



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 15, 2020 – 11:53 pm BST

PDB ID : 5ECO  
Title : Crystal Structure of FIN219-FIP1 complex with JA, Leu and Mg  
Authors : Chen, C.Y.; Cheng, Y.S.  
Deposited on : 2015-10-20  
Resolution : 1.80 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
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) : 2.11

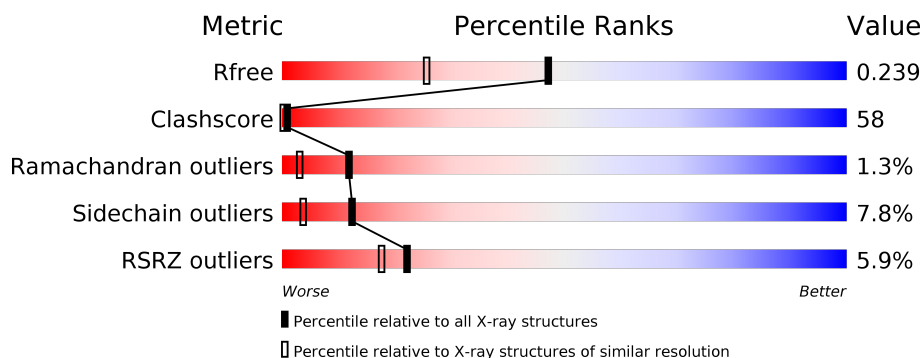
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.80 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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

Mol	Chain	Length	Quality of chain
1	A	575	<div> <div>9%</div> <div>25% 65% 8%</div> </div>
1	D	575	<div> <div>7%</div> <div>29% 60% 9%</div> </div>
2	B	223	<div> <div>2%</div> <div>37% 55%</div> </div>
2	C	223	<div> <div>2%</div> <div>36% 54% 6%</div> </div>
2	E	223	<div> <div>5%</div> <div>40% 49% 7%</div> </div>
2	F	223	<div> <div>3%</div> <div>32% 58% 5%</div> </div>

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
4	LEU	A	602	-	-	X	-

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 18387 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 Jasmonic acid-amido synthetase JAR1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	569	Total	C	N	O	S	0	0	0
			4479	2859	748	850	22			
1	D	569	Total	C	N	O	S	0	0	0
			4479	2859	748	850	22			

- Molecule 2 is a protein called Glutathione S-transferase U20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	214	Total	C	N	O	S	0	0	0
			1748	1136	284	323	5			
2	C	214	Total	C	N	O	S	0	0	0
			1748	1136	284	323	5			
2	E	214	Total	C	N	O	S	0	0	0
			1748	1136	284	323	5			
2	F	214	Total	C	N	O	S	0	0	0
			1748	1136	284	323	5			

There are 24 discrepancies between the modelled and reference sequences:

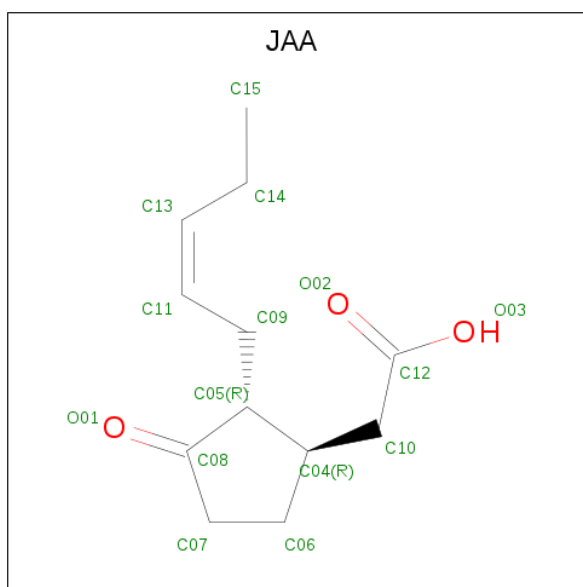
Chain	Residue	Modelled	Actual	Comment	Reference
B	-5	HIS	-	expression tag	UNP Q8L7C9
B	-4	HIS	-	expression tag	UNP Q8L7C9
B	-3	HIS	-	expression tag	UNP Q8L7C9
B	-2	HIS	-	expression tag	UNP Q8L7C9
B	-1	HIS	-	expression tag	UNP Q8L7C9
B	0	HIS	-	expression tag	UNP Q8L7C9
C	-5	HIS	-	expression tag	UNP Q8L7C9
C	-4	HIS	-	expression tag	UNP Q8L7C9
C	-3	HIS	-	expression tag	UNP Q8L7C9
C	-2	HIS	-	expression tag	UNP Q8L7C9
C	-1	HIS	-	expression tag	UNP Q8L7C9
C	0	HIS	-	expression tag	UNP Q8L7C9

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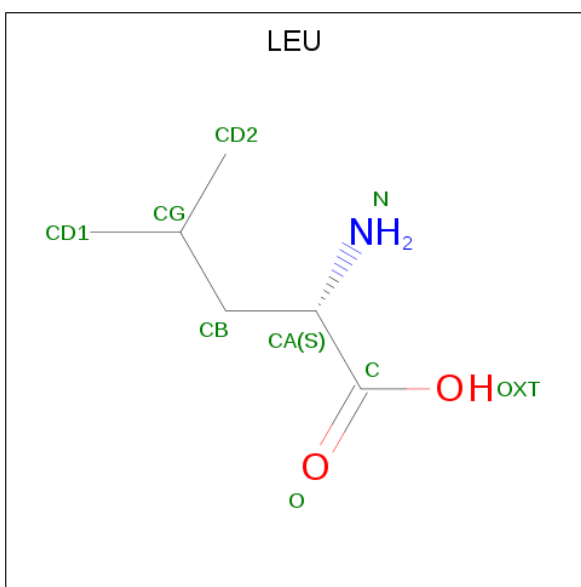
Chain	Residue	Modelled	Actual	Comment	Reference
E	-5	HIS	-	expression tag	UNP Q8L7C9
E	-4	HIS	-	expression tag	UNP Q8L7C9
E	-3	HIS	-	expression tag	UNP Q8L7C9
E	-2	HIS	-	expression tag	UNP Q8L7C9
E	-1	HIS	-	expression tag	UNP Q8L7C9
E	0	HIS	-	expression tag	UNP Q8L7C9
F	-5	HIS	-	expression tag	UNP Q8L7C9
F	-4	HIS	-	expression tag	UNP Q8L7C9
F	-3	HIS	-	expression tag	UNP Q8L7C9
F	-2	HIS	-	expression tag	UNP Q8L7C9
F	-1	HIS	-	expression tag	UNP Q8L7C9
F	0	HIS	-	expression tag	UNP Q8L7C9

- Molecule 3 is {(1R,2R)-3-oxo-2-[(2Z)-pent-2-en-1-yl]cyclopentyl}acetic acid (three-letter code: JAA) (formula: C<sub>12</sub>H<sub>18</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			15	12	3		
3	D	1	Total	C	O	0	0
			15	12	3		

- Molecule 4 is LEUCINE (three-letter code: LEU) (formula: C<sub>6</sub>H<sub>13</sub>NO<sub>2</sub>).

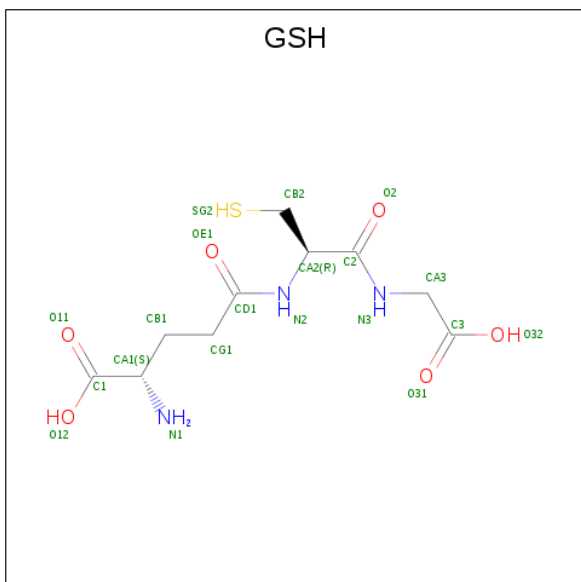


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			9	6	1	2		
4	D	1	Total	C	N	O	0	0
			9	6	1	2		

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Mg 1 1	0	0

- Molecule 6 is GLUTATHIONE (three-letter code: GSH) (formula:  $\text{C}_{10}\text{H}_{17}\text{N}_3\text{O}_6\text{S}$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	B	1	Total	C	N	O	S	0	0
			20	10	3	6	1		
6	C	1	Total	C	N	O	S	0	0
			20	10	3	6	1		
6	E	1	Total	C	N	O	S	0	0
			20	10	3	6	1		
6	F	1	Total	C	N	O	S	0	0
			20	10	3	6	1		

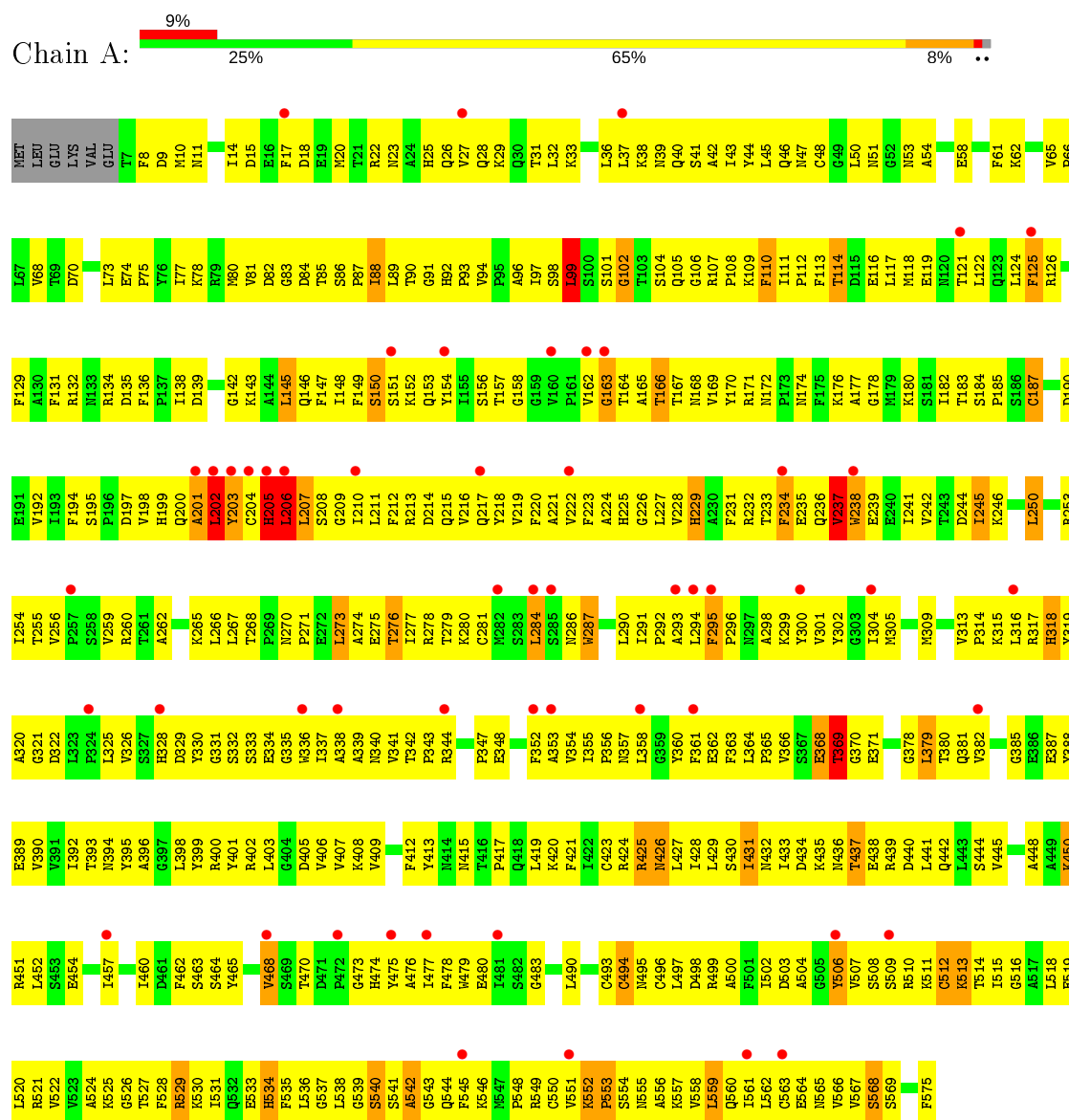
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	568	Total	O	0	0
			568	568		
7	B	270	Total	O	0	0
			270	270		
7	C	277	Total	O	0	0
			277	277		
7	D	651	Total	O	0	0
			651	651		
7	E	283	Total	O	0	0
			283	283		
7	F	259	Total	O	0	0
			259	259		

### 3 Residue-property plots

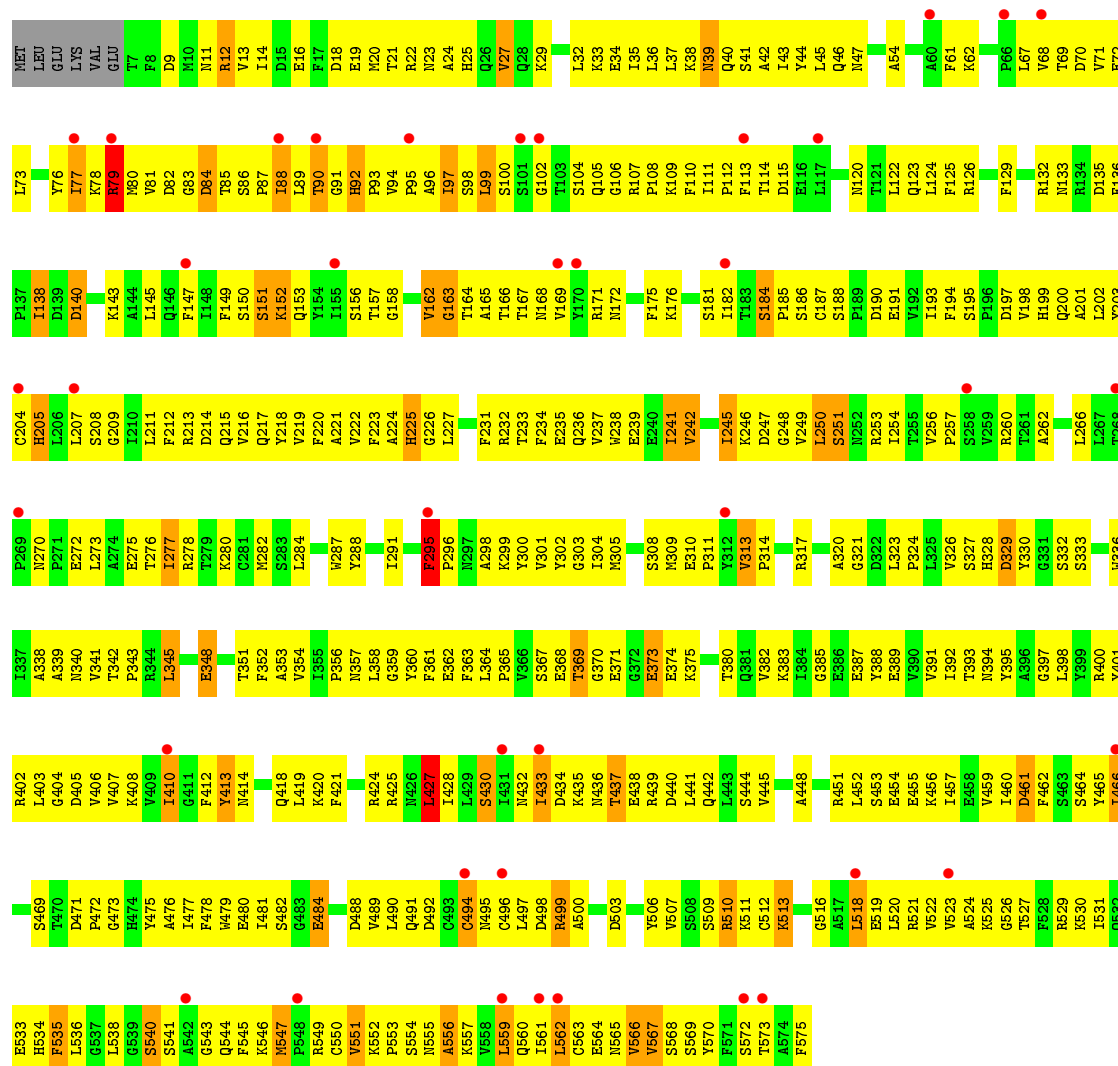
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: Jasmonic acid-amido synthetase JAR1

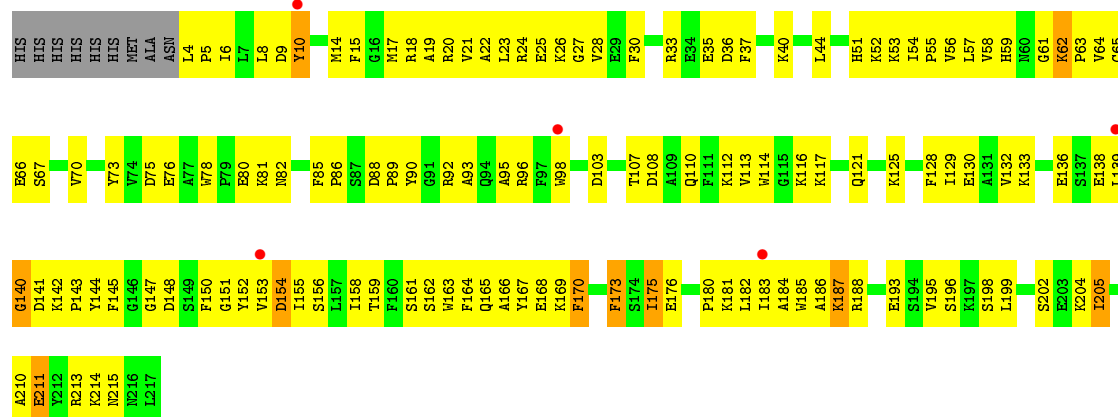


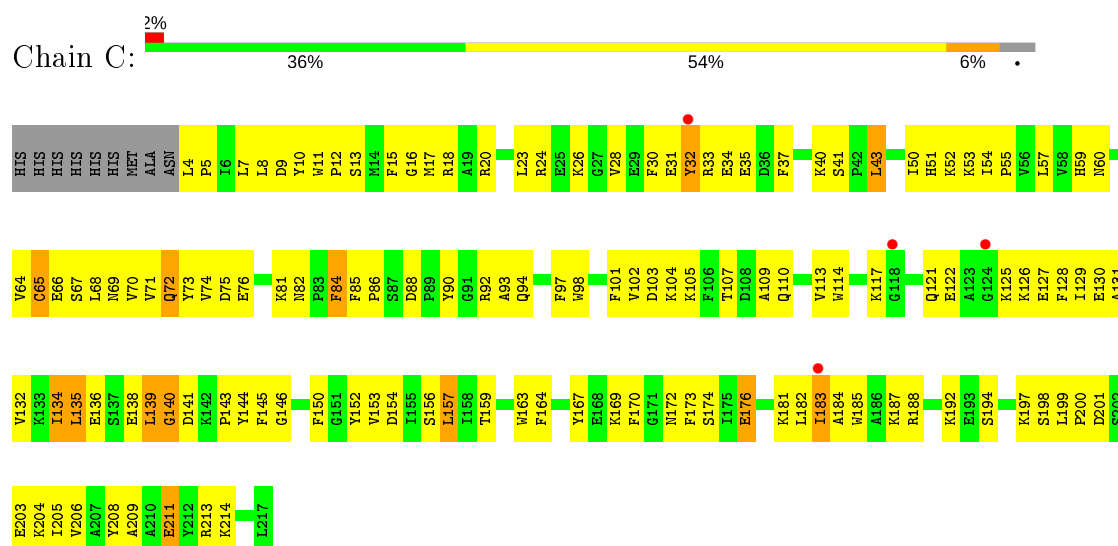
- Molecule 1: Jasmonic acid-amido synthetase JAR1



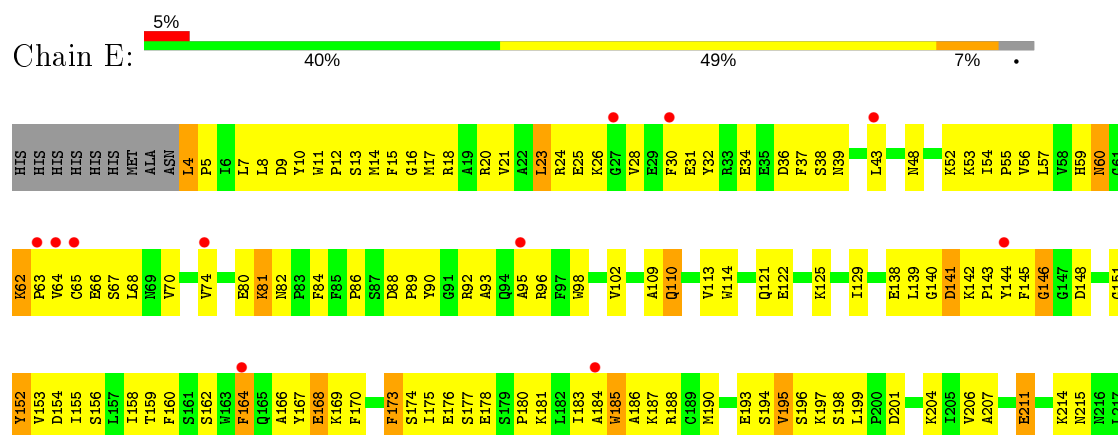


• Molecule 2: Glutathione S-transferase U20

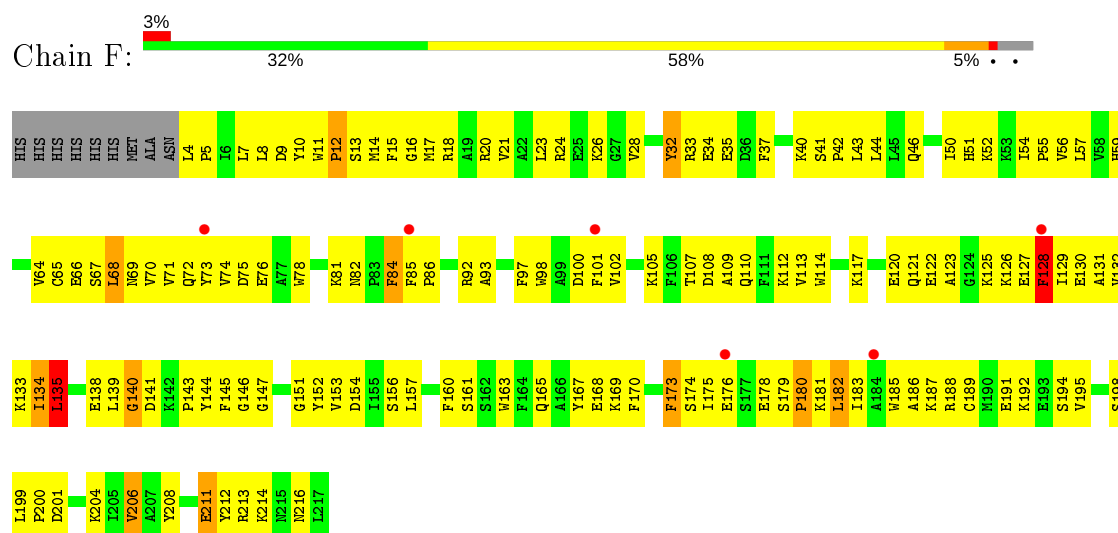




- Molecule 2: Glutathione S-transferase U20



- Molecule 2: Glutathione S-transferase U20



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	53.76Å 53.84Å 192.57Å 90.07° 89.96° 113.53°	Depositor
Resolution (Å)	23.48 – 1.80 23.48 – 1.80	Depositor EDS
% Data completeness (in resolution range)	95.4 (23.48-1.80) 95.4 (23.48-1.80)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.95 (at 1.80Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, $R_{free}$	0.222 , 0.239 0.222 , 0.239	Depositor DCC
$R_{free}$ test set	17478 reflections (9.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	8.6	Xtriage
Anisotropy	0.190	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.23 , 315.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.110 for -h,-k,l 0.104 for -k,-h,-l 0.088 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	18387	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	6.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 50.00 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.8822e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

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

## 5 Model quality

### 5.1 Standard geometry

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

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	0.47	1/4581 (0.0%)	0.94	19/6219 (0.3%)
1	D	0.47	1/4581 (0.0%)	0.89	16/6219 (0.3%)
2	B	0.33	0/1799	0.63	0/2428
2	C	0.39	0/1799	0.69	0/2428
2	E	0.41	0/1799	0.71	3/2428 (0.1%)
2	F	0.47	0/1799	0.77	4/2428 (0.2%)
All	All	0.44	2/16358 (0.0%)	0.83	42/22150 (0.2%)

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	A	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	205	HIS	N-CA	5.41	1.57	1.46
1	D	494	CYS	CB-SG	-5.23	1.73	1.81

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	202	LEU	CB-CA-C	12.83	134.58	110.20
1	A	201	ALA	C-N-CA	-10.72	94.91	121.70
1	D	79	ARG	NE-CZ-NH2	-7.87	116.36	120.30
1	D	466	ILE	CG1-CB-CG2	-7.48	94.94	111.40
1	A	99	LEU	CA-CB-CG	7.26	131.99	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	163	GLY	N-CA-C	7.11	130.88	113.10
1	D	428	ILE	N-CA-C	-7.06	91.95	111.00
1	A	206	LEU	CB-CG-CD2	-7.02	99.06	111.00
1	A	238	TRP	CA-CB-CG	6.97	126.95	113.70
1	D	494	CYS	CA-CB-SG	6.95	126.51	114.00
1	D	562	LEU	CA-CB-CG	6.70	130.72	115.30
1	A	202	LEU	CA-CB-CG	6.66	130.61	115.30
2	F	128	PHE	CB-CG-CD2	-6.47	116.27	120.80
1	D	77	ILE	CG1-CB-CG2	-6.47	97.17	111.40
1	D	295	PHE	CB-CG-CD1	-6.45	116.29	120.80
1	A	427	LEU	N-CA-C	6.32	128.06	111.00
1	D	102	GLY	N-CA-C	-6.29	97.37	113.10
1	A	202	LEU	N-CA-CB	-6.17	98.05	110.40
2	F	187	LYS	CD-CE-NZ	6.09	125.71	111.70
1	A	203	TYR	N-CA-C	-6.05	94.67	111.00
1	A	206	LEU	CA-CB-CG	6.00	129.09	115.30
1	A	163	GLY	N-CA-C	5.98	128.04	113.10
1	D	99	LEU	CA-CB-CG	5.84	128.73	115.30
1	A	102	GLY	N-CA-C	-5.76	98.69	113.10
1	D	427	LEU	CA-CB-CG	5.76	128.54	115.30
1	A	203	TYR	CB-CG-CD2	-5.70	117.58	121.00
1	A	203	TYR	CB-CG-CD1	5.62	124.37	121.00
1	A	202	LEU	CB-CG-CD2	5.61	120.53	111.00
2	E	152	TYR	N-CA-C	5.55	125.99	111.00
2	E	140	GLY	N-CA-C	-5.53	99.28	113.10
1	D	413	TYR	N-CA-C	-5.47	96.22	111.00
1	D	556	ALA	N-CA-C	5.47	125.76	111.00
2	E	146	GLY	N-CA-C	5.41	126.64	113.10
1	A	207	LEU	CA-CB-CG	5.39	127.71	115.30
2	F	128	PHE	CB-CG-CD1	5.36	124.55	120.80
1	A	237	VAL	N-CA-C	5.36	125.47	111.00
1	A	205	HIS	N-CA-CB	5.24	120.02	110.60
2	F	135	LEU	CB-CG-CD2	-5.12	102.29	111.00
1	D	295	PHE	CB-CG-CD2	5.11	124.38	120.80
1	A	552	LYS	N-CA-C	-5.11	97.20	111.00
1	D	559	LEU	CA-CB-CG	5.07	126.95	115.30
1	D	84	ASP	N-CA-C	-5.05	97.35	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	202	LEU	Peptide
1	A	318	HIS	Sidechain

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4479	0	4434	654	7
1	D	4479	0	4434	572	3
2	B	1748	0	1704	163	0
2	C	1748	0	1704	190	0
2	E	1748	0	1704	169	0
2	F	1748	0	1704	166	2
3	A	15	0	0	2	0
3	D	15	0	0	2	0
4	A	9	0	10	8	0
4	D	9	0	10	5	0
5	A	1	0	0	0	0
6	B	20	0	15	1	0
6	C	20	0	15	0	0
6	E	20	0	15	3	0
6	F	20	0	15	0	0
7	A	568	0	0	101	5
7	B	270	0	0	34	1
7	C	277	0	0	26	2
7	D	651	0	0	94	2
7	E	283	0	0	36	0
7	F	259	0	0	19	2
All	All	18387	0	15764	1837	17

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 58.

