:264:ILE:HD11	2.01	0.43
1:K:329:ASN:O	1:K:333:GLN:HG3	2.19	0.43
1:K:365:THR:C	1:K:367:ASP:H	2.22	0.43
1:L:230:TYR:CD2	1:L:269:LEU:HD23	2.54	0.43
1:L:318:LYS:O	1:L:322:VAL:HG23	2.19	0.43
1:A:58:HIS:CD2	3:A:647:HOH:O	2.72	0.43
1:A:91:ARG:HH21	1:B:282:ASP:N	2.16	0.43
1:B:53:TYR:CZ	1:B:96:VAL:HG21	2.54	0.43
1:E:245:ALA:HB1	1:E:254:VAL:HG21	2.01	0.43
1:F:360:ASN:OD1	1:F:361:VAL:N	2.52	0.43
1:K:14:ILE:HB	1:K:17:LEU:HD12	2.01	0.43
1:K:238:ARG:HB2	1:K:256:VAL:HG21	2.01	0.43
1:L:91:ARG:HG2	1:L:141:GLY:HA2	2.00	0.43
1:G:304:LEU:HD23	1:G:304:LEU:HA	1.69	0.42
1:H:357:LEU:HB2	3:H:666:HOH:O	2.19	0.42
1:H:374:THR:HA	3:H:644:HOH:O	2.17	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:136:TYR:HD2	1:K:138:ILE:HG12	1.84	0.42
1:K:163:PHE:HE1	1:K:344:GLN:HB3	1.84	0.42
1:K:326:LEU:CB	1:K:385:MET:HE1	2.49	0.42
1:L:51:LYS:NZ	3:L:651:HOH:O	2.49	0.42
1:L:266:LYS:HA	1:L:266:LYS:HD3	1.81	0.42
1:D:346:LEU:HA	1:D:346:LEU:HD12	1.66	0.42
1:F:6:VAL:HB	1:F:375:LYS:HE3	2.00	0.42
1:G:22:VAL:HG21	1:G:174:GLU:HG2	2.01	0.42
1:I:112:ILE:HD12	1:I:134:VAL:HB	2.00	0.42
1:L:294:GLY:HA3	3:L:642:HOH:O	2.17	0.42
1:A:125:TYR:HB2	1:A:274:THR:O	2.19	0.42
1:D:7:GLN:O	1:D:363:VAL:HG12	2.18	0.42
1:D:27:LEU:HA	1:D:32:TYR:CE1	2.55	0.42
1:E:19:VAL:HG11	1:F:360:ASN:HD22	1.85	0.42
1:F:23:GLU:HB3	1:F:296:ILE:HB	2.01	0.42
1:F:230:TYR:CD2	1:F:269:LEU:HD23	2.54	0.42
1:J:217:MET:HB3	1:J:217:MET:HE2	1.86	0.42
1:K:342:GLN:HG3	3:K:638:HOH:O	2.19	0.42
1:L:49:TYR:HB3	1:L:55:VAL:O	2.19	0.42
1:L:217:MET:CE	1:L:237:VAL:HG11	2.49	0.42
1:A:207:ARG:NE	1:B:5:ASN:HD22	2.15	0.42
1:B:163:PHE:CZ	1:B:165:VAL:HG22	2.55	0.42
1:C:76:LYS:HG3	1:C:225:GLU:HA	2.01	0.42
1:C:281:GLY:H	1:D:91:ARG:HE	1.66	0.42
1:C:357:LEU:HD23	1:C:357:LEU:O	2.20	0.42
1:D:27:LEU:HG	3:D:678:HOH:O	2.18	0.42
1:D:127:ASP:OD1	1:D:130:ARG:HG3	2.20	0.42
1:G:29:HIS:HA	1:G:30:PRO:HD2	1.91	0.42
1:H:25:LYS:HD2	1:H:289:GLY:HA2	2.00	0.42
1:H:311:ASN:ND2	1:H:314:ASN:OD1	2.53	0.42
1:I:235:GLU:O	1:I:239:ASN:ND2	2.52	0.42
1:J:263:LYS:HB2	1:J:268:ILE:HG13	2.01	0.42
1:K:205:LEU:HD12	1:K:206:ARG:N	2.35	0.42
1:L:354:ASP:HB2	1:L:386:LEU:O	2.19	0.42
1:A:12:SER:O	3:A:666:HOH:O	2.21	0.42
1:A:143:SER:HA	3:A:697:HOH:O	2.18	0.42
1:A:222:GLU:HG3	3:A:683:HOH:O	2.18	0.42
1:F:106:PRO:O	1:F:110:ILE:HG13	2.19	0.42
1:F:222:GLU:HB2	1:F:223:LEU:HD12	2.02	0.42
1:G:291:ARG:NH1	1:G:304:LEU:HA	2.35	0.42
1:I:346:LEU:HD11	1:J:21:LEU:HD11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:351:ARG:NH2	1:J:355:ASP:OD2	2.52	0.42
1:B:164:GLY:O	3:B:650:HOH:O	2.22	0.42
