



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 24, 2016 – 05:12 PM EDT

PDB ID : 5ECL  
Title : Crystal Structure of FIN219-FIP1 complex with JA, Ile and Mg  
Authors : Chen, C.Y.; Cheng, Y.S.  
Deposited on : 2015-10-20  
Resolution : 1.85 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20027939  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20027939

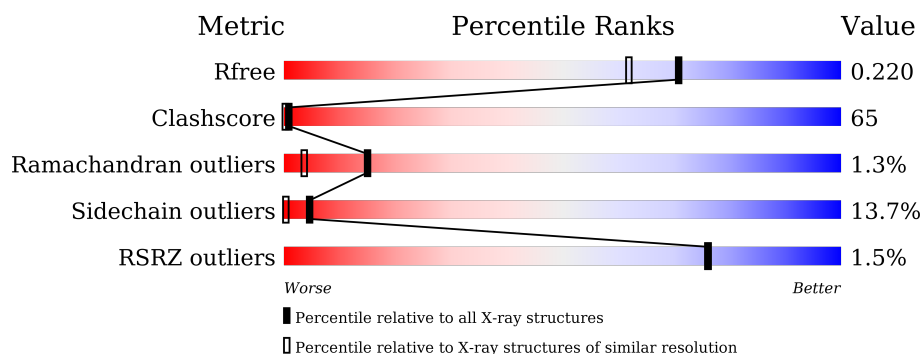
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.85 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	1745 (1.86-1.86)
Clashscore	102246	1898 (1.86-1.86)
Ramachandran outliers	100387	1875 (1.86-1.86)
Sidechain outliers	100360	1875 (1.86-1.86)
RSRZ outliers	91569	1747 (1.86-1.86)

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

Mol	Chain	Length	Quality of chain
1	A	575	<div> <div>3%</div> <div>22% 62% 14%</div> <div>..</div> </div>
1	D	575	<div> <div>%</div> <div>23% 62% 13%</div> <div>..</div> </div>
2	B	223	<div> <div>36% 52% 7%</div> <div>.</div> </div>
2	C	223	<div> <div>2%</div> <div>31% 55% 10%</div> <div>.</div> </div>
2	E	223	<div> <div>2%</div> <div>30% 57% 9%</div> <div>.</div> </div>
2	F	223	<div> <div>31% 52% 11%</div> <div>..</div> </div>

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 17172 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:

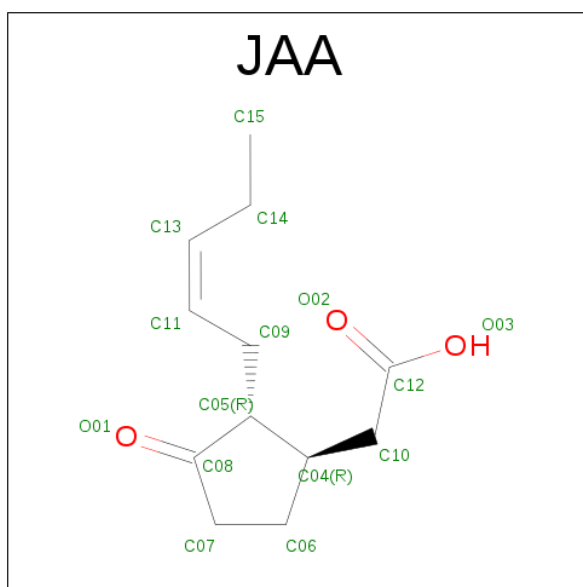
Chain	Residue	Modelled	Actual	Comment	Reference
B	-5	HIS	-	expression tag	UNP Q8L7C9
B	-4	HIS	-	expression tag	UNP Q8L7C9
B	-3	HIS	-	expression tag	UNP Q8L7C9
B	-2	HIS	-	expression tag	UNP Q8L7C9
B	-1	HIS	-	expression tag	UNP Q8L7C9
B	0	HIS	-	expression tag	UNP Q8L7C9
C	-5	HIS	-	expression tag	UNP Q8L7C9
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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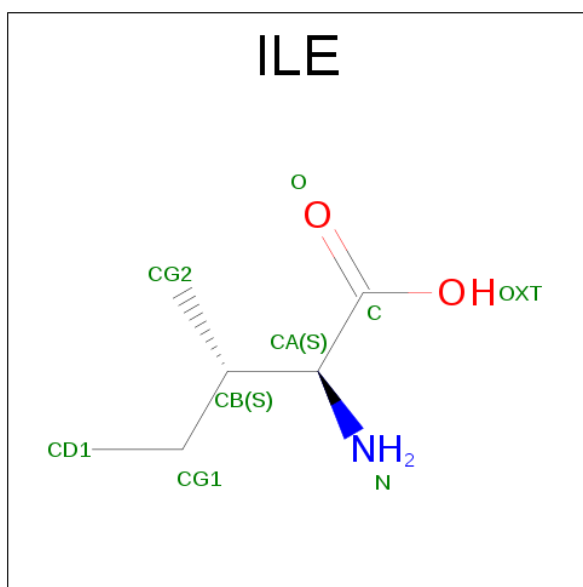
Chain	Residue	Modelled	Actual	Comment	Reference
E	-5	HIS	-	expression tag	UNP Q8L7C9
E	-4	HIS	-	expression tag	UNP Q8L7C9
E	-3	HIS	-	expression tag	UNP Q8L7C9
E	-2	HIS	-	expression tag	UNP Q8L7C9
E	-1	HIS	-	expression tag	UNP Q8L7C9
E	0	HIS	-	expression tag	UNP Q8L7C9
F	-5	HIS	-	expression tag	UNP Q8L7C9
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 ISOLEUCINE (three-letter code: ILE) (formula: C<sub>6</sub>H<sub>13</sub>NO<sub>2</sub>).

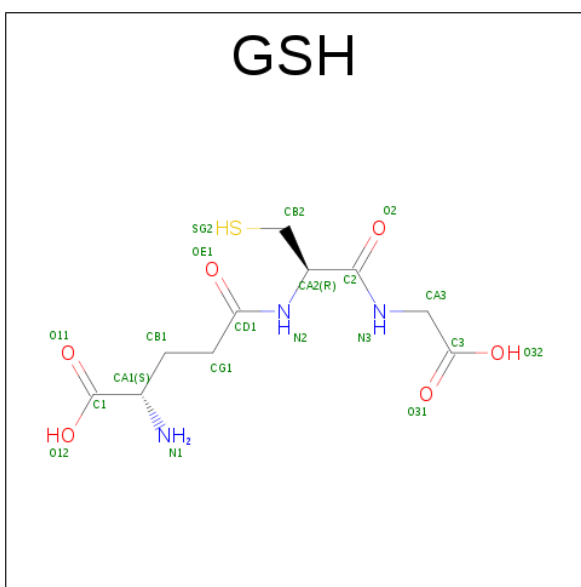


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			9	6	1	2		
4	D	1	Total	C	N	O	0	0
			9	6	1	2		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mg	0	0
			1	1		
5	D	3	Total	Mg	0	0
			3	3		

- Molecule 6 is GLUTATHIONE (three-letter code: GSH) (formula: C<sub>10</sub>H<sub>17</sub>N<sub>3</sub>O<sub>6</sub>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		

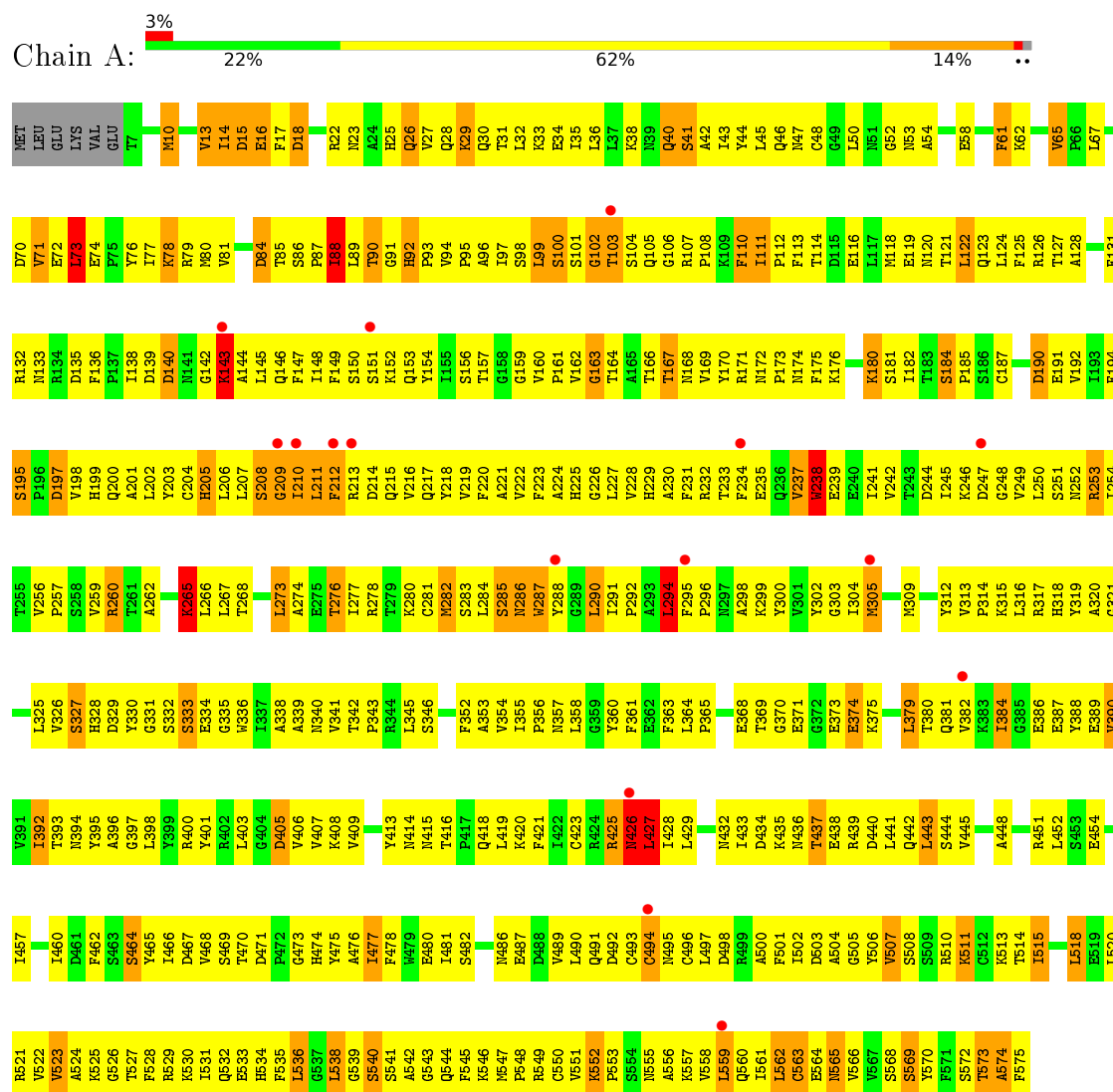
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	260	Total	O	0	0
			260	260		
7	B	162	Total	O	0	0
			162	162		
7	C	130	Total	O	0	0
			130	130		
7	D	276	Total	O	0	0
			276	276		
7	E	121	Total	O	0	0
			121	121		
7	F	141	Total	O	0	0
			141	141		

### 3 Residue-property plots

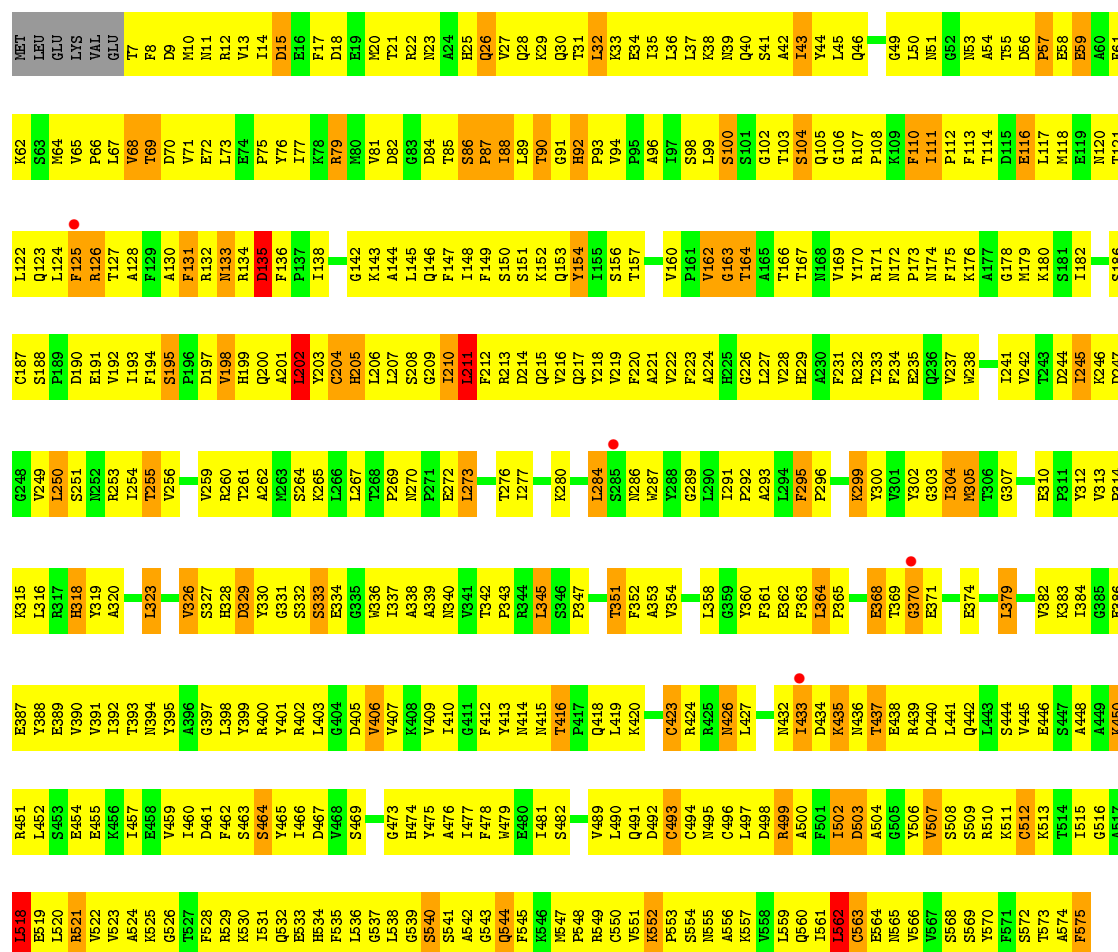
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

#### • Molecule 1: Jasmonic acid-amido synthetase JAR1



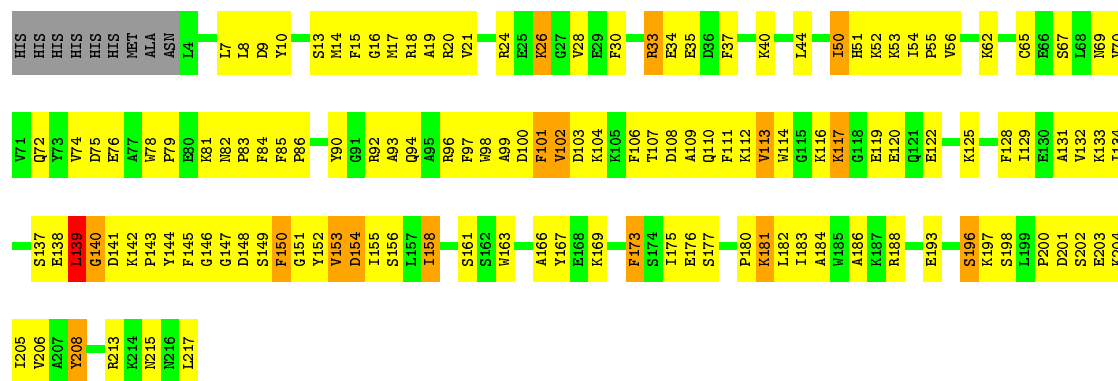
#### • Molecule 1: Jasmonic acid-amido synthetase JAR1





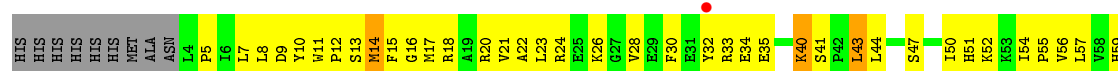
• Molecule 2: Glutathione S-transferase U20

Chain B: 36% 52% 7%

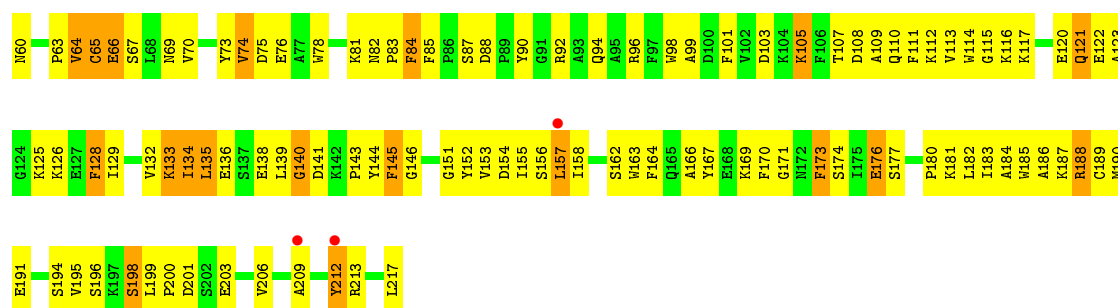


• Molecule 2: Glutathione S-transferase U20

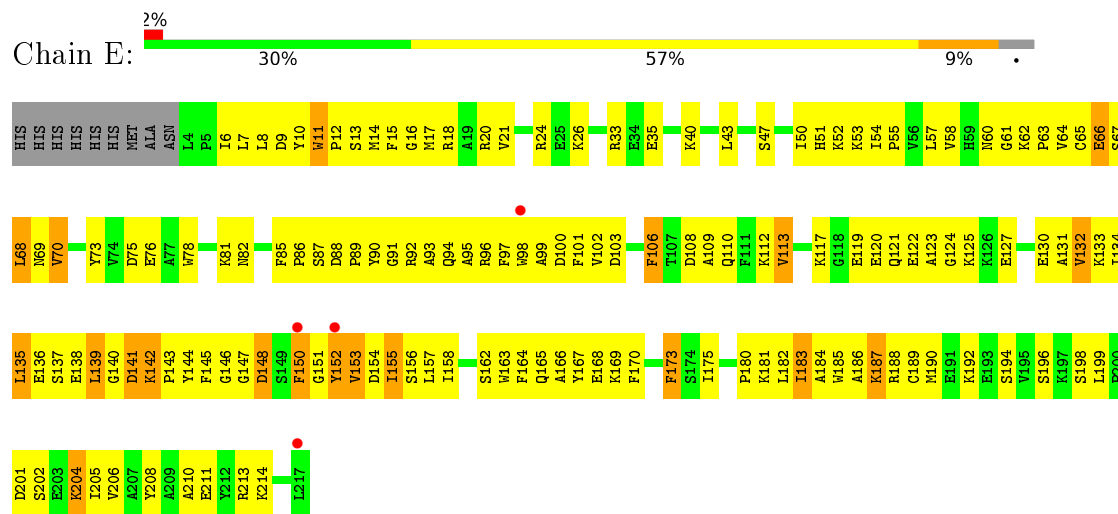
Chain C: 2% 31% 55% 10%



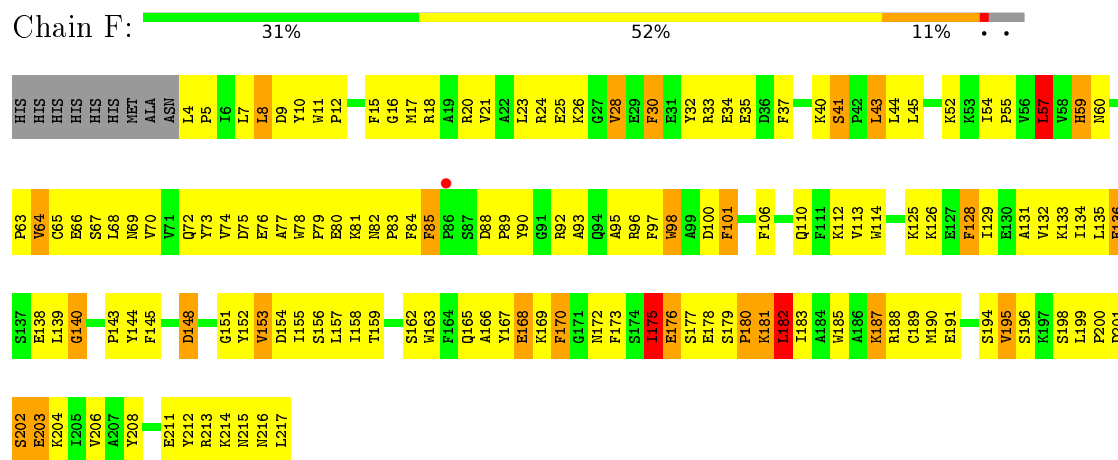




• Molecule 2: Glutathione S-transferase U20



• Molecule 2: Glutathione S-transferase U20



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	53.80Å 53.88Å 193.16Å 90.07° 90.03° 66.39°	Depositor
Resolution (Å)	24.15 – 1.85 24.15 – 1.85	Depositor EDS
% Data completeness (in resolution range)	97.5 (24.15-1.85) 97.4 (24.15-1.85)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.11 (at 1.85Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692+SVN)	Depositor
R, $R_{free}$	0.208 , 0.219 0.208 , 0.220	Depositor DCC
$R_{free}$ test set	16569 reflections (10.02%)	DCC
Wilson B-factor (Å <sup>2</sup> )	0.6	Xtriage
Anisotropy	2.777	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.50 , 142.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.095 for -h,-k,l 0.095 for k,h,-l 0.088 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.86	EDS
Total number of atoms	17172	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	4.0	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 27.03 % 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 2.3658e-03. 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	0.61	2/4581 (0.0%)	1.00	18/6219 (0.3%)
1	D	0.59	0/4581	0.96	16/6219 (0.3%)
2	B	0.50	0/1799	0.79	4/2428 (0.2%)
2	C	0.58	2/1799 (0.1%)	0.88	3/2428 (0.1%)
2	E	0.51	0/1799	0.78	3/2428 (0.1%)
2	F	0.56	0/1799	0.86	4/2428 (0.2%)
All	All	0.57	4/16358 (0.0%)	0.92	48/22150 (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 (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	212	TYR	CE2-CZ	-7.85	1.28	1.38
2	C	212	TYR	CD2-CE2	-6.67	1.29	1.39
1	A	143	LYS	CD-CE	-5.22	1.38	1.51
1	A	143	LYS	CG-CD	-5.12	1.35	1.52

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	392	ILE	CG1-CB-CG2	-10.95	87.30	111.40
1	D	210	ILE	CA-CB-CG1	10.53	131.00	111.00
2	C	212	TYR	CB-CG-CD2	-10.11	114.94	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	212	TYR	CB-CG-CD1	9.38	126.63	121.00
1	D	211	LEU	CA-CB-CG	9.10	136.23	115.30
2	B	139	LEU	CA-CB-CG	-8.16	96.54	115.30
1	A	265	LYS	CD-CE-NZ	8.14	130.42	111.70
1	D	135	ASP	CB-CG-OD1	7.40	124.96	118.30
2	E	139	LEU	CA-CB-CG	-7.37	98.34	115.30
1	A	290	LEU	CA-CB-CG	-7.33	98.43	115.30
1	A	273	LEU	CA-CB-CG	-7.27	98.58	115.30
1	A	282	MET	CG-SD-CE	7.22	111.75	100.20
1	A	427	LEU	CA-CB-CG	6.94	131.26	115.30
1	A	211	LEU	CA-CB-CG	6.86	131.07	115.30
2	F	175	ILE	N-CA-C	6.76	129.24	111.00
1	A	210	ILE	CG1-CB-CG2	-6.75	96.54	111.40
2	E	68	LEU	CB-CG-CD1	-6.74	99.54	111.00
1	D	86	SER	C-N-CD	-6.71	105.83	120.60
2	F	182	LEU	CA-CB-CG	6.65	130.59	115.30
1	D	563	CYS	CA-CB-SG	-6.54	102.23	114.00
1	D	163	GLY	N-CA-C	6.47	129.28	113.10
2	B	158	ILE	CB-CA-C	-6.40	98.80	111.60
2	B	140	GLY	N-CA-C	-6.26	97.45	113.10
1	D	563	CYS	N-CA-C	6.21	127.78	111.00
1	A	563	CYS	N-CA-C	6.20	127.74	111.00
2	C	157	LEU	CA-CB-CG	-6.19	101.06	115.30
1	D	102	GLY	N-CA-C	-6.02	98.05	113.10
2	F	187	LYS	CD-CE-NZ	5.93	125.33	111.70
1	A	163	GLY	N-CA-C	5.88	127.79	113.10
1	A	237	VAL	N-CA-C	5.85	126.78	111.00
1	D	32	LEU	CA-CB-CG	5.79	128.61	115.30
1	D	202	LEU	CA-CB-CG	5.75	128.54	115.30
1	D	370	GLY	N-CA-C	-5.70	98.86	113.10
1	D	255	THR	N-CA-C	5.69	126.36	111.00
1	A	238	TRP	CA-CB-CG	5.67	124.47	113.70
2	E	135	LEU	CB-CG-CD1	-5.58	101.51	111.00
1	D	518	LEU	CA-CB-CG	5.58	128.13	115.30
1	A	211	LEU	CB-CG-CD1	5.52	120.38	111.00
2	B	139	LEU	CB-CG-CD2	-5.35	101.91	111.00
1	D	135	ASP	CB-CG-OD2	-5.34	113.49	118.30
1	D	379	LEU	CA-CB-CG	5.34	127.58	115.30
1	A	294	LEU	CB-CG-CD1	-5.31	101.97	111.00
1	A	73	LEU	CA-CB-CG	5.22	127.32	115.30
1	A	15	ASP	CB-CG-OD1	5.17	122.96	118.30
1	A	102	GLY	N-CA-C	-5.17	100.18	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	562	LEU	CA-CB-CG	5.15	127.15	115.30
2	F	57	LEU	CA-CB-CG	5.14	127.12	115.30
1	A	559	LEU	CA-CB-CG	-5.09	103.60	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	209	GLY	Mainchain
1	A	426	ASN	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	2
1	D	4479	0	4434	690	0
2	B	1748	0	1704	184	0
2	C	1748	0	1704	210	0
2	E	1748	0	1704	227	1
2	F	1748	0	1704	213	2
3	A	15	0	0	1	0
3	D	15	0	0	1	0
4	A	9	0	10	4	0
4	D	9	0	10	1	0
5	A	1	0	0	0	0
5	D	3	0	0	0	0
6	B	20	0	15	3	0
6	C	20	0	15	1	0
6	E	20	0	15	2	0
6	F	20	0	15	0	0
7	A	260	0	0	45	2
7	B	162	0	0	17	1
7	C	130	0	0	22	1
7	D	276	0	0	47	2
7	E	121	0	0	27	0
7	F	141	0	0	19	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	17172	0	15764	2059	8

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 65.