All (1837) 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:D:176:LYS:NZ	1:D:190:ASP:OD2	1.71	1.21

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:LEU:O	1:A:205:HIS:ND1	1.81	1.10
1:A:202:LEU:HG	1:A:205:HIS:CB	1.86	1.05
1:D:86:SER:HB3	2:E:188:ARG:HB2	1.37	1.03
1:A:278:ARG:NH2	7:A:702:HOH:O	1.91	1.02
2:F:125:LYS:NZ	7:F:402:HOH:O	1.92	1.00
1:A:202:LEU:CG	1:A:205:HIS:HB3	1.90	1.00
2:E:24:ARG:NH1	2:E:24:ARG:O	1.97	0.98
2:C:204:LYS:NZ	7:C:401:HOH:O	1.96	0.97
2:E:66:GLU:OE2	7:E:401:HOH:O	1.83	0.96
1:A:202:LEU:HA	1:A:205:HIS:H	1.29	0.96
1:A:202:LEU:HG	1:A:205:HIS:HB3	0.98	0.96
1:A:176:LYS:NZ	1:A:190:ASP:OD2	1.98	0.96
1:D:76:TYR:O	1:D:79:ARG:NH2	2.00	0.94
1:D:90:THR:HG22	1:D:397:GLY:HA2	1.49	0.94
2:E:197:LYS:NZ	7:E:402:HOH:O	1.98	0.94
2:C:26:LYS:HG2	2:C:81:LYS:HZ3	1.30	0.93
2:F:26:LYS:NZ	2:F:82:ASN:O	2.02	0.93
1:A:199:HIS:HA	1:A:525:LYS:HG2	1.47	0.93
1:D:41:SER:HB3	2:E:144:TYR:HB3	1.52	0.92
2:E:125:LYS:HB3	2:E:173:PHE:HE2	1.34	0.91
2:B:145:PHE:HB3	2:B:153:VAL:HG13	1.53	0.91
1:D:88:ILE:O	7:D:701:HOH:O	1.85	0.91
1:D:100:SER:HB2	1:D:109:LYS:HD3	1.51	0.90
1:A:280:LYS:NZ	1:A:293:ALA:O	2.04	0.90
1:D:199:HIS:HB3	1:D:525:LYS:H	1.35	0.90
2:C:26:LYS:HG2	2:C:81:LYS:NZ	1.86	0.90
1:D:88:ILE:HG23	1:D:89:LEU:H	1.36	0.90
1:D:87:PRO:HB3	1:D:93:PRO:HD3	1.54	0.90
1:A:402:ARG:NH1	7:A:710:HOH:O	2.05	0.89
1:A:163:GLY:HA2	1:A:560:GLN:HB2	1.52	0.89
1:D:90:THR:OG1	1:D:91:GLY:N	1.96	0.89
1:A:99:LEU:HB3	1:A:557:LYS:H	1.36	0.89
2:B:187:LYS:NZ	7:B:405:HOH:O	2.05	0.89
2:C:26:LYS:NZ	2:C:82:ASN:O	2.05	0.89
2:B:116:LYS:NZ	7:B:403:HOH:O	1.99	0.88
2:C:136:GLU:HG3	2:C:181:LYS:HD3	1.56	0.88
1:D:98:SER:HB2	1:D:111:ILE:HB	1.55	0.88
2:F:76:GLU:OE2	7:F:401:HOH:O	1.91	0.88
1:A:38:LYS:HZ3	1:A:395:TYR:HD1	0.94	0.87
1:D:519:GLU:OE2	1:D:569:SER:OG	1.93	0.87
2:B:162:SER:HB3	2:B:199:LEU:HD23	1.57	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:117:LYS:HG2	2:B:213:ARG:HH11	1.39	0.86
4:D:602:LEU:O	7:D:702:HOH:O	1.93	0.86
1:A:105:GLN:HA	1:A:430:SER:HB3	1.57	0.86
1:D:251:SER:O	7:D:703:HOH:O	1.94	0.86
1:A:87:PRO:HB3	1:A:93:PRO:HD3	1.57	0.85
2:C:33:ARG:NH1	7:C:405:HOH:O	2.09	0.85
1:D:107:ARG:HH11	1:D:107:ARG:HG3	1.42	0.85
1:D:476:ALA:O	7:D:704:HOH:O	1.95	0.85
1:A:199:HIS:HB3	1:A:525:LYS:H	1.39	0.85
1:A:151:SER:HB3	1:A:565:ASN:HD21	1.39	0.85
1:D:424:ARG:HE	1:D:425:ARG:HD3	1.41	0.85
1:A:58:GLU:OE2	7:A:703:HOH:O	1.94	0.84
1:A:526:GLY:HA2	1:A:529:ARG:HD3	1.59	0.84
1:A:152:LYS:HE2	1:A:565:ASN:HB2	1.59	0.84
1:D:329:ASP:HB3	1:D:339:ALA:HA	1.59	0.84
1:D:95:PRO:HD3	2:E:181:LYS:HD3	1.56	0.84
2:C:135:LEU:HD22	2:C:182:LEU:HD12	1.59	0.84
1:A:145:LEU:HD13	1:A:209:GLY:HA3	1.60	0.84
1:D:198:VAL:HA	1:D:201:ALA:HB3	1.58	0.84
2:B:88:ASP:O	7:B:401:HOH:O	1.95	0.83
1:D:90:THR:HG22	1:D:397:GLY:CA	2.07	0.83
1:A:405:ASP:HB3	1:A:541:SER:HB3	1.60	0.83
1:D:77:ILE:HG21	1:D:110:PHE:HB3	1.61	0.83
1:A:344:ARG:NH1	7:A:721:HOH:O	2.11	0.83
1:A:498:ASP:O	7:A:704:HOH:O	1.95	0.83
2:B:138:GLU:OE2	7:B:402:HOH:O	1.96	0.83
1:A:143:LYS:HZ3	1:A:187:CYS:HA	1.43	0.83
1:A:389:GLU:OE2	1:A:405:ASP:N	2.12	0.83
1:A:442:GLN:HG2	1:A:462:PHE:HZ	1.42	0.83
2:C:203:GLU:OE2	7:C:401:HOH:O	1.96	0.82
1:D:405:ASP:HB2	1:D:541:SER:HB2	1.60	0.82
2:C:184:ALA:HB1	1:D:499:ARG:NH1	1.94	0.82
2:C:66:GLU:OE2	7:C:402:HOH:O	1.97	0.82
1:D:70:ASP:OD2	7:D:705:HOH:O	1.97	0.82
1:D:77:ILE:CG2	1:D:110:PHE:HB3	2.09	0.82
1:A:424:ARG:HB2	1:A:425:ARG:NH1	1.94	0.82
2:E:125:LYS:HB3	2:E:173:PHE:CE2	2.15	0.81
2:E:4:LEU:N	7:E:410:HOH:O	2.12	0.81
1:A:154:TYR:HD1	1:A:563:CYS:HB2	1.44	0.81
1:A:423:CYS:SG	1:A:541:SER:OG	2.37	0.81
1:D:494:CYS:HB3	1:D:520:LEU:HB3	1.60	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:LEU:H	1:A:557:LYS:HG3	1.46	0.81
1:A:201:ALA:O	1:A:204:CYS:HB2	1.79	0.81
1:A:368:GLU:OE2	7:A:705:HOH:O	1.98	0.81
1:A:147:PHE:CD1	1:A:205:HIS:CD2	2.69	0.81
1:D:219:VAL:HB	1:D:295:PHE:CZ	2.16	0.81
1:A:495:ASN:O	7:A:707:HOH:O	1.98	0.80
1:D:465:TYR:HB2	1:D:551:VAL:HG13	1.63	0.80
1:A:118:MET:SD	7:A:1034:HOH:O	2.39	0.80
1:A:317:ARG:HB2	1:A:325:LEU:HD11	1.64	0.80
2:C:117:LYS:NZ	7:C:409:HOH:O	2.13	0.80
2:F:140:GLY:C	2:F:181:LYS:HZ1	1.84	0.80
1:A:147:PHE:HD1	1:A:205:HIS:CD2	1.99	0.80
1:A:241:ILE:O	1:A:245:ILE:HG13	1.83	0.79
1:A:238:TRP:CH2	1:A:281:CYS:HB3	2.17	0.79
1:D:46:GLN:HB2	2:E:148:ASP:HB2	1.65	0.79
2:E:180:PRO:O	7:E:403:HOH:O	2.00	0.79
2:F:122:GLU:HA	2:F:125:LYS:HE2	1.64	0.79
2:C:127:GLU:OE1	7:C:403:HOH:O	2.00	0.79
1:A:87:PRO:HB2	2:B:143:PRO:HA	1.62	0.79
1:A:202:LEU:HA	1:A:205:HIS:N	1.95	0.79
1:A:229:HIS:CE1	1:A:529:ARG:HD2	2.17	0.79
2:E:64:VAL:HG13	2:E:70:VAL:HG22	1.63	0.79
1:A:202:LEU:CA	1:A:205:HIS:H	1.95	0.79
1:A:233:THR:HA	1:A:236:GLN:HB2	1.65	0.79
1:D:106:GLY:O	1:D:432:ASN:ND2	2.15	0.79
1:A:82:ASP:OD1	1:A:157:THR:OG1	2.01	0.78
1:A:39:ASN:ND2	1:A:399:TYR:OH	2.14	0.78
1:A:329:ASP:HB3	1:A:339:ALA:HA	1.64	0.78
1:A:33:LYS:NZ	7:A:730:HOH:O	2.13	0.78
2:B:168:GLU:OE2	7:B:404:HOH:O	2.01	0.78
1:A:199:HIS:H	1:A:524:ALA:HB1	1.48	0.78
2:C:188:ARG:NH1	1:D:499:ARG:O	2.17	0.77
1:A:221:ALA:HB3	1:A:227:LEU:HG	1.64	0.77
1:A:231:PHE:HA	1:A:234:PHE:HB3	1.65	0.77
2:E:178:GLU:OE2	7:E:405:HOH:O	2.03	0.77
2:E:48:ASN:OD1	7:E:404:HOH:O	2.02	0.77
2:B:96:ARG:NH1	2:C:76:GLU:OE2	2.17	0.77
1:D:132:ARG:HA	1:D:343:PRO:HG3	1.66	0.77
2:E:184:ALA:HB3	7:E:403:HOH:O	1.84	0.77
1:A:143:LYS:NZ	1:A:187:CYS:HA	1.98	0.77
1:D:162:VAL:O	1:D:560:GLN:HB2	1.85	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:152:LYS:HB2	1:D:561:ILE:HA	1.67	0.76
2:E:55:PRO:O	7:E:406:HOH:O	2.03	0.76
1:A:293:ALA:O	7:A:709:HOH:O	2.03	0.76
1:A:210:ILE:HG12	1:A:294:LEU:HD21	1.66	0.76
2:E:7:LEU:HD11	2:E:55:PRO:HB2	1.67	0.76
1:A:203:TYR:HD1	1:A:237:VAL:HG11	1.49	0.76
1:D:152:LYS:HG2	1:D:565:ASN:HB2	1.65	0.76
2:C:201:ASP:HB2	2:C:204:LYS:HG3	1.67	0.76
1:D:73:LEU:HD22	1:D:89:LEU:HD13	1.68	0.76
1:A:46:GLN:HB2	2:B:148:ASP:HB3	1.67	0.76
1:D:405:ASP:OD1	7:D:707:HOH:O	2.03	0.76
1:D:143:LYS:NZ	7:D:733:HOH:O	2.17	0.76
2:C:8:LEU:HD22	2:C:33:ARG:HH21	1.51	0.76
1:A:206:LEU:HG	1:A:234:PHE:HA	1.69	0.75
1:D:455:GLU:OE2	7:D:706:HOH:O	2.02	0.75
1:A:226:GLY:HA2	1:A:229:HIS:CE1	2.20	0.75
1:A:424:ARG:HB2	1:A:425:ARG:HH11	1.52	0.75
1:D:40:GLN:O	7:D:709:HOH:O	2.05	0.75
1:A:138:ILE:HB	1:A:217:GLN:HG3	1.69	0.75
1:D:254:ILE:O	7:D:703:HOH:O	2.04	0.75
1:D:444:SER:OG	7:D:708:HOH:O	2.05	0.75
2:E:53:LYS:HG2	6:E:301:GSH:HA31	1.66	0.75
2:B:125:LYS:HB3	2:B:173:PHE:HE2	1.49	0.75
1:A:110:PHE:CE1	1:A:556:ALA:HB2	2.22	0.74
1:A:218:TYR:HA	1:A:298:ALA:HB1	1.70	0.74
2:B:18:ARG:HH12	2:B:103:ASP:CG	1.89	0.74
1:D:521:ARG:HB3	1:D:566:VAL:HG12	1.70	0.74
1:A:198:VAL:HG22	1:A:524:ALA:HB3	1.69	0.74
2:E:138:GLU:OE2	2:E:142:LYS:NZ	2.13	0.74
1:A:29:LYS:HE3	1:A:58:GLU:HB2	1.69	0.74
1:D:76:TYR:HB3	1:D:88:ILE:HG12	1.69	0.74
2:E:10:TYR:O	7:E:407:HOH:O	2.04	0.74
1:A:480:GLU:HB2	1:A:528:PHE:CD2	2.23	0.73
1:A:480:GLU:HB2	1:A:528:PHE:HD2	1.53	0.73
2:F:26:LYS:HG2	2:F:81:LYS:HZ3	1.53	0.73
1:D:490:LEU:HD22	1:D:522:VAL:HG21	1.68	0.73
2:F:72:GLN:NE2	7:F:410:HOH:O	2.21	0.73
1:A:202:LEU:C	1:A:205:HIS:H	1.91	0.73
1:D:87:PRO:HD2	2:E:188:ARG:HB2	1.71	0.73
1:A:198:VAL:HA	1:A:201:ALA:HB3	1.70	0.73
1:A:239:GLU:OE1	7:A:711:HOH:O	2.07	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:507:VAL:HG13	1:A:511:LYS:HZ2	1.53	0.73
1:A:147:PHE:HD1	1:A:205:HIS:CG	2.05	0.72
2:B:18:ARG:NH1	2:B:103:ASP:OD2	2.15	0.72
1:A:17:PHE:HE1	1:A:355:ILE:HG12	1.54	0.72
1:D:199:HIS:HB2	1:D:525:LYS:HE3	1.69	0.72
1:A:81:VAL:HG11	1:A:110:PHE:HE2	1.55	0.72
1:A:444:SER:OG	7:A:706:HOH:O	1.98	0.72
1:A:253:ARG:NH2	7:A:748:HOH:O	2.21	0.72
1:D:231:PHE:O	7:D:710:HOH:O	2.06	0.72
1:A:28:GLN:HE21	1:A:361:PHE:H	1.37	0.72
1:D:143:LYS:HG3	1:D:216:VAL:HG12	1.71	0.72
1:D:534:HIS:CE1	1:D:557:LYS:HD3	2.25	0.72
1:A:362:GLU:OE2	7:A:712:HOH:O	2.07	0.72
1:A:305:MET:HB3	1:A:347:PRO:HB3	1.71	0.72
2:C:17:MET:SD	7:C:410:HOH:O	2.48	0.72
1:A:540:SER:OG	1:A:544:GLN:NE2	2.22	0.71
1:A:432:ASN:OD1	1:A:434:ASP:N	2.22	0.71
1:A:28:GLN:NE2	1:A:361:PHE:H	1.87	0.71
2:C:55:PRO:O	7:C:404:HOH:O	2.07	0.71
1:A:38:LYS:NZ	1:A:395:TYR:HD1	1.82	0.71
1:A:435:LYS:HZ1	1:A:438:GLU:HB3	1.55	0.71
1:A:452:LEU:HB3	1:A:457:ILE:HD11	1.72	0.71
1:A:15:ASP:OD2	7:A:716:HOH:O	2.09	0.71
1:A:126:ARG:NH2	1:A:178:GLY:O	2.22	0.71
1:A:329:ASP:O	7:A:714:HOH:O	2.09	0.71
2:B:98:TRP:CE2	2:B:138:GLU:HG2	2.25	0.71
1:D:96:ALA:HB3	1:D:113:PHE:HB3	1.72	0.71
1:D:152:LYS:O	7:D:711:HOH:O	2.07	0.71
1:D:442:GLN:HG2	1:D:462:PHE:HZ	1.55	0.71
1:D:152:LYS:HA	1:D:564:GLU:HB2	1.72	0.71
1:A:440:ASP:OD1	7:A:706:HOH:O	2.09	0.71
1:A:9:ASP:O	7:A:715:HOH:O	2.09	0.71
1:D:152:LYS:HZ3	1:D:561:ILE:HG23	1.56	0.71
2:F:10:TYR:O	2:F:20:ARG:NH2	2.20	0.71
1:A:331:GLY:HA3	1:A:336:TRP:CE3	2.24	0.71
1:A:222:VAL:HG23	1:A:223:PHE:CD1	2.26	0.71
1:A:236:GLN:NE2	7:A:751:HOH:O	2.23	0.71
1:A:68:VAL:HG13	1:A:401:TYR:HD1	1.56	0.71
1:A:507:VAL:HG13	1:A:511:LYS:NZ	2.06	0.71
1:D:212:PHE:HB3	1:D:215:GLN:HE21	1.56	0.71
1:D:435:LYS:HA	1:D:436:ASN:HB2	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:52:LYS:O	7:E:408:HOH:O	2.08	0.70
1:A:42:ALA:HA	2:B:143:PRO:HG3	1.73	0.70
2:E:175:ILE:HB	2:E:183:ILE:HD11	1.73	0.70
1:A:147:PHE:HB3	1:A:205:HIS:CD2	2.27	0.70
1:A:530:LYS:HE2	1:A:561:ILE:HD13	1.73	0.70
1:D:260:ARG:NH2	7:D:703:HOH:O	2.24	0.70
2:F:132:VAL:HG22	2:F:179:SER:HB2	1.73	0.70
1:A:498:ASP:OD2	1:A:510:ARG:NH1	2.25	0.70
1:A:552:LYS:O	1:A:554:SER:N	2.25	0.70
1:D:219:VAL:HB	1:D:295:PHE:HZ	1.56	0.70
1:D:478:PHE:HE1	1:D:521:ARG:HD2	1.56	0.70
2:E:20:ARG:NH1	2:E:198:SER:O	2.24	0.70
1:A:211:LEU:O	7:A:718:HOH:O	2.10	0.70
1:A:223:PHE:CZ	1:A:536:LEU:HB3	2.27	0.70
1:A:498:ASP:HB3	1:A:510:ARG:HH22	1.56	0.70
1:D:97:ILE:O	7:D:713:HOH:O	2.10	0.70
1:A:262:ALA:HA	1:A:265:LYS:NZ	2.07	0.70
1:A:525:LYS:O	7:A:720:HOH:O	2.10	0.70
1:D:111:ILE:O	7:D:712:HOH:O	2.08	0.70
1:A:102:GLY:HA2	1:A:546:LYS:HB3	1.73	0.69
1:D:19:GLU:O	1:D:23:ASN:ND2	2.24	0.69
1:D:81:VAL:HG11	1:D:110:PHE:CE2	2.27	0.69
2:F:11:TRP:CD1	2:F:12:PRO:HD3	2.27	0.69
2:F:151:GLY:N	2:F:154:ASP:OD2	2.25	0.69
1:A:329:ASP:OD1	1:A:340:ASN:N	2.21	0.69
2:C:24:ARG:O	7:C:406:HOH:O	2.09	0.69
1:A:132:ARG:O	1:A:136:PHE:N	2.15	0.69
1:A:394:ASN:ND2	7:A:756:HOH:O	2.25	0.69
2:E:139:LEU:C	2:E:141:ASP:H	1.95	0.69
2:F:147:GLY:O	7:F:403:HOH:O	2.11	0.69
1:A:90:THR:OG1	1:A:91:GLY:N	2.26	0.69
1:D:67:LEU:O	7:D:715:HOH:O	2.10	0.69
1:A:435:LYS:NZ	1:A:438:GLU:HB3	2.08	0.69
2:B:139:LEU:HG	2:B:142:LYS:HB2	1.75	0.69
1:A:22:ARG:O	7:A:719:HOH:O	2.10	0.69
1:D:552:LYS:O	1:D:554:SER:N	2.23	0.69
1:A:150:SER:HB2	1:A:167:THR:HA	1.74	0.69
1:A:339:ALA:O	7:A:722:HOH:O	2.11	0.69
1:D:112:PRO:O	7:D:716:HOH:O	2.11	0.69
2:F:125:LYS:HA	2:F:128:PHE:CE2	2.28	0.69
1:A:149:PHE:HD2	1:A:529:ARG:HH22	1.41	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:11:TRP:CD1	2:C:12:PRO:HD3	2.29	0.68
1:A:169:VAL:HG21	4:A:602:LEU:HD11	1.76	0.68
1:A:150:SER:HB3	1:A:170:TYR:CD2	2.28	0.68
1:D:39:ASN:ND2	1:D:90:THR:O	2.26	0.68
1:A:149:PHE:CE1	1:A:202:LEU:HD22	2.28	0.68
1:A:338:ALA:HA	1:A:354:VAL:HA	1.75	0.68
1:A:156:SER:HB3	1:A:162:VAL:HG13	1.76	0.68
1:D:342:THR:OG1	1:D:413:TYR:OH	2.11	0.68
1:D:562:LEU:O	7:D:717:HOH:O	2.11	0.68
2:F:135:LEU:HD22	2:F:182:LEU:HD12	1.74	0.68
2:B:176:GLU:OE2	7:B:407:HOH:O	2.11	0.68
2:B:40:LYS:HB3	2:B:44:LEU:HD23	1.76	0.68
1:D:353:ALA:HB2	1:D:413:TYR:HD2	1.58	0.68
1:A:134:ARG:NH2	7:A:761:HOH:O	2.26	0.68
2:C:156:SER:O	7:C:407:HOH:O	2.11	0.68
1:D:157:THR:HB	1:D:469:SER:HB3	1.76	0.68
1:D:80:MET:SD	7:D:1032:HOH:O	2.51	0.68
1:D:79:ARG:NH2	1:D:88:ILE:HB	2.09	0.68
2:E:26:LYS:NZ	2:E:82:ASN:O	2.24	0.68
1:A:163:GLY:O	7:A:725:HOH:O	2.12	0.68
2:C:64:VAL:HB	2:C:73:TYR:CD2	2.28	0.68
1:A:287:TRP:CE3	1:A:290:LEU:HD13	2.28	0.67
2:B:202:SER:O	2:B:205:ILE:HG13	1.94	0.67
1:D:199:HIS:CE1	1:D:567:VAL:HG21	2.28	0.67
1:D:572:SER:O	7:D:714:HOH:O	2.10	0.67
1:A:219:VAL:HG11	1:A:291:ILE:HD13	1.75	0.67
1:A:322:ASP:OD2	7:A:723:HOH:O	2.12	0.67
1:D:367:SER:O	7:D:720:HOH:O	2.13	0.67
1:D:46:GLN:NE2	7:D:759:HOH:O	2.26	0.67
1:A:208:SER:O	1:A:211:LEU:HB2	1.93	0.67
2:B:215:ASN:ND2	7:B:429:HOH:O	2.28	0.67
1:D:164:THR:HA	1:D:557:LYS:HG2	1.76	0.67
1:D:494:CYS:HB3	1:D:520:LEU:CB	2.24	0.67
1:D:498:ASP:OD2	7:D:719:HOH:O	2.12	0.67
1:A:166:THR:HA	4:A:602:LEU:HG	1.75	0.67
2:B:15:PHE:HB3	2:B:67:SER:HB3	1.76	0.67
2:C:31:GLU:OE2	7:C:408:HOH:O	2.12	0.67
1:A:145:LEU:O	7:A:727:HOH:O	2.13	0.67
1:A:106:GLY:C	1:A:432:ASN:HD22	1.98	0.67
2:B:121:GLN:NE2	7:B:422:HOH:O	2.23	0.67
2:C:187:LYS:HE3	1:D:492:ASP:C	2.14	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:99:LEU:HB2	1:D:556:ALA:H	1.59	0.67
1:D:435:LYS:HB3	1:D:436:ASN:C	2.14	0.67
1:A:145:LEU:HD23	1:A:295:PHE:HE2	1.60	0.67
1:A:238:TRP:NE1	7:A:763:HOH:O	2.27	0.67
1:A:98:SER:HB2	1:A:557:LYS:HE3	1.75	0.67
2:B:51:HIS:HB3	2:B:53:LYS:HG3	1.76	0.67
2:E:193:GLU:HA	2:E:196:SER:HB3	1.77	0.67
1:A:387:GLU:HG2	1:A:408:LYS:HB2	1.77	0.67
2:C:184:ALA:HA	2:C:187:LYS:NZ	2.09	0.67
1:D:35:ILE:HD11	1:D:359:GLY:HA2	1.76	0.67
1:D:373:GLU:OE2	7:D:721:HOH:O	2.13	0.67
1:D:191:GLU:OE1	7:D:718:HOH:O	2.12	0.67
1:A:440:ASP:O	7:A:706:HOH:O	2.13	0.66
1:A:284:LEU:HD13	1:A:287:TRP:H	1.60	0.66
1:A:548:PRO:O	7:A:724:HOH:O	2.12	0.66
1:A:87:PRO:HD2	2:B:188:ARG:HB2	1.77	0.66
1:A:74:GLU:OE2	7:A:717:HOH:O	2.12	0.66
2:E:215:ASN:ND2	7:E:426:HOH:O	2.27	0.66
1:A:332:SER:OG	1:A:333:SER:N	2.26	0.66
2:C:122:GLU:HA	2:C:125:LYS:HE2	1.76	0.66
2:C:201:ASP:OD2	2:C:204:LYS:HE2	1.95	0.66
1:D:550:CYS:O	7:D:722:HOH:O	2.13	0.66
2:F:84:PHE:CD1	2:F:152:TYR:HB2	2.31	0.66
2:F:194:SER:O	2:F:198:SER:OG	2.12	0.66
1:A:17:PHE:CE1	1:A:355:ILE:HG12	2.30	0.66
1:A:348:GLU:OE2	7:A:731:HOH:O	2.14	0.66
2:B:15:PHE:O	7:B:408:HOH:O	2.14	0.66
1:D:208:SER:O	7:D:723:HOH:O	2.14	0.66
1:D:22:ARG:HH11	1:D:414:ASN:CG	1.98	0.66
1:D:241:ILE:O	1:D:245:ILE:HG12	1.95	0.66
1:A:206:LEU:CG	1:A:234:PHE:HA	2.25	0.66
1:D:47:ASN:O	7:D:724:HOH:O	2.14	0.66
1:A:299:LYS:O	7:A:729:HOH:O	2.13	0.66
1:A:551:VAL:HG13	1:A:555:ASN:HB2	1.78	0.66
2:E:169:LYS:NZ	2:E:206:VAL:HG13	2.10	0.66
1:A:37:LEU:O	2:B:142:LYS:NZ	2.27	0.66
1:D:132:ARG:O	1:D:136:PHE:N	2.29	0.66
1:D:248:GLY:O	7:D:725:HOH:O	2.14	0.66
1:D:253:ARG:HH12	1:D:484:GLU:H	1.43	0.66
1:D:145:LEU:HD13	1:D:209:GLY:HA3	1.76	0.66
1:D:440:ASP:O	7:D:708:HOH:O	2.14	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:188:ARG:NH2	7:F:420:HOH:O	2.29	0.66
1:A:122:LEU:HD22	1:A:126:ARG:HH21	1.60	0.66
2:C:54:ILE:HB	2:C:55:PRO:HA	1.77	0.66
1:D:99:LEU:H	1:D:557:LYS:HD2	1.59	0.66
2:F:144:TYR:O	7:F:404:HOH:O	2.14	0.66
2:F:26:LYS:HE2	2:F:75:ASP:HA	1.77	0.66
1:A:360:TYR:HB3	1:A:393:THR:HB	1.78	0.65
1:A:510:ARG:NH2	7:A:704:HOH:O	2.28	0.65
1:A:526:GLY:CA	1:A:529:ARG:HD3	2.26	0.65
1:D:98:SER:O	1:D:110:PHE:HA	1.95	0.65
1:D:198:VAL:HG13	1:D:565:ASN:HD21	1.61	0.65
1:D:302:TYR:HH	1:D:328:HIS:HD1	1.43	0.65
1:A:132:ARG:HA	1:A:343:PRO:HG3	1.77	0.65
2:F:216:ASN:ND2	7:F:416:HOH:O	2.27	0.65
2:F:75:ASP:HB2	2:F:84:PHE:CE2	2.30	0.65
1:D:566:VAL:HB	1:D:569:SER:HB2	1.79	0.65
1:D:81:VAL:HB	1:D:97:ILE:HD12	1.78	0.65
1:A:134:ARG:NH1	1:A:135:ASP:OD1	2.28	0.65
1:A:473:GLY:O	1:A:516:GLY:N	2.29	0.65
1:D:451:ARG:NH1	1:D:454:GLU:OE2	2.30	0.65
1:D:295:PHE:HD1	1:D:298:ALA:HB2	1.62	0.65
2:C:144:TYR:HB3	2:C:154:ASP:OD2	1.96	0.65
1:A:91:GLY:HA3	2:B:141:ASP:C	2.16	0.65
1:A:38:LYS:HB2	2:B:140:GLY:HA3	1.78	0.65
2:F:132:VAL:HG23	2:F:182:LEU:HD13	1.79	0.65
1:A:147:PHE:HB3	1:A:205:HIS:HD2	1.61	0.65
2:B:193:GLU:HA	2:B:196:SER:HB3	1.77	0.65
1:D:223:PHE:CB	1:D:225:HIS:HD2	2.09	0.64
1:A:424:ARG:CB	1:A:425:ARG:NH1	2.59	0.64
1:A:99:LEU:HB2	1:A:556:ALA:H	1.61	0.64
2:C:132:VAL:HG23	2:C:182:LEU:HD13	1.79	0.64
2:C:187:LYS:HB2	2:C:187:LYS:HZ3	1.62	0.64
2:F:109:ALA:HB1	2:F:128:PHE:HB3	1.80	0.64
1:D:498:ASP:CG	1:D:510:ARG:HH22	2.00	0.64
2:F:140:GLY:CA	2:F:181:LYS:HZ1	2.11	0.64
1:A:114:THR:H	1:A:117:LEU:HD12	1.62	0.64
1:D:284:LEU:HD13	1:D:287:TRP:HA	1.80	0.64
1:D:503:ASP:O	1:D:507:VAL:HG23	1.97	0.64
2:E:89:PRO:HB3	2:F:76:GLU:HG3	1.78	0.64
2:B:204:LYS:NZ	7:B:428:HOH:O	2.26	0.64
1:A:526:GLY:O	1:A:529:ARG:NH1	2.29	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:130:GLU:OE2	7:B:410:HOH:O	2.15	0.64
1:D:143:LYS:HD2	1:D:212:PHE:HB2	1.79	0.64
1:D:38:LYS:HB2	1:D:395:TYR:HE1	1.63	0.64
1:D:434:ASP:OD1	1:D:435:LYS:NZ	2.28	0.64
2:E:4:LEU:N	7:E:429:HOH:O	2.29	0.64
2:F:26:LYS:HG2	2:F:81:LYS:NZ	2.13	0.64
1:A:344:ARG:O	7:A:735:HOH:O	2.15	0.64
1:A:381:GLN:NE2	7:A:775:HOH:O	2.29	0.64
1:A:22:ARG:HE	1:A:415:ASN:HB2	1.61	0.64
1:A:154:TYR:CD1	1:A:563:CYS:HB2	2.32	0.64
1:A:150:SER:O	7:A:732:HOH:O	2.15	0.64
1:A:219:VAL:O	7:A:736:HOH:O	2.15	0.64
1:A:253:ARG:O	7:A:733:HOH:O	2.15	0.64
2:B:211:GLU:OE2	2:B:214:LYS:HD2	1.97	0.64
1:D:99:LEU:HB3	1:D:557:LYS:HB2	1.80	0.64
2:F:11:TRP:CG	2:F:12:PRO:HD3	2.32	0.64
1:A:40:GLN:H	2:B:142:LYS:HE3	1.61	0.64
1:A:53:ASN:ND2	7:A:779:HOH:O	2.31	0.64
2:F:98:TRP:CD1	2:F:153:VAL:HG21	2.33	0.64
2:B:25:GLU:OE1	7:B:409:HOH:O	2.14	0.63
2:C:176:GLU:OE2	1:D:491:GLN:HG2	1.97	0.63
2:C:188:ARG:HH12	1:D:500:ALA:HA	1.63	0.63
1:D:402:ARG:NH2	7:D:768:HOH:O	2.29	0.63
1:D:445:VAL:HG22	1:D:479:TRP:HE1	1.62	0.63
2:E:11:TRP:CD1	2:E:12:PRO:HD3	2.33	0.63
1:A:403:LEU:HD23	1:A:540:SER:HB3	1.79	0.63
2:B:159:THR:HA	2:B:199:LEU:HD21	1.79	0.63
2:C:187:LYS:NZ	2:C:187:LYS:HB2	2.11	0.63
1:D:163:GLY:HA3	1:D:560:GLN:OE1	1.98	0.63
1:D:225:HIS:NE2	1:D:529:ARG:HG3	2.12	0.63
1:A:106:GLY:O	1:A:432:ASN:ND2	2.31	0.63
1:A:166:THR:HG23	4:A:602:LEU:C	2.17	0.63
2:C:26:LYS:HE2	2:C:75:ASP:HA	1.80	0.63
2:E:11:TRP:NE1	7:E:423:HOH:O	2.27	0.63
2:E:26:LYS:HZ3	2:E:82:ASN:C	2.02	0.63
1:A:109:LYS:NZ	1:A:111:ILE:HD11	2.12	0.63
1:A:205:HIS:CE1	1:A:206:LEU:HD13	2.34	0.63
1:A:565:ASN:ND2	7:A:783:HOH:O	2.32	0.63
1:D:437:THR:OG1	1:D:440:ASP:HB2	1.98	0.63
1:A:340:ASN:HB2	1:A:352:PHE:HD2	1.64	0.63
1:D:424:ARG:HH21	1:D:425:ARG:NE	1.95	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:169:LYS:HG3	2:E:170:PHE:N	2.13	0.63
2:F:72:GLN:NE2	2:F:152:TYR:OH	2.32	0.63
2:C:125:LYS:HA	2:C:128:PHE:CD2	2.33	0.63
2:C:98:TRP:CH2	2:C:135:LEU:HG	2.34	0.63
2:B:136:GLU:HG3	2:B:181:LYS:HE3	1.78	0.63
2:C:184:ALA:HB1	1:D:499:ARG:CZ	2.27	0.63
1:D:451:ARG:O	1:D:454:GLU:HG2	1.98	0.63
1:D:498:ASP:HB3	1:D:510:ARG:HH22	1.63	0.63
1:D:54:ALA:O	7:D:727:HOH:O	2.16	0.63
1:D:445:VAL:HG21	1:D:462:PHE:CG	2.33	0.63
2:E:139:LEU:C	2:E:141:ASP:N	2.50	0.63
1:A:536:LEU:HB2	1:A:545:PHE:CE1	2.33	0.63
1:D:114:THR:HG22	1:D:115:ASP:H	1.63	0.63
1:D:441:LEU:HD23	1:D:549:ARG:HB3	1.80	0.63
2:F:139:LEU:HB3	2:F:181:LYS:HE2	1.80	0.63
1:A:241:ILE:HG13	1:A:242:VAL:N	2.14	0.62
1:A:483:GLY:N	7:A:764:HOH:O	2.30	0.62
1:A:426:ASN:ND2	7:A:776:HOH:O	2.30	0.62
2:B:204:LYS:NZ	7:B:406:HOH:O	2.09	0.62
2:C:24:ARG:HB3	2:C:194:SER:HA	1.81	0.62
1:D:353:ALA:HB2	1:D:413:TYR:CD2	2.34	0.62
1:D:164:THR:OG1	1:D:557:LYS:O	2.15	0.62
2:E:121:GLN:O	2:E:125:LYS:HG3	1.99	0.62
1:A:208:SER:HA	1:A:211:LEU:HD12	1.80	0.62
1:A:424:ARG:CB	1:A:425:ARG:HH11	2.12	0.62
2:C:75:ASP:HB2	2:C:84:PHE:CE2	2.34	0.62
1:D:313:VAL:HG13	1:D:314:PRO:HD3	1.81	0.62
1:D:79:ARG:HH22	1:D:88:ILE:HB	1.62	0.62
1:D:84:ASP:O	7:D:728:HOH:O	2.16	0.62
2:F:16:GLY:HA2	2:F:55:PRO:HB3	1.82	0.62
1:A:535:PHE:HB3	1:A:544:GLN:O	1.99	0.62
1:A:145:LEU:HD11	1:A:147:PHE:CE1	2.35	0.62
1:A:215:GLN:NE2	7:A:788:HOH:O	2.33	0.62
1:A:238:TRP:HA	1:A:241:ILE:HG12	1.81	0.62
2:B:108:ASP:OD1	7:B:411:HOH:O	2.16	0.62
1:D:147:PHE:O	1:D:529:ARG:NH2	2.30	0.62
1:A:223:PHE:CZ	1:A:533:GLU:HA	2.35	0.62
1:D:522:VAL:HB	1:D:568:SER:OG	2.00	0.62
1:A:219:VAL:HB	1:A:295:PHE:CZ	2.34	0.62
1:D:507:VAL:O	7:D:726:HOH:O	2.16	0.62
2:C:5:PRO:HG3	2:C:59:HIS:CE1	2.35	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:213:ARG:HG3	1:D:214:ASP:N	2.15	0.62
1:D:466:ILE:HG13	1:D:552:LYS:HA	1.81	0.62
2:F:8:LEU:HD22	2:F:33:ARG:HH21	1.64	0.62
1:A:559:LEU:HD23	1:A:562:LEU:HD13	1.82	0.61
1:A:514:THR:O	7:A:737:HOH:O	2.16	0.61