1:C:340:PHE:O	1:C:364:ILE:N	2.52	0.42
1:F:161:THR:CG2	1:F:349:ILE:H	2.30	0.42
1:J:103:ASP:OD1	1:J:103:ASP:N	2.41	0.42
1:A:231:ILE:HD11	1:A:264:ILE:HG12	2.02	0.42
1:C:22:VAL:HG11	1:C:174:GLU:HA	2.01	0.42
1:E:290:ASN:HB2	1:E:404:PHE:O	2.20	0.42
1:E:391:LYS:HD2	1:E:394:GLU:HB3	2.02	0.42
1:F:2:ARG:HG3	3:F:702:HOH:O	2.20	0.42
1:H:164:GLY:HA2	1:H:321:ASN:ND2	2.35	0.42
1:I:270:TYR:CD1	3:J:633:HOH:O	2.56	0.42
1:J:357:LEU:HD23	1:J:357:LEU:O	2.20	0.42
1:J:382:VAL:O	1:J:386:LEU:HD13	2.20	0.42
1:A:231:ILE:HD11	1:A:264:ILE:CD1	2.50	0.42
1:C:52:LYS:HB3	1:C:52:LYS:HE3	1.86	0.42
1:C:53:TYR:O	1:C:55:VAL:HG22	2.20	0.42
1:C:207:ARG:HD2	1:D:358:ILE:HD12	2.02	0.42
1:D:64:THR:HB	1:D:286:THR:HG23	2.02	0.42
1:E:38:ALA:HB2	1:E:64:THR:OG1	2.20	0.42
1:F:161:THR:HG23	1:F:349:ILE:HG22	2.01	0.42
1:F:302:MET:HE2	1:F:302:MET:HB2	1.89	0.42
1:I:106:PRO:O	1:I:110:ILE:HG13	2.20	0.42
1:I:200:ILE:HA	1:I:216:ALA:O	2.19	0.42
1:J:171:THR:HG23	1:J:300:ARG:HH21	1.84	0.42
1:J:212:ASP:OD1	1:J:255:ARG:HD2	2.19	0.42
1:J:224:ILE:HG21	1:J:271:LEU:HD21	2.02	0.42
1:A:53:TYR:O	1:A:55:VAL:HG22	2.20	0.42
1:D:178:TYR:HE2	3:D:647:HOH:O	2.02	0.42
1:D:296:ILE:HG22	1:D:298:PRO:HD3	2.00	0.42
1:E:7:GLN:O	1:E:363:VAL:HG12	2.20	0.42
1:F:249:ALA:O	1:F:252:TYR:HB2	2.20	0.42
1:G:160:ASP:OD1	1:G:161:THR:N	2.52	0.42
1:H:165:VAL:HG12	1:H:166:GLY:N	2.35	0.42
1:I:257:TYR:HB3	1:I:260:THR:CG2	2.50	0.42
1:J:25:LYS:HD2	1:J:289:GLY:HA2	2.01	0.42
1:L:142:SER:HB3	1:L:145:LEU:CD1	2.50	0.42
1:A:158:SER:HA	1:A:316:VAL:HG11	2.02	0.42
1:A:206:ARG:HD2	1:A:252:TYR:CZ	2.55	0.42
1:B:375:LYS:HE2	1:B:375:LYS:HB3	1.76	0.42
1:D:39:GLU:HA	1:D:309:GLY:HA2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:63:LYS:N	3:D:641:HOH:O	2.52	0.42
1:D:64:THR:HB	1:D:286:THR:CG2	2.50	0.42
1:D:218:ALA:HA	1:D:270:TYR:HD2	1.84	0.42
1:D:318:LYS:O	1:D:322:VAL:HG23	2.20	0.42
1:E:130:ARG:NE	3:E:699:HOH:O	2.53	0.42
1:G:9:ASN:O	1:G:12:SER:HB3	2.20	0.42
1:G:281:GLY:H	1:H:91:ARG:HE	1.68	0.42
1:G:378:ILE:HG13	1:G:379:SER:N	2.34	0.42
1:H:22:VAL:HB	1:H:177:VAL:HG21	2.02	0.42
1:H:23:GLU:HB3	1:H:296:ILE:HB	2.02	0.42
1:L:22:VAL:HB	1:L:177:VAL:HG21	2.00	0.42
1:A:224:ILE:HG21	1:A:271:LEU:HD21	2.01	0.41
1:A:356:PRO:HG2	1:A:386:LEU:HD21	2.02	0.41
1:C:126:LEU:HD12	1:C:126:LEU:HA	1.85	0.41
1:D:8:LEU:HD12	1:D:363:VAL:HG13	2.00	0.41
1:D:354:ASP:HA	1:D:389:PHE:HE2	1.84	0.41
1:E:50:LEU:HD13	1:E:56:ILE:HG13	2.02	0.41
1:F:230:TYR:CG	1:F:269:LEU:HD23	2.54	0.41
1:F:305:GLU:HB2	3:F:656:HOH:O	2.19	0.41
1:G:62:ASP:OD2	1:G:310:LYS:NZ	2.43	0.41