All (2059) 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:143:LYS:NZ	7:D:701:HOH:O	1.72	1.21
1:A:163:GLY:HA3	1:A:560:GLN:HG3	1.24	1.17
1:A:213:ARG:NH1	1:A:294:LEU:HD13	1.66	1.10
2:B:20:ARG:HB3	2:B:24:ARG:HH22	1.23	1.04
2:E:143:PRO:O	2:E:188:ARG:NH1	1.90	1.04
2:C:188:ARG:HB2	1:D:499:ARG:NH2	1.76	1.01
2:E:185:TRP:HD1	2:E:188:ARG:NH1	1.59	1.00
2:E:145:PHE:HB3	2:E:153:VAL:HG13	1.44	1.00
1:D:498:ASP:OD2	7:D:702:HOH:O	1.77	1.00
1:A:42:ALA:HB3	1:A:45:LEU:HD12	1.44	1.00
1:D:451:ARG:NH1	1:D:489:VAL:O	1.95	0.99
1:D:143:LYS:HD2	1:D:212:PHE:HB2	1.42	0.98
1:A:426:ASN:H	1:A:426:ASN:ND2	1.61	0.97
2:F:176:GLU:HB2	2:F:183:ILE:HG12	1.46	0.97
2:E:53:LYS:HD3	6:E:301:GSH:HA1	1.49	0.95
2:C:136:GLU:HG3	2:C:181:LYS:HD3	1.46	0.95
1:D:199:HIS:H	1:D:524:ALA:HB1	1.31	0.95
1:A:164:THR:HG21	1:A:561:ILE:HG13	1.48	0.95
1:D:534:HIS:CE1	1:D:557:LYS:HG2	2.02	0.95
1:D:94:VAL:HG11	1:D:112:PRO:HB3	1.47	0.95
2:B:145:PHE:N	2:B:154:ASP:OD2	2.01	0.94
1:D:200:GLN:HB3	1:D:254:ILE:HG23	1.50	0.93
1:D:499:ARG:NH1	7:D:704:HOH:O	1.97	0.93
1:A:213:ARG:HA	1:A:216:VAL:HG23	1.48	0.93
1:D:150:SER:HB2	1:D:167:THR:HA	1.51	0.92
1:A:238:TRP:HZ3	1:A:277:ILE:HG12	1.32	0.92
2:F:98:TRP:CD1	2:F:153:VAL:HG21	2.03	0.92
1:A:157:THR:HG22	1:A:469:SER:HB3	1.49	0.92
2:C:132:VAL:HG23	2:C:182:LEU:HD13	1.51	0.92
1:D:206:LEU:O	1:D:210:ILE:HG22	1.70	0.92
1:A:213:ARG:HH12	1:A:294:LEU:HD13	1.30	0.91
1:A:211:LEU:O	7:A:701:HOH:O	1.89	0.91
1:A:238:TRP:CZ3	1:A:277:ILE:HG12	2.06	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:551:VAL:HB	1:D:555:ASN:HB2	1.53	0.90
2:C:10:TYR:HB3	2:C:13:SER:HB2	1.55	0.89
1:D:490:LEU:HD22	1:D:522:VAL:HG21	1.53	0.89
2:B:18:ARG:NH1	2:B:103:ASP:OD2	2.06	0.89
1:D:164:THR:HG23	1:D:557:LYS:HG3	1.55	0.89
1:A:135:ASP:OD2	1:A:343:PRO:HD2	1.73	0.89
2:B:51:HIS:HB3	2:B:53:LYS:HG2	1.54	0.89
1:A:432:ASN:HB3	1:A:435:LYS:HD2	1.55	0.88
1:A:426:ASN:N	1:A:426:ASN:HD22	1.70	0.88
2:B:112:LYS:HD2	2:B:116:LYS:HZ1	1.34	0.88
2:E:95:ALA:O	7:E:401:HOH:O	1.90	0.88
1:D:22:ARG:NH1	1:D:414:ASN:OD1	2.07	0.88
1:D:198:VAL:HG23	1:D:524:ALA:HB3	1.53	0.88
1:D:143:LYS:HD3	1:D:216:VAL:HG12	1.53	0.88
1:A:444:SER:HB3	1:A:497:LEU:HG	1.55	0.88
1:A:327:SER:HB2	1:A:352:PHE:HZ	1.38	0.87
1:A:41:SER:HB2	2:B:142:LYS:HG2	1.56	0.87
1:A:99:LEU:HB3	1:A:557:LYS:H	1.38	0.87
1:D:363:PHE:HD2	1:D:382:VAL:HG21	1.39	0.87
1:D:405:ASP:OD2	7:D:703:HOH:O	1.92	0.87
2:F:57:LEU:HG	2:F:64:VAL:HG22	1.58	0.86
1:D:93:PRO:HD2	2:E:181:LYS:HA	1.58	0.86
2:F:26:LYS:HG3	2:F:74:VAL:HG12	1.57	0.86
1:A:454:GLU:OE2	7:A:702:HOH:O	1.93	0.86
1:A:150:SER:HB2	1:A:167:THR:HA	1.56	0.85
1:D:540:SER:OG	1:D:544:GLN:NE2	2.09	0.85
2:F:57:LEU:HD23	2:F:70:VAL:HG13	1.58	0.85
1:D:403:LEU:HD13	1:D:540:SER:HB3	1.57	0.85
2:E:18:ARG:NH2	7:E:406:HOH:O	2.09	0.85
2:E:17:MET:O	7:E:402:HOH:O	1.94	0.85
1:A:143:LYS:HZ1	1:A:212:PHE:C	1.79	0.85
1:D:247:ASP:HB2	1:D:249:VAL:HG12	1.59	0.85
2:F:135:LEU:HD22	2:F:182:LEU:HD12	1.59	0.85
1:D:93:PRO:HD3	2:E:188:ARG:HH21	1.42	0.84
1:D:147:PHE:HA	1:D:205:HIS:CD2	2.11	0.84
1:D:93:PRO:HG2	2:E:184:ALA:HB3	1.60	0.84
2:F:98:TRP:HZ2	2:F:135:LEU:HG	1.40	0.84
2:B:20:ARG:HB3	2:B:24:ARG:NH2	1.93	0.83
2:C:176:GLU:OE2	1:D:573:THR:OG1	1.95	0.83
1:A:392:ILE:HG22	1:A:401:TYR:CE1	2.14	0.83
2:E:185:TRP:CD1	2:E:188:ARG:NH1	2.46	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:426:ASN:H	1:A:426:ASN:HD22	0.85	0.83
1:D:145:LEU:HD13	1:D:209:GLY:HA3	1.60	0.83
1:D:208:SER:O	7:D:701:HOH:O	1.97	0.82
2:B:20:ARG:NH2	2:B:198:SER:O	2.12	0.82
1:D:133:ASN:HD21	1:D:138:ILE:HG13	1.43	0.82
1:D:519:GLU:OE2	1:D:569:SER:OG	1.96	0.82
1:A:238:TRP:CH2	1:A:281:CYS:HB2	2.14	0.82
1:D:226:GLY:HA2	1:D:529:ARG:HD3	1.61	0.82
1:A:143:LYS:NZ	1:A:212:PHE:O	2.11	0.82
1:A:43:ILE:O	1:A:46:GLN:HG2	1.80	0.81
1:A:405:ASP:HB2	1:A:541:SER:HB3	1.60	0.81
1:A:477:ILE:HD13	1:A:497:LEU:HD22	1.62	0.81
1:D:96:ALA:HB1	1:D:163:GLY:H	1.45	0.81
1:A:226:GLY:O	1:A:229:HIS:ND1	2.12	0.81
1:D:81:VAL:HG21	1:D:110:PHE:CE2	2.15	0.81
2:C:209:ALA:HA	2:C:212:TYR:HE2	1.46	0.80
1:A:242:VAL:HG22	1:A:277:ILE:HD13	1.62	0.80
1:D:494:CYS:HB3	1:D:520:LEU:HB2	1.64	0.80
1:D:42:ALA:HB3	1:D:45:LEU:HD13	1.62	0.80
1:D:451:ARG:NH1	1:D:490:LEU:HA	1.95	0.80
1:A:334:GLU:O	1:A:394:ASN:ND2	2.15	0.80
1:D:99:LEU:HD11	1:D:548:PRO:HG3	1.62	0.80
2:B:85:PHE:HB2	2:B:92:ARG:HG2	1.64	0.80
2:F:98:TRP:CZ2	2:F:135:LEU:HG	2.17	0.80
1:A:138:ILE:HB	1:A:217:GLN:HG3	1.64	0.80
2:C:135:LEU:HD13	2:C:182:LEU:HD11	1.64	0.80
1:A:434:ASP:HB2	1:A:550:CYS:HB3	1.61	0.80
2:B:116:LYS:NZ	2:B:120:GLU:HB3	1.97	0.79
1:D:384:ILE:HA	1:D:409:VAL:HG13	1.64	0.79
1:A:282:MET:SD	1:A:282:MET:N	2.55	0.79
1:A:92:HIS:O	7:A:703:HOH:O	1.99	0.79
2:F:10:TYR:O	2:F:20:ARG:NH2	2.15	0.79
1:A:238:TRP:HA	1:A:241:ILE:HB	1.65	0.79
1:D:455:GLU:OE2	7:D:705:HOH:O	2.00	0.79
1:D:107:ARG:HG2	1:D:433:ILE:HG22	1.63	0.79
1:D:405:ASP:HB2	1:D:541:SER:HB3	1.65	0.78
1:D:332:SER:HB2	1:D:538:LEU:HA	1.63	0.78
2:E:96:ARG:NH1	2:F:72:GLN:HB2	1.97	0.78
1:D:507:VAL:HG23	1:D:511:LYS:HE2	1.65	0.78
1:A:221:ALA:HB3	1:A:227:LEU:HG	1.65	0.78
1:D:451:ARG:HH12	1:D:490:LEU:HA	1.49	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:451:ARG:NH1	1:D:493:CYS:HB3	1.97	0.78
1:A:143:LYS:NZ	1:A:212:PHE:C	2.36	0.78
1:D:435:LYS:HZ1	1:D:549:ARG:HB2	1.48	0.78
1:D:76:TYR:HA	1:D:79:ARG:HD3	1.66	0.78
2:C:209:ALA:HA	2:C:212:TYR:CE2	2.19	0.78
1:D:22:ARG:HA	1:D:415:ASN:HB2	1.66	0.78
1:D:452:LEU:HD23	1:D:481:ILE:HG21	1.66	0.78
2:E:139:LEU:HD21	2:E:145:PHE:CE1	2.19	0.78
1:A:489:VAL:O	7:A:704:HOH:O	2.01	0.77
1:D:401:TYR:CE2	1:D:403:LEU:HG	2.18	0.77
2:B:76:GLU:OE2	2:C:92:ARG:NH2	2.16	0.77
1:D:143:LYS:HD2	1:D:212:PHE:CB	2.13	0.77
1:A:132:ARG:O	1:A:136:PHE:N	2.18	0.77
1:A:405:ASP:OD2	7:A:705:HOH:O	2.02	0.77
2:B:33:ARG:NH1	7:B:408:HOH:O	2.17	0.77
1:D:440:ASP:O	7:D:706:HOH:O	2.02	0.77
2:C:54:ILE:HB	2:C:55:PRO:HA	1.67	0.77
2:F:18:ARG:NH2	2:F:159:THR:OG1	2.18	0.77
1:A:42:ALA:HA	2:B:143:PRO:HG3	1.66	0.77
1:D:369:THR:OG1	1:D:370:GLY:N	2.11	0.77
1:A:393:THR:O	7:A:706:HOH:O	2.03	0.76
2:C:7:LEU:HD21	2:C:23:LEU:HD12	1.67	0.76
1:D:138:ILE:HB	1:D:217:GLN:HG3	1.68	0.76
1:D:38:LYS:NZ	2:E:138:GLU:OE1	2.16	0.76
1:A:22:ARG:HA	1:A:415:ASN:HB2	1.66	0.76
1:D:242:VAL:HG22	1:D:277:ILE:HD13	1.68	0.76
2:E:106:PHE:CE2	2:E:131:ALA:HB1	2.20	0.76
2:E:145:PHE:HD2	2:E:153:VAL:HG22	1.50	0.76
2:F:85:PHE:HE1	2:F:95:ALA:HB3	1.49	0.75
2:E:26:LYS:HZ1	2:E:81:LYS:H	1.33	0.75
1:A:435:LYS:HE3	1:A:438:GLU:HG2	1.67	0.75
1:A:197:ASP:OD2	1:A:200:GLN:NE2	2.18	0.75
1:A:563:CYS:SG	1:A:564:GLU:N	2.60	0.75
1:A:153:GLN:H	1:A:564:GLU:HB2	1.50	0.75
1:D:401:TYR:HE2	1:D:403:LEU:HG	1.50	0.75
1:D:223:PHE:CZ	1:D:536:LEU:HB2	2.20	0.75
1:D:223:PHE:CE2	1:D:545:PHE:HZ	2.05	0.75
1:A:199:HIS:H	1:A:524:ALA:HB1	1.52	0.75
2:F:179:SER:OG	2:F:182:LEU:HB3	1.86	0.75
1:A:122:LEU:O	1:A:126:ARG:HG3	1.87	0.75
1:A:140:ASP:OD1	7:A:707:HOH:O	2.05	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:364:LEU:HD23	1:D:389:GLU:OE2	1.87	0.75
2:F:23:LEU:HA	2:F:74:VAL:HG11	1.67	0.75
1:A:204:CYS:SG	7:A:891:HOH:O	2.45	0.74
1:A:219:VAL:HB	1:A:295:PHE:CZ	2.21	0.74
2:B:24:ARG:HD3	2:B:197:LYS:HZ2	1.52	0.74
1:D:394:ASN:O	7:D:707:HOH:O	2.03	0.74
2:E:26:LYS:HA	2:E:82:ASN:HD21	1.51	0.74
2:E:94:GLN:HA	2:E:97:PHE:HD2	1.51	0.74
2:F:168:GLU:OE2	2:F:175:ILE:HG12	1.87	0.74
1:A:457:ILE:HB	1:A:482:SER:HB3	1.67	0.74
1:A:504:ALA:O	1:A:507:VAL:HG22	1.87	0.74
1:A:97:ILE:HD12	1:A:162:VAL:HG22	1.68	0.74
1:A:164:THR:HG1	1:A:167:THR:HG1	1.29	0.74
1:A:152:LYS:HA	1:A:564:GLU:HB3	1.68	0.74
1:A:152:LYS:NZ	1:A:527:THR:HG22	2.03	0.74
2:C:145:PHE:HB2	2:C:153:VAL:HG21	1.68	0.74
1:A:102:GLY:HA2	1:A:546:LYS:HG3	1.69	0.74
1:A:41:SER:OG	2:B:147:GLY:O	2.06	0.74
1:D:496:CYS:HA	1:D:499:ARG:NH1	2.02	0.74
1:D:87:PRO:HB3	1:D:91:GLY:O	1.88	0.74
1:A:111:ILE:HD12	1:A:334:GLU:OE2	1.88	0.74
1:D:521:ARG:HA	1:D:569:SER:HA	1.70	0.74
2:F:37:PHE:HZ	2:F:54:ILE:HG12	1.51	0.74
1:A:441:LEU:HD23	1:A:549:ARG:HB3	1.68	0.74
1:D:352:PHE:O	7:D:708:HOH:O	2.05	0.74
1:A:18:ASP:O	1:A:22:ARG:HG3	1.88	0.73
1:A:477:ILE:HD12	1:A:520:LEU:HD13	1.67	0.73
2:C:60:ASN:ND2	7:C:409:HOH:O	2.19	0.73
1:A:238:TRP:O	1:A:242:VAL:HG23	1.87	0.73
2:B:9:ASP:OD2	2:B:20:ARG:HD3	1.88	0.73
1:D:138:ILE:HA	1:D:217:GLN:HE21	1.54	0.73
1:D:87:PRO:HG2	2:E:188:ARG:NE	2.04	0.73
1:A:451:ARG:NH1	1:A:454:GLU:OE1	2.21	0.73
1:D:42:ALA:HA	2:E:143:PRO:HG3	1.69	0.73
1:A:364:LEU:HB3	1:A:389:GLU:HG2	1.70	0.73
1:D:339:ALA:N	1:D:353:ALA:O	2.19	0.73
1:D:387:GLU:HG2	1:D:406:VAL:HB	1.71	0.73
1:D:392:ILE:HB	1:D:401:TYR:CE1	2.23	0.73
1:D:143:LYS:HE3	1:D:187:CYS:HA	1.71	0.73
1:A:551:VAL:HG12	1:A:555:ASN:HD22	1.54	0.73
2:F:144:TYR:OH	7:F:401:HOH:O	2.05	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:460:ILE:HG22	1:D:461:ASP:OD2	1.89	0.72
1:D:510:ARG:HG2	1:D:515:ILE:HD11	1.71	0.72
2:B:53:LYS:HD3	6:B:301:GSH:HG12	1.68	0.72
2:B:21:VAL:HG11	2:B:158:ILE:HD11	1.71	0.72
1:D:563:CYS:SG	1:D:564:GLU:N	2.60	0.72
1:D:99:LEU:HB3	1:D:557:LYS:HB2	1.71	0.72
2:E:198:SER:HB3	7:E:402:HOH:O	1.89	0.72
1:D:114:THR:H	1:D:117:LEU:HD23	1.54	0.72
1:D:451:ARG:HH12	1:D:490:LEU:CA	2.03	0.72
2:E:100:ASP:OD2	7:E:404:HOH:O	2.07	0.72
1:D:302:TYR:HH	1:D:328:HIS:HD1	1.29	0.72
1:A:108:PRO:HD2	1:A:552:LYS:HD2	1.70	0.72
1:A:492:ASP:OD1	7:A:709:HOH:O	2.08	0.72
2:C:16:GLY:HA2	2:C:55:PRO:HB3	1.70	0.72
1:D:498:ASP:HB3	1:D:510:ARG:NH2	2.04	0.72
1:D:390:VAL:HG11	1:D:540:SER:HA	1.71	0.72
1:A:521:ARG:NH2	7:A:726:HOH:O	2.22	0.72
1:D:152:LYS:HA	1:D:564:GLU:HB3	1.72	0.71
2:E:146:GLY:H	2:E:151:GLY:HA3	1.53	0.71
1:A:200:GLN:HB3	1:A:254:ILE:HG13	1.70	0.71
1:A:390:VAL:O	7:A:708:HOH:O	2.08	0.71
1:A:401:TYR:HE2	1:A:403:LEU:HD13	1.55	0.71
2:F:98:TRP:CE2	2:F:138:GLU:OE2	2.43	0.71
2:B:112:LYS:HD2	2:B:116:LYS:NZ	2.05	0.71
2:C:26:LYS:NZ	2:C:82:ASN:O	2.21	0.71
1:D:326:VAL:HG21	1:D:343:PRO:HB3	1.72	0.71
1:D:451:ARG:CZ	1:D:493:CYS:HB3	2.19	0.71
1:A:226:GLY:HA2	1:A:529:ARG:HD3	1.71	0.71
1:A:92:HIS:CG	2:B:181:LYS:HG2	2.25	0.71
2:F:84:PHE:CD1	2:F:152:TYR:HB2	2.26	0.71
1:D:199:HIS:N	1:D:524:ALA:HB1	2.06	0.71
2:F:213:ARG:NH2	7:F:411:HOH:O	2.23	0.71
1:A:464:SER:OG	1:A:550:CYS:SG	2.48	0.71
1:D:448:ALA:O	1:D:451:ARG:HG2	1.91	0.71
1:A:552:LYS:HB2	1:A:553:PRO:HD2	1.72	0.70
2:B:26:LYS:NZ	2:B:28:VAL:HB	2.06	0.70
1:D:232:ARG:NH2	7:D:724:HOH:O	2.23	0.70
2:E:63:PRO:O	7:E:405:HOH:O	2.08	0.70
1:A:145:LEU:HD13	1:A:209:GLY:HA3	1.73	0.70
1:A:40:GLN:O	7:A:710:HOH:O	2.09	0.70
1:A:534:HIS:CE1	1:A:557:LYS:HG2	2.26	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:VAL:HG11	1:A:112:PRO:HB3	1.74	0.70
2:C:114:TRP:O	2:C:212:TYR:OH	2.09	0.70
1:D:45:LEU:O	1:D:49:GLY:N	2.23	0.70
2:E:95:ALA:HA	2:E:98:TRP:CE3	2.26	0.70
1:A:465:TYR:HD1	1:A:551:VAL:HG23	1.55	0.70
2:F:92:ARG:O	7:F:402:HOH:O	2.08	0.70
1:A:98:SER:HB3	1:A:113:PHE:CZ	2.26	0.70
1:A:126:ARG:NH1	7:A:728:HOH:O	2.23	0.70
1:A:371:GLU:N	1:A:371:GLU:OE2	2.24	0.70
1:A:551:VAL:HG11	1:A:558:VAL:HG11	1.72	0.70
1:D:253:ARG:NH2	7:D:726:HOH:O	2.24	0.70
1:D:44:TYR:HB2	1:D:89:LEU:HD22	1.72	0.70
2:E:40:LYS:NZ	2:E:52:LYS:HD2	2.06	0.70
1:A:551:VAL:HB	1:A:555:ASN:HB2	1.74	0.70
1:D:126:ARG:HH11	1:D:126:ARG:HG3	1.56	0.70
1:D:198:VAL:CG2	1:D:524:ALA:HB3	2.22	0.70
2:E:94:GLN:OE1	7:E:407:HOH:O	2.10	0.70
2:C:125:LYS:NZ	2:C:171:GLY:HA3	2.06	0.70
2:C:33:ARG:NH1	2:C:41:SER:OG	2.25	0.70
1:D:333:SER:OG	1:D:557:LYS:NZ	2.24	0.70
1:D:494:CYS:HB3	1:D:520:LEU:CB	2.21	0.70
1:D:99:LEU:HD13	1:D:555:ASN:OD1	1.92	0.70
1:A:145:LEU:HD22	1:A:213:ARG:NH2	2.07	0.70
1:A:207:LEU:HD21	1:A:245:ILE:HD11	1.73	0.70
1:D:451:ARG:HE	1:D:452:LEU:HD13	1.56	0.70
1:D:533:GLU:O	7:D:709:HOH:O	2.09	0.70
2:E:142:LYS:NZ	7:E:403:HOH:O	2.05	0.70
1:A:262:ALA:O	1:A:265:LYS:HE3	1.91	0.70
1:A:87:PRO:HB3	2:B:143:PRO:HA	1.74	0.70
1:D:392:ILE:HB	1:D:401:TYR:HE1	1.56	0.70
1:A:108:PRO:HD3	1:A:434:ASP:OD2	1.92	0.69
1:A:84:ASP:N	1:A:84:ASP:OD1	2.23	0.69
2:C:26:LYS:HD2	2:C:74:VAL:HG13	1.74	0.69
1:D:208:SER:HA	1:D:211:LEU:HG	1.73	0.69
1:D:223:PHE:CZ	1:D:533:GLU:HA	2.27	0.69
1:D:280:LYS:HE2	1:D:293:ALA:HB1	1.74	0.69
1:A:81:VAL:HB	1:A:110:PHE:HE2	1.57	0.69
1:A:152:LYS:HG3	1:A:565:ASN:HB2	1.72	0.69
1:D:342:THR:O	1:D:345:LEU:HG	1.92	0.69
2:F:8:LEU:HD22	2:F:43:LEU:HD13	1.75	0.69
1:D:353:ALA:HB2	1:D:413:TYR:CD2	2.27	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:165:GLN:NE2	7:E:414:HOH:O	2.20	0.69
1:A:520:LEU:O	7:A:711:HOH:O	2.09	0.69
2:B:169:LYS:HZ1	2:B:206:VAL:HG11	1.57	0.69
1:D:23:ASN:HB3	1:D:27:VAL:HG23	1.73	0.69
2:F:25:GLU:OE2	2:F:82:ASN:ND2	2.26	0.69
1:A:22:ARG:HH11	1:A:414:ASN:HB3	1.55	0.69
1:A:340:ASN:HB2	1:A:352:PHE:CD1	2.27	0.69
2:B:100:ASP:OD2	7:B:401:HOH:O	2.09	0.69
1:D:332:SER:OG	1:D:333:SER:N	2.22	0.69