2:C:16:GLY:HA2	2:C:55:PRO:HB3	1.82	0.61
2:F:121:GLN:O	2:F:125:LYS:HG3	2.00	0.61
1:A:222:VAL:HG23	1:A:223:PHE:HD1	1.64	0.61
1:A:199:HIS:N	1:A:524:ALA:HB1	2.14	0.61
2:C:117:LYS:HE3	2:C:213:ARG:NH1	2.16	0.61
1:D:473:GLY:O	1:D:516:GLY:N	2.33	0.61
4:A:602:LEU:N	7:A:789:HOH:O	2.33	0.61
1:A:43:ILE:HG12	1:A:88:ILE:HG23	1.81	0.61
2:E:154:ASP:O	2:E:158:ILE:HG12	2.00	0.61
1:A:143:LYS:HD2	1:A:212:PHE:HB2	1.82	0.61
2:C:164:PHE:HD2	2:C:183:ILE:HD12	1.66	0.61
1:A:212:PHE:O	1:A:216:VAL:HG23	2.00	0.61
2:B:85:PHE:HB3	2:B:92:ARG:HG2	1.82	0.61
1:D:108:PRO:HB3	1:D:555:ASN:CB	2.31	0.61
1:A:507:VAL:O	1:A:511:LYS:HB2	2.00	0.61
1:D:125:PHE:HE1	1:D:182:ILE:HD12	1.66	0.61
1:D:195:SER:OG	1:D:197:ASP:OD1	2.19	0.61
1:A:151:SER:HB3	1:A:565:ASN:ND2	2.14	0.61
1:A:528:PHE:HA	1:A:531:ILE:HG12	1.83	0.61
2:E:110:GLN:NE2	7:E:437:HOH:O	2.34	0.61
1:D:216:VAL:HG23	7:D:813:HOH:O	2.00	0.61
2:F:195:VAL:HG23	2:F:199:LEU:HD13	1.82	0.61
1:A:97:ILE:H	1:A:163:GLY:H	1.47	0.61
1:A:332:SER:HB2	1:A:538:LEU:HA	1.81	0.60
2:C:23:LEU:HD22	2:C:28:VAL:HG11	1.82	0.60
2:F:54:ILE:HB	2:F:55:PRO:HA	1.83	0.60
2:F:7:LEU:HD21	2:F:23:LEU:HD12	1.83	0.60
1:A:202:LEU:C	1:A:205:HIS:HD1	1.97	0.60
2:E:39:ASN:ND2	7:E:436:HOH:O	2.34	0.60
1:A:212:PHE:HB3	1:A:215:GLN:HE21	1.65	0.60
1:A:504:ALA:O	1:A:507:VAL:HB	2.01	0.60
1:A:70:ASP:HA	1:A:109:LYS:HE3	1.82	0.60
1:A:92:HIS:HB3	2:B:181:LYS:HB3	1.82	0.60
1:A:451:ARG:NH1	1:A:454:GLU:OE1	2.34	0.60
2:C:98:TRP:CD1	2:C:153:VAL:HG21	2.36	0.60
1:D:410:ILE:HG13	1:D:418:GLN:HB2	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:478:PHE:CZ	1:D:562:LEU:HB2	2.36	0.60
1:A:222:VAL:O	1:A:304:ILE:N	2.33	0.60
1:D:190:ASP:O	1:D:194:PHE:N	2.29	0.60
1:D:480:GLU:OE2	1:D:526:GLY:N	2.32	0.60
1:D:87:PRO:HD2	2:E:188:ARG:CB	2.32	0.60
1:A:435:LYS:HB3	1:A:436:ASN:C	2.22	0.60
2:B:125:LYS:HB3	2:B:173:PHE:CE2	2.35	0.60
2:C:68:LEU:HB2	2:C:152:TYR:OH	2.02	0.60
1:D:140:ASP:N	1:D:140:ASP:OD1	2.35	0.60
1:D:200:GLN:HB3	1:D:254:ILE:HG23	1.81	0.60
1:D:332:SER:OG	1:D:333:SER:N	2.34	0.60
1:D:369:THR:OG1	1:D:370:GLY:N	2.34	0.60
1:D:105:GLN:HA	1:D:430:SER:HB3	1.83	0.60
2:F:10:TYR:HB3	2:F:13:SER:HB2	1.84	0.60
1:A:232:ARG:NH2	7:A:781:HOH:O	2.32	0.60
1:A:305:MET:CB	1:A:347:PRO:HB3	2.31	0.60
2:E:114:TRP:HD1	2:E:167:TYR:HE1	1.48	0.60
2:E:63:PRO:O	7:E:412:HOH:O	2.16	0.60
1:A:442:GLN:HG2	1:A:462:PHE:CZ	2.31	0.60
2:C:18:ARG:NH2	2:C:103:ASP:OD1	2.23	0.60
1:D:107:ARG:HH21	1:D:434:ASP:HB3	1.67	0.60
1:D:329:ASP:N	1:D:329:ASP:OD1	2.35	0.59
1:A:107:ARG:HH11	1:A:433:ILE:HG13	1.67	0.59
1:A:164:THR:OG1	1:A:557:LYS:O	2.21	0.59
1:A:152:LYS:HA	1:A:564:GLU:HB2	1.83	0.59
2:C:57:LEU:HB3	2:C:64:VAL:CG2	2.32	0.59
1:D:552:LYS:C	1:D:554:SER:H	2.05	0.59
1:D:79:ARG:HD2	2:E:188:ARG:HH22	1.67	0.59
2:E:23:LEU:HG	2:E:28:VAL:HB	1.85	0.59
1:D:405:ASP:CB	1:D:541:SER:HB2	2.29	0.59
1:D:88:ILE:HG13	1:D:89:LEU:N	2.17	0.59
2:F:165:GLN:HG3	2:F:206:VAL:HG21	1.84	0.59
1:D:83:GLY:H	1:D:158:GLY:HA3	1.66	0.59
1:D:498:ASP:CB	1:D:510:ARG:HH22	2.15	0.59
2:F:33:ARG:NH2	2:F:35:GLU:OE2	2.35	0.59
1:D:288:TYR:O	7:D:730:HOH:O	2.16	0.59
2:F:40:LYS:HD2	2:F:52:LYS:HB3	1.85	0.59
1:A:213:ARG:HG3	1:A:214:ASP:N	2.18	0.59
1:A:441:LEU:HD23	1:A:549:ARG:HB3	1.84	0.59
1:D:152:LYS:NZ	1:D:561:ILE:HG23	2.17	0.59
2:F:143:PRO:O	2:F:185:TRP:HD1	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:181:SER:O	7:D:731:HOH:O	2.17	0.59
1:D:360:TYR:OH	1:D:362:GLU:OE2	2.11	0.59
1:D:535:PHE:O	1:D:538:LEU:HB3	2.02	0.59
1:A:424:ARG:CG	1:A:425:ARG:HH11	2.15	0.59
1:A:74:GLU:HG2	1:A:78:LYS:HD3	1.84	0.59
2:C:10:TYR:O	2:C:20:ARG:NH2	2.34	0.59
1:D:108:PRO:HB3	1:D:555:ASN:HB2	1.84	0.59
1:D:199:HIS:H	1:D:524:ALA:HB1	1.67	0.59
2:F:135:LEU:HD13	2:F:182:LEU:CD1	2.32	0.59
1:A:254:ILE:HG22	7:A:798:HOH:O	2.02	0.59
1:A:225:HIS:HB3	1:A:309:MET:SD	2.43	0.59
2:C:33:ARG:HH12	2:C:41:SER:HB2	1.67	0.59
2:F:110:GLN:HA	2:F:113:VAL:HG12	1.83	0.59
1:D:507:VAL:HG12	7:D:726:HOH:O	2.02	0.59
1:D:527:THR:O	7:D:729:HOH:O	2.16	0.59
1:D:90:THR:CG2	1:D:112:PRO:HG2	2.32	0.59
2:E:139:LEU:O	2:E:141:ASP:N	2.29	0.59
1:A:18:ASP:O	1:A:22:ARG:HG2	2.03	0.58
1:A:291:ILE:HD12	1:A:320:ALA:HB2	1.85	0.58
1:A:83:GLY:O	7:A:741:HOH:O	2.17	0.58
2:B:17:MET:SD	2:B:199:LEU:HG	2.43	0.58
2:B:184:ALA:HA	2:B:187:LYS:CG	2.33	0.58
1:D:526:GLY:O	1:D:530:LYS:HG3	2.03	0.58
2:F:24:ARG:HB3	2:F:194:SER:HA	1.85	0.58
2:F:64:VAL:HB	2:F:73:TYR:CE2	2.38	0.58
2:F:57:LEU:O	2:F:64:VAL:HG22	2.03	0.58
2:F:98:TRP:CE3	2:F:101:PHE:HB2	2.39	0.58
1:A:496:CYS:HA	1:A:499:ARG:HB2	1.85	0.58
1:A:450:LYS:HE3	7:A:1031:HOH:O	2.03	0.58
1:A:477:ILE:HG13	1:A:518:LEU:HD23	1.86	0.58
1:A:81:VAL:HG11	1:A:110:PHE:CE2	2.38	0.58
2:F:86:PRO:HD3	2:F:146:GLY:O	2.04	0.58
1:A:445:VAL:HG21	1:A:462:PHE:CG	2.38	0.58
2:C:86:PRO:HB2	7:C:434:HOH:O	2.04	0.58
2:F:114:TRP:HA	2:F:170:PHE:HD2	1.68	0.58
2:F:135:LEU:HD13	2:F:182:LEU:HD11	1.86	0.58
1:A:70:ASP:HB2	1:A:104:SER:HB2	1.86	0.58
1:A:559:LEU:O	1:A:562:LEU:HB3	2.03	0.58
2:B:169:LYS:HG3	2:B:170:PHE:N	2.18	0.58
1:A:87:PRO:HD2	2:B:188:ARG:CB	2.33	0.58
2:E:13:SER:O	2:E:17:MET:HG3	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:193:GLU:HB2	2:E:197:LYS:HD3	1.85	0.58
1:A:38:LYS:O	2:B:142:LYS:HG3	2.03	0.58
2:E:24:ARG:HE	2:E:193:GLU:HG3	1.68	0.58
1:A:340:ASN:HB2	1:A:352:PHE:CD2	2.39	0.58
1:D:166:THR:HG23	4:D:602:LEU:OXT	2.03	0.58
1:A:171:ARG:N	7:A:708:HOH:O	2.34	0.58
1:D:97:ILE:HG22	1:D:162:VAL:CG2	2.34	0.58
2:E:56:VAL:HA	7:E:406:HOH:O	2.04	0.58
2:B:26:LYS:NZ	2:B:78:TRP:CD2	2.72	0.58
2:F:33:ARG:NH2	2:F:43:LEU:HD11	2.19	0.58
2:F:43:LEU:HD12	2:F:44:LEU:N	2.18	0.58
1:A:342:THR:HG1	1:A:413:TYR:HH	1.52	0.57
2:C:176:GLU:OE2	1:D:573:THR:OG1	2.18	0.57
2:F:144:TYR:HB3	2:F:154:ASP:OD1	2.05	0.57
2:F:170:PHE:CD2	2:F:213:ARG:HD2	2.39	0.57
1:A:164:THR:HA	1:A:557:LYS:HG2	1.85	0.57
1:D:163:GLY:CA	1:D:560:GLN:OE1	2.52	0.57
1:D:135:ASP:OD2	1:D:343:PRO:HD2	2.04	0.57
1:D:152:LYS:HG2	1:D:565:ASN:CB	2.34	0.57
2:F:113:VAL:HB	2:F:128:PHE:CE2	2.39	0.57
1:A:150:SER:OG	1:A:150:SER:O	2.20	0.57
2:B:58:VAL:O	7:B:413:HOH:O	2.17	0.57
1:D:39:ASN:HA	2:E:142:LYS:HG2	1.85	0.57
1:D:432:ASN:O	1:D:433:ILE:HG23	2.04	0.57
1:A:478:PHE:CZ	1:A:562:LEU:HG	2.40	0.57
2:C:114:TRP:HA	2:C:170:PHE:HD2	1.69	0.57
1:D:518:LEU:N	7:D:719:HOH:O	2.36	0.57
2:E:139:LEU:O	2:E:142:LYS:HG3	2.04	0.57
1:A:165:ALA:HB1	4:A:602:LEU:HD12	1.86	0.57
1:A:284:LEU:HD13	1:A:287:TRP:N	2.19	0.57
1:A:428:ILE:HG13	1:A:428:ILE:O	2.03	0.57
1:A:452:LEU:HD13	1:A:493:CYS:SG	2.44	0.57
2:C:163:TRP:HB3	2:C:167:TYR:CZ	2.39	0.57
2:C:7:LEU:HD21	2:C:23:LEU:HD12	1.85	0.57
1:D:97:ILE:HG22	1:D:162:VAL:HG23	1.85	0.57
1:A:206:LEU:O	1:A:210:ILE:HG13	2.04	0.57
1:A:424:ARG:C	1:A:543:GLY:HA2	2.25	0.57
1:A:80:MET:HG3	1:A:88:ILE:HD12	1.86	0.57
2:B:158:ILE:HG12	2:B:195:VAL:HG21	1.87	0.57
2:B:20:ARG:NH1	2:B:198:SER:O	2.37	0.57
1:D:35:ILE:HD13	1:D:394:ASN:HA	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:169:LYS:HG3	2:E:170:PHE:H	1.69	0.57
2:F:72:GLN:HG2	2:F:152:TYR:HE1	1.69	0.57
1:A:465:TYR:HA	1:A:551:VAL:HB	1.87	0.57
1:D:382:VAL:HG13	1:D:388:TYR:CD2	2.40	0.57
1:A:148:ILE:HD12	1:A:170:TYR:CZ	2.39	0.57
2:C:84:PHE:CD1	2:C:152:TYR:HB2	2.39	0.57
1:D:496:CYS:HA	1:D:499:ARG:CZ	2.35	0.57
1:D:108:PRO:HG2	1:D:552:LYS:HB3	1.85	0.57
2:E:201:ASP:HB2	2:E:204:LYS:HG3	1.87	0.57
2:B:162:SER:O	2:B:205:ILE:HG12	2.05	0.57
2:C:102:VAL:O	2:C:107:THR:HG23	2.05	0.57
2:C:153:VAL:O	2:C:157:LEU:HD23	2.05	0.57
2:E:26:LYS:HE2	7:E:417:HOH:O	2.05	0.57
1:A:526:GLY:O	1:A:530:LYS:HG3	2.05	0.56
2:B:117:LYS:HG2	2:B:213:ARG:NH1	2.17	0.56
2:C:57:LEU:HB3	2:C:64:VAL:HG22	1.87	0.56
2:C:84:PHE:HB2	2:C:152:TYR:N	2.20	0.56
2:C:86:PRO:HD3	2:C:146:GLY:O	2.05	0.56
1:D:165:ALA:HB1	4:D:602:LEU:HD12	1.87	0.56
2:F:98:TRP:HE3	2:F:101:PHE:HB2	1.68	0.56
1:A:521:ARG:HB3	1:A:566:VAL:HG12	1.88	0.56
2:C:125:LYS:HA	2:C:128:PHE:CE2	2.40	0.56
2:C:184:ALA:HB1	1:D:499:ARG:HH11	1.68	0.56
2:C:18:ARG:NH1	2:C:67:SER:OG	2.38	0.56
1:D:340:ASN:HD21	1:D:345:LEU:HD11	1.71	0.56
2:E:166:ALA:HA	2:E:169:LYS:HG2	1.87	0.56
1:A:53:ASN:HD21	2:B:90:TYR:HB3	1.70	0.56
1:A:152:LYS:HG3	1:A:565:ASN:ND2	2.21	0.56
1:D:236:GLN:NE2	7:D:795:HOH:O	2.37	0.56
1:D:434:ASP:OD1	1:D:435:LYS:HG3	2.05	0.56
1:A:412:PHE:CZ	1:A:417:PRO:HB3	2.41	0.56
2:C:136:GLU:HG3	2:C:181:LYS:CD	2.31	0.56
1:D:247:ASP:HB2	1:D:249:VAL:HG22	1.86	0.56
1:D:438:GLU:O	1:D:442:GLN:HG3	2.06	0.56
2:C:53:LYS:O	7:C:411:HOH:O	2.17	0.56
1:D:110:PHE:CE2	1:D:554:SER:HA	2.40	0.56
2:E:145:PHE:HB2	2:E:154:ASP:OD1	2.05	0.56
2:F:140:GLY:CA	2:F:181:LYS:NZ	2.69	0.56
1:A:108:PRO:HB3	1:A:555:ASN:CG	2.26	0.56
1:A:96:ALA:HB3	1:A:113:PHE:CD2	2.40	0.56
2:C:64:VAL:HB	2:C:73:TYR:CE2	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:199:HIS:N	1:D:524:ALA:HB1	2.20	0.56
1:D:198:VAL:HG22	1:D:524:ALA:HB3	1.87	0.56
1:D:405:ASP:OD1	1:D:540:SER:HB2	2.05	0.56
1:A:97:ILE:N	1:A:163:GLY:H	2.04	0.56
1:A:315:LYS:O	1:A:318:HIS:HB3	2.06	0.56
1:A:506:TYR:OH	1:A:518:LEU:HD11	2.05	0.56
1:D:529:ARG:NH1	1:D:533:GLU:OE2	2.38	0.56
1:A:153:GLN:HG2	1:A:167:THR:HG21	1.88	0.56
2:B:139:LEU:O	2:B:141:ASP:N	2.38	0.56
2:B:8:LEU:HB2	2:B:56:VAL:HB	1.88	0.56
1:D:18:ASP:OD1	1:D:414:ASN:ND2	2.39	0.56
1:A:182:ILE:HG13	1:A:183:THR:HG23	1.86	0.56
1:A:319:TYR:HA	7:A:753:HOH:O	2.06	0.56
2:C:98:TRP:O	2:C:101:PHE:HB2	2.05	0.56
2:C:184:ALA:O	1:D:499:ARG:NH2	2.39	0.56
1:D:92:HIS:CG	2:E:139:LEU:HD23	2.40	0.56
1:A:105:GLN:OE1	7:A:743:HOH:O	2.18	0.56
1:A:267:LEU:HG	7:A:773:HOH:O	2.06	0.56
1:A:369:THR:HG23	1:A:370:GLY:H	1.71	0.56
2:C:10:TYR:HB3	2:C:13:SER:HB2	1.88	0.56
1:D:143:LYS:HB2	1:D:185:PRO:O	2.06	0.56
1:D:23:ASN:O	1:D:27:VAL:HG12	2.06	0.56
1:D:531:ILE:HG21	1:D:547:MET:HG2	1.87	0.56
1:D:76:TYR:HD2	1:D:88:ILE:HD11	1.70	0.56
2:F:72:GLN:HG2	2:F:152:TYR:CE1	2.40	0.56
2:C:140:GLY:N	2:C:181:LYS:HZ1	2.05	0.55
2:F:208:TYR:O	7:F:406:HOH:O	2.18	0.55
1:A:213:ARG:HH21	1:A:296:PRO:HG3	1.72	0.55
1:A:552:LYS:HD2	1:A:553:PRO:HD2	1.89	0.55
1:D:212:PHE:O	1:D:216:VAL:HG13	2.07	0.55
1:D:77:ILE:HG22	1:D:110:PHE:HB3	1.86	0.55
2:E:152:TYR:OH	7:E:411:HOH:O	2.13	0.55
2:E:53:LYS:HD3	6:E:301:GSH:HB13	1.88	0.55
1:A:152:LYS:HD3	1:A:561:ILE:O	2.06	0.55
2:B:58:VAL:HG22	2:B:63:PRO:HB3	1.88	0.55
1:A:94:VAL:HB	1:A:113:PHE:O	2.06	0.55
2:B:17:MET:HG2	2:B:20:ARG:NH1	2.21	0.55
1:D:410:ILE:HG21	1:D:420:LYS:HB3	1.89	0.55
1:D:90:THR:HG23	7:D:742:HOH:O	2.05	0.55
2:F:17:MET:HE2	2:F:200:PRO:HD2	1.87	0.55
2:E:64:VAL:HG23	2:F:93:ALA:HB1	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:197:LYS:NZ	7:C:433:HOH:O	2.39	0.55
2:B:76:GLU:OE2	2:C:92:ARG:NE	2.39	0.55
1:D:478:PHE:CE1	1:D:521:ARG:HD2	2.40	0.55
1:D:42:ALA:HA	2:E:143:PRO:HG3	1.87	0.55
1:A:202:LEU:CD2	1:A:205:HIS:HB3	2.36	0.55
1:A:300:TYR:CD2	1:A:302:TYR:HB2	2.41	0.55
1:A:32:LEU:HD22	1:A:360:TYR:CZ	2.42	0.55
1:D:12:ARG:NH2	7:D:803:HOH:O	2.39	0.55
1:D:76:TYR:C	1:D:79:ARG:HH21	2.07	0.55
2:F:37:PHE:O	2:F:40:LYS:NZ	2.40	0.55
1:A:164:THR:N	1:A:560:GLN:OE1	2.40	0.55
1:A:93:PRO:HG2	2:B:184:ALA:CB	2.37	0.55
2:E:174:SER:HB3	2:E:177:SER:HB2	1.89	0.55
1:A:250:LEU:HD11	1:A:260:ARG:CZ	2.37	0.55
1:A:238:TRP:HH2	1:A:281:CYS:HB3	1.69	0.55
1:A:315:LYS:HA	1:A:318:HIS:HB3	1.89	0.55
1:A:92:HIS:NE2	2:B:139:LEU:HB3	2.22	0.55
2:C:32:TYR:CD1	2:C:34:GLU:OE2	2.60	0.55
2:F:214:LYS:NZ	7:F:411:HOH:O	2.22	0.55
2:F:84:PHE:HB2	2:F:152:TYR:N	2.21	0.55
1:A:219:VAL:HB	1:A:295:PHE:HZ	1.71	0.55
1:A:363:PHE:HB3	1:A:388:TYR:HB3	1.87	0.55
1:A:42:ALA:HB3	1:A:45:LEU:HD22	1.88	0.55
1:D:104:SER:O	1:D:107:ARG:HB2	2.07	0.55
2:E:7:LEU:HB2	2:E:57:LEU:HD13	1.89	0.55
1:A:313:VAL:N	1:A:314:PRO:HD2	2.21	0.55
1:A:39:ASN:ND2	1:A:90:THR:O	2.40	0.55
2:E:195:VAL:HG23	2:E:199:LEU:HD22	1.88	0.55
2:F:98:TRP:CD2	2:F:138:GLU:OE2	2.59	0.55
1:A:468:VAL:O	7:A:744:HOH:O	2.18	0.54
2:B:33:ARG:NH1	7:B:444:HOH:O	2.40	0.54
2:C:117:LYS:HE3	2:C:213:ARG:HH11	1.72	0.54
2:C:64:VAL:HG23	2:C:70:VAL:HG22	1.88	0.54
2:C:98:TRP:O	2:C:102:VAL:HG23	2.07	0.54
1:D:79:ARG:NH2	1:D:88:ILE:CB	2.70	0.54
2:F:126:LYS:O	2:F:129:ILE:HG13	2.07	0.54
2:F:64:VAL:HB	2:F:73:TYR:CD2	2.42	0.54
1:A:162:VAL:HG21	1:A:559:LEU:HD13	1.89	0.54
1:A:424:ARG:HD2	1:A:425:ARG:NH1	2.23	0.54
2:C:140:GLY:O	7:C:412:HOH:O	2.18	0.54
1:D:302:TYR:HD1	1:D:326:VAL:HG13	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:98:TRP:O	2:F:101:PHE:HB2	2.06	0.54
2:F:178:GLU:OE1	7:F:407:HOH:O	2.18	0.54
2:E:96:ARG:NH2	2:F:69:ASN:OD1	2.40	0.54
2:C:141:ASP:N	2:C:141:ASP:OD1	2.40	0.54
1:D:223:PHE:HB2	1:D:225:HIS:HD2	1.71	0.54
1:A:31:THR:OG1	1:A:357:ASN:HA	2.07	0.54
1:D:13:VAL:HA	1:D:16:GLU:OE2	2.07	0.54
1:D:437:THR:O	1:D:440:ASP:N	2.41	0.54
1:D:82:ASP:N	7:D:728:HOH:O	2.39	0.54
1:D:114:THR:HG23	2:E:141:ASP:OD2	2.08	0.54
1:A:231:PHE:O	1:A:235:GLU:HB2	2.07	0.54
1:A:85:THR:N	7:A:804:HOH:O	2.40	0.54
1:D:506:TYR:CE2	1:D:510:ARG:NH1	2.75	0.54
1:A:124:LEU:HD12	1:A:355:ILE:HD12	1.89	0.54
1:A:81:VAL:O	7:A:742:HOH:O	2.17	0.54
2:C:184:ALA:HA	2:C:187:LYS:HZ1	1.71	0.54
1:D:496:CYS:N	1:D:499:ARG:NH1	2.56	0.54
1:D:163:GLY:HA2	1:D:560:GLN:HB2	1.90	0.54
2:E:159:THR:HA	2:E:199:LEU:HD21	1.90	0.54
2:E:201:ASP:OD2	2:E:204:LYS:HE2	2.07	0.54
2:E:26:LYS:NZ	2:E:82:ASN:C	2.61	0.54
2:E:15:PHE:HB3	2:E:67:SER:CB	2.38	0.54
2:E:8:LEU:HD21	2:E:43:LEU:HD23	1.90	0.54
1:A:557:LYS:O	1:A:561:ILE:HG13	2.07	0.54
2:E:144:TYR:OH	2:E:151:GLY:N	2.28	0.54
1:A:125:PHE:HB3	1:A:182:ILE:HD12	1.88	0.54
1:A:262:ALA:HA	1:A:265:LYS:HZ2	1.73	0.54
2:C:117:LYS:HA	2:C:121:GLN:HB2	1.89	0.54
2:C:201:ASP:OD2	1:D:456:LYS:NZ	2.34	0.54
1:D:162:VAL:HG23	1:D:556:ALA:HB1	1.90	0.54
2:F:9:ASP:HA	2:F:54:ILE:HD13	1.89	0.54
1:A:266:LEU:HB2	7:A:773:HOH:O	2.08	0.54
1:A:85:THR:O	2:B:184:ALA:HB1	2.08	0.54
1:D:221:ALA:HB3	1:D:227:LEU:HG	1.90	0.54
1:D:562:LEU:HD12	1:D:563:CYS:N	2.22	0.54
1:A:428:ILE:HG23	7:A:978:HOH:O	2.07	0.53
2:B:92:ARG:HG3	7:B:401:HOH:O	2.07	0.53
2:C:150:PHE:CD1	2:C:192:LYS:HG3	2.43	0.53
1:D:219:VAL:HG13	1:D:301:VAL:HG13	1.89	0.53
1:D:563:CYS:O	1:D:566:VAL:HG22	2.08	0.53
2:C:11:TRP:CG	2:C:12:PRO:HD3	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:107:THR:HG22	2:F:160:PHE:CZ	2.43	0.53
2:F:23:LEU:HD22	2:F:28:VAL:HG11	1.88	0.53
1:A:363:PHE:HE1	1:A:390:VAL:HG22	1.73	0.53
1:A:154:TYR:CE2	1:A:156:SER:HA	2.43	0.53
1:A:40:GLN:HG2	2:B:142:LYS:HE3	1.89	0.53
1:A:417:PRO:HB2	7:A:800:HOH:O	2.08	0.53
1:A:99:LEU:HD23	1:A:535:PHE:HZ	1.73	0.53
2:B:57:LEU:HD22	2:B:70:VAL:HG13	1.91	0.53
1:D:47:ASN:ND2	7:D:808:HOH:O	2.41	0.53
2:E:26:LYS:HE3	2:E:81:LYS:HZ1	1.73	0.53
1:A:302:TYR:CD2	1:A:328:HIS:NE2	2.77	0.53
1:D:151:SER:O	1:D:171:ARG:NH2	2.42	0.53
1:D:44:TYR:HD2	1:D:45:LEU:HD12	1.73	0.53
1:D:494:CYS:HB2	7:D:815:HOH:O	2.07	0.53
1:A:200:GLN:HE21	1:A:259:VAL:HG11	1.74	0.53
2:C:57:LEU:O	2:C:64:VAL:HG22	2.08	0.53
2:B:96:ARG:HE	2:C:73:TYR:HE1	1.57	0.53
1:D:169:VAL:O	1:D:175:PHE:HB2	2.09	0.53
2:E:176:GLU:HB2	2:E:183:ILE:HD12	1.90	0.53
2:F:192:LYS:NZ	7:F:436:HOH:O	2.41	0.53
1:A:200:GLN:OE1	7:A:733:HOH:O	2.18	0.53
1:D:36:LEU:HD22	1:D:61:PHE:CE1	2.44	0.53
2:E:68:LEU:HD11	2:E:152:TYR:CE1	2.43	0.53
1:A:83:GLY:H	1:A:158:GLY:HA3	1.72	0.53
1:A:314:PRO:HA	1:A:317:ARG:NH1	2.24	0.53
1:A:393:THR:HA	1:A:398:LEU:O	2.08	0.53
1:A:45:LEU:HG	1:A:50:LEU:HD22	1.90	0.53
2:F:120:GLU:O	7:F:405:HOH:O	2.17	0.53
1:A:151:SER:OG	1:A:195:SER:O	2.26	0.53
1:A:203:TYR:CE1	1:A:241:ILE:HG22	2.44	0.53
1:D:217:GLN:NE2	7:D:810:HOH:O	2.42	0.53
1:D:109:LYS:N	1:D:555:ASN:OD1	2.29	0.53
1:A:122:LEU:O	1:A:126:ARG:HB2	2.09	0.53
1:A:158:GLY:N	7:A:742:HOH:O	2.41	0.53
1:A:512:CYS:SG	1:A:514:THR:HG23	2.48	0.53
2:B:62:LYS:HB2	2:C:90:TYR:CZ	2.43	0.53
1:D:253:ARG:NH1	1:D:484:GLU:HB3	2.24	0.53
1:D:433:ILE:HD11	1:D:552:LYS:HE3	1.90	0.53
1:A:451:ARG:NE	7:A:812:HOH:O	2.42	0.52
1:A:460:ILE:HD11	1:A:480:GLU:HG2	1.91	0.52
2:B:108:ASP:O	2:B:112:LYS:HG2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:153:VAL:O	2:E:156:SER:OG	2.15	0.52
2:E:5:PRO:HB3	2:E:59:HIS:CD2	2.44	0.52
2:F:5:PRO:HG3	2:F:59:HIS:CE1	2.44	0.52
1:D:496:CYS:HA	1:D:499:ARG:NH1	2.24	0.52
2:E:154:ASP:HB3	2:E:158:ILE:HD11	1.90	0.52
1:A:522:VAL:O	1:A:567:VAL:HG22	2.09	0.52
1:A:92:HIS:CE1	2:B:139:LEU:HD23	2.44	0.52
2:B:169:LYS:HG3	2:B:170:PHE:H	1.74	0.52
1:A:260:ARG:HB2	7:A:798:HOH:O	2.08	0.52
1:D:88:ILE:HG13	1:D:89:LEU:HG	1.90	0.52
2:F:165:GLN:HG3	2:F:206:VAL:CG2	2.39	0.52
1:A:97:ILE:O	1:A:163:GLY:N	2.42	0.52
1:A:223:PHE:CE1	1:A:304:ILE:HD12	2.45	0.52
2:C:98:TRP:CD1	2:C:153:VAL:HG11	2.44	0.52
1:A:152:LYS:HG3	1:A:565:ASN:CG	2.30	0.52
1:A:301:VAL:HG22	7:A:889:HOH:O	2.08	0.52
1:D:208:SER:HA	1:D:211:LEU:HD12	1.92	0.52
2:F:201:ASP:HB2	2:F:204:LYS:HG3	1.92	0.52
2:E:96:ARG:HH21	2:F:69:ASN:HA	1.75	0.52
1:A:224:ALA:HB3	1:A:309:MET:HB3	1.92	0.52
1:A:302:TYR:HA	1:A:326:VAL:HG13	1.91	0.52
1:A:437:THR:O	1:A:440:ASP:N	2.42	0.52
1:A:73:LEU:HD22	1:A:89:LEU:HD13	1.91	0.52
2:C:145:PHE:HB3	2:C:153:VAL:HG13	1.91	0.52
2:E:74:VAL:HG12	7:E:516:HOH:O	2.09	0.52
1:A:149:PHE:CZ	1:A:202:LEU:HB2	2.44	0.52
1:A:172:ASN:ND2	7:A:817:HOH:O	2.43	0.52
1:A:538:LEU:HD12	1:A:539:GLY:N	2.25	0.52
1:A:552:LYS:CD	1:A:553:PRO:HD2	2.40	0.52
1:D:22:ARG:NH1	1:D:414:ASN:OD1	2.42	0.52
1:D:385:GLY:HA2	1:D:408:LYS:HE3	1.92	0.52
2:C:183:ILE:HD11	1:D:451:ARG:HE	1.74	0.52
1:A:107:ARG:HG3	1:A:107:ARG:HH11	1.74	0.52
1:A:423:CYS:SG	1:A:543:GLY:N	2.83	0.52
1:A:498:ASP:HB2	7:A:707:HOH:O	2.10	0.52
2:C:40:LYS:HD2	2:C:52:LYS:HB3	1.92	0.52
2:E:98:TRP:CZ2	2:E:138:GLU:HB2	2.45	0.52
2:E:26:LYS:HE3	2:E:81:LYS:NZ	2.25	0.52
2:F:68:LEU:O	2:F:72:GLN:HG3	2.09	0.52
2:F:84:PHE:CG	2:F:152:TYR:HB2	2.45	0.52
1:A:405:ASP:HB3	1:A:541:SER:CB	2.35	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:538:LEU:HD12	1:A:539:GLY:H	1.75	0.52
2:F:108:ASP:O	2:F:112:LYS:HG2	2.10	0.52
2:F:132:VAL:HG22	2:F:179:SER:CB	2.38	0.52
2:C:187:LYS:HE3	1:D:492:ASP:O	2.10	0.51
2:C:8:LEU:HD21	2:C:43:LEU:HD11	1.92	0.51
2:F:56:VAL:HG13	7:F:465:HOH:O	2.09	0.51
1:A:153:GLN:O	1:A:564:GLU:HG2	2.10	0.51
1:A:470:THR:HG21	1:A:474:HIS:CE1	2.45	0.51
1:D:330:TYR:HE2	1:D:540:SER:H	1.53	0.51
1:D:457:ILE:HD11	1:D:481:ILE:HB	1.92	0.51
1:A:32:LEU:HB2	1:A:360:TYR:CD1	2.46	0.51
1:A:331:GLY:N	1:A:537:GLY:O	2.43	0.51
1:A:405:ASP:CB	1:A:541:SER:HB3	2.35	0.51
1:A:58:GLU:HG2	1:A:62:LYS:HE2	1.91	0.51
1:A:81:VAL:HG13	1:A:82:ASP:OD2	2.09	0.51
2:B:107:THR:HA	2:B:110:GLN:HG2	1.92	0.51
2:B:19:ALA:N	7:B:408:HOH:O	2.43	0.51
2:B:92:ARG:N	7:B:401:HOH:O	2.42	0.51
1:D:291:ILE:HB	1:D:320:ALA:HA	1.92	0.51
1:D:511:LYS:HB2	7:D:726:HOH:O	2.09	0.51
2:F:165:GLN:NE2	2:F:165:GLN:O	2.44	0.51
1:A:424:ARG:CG	1:A:425:ARG:NH1	2.74	0.51
1:A:531:ILE:HA	1:A:534:HIS:NE2	2.25	0.51
1:A:77:ILE:HD13	1:A:112:PRO:HD3	1.92	0.51
2:B:96:ARG:HH11	2:C:73:TYR:HE1	1.56	0.51
1:D:167:THR:OG1	7:D:735:HOH:O	2.19	0.51
1:D:22:ARG:NH1	1:D:414:ASN:CG	2.64	0.51
1:D:152:LYS:HD3	1:D:561:ILE:HG23	1.90	0.51
2:F:131:ALA:O	2:F:135:LEU:HB2	2.11	0.51
2:F:145:PHE:HB3	2:F:153:VAL:HG13	1.91	0.51
2:F:26:LYS:HD3	2:F:78:TRP:HB2	1.91	0.51
2:B:188:ARG:HG2	7:B:454:HOH:O	2.10	0.51
1:D:138:ILE:O	7:D:734:HOH:O	2.19	0.51
1:D:223:PHE:HD2	1:D:225:HIS:CD2	2.28	0.51
1:D:225:HIS:HE2	1:D:529:ARG:HG3	1.73	0.51
1:D:424:ARG:HB3	1:D:424:ARG:NH1	2.25	0.51
2:E:145:PHE:N	2:E:154:ASP:OD1	2.41	0.51
2:F:110:GLN:O	2:F:113:VAL:HG12	2.10	0.51
2:F:188:ARG:HD2	2:F:191:GLU:OE2	2.09	0.51
1:A:438:GLU:O	1:A:442:GLN:HG3	2.11	0.51
1:A:476:ALA:HA	1:A:519:GLU:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:222:VAL:HB	1:D:533:GLU:HB3	1.93	0.51
1:A:147:PHE:CB	1:A:205:HIS:CD2	2.94	0.51
1:A:147:PHE:CB	1:A:205:HIS:HD2	2.24	0.51
1:A:96:ALA:O	1:A:113:PHE:HB3	2.11	0.51
2:C:187:LYS:NZ	1:D:496:CYS:HB2	2.26	0.51
1:D:122:LEU:HD23	1:D:125:PHE:CZ	2.46	0.51
1:D:20:MET:SD	7:D:757:HOH:O	2.58	0.51
1:D:295:PHE:CD1	1:D:298:ALA:HB2	2.43	0.51
1:D:541:SER:O	1:D:543:GLY:N	2.41	0.51
1:D:69:THR:N	1:D:72:GLU:OE1	2.43	0.51
1:A:147:PHE:CD1	1:A:205:HIS:CG	2.93	0.51
2:B:166:ALA:O	2:B:170:PHE:HB2	2.10	0.51
1:D:11:ASN:O	1:D:14:ILE:HG13	2.11	0.51