1:G:70:GLN:HA	1:G:280:HIS:CD2	2.55	0.41
1:I:11:LEU:HD23	1:J:11:LEU:HG	2.01	0.41
1:I:19:VAL:HG11	1:J:360:ASN:HD22	1.85	0.41
1:I:207:ARG:HE	1:J:5:ASN:ND2	2.16	0.41
1:J:38:ALA:HB1	1:J:61:LEU:O	2.20	0.41
1:K:291:ARG:HA	1:K:291:ARG:NE	2.35	0.41
1:L:52:LYS:C	1:L:54:GLY:H	2.19	0.41
1:B:80:ILE:HG13	1:B:131:HIS:CD2	2.55	0.41
1:C:335:VAL:O	1:C:338:VAL:HG22	2.21	0.41
1:D:22:VAL:HB	1:D:177:VAL:HG21	2.02	0.41
1:D:76:LYS:HG3	1:D:225:GLU:HA	2.01	0.41
1:D:163:PHE:CE1	1:D:165:VAL:HG22	2.55	0.41
1:D:213:LEU:HB3	1:D:256:VAL:HG12	2.02	0.41
1:D:238:ARG:HB2	1:D:256:VAL:CG2	2.50	0.41
1:F:15:GLU:CG	1:F:171:THR:HB	2.51	0.41
1:F:375:LYS:HE2	1:F:375:LYS:HB3	1.81	0.41
1:H:74:ARG:HD3	3:H:621:HOH:O	2.20	0.41
1:H:165:VAL:HG23	1:H:303:SER:HB2	2.02	0.41
1:H:223:LEU:HD12	1:H:223:LEU:N	2.35	0.41
1:H:270:TYR:OH	1:H:277:SER:HB3	2.20	0.41
1:H:354:ASP:HA	1:H:389:PHE:CE2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:245:ALA:HB1	1:K:254:VAL:HG21	2.01	0.41
1:K:354:ASP:C	1:K:356:PRO:HD3	2.39	0.41
1:L:281:GLY:N	3:L:632:HOH:O	2.53	0.41
1:A:19:VAL:HG21	1:B:360:ASN:HD21	1.83	0.41
1:C:222:GLU:HG3	3:C:683:HOH:O	2.20	0.41
1:D:62:ASP:CG	1:D:310:LYS:HD3	2.41	0.41
1:D:165:VAL:HG12	1:D:166:GLY:N	2.35	0.41
1:D:357:LEU:O	1:D:357:LEU:HD23	2.20	0.41
1:E:91:ARG:HH21	1:F:282:ASP:N	2.18	0.41
1:F:217:MET:HB3	1:F:217:MET:HE2	1.87	0.41
1:H:71:ALA:HB2	1:H:80:ILE:HD13	2.02	0.41
1:H:199:ASP:HB2	1:H:276:THR:HA	2.01	0.41
1:I:85:TYR:CD2	1:J:137:LYS:HD2	2.55	0.41
1:J:90:GLY:O	1:J:91:ARG:HD2	2.20	0.41
1:J:222:GLU:HB2	1:J:223:LEU:HD12	2.02	0.41
1:K:57:LEU:HD22	1:K:93:THR:HG21	2.01	0.41
1:C:319:LEU:HD23	1:C:319:LEU:HA	1.78	0.41
1:D:165:VAL:HG23	1:D:303:SER:HB2	2.02	0.41
1:E:53:TYR:CZ	1:E:96:VAL:HG21	2.54	0.41
1:E:80:ILE:HG13	1:E:131:HIS:CD2	2.55	0.41
1:H:95:GLU:HG2	3:H:658:HOH:O	2.21	0.41
1:H:373:GLU:HG2	1:H:374:THR:N	2.34	0.41
1:J:218:ALA:HA	1:J:270:TYR:CD2	2.55	0.41
1:L:9:ASN:HA	1:L:10:PRO:HD3	1.77	0.41
1:L:183:HIS:O	1:L:186:SER:HB3	2.20	0.41
1:B:120:ARG:NH2	3:B:654:HOH:O	2.28	0.41
1:B:217:MET:HB3	1:B:217:MET:HE2	1.85	0.41
1:D:49:TYR:O	1:D:52:LYS:O	2.39	0.41
1:E:217:MET:CE	1:E:237:VAL:HG11	2.50	0.41
1:F:268:ILE:HD13	1:F:268:ILE:HG21	1.84	0.41
1:H:170:LEU:HB3	1:H:174:GLU:HB2	2.01	0.41
1:H:274:THR:N	1:H:279:GLU:OE1	2.50	0.41
1:H:328:ALA:HB2	1:H:343:VAL:HG23	2.02	0.41
1:H:360:ASN:OD1	1:H:361:VAL:N	2.54	0.41
1:K:71:ALA:N	1:K:280:HIS:HD2	2.03	0.41
1:L:237:VAL:O	1:L:240:GLN:HB2	2.20	0.41
1:F:33:ILE:O	1:F:37:VAL:HG22	2.20	0.41
1:F:53:TYR:O	1:F:55:VAL:N	2.52	0.41