2:F:154:ASP:HA	2:F:185:TRP:HZ2	1.57	0.69
2:F:128:PHE:CE1	2:F:175:ILE:HG22	2.27	0.69
1:A:154:TYR:HB2	1:A:563:CYS:SG	2.32	0.69
1:A:77:ILE:HG22	1:A:110:PHE:HD2	1.57	0.69
2:B:24:ARG:HH21	2:B:30:PHE:HZ	1.39	0.69
2:B:35:GLU:O	7:B:402:HOH:O	2.11	0.69
2:F:11:TRP:CD1	2:F:12:PRO:HD3	2.28	0.69
1:A:163:GLY:CA	1:A:560:GLN:HG3	2.15	0.69
1:A:87:PRO:HG3	1:A:93:PRO:HD3	1.75	0.69
2:C:121:GLN:O	2:C:125:LYS:HG3	1.93	0.69
2:E:154:ASP:O	2:E:158:ILE:HG23	1.93	0.69
1:A:164:THR:HG22	1:A:557:LYS:O	1.92	0.69
1:D:154:TYR:HB3	1:D:563:CYS:SG	2.33	0.69
1:A:152:LYS:HZ1	1:A:198:VAL:HG21	1.58	0.68
2:C:184:ALA:O	7:D:704:HOH:O	2.11	0.68
1:A:41:SER:HA	2:B:148:ASP:HA	1.75	0.68
1:A:81:VAL:O	7:A:712:HOH:O	2.11	0.68
2:B:201:ASP:O	7:B:403:HOH:O	2.12	0.68
2:C:146:GLY:O	7:C:403:HOH:O	2.11	0.68
2:C:163:TRP:HB3	2:C:167:TYR:CZ	2.28	0.68
2:C:174:SER:O	7:C:402:HOH:O	2.09	0.68
1:D:51:ASN:ND2	2:E:87:SER:OG	2.26	0.68
2:F:168:GLU:OE1	7:F:403:HOH:O	2.11	0.68
1:D:202:LEU:HA	1:D:205:HIS:HB2	1.74	0.68
1:D:462:PHE:O	1:D:549:ARG:NH1	2.27	0.68
1:D:544:GLN:NE2	7:D:703:HOH:O	2.17	0.68
2:F:57:LEU:HG	2:F:64:VAL:CG2	2.23	0.68
1:A:418:GLN:N	7:A:730:HOH:O	2.26	0.68
1:A:48:CYS:SG	1:A:65:VAL:HB	2.33	0.68
2:F:191:GLU:OE2	7:F:401:HOH:O	2.12	0.68
1:A:390:VAL:HG11	1:A:540:SER:HA	1.75	0.68
1:D:477:ILE:HD11	1:D:497:LEU:HD13	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:188:ARG:NH1	1:D:499:ARG:O	2.26	0.68
2:F:139:LEU:O	7:F:404:HOH:O	2.11	0.68
1:A:180:LYS:O	7:A:713:HOH:O	2.11	0.68
1:A:421:PHE:CE1	1:A:541:SER:HA	2.29	0.68
2:C:187:LYS:HE3	1:D:493:CYS:HA	1.73	0.68
2:C:18:ARG:HD2	2:C:67:SER:HB2	1.74	0.67
2:E:182:LEU:O	2:E:185:TRP:HB3	1.94	0.67
2:F:33:ARG:NH1	2:F:35:GLU:OE2	2.27	0.67
2:B:75:ASP:OD2	2:B:85:PHE:HD1	1.78	0.67
1:D:172:ASN:HB3	1:D:175:PHE:CE2	2.30	0.67
2:E:190:MET:SD	7:E:471:HOH:O	2.51	0.67
1:A:480:GLU:HG3	1:A:525:LYS:HA	1.74	0.67
1:A:114:THR:OG1	2:B:141:ASP:OD2	2.10	0.67
1:D:305:MET:HG3	1:D:347:PRO:HB3	1.75	0.67
1:D:423:CYS:SG	1:D:541:SER:OG	2.49	0.67
1:A:169:VAL:HG13	1:A:170:TYR:CD1	2.29	0.67
1:A:143:LYS:HZ2	1:A:212:PHE:CA	2.07	0.67
1:A:360:TYR:N	7:A:706:HOH:O	2.27	0.67
1:A:38:LYS:O	2:B:142:LYS:HB2	1.94	0.67
2:B:76:GLU:OE1	2:C:92:ARG:NE	2.28	0.67
1:D:435:LYS:NZ	1:D:549:ARG:HB2	2.08	0.67
1:A:363:PHE:HB3	1:A:388:TYR:HB3	1.74	0.67
1:A:471:ASP:OD1	7:A:714:HOH:O	2.13	0.67
1:D:110:PHE:CE1	1:D:556:ALA:HB2	2.29	0.67
1:D:39:ASN:HA	2:E:142:LYS:HE3	1.75	0.67
1:A:106:GLY:HA3	1:A:432:ASN:HB2	1.77	0.67
1:A:46:GLN:HB3	2:B:148:ASP:HB3	1.75	0.67
2:C:11:TRP:CD1	2:C:12:PRO:HD3	2.29	0.67
1:D:25:HIS:HA	1:D:28:GLN:HG2	1.77	0.67
1:D:135:ASP:OD2	1:D:343:PRO:HB2	1.94	0.67
2:E:185:TRP:HD1	2:E:188:ARG:HH12	1.43	0.67
2:C:98:TRP:HE1	2:C:145:PHE:HD2	1.41	0.67
1:A:108:PRO:HG2	1:A:552:LYS:HG2	1.77	0.67
2:C:144:TYR:HB3	2:C:154:ASP:OD2	1.95	0.67
1:D:331:GLY:HA3	1:D:336:TRP:CE3	2.28	0.67
1:A:166:THR:HA	1:A:169:VAL:HG12	1.77	0.66
1:A:363:PHE:HD2	1:A:382:VAL:HG21	1.59	0.66
1:A:409:VAL:HG13	7:A:730:HOH:O	1.95	0.66
2:B:204:LYS:HB2	7:B:403:HOH:O	1.95	0.66
2:F:125:LYS:HA	2:F:128:PHE:CD2	2.30	0.66
1:D:199:HIS:H	1:D:524:ALA:CB	2.05	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:96:ALA:HA	1:D:162:VAL:HA	1.75	0.66
2:E:150:PHE:CE2	2:E:192:LYS:HG3	2.30	0.66
1:A:90:THR:HG23	1:A:397:GLY:HA2	1.75	0.66
1:D:99:LEU:HB3	1:D:557:LYS:H	1.60	0.66
2:B:142:LYS:O	7:B:405:HOH:O	2.14	0.66
2:C:40:LYS:HD3	2:C:52:LYS:HB3	1.77	0.66
2:F:23:LEU:HD11	2:F:30:PHE:CD2	2.30	0.66
2:B:150:PHE:HZ	2:B:158:ILE:HG21	1.60	0.66
1:A:116:GLU:OE2	1:A:395:TYR:HB3	1.95	0.66
1:D:224:ALA:HA	1:D:316:LEU:HD22	1.78	0.66
2:C:201:ASP:HB3	1:D:454:GLU:O	1.96	0.66
2:E:11:TRP:HZ2	2:E:204:LYS:HB3	1.60	0.66
2:F:162:SER:O	7:F:405:HOH:O	2.13	0.66
2:F:98:TRP:NE1	2:F:138:GLU:OE2	2.29	0.66
1:A:143:LYS:NZ	1:A:212:PHE:CB	2.59	0.66
1:D:451:ARG:NH1	1:D:490:LEU:CA	2.58	0.66
1:D:534:HIS:CD2	1:D:557:LYS:HE2	2.30	0.66
1:A:390:VAL:HG11	1:A:540:SER:CA	2.26	0.66
2:C:17:MET:SD	2:C:199:LEU:HG	2.36	0.66
2:E:145:PHE:O	7:E:408:HOH:O	2.14	0.66
2:E:136:GLU:HG3	2:E:181:LYS:HE2	1.78	0.66
1:A:126:ARG:HA	1:A:182:ILE:HG21	1.77	0.66
1:A:223:PHE:HD2	1:A:225:HIS:CE1	2.14	0.66
1:A:23:ASN:HB3	1:A:27:VAL:HG23	1.77	0.66
1:A:213:ARG:HH11	1:A:294:LEU:HD13	1.59	0.66
1:A:90:THR:HG22	2:B:141:ASP:HB3	1.78	0.66
2:E:157:LEU:HD21	2:E:182:LEU:HD11	1.77	0.66
1:A:163:GLY:HA3	1:A:560:GLN:CG	2.16	0.65
1:A:143:LYS:HZ2	1:A:212:PHE:CB	2.09	0.65
1:A:237:VAL:HG11	1:A:253:ARG:NH2	2.11	0.65
1:A:427:LEU:O	7:A:715:HOH:O	2.13	0.65
2:B:33:ARG:O	7:B:404:HOH:O	2.13	0.65
2:E:99:ALA:N	7:E:401:HOH:O	2.28	0.65
1:A:116:GLU:O	1:A:119:GLU:HG2	1.96	0.65
2:C:60:ASN:O	7:C:406:HOH:O	2.15	0.65
1:D:273:LEU:HD12	1:D:273:LEU:H	1.61	0.65
2:F:98:TRP:CZ3	2:F:101:PHE:HB2	2.31	0.65
2:E:13:SER:O	2:E:17:MET:HG3	1.96	0.65
2:E:211:GLU:HA	2:E:214:LYS:HG3	1.78	0.65
1:A:239:GLU:OE1	7:A:716:HOH:O	2.13	0.65
1:A:475:TYR:O	1:A:518:LEU:HD23	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:24:ARG:NH1	2:B:198:SER:OG	2.29	0.65
1:D:38:LYS:C	2:E:142:LYS:HZ2	2.00	0.65
2:F:215:ASN:OD1	7:F:406:HOH:O	2.14	0.65
1:D:116:GLU:OE2	1:D:395:TYR:HB2	1.96	0.65
1:D:478:PHE:HZ	1:D:562:LEU:HD12	1.61	0.65
2:F:158:ILE:HG12	2:F:195:VAL:HG11	1.79	0.65
1:A:575:PHE:O	7:A:718:HOH:O	2.14	0.65
1:A:97:ILE:HG21	1:A:110:PHE:CD2	2.32	0.65
1:D:69:THR:OG1	1:D:72:GLU:OE2	2.15	0.65
2:F:201:ASP:HB2	2:F:204:LYS:HE3	1.79	0.65
1:A:353:ALA:HB2	1:A:413:TYR:CD2	2.31	0.65
1:A:551:VAL:HB	1:A:555:ASN:CB	2.27	0.65
2:C:196:SER:O	7:C:404:HOH:O	2.14	0.65
2:E:21:VAL:HG11	2:E:158:ILE:HD11	1.79	0.65
2:F:11:TRP:CG	2:F:12:PRO:HD3	2.31	0.65
1:A:152:LYS:NZ	1:A:198:VAL:HG21	2.11	0.65
1:A:87:PRO:HD3	1:A:93:PRO:HG3	1.78	0.65
2:C:152:TYR:O	7:C:407:HOH:O	2.15	0.65
1:A:108:PRO:HG2	1:A:552:LYS:H	1.61	0.64
2:B:116:LYS:HZ2	2:B:120:GLU:HB3	1.61	0.64
1:D:132:ARG:O	1:D:136:PHE:N	2.20	0.64
1:A:110:PHE:CE1	1:A:556:ALA:HB2	2.32	0.64
2:B:166:ALA:HA	2:B:169:LYS:HZ3	1.61	0.64
2:F:63:PRO:O	7:F:407:HOH:O	2.14	0.64
1:A:211:LEU:HD12	1:A:212:PHE:CD2	2.32	0.64
2:B:24:ARG:HD3	2:B:197:LYS:NZ	2.12	0.64
2:B:193:GLU:HA	2:B:196:SER:HB3	1.80	0.64
2:B:40:LYS:NZ	2:B:52:LYS:HD2	2.13	0.64
2:C:177:SER:HA	1:D:573:THR:HG21	1.78	0.64
1:D:17:PHE:HA	1:D:20:MET:HG2	1.79	0.64
2:F:10:TYR:CG	2:F:12:PRO:HD2	2.33	0.64
1:A:149:PHE:HB2	1:A:530:LYS:NZ	2.13	0.64
1:A:246:LYS:HG3	1:A:274:ALA:HB2	1.80	0.64
2:C:109:ALA:HB1	2:C:128:PHE:HB3	1.78	0.64
2:C:203:GLU:OE2	7:C:405:HOH:O	2.14	0.64
2:C:24:ARG:HB3	2:C:194:SER:HA	1.79	0.64
2:F:208:TYR:O	7:F:408:HOH:O	2.15	0.64
1:A:498:ASP:HB3	1:A:510:ARG:NH2	2.13	0.64
1:A:96:ALA:O	1:A:113:PHE:HB2	1.98	0.64
2:B:110:GLN:O	2:B:113:VAL:HG12	1.98	0.64
1:D:254:ILE:O	7:D:714:HOH:O	2.15	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:492:ASP:O	1:D:495:ASN:HB2	1.98	0.64
2:E:166:ALA:HB2	2:E:206:VAL:HG12	1.79	0.64
1:A:336:TRP:HB3	1:A:358:LEU:HD13	1.80	0.64
1:A:364:LEU:HD23	1:A:389:GLU:OE2	1.97	0.64
1:A:92:HIS:CD2	2:B:181:LYS:HG2	2.32	0.64
2:B:125:LYS:HB2	2:B:173:PHE:CE2	2.32	0.64
1:D:18:ASP:O	1:D:22:ARG:HG3	1.96	0.64
1:D:29:LYS:NZ	1:D:58:GLU:OE2	2.31	0.64
1:A:81:VAL:HB	1:A:110:PHE:CE2	2.32	0.64
2:C:180:PRO:HB3	1:D:573:THR:HG22	1.80	0.64
1:D:40:GLN:NE2	1:D:51:ASN:O	2.31	0.64
1:D:73:LEU:HD23	1:D:89:LEU:HD12	1.79	0.64
2:E:142:LYS:HD3	2:E:143:PRO:HD2	1.78	0.64
1:A:108:PRO:HB3	1:A:555:ASN:CG	2.18	0.64
2:B:9:ASP:N	7:B:404:HOH:O	2.26	0.64
2:C:125:LYS:HZ2	2:C:171:GLY:HA3	1.61	0.63
2:B:9:ASP:OD1	2:B:10:TYR:N	2.30	0.63
1:D:42:ALA:N	7:D:739:HOH:O	2.32	0.63
1:A:392:ILE:HG22	1:A:401:TYR:HE1	1.64	0.63
1:D:504:ALA:O	1:D:507:VAL:HG13	1.99	0.63
2:E:145:PHE:CD2	2:E:153:VAL:HG22	2.32	0.63
1:A:191:GLU:O	1:A:195:SER:N	2.32	0.63
1:A:40:GLN:HE21	1:A:52:GLY:HA3	1.62	0.63
1:A:407:VAL:HG21	1:A:419:LEU:HD23	1.80	0.63
2:C:12:PRO:O	2:C:163:TRP:HZ2	1.81	0.63
1:D:172:ASN:HB3	1:D:175:PHE:CZ	2.32	0.63
1:A:197:ASP:N	1:A:197:ASP:OD1	2.30	0.63
1:A:250:LEU:HD22	1:A:260:ARG:HE	1.63	0.63
1:A:219:VAL:HB	1:A:295:PHE:CE2	2.33	0.63
1:A:486:ASN:ND2	7:A:739:HOH:O	2.30	0.63
2:E:103:ASP:OD2	7:E:409:HOH:O	2.14	0.63
2:E:132:VAL:HG21	2:E:175:ILE:HG23	1.79	0.63
2:E:26:LYS:NZ	2:E:81:LYS:H	1.95	0.63
2:E:62:LYS:HB3	2:F:90:TYR:CZ	2.34	0.63
1:A:223:PHE:HB3	1:A:309:MET:HE3	1.81	0.63
1:A:252:ASN:HA	1:A:260:ARG:HH22	1.63	0.63
1:A:494:CYS:SG	1:A:495:ASN:N	2.72	0.63
2:B:215:ASN:O	7:B:407:HOH:O	2.16	0.63
1:D:93:PRO:HD2	2:E:181:LYS:CA	2.27	0.63
2:F:167:TYR:HB2	2:F:168:GLU:OE1	1.99	0.63
1:A:218:TYR:HA	1:A:298:ALA:HB1	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:315:LYS:HA	1:A:318:HIS:HB3	1.81	0.63
1:D:145:LEU:O	7:D:715:HOH:O	2.16	0.63
1:D:146:GLN:O	1:D:205:HIS:NE2	2.31	0.63
2:C:98:TRP:CH2	2:C:135:LEU:HG	2.33	0.63
2:C:14:MET:HG3	2:C:163:TRP:CH2	2.33	0.63
1:D:383:LYS:O	1:D:386:GLU:HG2	1.98	0.63
1:D:87:PRO:HG2	2:E:188:ARG:CZ	2.28	0.63
2:E:6:ILE:HD12	2:E:6:ILE:H	1.63	0.63
1:A:190:ASP:O	1:A:194:PHE:HD2	1.81	0.62
1:D:473:GLY:O	1:D:516:GLY:N	2.29	0.62
2:F:21:VAL:HG12	2:F:155:ILE:HG12	1.80	0.62
1:A:503:ASP:OD1	1:A:504:ALA:N	2.32	0.62
1:D:228:VAL:HG11	1:D:315:LYS:HD3	1.79	0.62
2:F:4:LEU:HD12	2:F:5:PRO:HD2	1.79	0.62
1:D:146:GLN:NE2	7:D:720:HOH:O	2.19	0.62
1:D:371:GLU:N	1:D:371:GLU:OE2	2.32	0.62
2:E:66:GLU:OE2	2:F:97:PHE:HD1	1.82	0.62
1:D:153:GLN:NE2	1:D:171:ARG:HG3	2.14	0.62
1:D:20:MET:HA	1:D:23:ASN:HB2	1.80	0.62
1:D:212:PHE:N	7:D:701:HOH:O	2.12	0.62
1:D:433:ILE:HG13	1:D:433:ILE:O	1.98	0.62
2:E:143:PRO:C	2:E:188:ARG:NH1	2.52	0.62
2:F:140:GLY:HA2	2:F:181:LYS:NZ	2.15	0.62
1:A:152:LYS:HD3	1:A:561:ILE:HA	1.82	0.62
1:A:238:TRP:CZ2	1:A:281:CYS:HB2	2.35	0.62
1:A:526:GLY:O	1:A:530:LYS:HG2	2.00	0.62
2:F:40:LYS:HD2	2:F:52:LYS:HD2	1.80	0.62
2:C:117:LYS:HE3	2:C:213:ARG:HH11	1.65	0.62
1:D:150:SER:HB2	1:D:167:THR:CA	2.28	0.62
1:D:198:VAL:HG22	1:D:565:ASN:HD22	1.62	0.62
2:F:112:LYS:O	7:F:409:HOH:O	2.16	0.62
2:F:35:GLU:OE2	2:F:41:SER:HB2	1.99	0.62
1:A:118:MET:HG2	1:A:174:ASN:ND2	2.15	0.62
1:A:247:ASP:CG	1:A:249:VAL:HG12	2.20	0.62
2:B:119:GLU:N	2:B:119:GLU:OE1	2.33	0.62
1:D:315:LYS:HA	1:D:318:HIS:HB3	1.82	0.62
1:D:442:GLN:HA	1:D:462:PHE:CZ	2.34	0.62
1:D:29:LYS:HZ1	1:D:58:GLU:CD	2.03	0.62
2:E:24:ARG:HG3	2:E:194:SER:HA	1.79	0.62
1:A:315:LYS:O	1:A:318:HIS:HB3	2.00	0.62
1:A:507:VAL:O	1:A:511:LYS:HB2	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:523:VAL:HG22	1:A:524:ALA:H	1.64	0.62
2:C:194:SER:O	2:C:198:SER:OG	2.18	0.62
1:A:242:VAL:O	1:A:246:LYS:HB2	2.00	0.61
2:E:163:TRP:HB3	2:E:167:TYR:CZ	2.35	0.61
2:C:125:LYS:HA	2:C:128:PHE:CE2	2.35	0.61
2:F:166:ALA:HB2	2:F:206:VAL:HA	1.82	0.61
2:B:205:ILE:HA	2:B:208:TYR:CE2	2.35	0.61
2:B:65:CYS:SG	7:B:458:HOH:O	2.53	0.61
2:B:75:ASP:OD2	2:B:85:PHE:CD1	2.53	0.61
1:D:105:GLN:NE2	7:D:736:HOH:O	2.28	0.61
1:D:566:VAL:HG21	1:D:569:SER:HB2	1.81	0.61
2:F:40:LYS:H	2:F:40:LYS:NZ	1.98	0.61
1:D:292:PRO:HB3	1:D:323:LEU:HD12	1.82	0.61
1:D:463:SER:HB3	1:D:478:PHE:HD2	1.65	0.61
1:D:226:GLY:CA	1:D:529:ARG:HD3	2.29	0.61
2:E:11:TRP:HZ2	2:E:204:LYS:CB	2.13	0.61
2:F:133:LYS:O	2:F:136:GLU:HG3	2.00	0.61
1:A:274:ALA:O	1:A:278:ARG:HD2	2.00	0.61
1:A:398:LEU:HB3	1:A:401:TYR:CD1	2.36	0.61
2:B:86:PRO:HD3	2:B:146:GLY:O	2.00	0.61
1:A:338:ALA:HA	1:A:354:VAL:HA	1.80	0.61
1:A:77:ILE:HG23	1:A:80:MET:HE3	1.83	0.61
2:B:109:ALA:HA	2:B:112:LYS:HG2	1.81	0.61
2:C:98:TRP:CZ2	2:C:157:LEU:HD22	2.35	0.61
1:D:108:PRO:HB2	1:D:554:SER:HB2	1.80	0.61
2:E:18:ARG:HD3	2:E:156:SER:HA	1.82	0.61
2:B:112:LYS:CD	2:B:116:LYS:HZ1	2.11	0.61
2:C:145:PHE:N	2:C:145:PHE:CD1	2.64	0.61
2:C:84:PHE:HB2	2:C:152:TYR:N	2.16	0.61
1:D:464:SER:HB2	1:D:477:ILE:HG22	1.83	0.61
1:D:93:PRO:HD3	2:E:188:ARG:NH2	2.14	0.61
2:B:90:TYR:O	2:B:93:ALA:HB3	2.01	0.61
2:C:176:GLU:OE2	1:D:491:GLN:HG2	2.01	0.61
1:D:329:ASP:HB3	1:D:339:ALA:HA	1.81	0.61
1:A:153:GLN:HE22	1:A:171:ARG:HG2	1.66	0.61
1:D:330:TYR:O	1:D:338:ALA:N	2.32	0.61
1:D:38:LYS:HB3	2:E:140:GLY:HA3	1.82	0.61
1:A:38:LYS:HB3	2:B:140:GLY:HA3	1.82	0.61
1:D:108:PRO:HG2	1:D:552:LYS:HG2	1.82	0.61
1:D:149:PHE:CE2	1:D:202:LEU:HD22	2.35	0.60
1:D:509:SER:OG	1:D:515:ILE:HG12	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:60:ASN:ND2	7:F:418:HOH:O	2.26	0.60
2:C:177:SER:HA	1:D:573:THR:CG2	2.31	0.60
1:D:8:PHE:HA	1:D:126:ARG:CZ	2.31	0.60
1:A:278:ARG:O	1:A:282:MET:HG2	2.00	0.60
1:A:305:MET:SD	1:A:325:LEU:HB3	2.41	0.60
2:B:20:ARG:HH22	2:B:200:PRO:HD3	1.67	0.60
1:D:363:PHE:HE1	1:D:390:VAL:HG23	1.65	0.60
1:D:394:ASN:ND2	7:D:744:HOH:O	2.33	0.60
2:E:144:TYR:HB3	2:E:154:ASP:OD2	2.02	0.60
1:A:209:GLY:C	1:A:213:ARG:HE	2.05	0.60
2:C:108:ASP:O	2:C:112:LYS:HG2	2.02	0.60
2:C:98:TRP:O	2:C:101:PHE:HB2	2.01	0.60
1:D:351:THR:HG21	1:D:410:ILE:HG12	1.83	0.60
1:A:274:ALA:HB1	1:A:278:ARG:NH2	2.16	0.60