1:D:218:TYR:N	7:D:813:HOH:O	2.42	0.51
1:D:383:LYS:NZ	7:D:819:HOH:O	2.44	0.51
1:D:62:LYS:HB3	1:D:400:ARG:HH12	1.75	0.51
1:D:9:ASP:N	7:D:812:HOH:O	2.42	0.51
2:E:57:LEU:HG	2:E:59:HIS:NE2	2.26	0.51
2:E:8:LEU:HB2	7:E:438:HOH:O	2.11	0.51
2:F:102:VAL:O	2:F:107:THR:HG23	2.11	0.51
2:F:70:VAL:O	2:F:73:TYR:HB2	2.10	0.51
1:A:220:PHE:CE1	1:A:328:HIS:HE1	2.29	0.51
1:D:153:GLN:H	1:D:564:GLU:HB2	1.76	0.51
1:D:70:ASP:OD1	1:D:71:VAL:N	2.44	0.51
2:F:144:TYR:HA	2:F:185:TRP:NE1	2.25	0.51
1:A:149:PHE:HZ	1:A:202:LEU:HB2	1.76	0.51
1:A:334:GLU:O	1:A:394:ASN:ND2	2.44	0.51
1:D:204:CYS:HA	1:D:207:LEU:HB3	1.93	0.51
1:D:365:PRO:HG3	1:D:388:TYR:CE2	2.46	0.51
1:D:527:THR:O	1:D:530:LYS:HB2	2.12	0.51
1:A:435:LYS:HA	1:A:436:ASN:HB2	1.93	0.50
1:A:556:ALA:HA	1:A:559:LEU:HB2	1.93	0.50
1:A:77:ILE:HG13	1:A:89:LEU:HD12	1.93	0.50
2:B:96:ARG:HH12	2:C:76:GLU:CD	2.14	0.50
1:D:99:LEU:CB	1:D:557:LYS:H	2.24	0.50
1:A:94:VAL:HG21	1:A:112:PRO:HA	1.94	0.50
1:A:22:ARG:NH2	1:A:415:ASN:OD1	2.44	0.50
2:B:26:LYS:NZ	2:B:78:TRP:CG	2.78	0.50
1:D:223:PHE:HZ	1:D:536:LEU:CB	2.24	0.50
1:D:235:GLU:OE1	7:D:736:HOH:O	2.20	0.50
2:E:214:LYS:NZ	7:E:409:HOH:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:PRO:HD2	1:A:396:ALA:O	2.11	0.50
1:A:149:PHE:CZ	1:A:202:LEU:CB	2.94	0.50
2:B:65:CYS:O	2:B:66:GLU:HB2	2.11	0.50
1:D:94:VAL:HB	1:D:113:PHE:O	2.11	0.50
1:D:20:MET:HE2	1:D:356:PRO:HD2	1.93	0.50
1:D:299:LYS:HG3	7:D:823:HOH:O	2.12	0.50
1:D:424:ARG:HE	1:D:425:ARG:CD	2.20	0.50
1:D:510:ARG:NH1	1:D:518:LEU:HG	2.26	0.50
2:E:141:ASP:OD2	2:E:181:LYS:NZ	2.43	0.50
2:E:10:TYR:HA	2:E:34:GLU:OE2	2.12	0.50
1:A:152:LYS:HD3	1:A:561:ILE:C	2.32	0.50
1:A:223:PHE:CE1	1:A:533:GLU:HA	2.46	0.50
1:D:200:GLN:HG2	1:D:254:ILE:HA	1.93	0.50
2:E:109:ALA:O	2:E:113:VAL:HG23	2.12	0.50
1:A:237:VAL:O	1:A:241:ILE:HG23	2.11	0.50
1:A:273:LEU:HA	1:A:276:THR:HG23	1.92	0.50
1:A:276:THR:O	1:A:279:THR:OG1	2.23	0.50
1:A:152:LYS:HE3	1:A:527:THR:HG21	1.93	0.50
1:D:276:THR:OG1	1:D:277:ILE:N	2.44	0.50
1:D:303:GLY:O	1:D:327:SER:HA	2.12	0.50
1:D:464:SER:HB2	1:D:550:CYS:HB2	1.93	0.50
2:F:50:ILE:HG13	2:F:51:HIS:H	1.76	0.50
2:F:97:PHE:CE1	2:F:101:PHE:HE1	2.29	0.50
1:D:208:SER:O	1:D:211:LEU:HB2	2.11	0.50
1:D:296:PRO:HD2	7:D:861:HOH:O	2.11	0.50
1:D:391:VAL:HG22	1:D:402:ARG:HA	1.93	0.50
2:B:130:GLU:OE2	2:B:133:LYS:HD2	2.11	0.50
1:A:93:PRO:HG2	2:B:184:ALA:HB3	1.94	0.50
1:D:90:THR:HG23	1:D:112:PRO:HG2	1.93	0.50
1:D:114:THR:HG23	2:E:181:LYS:HZ2	1.77	0.50
1:D:522:VAL:O	1:D:567:VAL:HG12	2.12	0.50
1:D:531:ILE:HA	1:D:534:HIS:CD2	2.46	0.50
1:D:98:SER:C	1:D:556:ALA:HB3	2.31	0.50
2:E:144:TYR:CZ	2:E:151:GLY:N	2.79	0.50
2:F:141:ASP:N	2:F:141:ASP:OD1	2.45	0.50
1:A:138:ILE:HB	1:A:217:GLN:CG	2.39	0.50
1:A:135:ASP:OD2	1:A:343:PRO:HD2	2.12	0.50
1:A:20:MET:HG2	1:A:356:PRO:CG	2.42	0.50
1:A:77:ILE:CG2	1:A:110:PHE:HB3	2.41	0.50
1:D:122:LEU:HA	1:D:125:PHE:CE2	2.47	0.50
1:D:551:VAL:HG23	1:D:555:ASN:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:LEU:HD21	1:A:61:PHE:HD2	1.76	0.50
2:B:54:ILE:HB	2:B:55:PRO:HA	1.93	0.50
2:B:90:TYR:O	2:B:93:ALA:HB3	2.12	0.50
2:C:135:LEU:HD22	2:C:182:LEU:CD1	2.34	0.50
1:D:231:PHE:CZ	1:D:291:ILE:HG12	2.47	0.50
1:D:34:GLU:O	1:D:38:LYS:HG2	2.11	0.50
1:D:491:GLN:NE2	1:D:570:TYR:HB3	2.27	0.50
1:D:85:THR:HA	7:D:866:HOH:O	2.12	0.50
2:F:17:MET:SD	2:F:199:LEU:HG	2.52	0.50
1:A:163:GLY:HA2	1:A:560:GLN:CB	2.33	0.49
2:B:161:SER:HA	2:B:164:PHE:CD2	2.47	0.49
1:D:273:LEU:HA	1:D:276:THR:HG23	1.93	0.49
1:D:35:ILE:HA	1:D:395:TYR:CE1	2.47	0.49
2:E:14:MET:O	2:E:17:MET:HB2	2.12	0.49
2:E:95:ALA:HB1	2:E:152:TYR:HD2	1.77	0.49
2:F:98:TRP:CD1	2:F:153:VAL:HG11	2.47	0.49
1:A:510:ARG:NH1	1:A:575:PHE:CE2	2.80	0.49
1:D:43:ILE:HD11	1:D:88:ILE:HD11	1.94	0.49
1:A:250:LEU:HD11	1:A:260:ARG:NH1	2.28	0.49
2:C:15:PHE:O	7:C:413:HOH:O	2.19	0.49
1:D:143:LYS:O	1:D:216:VAL:HA	2.12	0.49
2:F:140:GLY:O	2:F:181:LYS:NZ	2.45	0.49
1:A:166:THR:HG23	4:A:602:LEU:O	2.11	0.49
1:A:421:PHE:CE1	1:A:541:SER:HA	2.47	0.49
1:D:342:THR:O	1:D:345:LEU:HG	2.12	0.49
1:D:39:ASN:O	7:D:737:HOH:O	2.20	0.49
1:A:330:TYR:HE2	1:A:352:PHE:CE1	2.31	0.49
3:A:601:JAA:C05	4:A:602:LEU:HB2	2.42	0.49
1:D:197:ASP:HB2	1:D:200:GLN:OE1	2.13	0.49
1:A:17:PHE:CE2	1:A:341:VAL:HG11	2.47	0.49
1:A:199:HIS:CD2	1:A:200:GLN:H	2.30	0.49
1:A:23:ASN:O	1:A:27:VAL:HG12	2.13	0.49
1:A:434:ASP:HB2	1:A:550:CYS:HB3	1.93	0.49
1:A:506:TYR:CE2	1:A:510:ARG:NE	2.81	0.49
2:C:126:LYS:O	2:C:129:ILE:HG13	2.12	0.49
2:C:159:THR:HA	2:C:199:LEU:HD21	1.95	0.49
1:D:387:GLU:HB3	1:D:406:VAL:CG1	2.42	0.49
2:F:143:PRO:O	2:F:185:TRP:CD1	2.65	0.49
1:A:244:ASP:HB3	1:A:250:LEU:HA	1.94	0.49
1:A:490:LEU:HD22	1:A:522:VAL:HG11	1.94	0.49
2:B:75:ASP:OD1	7:B:416:HOH:O	2.20	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:104:LYS:HG3	2:C:105:LYS:N	2.28	0.49
2:C:201:ASP:OD2	1:D:456:LYS:HG3	2.12	0.49
1:D:143:LYS:CG	1:D:216:VAL:HG12	2.42	0.49
1:D:253:ARG:NH2	7:D:756:HOH:O	2.26	0.49
1:D:303:GLY:O	1:D:328:HIS:N	2.44	0.49
1:D:510:ARG:HH21	1:D:575:PHE:HE2	1.56	0.49
1:D:89:LEU:O	7:D:738:HOH:O	2.20	0.49
1:A:378:GLY:N	1:A:381:GLN:HB2	2.28	0.49
1:A:462:PHE:O	1:A:549:ARG:NH1	2.46	0.49
1:A:528:PHE:HA	1:A:531:ILE:CG1	2.43	0.49
2:C:50:ILE:HG13	2:C:51:HIS:H	1.78	0.49
1:D:253:ARG:NH1	1:D:484:GLU:H	2.10	0.49
2:E:15:PHE:O	2:E:18:ARG:HB2	2.12	0.49
2:C:188:ARG:NH1	1:D:500:ALA:HA	2.27	0.49
1:D:407:VAL:HG11	1:D:419:LEU:HD13	1.94	0.49
1:D:441:LEU:HG	1:D:462:PHE:CE1	2.48	0.49
2:E:184:ALA:HA	2:E:187:LYS:HB2	1.95	0.49
2:E:24:ARG:NE	2:E:193:GLU:HG3	2.28	0.49
2:E:92:ARG:NH1	2:F:76:GLU:OE1	2.46	0.49
1:A:149:PHE:CB	1:A:530:LYS:HD3	2.43	0.49
1:A:149:PHE:HD2	1:A:529:ARG:NH2	2.09	0.49
1:A:445:VAL:HA	1:A:479:TRP:CZ2	2.48	0.49
1:A:99:LEU:HB3	1:A:557:LYS:N	2.18	0.49
2:C:17:MET:SD	2:C:199:LEU:HG	2.53	0.49
1:D:465:TYR:CB	1:D:551:VAL:HG13	2.37	0.49
2:E:90:TYR:O	2:E:93:ALA:HB3	2.13	0.49
1:D:538:LEU:HD23	1:D:544:GLN:HG2	1.94	0.48
1:D:88:ILE:HG23	1:D:89:LEU:N	2.15	0.48
2:B:151:GLY:O	2:B:154:ASP:HB2	2.13	0.48
2:C:169:LYS:HD3	2:C:206:VAL:HG13	1.95	0.48
1:D:453:SER:HA	1:D:457:ILE:HG22	1.95	0.48
1:D:506:TYR:OH	1:D:518:LEU:HD21	2.14	0.48
1:D:480:GLU:HG3	1:D:525:LYS:HA	1.94	0.48
2:E:54:ILE:HG22	7:E:438:HOH:O	2.13	0.48
2:F:113:VAL:HB	2:F:128:PHE:HE2	1.77	0.48
1:A:224:ALA:O	1:A:228:VAL:HG23	2.12	0.48
2:B:30:PHE:O	7:B:417:HOH:O	2.20	0.48
1:D:151:SER:HB2	1:D:194:PHE:HA	1.96	0.48
1:D:223:PHE:CZ	1:D:536:LEU:HB3	2.48	0.48
1:D:475:TYR:HB2	1:D:518:LEU:HD22	1.95	0.48
2:E:169:LYS:HZ2	2:E:206:VAL:HG13	1.76	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:352:PHE:HD1	7:A:805:HOH:O	1.97	0.48
1:A:366:VAL:HG22	1:A:387:GLU:O	2.13	0.48
2:C:98:TRP:HE3	2:C:101:PHE:HB2	1.78	0.48
1:D:151:SER:HB2	1:D:194:PHE:C	2.34	0.48
1:D:465:TYR:O	1:D:475:TYR:HA	2.13	0.48
1:A:199:HIS:CD2	1:A:200:GLN:N	2.81	0.48
1:A:202:LEU:C	1:A:205:HIS:ND1	2.62	0.48
1:A:99:LEU:HD12	1:A:555:ASN:CG	2.33	0.48
2:B:9:ASP:OD2	2:B:20:ARG:NE	2.43	0.48
2:C:139:LEU:O	2:C:141:ASP:N	2.46	0.48
1:D:126:ARG:HA	1:D:182:ILE:HG21	1.94	0.48
1:D:314:PRO:HB3	1:D:317:ARG:HH12	1.77	0.48
1:D:79:ARG:HH22	1:D:88:ILE:CB	2.27	0.48
2:E:154:ASP:OD2	2:E:185:TRP:NE1	2.45	0.48
1:A:291:ILE:HB	1:A:292:PRO:HD3	1.95	0.48
1:A:316:LEU:O	1:A:320:ALA:N	2.38	0.48
1:A:496:CYS:HA	1:A:499:ARG:CB	2.44	0.48
2:B:199:LEU:O	7:B:414:HOH:O	2.19	0.48
2:C:110:GLN:O	2:C:113:VAL:HG12	2.13	0.48
2:C:70:VAL:O	2:C:73:TYR:HB2	2.13	0.48
1:D:197:ASP:OD1	1:D:197:ASP:N	2.45	0.48
1:D:407:VAL:HG23	1:D:541:SER:OG	2.14	0.48
2:B:133:LYS:HE2	2:B:133:LYS:HB3	1.62	0.48
2:B:114:TRP:HB3	2:B:167:TYR:HE1	1.78	0.48
1:D:124:LEU:HB3	3:D:601:JAA:C15	2.44	0.48
1:D:32:LEU:HD21	1:D:61:PHE:HD2	1.79	0.48
1:D:451:ARG:NH1	1:D:454:GLU:CD	2.67	0.48
2:F:46:GLN:O	7:F:409:HOH:O	2.20	0.48
1:A:20:MET:HG2	1:A:356:PRO:HG2	1.94	0.48
2:C:31:GLU:N	7:C:429:HOH:O	2.47	0.48
2:C:33:ARG:NH2	2:C:35:GLU:OE2	2.47	0.48
1:D:222:VAL:O	1:D:304:ILE:N	2.47	0.48
1:D:521:ARG:NH1	1:D:562:LEU:HD13	2.29	0.48
2:E:144:TYR:CE2	2:E:151:GLY:N	2.81	0.48
1:A:142:GLY:HA2	1:A:215:GLN:HB2	1.94	0.48
1:A:464:SER:O	1:A:551:VAL:HG23	2.14	0.48
1:A:97:ILE:O	1:A:556:ALA:HB1	2.14	0.48
1:A:164:THR:HG21	1:A:561:ILE:HD11	1.95	0.48
2:C:10:TYR:CD2	2:C:12:PRO:HD2	2.49	0.48
1:D:143:LYS:CD	1:D:212:PHE:HB2	2.44	0.48
1:D:405:ASP:OD1	1:D:405:ASP:N	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:PHE:O	1:A:134:ARG:HB3	2.14	0.48
1:A:41:SER:HA	2:B:148:ASP:HA	1.95	0.48
1:A:432:ASN:CG	1:A:433:ILE:N	2.67	0.48
2:B:145:PHE:CD2	2:B:153:VAL:HG22	2.49	0.48
2:B:86:PRO:HG2	7:B:401:HOH:O	2.13	0.48
1:A:53:ASN:ND2	2:B:90:TYR:HB3	2.29	0.48
2:C:10:TYR:HH	2:C:208:TYR:HH	1.57	0.48
1:D:153:GLN:HG3	1:D:171:ARG:HD2	1.96	0.48
1:D:374:GLU:HB2	7:D:720:HOH:O	2.12	0.48
2:F:105:LYS:NZ	7:F:419:HOH:O	2.29	0.48
1:A:330:TYR:HD1	1:A:537:GLY:HA2	1.78	0.47
1:A:335:GLY:HA2	1:A:394:ASN:ND2	2.29	0.47
1:A:47:ASN:O	7:A:747:HOH:O	2.20	0.47
1:A:99:LEU:HD23	1:A:535:PHE:CZ	2.49	0.47
2:C:131:ALA:O	2:C:135:LEU:HB2	2.14	0.47
1:D:460:ILE:HD11	1:D:482:SER:HB3	1.95	0.47
1:D:79:ARG:HB3	1:D:79:ARG:HE	1.63	0.47
1:D:168:ASN:O	1:D:172:ASN:HB2	2.14	0.47
1:D:29:LYS:HB2	1:D:29:LYS:HE3	1.57	0.47
2:F:100:ASP:OD1	7:F:408:HOH:O	2.20	0.47
1:A:406:VAL:O	1:A:541:SER:OG	2.31	0.47
2:C:32:TYR:HD2	2:C:32:TYR:H	1.62	0.47
1:D:295:PHE:HA	7:D:861:HOH:O	2.15	0.47
1:D:336:TRP:HB2	1:D:358:LEU:HD13	1.96	0.47
1:D:45:LEU:HD22	7:D:737:HOH:O	2.14	0.47
1:D:253:ARG:HH11	1:D:484:GLU:HB3	1.79	0.47
1:D:552:LYS:HG3	1:D:553:PRO:HD2	1.97	0.47
1:D:87:PRO:CB	1:D:93:PRO:HD3	2.37	0.47
2:E:30:PHE:HD1	7:E:441:HOH:O	1.96	0.47
2:E:70:VAL:HG21	7:E:406:HOH:O	2.15	0.47
1:A:412:PHE:HA	1:A:417:PRO:HA	1.95	0.47
1:A:460:ILE:HG12	1:A:480:GLU:O	2.14	0.47
1:A:152:LYS:CE	1:A:565:ASN:HB2	2.37	0.47
2:B:144:TYR:HB3	2:B:154:ASP:OD2	2.14	0.47
2:B:30:PHE:HA	7:B:427:HOH:O	2.13	0.47
2:B:8:LEU:HD22	2:B:35:GLU:OE2	2.14	0.47
2:C:169:LYS:HG3	2:C:170:PHE:N	2.29	0.47
1:D:451:ARG:HH11	1:D:454:GLU:CD	2.17	0.47
2:E:17:MET:HB2	2:E:159:THR:HB	1.95	0.47
1:A:138:ILE:HA	1:A:217:GLN:NE2	2.29	0.47
1:A:480:GLU:OE2	1:A:526:GLY:N	2.35	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:193:ILE:HG12	1:D:205:HIS:NE2	2.30	0.47
1:D:92:HIS:HB2	2:E:141:ASP:HA	1.95	0.47
2:F:211:GLU:HA	2:F:214:LYS:HE3	1.97	0.47
2:F:98:TRP:NE1	2:F:153:VAL:HG21	2.29	0.47
1:A:432:ASN:HD21	1:A:434:ASP:CG	2.17	0.47
1:A:480:GLU:OE1	1:A:528:PHE:N	2.43	0.47
2:B:181:LYS:HB2	2:B:181:LYS:HE2	1.50	0.47
2:B:183:ILE:O	2:B:186:ALA:HB3	2.15	0.47
2:B:23:LEU:HD11	2:B:57:LEU:HD11	1.95	0.47
2:C:37:PHE:O	2:C:40:LYS:NZ	2.46	0.47
1:D:361:PHE:CD1	1:D:392:ILE:HD13	2.49	0.47
1:D:435:LYS:HB3	1:D:436:ASN:O	2.14	0.47
1:D:461:ASP:HB2	7:D:787:HOH:O	2.14	0.47
1:D:330:TYR:OH	1:D:541:SER:N	2.47	0.47
1:D:464:SER:N	1:D:549:ARG:O	2.48	0.47
2:F:107:THR:HG22	2:F:160:PHE:CE2	2.49	0.47
2:F:32:TYR:CD1	2:F:34:GLU:OE2	2.68	0.47
1:A:107:ARG:NH1	1:A:107:ARG:HG3	2.30	0.47
1:A:238:TRP:CZ2	1:A:281:CYS:SG	3.07	0.47
1:A:43:ILE:HG13	1:A:44:TYR:N	2.30	0.47
2:C:187:LYS:HE2	1:D:496:CYS:HB2	1.96	0.47
1:D:401:TYR:HB2	7:D:817:HOH:O	2.15	0.47
1:D:432:ASN:OD1	1:D:433:ILE:N	2.38	0.47
2:E:21:VAL:HG12	2:E:155:ILE:HG12	1.97	0.47
2:E:187:LYS:HA	2:E:190:MET:HG3	1.96	0.47
2:C:90:TYR:O	2:C:94:GLN:HG3	2.15	0.47
1:D:187:CYS:O	7:D:733:HOH:O	2.21	0.47
1:D:530:LYS:HB3	7:D:797:HOH:O	2.14	0.47
1:A:149:PHE:HZ	1:A:202:LEU:CB	2.28	0.47
1:A:256:VAL:N	7:A:798:HOH:O	2.47	0.47
1:A:362:GLU:HG3	1:A:400:ARG:CZ	2.44	0.47
1:D:107:ARG:HG3	1:D:107:ARG:NH1	2.17	0.47
2:C:10:TYR:CG	2:C:12:PRO:HD2	2.50	0.47
1:D:317:ARG:O	1:D:321:GLY:N	2.36	0.47
1:D:420:LYS:NZ	7:D:783:HOH:O	2.34	0.47
1:D:437:THR:HG21	1:D:439:ARG:HH21	1.79	0.47
1:D:442:GLN:HG2	1:D:462:PHE:CZ	2.44	0.47
1:D:92:HIS:CD2	1:D:93:PRO:HD2	2.49	0.47
1:A:353:ALA:HB2	1:A:413:TYR:CD2	2.50	0.47
2:C:73:TYR:HD1	2:C:76:GLU:OE2	1.98	0.47
1:D:107:ARG:HH22	1:D:552:LYS:HB2	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:393:THR:HA	1:D:398:LEU:O	2.15	0.47
1:D:451:ARG:NH1	1:D:454:GLU:OE1	2.48	0.47
2:E:15:PHE:HB3	2:E:67:SER:HB3	1.96	0.47
2:E:17:MET:O	2:E:21:VAL:HG23	2.15	0.47
2:F:182:LEU:HD23	2:F:183:ILE:N	2.30	0.47
1:A:344:ARG:NH1	7:A:824:HOH:O	2.47	0.46
1:A:477:ILE:HD12	1:A:497:LEU:HD22	1.97	0.46
1:A:198:VAL:CG2	1:A:524:ALA:HB3	2.43	0.46
1:D:278:ARG:O	1:D:282:MET:HE2	2.15	0.46
2:C:184:ALA:CB	1:D:499:ARG:NH1	2.74	0.46
2:E:21:VAL:CG1	2:E:155:ILE:HG12	2.45	0.46
2:F:165:GLN:O	2:F:168:GLU:HB2	2.15	0.46
1:A:255:THR:OG1	7:A:738:HOH:O	2.17	0.46
1:A:365:PRO:HG3	1:A:388:TYR:CZ	2.50	0.46
1:A:421:PHE:HB3	1:A:542:ALA:HB2	1.96	0.46
2:B:14:MET:O	2:B:17:MET:HB2	2.15	0.46
2:C:33:ARG:CZ	2:C:35:GLU:OE2	2.62	0.46
1:D:202:LEU:HD23	1:D:525:LYS:HD2	1.97	0.46
1:D:90:THR:HG1	1:D:91:GLY:H	1.59	0.46
2:E:144:TYR:CZ	2:E:154:ASP:HB2	2.49	0.46
1:A:167:THR:HB	1:A:560:GLN:CD	2.36	0.46
2:B:107:THR:O	2:B:110:GLN:HG3	2.15	0.46
2:B:4:LEU:HA	2:B:5:PRO:HD3	1.79	0.46
1:D:149:PHE:HZ	1:D:202:LEU:HD13	1.80	0.46
1:D:531:ILE:CG2	1:D:547:MET:HG2	2.45	0.46
1:D:552:LYS:HE2	7:D:882:HOH:O	2.14	0.46
2:E:144:TYR:CE2	2:E:154:ASP:OD1	2.68	0.46
1:A:177:ALA:O	1:A:180:LYS:HG2	2.15	0.46
2:B:176:GLU:O	2:B:180:PRO:N	2.48	0.46
2:C:68:LEU:HD23	2:C:103:ASP:OD2	2.14	0.46
1:D:496:CYS:CA	1:D:499:ARG:NH1	2.78	0.46
1:D:510:ARG:HE	1:D:510:ARG:HB3	1.50	0.46
1:D:99:LEU:HG	1:D:555:ASN:OD1	2.15	0.46
1:D:559:LEU:O	1:D:562:LEU:HG	2.15	0.46
2:E:86:PRO:HB2	2:E:88:ASP:OD1	2.16	0.46
2:F:71:VAL:O	2:F:74:VAL:HB	2.15	0.46
1:A:101:SER:HB3	1:A:535:PHE:CD2	2.51	0.46
2:B:65:CYS:HB2	2:C:97:PHE:CE1	2.50	0.46
1:D:239:GLU:O	1:D:242:VAL:HG13	2.16	0.46
1:D:262:ALA:O	1:D:266:LEU:HG	2.15	0.46
1:A:444:SER:HB3	1:A:497:LEU:HD23	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:THR:HB	1:A:560:GLN:OE1	2.15	0.46
1:A:74:GLU:N	1:A:75:PRO:HD2	2.31	0.46
2:B:37:PHE:CE1	6:B:301:GSH:HA32	2.50	0.46
1:D:156:SER:HB3	1:D:162:VAL:CG1	2.46	0.46
1:D:199:HIS:NE2	1:D:200:GLN:OE1	2.49	0.46
1:D:547:MET:H	1:D:547:MET:HE3	1.80	0.46
1:A:300:TYR:CE2	1:A:302:TYR:HB2	2.51	0.46
1:A:394:ASN:HD21	1:A:396:ALA:HB3	1.79	0.46
1:A:527:THR:HA	1:A:530:LYS:NZ	2.31	0.46
1:A:421:PHE:CD1	1:A:541:SER:HA	2.51	0.46
1:A:53:ASN:HB3	1:A:54:ALA:H	1.44	0.46
1:A:108:PRO:HG2	1:A:552:LYS:HB3	1.98	0.46
1:A:531:ILE:HD11	1:A:558:VAL:HG23	1.98	0.46
2:C:13:SER:O	2:C:17:MET:HG3	2.15	0.46
2:C:73:TYR:HA	2:C:76:GLU:OE2	2.16	0.46
2:C:98:TRP:CE3	2:C:101:PHE:HB2	2.51	0.46
1:D:200:GLN:O	1:D:203:TYR:HB3	2.16	0.46
1:D:314:PRO:HA	1:D:317:ARG:NH1	2.30	0.46
1:D:340:ASN:HB2	1:D:352:PHE:CD1	2.51	0.46
1:D:561:ILE:HG22	7:D:772:HOH:O	2.15	0.46
2:E:62:LYS:HA	2:E:63:PRO:HD3	1.83	0.46
1:A:147:PHE:CE1	1:A:206:LEU:HD12	2.51	0.46
1:A:450:LYS:H	1:A:450:LYS:HG2	1.44	0.46
2:B:150:PHE:O	7:B:418:HOH:O	2.21	0.46
2:C:121:GLN:O	2:C:125:LYS:HG3	2.16	0.46
1:D:235:GLU:HG3	7:D:710:HOH:O	2.15	0.46
1:D:78:LYS:HG3	1:D:553:PRO:O	2.14	0.46
1:D:98:SER:HA	7:D:713:HOH:O	2.16	0.46
2:E:20:ARG:HB2	7:E:425:HOH:O	2.15	0.46
1:A:295:PHE:CD1	1:A:298:ALA:HB2	2.50	0.46
1:A:522:VAL:HG23	1:A:567:VAL:HG23	1.98	0.46
1:A:552:LYS:CG	1:A:553:PRO:HD2	2.46	0.46
2:B:52:LYS:O	7:B:415:HOH:O	2.20	0.46
1:D:498:ASP:HB3	1:D:510:ARG:NH2	2.30	0.46
1:D:69:THR:OG1	1:D:72:GLU:OE1	2.26	0.46
2:F:123:ALA:O	2:F:127:GLU:HG3	2.15	0.46
2:F:183:ILE:O	2:F:186:ALA:HB3	2.16	0.46
2:F:17:MET:CE	2:F:200:PRO:HD2	2.46	0.46
2:F:33:ARG:CZ	2:F:35:GLU:OE2	2.64	0.46
1:A:522:VAL:HG23	1:A:567:VAL:CG2	2.46	0.46
2:B:26:LYS:HE2	2:B:26:LYS:HB3	1.57	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:ASN:ND2	2:B:88:ASP:OD2	2.46	0.46
2:C:24:ARG:HD2	2:C:198:SER:OG	2.15	0.46
2:C:18:ARG:HD2	2:C:67:SER:HB2	1.96	0.46
2:E:169:LYS:HD3	2:E:206:VAL:HG13	1.98	0.46
2:E:70:VAL:HG13	7:E:498:HOH:O	2.16	0.46
1:A:203:TYR:CD1	1:A:237:VAL:HG11	2.39	0.45
1:A:370:GLY:HA2	1:A:371:GLU:HA	1.78	0.45
1:A:25:HIS:CE1	1:A:380:THR:HG1	2.34	0.45
1:A:424:ARG:HG3	1:A:425:ARG:HH11	1.82	0.45
1:A:460:ILE:HD11	1:A:480:GLU:OE2	2.16	0.45
2:B:14:MET:HG2	2:B:163:TRP:CD1	2.52	0.45
2:C:187:LYS:CE	1:D:496:CYS:HB2	2.46	0.45
1:D:129:PHE:O	1:D:133:ASN:HB2	2.16	0.45
1:D:328:HIS:CG	1:D:329:ASP:N	2.84	0.45
1:D:526:GLY:HA2	1:D:529:ARG:HB3	1.98	0.45
2:F:144:TYR:HA	2:F:185:TRP:HE1	1.81	0.45
1:A:116:GLU:O	1:A:119:GLU:HB2	2.16	0.45
1:A:146:GLN:HB2	1:A:148:ILE:HG23	1.98	0.45
1:A:237:VAL:HB	1:A:241:ILE:HG23	1.98	0.45
1:A:385:GLY:N	1:A:409:VAL:O	2.33	0.45
1:A:48:CYS:SG	1:A:65:VAL:HG23	2.57	0.45
1:A:62:LYS:HD3	7:A:712:HOH:O	2.16	0.45
2:B:181:LYS:H	2:B:181:LYS:HG3	1.48	0.45
2:B:66:GLU:O	2:B:70:VAL:HG23	2.16	0.45
2:C:169:LYS:HE3	2:C:169:LYS:HB2	1.78	0.45
1:D:444:SER:HA	1:D:500:ALA:CB	2.46	0.45
1:D:531:ILE:HG12	7:D:729:HOH:O	2.16	0.45
1:D:107:ARG:NH2	1:D:552:LYS:HB2	2.32	0.45
2:E:211:GLU:O	2:E:214:LYS:HB2	2.16	0.45
2:F:138:GLU:HG3	2:F:145:PHE:HE1	1.79	0.45
2:F:140:GLY:N	2:F:181:LYS:NZ	2.65	0.45
1:A:150:SER:HG	1:A:170:TYR:HB2	1.81	0.45
2:C:18:ARG:NH2	7:C:407:HOH:O	2.49	0.45
1:D:223:PHE:CD1	1:D:304:ILE:HB	2.50	0.45
1:D:239:GLU:HA	1:D:242:VAL:HG13	1.98	0.45
1:D:451:ARG:CZ	1:D:489:VAL:HG12	2.46	0.45
1:D:510:ARG:NH2	1:D:575:PHE:CE2	2.79	0.45
1:A:222:VAL:HG21	7:A:789:HOH:O	2.17	0.45
1:A:437:THR:OG1	1:A:440:ASP:HB2	2.16	0.45
2:B:184:ALA:HA	2:B:187:LYS:HG2	1.98	0.45
2:C:132:VAL:HG22	7:C:414:HOH:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:170:PHE:CD2	2:C:213:ARG:HD2	2.52	0.45
1:D:223:PHE:HB3	1:D:225:HIS:HD2	1.82	0.45
1:D:340:ASN:HB2	1:D:352:PHE:HD1	1.80	0.45
1:D:427:LEU:HD12	1:D:427:LEU:O	2.16	0.45
1:D:448:ALA:HB2	1:D:496:CYS:HB3	1.99	0.45
1:D:91:GLY:HA3	2:E:141:ASP:O	2.16	0.45
2:F:32:TYR:HD2	2:F:32:TYR:H	1.65	0.45
1:A:164:THR:OG1	1:A:561:ILE:HG13	2.17	0.45
1:A:302:TYR:CG	1:A:328:HIS:NE2	2.83	0.45
1:A:77:ILE:HA	1:A:80:MET:SD	2.56	0.45
2:C:144:TYR:HB3	2:C:154:ASP:CG	2.37	0.45
2:C:24:ARG:HG3	2:C:30:PHE:CZ	2.50	0.45
1:D:498:ASP:OD2	1:D:510:ARG:NH2	2.50	0.45
1:D:68:VAL:HG11	1:D:73:LEU:HD21	1.98	0.45
2:E:86:PRO:HD3	2:E:146:GLY:O	2.17	0.45
2:F:163:TRP:HB3	2:F:167:TYR:CZ	2.51	0.45
1:A:61:PHE:O	1:A:65:VAL:HG12	2.17	0.45
2:C:114:TRP:HA	2:C:170:PHE:CD2	2.51	0.45
2:C:138:GLU:HG3	2:C:145:PHE:HE1	1.81	0.45
2:C:173:PHE:HB3	2:C:174:SER:H	1.63	0.45
1:D:220:PHE:HD1	1:D:302:TYR:HB3	1.81	0.45
1:D:551:VAL:HG23	1:D:555:ASN:CB	2.46	0.45
1:D:491:GLN:HE22	1:D:570:TYR:HB3	1.81	0.45
1:A:150:SER:HB2	1:A:167:THR:CA	2.45	0.45
1:A:174:ASN:O	1:A:178:GLY:N	2.40	0.45
1:A:200:GLN:OE1	1:A:254:ILE:HA	2.17	0.45
1:A:382:VAL:HG13	1:A:388:TYR:CD2	2.52	0.45
1:A:102:GLY:HA3	1:A:426:ASN:ND2	2.32	0.45
1:A:478:PHE:CE2	1:A:562:LEU:HA	2.51	0.45
1:A:498:ASP:HB3	1:A:510:ARG:NH2	2.28	0.45
1:A:99:LEU:CD2	1:A:535:PHE:HZ	2.28	0.45
1:A:53:ASN:HB2	2:B:88:ASP:CG	2.37	0.45
2:C:109:ALA:HA	7:C:403:HOH:O	2.17	0.45
1:D:110:PHE:CD1	1:D:556:ALA:HB2	2.52	0.45
2:E:11:TRP:CG	2:E:12:PRO:HD3	2.52	0.45
2:E:37:PHE:HZ	2:E:53:LYS:HA	1.82	0.45
2:F:68:LEU:HD12	2:F:69:ASN:N	2.32	0.45
1:A:125:PHE:O	1:A:129:PHE:HB2	2.16	0.45
1:A:168:ASN:O	1:A:172:ASN:HB2	2.17	0.45
1:A:171:ARG:HG3	1:A:194:PHE:CE1	2.52	0.45
1:A:253:ARG:O	7:A:746:HOH:O	2.20	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:390:VAL:HG23	7:A:777:HOH:O	2.16	0.45
1:A:53:ASN:HD22	2:B:88:ASP:CG	2.19	0.45
2:C:26:LYS:HG2	2:C:81:LYS:HZ1	1.77	0.45
1:D:12:ARG:HD2	1:D:12:ARG:HA	1.68	0.45
2:E:162:SER:HB3	2:E:199:LEU:HD23	1.98	0.45
2:F:26:LYS:HE3	2:F:78:TRP:O	2.16	0.45
1:A:149:PHE:HB2	1:A:530:LYS:HD3	1.99	0.45
1:A:315:LYS:HD2	1:A:319:TYR:CE2	2.52	0.45
1:A:444:SER:HA	1:A:500:ALA:HB3	1.98	0.45
2:C:71:VAL:O	2:C:74:VAL:HB	2.17	0.45
1:D:149:PHE:HB3	1:D:198:VAL:HG11	1.99	0.45
1:D:149:PHE:O	1:D:530:LYS:HE3	2.17	0.45
1:D:232:ARG:HG3	7:D:795:HOH:O	2.16	0.45
2:F:86:PRO:HB2	7:F:441:HOH:O	2.16	0.45
1:A:403:LEU:HA	1:A:403:LEU:HD12	1.84	0.45
1:A:22:ARG:HH21	1:A:415:ASN:CG	2.20	0.45
1:A:502:ILE:HD12	1:A:503:ASP:N	2.31	0.45
2:C:145:PHE:HB3	2:C:153:VAL:CG1	2.46	0.45
2:C:184:ALA:HA	2:C:187:LYS:HZ2	1.80	0.45
1:D:125:PHE:CE1	1:D:182:ILE:HD12	2.49	0.45
1:D:223:PHE:HZ	1:D:536:LEU:HB3	1.82	0.45
2:E:7:LEU:HB3	7:E:441:HOH:O	2.17	0.45