1:F:209:ASN:O	1:F:253:ASN:N	2.43	0.41
1:F:305:GLU:HG3	3:F:627:HOH:O	2.21	0.41
1:F:394:GLU:HG3	3:F:680:HOH:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:281:GLY:H	1:H:91:ARG:HH21	1.68	0.41
1:H:81:ILE:HD13	1:H:81:ILE:HA	1.70	0.41
1:H:234:LYS:NZ	1:H:259:ASN:HB2	2.35	0.41
1:H:365:THR:O	1:H:367:ASP:N	2.49	0.41
1:J:263:LYS:HB2	1:J:268:ILE:CG1	2.50	0.41
1:J:365:THR:C	1:J:367:ASP:N	2.74	0.41
1:K:69:GLY:O	1:K:70:GLN:HG3	2.20	0.41
1:K:212:ASP:OD2	1:L:357:LEU:HD21	2.20	0.41
1:K:222:GLU:HB2	1:K:223:LEU:HD12	2.01	0.41
1:L:161:THR:HG22	1:L:348:GLN:HA	2.03	0.41
1:B:105:ILE:HG23	1:B:105:ILE:HD12	1.71	0.41
1:D:29:HIS:HA	1:D:30:PRO:HD2	1.90	0.41
1:E:199:ASP:OD2	1:E:277:SER:OG	2.23	0.41
1:G:60:ASN:OD1	1:G:60:ASN:C	2.58	0.41
1:G:140:LYS:NZ	3:G:638:HOH:O	2.33	0.41
1:H:377:GLU:HB2	3:H:644:HOH:O	2.21	0.41
1:I:9:ASN:O	1:I:12:SER:HB3	2.21	0.41
1:I:201:LYS:NZ	1:J:160:ASP:OD2	2.53	0.41
1:I:238:ARG:HB2	1:I:256:VAL:CG2	2.51	0.41
1:J:310:LYS:HB2	1:J:318:LYS:HB2	2.03	0.41
1:J:329:ASN:O	1:J:333:GLN:HG3	2.20	0.41
1:K:138:ILE:HG22	1:K:139:GLY:O	2.20	0.41
1:K:210:GLU:HG2	1:K:253:ASN:HB3	2.03	0.41
1:L:80:ILE:HD12	1:L:80:ILE:HG23	1.82	0.41
1:L:184:LEU:HB3	1:L:200:ILE:HD13	2.01	0.41
1:L:363:VAL:HG22	1:L:364:ILE:N	2.36	0.41
1:A:15:GLU:HG3	1:A:171:THR:HB	2.01	0.41
1:A:103:ASP:OD1	1:A:103:ASP:N	2.44	0.41
1:D:53:TYR:CZ	1:D:96:VAL:HG21	2.55	0.41
1:E:318:LYS:O	1:E:322:VAL:HG23	2.21	0.41
3:E:650:HOH:O	1:F:288:ARG:HG2	2.19	0.41
1:F:356:PRO:HG2	1:F:386:LEU:HD21	2.03	0.41
1:H:310:LYS:HB2	1:H:318:LYS:HB2	2.02	0.41
1:I:197:GLY:HA3	1:I:218:ALA:CB	2.51	0.41
1:A:53:TYR:CZ	1:A:96:VAL:HG21	2.56	0.41
1:A:68:GLY:HA2	1:A:278:ALA:O	2.21	0.41
1:A:394:GLU:O	1:A:394:GLU:HG2	2.21	0.41
1:B:14:ILE:HB	1:B:17:LEU:HD12	2.02	0.41
1:B:162:SER:O	1:B:346:LEU:HD12	2.21	0.41
1:B:181:GLU:OE1	1:B:182:ARG:HD2	2.21	0.41
1:B:306:ALA:O	1:B:310:LYS:NZ	2.32	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:84:ILE:N	1:C:131:HIS:O	2.42	0.41
1:C:237:VAL:O	1:C:240:GLN:HB2	2.20	0.41
1:C:297:THR:HA	1:C:298:PRO:HD2	1.93	0.41
1:C:351:ARG:HD3	1:C:355:ASP:O	2.21	0.41
1:E:43:ARG:NH1	1:E:398:GLU:HA	2.36	0.41
1:F:163:PHE:CE1	1:F:165:VAL:CG2	3.04	0.41
1:G:20:GLU:HA	1:G:299:MET:SD	2.61	0.41
1:G:71:ALA:HB2	1:G:80:ILE:HD13	2.02	0.41
1:G:96:VAL:HG21	3:G:616:HOH:O	2.20	0.41
1:H:193:LEU:HD23	1:H:193:LEU:HA	1.86	0.41
1:I:186:SER:HB3	1:I:189:PHE:HB3	2.02	0.41
1:I:210:GLU:HG2	1:I:253:ASN:HB3	2.01	0.41
1:I:353:ILE:HG13	1:I:389:PHE:CE2	2.56	0.41
1:J:53:TYR:CZ	1:J:96:VAL:HG21	2.56	0.41
1:K:22:VAL:HG21	1:K:174:GLU:CG	2.50	0.41