1:A:365:PRO:HG3	1:A:374:GLU:HG2	1.82	0.60
1:D:87:PRO:HD3	1:D:93:PRO:HG3	1.82	0.60
2:F:163:TRP:HB3	2:F:167:TYR:CZ	2.37	0.60
1:A:312:TYR:CD2	1:A:315:LYS:HE2	2.36	0.60
1:D:118:MET:HE3	1:D:169:VAL:HG23	1.84	0.60
1:D:273:LEU:N	1:D:273:LEU:HD12	2.16	0.60
2:C:188:ARG:HE	1:D:499:ARG:HH21	1.50	0.60
1:D:435:LYS:HZ1	1:D:549:ARG:CB	2.14	0.60
1:A:13:VAL:HG22	1:A:17:PHE:CZ	2.37	0.60
2:B:96:ARG:HA	2:B:152:TYR:HE2	1.66	0.60
1:D:526:GLY:HA2	1:D:529:ARG:NH1	2.17	0.60
1:A:42:ALA:HB1	1:A:44:TYR:CE1	2.37	0.60
1:A:435:LYS:HG2	1:A:438:GLU:OE2	2.01	0.60
1:D:432:ASN:OD1	1:D:433:ILE:N	2.35	0.60
1:D:498:ASP:HB3	1:D:510:ARG:HH21	1.67	0.60
2:E:119:GLU:HA	2:E:122:GLU:HG2	1.83	0.60
2:F:114:TRP:HZ3	2:F:212:TYR:HD2	1.50	0.60
1:D:79:ARG:NH2	1:D:87:PRO:O	2.35	0.60
1:D:93:PRO:HG2	2:E:184:ALA:CB	2.30	0.60
1:A:29:LYS:HG3	1:A:30:GLN:H	1.67	0.59
1:D:234:PHE:CD2	1:D:287:TRP:HH2	2.20	0.59
1:D:46:GLN:HB2	2:E:148:ASP:HB2	1.84	0.59
1:D:87:PRO:HG2	2:E:188:ARG:HE	1.65	0.59
1:D:46:GLN:HE21	2:E:148:ASP:HB2	1.66	0.59
1:A:451:ARG:NH1	1:A:489:VAL:HG12	2.17	0.59
2:F:169:LYS:HG3	2:F:170:PHE:H	1.67	0.59
1:A:531:ILE:HA	1:A:534:HIS:CD2	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:GLU:O	1:A:61:PHE:HB2	2.02	0.59
2:C:98:TRP:NE1	2:C:145:PHE:HD2	2.01	0.59
1:D:104:SER:O	1:D:107:ARG:HB2	2.02	0.59
2:E:65:CYS:O	2:E:66:GLU:HB2	2.02	0.59
1:A:118:MET:HE3	1:A:169:VAL:HA	1.85	0.59
2:B:146:GLY:HA3	2:B:151:GLY:HA3	1.84	0.59
2:B:202:SER:O	2:B:206:VAL:HG13	2.01	0.59
1:D:273:LEU:CD1	1:D:273:LEU:H	2.15	0.59
1:D:276:THR:OG1	1:D:277:ILE:N	2.33	0.59
1:A:292:PRO:O	1:A:296:PRO:HA	2.02	0.59
1:A:435:LYS:HB3	1:A:436:ASN:C	2.23	0.59
1:A:46:GLN:OE1	2:B:149:SER:OG	2.20	0.59
1:A:506:TYR:CE1	1:A:510:ARG:HD3	2.37	0.59
2:B:13:SER:O	2:B:17:MET:HG3	2.03	0.59
2:C:20:ARG:HB3	2:C:198:SER:HB3	1.85	0.59
1:D:87:PRO:HG2	2:E:188:ARG:NH2	2.17	0.59
1:A:247:ASP:OD2	1:A:249:VAL:HG12	2.03	0.59
2:B:17:MET:HG2	2:B:20:ARG:NH2	2.18	0.59
1:D:108:PRO:HG2	1:D:552:LYS:H	1.68	0.59
1:D:152:LYS:HD3	1:D:561:ILE:HG23	1.83	0.59
1:D:92:HIS:HE1	2:E:185:TRP:HB2	1.68	0.59
1:A:225:HIS:CD2	1:A:529:ARG:HE	2.21	0.59
1:A:53:ASN:OD1	1:A:54:ALA:N	2.36	0.59
1:A:22:ARG:NH1	1:A:414:ASN:HB3	2.18	0.59
1:D:149:PHE:CZ	1:D:202:LEU:HD22	2.38	0.59
1:D:229:HIS:O	1:D:233:THR:HG23	2.02	0.59
1:D:328:HIS:CG	1:D:329:ASP:N	2.71	0.59
1:A:99:LEU:HD11	1:A:548:PRO:HG2	1.85	0.59
1:D:451:ARG:O	1:D:454:GLU:HG2	2.02	0.59
2:B:116:LYS:HZ3	2:B:120:GLU:HB3	1.66	0.58
1:D:92:HIS:CG	2:E:181:LYS:HB2	2.38	0.58
1:A:143:LYS:HB2	1:A:185:PRO:O	2.02	0.58
1:A:159:GLY:N	7:A:725:HOH:O	2.36	0.58
1:A:316:LEU:O	1:A:320:ALA:N	2.24	0.58
1:D:178:GLY:O	7:D:713:HOH:O	2.15	0.58
1:D:451:ARG:HG3	1:D:452:LEU:N	2.19	0.58
1:D:572:SER:OG	7:D:702:HOH:O	2.09	0.58
1:D:38:LYS:HE3	2:E:138:GLU:O	2.02	0.58
2:E:57:LEU:O	7:E:412:HOH:O	2.17	0.58
2:F:98:TRP:HZ3	2:F:101:PHE:HB2	1.68	0.58
2:B:176:GLU:HG3	2:B:180:PRO:HA	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:153:VAL:HB	7:E:401:HOH:O	2.03	0.58
2:F:54:ILE:HB	2:F:55:PRO:HA	1.84	0.58
1:D:368:GLU:OE2	7:D:716:HOH:O	2.16	0.58
1:D:228:VAL:HA	1:D:319:TYR:CE2	2.38	0.58
2:F:203:GLU:HA	2:F:206:VAL:HG22	1.86	0.58
1:A:327:SER:HB2	1:A:352:PHE:CZ	2.29	0.58
1:D:146:GLN:NE2	7:D:738:HOH:O	2.31	0.58
1:D:195:SER:OG	1:D:197:ASP:OD1	2.22	0.58
1:D:465:TYR:HD1	1:D:551:VAL:HG23	1.69	0.58
1:A:284:LEU:HD13	1:A:287:TRP:N	2.19	0.58
1:A:342:THR:HB	1:A:345:LEU:HD13	1.84	0.58
1:D:204:CYS:HA	1:D:207:LEU:HB3	1.85	0.58
2:F:135:LEU:HD22	2:F:182:LEU:HB2	1.84	0.58
1:A:207:LEU:HD11	1:A:245:ILE:HG13	1.84	0.58
1:A:331:GLY:HA2	1:A:539:GLY:N	2.18	0.58
1:D:153:GLN:HE21	1:D:171:ARG:HG3	1.68	0.58
1:D:503:ASP:OD1	1:D:504:ALA:N	2.36	0.58
1:D:114:THR:OG1	2:E:141:ASP:OD2	2.18	0.58
2:C:14:MET:HB3	7:C:401:HOH:O	2.03	0.58
2:C:84:PHE:HD1	2:C:85:PHE:N	2.02	0.58
1:D:148:ILE:HB	1:D:170:TYR:CE2	2.39	0.58
1:D:231:PHE:CZ	1:D:291:ILE:HG12	2.39	0.58
1:D:445:VAL:HG21	1:D:462:PHE:CG	2.38	0.58
1:A:276:THR:OG1	1:A:277:ILE:N	2.35	0.58
1:A:32:LEU:HD22	1:A:61:PHE:CE2	2.39	0.58
2:B:153:VAL:O	2:B:156:SER:OG	2.19	0.58
2:B:35:GLU:HG2	7:B:404:HOH:O	2.04	0.58
1:D:10:MET:O	1:D:14:ILE:HG23	2.04	0.58
1:D:197:ASP:OD2	1:D:256:VAL:HB	2.04	0.58
1:D:510:ARG:HH11	1:D:510:ARG:HG3	1.69	0.58
2:E:62:LYS:HB3	2:F:90:TYR:CE1	2.39	0.58
1:A:143:LYS:NZ	1:A:212:PHE:CG	2.72	0.57
1:D:244:ASP:OD1	1:D:251:SER:HB3	2.03	0.57
2:E:169:LYS:O	7:E:411:HOH:O	2.17	0.57
2:B:122:GLU:O	2:B:125:LYS:HG3	2.04	0.57
1:D:506:TYR:CE1	1:D:510:ARG:HD3	2.39	0.57
1:D:562:LEU:HD23	1:D:563:CYS:N	2.19	0.57
1:D:153:GLN:H	1:D:564:GLU:HB2	1.69	0.57
1:A:152:LYS:HZ1	1:A:527:THR:HG22	1.69	0.57
1:D:138:ILE:HA	1:D:217:GLN:NE2	2.18	0.57
2:F:166:ALA:HA	2:F:169:LYS:HG2	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:81:LYS:O	2:B:83:PRO:HD3	2.03	0.57
1:D:31:THR:HA	1:D:34:GLU:HG2	1.86	0.57
2:B:21:VAL:HG11	2:B:158:ILE:CD1	2.33	0.57
1:D:172:ASN:H	1:D:175:PHE:HE2	1.52	0.57
1:D:520:LEU:HG	1:D:522:VAL:HG23	1.85	0.57
2:E:169:LYS:NZ	2:E:206:VAL:HG21	2.18	0.57
1:A:225:HIS:HB3	1:A:309:MET:SD	2.45	0.57
2:C:110:GLN:O	2:C:114:TRP:HD1	1.87	0.57
1:D:451:ARG:NE	1:D:452:LEU:HD13	2.18	0.57
1:D:518:LEU:N	7:D:702:HOH:O	2.31	0.57
2:E:180:PRO:HD2	2:E:181:LYS:HG2	1.85	0.57
2:E:68:LEU:HD11	2:E:152:TYR:CE1	2.40	0.57
7:E:404:HOH:O	2:F:68:LEU:HD11	2.04	0.57
2:B:112:LYS:HD2	2:B:116:LYS:CE	2.34	0.57
2:C:164:PHE:CD2	2:C:183:ILE:HG22	2.40	0.57
1:D:56:ASP:O	1:D:59:GLU:HG2	2.05	0.57
2:F:43:LEU:HD12	2:F:44:LEU:H	1.69	0.57
1:A:148:ILE:HB	1:A:170:TYR:CE2	2.40	0.57
1:A:95:PRO:O	1:A:161:PRO:HG2	2.04	0.57
1:A:353:ALA:HB2	1:A:413:TYR:HD2	1.68	0.57
1:A:361:PHE:CZ	1:A:379:LEU:HD13	2.40	0.57
1:A:528:PHE:O	1:A:532:GLN:HG3	2.05	0.57
4:A:602:ILE:O	4:A:602:ILE:HG23	2.04	0.57
1:A:86:SER:HB2	2:B:188:ARG:HH21	1.68	0.57
2:B:169:LYS:NZ	2:B:206:VAL:HG11	2.18	0.57
1:D:98:SER:HG	1:D:113:PHE:HE1	1.51	0.57
1:D:330:TYR:HB3	1:D:338:ALA:HB3	1.87	0.57
1:D:77:ILE:O	1:D:81:VAL:HG23	2.05	0.57
2:E:16:GLY:HA2	2:E:55:PRO:HB3	1.86	0.57
2:C:112:LYS:HB3	7:C:421:HOH:O	2.03	0.57
1:D:250:LEU:HD21	1:D:254:ILE:HB	1.86	0.57
2:E:121:GLN:O	2:E:125:LYS:HG2	2.04	0.57
2:F:187:LYS:HA	2:F:190:MET:HB2	1.87	0.57
2:F:70:VAL:O	2:F:74:VAL:HG23	2.05	0.57
2:F:110:GLN:O	2:F:114:TRP:HD1	1.88	0.56
2:F:154:ASP:HA	2:F:185:TRP:CZ2	2.40	0.56
1:A:228:VAL:HG12	1:A:232:ARG:NH1	2.20	0.56
1:A:41:SER:N	2:B:142:LYS:HE3	2.20	0.56
2:B:202:SER:O	2:B:205:ILE:HG13	2.06	0.56
2:C:121:GLN:HA	7:C:421:HOH:O	2.05	0.56
2:C:35:GLU:HB3	7:C:451:HOH:O	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:528:PHE:HE2	1:D:549:ARG:HH12	1.53	0.56
1:D:76:TYR:HB3	1:D:88:ILE:HB	1.87	0.56
1:A:361:PHE:CE1	1:A:379:LEU:HB2	2.41	0.56
1:A:99:LEU:HD13	1:A:555:ASN:OD1	2.04	0.56
1:D:65:VAL:HG11	1:D:400:ARG:NH1	2.20	0.56
2:E:130:GLU:O	2:E:134:ILE:HG12	2.05	0.56
1:A:222:VAL:O	1:A:223:PHE:HD1	1.89	0.56
1:A:478:PHE:CE1	1:A:521:ARG:HB2	2.40	0.56
2:C:64:VAL:HG13	2:C:73:TYR:HD2	1.70	0.56
2:C:75:ASP:HB2	2:C:84:PHE:CE2	2.40	0.56
1:D:172:ASN:CG	1:D:173:PRO:HD2	2.25	0.56
1:D:416:THR:N	7:D:722:HOH:O	2.37	0.56
2:F:125:LYS:NZ	2:F:129:ILE:HG21	2.21	0.56
2:F:135:LEU:CD2	2:F:182:LEU:HD12	2.34	0.56
2:E:68:LEU:HD11	2:E:152:TYR:OH	2.05	0.56
1:A:153:GLN:NE2	1:A:171:ARG:HG2	2.19	0.56
1:A:219:VAL:HG21	1:A:231:PHE:CZ	2.41	0.56
1:A:25:HIS:HA	1:A:28:GLN:HG2	1.86	0.56
1:A:112:PRO:HG2	1:A:397:GLY:HA3	1.86	0.56
1:D:92:HIS:CE1	2:E:185:TRP:HB2	2.41	0.56
2:E:150:PHE:HE2	2:E:192:LYS:HG3	1.70	0.56
2:E:85:PHE:HB2	2:E:92:ARG:HG2	1.87	0.56
1:A:522:VAL:HB	1:A:568:SER:OG	2.06	0.56
1:D:203:TYR:HA	1:D:206:LEU:HD12	1.88	0.56
1:D:364:LEU:HB3	1:D:389:GLU:HG2	1.87	0.56
1:D:32:LEU:HD22	1:D:61:PHE:CE2	2.41	0.56
1:D:96:ALA:HB3	1:D:113:PHE:CD2	2.41	0.56
1:A:150:SER:OG	1:A:170:TYR:HB2	2.06	0.56
2:B:40:LYS:HZ3	2:B:52:LYS:HD2	1.70	0.56
1:D:111:ILE:HD11	1:D:334:GLU:OE2	2.06	0.56
1:D:213:ARG:HA	1:D:216:VAL:HG13	1.86	0.56
2:F:84:PHE:HE1	2:F:85:PHE:CE2	2.23	0.56
1:A:13:VAL:HA	1:A:16:GLU:OE2	2.04	0.56
1:A:143:LYS:NZ	1:A:212:PHE:CA	2.69	0.56
1:A:228:VAL:HA	1:A:319:TYR:CE2	2.41	0.56
2:E:26:LYS:HE2	2:E:78:TRP:HB3	1.88	0.56
1:A:286:ASN:O	1:A:287:TRP:HB3	2.06	0.56
2:B:203:GLU:O	2:B:206:VAL:HG22	2.06	0.56
2:C:40:LYS:HA	7:C:451:HOH:O	2.05	0.56
2:C:85:PHE:CD2	2:C:92:ARG:HG2	2.41	0.56
1:D:151:SER:HB2	1:D:194:PHE:HA	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:365:PRO:HB2	1:D:374:GLU:HG2	1.88	0.56
1:D:90:THR:HG23	1:D:397:GLY:HA2	1.88	0.56
1:A:199:HIS:HB2	1:A:525:LYS:HE3	1.88	0.56
1:A:87:PRO:HD2	2:B:188:ARG:CB	2.35	0.56
1:D:150:SER:OG	1:D:170:TYR:HB2	2.06	0.56
1:D:46:GLN:HB2	2:E:148:ASP:CB	2.36	0.56
1:A:111:ILE:HG21	1:A:398:LEU:HD21	1.87	0.55
1:A:152:LYS:HE3	1:A:565:ASN:HB2	1.88	0.55
1:D:238:TRP:O	1:D:242:VAL:HG23	2.06	0.55
1:D:361:PHE:HD1	1:D:392:ILE:HG12	1.71	0.55
2:C:176:GLU:HG2	1:D:573:THR:HG21	1.88	0.55
1:D:9:ASP:OD1	7:D:717:HOH:O	2.18	0.55
1:A:203:TYR:CE1	1:A:241:ILE:HG13	2.42	0.55
1:A:222:VAL:HA	1:A:328:HIS:NE2	2.22	0.55
1:A:445:VAL:HG21	1:A:462:PHE:CG	2.41	0.55
1:A:423:CYS:HG	1:A:541:SER:HG	1.54	0.55
1:A:555:ASN:O	1:A:559:LEU:HD22	2.05	0.55
2:C:110:GLN:O	2:C:114:TRP:CD1	2.59	0.55
1:D:446:GLU:O	1:D:450:LYS:NZ	2.35	0.55
1:D:574:ALA:O	1:D:575:PHE:HB2	2.06	0.55
2:C:188:ARG:HB2	1:D:499:ARG:HH22	1.68	0.55
2:B:62:LYS:HD3	2:C:90:TYR:CD2	2.41	0.55
1:D:26:GLN:HG3	1:D:27:VAL:N	2.22	0.55
1:D:228:VAL:HA	1:D:319:TYR:HE2	1.72	0.55
1:D:563:CYS:O	1:D:566:VAL:HG12	2.05	0.55
1:A:114:THR:HB	1:A:116:GLU:CD	2.27	0.55
1:A:29:LYS:HG3	1:A:30:GLN:N	2.21	0.55
1:A:361:PHE:HZ	1:A:379:LEU:HD13	1.70	0.55
1:A:22:ARG:HA	1:A:415:ASN:CB	2.35	0.55
2:B:116:LYS:O	2:B:213:ARG:NH2	2.40	0.55
2:C:139:LEU:HG	2:C:145:PHE:CE1	2.42	0.55
1:D:105:GLN:HB2	1:D:107:ARG:NH1	2.21	0.55
1:D:15:ASP:HA	1:D:18:ASP:OD2	2.06	0.55
1:D:368:GLU:HG3	1:D:369:THR:HG23	1.89	0.55
2:E:89:PRO:HB3	2:F:76:GLU:HG2	1.87	0.55
1:A:223:PHE:HZ	1:A:536:LEU:HB2	1.69	0.55
2:B:150:PHE:CZ	2:B:158:ILE:HG21	2.40	0.55
2:C:8:LEU:HG	2:C:56:VAL:HB	1.88	0.55
2:C:28:VAL:HG21	2:C:78:TRP:CZ3	2.41	0.55
1:D:128:ALA:HA	1:D:131:PHE:CE2	2.41	0.55
1:D:338:ALA:HA	1:D:354:VAL:HA	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:40:LYS:HZ2	2:E:52:LYS:HD2	1.70	0.55
2:F:195:VAL:O	2:F:199:LEU:HG	2.06	0.55
2:F:81:LYS:HG3	2:F:82:ASN:H	1.71	0.55
1:A:41:SER:H	2:B:142:LYS:HE3	1.71	0.55
1:D:519:GLU:OE2	1:D:521:ARG:NH2	2.37	0.55
1:D:551:VAL:HG12	1:D:555:ASN:HD22	1.71	0.55
2:B:19:ALA:HB2	2:B:70:VAL:HG11	1.89	0.55
1:D:451:ARG:HH12	1:D:490:LEU:C	2.09	0.55
2:F:32:TYR:HD2	2:F:34:GLU:OE2	1.90	0.55
1:A:152:LYS:CG	1:A:565:ASN:HB2	2.35	0.55
1:A:478:PHE:HE1	1:A:521:ARG:HB2	1.72	0.55
1:D:234:PHE:HD2	1:D:287:TRP:HH2	1.54	0.55
1:D:269:PRO:O	1:D:270:ASN:ND2	2.40	0.55
1:D:199:HIS:HB2	1:D:525:LYS:HE3	1.89	0.55
1:D:223:PHE:CE2	1:D:533:GLU:HA	2.42	0.55
2:F:151:GLY:N	2:F:154:ASP:OD2	2.40	0.55
2:F:37:PHE:CZ	2:F:54:ILE:HG12	2.39	0.55
2:F:96:ARG:NH2	7:F:424:HOH:O	2.38	0.55
2:C:5:PRO:HG2	2:C:30:PHE:HB3	1.89	0.54
1:D:22:ARG:HG2	1:D:414:ASN:HB3	1.88	0.54
1:D:132:ARG:HA	1:D:343:PRO:HG2	1.88	0.54
2:F:132:VAL:HG22	2:F:179:SER:HB3	1.89	0.54
1:A:250:LEU:HD21	1:A:254:ILE:HB	1.89	0.54
1:A:281:CYS:O	1:A:284:LEU:HG	2.06	0.54
1:D:223:PHE:CE1	1:D:536:LEU:HB2	2.41	0.54
1:D:336:TRP:HB2	1:D:358:LEU:HD13	1.90	0.54
1:D:76:TYR:HB3	1:D:88:ILE:CG2	2.38	0.54
2:E:11:TRP:HH2	2:E:208:TYR:CD1	2.25	0.54
1:A:152:LYS:HZ3	1:A:527:THR:HG22	1.72	0.54
1:A:224:ALA:O	1:A:228:VAL:HG23	2.07	0.54
1:A:445:VAL:HG21	1:A:462:PHE:CD1	2.43	0.54
2:B:108:ASP:O	2:B:111:PHE:HB3	2.06	0.54
1:D:164:THR:OG1	1:D:557:LYS:O	2.15	0.54
1:D:8:PHE:HE1	1:D:130:ALA:HB2	1.72	0.54
1:A:120:ASN:O	1:A:124:LEU:HG	2.08	0.54
1:D:154:TYR:OH	1:D:162:VAL:HG22	2.07	0.54
1:D:34:GLU:O	1:D:38:LYS:HG2	2.05	0.54
1:D:405:ASP:OD2	1:D:540:SER:HB2	2.08	0.54
1:A:211:LEU:HD12	1:A:212:PHE:HD2	1.72	0.54
2:B:139:LEU:O	2:B:141:ASP:N	2.41	0.54
2:C:188:ARG:HE	1:D:499:ARG:NH2	2.04	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:212:TYR:CZ	2:C:213:ARG:HG3	2.43	0.54
1:D:8:PHE:CE1	1:D:130:ALA:HB2	2.41	0.54
1:D:179:MET:SD	7:D:811:HOH:O	2.58	0.54
1:D:171:ARG:HH21	1:D:194:PHE:HB3	1.73	0.54
1:D:506:TYR:CZ	1:D:510:ARG:HD3	2.41	0.54
2:E:122:GLU:HG3	2:E:123:ALA:N	2.23	0.54
1:A:317:ARG:O	1:A:321:GLY:N	2.37	0.54
2:B:176:GLU:HB2	2:B:183:ILE:HG21	1.89	0.54
1:D:365:PRO:HG2	1:D:374:GLU:HG2	1.89	0.54
1:D:365:PRO:HG3	1:D:388:TYR:CE2	2.42	0.54
1:D:475:TYR:CE1	1:D:515:ILE:HD12	2.43	0.54
1:D:332:SER:CB	1:D:538:LEU:HA	2.35	0.54
2:F:66:GLU:O	2:F:70:VAL:HG23	2.08	0.54
1:A:200:GLN:HE21	1:A:254:ILE:HG23	1.72	0.54
1:A:444:SER:HA	1:A:500:ALA:HB1	1.90	0.54
1:D:224:ALA:O	1:D:228:VAL:HG23	2.08	0.54
1:D:445:VAL:HG21	1:D:462:PHE:CB	2.37	0.54
1:D:465:TYR:HB2	1:D:551:VAL:HG22	1.90	0.54