2:E:9:ASP:OD1	2:E:10:TYR:N	2.37	0.45
1:A:11:ASN:O	1:A:14:ILE:HG13	2.16	0.44
1:D:225:HIS:HB3	1:D:309:MET:SD	2.56	0.44
1:D:47:ASN:O	7:D:740:HOH:O	2.21	0.44
1:D:226:GLY:HA3	1:D:529:ARG:HD2	1.99	0.44
1:A:192:VAL:HG12	1:A:202:LEU:CD1	2.47	0.44
1:A:242:VAL:O	1:A:246:LYS:HB2	2.17	0.44
1:A:124:LEU:HD13	1:A:336:TRP:CE3	2.52	0.44
1:A:531:ILE:HA	1:A:534:HIS:CD2	2.53	0.44
1:A:97:ILE:H	1:A:163:GLY:N	2.14	0.44
2:B:17:MET:O	2:B:21:VAL:HG23	2.18	0.44
1:D:223:PHE:CZ	1:D:533:GLU:HA	2.52	0.44
1:A:150:SER:OG	1:A:170:TYR:HB2	2.17	0.44
1:A:365:PRO:HG3	1:A:388:TYR:CE2	2.53	0.44
1:A:451:ARG:HA	7:A:991:HOH:O	2.17	0.44
1:A:451:ARG:NH1	1:A:454:GLU:CD	2.70	0.44
1:A:527:THR:HB	1:A:561:ILE:CG2	2.47	0.44
1:A:41:SER:HA	2:B:147:GLY:O	2.18	0.44
1:D:407:VAL:HG12	7:D:794:HOH:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:466:ILE:HD11	1:D:552:LYS:HG3	1.98	0.44
1:D:498:ASP:OD1	1:D:518:LEU:HB2	2.18	0.44
2:E:139:LEU:HA	2:E:139:LEU:HD12	1.59	0.44
2:E:183:ILE:O	2:E:186:ALA:HB3	2.17	0.44
1:A:206:LEU:HA	7:A:1013:HOH:O	2.17	0.44
1:A:315:LYS:O	1:A:319:TYR:N	2.50	0.44
1:A:405:ASP:OD1	1:A:426:ASN:HB3	2.18	0.44
1:A:511:LYS:NZ	7:A:701:HOH:O	1.91	0.44
1:A:121:THR:HG23	3:A:601:JAA:C13	2.47	0.44
1:D:362:GLU:O	1:D:391:VAL:HB	2.16	0.44
1:D:96:ALA:HB1	1:D:163:GLY:H	1.82	0.44
2:E:95:ALA:HB1	2:E:152:TYR:CD2	2.52	0.44
2:F:130:GLU:O	2:F:134:ILE:HG22	2.18	0.44
1:A:223:PHE:HE2	1:A:545:PHE:CZ	2.36	0.44
1:A:23:ASN:C	1:A:27:VAL:HG12	2.38	0.44
1:A:336:TRP:HB2	1:A:358:LEU:HB3	1.99	0.44
1:A:62:LYS:HG2	1:A:400:ARG:NH1	2.32	0.44
1:A:499:ARG:N	7:A:707:HOH:O	2.51	0.44
1:A:39:ASN:HA	2:B:142:LYS:CG	2.48	0.44
2:C:132:VAL:O	7:C:414:HOH:O	2.21	0.44
1:D:83:GLY:N	1:D:158:GLY:HA3	2.32	0.44
1:D:363:PHE:HB3	1:D:388:TYR:HB3	1.99	0.44
1:D:70:ASP:HB2	1:D:104:SER:OG	2.18	0.44
1:A:233:THR:HG23	1:A:525:LYS:NZ	2.32	0.44
1:A:526:GLY:HA2	1:A:529:ARG:HB3	1.98	0.44
1:A:540:SER:HG	1:A:544:GLN:HE21	1.61	0.44
2:B:196:SER:O	7:B:419:HOH:O	2.21	0.44
2:C:113:VAL:HG21	2:C:128:PHE:CE2	2.53	0.44
2:C:4:LEU:HA	2:C:5:PRO:HD3	1.74	0.44
1:D:107:ARG:CG	1:D:107:ARG:HH11	2.19	0.44
1:D:138:ILE:HD12	7:D:823:HOH:O	2.18	0.44
1:D:190:ASP:HB2	7:D:718:HOH:O	2.18	0.44
2:E:139:LEU:HG	2:E:142:LYS:H	1.83	0.44
2:E:114:TRP:CD1	2:E:167:TYR:HE1	2.31	0.44
2:E:24:ARG:HG2	2:E:194:SER:HA	1.99	0.44
2:E:65:CYS:HA	7:E:406:HOH:O	2.17	0.44
2:E:26:LYS:HZ2	2:E:82:ASN:H	1.66	0.44
1:A:87:PRO:C	1:A:88:ILE:HG13	2.38	0.44
1:D:233:THR:O	1:D:237:VAL:HG22	2.18	0.44
1:D:120:ASN:CG	1:D:358:LEU:HD22	2.38	0.44
1:D:393:THR:OG1	1:D:400:ARG:N	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:523:VAL:HG12	1:D:524:ALA:H	1.83	0.44
2:E:125:LYS:O	2:E:129:ILE:HG12	2.17	0.44
2:F:109:ALA:CB	2:F:128:PHE:HB3	2.46	0.44
1:A:440:ASP:OD1	1:A:502:ILE:HG13	2.17	0.44
2:B:57:LEU:HG	7:B:413:HOH:O	2.17	0.44
2:B:58:VAL:HA	2:B:63:PRO:HA	1.99	0.44
1:D:107:ARG:CZ	1:D:433:ILE:HG13	2.47	0.44
1:D:462:PHE:O	1:D:549:ARG:NH1	2.51	0.44
1:D:77:ILE:CG2	1:D:97:ILE:HD11	2.47	0.44
1:D:84:ASP:C	1:D:86:SER:H	2.20	0.44
2:F:9:ASP:HB2	2:F:20:ARG:HH21	1.83	0.44
1:A:143:LYS:HZ2	1:A:187:CYS:HB3	1.82	0.44
1:A:432:ASN:O	1:A:433:ILE:HG23	2.17	0.44
2:B:10:TYR:O	2:B:20:ARG:NH2	2.51	0.44
2:C:66:GLU:O	2:C:70:VAL:HG23	2.18	0.44
2:C:65:CYS:O	2:C:69:ASN:HB3	2.18	0.44
1:D:114:THR:HG22	1:D:115:ASP:N	2.31	0.44
1:D:253:ARG:HG2	1:D:254:ILE:HD13	2.00	0.44
1:D:362:GLU:C	1:D:363:PHE:HD1	2.21	0.44
1:D:507:VAL:C	7:D:726:HOH:O	2.55	0.44
2:E:9:ASP:OD1	2:E:16:GLY:HA3	2.18	0.44
2:F:8:LEU:HB2	2:F:56:VAL:HB	2.00	0.44
1:A:117:LEU:HD21	7:A:756:HOH:O	2.17	0.43
1:A:205:HIS:CE1	1:A:206:LEU:CD1	3.01	0.43
1:A:317:ARG:O	1:A:321:GLY:N	2.51	0.43
1:A:337:ILE:O	1:A:354:VAL:HG23	2.18	0.43
1:A:451:ARG:NH1	1:A:454:GLU:OE2	2.51	0.43
2:B:144:TYR:O	2:B:145:PHE:HD1	2.01	0.43
2:C:209:ALA:HB2	7:C:470:HOH:O	2.18	0.43
1:D:94:VAL:HG21	1:D:112:PRO:HB3	1.98	0.43
7:C:416:HOH:O	1:D:489:VAL:HG13	2.18	0.43
1:D:444:SER:HA	1:D:500:ALA:HB1	2.00	0.43
1:D:507:VAL:O	1:D:511:LYS:HB2	2.18	0.43
1:D:77:ILE:HG23	1:D:77:ILE:HD12	1.42	0.43
1:A:26:GLN:NE2	7:A:787:HOH:O	2.32	0.43
1:A:132:ARG:HD2	1:A:326:VAL:HG21	1.99	0.43
1:A:48:CYS:SG	1:A:66:PRO:HD2	2.58	0.43
1:A:552:LYS:HA	1:A:552:LYS:HD2	1.77	0.43
2:B:188:ARG:HD3	2:B:188:ARG:O	2.17	0.43
2:B:64:VAL:HG13	2:C:93:ALA:HB1	1.99	0.43
2:B:65:CYS:HB2	2:C:97:PHE:CZ	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:7:LEU:HD13	2:C:30:PHE:CD2	2.53	0.43
1:D:153:GLN:HG3	1:D:171:ARG:NH1	2.33	0.43
1:D:256:VAL:HA	1:D:257:PRO:HD3	1.79	0.43
2:E:36:ASP:OD2	2:E:38:SER:HB2	2.17	0.43
2:F:133:LYS:HB3	2:F:133:LYS:HE2	1.68	0.43
2:F:173:PHE:HB3	2:F:174:SER:H	1.72	0.43
1:A:109:LYS:CE	1:A:111:ILE:HD11	2.48	0.43
1:A:114:THR:O	1:A:117:LEU:HB2	2.18	0.43
1:A:368:GLU:HG3	1:A:369:THR:HG22	1.99	0.43
1:A:463:SER:HB2	1:A:528:PHE:HE1	1.83	0.43
1:A:164:THR:HG1	1:A:561:ILE:HG13	1.83	0.43
2:B:128:PHE:O	2:B:132:VAL:HG13	2.17	0.43
2:C:130:GLU:O	2:C:134:ILE:HG22	2.19	0.43
1:D:238:TRP:CE2	1:D:239:GLU:HG3	2.53	0.43
1:D:401:TYR:HE2	1:D:403:LEU:HD13	1.83	0.43
1:D:441:LEU:HG	1:D:462:PHE:HE1	1.84	0.43
3:D:601:JAA:O02	4:D:602:LEU:N	2.52	0.43
2:F:114:TRP:HA	2:F:170:PHE:CD2	2.53	0.43
2:F:185:TRP:CE2	2:F:189:CYS:SG	3.11	0.43
1:A:284:LEU:HG	1:A:284:LEU:H	1.45	0.43
2:B:153:VAL:HA	2:B:156:SER:HB3	2.01	0.43
2:C:143:PRO:HB2	2:C:144:TYR:CD2	2.54	0.43
1:D:323:LEU:HD23	1:D:324:PRO:HD2	1.99	0.43
1:D:575:PHE:HB2	7:D:714:HOH:O	2.19	0.43
2:F:17:MET:HE3	2:F:163:TRP:HH2	1.83	0.43
2:F:73:TYR:HD1	2:F:76:GLU:OE2	2.01	0.43
1:A:195:SER:OG	7:A:726:HOH:O	2.12	0.43
1:A:227:LEU:HB2	1:A:316:LEU:HD22	2.00	0.43
1:A:568:SER:OG	7:A:749:HOH:O	2.21	0.43
1:A:77:ILE:O	1:A:80:MET:HB2	2.18	0.43
2:B:18:ARG:HG2	2:B:155:ILE:O	2.19	0.43
1:D:122:LEU:HD23	1:D:125:PHE:HZ	1.83	0.43
1:D:387:GLU:HB3	1:D:406:VAL:HG12	2.00	0.43
2:E:145:PHE:CB	2:E:153:VAL:HB	2.49	0.43
2:E:14:MET:HB3	2:E:159:THR:OG1	2.18	0.43
2:F:169:LYS:HD3	2:F:206:VAL:HG13	2.00	0.43
1:A:387:GLU:C	1:A:388:TYR:HD1	2.21	0.43
1:A:74:GLU:HA	7:A:826:HOH:O	2.17	0.43
1:D:224:ALA:HB2	1:D:305:MET:SD	2.59	0.43
1:D:308:SER:O	1:D:311:PRO:HD2	2.18	0.43
2:E:122:GLU:O	2:E:125:LYS:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:292:PRO:O	1:A:296:PRO:HA	2.19	0.43
2:B:6:ILE:O	2:B:57:LEU:HA	2.18	0.43
7:C:416:HOH:O	1:D:488:ASP:HB3	2.17	0.43
1:D:223:PHE:CG	1:D:533:GLU:HG2	2.54	0.43
2:F:4:LEU:HA	2:F:5:PRO:HD3	1.80	0.43
1:A:118:MET:SD	7:A:831:HOH:O	2.62	0.43
1:A:426:ASN:N	1:A:426:ASN:OD1	2.44	0.43
1:A:549:ARG:NE	7:A:791:HOH:O	2.47	0.43
2:C:104:LYS:CG	2:C:105:LYS:N	2.81	0.43
2:C:129:ILE:O	2:C:132:VAL:HG12	2.19	0.43
2:C:211:GLU:HA	2:C:214:LYS:HG2	2.01	0.43
1:D:186:SER:OG	7:D:739:HOH:O	2.20	0.43
2:F:65:CYS:O	2:F:66:GLU:HB2	2.18	0.43
1:A:229:HIS:HA	1:A:232:ARG:HG2	2.00	0.43
2:B:113:VAL:O	7:B:420:HOH:O	2.22	0.43
2:B:95:ALA:HB1	2:B:152:TYR:HD2	1.83	0.43
1:D:389:GLU:OE2	1:D:404:GLY:HA2	2.19	0.43
1:D:391:VAL:HG23	7:D:828:HOH:O	2.19	0.43
2:F:117:LYS:HE3	2:F:213:ARG:NH1	2.33	0.43
1:A:552:LYS:C	1:A:554:SER:H	2.23	0.42
1:A:80:MET:HA	1:A:86:SER:O	2.19	0.42
2:C:164:PHE:CD2	2:C:183:ILE:HD12	2.52	0.42
2:C:15:PHE:O	2:C:18:ARG:HB2	2.18	0.42
1:D:207:LEU:HD13	1:D:241:ILE:HD12	2.01	0.42
1:D:291:ILE:HG23	1:D:295:PHE:CZ	2.53	0.42
1:D:295:PHE:CD1	1:D:295:PHE:O	2.72	0.42
1:D:348:GLU:OE2	7:D:743:HOH:O	2.21	0.42
1:D:370:GLY:HA2	1:D:371:GLU:HA	1.69	0.42
2:E:30:PHE:N	2:E:30:PHE:CD2	2.86	0.42
1:A:231:PHE:CZ	1:A:291:ILE:HG12	2.54	0.42
1:A:513:LYS:NZ	1:A:575:PHE:HB3	2.33	0.42
1:D:253:ARG:NH1	7:D:840:HOH:O	2.53	0.42
1:D:495:ASN:C	1:D:499:ARG:NH1	2.73	0.42
1:D:99:LEU:HB3	1:D:557:LYS:H	1.83	0.42
1:D:93:PRO:HG2	7:E:403:HOH:O	2.18	0.42
2:E:110:GLN:OE1	2:E:160:PHE:HD2	2.02	0.42
2:E:18:ARG:HG3	2:E:159:THR:HG21	1.99	0.42
2:F:151:GLY:CA	2:F:154:ASP:OD2	2.67	0.42
1:A:131:PHE:CD1	1:A:341:VAL:HB	2.54	0.42
1:A:353:ALA:HB3	7:A:722:HOH:O	2.19	0.42
2:B:170:PHE:HZ	2:B:210:ALA:HA	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:26:LYS:HZ3	2:B:28:VAL:HG21	1.83	0.42
2:C:129:ILE:HA	2:C:132:VAL:HG12	2.01	0.42
1:D:202:LEU:HA	1:D:205:HIS:HB2	2.00	0.42
1:D:245:ILE:HG12	1:D:245:ILE:H	1.33	0.42
1:D:403:LEU:HD23	1:D:540:SER:HB3	2.01	0.42
1:D:552:LYS:C	1:D:554:SER:N	2.68	0.42
2:E:53:LYS:NZ	6:E:301:GSH:N3	2.67	0.42
2:F:12:PRO:O	2:F:163:TRP:CZ2	2.73	0.42
2:F:144:TYR:HB3	2:F:154:ASP:CG	2.40	0.42
1:A:212:PHE:CB	1:A:215:GLN:HE21	2.32	0.42
1:A:503:ASP:CG	1:A:504:ALA:N	2.73	0.42
1:A:223:PHE:HE2	1:A:545:PHE:HZ	1.67	0.42
2:C:113:VAL:HG23	2:C:125:LYS:HG2	2.01	0.42
2:C:114:TRP:CD1	2:C:167:TYR:HE1	2.38	0.42
2:C:24:ARG:NE	7:C:440:HOH:O	2.43	0.42
1:D:182:ILE:HG13	1:D:182:ILE:H	1.62	0.42
1:D:563:CYS:O	1:D:566:VAL:N	2.52	0.42
2:E:31:GLU:HB3	7:E:457:HOH:O	2.19	0.42
2:F:125:LYS:O	2:F:129:ILE:HG23	2.19	0.42
2:F:21:VAL:HG22	2:F:195:VAL:HA	2.01	0.42
1:A:122:LEU:HD22	1:A:126:ARG:NH2	2.31	0.42
1:A:197:ASP:O	1:A:201:ALA:HB2	2.20	0.42
1:A:205:HIS:ND1	1:A:206:LEU:HD13	2.34	0.42
1:A:27:VAL:O	1:A:31:THR:OG1	2.30	0.42
2:C:104:LYS:HG3	2:C:105:LYS:H	1.83	0.42
1:D:150:SER:HB3	1:D:166:THR:HB	2.02	0.42
1:D:109:LYS:O	1:D:555:ASN:HA	2.19	0.42
2:E:24:ARG:HE	2:E:193:GLU:CG	2.32	0.42
1:A:102:GLY:HA3	1:A:426:ASN:HD21	1.85	0.42
1:A:104:SER:O	1:A:107:ARG:HB2	2.18	0.42
1:A:277:ILE:HG23	1:A:278:ARG:N	2.34	0.42
1:A:330:TYR:N	7:A:786:HOH:O	2.52	0.42
1:A:8:PHE:HD1	1:A:126:ARG:HG3	1.85	0.42
1:A:91:GLY:HA2	2:B:143:PRO:HD3	2.00	0.42
1:A:41:SER:HB3	2:B:144:TYR:H	1.84	0.42
2:B:59:HIS:ND1	2:B:73:TYR:OH	2.42	0.42
2:C:84:PHE:HE1	2:C:85:PHE:CD2	2.38	0.42
1:D:389:GLU:CD	1:D:402:ARG:HH21	2.23	0.42
1:D:471:ASP:HA	1:D:472:PRO:HA	1.87	0.42
1:D:223:PHE:CZ	1:D:536:LEU:CB	3.03	0.42
1:D:495:ASN:HD22	1:D:572:SER:HB3	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:68:VAL:HG22	1:D:69:THR:H	1.85	0.42
2:E:102:VAL:HG23	7:E:450:HOH:O	2.20	0.42
2:E:17:MET:SD	2:E:199:LEU:HG	2.59	0.42
2:F:153:VAL:HA	2:F:156:SER:HB2	2.00	0.42
2:F:7:LEU:HD11	2:F:23:LEU:CD1	2.48	0.42
1:A:234:PHE:HE2	1:A:290:LEU:HD11	1.85	0.42
1:A:220:PHE:CE1	1:A:328:HIS:CE1	3.08	0.42
1:A:363:PHE:CE1	1:A:390:VAL:HG22	2.53	0.42
1:A:448:ALA:HB3	1:A:479:TRP:CH2	2.54	0.42
1:A:97:ILE:HG21	1:A:110:PHE:CG	2.55	0.42
2:B:22:ALA:HB2	2:B:155:ILE:HD13	2.01	0.42
2:C:88:ASP:O	2:C:92:ARG:HG3	2.18	0.42
1:D:143:LYS:C	1:D:184:SER:HB3	2.40	0.42
1:D:153:GLN:HB2	1:D:171:ARG:NH1	2.35	0.42
1:D:299:LYS:HB2	1:D:300:TYR:HD1	1.84	0.42
1:D:555:ASN:ND2	7:D:722:HOH:O	2.50	0.42
1:D:76:TYR:HB2	1:D:89:LEU:HD11	2.00	0.42
1:A:149:PHE:CZ	1:A:202:LEU:HD22	2.54	0.42
1:A:36:LEU:HD22	1:A:61:PHE:CZ	2.54	0.42
1:A:503:ASP:O	1:A:507:VAL:HG23	2.20	0.42
2:B:98:TRP:CZ2	2:B:138:GLU:HG2	2.55	0.42
2:C:9:ASP:OD1	2:C:9:ASP:N	2.52	0.42
1:D:302:TYR:CD1	1:D:326:VAL:HG13	2.52	0.42
1:D:36:LEU:O	1:D:40:GLN:N	2.52	0.42
1:D:563:CYS:N	7:D:822:HOH:O	2.52	0.42
2:E:164:PHE:HA	2:E:164:PHE:HD1	1.62	0.42
2:F:114:TRP:CD1	2:F:167:TYR:HE1	2.38	0.42
1:A:150:SER:OG	7:A:708:HOH:O	2.02	0.42
1:A:246:LYS:HD2	1:A:274:ALA:HB2	2.01	0.42
1:A:36:LEU:HD22	1:A:61:PHE:CE2	2.55	0.42
2:B:167:TYR:N	2:B:167:TYR:CD1	2.84	0.42
2:C:97:PHE:CE1	2:C:101:PHE:HE1	2.37	0.42
1:D:405:ASP:O	7:D:707:HOH:O	2.21	0.42
2:C:187:LYS:HG2	1:D:451:ARG:HD3	2.01	0.42
1:D:477:ILE:HG21	1:D:497:LEU:HD13	2.02	0.42
1:D:509:SER:O	1:D:513:LYS:N	2.22	0.42
1:D:82:ASP:C	1:D:84:ASP:H	2.23	0.42
1:D:83:GLY:O	1:D:85:THR:HG23	2.20	0.42
2:F:110:GLN:HB3	2:F:167:TYR:CE1	2.55	0.42
1:A:109:LYS:HZ1	1:A:111:ILE:HD11	1.84	0.42
1:A:480:GLU:CD	1:A:526:GLY:H	2.21	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:165:GLN:HB2	7:B:491:HOH:O	2.20	0.42
2:C:68:LEU:HA	2:C:71:VAL:HG12	2.02	0.42
2:C:98:TRP:CD2	2:C:138:GLU:OE2	2.73	0.42
1:D:110:PHE:CE1	1:D:555:ASN:C	2.92	0.42
1:D:232:ARG:O	1:D:235:GLU:HB2	2.20	0.42
1:D:46:GLN:NE2	7:D:845:HOH:O	2.53	0.42
1:D:499:ARG:CB	1:D:499:ARG:CZ	2.95	0.42
2:F:143:PRO:HB2	2:F:144:TYR:CD2	2.54	0.42
2:F:179:SER:HA	2:F:180:PRO:HD3	1.84	0.42
2:F:18:ARG:HH21	2:F:160:PHE:HE1	1.68	0.42
2:F:98:TRP:CZ2	2:F:157:LEU:HD22	2.54	0.42
1:A:364:LEU:HB2	1:A:389:GLU:HB3	2.01	0.41
1:A:39:ASN:HA	2:B:142:LYS:HG2	2.01	0.41
1:A:552:LYS:HG3	1:A:553:PRO:HD2	2.02	0.41
2:C:11:TRP:HZ3	2:C:205:ILE:HG13	1.84	0.41
2:C:60:ASN:ND2	2:C:60:ASN:O	2.52	0.41
1:D:149:PHE:CZ	1:D:202:LEU:HD13	2.55	0.41
1:D:445:VAL:HG13	1:D:479:TRP:NE1	2.35	0.41
1:A:139:ASP:H	1:A:217:GLN:CD	2.23	0.41
1:A:361:PHE:CE2	1:A:392:ILE:HG12	2.55	0.41
1:A:568:SER:HB3	7:A:882:HOH:O	2.20	0.41
1:A:165:ALA:HB3	4:A:602:LEU:OXT	2.19	0.41
2:C:24:ARG:HG3	2:C:30:PHE:CE1	2.55	0.41
1:D:412:PHE:HB3	1:D:414:ASN:O	2.20	0.41
1:D:433:ILE:C	1:D:435:LYS:H	2.21	0.41
1:D:197:ASP:HB3	1:D:567:VAL:HG23	2.01	0.41
2:F:70:VAL:HA	2:F:73:TYR:CD2	2.55	0.41
1:A:10:MET:HG2	7:A:853:HOH:O	2.19	0.41
1:A:305:MET:HE3	1:A:325:LEU:HB3	2.02	0.41
1:A:437:THR:HG21	1:A:439:ARG:HH21	1.84	0.41
1:A:87:PRO:CB	1:A:93:PRO:HD3	2.40	0.41
2:B:35:GLU:HG3	2:B:44:LEU:HD22	2.01	0.41
1:D:123:GLN:HG2	7:D:864:HOH:O	2.19	0.41
1:D:152:LYS:HZ3	1:D:561:ILE:CG2	2.28	0.41
1:D:169:VAL:HG21	4:D:602:LEU:HD11	2.02	0.41
1:D:13:VAL:O	1:D:16:GLU:HG2	2.20	0.41
1:D:250:LEU:HG	7:D:800:HOH:O	2.20	0.41
1:D:272:GLU:O	1:D:275:GLU:HB3	2.20	0.41
1:D:301:VAL:HG23	1:D:323:LEU:HD13	2.01	0.41
2:E:168:GLU:CD	2:E:174:SER:HA	2.40	0.41
1:A:200:GLN:O	1:A:203:TYR:HB3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:325:LEU:O	7:A:750:HOH:O	2.21	0.41
1:A:337:ILE:HG22	1:A:338:ALA:N	2.34	0.41
1:A:108:PRO:HB3	1:A:555:ASN:CB	2.51	0.41
2:B:85:PHE:HE1	2:B:152:TYR:HB2	1.85	0.41
1:D:338:ALA:HA	1:D:354:VAL:HA	2.02	0.41
2:E:98:TRP:CE2	2:E:138:GLU:HG2	2.55	0.41
2:F:68:LEU:HG	7:F:476:HOH:O	2.19	0.41
1:A:101:SER:HB3	1:A:535:PHE:CG	2.55	0.41
1:A:170:TYR:N	1:A:170:TYR:CD1	2.88	0.41
1:A:25:HIS:HB2	7:A:866:HOH:O	2.20	0.41
1:A:363:PHE:HD2	1:A:382:VAL:HG21	1.86	0.41
1:A:362:GLU:HG3	1:A:400:ARG:NH2	2.35	0.41
1:A:528:PHE:O	1:A:531:ILE:HB	2.21	0.41
2:B:129:ILE:O	2:B:132:VAL:HG22	2.21	0.41
2:C:32:TYR:HD1	2:C:34:GLU:OE2	2.02	0.41
1:D:235:GLU:HG2	1:D:287:TRP:CG	2.56	0.41
1:D:33:LYS:O	1:D:37:LEU:HB2	2.21	0.41
1:D:99:LEU:HB2	1:D:557:LYS:H	1.86	0.41
2:E:21:VAL:HG23	7:E:425:HOH:O	2.20	0.41
2:F:64:VAL:HG23	2:F:70:VAL:HG22	2.01	0.41
2:F:15:PHE:HB3	2:F:67:SER:HB3	2.03	0.41
2:F:26:LYS:HD2	2:F:74:VAL:CG1	2.51	0.41
1:A:336:TRP:CB	1:A:358:LEU:HB3	2.50	0.41
1:A:510:ARG:HG2	1:A:515:ILE:O	2.21	0.41
1:A:527:THR:O	1:A:530:LYS:HB2	2.21	0.41
1:A:93:PRO:HG2	2:B:184:ALA:HB1	2.01	0.41
2:B:18:ARG:NH1	2:B:103:ASP:CG	2.67	0.41
2:B:183:ILE:O	2:B:187:LYS:HG2	2.21	0.41
1:D:104:SER:OG	1:D:109:LYS:HG3	2.20	0.41
1:D:234:PHE:HB3	7:D:710:HOH:O	2.20	0.41
1:D:351:THR:HG22	1:D:420:LYS:HB3	2.03	0.41
2:E:53:LYS:O	7:E:413:HOH:O	2.20	0.41
2:E:60:ASN:OD1	2:E:60:ASN:N	2.53	0.41
2:F:98:TRP:O	2:F:98:TRP:CE3	2.73	0.41
1:A:197:ASP:O	1:A:201:ALA:N	2.52	0.41
1:A:28:GLN:HE21	1:A:361:PHE:N	2.12	0.41
1:A:407:VAL:HG22	1:A:419:LEU:HD22	2.01	0.41
1:D:153:GLN:HG2	1:D:167:THR:HG21	2.02	0.41
1:D:25:HIS:CE1	1:D:380:THR:HG21	2.55	0.41
1:D:495:ASN:ND2	1:D:572:SER:HB3	2.36	0.41
1:A:134:ARG:NH2	7:A:825:HOH:O	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:TYR:CE2	1:A:220:PHE:HB2	2.55	0.41
1:A:407:VAL:HG23	1:A:420:LYS:O	2.21	0.41
1:A:42:ALA:HA	2:B:143:PRO:CG	2.47	0.41
1:A:526:GLY:C	1:A:529:ARG:HH11	2.19	0.41
1:A:555:ASN:HB3	7:A:841:HOH:O	2.19	0.41
2:B:125:LYS:O	2:B:129:ILE:HG12	2.21	0.41
2:C:98:TRP:HD1	2:C:153:VAL:HG11	1.85	0.41
2:C:23:LEU:CD2	2:C:28:VAL:HG11	2.49	0.41
2:C:5:PRO:HB3	2:C:57:LEU:HD11	2.03	0.41
2:E:93:ALA:HB1	2:F:73:TYR:CZ	2.56	0.41
2:F:98:TRP:CH2	2:F:135:LEU:HG	2.55	0.41
2:F:151:GLY:O	2:F:154:ASP:HB2	2.21	0.41
1:A:113:PHE:CZ	1:A:168:ASN:HB3	2.56	0.41
1:A:225:HIS:ND1	1:A:309:MET:SD	2.92	0.41
1:A:500:ALA:O	1:A:502:ILE:N	2.54	0.41
2:B:89:PRO:HB3	2:C:76:GLU:HG3	2.02	0.41
2:C:71:VAL:HG13	2:C:152:TYR:CE1	2.56	0.41
1:D:227:LEU:O	1:D:231:PHE:HD2	2.03	0.41
1:D:238:TRP:CZ2	1:D:239:GLU:HG3	2.56	0.41
1:D:364:LEU:HB2	7:D:828:HOH:O	2.21	0.41
1:D:437:THR:CG2	1:D:439:ARG:HH21	2.34	0.41
1:D:464:SER:HA	1:D:476:ALA:O	2.21	0.41
1:D:563:CYS:HA	1:D:566:VAL:HG13	2.01	0.41
2:F:129:ILE:O	2:F:132:VAL:HG12	2.21	0.41
2:F:85:PHE:HD2	2:F:92:ARG:NH1	2.19	0.41
1:A:387:GLU:HA	1:A:407:VAL:O	2.21	0.41
1:A:494:CYS:SG	1:A:495:ASN:N	2.94	0.41
1:A:149:PHE:HB3	1:A:530:LYS:HD3	2.03	0.41
1:A:567:VAL:HA	7:A:834:HOH:O	2.21	0.41
1:A:520:LEU:O	1:A:569:SER:HA	2.21	0.41
2:B:142:LYS:HG3	2:B:142:LYS:HZ2	1.72	0.41
2:B:81:LYS:HB2	2:B:82:ASN:H	1.73	0.41
1:D:238:TRP:HZ3	1:D:278:ARG:HA	1.85	0.41
1:D:413:TYR:O	1:D:414:ASN:HB2	2.21	0.41
2:E:36:ASP:OD1	7:E:415:HOH:O	2.21	0.41
1:A:113:PHE:HA	1:A:117:LEU:HD12	2.02	0.41
1:A:134:ARG:NH1	1:A:135:ASP:CG	2.74	0.41
1:A:202:LEU:HG	1:A:205:HIS:CA	2.48	0.41
1:A:202:LEU:O	1:A:205:HIS:N	2.54	0.41
1:A:241:ILE:HG13	1:A:242:VAL:H	1.84	0.41
1:A:238:TRP:CZ2	1:A:281:CYS:HB3	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:354:VAL:HG11	1:A:379:LEU:HD11	2.03	0.41
1:A:379:LEU:HD23	1:A:380:THR:HG23	2.03	0.41
1:D:21:THR:O	1:D:24:ALA:HB2	2.21	0.41
1:D:566:VAL:C	1:D:568:SER:N	2.74	0.41
2:E:25:GLU:HG2	2:E:84:PHE:HE1	1.86	0.41
2:E:88:ASP:HA	2:E:89:PRO:HD2	1.87	0.41
2:F:14:MET:N	7:F:433:HOH:O	2.40	0.41
1:A:143:LYS:HB2	1:A:185:PRO:O	2.22	0.40
1:A:27:VAL:HG13	1:A:356:PRO:HB2	2.03	0.40
1:A:426:ASN:HB2	7:A:810:HOH:O	2.21	0.40
1:A:452:LEU:O	1:A:457:ILE:HG12	2.21	0.40
2:B:164:PHE:CD2	2:B:183:ILE:HG13	2.57	0.40
2:B:61:GLY:N	7:B:453:HOH:O	2.53	0.40
2:C:11:TRP:O	2:C:200:PRO:HG2	2.21	0.40
1:D:126:ARG:CZ	1:D:182:ILE:HD11	2.51	0.40
1:D:332:SER:CB	1:D:538:LEU:HA	2.50	0.40
1:D:332:SER:HB3	1:D:538:LEU:HA	2.04	0.40
1:D:341:VAL:HG23	1:D:342:THR:HG23	2.02	0.40
2:E:207:ALA:O	2:E:211:GLU:HB2	2.20	0.40
1:A:94:VAL:HG11	1:A:112:PRO:HB3	2.03	0.40
1:A:142:GLY:CA	1:A:215:GLN:HB2	2.52	0.40
1:A:70:ASP:HB2	1:A:109:LYS:HG3	2.04	0.40
1:A:74:GLU:O	1:A:78:LYS:HB2	2.20	0.40
1:D:143:LYS:NZ	1:D:187:CYS:HA	2.36	0.40
1:D:284:LEU:HD13	1:D:287:TRP:CA	2.51	0.40
1:D:29:LYS:O	1:D:33:LYS:HG3	2.21	0.40
1:D:336:TRP:HB2	1:D:358:LEU:CD1	2.52	0.40
1:D:92:HIS:CD2	2:E:185:TRP:HB2	2.56	0.40
1:D:92:HIS:CD2	2:E:139:LEU:HD23	2.57	0.40
2:E:144:TYR:C	2:E:145:PHE:HD1	2.23	0.40
1:A:275:GLU:O	1:A:279:THR:HG23	2.21	0.40
1:A:27:VAL:HB	7:A:862:HOH:O	2.21	0.40
1:A:84:ASP:C	1:A:86:SER:H	2.25	0.40
2:B:128:PHE:HE2	2:B:175:ILE:HG21	1.85	0.40
2:B:24:ARG:NH1	7:B:436:HOH:O	2.32	0.40
2:C:159:THR:O	7:C:410:HOH:O	2.22	0.40
2:C:68:LEU:O	2:C:72:GLN:HG2	2.21	0.40
1:D:27:VAL:HG21	1:D:356:PRO:HG2	2.02	0.40
1:D:27:VAL:HG23	1:D:357:ASN:HB3	2.03	0.40
1:D:391:VAL:HG22	1:D:402:ARG:HG2	2.04	0.40
1:D:107:ARG:NH1	1:D:433:ILE:HD11	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:565:ASN:O	1:D:567:VAL:N	2.53	0.40
2:E:48:ASN:ND2	2:E:65:CYS:SG	2.94	0.40
2:E:9:ASP:HB3	2:E:32:TYR:CE1	2.56	0.40
1:A:213:ARG:CG	1:A:214:ASP:N	2.85	0.40
1:A:217:GLN:O	1:A:299:LYS:N	2.51	0.40
1:A:313:VAL:N	1:A:314:PRO:CD	2.85	0.40
1:A:477:ILE:O	1:A:520:LEU:HD12	2.22	0.40
1:A:490:LEU:HD13	1:A:522:VAL:HG21	2.03	0.40
1:A:559:LEU:HD23	1:A:559:LEU:HA	1.86	0.40
1:A:96:ALA:HB1	1:A:163:GLY:HA3	2.03	0.40
2:B:117:LYS:O	7:B:421:HOH:O	2.22	0.40
2:B:26:LYS:HZ3	2:B:28:VAL:CG2	2.34	0.40
1:D:18:ASP:O	1:D:21:THR:OG1	2.33	0.40
1:D:235:GLU:HG2	1:D:287:TRP:CD2	2.56	0.40
1:D:405:ASP:OD2	1:D:541:SER:O	2.40	0.40
2:E:145:PHE:N	2:E:145:PHE:CD1	2.90	0.40
2:E:26:LYS:HD2	2:E:26:LYS:HA	1.62	0.40
2:E:74:VAL:O	7:E:417:HOH:O	2.22	0.40
2:F:12:PRO:O	2:F:163:TRP:HZ2	2.04	0.40
2:F:41:SER:HA	2:F:42:PRO:HD3	2.00	0.40
1:A:233:THR:C	1:A:236:GLN:H	2.25	0.40
1:A:260:ARG:HH11	1:A:260:ARG:HG2	1.86	0.40
1:A:475:TYR:OH	7:A:728:HOH:O	2.13	0.40
1:A:110:PHE:HE1	1:A:556:ALA:HB2	1.75	0.40
2:B:182:LEU:O	2:B:185:TRP:HB3	2.21	0.40
2:C:110:GLN:HG2	2:C:167:TYR:CE2	2.57	0.40
2:C:4:LEU:HA	2:C:4:LEU:HD23	1.82	0.40
1:D:246:LYS:HB3	1:D:246:LYS:HE3	1.84	0.40
1:D:310:GLU:N	1:D:311:PRO:CD	2.84	0.40
1:D:464:SER:O	1:D:550:CYS:HA	2.21	0.40
1:D:497:LEU:HD12	1:D:520:LEU:HD22	2.02	0.40
2:E:16:GLY:HA2	2:E:55:PRO:HG3	2.04	0.40