1:K:292:GLY:O	1:K:402:THR:OG1	2.31	0.41
1:L:8:LEU:HD12	1:L:363:VAL:HG13	2.03	0.41
1:L:29:HIS:HA	1:L:30:PRO:HD2	1.87	0.41
1:L:205:LEU:HD12	1:L:206:ARG:N	2.36	0.41
1:L:320:TYR:HE2	1:L:347:GLY:CA	2.34	0.41
1:A:257:TYR:HB3	1:A:260:THR:CG2	2.51	0.41
1:B:155:VAL:HA	1:B:156:PRO:HD3	1.87	0.41
1:B:238:ARG:HB2	1:B:256:VAL:CG2	2.51	0.41
1:D:311:ASN:ND2	1:D:314:ASN:OD1	2.54	0.41
1:D:325:ASN:HB2	3:D:630:HOH:O	2.19	0.41
1:E:169:PRO:HD2	1:E:340:PHE:HD1	1.85	0.41
1:E:259:ASN:HA	3:E:714:HOH:O	2.21	0.41
1:E:351:ARG:HG2	1:E:355:ASP:O	2.21	0.41
1:F:90:GLY:O	1:F:91:ARG:HD2	2.20	0.41
1:F:340:PHE:O	1:F:364:ILE:N	2.54	0.41
1:G:260:THR:HG21	1:H:348:GLN:NE2	2.36	0.41
1:K:304:LEU:HD23	1:K:304:LEU:HA	1.81	0.41
1:L:339:LYS:HG3	1:L:366:TYR:CE1	2.56	0.41
1:C:268:ILE:O	1:C:268:ILE:HG13	2.21	0.40
1:D:218:ALA:HA	1:D:270:TYR:CD2	2.56	0.40
1:E:264:ILE:HD12	1:E:264:ILE:HA	1.94	0.40
1:F:268:ILE:C	1:F:269:LEU:HD12	2.42	0.40
1:G:217:MET:CE	1:G:237:VAL:HG11	2.51	0.40
1:H:217:MET:HB3	1:H:217:MET:HE2	1.95	0.40
1:H:356:PRO:HG2	1:H:386:LEU:HD21	2.03	0.40
1:I:356:PRO:HG2	1:I:386:LEU:HD21	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:ALA:HB2	1:A:80:ILE:HD13	2.03	0.40
1:A:95:GLU:O	1:A:142:SER:HA	2.22	0.40
1:B:127:ASP:OD1	1:B:130:ARG:HG3	2.21	0.40
1:F:64:THR:HB	1:F:286:THR:HG23	2.04	0.40
1:J:217:MET:O	1:J:270:TYR:CD2	2.73	0.40
1:L:161:THR:CG2	1:L:349:ILE:H	2.34	0.40
1:L:323:LEU:HD21	1:L:386:LEU:HD12	2.04	0.40
1:A:60:ASN:O	1:A:90:GLY:HA3	2.22	0.40
1:A:280:HIS:CE1	1:B:140:LYS:O	2.75	0.40
1:B:3:ASN:HB2	3:B:642:HOH:O	2.22	0.40
1:D:195:GLU:OE1	1:D:195:GLU:N	2.47	0.40
1:D:319:LEU:HA	1:D:319:LEU:HD23	1.93	0.40
1:F:394:GLU:O	1:F:394:GLU:HG2	2.22	0.40
1:G:211:VAL:HB	1:G:254:VAL:HG12	2.03	0.40
1:H:329:ASN:O	1:H:333:GLN:HG3	2.20	0.40
1:I:222:GLU:HB2	1:I:223:LEU:HD12	2.03	0.40
1:J:46:SER:OG	1:J:59:HIS:CE1	2.74	0.40
1:L:224:ILE:HD12	3:L:662:HOH:O	2.21	0.40
1:A:167:PHE:CZ	1:A:293:VAL:HG21	2.56	0.40
1:B:142:SER:N	3:B:630:HOH:O	2.48	0.40
1:B:229:HIS:CE1	3:B:690:HOH:O	2.74	0.40
1:B:230:TYR:CD2	1:B:269:LEU:HD23	2.57	0.40
1:C:138:ILE:HD13	1:C:138:ILE:HA	1.85	0.40
1:C:205:LEU:HD12	1:C:206:ARG:H	1.87	0.40
1:D:322:VAL:O	1:D:326:LEU:HD13	2.22	0.40
1:E:206:ARG:NH1	1:E:208:GLY:O	2.54	0.40
1:F:217:MET:O	1:F:270:TYR:CD2	2.75	0.40
1:F:365:THR:C	1:F:367:ASP:H	2.24	0.40
1:G:283:ASP:OD2	1:H:90:GLY:HA2	2.21	0.40
1:H:56:ILE:HD11	1:H:397:LEU:HD11	2.01	0.40
1:J:155:VAL:HA	1:J:156:PRO:HD3	1.82	0.40
3:K:654:HOH:O	1:L:25:LYS:NZ	2.55	0.40
1:L:21:LEU:O	1:L:298:PRO:HD2	2.22	0.40