1:D:152:LYS:HB3	1:D:560:GLN:O	2.07	0.54
2:E:169:LYS:HZ1	2:E:206:VAL:HG21	1.73	0.54
2:E:75:ASP:OD2	2:E:85:PHE:CD2	2.61	0.54
2:F:140:GLY:HA2	2:F:181:LYS:HZ1	1.72	0.54
1:A:160:VAL:N	7:A:725:HOH:O	2.20	0.54
1:D:151:SER:OG	1:D:151:SER:O	2.25	0.54
1:D:41:SER:H	2:E:142:LYS:HE2	1.72	0.54
2:F:125:LYS:HA	2:F:128:PHE:CE2	2.42	0.54
2:B:110:GLN:HB2	2:B:167:TYR:CZ	2.43	0.54
2:C:98:TRP:CE3	2:C:101:PHE:HB2	2.42	0.54
1:D:504:ALA:C	1:D:507:VAL:HG13	2.27	0.54
2:F:16:GLY:HA2	2:F:55:PRO:HG3	1.89	0.54
1:A:265:LYS:NZ	1:A:266:LEU:HG	2.22	0.54
1:A:541:SER:O	1:A:544:GLN:NE2	2.41	0.54
2:C:206:VAL:O	2:C:209:ALA:HB3	2.08	0.54
1:D:186:SER:HA	7:D:720:HOH:O	2.08	0.54
1:D:143:LYS:HE3	1:D:187:CYS:CA	2.38	0.54
1:D:477:ILE:HD13	1:D:497:LEU:HD22	1.89	0.54
2:E:185:TRP:O	2:E:188:ARG:HG2	2.08	0.54
2:B:133:LYS:O	2:B:137:SER:N	2.39	0.53
1:D:198:VAL:HG23	1:D:524:ALA:CB	2.33	0.53
1:D:213:ARG:HG3	1:D:214:ASP:N	2.23	0.53
1:D:493:CYS:SG	1:D:520:LEU:HD22	2.48	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:125:LYS:O	2:F:129:ILE:HG23	2.07	0.53
1:A:403:LEU:HD21	1:A:538:LEU:HD21	1.89	0.53
2:B:150:PHE:CZ	2:B:158:ILE:HD13	2.43	0.53
2:C:11:TRP:CG	2:C:12:PRO:HD3	2.43	0.53
2:C:21:VAL:HG12	2:C:155:ILE:HG12	1.89	0.53
1:D:200:GLN:OE1	1:D:255:THR:N	2.40	0.53
1:D:221:ALA:HB2	1:D:227:LEU:HG	1.91	0.53
1:A:104:SER:O	1:A:107:ARG:HB2	2.09	0.53
1:A:10:MET:O	1:A:14:ILE:HG22	2.07	0.53
1:A:508:SER:HB2	7:A:831:HOH:O	2.07	0.53
1:A:223:PHE:CZ	1:A:536:LEU:HB2	2.43	0.53
2:B:15:PHE:HB3	2:B:67:SER:HB3	1.90	0.53
2:C:176:GLU:CD	1:D:491:GLN:HG2	2.28	0.53
1:D:536:LEU:HG	1:D:545:PHE:CE1	2.43	0.53
1:A:425:ARG:HE	1:A:546:LYS:HD2	1.73	0.53
2:C:66:GLU:HB2	2:C:69:ASN:HB2	1.89	0.53
1:D:198:VAL:HB	1:D:202:LEU:HD21	1.89	0.53
2:E:15:PHE:HB3	2:E:67:SER:HB3	1.90	0.53
1:A:31:THR:OG1	1:A:357:ASN:HA	2.08	0.53
2:C:133:LYS:O	2:C:136:GLU:HB3	2.08	0.53
2:C:81:LYS:HG3	2:C:82:ASN:H	1.74	0.53
2:E:110:GLN:OE1	2:E:167:TYR:OH	2.26	0.53
1:A:142:GLY:O	1:A:185:PRO:HD2	2.09	0.53
1:A:219:VAL:HG21	1:A:231:PHE:HZ	1.72	0.53
1:D:235:GLU:HG2	1:D:287:TRP:CD2	2.43	0.53
1:D:496:CYS:CA	1:D:499:ARG:NH1	2.72	0.53
1:A:441:LEU:HA	1:A:501:PHE:HE1	1.72	0.53
1:A:448:ALA:CB	1:A:496:CYS:HB3	2.39	0.53
1:A:86:SER:HA	2:B:188:ARG:HB2	1.89	0.53
2:C:84:PHE:HB2	2:C:151:GLY:C	2.28	0.53
2:C:70:VAL:O	2:C:73:TYR:HB2	2.09	0.53
1:D:14:ILE:HG21	1:D:134:ARG:NH1	2.24	0.53
1:D:233:THR:O	1:D:237:VAL:HG22	2.08	0.53
1:D:329:ASP:N	1:D:329:ASP:OD1	2.42	0.53
1:D:451:ARG:CZ	1:D:490:LEU:HA	2.39	0.53
1:D:509:SER:O	1:D:513:LYS:N	2.42	0.53
2:E:142:LYS:HD2	2:E:144:TYR:O	2.08	0.53
2:E:88:ASP:OD1	2:E:91:GLY:N	2.36	0.53
2:F:10:TYR:CG	2:F:37:PHE:HE1	2.27	0.53
2:F:183:ILE:O	2:F:183:ILE:HG13	2.09	0.53
1:A:413:TYR:CD2	1:A:418:GLN:HG2	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:435:LYS:HE2	1:A:437:THR:HA	1.91	0.53
1:A:440:ASP:HA	1:A:443:LEU:HB2	1.90	0.53
1:A:79:ARG:HG2	1:A:86:SER:OG	2.09	0.53
1:D:365:PRO:HA	1:D:388:TYR:CD1	2.42	0.53
1:D:37:LEU:O	7:E:403:HOH:O	2.19	0.53
1:D:526:GLY:HA2	1:D:529:ARG:CZ	2.39	0.53
1:D:538:LEU:HD23	1:D:544:GLN:HG2	1.90	0.53
1:A:47:ASN:O	7:A:721:HOH:O	2.18	0.53
1:A:199:HIS:N	1:A:524:ALA:HB1	2.21	0.53
1:A:466:ILE:CG1	1:A:552:LYS:HA	2.38	0.53
1:D:110:PHE:HE1	1:D:556:ALA:HB2	1.74	0.53
1:D:92:HIS:ND1	2:E:188:ARG:NH2	2.56	0.53
2:E:73:TYR:HE1	2:F:90:TYR:HA	1.73	0.53
1:A:231:PHE:O	1:A:235:GLU:HG3	2.08	0.53
1:A:386:GLU:N	7:A:733:HOH:O	2.42	0.53
2:B:96:ARG:NH1	2:C:76:GLU:OE2	2.41	0.53
1:D:152:LYS:HD3	1:D:561:ILE:HA	1.91	0.53
1:D:154:TYR:HE2	1:D:162:VAL:O	1.92	0.53
1:D:211:LEU:HD13	1:D:212:PHE:HD1	1.74	0.53
1:D:365:PRO:HG3	1:D:388:TYR:CZ	2.44	0.53
2:E:130:GLU:HA	2:E:133:LYS:HE3	1.90	0.53
2:E:155:ILE:HA	2:E:158:ILE:HG12	1.91	0.53
2:F:128:PHE:HE1	2:F:175:ILE:HG22	1.71	0.53
2:F:165:GLN:HG3	2:F:202:SER:OG	2.09	0.53
2:F:40:LYS:HB2	2:F:45:LEU:HD11	1.90	0.53
1:A:143:LYS:CA	1:A:184:SER:HB2	2.40	0.52
1:A:164:THR:HG23	1:A:560:GLN:HB2	1.91	0.52
2:B:67:SER:O	2:B:70:VAL:HG12	2.09	0.52
1:D:162:VAL:HG23	1:D:556:ALA:HB1	1.90	0.52
1:D:312:TYR:CD1	1:D:315:LYS:HD2	2.44	0.52
1:D:29:LYS:NZ	1:D:58:GLU:CD	2.61	0.52
1:D:91:GLY:HA3	2:E:141:ASP:O	2.08	0.52
2:E:20:ARG:HB2	7:E:402:HOH:O	2.08	0.52
1:A:41:SER:HB2	2:B:142:LYS:CG	2.35	0.52
1:A:451:ARG:O	1:A:454:GLU:HG2	2.09	0.52
1:D:12:ARG:HH12	1:D:126:ARG:HH21	1.57	0.52
1:A:224:ALA:HA	1:A:316:LEU:HD22	1.91	0.52
1:A:437:THR:O	1:A:440:ASP:N	2.42	0.52
1:A:521:ARG:HG2	1:A:569:SER:OG	2.09	0.52
2:B:18:ARG:NE	2:B:156:SER:O	2.42	0.52
2:C:8:LEU:HD13	2:C:44:LEU:HB2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:217:GLN:OE1	1:D:217:GLN:HA	2.08	0.52
1:D:234:PHE:HD2	1:D:287:TRP:CH2	2.28	0.52
1:D:493:CYS:O	1:D:497:LEU:HD12	2.10	0.52
1:D:199:HIS:HB3	1:D:525:LYS:H	1.74	0.52
1:D:531:ILE:HA	1:D:534:HIS:ND1	2.25	0.52
2:E:122:GLU:HG3	2:E:123:ALA:H	1.74	0.52
2:E:97:PHE:HE1	2:F:65:CYS:O	1.93	0.52
1:A:294:LEU:HD12	1:A:295:PHE:N	2.24	0.52
1:A:303:GLY:O	1:A:327:SER:HA	2.09	0.52
1:D:435:LYS:HA	1:D:436:ASN:HB2	1.92	0.52
1:D:87:PRO:CD	1:D:93:PRO:HG3	2.40	0.52
2:E:86:PRO:HD3	2:E:146:GLY:O	2.09	0.52
1:A:238:TRP:HZ2	1:A:282:MET:CE	2.23	0.52
1:A:86:SER:HB2	2:B:188:ARG:NH2	2.25	0.52
1:D:442:GLN:HG2	1:D:462:PHE:HZ	1.72	0.52
2:E:99:ALA:HA	2:E:102:VAL:HG12	1.92	0.52
2:E:150:PHE:HE2	2:E:192:LYS:CG	2.21	0.52
6:E:301:GSH:OE1	7:E:413:HOH:O	2.19	0.52
1:A:192:VAL:HG22	1:A:259:VAL:HG23	1.91	0.52
1:A:26:GLN:O	1:A:29:LYS:HG3	2.10	0.52
1:A:223:PHE:CZ	1:A:533:GLU:HA	2.45	0.52
1:A:96:ALA:C	1:A:97:ILE:HG13	2.28	0.52
1:D:126:ARG:NH1	1:D:126:ARG:HG3	2.24	0.52
1:D:149:PHE:HB2	1:D:530:LYS:HE3	1.92	0.52
1:D:219:VAL:HB	1:D:295:PHE:CZ	2.45	0.52
1:D:307:GLY:O	1:D:310:GLU:HG3	2.10	0.52
1:D:32:LEU:HD22	1:D:61:PHE:HE2	1.74	0.52
2:C:187:LYS:HD3	1:D:492:ASP:HB3	1.91	0.52
2:F:110:GLN:O	2:F:114:TRP:CD1	2.63	0.52
2:F:9:ASP:N	2:F:9:ASP:OD1	2.42	0.52
1:A:138:ILE:O	7:A:723:HOH:O	2.19	0.52
1:A:71:VAL:HG23	1:A:107:ARG:HH22	1.74	0.52
2:C:139:LEU:O	2:C:141:ASP:N	2.43	0.52
2:C:191:GLU:HA	1:D:450:LYS:CE	2.40	0.52
2:C:88:ASP:HB2	7:C:457:HOH:O	2.09	0.52
1:D:213:ARG:HH21	1:D:296:PRO:HD3	1.74	0.52
1:D:30:GLN:HA	1:D:30:GLN:OE1	2.09	0.52
1:D:163:GLY:HA3	1:D:560:GLN:HB2	1.91	0.52
1:D:7:THR:OG1	7:D:718:HOH:O	2.19	0.52
2:E:185:TRP:HA	2:E:188:ARG:CZ	2.39	0.52
2:E:64:VAL:HG13	2:F:93:ALA:HB1	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:602:ILE:O	7:A:722:HOH:O	2.19	0.52
2:B:107:THR:HA	2:B:110:GLN:HE21	1.73	0.52
2:B:98:TRP:CE2	2:B:138:GLU:HG2	2.45	0.52
2:C:10:TYR:CG	2:C:12:PRO:HD2	2.44	0.52
2:C:111:PHE:HA	2:C:114:TRP:NE1	2.25	0.52
2:C:140:GLY:O	2:C:181:LYS:NZ	2.40	0.52
1:D:45:LEU:HB3	1:D:50:LEU:HB2	1.90	0.52
1:D:445:VAL:HG22	1:D:479:TRP:HE1	1.75	0.52
1:D:51:ASN:OD1	1:D:51:ASN:N	2.41	0.52
2:E:125:LYS:HB2	2:E:173:PHE:CE2	2.44	0.52
2:E:8:LEU:HD22	2:E:35:GLU:OE2	2.09	0.52
2:E:51:HIS:HB3	2:E:53:LYS:HE3	1.91	0.52
2:E:67:SER:HA	2:E:70:VAL:HG12	1.92	0.52
1:A:143:LYS:HA	1:A:184:SER:HB2	1.91	0.52
1:A:445:VAL:HG11	1:A:462:PHE:CD2	2.45	0.52
2:B:106:PHE:O	2:B:110:GLN:HG2	2.10	0.52
1:D:57:PRO:HD2	1:D:58:GLU:OE2	2.10	0.52
1:D:8:PHE:CD1	1:D:126:ARG:NH1	2.77	0.52
2:E:164:PHE:O	2:E:168:GLU:HG2	2.10	0.52
2:E:201:ASP:OD2	2:E:204:LYS:HE2	2.10	0.52
2:F:8:LEU:HD22	2:F:33:ARG:HD3	1.92	0.52
1:A:315:LYS:O	1:A:319:TYR:N	2.40	0.52
1:D:174:ASN:OD1	7:D:719:HOH:O	2.19	0.52
1:D:476:ALA:HB1	1:D:521:ARG:HD2	1.92	0.52
1:D:526:GLY:O	1:D:530:LYS:HG3	2.09	0.52
1:D:559:LEU:O	1:D:562:LEU:HB3	2.09	0.52
1:D:523:VAL:HG12	1:D:566:VAL:HA	1.92	0.52
2:F:158:ILE:HG23	2:F:159:THR:HG23	1.92	0.52
1:A:77:ILE:HG22	1:A:110:PHE:CD2	2.42	0.51
2:B:26:LYS:HZ3	2:B:28:VAL:HB	1.74	0.51
2:B:54:ILE:HB	2:B:55:PRO:HA	1.92	0.51
2:C:64:VAL:HG13	2:C:73:TYR:CD2	2.45	0.51
1:D:105:GLN:HB2	1:D:107:ARG:HH12	1.75	0.51
1:D:478:PHE:O	1:D:479:TRP:HD1	1.93	0.51
1:D:142:GLY:HA2	1:D:215:GLN:HB2	1.90	0.51
1:D:506:TYR:O	1:D:510:ARG:HG3	2.09	0.51
1:D:506:TYR:CD2	1:D:510:ARG:NH1	2.78	0.51
1:A:229:HIS:CG	1:A:230:ALA:N	2.77	0.51
1:A:406:VAL:O	1:A:541:SER:OG	2.27	0.51
1:D:13:VAL:HB	1:D:126:ARG:CZ	2.41	0.51
1:D:448:ALA:HB1	1:D:493:CYS:HB2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:131:ALA:HA	2:F:134:ILE:HG12	1.92	0.51
2:F:163:TRP:HB3	2:F:167:TYR:CE1	2.46	0.51
2:F:24:ARG:HB3	2:F:194:SER:HA	1.92	0.51
1:A:168:ASN:O	1:A:172:ASN:HB2	2.10	0.51
1:A:38:LYS:HD2	2:B:138:GLU:O	2.11	0.51
2:C:196:SER:OG	7:C:408:HOH:O	2.18	0.51
1:D:147:PHE:HA	1:D:205:HIS:HD2	1.70	0.51
1:D:363:PHE:HD1	1:D:390:VAL:HA	1.74	0.51
2:F:33:ARG:HH12	2:F:35:GLU:CG	2.23	0.51
1:A:251:SER:O	1:A:260:ARG:NH2	2.34	0.51
1:D:133:ASN:HB3	7:D:845:HOH:O	2.10	0.51
1:D:166:THR:O	1:D:169:VAL:HG12	2.11	0.51
1:D:535:PHE:O	1:D:538:LEU:HB3	2.10	0.51
2:E:69:ASN:OD1	2:F:96:ARG:NE	2.38	0.51
2:F:17:MET:HE2	2:F:200:PRO:HD2	1.93	0.51
1:A:219:VAL:HB	1:A:295:PHE:HZ	1.71	0.51
1:A:316:LEU:HD12	1:A:319:TYR:HB2	1.92	0.51
2:C:75:ASP:HB2	2:C:84:PHE:CZ	2.45	0.51
1:D:187:CYS:O	1:D:208:SER:HB3	2.10	0.51
1:D:228:VAL:O	1:D:232:ARG:HG2	2.10	0.51
1:D:92:HIS:H	2:E:142:LYS:N	2.09	0.51
2:E:94:GLN:HB3	2:E:98:TRP:CZ2	2.46	0.51
1:A:156:SER:OG	1:A:157:THR:N	2.43	0.51
1:A:212:PHE:HD1	1:A:215:GLN:HE21	1.58	0.51
2:B:35:GLU:HG3	2:B:44:LEU:HD21	1.92	0.51
1:A:116:GLU:CD	1:A:395:TYR:HB3	2.31	0.51
1:A:334:GLU:HG3	1:A:538:LEU:HD13	1.92	0.51
1:A:532:GLN:HG2	1:A:547:MET:HE3	1.93	0.51
1:A:466:ILE:HG13	1:A:552:LYS:HA	1.92	0.51
1:A:556:ALA:HA	1:A:559:LEU:HB2	1.93	0.51
2:C:90:TYR:O	2:C:94:GLN:HG3	2.10	0.51
1:D:77:ILE:HG21	1:D:110:PHE:HB3	1.93	0.51
1:D:255:THR:HA	1:D:260:ARG:HD2	1.92	0.51
2:E:183:ILE:HG13	2:E:187:LYS:HZ1	1.74	0.51
2:E:210:ALA:O	2:E:213:ARG:HB3	2.11	0.51
2:F:43:LEU:HD12	2:F:44:LEU:N	2.25	0.51
1:D:33:LYS:O	1:D:37:LEU:HB2	2.11	0.51
1:D:363:PHE:CD2	1:D:382:VAL:HG21	2.31	0.51
1:A:287:TRP:NE1	1:A:319:TYR:CD1	2.79	0.51
1:A:32:LEU:HB3	1:A:61:PHE:HE2	1.76	0.51
1:A:448:ALA:HB2	1:A:496:CYS:HB3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:97:PHE:CE2	2:B:101:PHE:HE2	2.29	0.51
2:B:72:GLN:O	2:B:76:GLU:HG3	2.11	0.51
1:D:164:THR:OG1	1:D:561:ILE:HG12	2.11	0.51
2:F:7:LEU:HD22	2:F:30:PHE:CD1	2.46	0.51
1:A:77:ILE:CG2	1:A:110:PHE:HB3	2.41	0.50
1:A:172:ASN:OD1	1:A:173:PRO:HD2	2.09	0.50
1:A:149:PHE:HD2	1:A:530:LYS:HE2	1.77	0.50
2:C:170:PHE:HD1	2:C:213:ARG:HH21	1.59	0.50
2:C:8:LEU:HD22	2:C:33:ARG:NH2	2.26	0.50
2:C:57:LEU:HB3	2:C:64:VAL:HG12	1.93	0.50
1:D:124:LEU:HD13	1:D:336:TRP:CE3	2.45	0.50
2:E:109:ALA:HB3	7:E:416:HOH:O	2.11	0.50
2:E:163:TRP:HA	2:E:205:ILE:CD1	2.42	0.50
2:E:185:TRP:HA	2:E:188:ARG:NE	2.26	0.50
2:E:54:ILE:HB	2:E:55:PRO:HA	1.93	0.50
1:A:203:TYR:HD1	1:A:237:VAL:HG21	1.74	0.50
2:B:24:ARG:HG2	2:B:197:LYS:HZ1	1.76	0.50
1:D:70:ASP:OD1	1:D:71:VAL:N	2.44	0.50
1:A:206:LEU:O	1:A:210:ILE:HG13	2.11	0.50
1:A:42:ALA:O	1:A:45:LEU:HB2	2.11	0.50
1:A:97:ILE:HG21	1:A:110:PHE:CE2	2.46	0.50
2:C:185:TRP:NE1	2:C:189:CYS:SG	2.85	0.50
2:C:92:ARG:O	2:C:96:ARG:HG3	2.11	0.50
1:A:76:TYR:O	1:A:79:ARG:HB3	2.11	0.50
1:D:328:HIS:CG	1:D:329:ASP:H	2.28	0.50
1:D:90:THR:OG1	1:D:112:PRO:HG2	2.10	0.50
2:E:75:ASP:OD2	2:E:85:PHE:HD2	1.94	0.50
2:F:110:GLN:HA	2:F:113:VAL:HG12	1.93	0.50
1:A:146:GLN:HB2	1:A:148:ILE:HG23	1.93	0.50
1:A:341:VAL:O	1:A:343:PRO:HD3	2.11	0.50
1:A:398:LEU:HD22	1:A:401:TYR:CZ	2.45	0.50
2:B:117:LYS:HG3	2:B:213:ARG:NH1	2.27	0.50
2:C:111:PHE:O	2:C:115:GLY:HA3	2.11	0.50
2:C:99:ALA:CB	2:C:152:TYR:HE1	2.24	0.50
1:D:174:ASN:N	7:D:719:HOH:O	2.37	0.50
1:D:41:SER:HB2	2:E:147:GLY:O	2.12	0.50
1:D:569:SER:C	1:D:570:TYR:HD1	2.14	0.50
1:D:69:THR:HB	1:D:71:VAL:HG12	1.93	0.50
2:F:133:LYS:HA	2:F:136:GLU:HG2	1.94	0.50
2:F:135:LEU:O	2:F:138:GLU:HG3	2.11	0.50
1:A:252:ASN:HA	1:A:260:ARG:NH2	2.25	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:340:ASN:HB2	1:A:352:PHE:CE1	2.46	0.50
2:C:73:TYR:HD1	2:C:76:GLU:OE2	1.94	0.50
1:D:118:MET:SD	1:D:175:PHE:HE1	2.34	0.50
1:D:12:ARG:HH12	1:D:126:ARG:NH2	2.09	0.50
1:D:148:ILE:HB	1:D:170:TYR:HE2	1.77	0.50
1:D:227:LEU:HB3	1:D:316:LEU:HD11	1.93	0.50
1:D:434:ASP:O	1:D:550:CYS:HB3	2.11	0.50
1:D:55:THR:C	1:D:57:PRO:HD3	2.32	0.50
1:D:59:GLU:HA	1:D:62:LYS:NZ	2.26	0.50
2:F:17:MET:SD	2:F:163:TRP:HZ3	2.35	0.50
2:F:169:LYS:HG3	2:F:170:PHE:N	2.26	0.50
1:A:393:THR:HG22	1:A:400:ARG:H	1.76	0.50
1:A:563:CYS:O	1:A:566:VAL:HG12	2.12	0.50
1:D:94:VAL:HG21	1:D:112:PRO:HA	1.94	0.50
1:D:541:SER:O	1:D:543:GLY:N	2.44	0.50
1:D:154:TYR:OH	1:D:559:LEU:HD13	2.11	0.50
1:D:99:LEU:HD12	1:D:100:SER:N	2.27	0.50
2:E:96:ARG:NE	2:F:69:ASN:OD1	2.44	0.50
1:A:114:THR:HB	1:A:116:GLU:OE2	2.10	0.50
1:A:562:LEU:HD12	1:A:563:CYS:N	2.27	0.50
1:D:191:GLU:O	1:D:195:SER:N	2.45	0.50
1:D:82:ASP:OD2	1:D:553:PRO:HB3	2.12	0.50
2:F:139:LEU:HB2	2:F:145:PHE:CZ	2.47	0.50