All (17) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:270:ASN:O	1:D:511:LYS:NZ[1_655]	1.97	0.23
1:A:299:LYS:NZ	1:A:431:ILE:O[1_655]	2.01	0.19
1:A:239:GLU:OE2	2:F:174:SER:N[1_554]	2.02	0.18

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:286:ASN:ND2	2:F:161:SER:OG[1_554]	2.03	0.17
1:A:213:ARG:NH1	1:A:436:ASN:OD1[1_655]	2.07	0.13
1:D:270:ASN:ND2	1:D:510:ARG:O[1_655]	2.08	0.12
1:A:139:ASP:OD2	7:A:717:HOH:O[1_655]	2.10	0.10
1:A:270:ASN:ND2	1:A:510:ARG:O[1_655]	2.11	0.09
7:A:748:HOH:O	7:F:423:HOH:O[1_554]	2.15	0.05
1:D:213:ARG:NH1	1:D:436:ASN:OD1[1_655]	2.16	0.04
7:A:788:HOH:O	7:A:846:HOH:O[1_655]	2.16	0.04
1:A:207:LEU:O	1:A:508:SER:OG[1_655]	2.17	0.03
7:A:1258:HOH:O	7:A:1259:HOH:O[1_655]	2.18	0.02
7:D:1340:HOH:O	7:D:1343:HOH:O[1_445]	2.18	0.02
7:B:483:HOH:O	7:C:472:HOH:O[1_565]	2.19	0.01
7:A:927:HOH:O	7:F:542:HOH:O[1_554]	2.19	0.01
7:C:626:HOH:O	7:D:1268:HOH:O[1_455]	2.19	0.01