1:C:280:HIS:CE1	1:D:142:SER:HA	2.56	0.40
1:D:14:ILE:HD13	3:D:654:HOH:O	2.21	0.40
1:E:192:LYS:HA	1:E:192:LYS:HD2	1.75	0.40
1:E:205:LEU:HD12	1:E:206:ARG:H	1.86	0.40
1:E:269:LEU:HD12	1:E:269:LEU:N	2.37	0.40
1:E:348:GLN:HB2	1:E:357:LEU:HD12	2.02	0.40
1:E:356:PRO:HG2	1:E:386:LEU:HD21	2.03	0.40
1:G:252:TYR:HD1	1:G:252:TYR:HA	1.77	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:106:PRO:O	1:H:110:ILE:HG13	2.22	0.40
1:I:268:ILE:C	1:I:269:LEU:HD12	2.42	0.40
1:K:167:PHE:CE2	1:K:293:VAL:HG21	2.56	0.40
1:K:288:ARG:NH2	1:L:62:ASP:O	2.48	0.40
1:L:155:VAL:N	3:L:647:HOH:O	2.53	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	385/413 (93%)	371 (96%)	13 (3%)	1 (0%)	41	72
1	B	386/413 (94%)	372 (96%)	12 (3%)	2 (0%)	29	61
1	C	385/413 (93%)	370 (96%)	14 (4%)	1 (0%)	41	72
1	D	386/413 (94%)	372 (96%)	12 (3%)	2 (0%)	29	61
1	E	385/413 (93%)	372 (97%)	12 (3%)	1 (0%)	41	72
1	F	386/413 (94%)	369 (96%)	14 (4%)	3 (1%)	19	49
1	G	385/413 (93%)	370 (96%)	13 (3%)	2 (0%)	29	61
1	H	386/413 (94%)	371 (96%)	13 (3%)	2 (0%)	29	61
1	I	385/413 (93%)	370 (96%)	14 (4%)	1 (0%)	41	72
1	J	386/413 (94%)	371 (96%)	13 (3%)	2 (0%)	29	61
1	K	385/413 (93%)	369 (96%)	14 (4%)	2 (0%)	29	61
1	L	386/413 (94%)	372 (96%)	12 (3%)	2 (0%)	29	61
All	All	4626/4956 (93%)	4449 (96%)	156 (3%)	21 (0%)	29	61

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	53	TYR
1	D	53	TYR
1	F	53	TYR
1	G	3	ASN
1	H	53	TYR
1	J	53	TYR
1	L	53	TYR
1	F	54	GLY
1	A	366	TYR
1	D	366	TYR
1	H	366	TYR
1	K	3	ASN
1	K	366	TYR
1	L	366	TYR
1	B	366	TYR
1	C	366	TYR
1	E	366	TYR
1	G	366	TYR
1	I	366	TYR
1	J	366	TYR
1	F	366	TYR

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	336/354 (95%)	332 (99%)	4 (1%)	71	92
1	B	336/354 (95%)	333 (99%)	3 (1%)	78	94
1	C	336/354 (95%)	331 (98%)	5 (2%)	65	89
1	D	336/354 (95%)	333 (99%)	3 (1%)	78	94
1	E	336/354 (95%)	332 (99%)	4 (1%)	71	92
1	F	336/354 (95%)	333 (99%)	3 (1%)	78	94
1	G	336/354 (95%)	329 (98%)	7 (2%)	53	84
1	H	336/354 (95%)	328 (98%)	8 (2%)	49	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	I	336/354 (95%)	334 (99%)	2 (1%)	86 96
1	J	336/354 (95%)	333 (99%)	3 (1%)	78 94
1	K	336/354 (95%)	330 (98%)	6 (2%)	59 86
1	L	336/354 (95%)	333 (99%)	3 (1%)	78 94
All	All	4032/4248 (95%)	3981 (99%)	51 (1%)	69 91

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	60	ASN
1	A	299	MET
1	A	365	THR
1	B	91	ARG
1	B	276	THR
1	B	299	MET
1	C	1	MET
1	C	2	ARG
1	C	60	ASN
1	C	299	MET
1	C	316	VAL
1	D	91	ARG
1	D	276	THR
1	D	299	MET
1	E	60	ASN
1	E	87	ILE
1	E	276	THR
1	E	299	MET
1	F	91	ARG