1:A:17:PHE:CE2	1:A:127:THR:HG23	2.47	0.50
1:A:352:PHE:N	1:A:352:PHE:CD2	2.80	0.50
2:C:169:LYS:HG3	2:C:170:PHE:N	2.27	0.50
2:C:183:ILE:HD13	1:D:492:ASP:OD1	2.12	0.50
1:A:304:ILE:HG13	1:A:328:HIS:CD2	2.47	0.49
1:A:77:ILE:O	1:A:80:MET:HG2	2.11	0.49
2:B:150:PHE:CE2	2:B:158:ILE:HD13	2.47	0.49
2:B:18:ARG:HH12	2:B:103:ASP:CG	2.08	0.49
1:D:148:ILE:HG23	1:D:220:PHE:HE2	1.77	0.49
1:D:313:VAL:N	1:D:314:PRO:HD2	2.27	0.49
1:D:441:LEU:HD23	1:D:549:ARG:HB3	1.94	0.49
2:E:106:PHE:CE2	2:E:135:LEU:HD11	2.47	0.49
2:E:202:SER:O	2:E:206:VAL:HG13	2.11	0.49
2:B:139:LEU:HD11	2:B:145:PHE:CE1	2.47	0.49
1:D:135:ASP:OD1	1:D:136:PHE:N	2.44	0.49
1:D:138:ILE:CB	1:D:217:GLN:HG3	2.40	0.49
1:D:13:VAL:HB	1:D:126:ARG:NH2	2.27	0.49
2:E:143:PRO:O	2:E:188:ARG:HD2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:17:MET:CE	2:F:200:PRO:HD2	2.42	0.49
1:A:534:HIS:HB3	4:A:602:ILE:O	2.12	0.49
1:A:121:THR:HG23	3:A:601:JAA:C14	2.42	0.49
2:B:166:ALA:HB2	2:B:206:VAL:HG12	1.93	0.49
1:A:85:THR:HB	2:B:184:ALA:HB1	1.94	0.49
1:A:176:LYS:HE3	1:A:190:ASP:OD2	2.12	0.49
1:A:244:ASP:OD1	1:A:251:SER:HB3	2.11	0.49
1:A:285:SER:O	1:A:286:ASN:CB	2.59	0.49
1:D:56:ASP:HA	1:D:59:GLU:OE2	2.13	0.49
1:A:294:LEU:HD12	1:A:295:PHE:H	1.76	0.49
1:A:27:VAL:HB	1:A:356:PRO:HB2	1.93	0.49
1:D:143:LYS:HG2	1:D:144:ALA:H	1.77	0.49
1:D:445:VAL:HG21	1:D:462:PHE:HB2	1.95	0.49
2:F:125:LYS:HD2	2:F:128:PHE:CE2	2.47	0.49
2:F:23:LEU:HD11	2:F:30:PHE:CE2	2.47	0.49
1:A:309:MET:SD	1:A:312:TYR:HB2	2.53	0.49
1:A:199:HIS:HB3	1:A:525:LYS:H	1.76	0.49
2:B:145:PHE:HB2	2:B:153:VAL:HG13	1.93	0.49
2:B:15:PHE:CD2	6:B:301:GSH:HB12	2.46	0.49
1:D:241:ILE:O	1:D:245:ILE:HG12	2.13	0.49
1:D:312:TYR:HD1	1:D:315:LYS:HD2	1.78	0.49
1:D:363:PHE:CE1	1:D:390:VAL:HG23	2.46	0.49
1:D:507:VAL:O	1:D:511:LYS:HG3	2.12	0.49
2:F:20:ARG:O	2:F:24:ARG:HB2	2.13	0.49
2:F:33:ARG:NH2	7:F:428:HOH:O	2.43	0.49
1:A:146:GLN:HA	1:A:220:PHE:HB3	1.94	0.49
1:A:379:LEU:HG	1:A:380:THR:N	2.26	0.49
1:A:534:HIS:HE1	1:A:535:PHE:CE1	2.30	0.49
2:C:139:LEU:HD13	2:C:181:LYS:HE2	1.94	0.49
2:C:7:LEU:HA	2:C:56:VAL:O	2.13	0.49
1:D:126:ARG:HA	1:D:182:ILE:HG21	1.95	0.49
2:E:135:LEU:HD12	2:E:135:LEU:N	2.27	0.49
2:F:110:GLN:HB3	2:F:167:TYR:CZ	2.48	0.49
2:F:41:SER:HB3	2:F:43:LEU:CD1	2.43	0.49
1:A:104:SER:O	1:A:104:SER:OG	2.22	0.49
1:A:210:ILE:HA	1:A:213:ARG:NE	2.28	0.49
2:C:110:GLN:HB3	2:C:167:TYR:CZ	2.48	0.49
1:D:231:PHE:HD1	1:D:287:TRP:HZ2	1.60	0.49
2:E:14:MET:O	2:E:17:MET:HB2	2.12	0.49
2:E:188:ARG:HG3	2:E:189:CYS:N	2.27	0.49
2:F:170:PHE:CD2	2:F:213:ARG:HD2	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:ARG:HG2	1:A:182:ILE:HD12	1.95	0.49
1:A:143:LYS:HD3	1:A:212:PHE:CD1	2.48	0.49
1:A:315:LYS:HA	1:A:318:HIS:CB	2.43	0.49
2:B:8:LEU:HD13	2:B:44:LEU:HG	1.95	0.49
2:C:136:GLU:HG3	2:C:181:LYS:CD	2.33	0.49
2:C:184:ALA:HA	2:C:187:LYS:NZ	2.27	0.49
2:C:5:PRO:HB3	2:C:59:HIS:CE1	2.48	0.49
1:D:212:PHE:HD2	1:D:215:GLN:CD	2.16	0.49
1:A:119:GLU:O	1:A:123:GLN:HG2	2.12	0.49
1:A:143:LYS:NZ	1:A:212:PHE:CD1	2.80	0.49
1:A:302:TYR:HA	1:A:326:VAL:HG13	1.95	0.49
1:A:420:LYS:HG2	1:A:421:PHE:N	2.28	0.49
1:A:444:SER:HA	1:A:500:ALA:CB	2.42	0.49
2:B:19:ALA:CB	2:B:70:VAL:HG11	2.43	0.49
2:B:16:GLY:O	2:B:20:ARG:HG3	2.12	0.49
2:B:13:SER:CB	2:B:54:ILE:HD11	2.43	0.49
2:C:98:TRP:CE3	2:C:138:GLU:OE2	2.66	0.49
1:D:445:VAL:HG13	1:D:479:TRP:CE2	2.48	0.49
2:E:148:ASP:OD1	2:E:148:ASP:N	2.43	0.49
2:E:24:ARG:NH1	2:E:198:SER:OG	2.38	0.49
1:A:45:LEU:CD2	1:A:50:LEU:HD23	2.42	0.48
2:B:18:ARG:O	2:B:21:VAL:HG12	2.13	0.48
2:C:184:ALA:HA	2:C:187:LYS:HZ1	1.78	0.48
2:C:32:TYR:CD1	2:C:34:GLU:OE2	2.66	0.48
1:D:163:GLY:CA	1:D:560:GLN:HB2	2.43	0.48
1:D:426:ASN:N	1:D:426:ASN:OD1	2.41	0.48
1:D:108:PRO:CG	1:D:552:LYS:H	2.26	0.48
1:D:76:TYR:HB3	1:D:88:ILE:CB	2.43	0.48
1:A:152:LYS:HA	1:A:564:GLU:CB	2.41	0.48
1:A:295:PHE:CD1	1:A:295:PHE:O	2.66	0.48
2:C:184:ALA:O	1:D:499:ARG:NH1	2.47	0.48
1:D:36:LEU:O	1:D:40:GLN:N	2.46	0.48
1:A:103:THR:HB	1:A:106:GLY:CA	2.44	0.48
2:C:24:ARG:NH2	7:C:420:HOH:O	2.45	0.48
1:D:35:ILE:O	1:D:39:ASN:HB2	2.13	0.48
1:D:331:GLY:N	1:D:537:GLY:O	2.44	0.48
2:E:58:VAL:HG23	7:E:418:HOH:O	2.13	0.48
2:E:66:GLU:HB2	2:E:69:ASN:HB3	1.95	0.48
2:F:125:LYS:HD3	2:F:173:PHE:CG	2.47	0.48
2:F:143:PRO:HB2	2:F:144:TYR:CD2	2.48	0.48
2:F:15:PHE:HB3	2:F:67:SER:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:136:GLU:HB3	2:F:179:SER:OG	2.13	0.48
2:F:68:LEU:O	2:F:72:GLN:HG3	2.12	0.48
1:A:192:VAL:HG12	1:A:205:HIS:HD2	1.79	0.48
1:A:22:ARG:HG2	1:A:22:ARG:HH11	1.78	0.48
1:A:273:LEU:HA	1:A:276:THR:HG23	1.95	0.48
1:A:335:GLY:HA3	1:A:394:ASN:HD22	1.79	0.48
2:B:34:GLU:OE2	7:B:402:HOH:O	2.20	0.48
1:D:121:THR:HG23	3:D:601:JAA:C15	2.43	0.48
1:D:231:PHE:O	1:D:235:GLU:HG3	2.13	0.48
1:D:303:GLY:O	1:D:327:SER:HA	2.13	0.48
1:D:441:LEU:CD2	1:D:549:ARG:HB3	2.43	0.48
1:A:213:ARG:HD3	1:A:216:VAL:HG21	1.94	0.48
2:F:7:LEU:HD11	2:F:57:LEU:HB2	1.96	0.48
1:A:113:PHE:HE2	1:A:163:GLY:O	1.97	0.48
2:B:14:MET:O	2:B:17:MET:HB2	2.14	0.48
2:B:34:GLU:HG3	2:B:35:GLU:N	2.28	0.48
1:D:549:ARG:NH2	7:D:725:HOH:O	2.46	0.48
2:E:154:ASP:HA	2:E:185:TRP:HZ2	1.78	0.48
2:E:17:MET:HG2	2:E:20:ARG:HH21	1.79	0.48
2:F:114:TRP:CZ3	2:F:212:TYR:HD2	2.29	0.48
1:A:211:LEU:HD12	1:A:212:PHE:CE2	2.48	0.48
1:A:534:HIS:HB3	4:A:602:ILE:C	2.34	0.48
1:A:491:GLN:OE1	1:A:573:THR:N	2.47	0.48
1:A:97:ILE:HD13	1:A:110:PHE:CE2	2.48	0.48
2:B:15:PHE:HA	2:B:18:ARG:HD2	1.96	0.48
1:D:190:ASP:O	1:D:194:PHE:N	2.44	0.48
1:D:191:GLU:N	1:D:191:GLU:OE1	2.47	0.48
1:D:235:GLU:HG2	1:D:287:TRP:CE3	2.49	0.48
1:D:132:ARG:HD3	1:D:300:TYR:CZ	2.49	0.48
1:D:365:PRO:CG	1:D:374:GLU:HG2	2.42	0.48
1:A:169:VAL:O	1:A:175:PHE:HB2	2.13	0.48
1:A:238:TRP:CZ2	1:A:282:MET:SD	3.07	0.48
1:A:510:ARG:HG2	1:A:515:ILE:HG13	1.94	0.48
1:A:96:ALA:HB3	1:A:113:PHE:HD2	1.78	0.48
2:B:117:LYS:HG3	2:B:213:ARG:HH11	1.78	0.48
2:B:120:GLU:HG2	7:B:454:HOH:O	2.14	0.48
2:C:8:LEU:HD21	2:C:43:LEU:HD21	1.95	0.48
1:D:508:SER:O	1:D:512:CYS:HB3	2.13	0.48
1:D:50:LEU:HD13	1:D:61:PHE:HE1	1.77	0.48
2:F:211:GLU:O	2:F:214:LYS:HG2	2.14	0.48
2:E:66:GLU:OE2	2:F:97:PHE:CD1	2.65	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:332:SER:HB2	1:A:538:LEU:HA	1.96	0.48
1:A:354:VAL:HG11	1:A:361:PHE:CZ	2.48	0.48
1:A:432:ASN:OD1	1:A:433:ILE:N	2.46	0.48
1:A:492:ASP:HB2	7:A:704:HOH:O	2.14	0.48
2:C:117:LYS:HE3	2:C:213:ARG:NH1	2.28	0.48
2:C:136:GLU:OE2	2:C:180:PRO:HD2	2.14	0.48
1:D:131:PHE:CD1	1:D:132:ARG:N	2.81	0.48
1:A:465:TYR:CE2	1:A:467:ASP:HB3	2.49	0.48
2:B:97:PHE:CE1	2:C:65:CYS:HB2	2.49	0.48
2:C:73:TYR:HA	2:C:76:GLU:HG2	1.96	0.48
1:D:398:LEU:HB3	1:D:401:TYR:CD1	2.49	0.48
1:D:441:LEU:O	1:D:444:SER:HB2	2.14	0.48
2:E:98:TRP:HE3	2:E:153:VAL:HG11	1.78	0.48
1:A:340:ASN:ND2	1:A:343:PRO:HA	2.29	0.47
2:B:8:LEU:HB2	2:B:56:VAL:HB	1.96	0.47
1:D:122:LEU:HD12	1:D:123:GLN:N	2.28	0.47
1:D:336:TRP:CB	1:D:358:LEU:HD13	2.44	0.47
1:D:337:ILE:HG22	1:D:338:ALA:N	2.29	0.47
1:D:393:THR:HG22	1:D:400:ARG:H	1.79	0.47
1:D:41:SER:H	2:E:142:LYS:CE	2.27	0.47
2:F:168:GLU:CD	2:F:175:ILE:HG12	2.35	0.47
1:A:331:GLY:HA2	1:A:539:GLY:CA	2.44	0.47
1:A:421:PHE:CD1	1:A:541:SER:HA	2.49	0.47
1:D:507:VAL:HG23	1:D:511:LYS:CE	2.40	0.47
1:A:201:ALA:O	1:A:205:HIS:HB2	2.14	0.47
1:A:370:GLY:HA2	1:A:371:GLU:HA	1.69	0.47
1:A:152:LYS:HG2	1:A:561:ILE:O	2.15	0.47
1:A:562:LEU:HD12	1:A:563:CYS:HB3	1.96	0.47
1:D:117:LEU:HB2	7:D:793:HOH:O	2.14	0.47
1:D:525:LYS:NZ	7:D:755:HOH:O	2.42	0.47
1:D:528:PHE:O	1:D:532:GLN:HG2	2.14	0.47
2:F:33:ARG:HH12	2:F:35:GLU:CD	2.15	0.47
2:E:96:ARG:NH1	2:F:73:TYR:CE1	2.82	0.47
2:C:187:LYS:HB2	2:C:187:LYS:HE2	1.69	0.47
1:D:17:PHE:CD2	1:D:127:THR:HG21	2.50	0.47
2:E:43:LEU:HD21	2:E:58:VAL:HG21	1.96	0.47
1:A:149:PHE:HB2	1:A:530:LYS:HZ3	1.79	0.47
1:A:118:MET:HG2	1:A:174:ASN:HD21	1.78	0.47
1:A:210:ILE:O	1:A:210:ILE:HG22	2.15	0.47
2:B:15:PHE:HB3	2:B:67:SER:CB	2.45	0.47
2:C:10:TYR:H	2:C:20:ARG:NH2	2.12	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:223:PHE:CE2	1:D:545:PHE:CZ	2.95	0.47
1:D:412:PHE:N	1:D:418:GLN:HE21	2.12	0.47
2:E:60:ASN:HD21	2:E:62:LYS:HD2	1.79	0.47
2:E:7:LEU:HD13	2:E:9:ASP:HB2	1.97	0.47
2:F:175:ILE:HG13	2:F:176:GLU:N	2.27	0.47
1:A:209:GLY:O	1:A:213:ARG:NE	2.34	0.47
1:A:284:LEU:HD23	1:A:290:LEU:HD13	1.97	0.47
1:A:35:ILE:HA	1:A:395:TYR:CE1	2.50	0.47
1:A:546:LYS:HG3	1:A:546:LYS:O	2.15	0.47
2:B:50:ILE:HD11	2:C:101:PHE:CZ	2.50	0.47
1:D:329:ASP:HB3	1:D:338:ALA:O	2.15	0.47
1:D:452:LEU:HD22	1:D:479:TRP:HZ3	1.79	0.47
2:F:152:TYR:O	2:F:155:ILE:HB	2.14	0.47
1:A:223:PHE:HD2	1:A:225:HIS:ND1	2.12	0.47
1:A:154:TYR:HB2	1:A:563:CYS:CB	2.45	0.47
1:D:405:ASP:CG	1:D:540:SER:HB2	2.35	0.47
2:F:136:GLU:HB3	2:F:179:SER:HG	1.78	0.47
1:A:105:GLN:HG3	1:A:107:ARG:HH21	1.80	0.47
1:A:120:ASN:OD1	1:A:121:THR:N	2.47	0.47
1:A:97:ILE:O	1:A:556:ALA:HB1	2.15	0.47
2:B:144:TYR:OH	2:B:188:ARG:HD2	2.15	0.47
1:A:93:PRO:HG2	2:B:184:ALA:HB3	1.96	0.47
1:D:148:ILE:HG21	1:D:170:TYR:OH	2.15	0.47
1:D:552:LYS:HB2	1:D:553:PRO:HD2	1.95	0.47
2:E:202:SER:O	2:E:205:ILE:HG13	2.15	0.47
2:E:85:PHE:HB2	2:E:92:ARG:CG	2.45	0.47
2:F:148:ASP:O	7:F:410:HOH:O	2.20	0.47
1:A:208:SER:HA	1:A:211:LEU:CD2	2.45	0.47
1:D:340:ASN:HD21	1:D:345:LEU:HD11	1.80	0.47
2:E:108:ASP:O	2:E:112:LYS:HG2	2.14	0.47
2:E:11:TRP:CZ2	2:E:204:LYS:HB3	2.44	0.47
2:E:60:ASN:ND2	2:E:62:LYS:HD2	2.30	0.47
2:F:110:GLN:O	2:F:113:VAL:HG12	2.14	0.47
2:F:180:PRO:HA	2:F:183:ILE:HG22	1.96	0.47
2:F:201:ASP:O	2:F:204:LYS:HG2	2.13	0.47
1:A:139:ASP:OD1	1:A:142:GLY:HA3	2.14	0.47
1:A:291:ILE:HB	1:A:320:ALA:HA	1.97	0.47
1:A:228:VAL:HG13	1:A:319:TYR:HE2	1.79	0.47
1:D:438:GLU:HG2	1:D:442:GLN:OE1	2.15	0.47
1:D:451:ARG:NH1	1:D:489:VAL:C	2.66	0.47
1:A:171:ARG:HD3	1:A:171:ARG:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:33:ARG:NE	2:C:35:GLU:OE2	2.48	0.47
1:D:246:LYS:HB3	1:D:246:LYS:HE3	1.60	0.47
1:D:326:VAL:CG2	1:D:343:PRO:HB3	2.43	0.47
1:D:444:SER:HA	1:D:500:ALA:HB1	1.96	0.47
1:D:67:LEU:HD23	1:D:400:ARG:HB3	1.97	0.47
2:F:23:LEU:HD21	2:F:30:PHE:CD1	2.50	0.47
1:A:339:ALA:O	1:A:353:ALA:N	2.40	0.46
2:B:163:TRP:HB3	2:B:167:TYR:CZ	2.49	0.46
2:B:50:ILE:HG21	2:C:134:ILE:HD12	1.97	0.46
2:C:47:SER:HB2	2:C:63:PRO:HB3	1.97	0.46
1:D:131:PHE:HD1	1:D:132:ARG:N	2.12	0.46
1:D:394:ASN:O	1:D:399:TYR:HE1	1.96	0.46
1:D:434:ASP:HB2	1:D:550:CYS:HB3	1.96	0.46
1:D:70:ASP:OD2	1:D:104:SER:HA	2.15	0.46
2:E:70:VAL:O	2:E:73:TYR:HB3	2.15	0.46
1:A:314:PRO:O	1:A:318:HIS:N	2.40	0.46
1:A:435:LYS:HB3	1:A:436:ASN:O	2.16	0.46
1:A:440:ASP:OD1	1:A:441:LEU:N	2.48	0.46
1:A:503:ASP:CG	1:A:505:GLY:H	2.18	0.46
1:A:434:ASP:CB	1:A:550:CYS:HB3	2.40	0.46
2:B:92:ARG:NH1	7:B:412:HOH:O	2.27	0.46
2:C:116:LYS:O	2:C:121:GLN:HG3	2.15	0.46
2:C:195:VAL:HG23	2:C:199:LEU:HD13	1.96	0.46
1:D:529:ARG:HB2	1:D:529:ARG:CZ	2.45	0.46
1:D:534:HIS:NE2	1:D:557:LYS:HG2	2.30	0.46
2:E:90:TYR:HE1	7:F:407:HOH:O	1.98	0.46
2:F:64:VAL:HB	2:F:73:TYR:CE2	2.50	0.46
1:A:118:MET:HG2	1:A:174:ASN:CG	2.36	0.46
1:A:413:TYR:N	1:A:416:THR:O	2.48	0.46
1:A:549:ARG:HD3	1:A:549:ARG:HA	1.47	0.46
1:D:304:ILE:HG12	1:D:536:LEU:HD13	1.96	0.46
1:D:405:ASP:CB	1:D:541:SER:HB3	2.39	0.46
1:D:59:GLU:HB3	1:D:62:LYS:HZ1	1.80	0.46
2:F:162:SER:O	2:F:165:GLN:HG3	2.15	0.46
1:A:172:ASN:OD1	1:A:174:ASN:ND2	2.49	0.46
1:D:234:PHE:HB3	1:D:287:TRP:CH2	2.50	0.46
1:D:452:LEU:HG	1:D:457:ILE:HD11	1.97	0.46
2:F:84:PHE:CG	2:F:152:TYR:HB2	2.50	0.46
1:A:202:LEU:HD13	1:A:229:HIS:NE2	2.31	0.46
1:A:234:PHE:CD2	1:A:234:PHE:C	2.88	0.46
1:A:442:GLN:HG2	1:A:462:PHE:HZ	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199:HIS:HA	1:A:525:LYS:HG2	1.97	0.46
1:D:242:VAL:HG22	1:D:277:ILE:CD1	2.42	0.46
1:D:254:ILE:O	1:D:260:ARG:HD2	2.15	0.46
1:D:364:LEU:HB3	1:D:389:GLU:CG	2.45	0.46
2:E:96:ARG:HH11	2:F:69:ASN:HA	1.80	0.46
1:A:206:LEU:HD11	1:A:234:PHE:HD1	1.81	0.46
1:A:341:VAL:C	1:A:343:PRO:HD3	2.35	0.46
1:A:330:TYR:CE2	1:A:352:PHE:CD2	3.03	0.46
1:A:436:ASN:HA	1:A:440:ASP:OD2	2.15	0.46
1:D:110:PHE:CE2	1:D:553:PRO:O	2.69	0.46
1:D:125:PHE:HD1	1:D:125:PHE:HA	1.63	0.46
1:D:413:TYR:CD2	1:D:418:GLN:HG2	2.50	0.46
1:D:552:LYS:NZ	7:D:711:HOH:O	2.13	0.46
1:D:552:LYS:HG3	1:D:553:PRO:N	2.30	0.46
2:E:68:LEU:HD12	2:E:68:LEU:HA	1.52	0.46
1:A:143:LYS:NZ	1:A:212:PHE:HB2	2.31	0.46
1:A:215:GLN:O	1:A:217:GLN:NE2	2.43	0.46
1:A:27:VAL:O	1:A:31:THR:OG1	2.27	0.46
1:A:295:PHE:CD1	1:A:298:ALA:HB3	2.51	0.46
2:C:116:LYS:HB2	7:C:436:HOH:O	2.15	0.46
1:D:405:ASP:OD1	1:D:540:SER:HB2	2.15	0.46
1:D:531:ILE:O	1:D:534:HIS:CE1	2.68	0.46
1:D:494:CYS:SG	1:D:572:SER:HA	2.56	0.46
1:D:43:ILE:HD11	1:D:76:TYR:CE2	2.50	0.46
2:E:169:LYS:HG3	2:E:170:PHE:CD1	2.50	0.46
6:C:301:GSH:O32	7:C:410:HOH:O	2.20	0.46
1:D:235:GLU:O	1:D:238:TRP:CD1	2.69	0.46