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	567/575 (99%)	526 (93%)	29 (5%)	12 (2%)	7	1
1	D	567/575 (99%)	530 (94%)	30 (5%)	7 (1%)	13	3
2	B	212/223 (95%)	196 (92%)	14 (7%)	2 (1%)	17	6
2	C	212/223 (95%)	196 (92%)	15 (7%)	1 (0%)	29	15
2	E	212/223 (95%)	198 (93%)	13 (6%)	1 (0%)	29	15
2	F	212/223 (95%)	197 (93%)	12 (6%)	3 (1%)	11	3
All	All	1982/2042 (97%)	1843 (93%)	113 (6%)	26 (1%)	12	3

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	287	TRP

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Mol	Chain	Res	Type
1	A	513	LYS
1	A	540	SER
1	D	369	THR
1	D	433	ILE
1	D	437	THR
1	D	513	LYS
1	D	540	SER
2	E	141	ASP
1	A	368	GLU
1	A	437	THR
1	A	553	PRO
2	B	140	GLY
2	C	140	GLY
1	D	88	ILE
1	D	368	GLU
2	F	140	GLY
2	F	180	PRO
1	A	237	VAL
2	B	27	GLY
1	A	51	ASN
1	A	369	THR
1	A	542	ALA
1	A	271	PRO
1	A	88	ILE
2	F	12	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	499/505 (99%)	462 (93%)	37 (7%)	13	4
1	D	499/505 (99%)	450 (90%)	49 (10%)	8	2
2	B	187/195 (96%)	176 (94%)	11 (6%)	19	7
2	C	187/195 (96%)	173 (92%)	14 (8%)	13	4
2	E	187/195 (96%)	174 (93%)	13 (7%)	15	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	F	187/195 (96%)	174 (93%)	13 (7%)	15	5
All	All	1746/1790 (98%)	1609 (92%)	137 (8%)	12	4

All (137) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	99	LEU
1	A	110	PHE
1	A	114	THR
1	A	125	PHE
1	A	145	LEU
1	A	150	SER
1	A	166	THR
1	A	184	SER
1	A	187	CYS
1	A	205	HIS
1	A	206	LEU
1	A	229	HIS
1	A	234	PHE
1	A	237	VAL
1	A	245	ILE
1	A	250	LEU
1	A	268	THR
1	A	273	LEU
1	A	276	THR
1	A	284	LEU
1	A	295	PHE
1	A	369	THR
1	A	379	LEU
1	A	425	ARG
1	A	426	ASN
1	A	429	LEU
1	A	431	ILE
1	A	450	LYS
1	A	468	VAL
1	A	494	CYS
1	A	506	TYR
1	A	509	SER
1	A	512	CYS
1	A	529	ARG
1	A	534	HIS
1	A	559	LEU

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Mol	Chain	Res	Type
1	A	568	SER
2	B	10	TYR
2	B	36	ASP
2	B	62	LYS
2	B	80	GLU
2	B	154	ASP
2	B	170	PHE
2	B	173	PHE
2	B	175	ILE
2	B	187	LYS
2	B	205	ILE
2	B	211	GLU
2	C	32	TYR
2	C	43	LEU
2	C	65	CYS
2	C	72	GLN
2	C	84	PHE
2	C	134	ILE
2	C	135	LEU
2	C	139	LEU
2	C	157	LEU
2	C	172	ASN
2	C	176	GLU
2	C	183	ILE
2	C	185	TRP
2	C	211	GLU
1	D	12	ARG
1	D	27	VAL
1	D	39	ASN
1	D	79	ARG
1	D	90	THR
1	D	92	HIS
1	D	97	ILE
1	D	138	ILE
1	D	140	ASP
1	D	151	SER
1	D	152	LYS
1	D	162	VAL
1	D	184	SER
1	D	188	SER
1	D	205	HIS
1	D	225	HIS

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Mol	Chain	Res	Type
1	D	241	ILE
1	D	242	VAL
1	D	245	ILE
1	D	250	LEU
1	D	251	SER
1	D	277	ILE
1	D	280	LYS
1	D	295	PHE
1	D	313	VAL
1	D	329	ASP
1	D	345	LEU
1	D	348	GLU
1	D	373	GLU
1	D	375	LYS
1	D	410	ILE
1	D	421	PHE
1	D	427	LEU
1	D	430	SER
1	D	452	LEU
1	D	459	VAL
1	D	461	ASP
1	D	484	GLU
1	D	499	ARG
1	D	510	ARG
1	D	512	CYS
1	D	518	LEU
1	D	535	PHE
1	D	545	PHE
1	D	546	LYS
1	D	547	MET
1	D	551	VAL
1	D	566	VAL
1	D	567	VAL
2	E	4	LEU
2	E	23	LEU
2	E	60	ASN
2	E	62	LYS
2	E	80	GLU
2	E	81	LYS
2	E	110	GLN
2	E	164	PHE
2	E	168	GLU

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Mol	Chain	Res	Type
2	E	173	PHE
2	E	185	TRP
2	E	195	VAL
2	E	211	GLU
2	F	32	TYR
2	F	68	LEU
2	F	84	PHE
2	F	128	PHE
2	F	134	ILE
2	F	135	LEU
2	F	173	PHE
2	F	175	ILE
2	F	176	GLU
2	F	182	LEU
2	F	206	VAL
2	F	211	GLU
2	F	212	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	GLN
1	A	53	ASN
1	A	172	ASN
1	A	215	GLN
1	A	217	GLN
1	A	318	HIS
1	D	47	ASN
1	D	215	GLN
1	D	225	HIS
1	D	340	ASN
2	E	48	ASN
2	F	72	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 1 is monoatomic - leaving 8 for Mogul analysis.