1	F	163	PHE
1	F	299	MET
1	G	1	MET
1	G	2	ARG
1	G	3	ASN
1	G	60	ASN
1	G	87	ILE
1	G	299	MET
1	G	316	VAL
1	H	2	ARG
1	H	5	ASN
1	H	87	ILE

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Mol	Chain	Res	Type
1	H	91	ARG
1	H	299	MET
1	H	316	VAL
1	H	374	THR
1	H	383	ASP
1	I	299	MET
1	I	365	THR
1	J	87	ILE
1	J	91	ARG
1	J	299	MET
1	K	1	MET
1	K	2	ARG
1	K	87	ILE
1	K	186	SER
1	K	299	MET
1	K	316	VAL
1	L	91	ARG
1	L	299	MET
1	L	374	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	280	HIS
1	B	70	GLN
1	C	121	ASN
1	C	280	HIS
1	D	5	ASN
1	E	60	ASN
1	E	280	HIS
1	F	315	HIS
1	F	348	GLN
1	G	280	HIS
1	I	60	ASN
1	I	280	HIS
1	J	5	ASN
1	K	60	ASN
1	K	280	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

18 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	PO4	B	501	-	4,4,4	1.02	0	6,6,6	0.47	0
2	PO4	D	501	-	4,4,4	1.05	0	6,6,6	0.79	0
2	PO4	E	502	-	4,4,4	1.04	0	6,6,6	0.50	0
2	PO4	H	501	-	4,4,4	1.01	0	6,6,6	0.58	0
2	PO4	E	501	-	4,4,4	1.07	0	6,6,6	0.57	0
2	PO4	A	501	-	4,4,4	1.16	0	6,6,6	0.29	0
2	PO4	I	502	-	4,4,4	0.99	0	6,6,6	0.47	0
2	PO4	G	501	-	4,4,4	1.12	0	6,6,6	0.77	0
2	PO4	J	501	-	4,4,4	1.00	0	6,6,6	0.49	0
2	PO4	L	501	-	4,4,4	1.22	0	6,6,6	0.59	0
2	PO4	F	501	-	4,4,4	1.10	0	6,6,6	0.57	0
2	PO4	I	501	-	4,4,4	1.07	0	6,6,6	0.41	0
2	PO4	D	502	-	4,4,4	0.96	0	6,6,6	0.44	0
2	PO4	K	501	-	4,4,4	1.12	0	6,6,6	0.50	0
2	PO4	G	502	-	4,4,4	0.99	0	6,6,6	0.50	0
2	PO4	A	502	-	4,4,4	1.04	0	6,6,6	0.46	0
2	PO4	C	501	-	4,4,4	1.08	0	6,6,6	0.65	0
2	PO4	K	502	-	4,4,4	0.98	0	6,6,6	0.46	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	501	PO4	1	0
2	A	501	PO4	1	0
2	G	501	PO4	2	0
2	J	501	PO4	1	0
2	L	501	PO4	2	0
2	F	501	PO4	1	0
2	A	502	PO4	2	0
2	C	501	PO4	1	0

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

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	391/413 (94%)	-0.37	5 (1%)	77	72	23, 40, 71, 132	0
1	B	392/413 (94%)	-0.37	3 (0%)	86	81	25, 46, 75, 116	0
1	C	391/413 (94%)	-0.30	3 (0%)	86	81	32, 53, 83, 119	0
1	D	392/413 (94%)	-0.26	8 (2%)	65	56	31, 53, 83, 126	0
1	E	391/413 (94%)	-0.42	9 (2%)	60	51	18, 35, 67, 126	0
1	F	392/413 (94%)	-0.35	10 (2%)	56	46	22, 42, 71, 120	0
1	G	391/413 (94%)	-0.28	7 (1%)	68	61	23, 49, 85, 125	0
1	H	392/413 (94%)	-0.25	11 (2%)	53	43	26, 53, 90, 126	0
1	I	391/413 (94%)	-0.17	7 (1%)	68	61	40, 60, 91, 128	0
1	J	392/413 (94%)	-0.20	7 (1%)	68	61	35, 61, 95, 126	0
1	K	391/413 (94%)	-0.25	5 (1%)	77	72	33, 54, 87, 125	0
1	L	392/413 (94%)	-0.24	9 (2%)	60	51	32, 58, 94, 146	0
All	All	4698/4956 (94%)	-0.29	84 (1%)	68	61	18, 50, 87, 146	0