1:D:154:TYR:HD2	1:D:560:GLN:HA	1.80	0.46
2:E:9:ASP:OD1	2:E:10:TYR:N	2.49	0.46
2:E:96:ARG:HH12	2:F:72:GLN:HB2	1.79	0.46
1:A:181:SER:OG	1:A:182:ILE:HG13	2.16	0.46
1:A:195:SER:O	1:A:565:ASN:ND2	2.45	0.46
1:A:30:GLN:OE1	1:A:30:GLN:HA	2.15	0.46
2:B:128:PHE:HE2	2:B:175:ILE:HG12	1.81	0.46
2:C:187:LYS:O	7:C:411:HOH:O	2.21	0.46
1:D:207:LEU:O	1:D:210:ILE:HG23	2.15	0.46
1:D:452:LEU:HD21	1:D:481:ILE:HD13	1.97	0.46
1:D:497:LEU:O	1:D:500:ALA:HB3	2.15	0.46
2:F:135:LEU:HD13	2:F:182:LEU:HD12	1.98	0.46
2:F:8:LEU:HA	2:F:33:ARG:HG3	1.98	0.46
1:A:100:SER:HA	1:A:535:PHE:HE1	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:313:VAL:HG23	1:A:325:LEU:HD12	1.98	0.46
2:C:57:LEU:O	2:C:64:VAL:HB	2.16	0.46
1:D:53:ASN:OD1	1:D:54:ALA:N	2.49	0.46
2:F:57:LEU:HD13	2:F:59:HIS:HD2	1.81	0.46
1:A:103:THR:HB	1:A:106:GLY:C	2.37	0.45
1:A:248:GLY:O	1:A:267:LEU:HB3	2.16	0.45
1:A:28:GLN:HG3	1:A:29:LYS:N	2.31	0.45
1:A:224:ALA:HB3	1:A:309:MET:HG3	1.98	0.45
1:A:346:SER:N	7:A:749:HOH:O	2.41	0.45
1:A:470:THR:OG1	1:A:473:GLY:HA2	2.17	0.45
2:C:190:MET:C	1:D:450:LYS:HD2	2.36	0.45
2:C:166:ALA:CA	2:C:206:VAL:HG22	2.46	0.45
2:C:16:GLY:HA3	2:C:20:ARG:NH2	2.31	0.45
2:C:50:ILE:HG13	2:C:51:HIS:H	1.81	0.45
1:D:391:VAL:HA	1:D:401:TYR:O	2.16	0.45
2:E:188:ARG:N	7:E:419:HOH:O	2.49	0.45
2:E:201:ASP:HB2	2:E:204:LYS:HG2	1.98	0.45
2:E:65:CYS:HB2	2:F:97:PHE:CZ	2.51	0.45
1:A:355:ILE:HA	1:A:356:PRO:HD3	1.75	0.45
1:A:46:GLN:HB3	2:B:148:ASP:CB	2.41	0.45
1:A:500:ALA:O	1:A:502:ILE:HG23	2.15	0.45
1:A:73:LEU:HD22	1:A:89:LEU:HD13	1.97	0.45
1:A:91:GLY:HA3	2:B:141:ASP:C	2.36	0.45
2:B:34:GLU:HG3	2:B:35:GLU:H	1.81	0.45
2:B:76:GLU:O	2:B:79:PRO:HD3	2.17	0.45
2:C:110:GLN:HA	2:C:113:VAL:HG12	1.98	0.45
2:C:188:ARG:N	7:D:704:HOH:O	2.49	0.45
1:D:273:LEU:N	1:D:273:LEU:CD1	2.78	0.45
1:D:289:GLY:N	1:D:318:HIS:O	2.35	0.45
1:D:334:GLU:HG3	1:D:538:LEU:HD13	1.98	0.45
1:D:41:SER:N	2:E:142:LYS:HE2	2.31	0.45
1:D:467:ASP:OD2	1:D:474:HIS:CE1	2.69	0.45
2:F:7:LEU:HD22	2:F:30:PHE:CE1	2.52	0.45
2:F:75:ASP:HB2	2:F:84:PHE:CE2	2.52	0.45
1:A:491:GLN:HE22	1:A:570:TYR:HB3	1.80	0.45
2:B:96:ARG:HH12	2:C:76:GLU:CD	2.20	0.45
2:C:141:ASP:N	2:C:141:ASP:OD1	2.50	0.45
2:C:34:GLU:CD	2:C:34:GLU:N	2.69	0.45
2:F:98:TRP:CE3	2:F:101:PHE:HB2	2.51	0.45
1:A:14:ILE:HG13	1:A:131:PHE:HE1	1.81	0.45
1:A:145:LEU:O	1:A:220:PHE:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:313:VAL:HG13	1:A:314:PRO:HD3	1.97	0.45
1:A:389:GLU:HA	1:A:405:ASP:O	2.17	0.45
1:A:465:TYR:N	1:A:476:ALA:O	2.47	0.45
2:B:177:SER:OG	7:B:406:HOH:O	2.15	0.45
2:C:117:LYS:HA	2:C:121:GLN:HB2	1.98	0.45
2:C:84:PHE:CD1	2:C:152:TYR:HB2	2.52	0.45
1:D:452:LEU:HD22	1:D:479:TRP:CZ3	2.52	0.45
2:C:125:LYS:HB3	2:C:125:LYS:HE3	1.62	0.45
1:D:143:LYS:O	1:D:216:VAL:HA	2.17	0.45
1:D:466:ILE:HD11	1:D:552:LYS:HB2	1.99	0.45
1:D:59:GLU:HA	1:D:62:LYS:HZ3	1.81	0.45
2:E:106:PHE:CE2	2:E:135:LEU:CD1	2.99	0.45
2:F:18:ARG:HG3	2:F:67:SER:OG	2.16	0.45
1:A:143:LYS:C	1:A:184:SER:HB2	2.37	0.45
1:A:132:ARG:NH2	1:A:300:TYR:OH	2.50	0.45
1:A:329:ASP:OD2	7:A:724:HOH:O	2.20	0.45
1:A:493:CYS:N	7:A:704:HOH:O	2.48	0.45
1:A:53:ASN:ND2	7:A:760:HOH:O	2.49	0.45
1:A:552:LYS:HB2	1:A:553:PRO:CD	2.45	0.45
2:B:37:PHE:CZ	6:B:301:GSH:HA32	2.52	0.45
2:C:213:ARG:O	2:C:217:LEU:HG	2.16	0.45
1:D:451:ARG:NH2	1:D:490:LEU:HD23	2.31	0.45
2:F:135:LEU:HD11	2:F:157:LEU:HD13	1.99	0.45
2:F:188:ARG:O	2:F:191:GLU:HG2	2.17	0.45
1:A:452:LEU:HD13	1:A:493:CYS:SG	2.57	0.45
2:C:157:LEU:CD1	2:C:185:TRP:CH2	2.99	0.45
2:E:122:GLU:HA	2:E:125:LYS:HE3	1.99	0.45
1:A:290:LEU:O	1:A:290:LEU:HG	2.17	0.45
1:A:560:GLN:HG2	7:A:734:HOH:O	2.16	0.45
1:D:29:LYS:HD3	7:D:813:HOH:O	2.17	0.45
2:F:101:PHE:CD1	2:F:101:PHE:N	2.84	0.45
2:F:136:GLU:OE1	2:F:179:SER:HA	2.17	0.45
2:F:144:TYR:HE1	2:F:189:CYS:HG	1.63	0.45
1:A:256:VAL:HA	1:A:257:PRO:HD3	1.83	0.45
1:A:477:ILE:H	1:A:477:ILE:HG13	1.59	0.45
1:A:538:LEU:HB3	1:A:544:GLN:OE1	2.17	0.45
2:B:97:PHE:CZ	2:B:101:PHE:HE2	2.35	0.45
2:C:164:PHE:HD2	2:C:183:ILE:HG22	1.79	0.45
2:C:183:ILE:HD12	2:C:184:ALA:N	2.32	0.45
2:C:158:ILE:HD11	2:C:186:ALA:O	2.16	0.45
1:D:413:TYR:HD2	1:D:418:GLN:HG2	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:462:PHE:C	1:D:528:PHE:HZ	2.20	0.45
1:D:152:LYS:CB	1:D:561:ILE:HA	2.46	0.45
2:F:23:LEU:CA	2:F:74:VAL:HG11	2.43	0.45
1:A:104:SER:N	1:A:107:ARG:O	2.49	0.45
1:A:235:GLU:OE2	1:A:287:TRP:CG	2.70	0.45
1:A:265:LYS:HZ2	1:A:266:LEU:HG	1.80	0.45
1:A:224:ALA:HB3	1:A:309:MET:CG	2.47	0.45
1:A:79:ARG:HG3	1:A:84:ASP:OD2	2.17	0.45
2:C:156:SER:OG	7:C:407:HOH:O	2.20	0.45
2:C:16:GLY:HA3	2:C:20:ARG:HH21	1.82	0.45
2:C:187:LYS:CE	1:D:496:CYS:HB2	2.47	0.45
1:D:29:LYS:O	1:D:32:LEU:HB2	2.17	0.45
1:D:393:THR:CG2	1:D:400:ARG:H	2.30	0.45
1:D:500:ALA:HB1	7:D:706:HOH:O	2.17	0.45
2:F:135:LEU:HD23	2:F:145:PHE:HZ	1.82	0.45
1:A:286:ASN:O	1:A:287:TRP:CB	2.63	0.44
1:A:510:ARG:NH1	1:A:518:LEU:H	2.15	0.44
2:B:14:MET:HG3	2:B:163:TRP:NE1	2.32	0.44
2:B:21:VAL:HG21	2:B:158:ILE:HD12	1.99	0.44
2:C:10:TYR:O	2:C:20:ARG:NH2	2.42	0.44
1:D:364:LEU:CD2	1:D:402:ARG:HH12	2.30	0.44
1:D:407:VAL:HG23	1:D:420:LYS:O	2.16	0.44
1:D:198:VAL:HG13	1:D:565:ASN:ND2	2.32	0.44
2:F:41:SER:HB3	2:F:43:LEU:HD11	1.98	0.44
2:F:98:TRP:O	2:F:98:TRP:CE3	2.70	0.44
1:A:133:ASN:HA	1:A:136:PHE:O	2.17	0.44
1:A:192:VAL:HG12	1:A:205:HIS:CD2	2.53	0.44
1:A:278:ARG:O	1:A:282:MET:SD	2.75	0.44
1:A:507:VAL:CG2	1:A:508:SER:N	2.81	0.44
2:B:161:SER:HB2	2:B:186:ALA:HB1	2.00	0.44
2:C:5:PRO:HB3	2:C:59:HIS:NE2	2.32	0.44
1:D:192:VAL:HG23	1:D:259:VAL:HG21	1.98	0.44
1:D:360:TYR:HB3	1:D:393:THR:OG1	2.17	0.44
2:F:44:LEU:HD21	2:F:52:LYS:C	2.37	0.44
1:A:145:LEU:HD11	1:A:147:PHE:CE1	2.51	0.44
1:A:238:TRP:HE3	1:A:277:ILE:HD11	1.82	0.44
1:D:369:THR:HG1	1:D:370:GLY:H	1.53	0.44
1:D:38:LYS:O	2:E:142:LYS:HG2	2.18	0.44
1:D:86:SER:HA	1:D:87:PRO:HD2	1.86	0.44
1:A:233:THR:O	1:A:237:VAL:HG22	2.17	0.44
1:A:423:CYS:HA	7:A:782:HOH:O	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:487:GLU:O	1:A:490:LEU:HG	2.17	0.44
1:A:506:TYR:CZ	1:A:510:ARG:HD3	2.53	0.44
2:B:74:VAL:HA	2:B:78:TRP:CE3	2.52	0.44
2:C:10:TYR:HB3	2:C:13:SER:CB	2.36	0.44
2:C:14:MET:HG3	2:C:163:TRP:CZ2	2.52	0.44
1:D:133:ASN:ND2	1:D:138:ILE:HG13	2.22	0.44
1:D:210:ILE:HD12	1:D:234:PHE:CZ	2.52	0.44
1:D:206:LEU:HD22	1:D:234:PHE:HD1	1.82	0.44
1:D:407:VAL:HG21	1:D:419:LEU:HD23	2.00	0.44
2:E:98:TRP:HB2	7:E:401:HOH:O	2.16	0.44
2:F:136:GLU:HG2	2:F:179:SER:HB2	2.00	0.44
1:A:213:ARG:HD3	1:A:216:VAL:CG2	2.48	0.44
1:A:32:LEU:HG	1:A:360:TYR:HB2	2.00	0.44
1:A:464:SER:O	1:A:551:VAL:N	2.46	0.44
1:A:534:HIS:CE1	1:A:535:PHE:CE1	3.06	0.44
1:A:545:PHE:HE1	7:A:919:HOH:O	2.00	0.44
1:A:90:THR:HB	1:A:91:GLY:H	1.55	0.44
2:C:128:PHE:O	2:C:132:VAL:HG12	2.16	0.44
2:C:163:TRP:HB3	2:C:167:TYR:CE2	2.52	0.44
2:C:209:ALA:CA	2:C:212:TYR:HE2	2.26	0.44
1:D:21:THR:HB	1:D:416:THR:HB	2.00	0.44
1:D:310:GLU:O	1:D:313:VAL:HG12	2.18	0.44
1:D:121:THR:HG1	1:D:336:TRP:HE1	1.65	0.44
2:E:145:PHE:N	2:E:154:ASP:OD2	2.39	0.44
2:F:144:TYR:HB3	2:F:154:ASP:OD2	2.17	0.44
2:F:190:MET:O	2:F:196:SER:HB2	2.17	0.44
1:A:284:LEU:HB2	1:A:287:TRP:H	1.81	0.44
1:A:477:ILE:HG21	1:A:497:LEU:HD23	1.99	0.44
1:A:558:VAL:HG22	7:A:829:HOH:O	2.17	0.44
1:A:76:TYR:HB2	1:A:89:LEU:HD11	1.99	0.44
2:C:114:TRP:CE3	2:C:212:TYR:CE2	3.06	0.44
2:C:209:ALA:HA	2:C:212:TYR:CD2	2.51	0.44
1:D:242:VAL:O	1:D:246:LYS:HG3	2.17	0.44
1:D:360:TYR:OH	1:D:362:GLU:OE2	2.24	0.44
1:D:494:CYS:HB3	1:D:520:LEU:HB3	2.00	0.44
1:A:27:VAL:CG1	1:A:357:ASN:HB3	2.48	0.44
1:A:387:GLU:HG2	1:A:408:LYS:HB2	1.98	0.44
2:C:166:ALA:HB2	2:C:206:VAL:HG22	2.00	0.44
2:C:57:LEU:HB3	2:C:64:VAL:CG1	2.47	0.44
1:D:218:TYR:CE1	1:D:220:PHE:HB2	2.52	0.44
1:D:440:ASP:OD1	1:D:441:LEU:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:50:ILE:HD12	2:E:51:HIS:N	2.33	0.44
2:F:113:VAL:HG22	2:F:167:TYR:O	2.17	0.44
1:A:151:SER:O	1:A:565:ASN:ND2	2.50	0.44
1:A:280:LYS:O	1:A:283:SER:OG	2.31	0.44
1:A:313:VAL:N	1:A:314:PRO:HD2	2.32	0.44
1:A:74:GLU:O	1:A:78:LYS:HB2	2.18	0.44
2:C:177:SER:HB2	7:C:402:HOH:O	2.16	0.44
2:C:187:LYS:O	2:C:190:MET:HB2	2.18	0.44
2:C:98:TRP:CE2	2:C:157:LEU:HD22	2.52	0.44
2:C:187:LYS:HE3	1:D:492:ASP:C	2.38	0.44
1:D:493:CYS:SG	1:D:497:LEU:HD11	2.58	0.44
1:D:475:TYR:HB2	1:D:518:LEU:HB2	2.00	0.44
1:D:518:LEU:HD12	1:D:519:GLU:N	2.33	0.44
1:D:77:ILE:HG13	1:D:88:ILE:CD1	2.48	0.44
1:D:76:TYR:O	1:D:88:ILE:HG21	2.17	0.44
2:F:10:TYR:CD1	2:F:12:PRO:HD2	2.52	0.44
2:E:93:ALA:HA	2:F:73:TYR:CE1	2.53	0.44
1:A:96:ALA:HA	1:A:161:PRO:O	2.18	0.44
1:A:210:ILE:HD13	1:A:210:ILE:HG21	1.55	0.44
1:A:315:LYS:CA	1:A:318:HIS:HB3	2.46	0.44
1:A:332:SER:HB3	1:A:538:LEU:HD12	1.99	0.44
1:A:408:LYS:HE3	1:A:420:LYS:NZ	2.33	0.44
1:A:429:LEU:HD13	1:A:546:LYS:NZ	2.33	0.44
2:C:21:VAL:O	2:C:194:SER:HB2	2.18	0.44
1:D:104:SER:O	1:D:105:GLN:HB2	2.18	0.44
1:D:154:TYR:CD2	1:D:560:GLN:HA	2.53	0.44
1:D:383:LYS:N	1:D:386:GLU:OE2	2.49	0.44
1:D:79:ARG:O	1:D:84:ASP:HB3	2.17	0.44
2:E:165:GLN:HG3	2:E:168:GLU:OE2	2.17	0.44
2:E:192:LYS:O	2:E:196:SER:HB2	2.17	0.44
2:F:77:ALA:HB3	2:F:78:TRP:CE3	2.53	0.44
2:F:89:PRO:O	2:F:92:ARG:HB3	2.17	0.44
1:A:148:ILE:HB	1:A:170:TYR:HE2	1.83	0.43
1:A:198:VAL:HA	1:A:201:ALA:HB3	2.00	0.43
1:A:354:VAL:HG23	1:A:419:LEU:HD13	2.00	0.43
1:A:460:ILE:HD12	1:A:481:ILE:C	2.39	0.43
1:A:551:VAL:CG1	1:A:555:ASN:HD22	2.26	0.43
1:A:113:PHE:HZ	1:A:557:LYS:HZ2	1.65	0.43
2:B:70:VAL:O	2:B:74:VAL:HG23	2.18	0.43
1:D:198:VAL:HA	1:D:201:ALA:HB3	1.99	0.43
1:D:370:GLY:HA2	1:D:371:GLU:HA	1.77	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:163:TRP:HA	2:E:205:ILE:HD13	1.98	0.43
2:F:182:LEU:HD23	2:F:183:ILE:N	2.32	0.43
2:F:40:LYS:H	2:F:40:LYS:HZ1	1.65	0.43
1:A:214:ASP:N	1:A:214:ASP:OD1	2.50	0.43
1:A:329:ASP:HA	1:A:352:PHE:HD1	1.82	0.43
1:A:365:PRO:HB3	1:A:388:TYR:CE1	2.53	0.43
2:B:20:ARG:NH2	2:B:200:PRO:HD3	2.32	0.43
1:D:136:PHE:CD1	1:D:299:LYS:HD2	2.52	0.43
1:D:273:LEU:O	1:D:277:ILE:HG22	2.18	0.43
1:D:56:ASP:N	1:D:57:PRO:HD3	2.33	0.43
2:E:99:ALA:HB3	2:E:152:TYR:OH	2.18	0.43
2:E:26:LYS:NZ	2:E:78:TRP:O	2.34	0.43
1:A:232:ARG:HG3	1:A:233:THR:N	2.33	0.43
1:A:295:PHE:CE1	1:A:298:ALA:HB3	2.54	0.43
1:A:379:LEU:HG	1:A:380:THR:HG23	2.01	0.43
1:A:408:LYS:HE3	1:A:420:LYS:HE2	2.00	0.43
1:A:87:PRO:HA	1:A:91:GLY:O	2.18	0.43
2:C:129:ILE:HA	2:C:132:VAL:HG12	1.99	0.43
1:D:128:ALA:HA	1:D:131:PHE:CZ	2.53	0.43
1:D:156:SER:OG	1:D:160:VAL:O	2.19	0.43
1:A:145:LEU:HD22	1:A:213:ARG:CZ	2.47	0.43
1:A:152:LYS:HE3	1:A:565:ASN:CB	2.49	0.43
1:A:250:LEU:HD11	7:A:891:HOH:O	2.17	0.43
1:A:128:ALA:HB2	1:A:329:ASP:OD2	2.18	0.43
1:A:381:GLN:NE2	7:A:762:HOH:O	2.50	0.43
2:B:217:LEU:O	7:B:409:HOH:O	2.21	0.43
2:B:94:GLN:O	2:B:98:TRP:HD1	2.01	0.43
2:C:103:ASP:HA	2:C:107:THR:HG23	2.00	0.43
1:D:7:THR:O	1:D:126:ARG:NE	2.52	0.43
2:E:102:VAL:HG13	7:E:406:HOH:O	2.18	0.43
1:A:274:ALA:O	1:A:278:ARG:HB2	2.18	0.43
1:A:302:TYR:CG	1:A:328:HIS:CE1	3.07	0.43
1:A:70:ASP:OD2	1:A:104:SER:HA	2.19	0.43
1:A:77:ILE:HG21	1:A:110:PHE:HB3	2.00	0.43
2:B:169:LYS:NZ	2:B:206:VAL:CG1	2.82	0.43
2:B:96:ARG:HA	2:B:152:TYR:CE2	2.51	0.43
2:C:126:LYS:O	2:C:129:ILE:HG13	2.18	0.43
1:D:152:LYS:CG	1:D:565:ASN:HB2	2.48	0.43
1:D:444:SER:HB3	1:D:497:LEU:HD23	1.99	0.43
1:D:502:ILE:H	1:D:502:ILE:HG13	1.56	0.43
1:D:575:PHE:N	1:D:575:PHE:CD1	2.87	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:85:THR:O	1:D:87:PRO:HD3	2.18	0.43
2:F:129:ILE:O	2:F:132:VAL:HG12	2.18	0.43
2:F:170:PHE:CE2	2:F:213:ARG:HD2	2.54	0.43
2:B:93:ALA:HA	2:B:96:ARG:HE	1.83	0.43
2:C:105:LYS:HZ2	2:C:105:LYS:CB	2.31	0.43
1:D:213:ARG:HG3	1:D:214:ASP:H	1.83	0.43
1:D:457:ILE:HD12	1:D:481:ILE:HB	2.00	0.43
1:A:167:THR:O	1:A:171:ARG:HB3	2.19	0.43
1:A:208:SER:O	1:A:211:LEU:HG	2.19	0.43
1:A:476:ALA:HB1	1:A:521:ARG:HD2	2.00	0.43
1:D:187:CYS:HB2	1:D:209:GLY:HA2	2.00	0.43
1:D:330:TYR:N	1:D:338:ALA:O	2.29	0.43
2:E:8:LEU:HG	7:E:418:HOH:O	2.19	0.43
1:A:149:PHE:CD2	1:A:530:LYS:HE2	2.53	0.43
1:A:238:TRP:CE3	1:A:277:ILE:HG12	2.52	0.43
1:A:384:ILE:H	1:A:384:ILE:HG23	1.58	0.43
1:A:98:SER:C	1:A:556:ALA:HB3	2.39	0.43
2:B:13:SER:HB3	2:B:54:ILE:HD11	2.00	0.43
2:C:81:LYS:HG3	2:C:82:ASN:N	2.33	0.43
1:D:103:THR:HG22	1:D:548:PRO:HB3	2.00	0.43
1:D:193:ILE:HG12	1:D:205:HIS:HE1	1.82	0.43
1:D:207:LEU:HA	1:D:210:ILE:CG2	2.48	0.43
1:D:87:PRO:HG2	2:E:188:ARG:HH21	1.83	0.43
2:E:135:LEU:O	2:E:139:LEU:HB2	2.19	0.43
2:F:114:TRP:CD1	2:F:167:TYR:CD1	3.06	0.43
1:A:213:ARG:HA	1:A:213:ARG:HD3	1.94	0.43
1:A:33:LYS:O	1:A:36:LEU:HG	2.19	0.43
1:A:423:CYS:HB2	1:A:542:ALA:HB3	2.01	0.43
2:C:114:TRP:CD1	2:C:167:TYR:CE1	3.06	0.43
2:C:15:PHE:O	2:C:18:ARG:HB2	2.19	0.43
2:C:209:ALA:O	2:C:212:TYR:CE2	2.72	0.43
2:C:65:CYS:O	2:C:66:GLU:HB2	2.18	0.43
1:D:146:GLN:O	1:D:205:HIS:CD2	2.71	0.43