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$
3	JAA	D	601	-	12,15,15	5.94	6 (50%)	12,19,19	3.20	6 (50%)
6	GSH	F	301	-	12,19,19	1.65	3 (25%)	15,24,24	2.91	6 (40%)
6	GSH	E	301	-	12,19,19	1.72	3 (25%)	15,24,24	3.19	7 (46%)
3	JAA	A	601	-	12,15,15	5.81	6 (50%)	12,19,19	3.27	6 (50%)
6	GSH	C	301	-	12,19,19	1.71	3 (25%)	15,24,24	3.23	5 (33%)
6	GSH	B	301	-	12,19,19	1.71	3 (25%)	15,24,24	2.95	5 (33%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	JAA	D	601	-	-	4/7/22/22	0/1/1/1
6	GSH	F	301	-	-	3/18/24/24	-
6	GSH	E	301	-	-	5/18/24/24	-
3	JAA	A	601	-	-	7/7/22/22	0/1/1/1
6	GSH	C	301	-	-	3/18/24/24	-
6	GSH	B	301	-	-	0/18/24/24	-

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	601	JAA	C05-C08	-13.01	1.30	1.52
3	A	601	JAA	C05-C08	-12.50	1.31	1.52
3	D	601	JAA	C06-C04	-11.21	1.24	1.53
3	A	601	JAA	C06-C04	-11.10	1.24	1.53
3	A	601	JAA	C10-C04	-6.85	1.45	1.53
3	D	601	JAA	C10-C04	-6.47	1.45	1.53
3	D	601	JAA	C07-C08	6.31	1.61	1.51
3	A	601	JAA	C07-C08	6.23	1.61	1.51
3	D	601	JAA	C05-C04	4.77	1.66	1.54
3	A	601	JAA	C05-C04	4.54	1.66	1.54
3	D	601	JAA	C09-C05	-4.18	1.48	1.54
3	A	601	JAA	C09-C05	-3.60	1.49	1.54
6	E	301	GSH	C2-N3	3.12	1.40	1.33
6	B	301	GSH	C2-N3	3.03	1.40	1.33
6	C	301	GSH	C2-N3	3.01	1.40	1.33
6	F	301	GSH	C2-N3	3.00	1.40	1.33
6	C	301	GSH	CA2-N2	-2.83	1.39	1.45
6	E	301	GSH	CD1-N2	2.74	1.39	1.34
6	B	301	GSH	CD1-N2	2.71	1.39	1.34
6	B	301	GSH	CA2-N2	-2.69	1.40	1.45
6	E	301	GSH	CA2-N2	-2.67	1.40	1.45
6	F	301	GSH	CA2-N2	-2.66	1.40	1.45
6	F	301	GSH	CD1-N2	2.62	1.39	1.34
6	C	301	GSH	CD1-N2	2.40	1.39	1.34

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	301	GSH	CA2-CB2-SG2	-10.60	102.28	114.19
6	B	301	GSH	CA2-CB2-SG2	-9.36	103.67	114.19
6	F	301	GSH	CA2-CB2-SG2	-8.46	104.69	114.19
6	E	301	GSH	CA2-CB2-SG2	-7.88	105.34	114.19
3	D	601	JAA	C07-C06-C04	-6.24	97.89	104.41
6	E	301	GSH	CB2-CA2-N2	-5.95	102.80	111.28
3	A	601	JAA	C07-C06-C04	-5.92	98.22	104.41
3	A	601	JAA	C09-C11-C13	-5.64	105.46	126.40
3	D	601	JAA	C09-C11-C13	-5.07	107.59	126.40
3	D	601	JAA	C06-C07-C08	-4.75	100.65	105.42
3	A	601	JAA	C06-C07-C08	-4.71	100.69	105.42
6	B	301	GSH	CB2-CA2-N2	-4.02	105.56	111.28
6	F	301	GSH	CB2-CA2-N2	-3.88	105.76	111.28
6	E	301	GSH	CA3-N3-C2	-3.71	117.00	122.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	301	GSH	CA3-N3-C2	-3.68	117.04	122.34
3	A	601	JAA	C06-C04-C10	-3.68	107.08	113.67
3	D	601	JAA	C06-C04-C10	-3.65	107.13	113.67
6	E	301	GSH	CB1-CG1-CD1	3.60	121.07	113.04
3	A	601	JAA	O01-C08-C05	3.59	130.21	125.58
6	E	301	GSH	CG1-CD1-N2	-3.35	110.03	115.83
3	D	601	JAA	C07-C08-C05	-3.19	103.66	109.05
3	A	601	JAA	C07-C08-C05	-3.15	103.72	109.05
6	C	301	GSH	CB2-CA2-N2	-3.08	106.90	111.28
6	F	301	GSH	CG1-CD1-N2	-2.99	110.65	115.83
6	F	301	GSH	CB1-CG1-CD1	2.94	119.61	113.04
6	B	301	GSH	CA3-N3-C2	-2.71	118.44	122.34
6	C	301	GSH	C2-CA2-N2	-2.60	104.09	111.16
3	D	601	JAA	O01-C08-C05	2.48	128.77	125.58
6	E	301	GSH	CB2-CA2-C2	-2.40	104.82	109.76
6	B	301	GSH	CG1-CD1-N2	-2.31	111.83	115.83
6	E	301	GSH	OE1-CD1-CG1	2.30	126.21	122.02
6	F	301	GSH	OE1-CD1-CG1	2.27	126.17	122.02
6	F	301	GSH	CA3-N3-C2	-2.22	119.14	122.34
6	B	301	GSH	CB1-CG1-CD1	2.16	117.87	113.04
6	C	301	GSH	CG1-CD1-N2	-2.16	112.09	115.83

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	F	301	GSH	N2-CA2-CB2-SG2
6	F	301	GSH	C2-CA2-CB2-SG2
6	E	301	GSH	N1-CA1-CB1-CG1
6	E	301	GSH	C1-CA1-CB1-CG1
6	E	301	GSH	N2-CA2-CB2-SG2
6	E	301	GSH	C2-CA2-CB2-SG2
3	A	601	JAA	C05-C04-C10-C12
3	A	601	JAA	C06-C04-C10-C12
3	A	601	JAA	C08-C05-C09-C11
3	A	601	JAA	C09-C11-C13-C14
3	A	601	JAA	C11-C13-C14-C15
6	C	301	GSH	N2-CA2-CB2-SG2
6	C	301	GSH	C2-CA2-CB2-SG2
6	E	301	GSH	CA1-CB1-CG1-CD1
3	D	601	JAA	C09-C11-C13-C14
3	D	601	JAA	C05-C09-C11-C13

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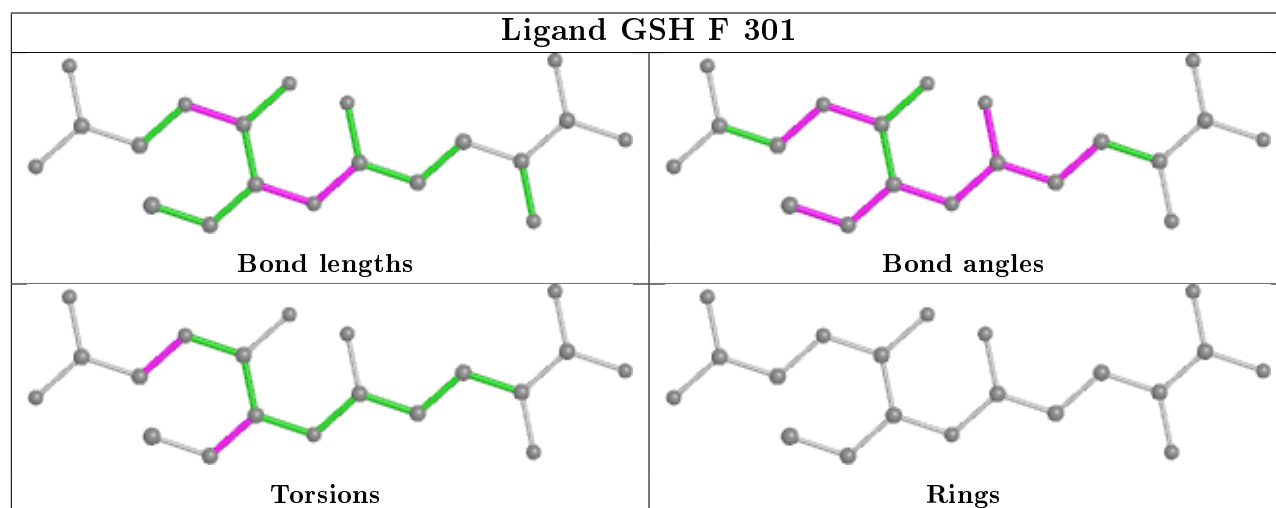
Mol	Chain	Res	Type	Atoms
3	A	601	JAA	C04-C05-C09-C11
3	A	601	JAA	C05-C09-C11-C13
6	F	301	GSH	C3-CA3-N3-C2
3	D	601	JAA	C04-C05-C09-C11
3	D	601	JAA	C08-C05-C09-C11
6	C	301	GSH	CA1-CB1-CG1-CD1

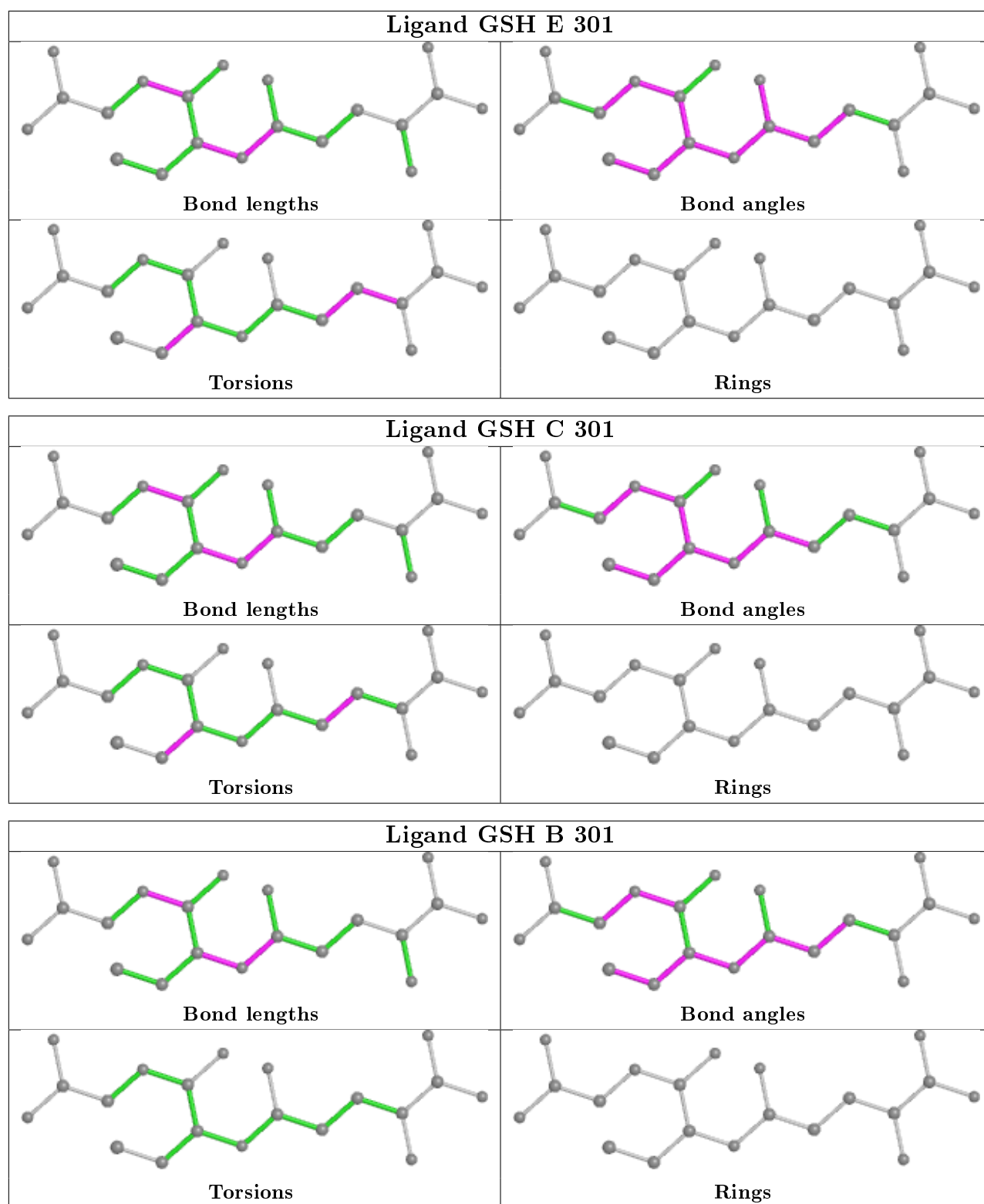
There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	601	JAA	2	0
6	E	301	GSH	3	0
3	A	601	JAA	2	0
6	B	301	GSH	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	569/575 (98%)	0.84	53 (9%) 8 6	3, 9, 15, 21	0
1	D	569/575 (98%)	0.71	39 (6%) 16 13	3, 8, 13, 20	0
2	B	214/223 (95%)	0.34	5 (2%) 60 56	3, 6, 11, 13	0
2	C	214/223 (95%)	0.30	4 (1%) 66 63	2, 3, 7, 11	0
2	E	214/223 (95%)	0.45	11 (5%) 28 22	3, 7, 11, 15	0
2	F	214/223 (95%)	0.33	6 (2%) 53 47	2, 3, 7, 11	0
All	All	1994/2042 (97%)	0.59	118 (5%) 22 17	2, 7, 13, 21	0

All (118) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	202	LEU	10.2
1	D	494	CYS	6.3
1	A	201	ALA	6.2
1	A	506	TYR	5.5
1	A	205	HIS	5.1
1	A	210	ILE	4.3
1	D	433	ILE	4.0
1	A	294	LEU	3.9
1	D	88	ILE	3.8
1	A	17	PHE	3.8
1	D	295	PHE	3.7
1	A	382	VAL	3.6
1	D	523	VAL	3.5
1	A	151	SER	3.5
2	F	128	PHE	3.5
1	A	203	TYR	3.4
1	A	481	ILE	3.4
1	A	37	LEU	3.4
1	D	90	THR	3.3

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Mol	Chain	Res	Type	RSRZ
2	E	27	GLY	3.3
1	A	284	LEU	3.3
2	C	32	TYR	3.3
1	A	304	ILE	3.2
1	D	410	ILE	3.2
1	D	77	ILE	3.2
1	D	113	PHE	3.2
1	D	573	THR	3.2
1	D	559	LEU	3.1
1	A	257	PRO	3.0
1	D	562	LEU	3.0
1	A	163	GLY	3.0
1	A	352	PHE	2.9
1	A	328	HIS	2.9
1	A	551	VAL	2.9
1	D	258	SER	2.9
2	B	153	VAL	2.8
1	A	358	LEU	2.8
1	A	222	VAL	2.8
1	D	117	LEU	2.8
1	D	572	SER	2.8
1	A	206	LEU	2.8
2	C	118	GLY	2.7
1	D	68	VAL	2.7
2	B	98	TRP	2.7
1	A	338	ALA	2.7
1	A	561	ILE	2.7
1	A	472	PRO	2.7
1	A	282	MET	2.6
1	D	169	VAL	2.6
2	B	139	LEU	2.6
2	B	10	TYR	2.6
2	C	183	ILE	2.6
1	A	27	VAL	2.6
1	D	496	CYS	2.5
1	A	285	SER	2.5
1	A	293	ALA	2.5
1	D	542	ALA	2.5
2	E	64	VAL	2.5
2	E	184	ALA	2.5
2	C	124	GLY	2.5
1	D	60	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	457	ILE	2.4
1	A	154	TYR	2.4
1	D	95	PRO	2.4
2	E	65	CYS	2.4
1	D	182	ILE	2.4
1	A	477	ILE	2.3
1	A	238	TRP	2.3
1	A	509	SER	2.3
1	D	102	GLY	2.3
1	A	160	VAL	2.3
1	D	548	PRO	2.3
1	D	101	SER	2.3
2	E	63	PRO	2.3
1	A	563	CYS	2.2
1	D	147	PHE	2.2
1	D	155	ILE	2.2
1	D	518	LEU	2.2
1	D	170	TYR	2.2
2	E	95	ALA	2.2
1	A	324	PRO	2.2
1	A	300	TYR	2.2
1	A	545	PHE	2.2
1	D	204	CYS	2.2
2	F	85	PHE	2.2
1	A	344	ARG	2.2
1	A	475	TYR	2.2
1	A	125	PHE	2.2
1	A	295	PHE	2.2
2	E	164	PHE	2.2
2	F	101	PHE	2.2
1	A	162	VAL	2.2
2	E	74	VAL	2.2
1	D	431	ILE	2.1
2	B	183	ILE	2.1
1	A	316	LEU	2.1
1	D	207	LEU	2.1
1	A	234	PHE	2.1
1	D	66	PRO	2.1
1	A	121	THR	2.1
2	E	43	LEU	2.1
1	D	79	ARG	2.1
1	D	312	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
2	E	30	PHE	2.1
1	A	353	ALA	2.1
2	E	144	TYR	2.1
2	F	73	TYR	2.1
1	A	217	GLN	2.1
1	A	204	CYS	2.1
1	A	468	VAL	2.0
1	D	466	ILE	2.0
1	A	361	PHE	2.0
1	D	269	PRO	2.0
2	F	184	ALA	2.0
1	A	336	TRP	2.0
1	D	561	ILE	2.0
1	D	268	THR	2.0
2	F	176	GLU	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	LEU	D	602	9/9	0.78	0.17	6,8,11,22	0
3	JAA	A	601	15/15	0.81	0.21	7,11,17,18	0
3	JAA	D	601	15/15	0.85	0.16	5,9,12,15	0
4	LEU	A	602	9/9	0.88	0.13	8,10,14,15	0
6	GSH	F	301	20/20	0.92	0.10	3,5,10,10	0
6	GSH	C	301	20/20	0.93	0.10	2,4,6,7	0
6	GSH	B	301	20/20	0.93	0.10	2,5,14,15	0
6	GSH	E	301	20/20	0.95	0.11	3,9,13,17	0

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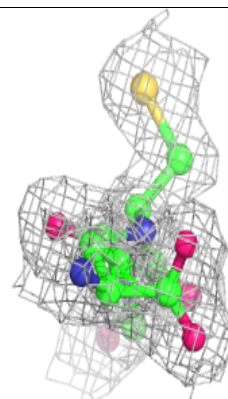
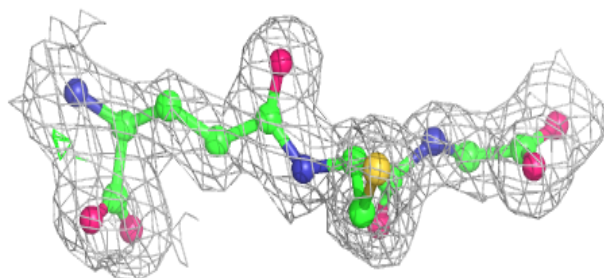
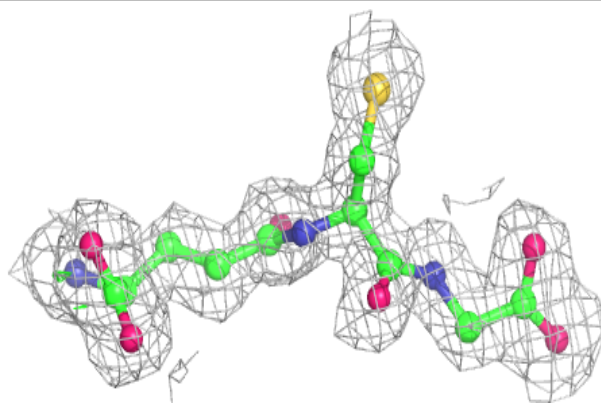
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	MG	A	603	1/1	0.95	0.15	16,16,16,16	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

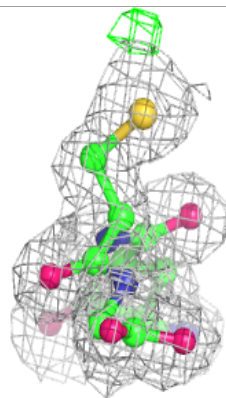
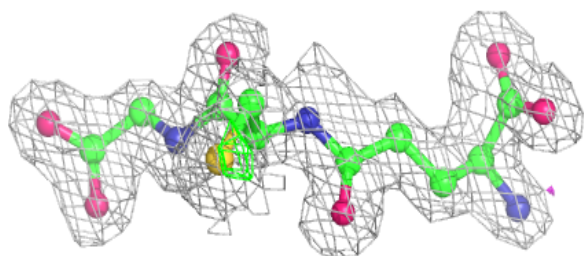
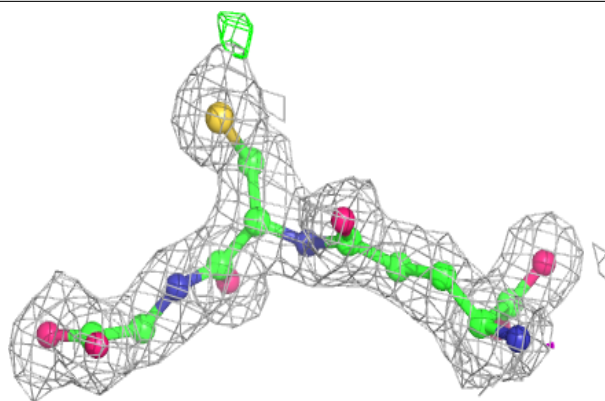
**Electron density around GSH F 301:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)

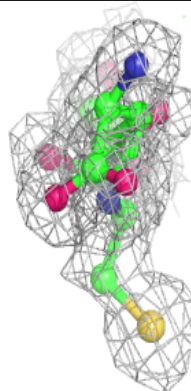
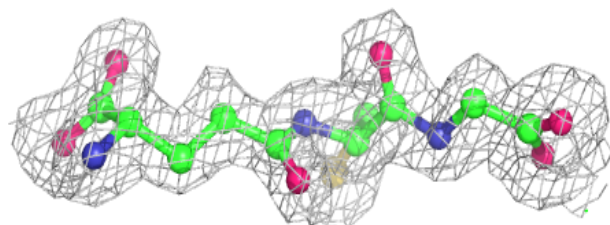
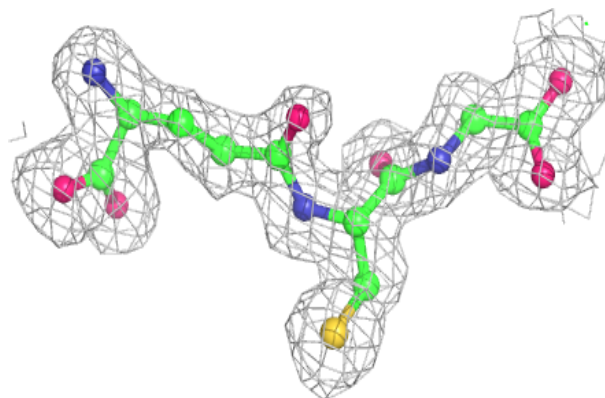


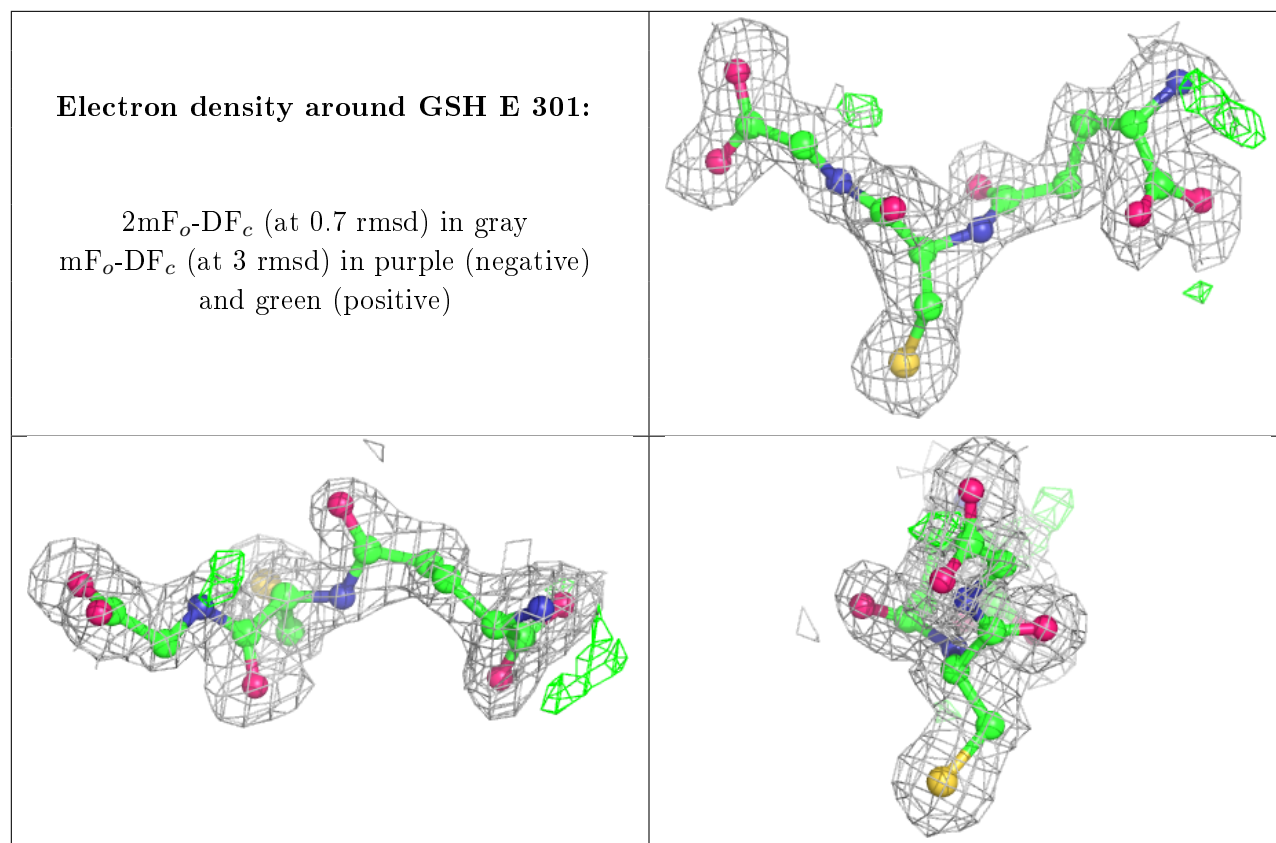
**Electron density around GSH C 301:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around GSH B 301:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





## 6.5 Other polymers [i](#)

There are no such residues in this entry.