All (84) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	10	PRO	4.9
1	L	336	LYS	4.7
1	L	99	GLU	4.6
1	H	10	PRO	4.3
1	L	10	PRO	4.0
1	L	101	GLY	3.8
1	F	99	GLU	3.7
1	L	100	SER	3.6
1	G	265	ASP	3.6
1	F	265	ASP	3.4
1	A	99	GLU	3.4

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Mol	Chain	Res	Type	RSRZ
1	J	187	LYS	3.3
1	D	8	LEU	3.3
1	I	100	SER	3.2
1	B	336	LYS	3.1
1	A	98	THR	3.1
1	F	10	PRO	3.1
1	I	99	GLU	3.0
1	J	376	ASN	2.9
1	D	99	GLU	2.9
1	J	337	ASP	2.8
1	E	188	GLN	2.8
1	H	336	LYS	2.8
1	H	187	LYS	2.8
1	G	400	LYS	2.7
1	F	336	LYS	2.7
1	H	99	GLU	2.6
1	G	188	GLN	2.6
1	G	336	LYS	2.6
1	H	374	THR	2.6
1	F	372	ASP	2.6
1	A	100	SER	2.6
1	F	12	SER	2.6
1	L	98	THR	2.5
1	I	265	ASP	2.5
1	I	350	GLY	2.5
1	D	267	ASN	2.5
1	F	98	THR	2.5
1	C	100	SER	2.4
1	F	100	SER	2.4
1	D	336	LYS	2.4
1	K	155	VAL	2.4
1	J	336	LYS	2.4
1	H	366	TYR	2.4
1	E	98	THR	2.4
1	E	159	GLY	2.4
1	H	101	GLY	2.4
1	K	99	GLU	2.3
1	J	98	THR	2.3
1	A	97	LYS	2.3
1	K	96	VAL	2.3
1	F	101	GLY	2.3
1	B	265	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	J	99	GLU	2.3
1	K	192	LYS	2.2
1	J	366	TYR	2.2
1	H	334	GLU	2.2
1	I	267	ASN	2.2
1	D	376	ASN	2.2
1	G	239	ASN	2.2
1	L	264	ILE	2.2
1	G	372	ASP	2.2
1	E	101	GLY	2.2
1	E	100	SER	2.1
1	H	98	THR	2.1
1	H	265	ASP	2.1
1	E	155	VAL	2.1
1	D	264	ILE	2.1
1	H	372	ASP	2.1
1	E	102	ILE	2.1
1	D	100	SER	2.1
1	K	102	ILE	2.1
1	E	99	GLU	2.1
1	B	266	LYS	2.1
1	C	192	LYS	2.1
1	L	366	TYR	2.1
1	E	336	LYS	2.1
1	I	372	ASP	2.0
1	C	267	ASN	2.0
1	A	0	ILE	2.0
1	F	264	ILE	2.0
1	L	12	SER	2.0
1	I	157	LEU	2.0
1	G	365	THR	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)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	PO4	D	502	5/5	0.59	1.48	211,313,334,380	0
2	PO4	I	502	5/5	0.77	0.75	180,183,195,202	0
2	PO4	A	502	5/5	0.82	0.39	146,149,158,159	0
2	PO4	E	501	5/5	0.84	0.36	108,122,130,136	0
2	PO4	J	501	5/5	0.84	0.28	114,118,154,157	0
2	PO4	E	502	5/5	0.85	0.30	137,138,146,154	0
2	PO4	G	501	5/5	0.86	0.31	95,109,127,148	0
2	PO4	G	502	5/5	0.88	0.30	101,104,132,148	0
2	PO4	K	502	5/5	0.90	0.38	117,119,177,181	0
2	PO4	K	501	5/5	0.91	0.43	117,135,139,142	0
2	PO4	D	501	5/5	0.91	0.22	84,84,88,93	0
2	PO4	L	501	5/5	0.92	0.21	98,103,107,117	0
2	PO4	I	501	5/5	0.94	0.27	98,98,105,115	0
2	PO4	F	501	5/5	0.94	0.27	103,112,123,124	0
2	PO4	H	501	5/5	0.94	0.28	21,79,121,136	0
2	PO4	C	501	5/5	0.95	0.11	70,77,83,85	0
2	PO4	A	501	5/5	0.95	0.22	62,77,90,99	0
2	PO4	B	501	5/5	0.95	0.16	72,75,81,84	0

6.5 Other polymers (i)

There are no such residues in this entry.