1:D:170:TYR:HB3	1:D:194:PHE:CZ	2.53	0.43
2:C:187:LYS:HD3	1:D:492:ASP:CB	2.49	0.43
2:E:26:LYS:HA	2:E:82:ASN:ND2	2.28	0.43
1:A:235:GLU:OE2	1:A:287:TRP:CD1	2.72	0.43
1:A:448:ALA:CB	1:A:497:LEU:HD12	2.49	0.43
1:D:120:ASN:CB	1:D:358:LEU:HD22	2.49	0.43
1:D:219:VAL:HB	1:D:295:PHE:HZ	1.84	0.43
1:D:442:GLN:HG2	1:D:462:PHE:CZ	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:87:PRO:CG	2:E:188:ARG:NE	2.78	0.43
2:E:15:PHE:HB3	2:E:67:SER:CB	2.48	0.43
2:F:213:ARG:NH1	2:F:217:LEU:HD21	2.34	0.43
2:F:81:LYS:O	2:F:83:PRO:HD3	2.19	0.43
1:A:273:LEU:O	1:A:277:ILE:HG22	2.19	0.42
1:A:336:TRP:CB	1:A:358:LEU:HD13	2.46	0.42
1:A:34:GLU:O	1:A:38:LYS:HG2	2.19	0.42
2:B:8:LEU:HD12	2:B:56:VAL:HB	2.00	0.42
1:D:151:SER:HB2	1:D:194:PHE:C	2.40	0.42
1:D:538:LEU:HD12	1:D:539:GLY:N	2.34	0.42
2:F:190:MET:HA	2:F:195:VAL:CG2	2.48	0.42
1:A:111:ILE:HG21	1:A:398:LEU:CD2	2.49	0.42
1:A:152:LYS:O	1:A:167:THR:HG21	2.19	0.42
1:A:31:THR:O	1:A:34:GLU:HG3	2.19	0.42
1:A:365:PRO:CG	1:A:374:GLU:HG2	2.48	0.42
1:A:466:ILE:O	1:A:466:ILE:HG13	2.19	0.42
1:A:108:PRO:CG	1:A:552:LYS:HG2	2.48	0.42
1:A:87:PRO:HD2	2:B:188:ARG:HB3	2.00	0.42
1:D:157:THR:OG1	1:D:469:SER:HB3	2.19	0.42
1:D:20:MET:HG3	1:D:21:THR:N	2.33	0.42
1:D:218:TYR:HE1	1:D:220:PHE:HB2	1.84	0.42
1:D:510:ARG:NH1	1:D:510:ARG:HG3	2.34	0.42
1:D:531:ILE:O	1:D:534:HIS:ND1	2.52	0.42
1:D:222:VAL:HG21	4:D:602:ILE:N	2.34	0.42
2:E:151:GLY:O	2:E:154:ASP:HB2	2.19	0.42
2:E:7:LEU:O	2:E:33:ARG:HB2	2.19	0.42
1:A:182:ILE:O	1:A:182:ILE:HG22	2.19	0.42
1:A:242:VAL:HG11	1:A:278:ARG:NE	2.34	0.42
1:A:432:ASN:CB	1:A:435:LYS:HD2	2.38	0.42
1:A:108:PRO:HB3	1:A:555:ASN:CB	2.48	0.42
1:A:91:GLY:HA2	2:B:143:PRO:N	2.34	0.42
2:B:183:ILE:O	2:B:186:ALA:HB3	2.19	0.42
1:D:77:ILE:CG2	1:D:110:PHE:HB3	2.49	0.42
1:D:143:LYS:HZ1	1:D:187:CYS:HB2	1.85	0.42
1:D:211:LEU:HD12	7:D:701:HOH:O	2.19	0.42
1:D:365:PRO:CB	1:D:374:GLU:HG2	2.48	0.42
1:D:522:VAL:O	1:D:566:VAL:HG23	2.19	0.42
2:E:124:GLY:HA2	2:E:127:GLU:OE1	2.19	0.42
2:E:65:CYS:HB2	2:F:97:PHE:CE1	2.55	0.42
2:F:126:LYS:O	2:F:129:ILE:HG13	2.18	0.42
2:F:153:VAL:HA	2:F:156:SER:OG	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:20:ARG:HB2	2:F:198:SER:OG	2.19	0.42
2:F:23:LEU:HA	2:F:74:VAL:CG1	2.44	0.42
2:F:77:ALA:C	2:F:79:PRO:HD3	2.39	0.42
1:A:113:PHE:CE1	1:A:333:SER:HB2	2.55	0.42
2:B:40:LYS:HE2	2:B:40:LYS:HB3	1.83	0.42
2:C:185:TRP:O	2:C:188:ARG:HB3	2.19	0.42
2:C:17:MET:CE	2:C:200:PRO:HD2	2.48	0.42
1:D:210:ILE:HD12	1:D:234:PHE:HZ	1.85	0.42
1:D:199:HIS:HA	1:D:525:LYS:HG2	2.01	0.42
1:D:94:VAL:HG11	1:D:112:PRO:CB	2.33	0.42
2:E:204:LYS:O	2:E:208:TYR:HD1	2.03	0.42
2:F:17:MET:O	2:F:21:VAL:HG23	2.18	0.42
1:A:245:ILE:HD13	1:A:267:LEU:HD21	2.01	0.42
1:A:23:ASN:O	1:A:27:VAL:HG23	2.19	0.42
1:A:302:TYR:HD1	1:A:326:VAL:HG13	1.85	0.42
1:A:328:HIS:O	1:A:352:PHE:CE1	2.72	0.42
1:A:396:ALA:HB2	7:A:808:HOH:O	2.19	0.42
1:A:78:LYS:HB3	1:A:78:LYS:HE3	1.74	0.42
1:A:98:SER:HB3	1:A:113:PHE:CE1	2.54	0.42
2:B:67:SER:HA	2:B:70:VAL:HG12	2.02	0.42
2:C:122:GLU:HA	2:C:125:LYS:HG3	2.02	0.42
2:C:143:PRO:HB2	2:C:144:TYR:CD2	2.54	0.42
2:C:81:LYS:HB3	2:C:81:LYS:HE2	1.79	0.42
1:D:166:THR:HA	1:D:169:VAL:HG12	2.02	0.42
1:D:227:LEU:HA	1:D:227:LEU:HD23	1.73	0.42
1:D:256:VAL:O	1:D:260:ARG:HG3	2.19	0.42
1:D:261:THR:HB	1:D:265:LYS:HZ1	1.83	0.42
1:D:305:MET:CG	1:D:347:PRO:HB3	2.48	0.42
1:D:87:PRO:HD2	2:E:188:ARG:HE	1.84	0.42
2:E:73:TYR:CE1	2:F:90:TYR:HA	2.54	0.42
2:F:98:TRP:HZ2	2:F:135:LEU:CG	2.21	0.42
1:A:388:TYR:O	1:A:407:VAL:HG12	2.19	0.42
1:A:408:LYS:HE3	1:A:420:LYS:CE	2.50	0.42
1:D:152:LYS:HE3	1:D:530:LYS:HE2	2.02	0.42
1:D:197:ASP:OD1	1:D:197:ASP:N	2.43	0.42
1:D:261:THR:C	1:D:265:LYS:HZ3	2.23	0.42
1:D:287:TRP:CD1	1:D:319:TYR:CD1	3.07	0.42
1:D:402:ARG:NH2	7:D:731:HOH:O	2.53	0.42
1:D:99:LEU:HB3	1:D:557:LYS:CB	2.43	0.42
2:E:152:TYR:O	2:E:155:ILE:HG13	2.20	0.42
2:E:52:LYS:HE3	2:E:52:LYS:HB2	1.91	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:PRO:HB2	7:A:755:HOH:O	2.20	0.42
1:A:203:TYR:HE1	1:A:237:VAL:HB	1.84	0.42
1:A:420:LYS:HB3	1:A:420:LYS:HE3	1.80	0.42
1:A:477:ILE:HG12	1:A:518:LEU:HD21	2.01	0.42
2:B:7:LEU:HG	7:B:418:HOH:O	2.20	0.42
2:B:99:ALA:O	2:B:102:VAL:HG13	2.20	0.42
1:D:437:THR:N	1:D:440:ASP:OD2	2.53	0.42
1:D:475:TYR:CD1	1:D:475:TYR:N	2.88	0.42
2:F:18:ARG:N	2:F:159:THR:HG21	2.34	0.42
1:A:62:LYS:HE3	1:A:62:LYS:HB3	1.87	0.42
1:D:10:MET:HG3	1:D:11:ASN:H	1.85	0.42
2:E:11:TRP:CE3	2:E:12:PRO:HD3	2.55	0.42
1:D:87:PRO:CG	2:E:188:ARG:HE	2.30	0.42
2:F:5:PRO:HB3	2:F:59:HIS:NE2	2.35	0.42
1:A:145:LEU:HD13	1:A:209:GLY:CA	2.48	0.42
1:A:118:MET:CE	1:A:169:VAL:HA	2.49	0.42
1:A:452:LEU:HD23	1:A:481:ILE:HG21	2.02	0.42
1:D:36:LEU:C	1:D:39:ASN:H	2.23	0.42
2:E:10:TYR:H	2:E:54:ILE:HD13	1.85	0.42
2:E:68:LEU:HD11	2:E:152:TYR:CZ	2.55	0.42
2:F:106:PHE:O	2:F:110:GLN:HG3	2.20	0.42
1:A:42:ALA:HA	2:B:143:PRO:CG	2.43	0.42
2:F:23:LEU:HD13	2:F:28:VAL:HG13	2.02	0.42
1:A:167:THR:HG21	1:A:560:GLN:HB3	2.02	0.41
1:A:295:PHE:HD1	1:A:295:PHE:O	2.02	0.41
1:A:227:LEU:HD13	1:A:316:LEU:HD21	2.02	0.41
1:A:527:THR:HB	1:A:561:ILE:HG21	2.02	0.41
1:D:127:THR:O	1:D:130:ALA:HB3	2.20	0.41
2:C:183:ILE:HD13	1:D:492:ASP:HA	2.02	0.41
1:D:94:VAL:HB	1:D:113:PHE:H	1.84	0.41
2:F:203:GLU:O	2:F:206:VAL:HG22	2.19	0.41
1:A:136:PHE:HD1	1:A:299:LYS:HE2	1.84	0.41
1:A:29:LYS:O	1:A:32:LEU:HB2	2.20	0.41
1:A:339:ALA:N	1:A:353:ALA:O	2.27	0.41
1:A:498:ASP:OD1	1:A:518:LEU:HB3	2.20	0.41
1:A:477:ILE:HG12	1:A:518:LEU:CD2	2.50	0.41
1:A:494:CYS:SG	1:A:572:SER:HA	2.59	0.41
2:C:98:TRP:HE3	2:C:101:PHE:HB2	1.85	0.41
2:C:166:ALA:O	2:C:170:PHE:HD2	2.03	0.41
2:C:188:ARG:HB2	2:C:188:ARG:HE	1.68	0.41
2:C:9:ASP:HB2	2:C:20:ARG:NH2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:149:PHE:CD2	1:D:202:LEU:HD22	2.55	0.41
1:D:151:SER:HB2	1:D:194:PHE:CA	2.50	0.41
1:D:358:LEU:H	1:D:358:LEU:HG	1.59	0.41
1:D:382:VAL:HG22	1:D:388:TYR:CD2	2.55	0.41
1:D:451:ARG:NH1	1:D:493:CYS:H	2.18	0.41
1:D:67:LEU:HB2	7:D:878:HOH:O	2.19	0.41
1:D:76:TYR:HB3	1:D:88:ILE:HG21	2.02	0.41
2:E:169:LYS:HE2	2:E:169:LYS:HB3	1.82	0.41
2:F:211:GLU:HA	2:F:214:LYS:HG2	2.01	0.41
1:A:210:ILE:HD12	7:A:847:HOH:O	2.20	0.41
1:A:80:MET:HE2	1:A:88:ILE:HD11	2.01	0.41
2:B:65:CYS:O	2:B:69:ASN:HB3	2.20	0.41
2:C:120:GLU:HB3	7:C:436:HOH:O	2.20	0.41
2:C:169:LYS:HB2	2:C:169:LYS:HE2	1.69	0.41
1:D:190:ASP:O	1:D:193:ILE:HB	2.20	0.41
1:D:223:PHE:HZ	1:D:536:LEU:HB2	1.76	0.41
1:D:46:GLN:NE2	2:E:148:ASP:OD2	2.54	0.41
2:E:183:ILE:HG13	2:E:184:ALA:N	2.34	0.41
1:A:103:THR:HB	1:A:106:GLY:HA2	2.02	0.41
1:A:143:LYS:HG3	1:A:144:ALA:N	2.34	0.41
1:A:574:ALA:O	1:A:575:PHE:HB2	2.21	0.41
2:C:123:ALA:HA	7:C:454:HOH:O	2.20	0.41
1:D:211:LEU:HD13	1:D:212:PHE:CD1	2.55	0.41
1:D:316:LEU:O	1:D:320:ALA:N	2.48	0.41
1:D:46:GLN:HE21	2:E:148:ASP:CB	2.33	0.41
2:F:125:LYS:HZ3	2:F:129:ILE:HG21	1.85	0.41
2:F:176:GLU:O	2:F:183:ILE:HG21	2.19	0.41
2:F:213:ARG:HH11	2:F:217:LEU:HD21	1.85	0.41
1:A:303:GLY:N	1:A:328:HIS:CE1	2.89	0.41
1:A:543:GLY:C	1:A:544:GLN:HG3	2.40	0.41
1:D:510:ARG:HB3	1:D:575:PHE:CE2	2.55	0.41
1:D:64:MET:O	1:D:66:PRO:HD3	2.20	0.41
2:E:99:ALA:O	2:E:102:VAL:HG12	2.21	0.41
2:E:125:LYS:HD2	2:E:173:PHE:CE2	2.54	0.41
2:E:93:ALA:HA	2:F:73:TYR:HE1	1.86	0.41
2:F:114:TRP:CD1	2:F:167:TYR:CE1	3.09	0.41
2:F:212:TYR:HD1	2:F:212:TYR:HA	1.78	0.41
1:A:222:VAL:HB	1:A:533:GLU:HB3	2.02	0.41
1:A:110:PHE:CD1	1:A:556:ALA:HB2	2.56	0.41
2:B:146:GLY:CA	2:B:151:GLY:HA3	2.50	0.41
2:C:73:TYR:HA	2:C:76:GLU:CD	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:75:PRO:O	1:D:79:ARG:HG3	2.20	0.41
1:D:39:ASN:OD1	2:E:141:ASP:O	2.38	0.41
2:E:183:ILE:O	2:E:186:ALA:HB3	2.20	0.41
2:E:68:LEU:HD11	2:E:152:TYR:HE1	1.84	0.41
2:E:76:GLU:OE2	2:F:92:ARG:HD3	2.21	0.41
1:A:77:ILE:HD12	1:A:112:PRO:HD3	2.03	0.41
1:A:119:GLU:CG	1:A:120:ASN:N	2.83	0.41
1:A:439:ARG:O	1:A:443:LEU:HB2	2.21	0.41
1:A:467:ASP:OD1	1:A:474:HIS:N	2.46	0.41
1:A:491:GLN:NE2	1:A:570:TYR:HB3	2.36	0.41
2:B:151:GLY:O	2:B:154:ASP:HB2	2.20	0.41
2:C:22:ALA:HB1	2:C:74:VAL:HG11	2.03	0.41
2:C:84:PHE:CZ	2:C:152:TYR:HD2	2.38	0.41
1:D:13:VAL:HG22	1:D:127:THR:HG23	2.03	0.41
1:D:11:ASN:O	1:D:14:ILE:HG13	2.21	0.41
1:D:286:ASN:O	1:D:287:TRP:HB3	2.21	0.41
1:D:316:LEU:HD12	1:D:316:LEU:HA	1.71	0.41
2:E:66:GLU:OE2	2:F:100:ASP:CB	2.69	0.41
2:F:10:TYR:CG	2:F:37:PHE:CE1	3.09	0.41
2:F:23:LEU:HD23	7:F:442:HOH:O	2.21	0.41
1:A:163:GLY:HA2	1:A:556:ALA:O	2.21	0.41
1:A:187:CYS:HB2	1:A:208:SER:O	2.21	0.41
1:A:225:HIS:NE2	1:A:529:ARG:HG3	2.36	0.41
1:A:312:TYR:HA	1:A:315:LYS:HZ3	1.86	0.41
1:A:433:ILE:HG21	1:A:552:LYS:NZ	2.36	0.41
2:B:114:TRP:HD1	2:B:167:TYR:HE1	1.67	0.41
2:C:125:LYS:HA	2:C:128:PHE:CD2	2.56	0.41
1:D:111:ILE:HD12	7:D:815:HOH:O	2.20	0.41
1:D:154:TYR:CZ	1:D:559:LEU:HB3	2.56	0.41
1:D:227:LEU:HD22	1:D:231:PHE:CE2	2.56	0.41
1:D:503:ASP:CG	1:D:504:ALA:N	2.73	0.41
1:D:510:ARG:HG2	1:D:515:ILE:CD1	2.46	0.41
1:D:528:PHE:O	1:D:531:ILE:HG12	2.20	0.41
1:D:99:LEU:HD12	1:D:100:SER:H	1.86	0.41
2:E:110:GLN:O	2:E:113:VAL:HG12	2.21	0.41
1:D:41:SER:HG	2:E:144:TYR:H	1.69	0.41
2:E:180:PRO:HD2	2:E:181:LYS:H	1.85	0.41
2:E:40:LYS:HZ1	2:E:52:LYS:HD2	1.81	0.41
1:A:27:VAL:CG1	1:A:356:PRO:HB2	2.51	0.41
1:A:234:PHE:CD2	1:A:287:TRP:CZ3	3.09	0.41
1:A:33:LYS:HA	1:A:36:LEU:CD2	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:546:LYS:HB2	1:A:546:LYS:HE3	1.73	0.41
1:A:95:PRO:HD2	1:A:113:PHE:O	2.20	0.41
2:B:151:GLY:O	2:B:155:ILE:HG13	2.21	0.41
2:C:140:GLY:C	2:C:181:LYS:HZ1	2.23	0.41
1:D:8:PHE:CD1	1:D:182:ILE:HG23	2.56	0.41
1:D:207:LEU:HD13	1:D:241:ILE:HG23	2.02	0.41
1:D:272:GLU:O	1:D:276:THR:HG23	2.21	0.41
1:D:333:SER:HG	1:D:333:SER:H	1.53	0.41
1:D:363:PHE:HB3	1:D:388:TYR:HB3	2.03	0.41
1:D:79:ARG:HB2	1:D:79:ARG:HE	1.65	0.41
2:E:15:PHE:CD1	2:E:15:PHE:N	2.88	0.41
2:F:135:LEU:HD13	2:F:182:LEU:CD1	2.51	0.41
2:F:92:ARG:HG3	7:F:402:HOH:O	2.20	0.41
1:A:374:GLU:HG3	1:A:375:LYS:N	2.35	0.41
1:A:433:ILE:HG21	1:A:552:LYS:HZ1	1.86	0.41
2:B:158:ILE:HG12	2:B:158:ILE:H	1.64	0.41
2:B:98:TRP:CZ2	2:B:138:GLU:HG2	2.56	0.41
2:C:14:MET:O	2:C:18:ARG:HG3	2.21	0.41
2:C:125:LYS:HE2	2:C:173:PHE:CE2	2.55	0.41
1:D:106:GLY:O	1:D:432:ASN:ND2	2.54	0.41
1:D:163:GLY:HA3	1:D:560:GLN:OE1	2.20	0.41
1:D:175:PHE:O	1:D:179:MET:HB2	2.21	0.41
1:D:434:ASP:HB2	1:D:550:CYS:CB	2.50	0.41
1:D:575:PHE:N	1:D:575:PHE:HD1	2.19	0.41
1:D:68:VAL:HG12	1:D:401:TYR:CB	2.50	0.41
1:D:76:TYR:C	1:D:88:ILE:HG21	2.42	0.41
1:A:551:VAL:HG11	1:A:558:VAL:CG1	2.47	0.41
2:B:110:GLN:HB2	2:B:167:TYR:OH	2.20	0.41
2:B:198:SER:O	2:B:200:PRO:HD3	2.21	0.41
2:B:24:ARG:HD2	2:B:24:ARG:HH11	1.69	0.41
2:C:114:TRP:CD1	2:C:167:TYR:HE1	2.39	0.41
2:C:70:VAL:HA	2:C:73:TYR:CD2	2.57	0.41
1:D:154:TYR:CE2	1:D:559:LEU:HB3	2.56	0.41
1:D:284:LEU:HD22	1:D:287:TRP:HA	2.03	0.41
1:D:38:LYS:HE2	7:D:862:HOH:O	2.21	0.41
1:D:390:VAL:HG11	1:D:540:SER:CA	2.46	0.41
1:D:398:LEU:N	1:D:398:LEU:HD12	2.36	0.41
1:D:496:CYS:CB	1:D:499:ARG:NH1	2.83	0.41
2:E:62:LYS:HB3	2:F:90:TYR:CE2	2.56	0.41
2:F:134:ILE:HG13	2:F:135:LEU:N	2.36	0.41
2:F:187:LYS:HB3	2:F:187:LYS:HE3	1.78	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:TYR:OH	1:A:241:ILE:HA	2.22	0.40
1:A:302:TYR:CG	1:A:328:HIS:HE1	2.38	0.40
1:A:67:LEU:HD23	1:A:400:ARG:HB3	2.02	0.40
1:A:98:SER:O	1:A:111:ILE:HG13	2.21	0.40
2:B:106:PHE:CZ	2:B:131:ALA:HB1	2.57	0.40
2:B:24:ARG:CD	2:B:197:LYS:NZ	2.81	0.40
1:D:116:GLU:N	7:D:768:HOH:O	2.54	0.40
1:D:192:VAL:HG23	1:D:259:VAL:CG2	2.52	0.40
1:D:262:ALA:O	1:D:265:LYS:HB2	2.21	0.40
1:D:108:PRO:HG3	1:D:551:VAL:HA	2.03	0.40
2:E:173:PHE:HA	2:E:173:PHE:HD1	1.80	0.40
2:E:162:SER:HB3	2:E:199:LEU:HD11	2.03	0.40
1:A:169:VAL:HG13	1:A:170:TYR:CE1	2.56	0.40
1:A:390:VAL:HG11	1:A:540:SER:C	2.41	0.40
1:A:152:LYS:HB3	1:A:563:CYS:SG	2.61	0.40
1:A:41:SER:HB3	2:B:144:TYR:H	1.86	0.40
2:C:105:LYS:HB2	2:C:105:LYS:HE3	1.84	0.40
1:D:213:ARG:HA	1:D:216:VAL:CG1	2.51	0.40
2:E:120:GLU:OE1	7:E:415:HOH:O	2.21	0.40
2:E:162:SER:HB3	2:E:199:LEU:CG	2.51	0.40
1:A:208:SER:HA	1:A:211:LEU:HG	2.04	0.40
1:A:274:ALA:C	1:A:278:ARG:HD2	2.42	0.40
1:A:290:LEU:HA	1:A:290:LEU:HD12	1.70	0.40
1:A:299:LYS:HB2	1:A:299:LYS:HE3	1.53	0.40
1:A:86:SER:HA	1:A:87:PRO:HD2	1.94	0.40
1:A:44:TYR:CD1	1:A:89:LEU:HA	2.56	0.40
2:B:84:PHE:CD1	2:B:84:PHE:N	2.89	0.40
1:D:226:GLY:HA2	1:D:529:ARG:CD	2.43	0.40
1:D:264:SER:HA	1:D:267:LEU:HD12	2.03	0.40
1:D:499:ARG:CZ	1:D:499:ARG:CB	2.98	0.40
1:D:559:LEU:HD23	1:D:559:LEU:HA	1.69	0.40
1:D:87:PRO:CG	1:D:93:PRO:HG3	2.51	0.40
1:A:111:ILE:HA	1:A:112:PRO:HD3	1.69	0.40
1:A:228:VAL:HG22	1:A:319:TYR:CE2	2.56	0.40
1:A:238:TRP:HZ2	1:A:282:MET:SD	2.43	0.40
1:A:375:LYS:H	1:A:375:LYS:HG2	1.53	0.40
1:A:437:THR:HG21	1:A:439:ARG:NH1	2.36	0.40
1:A:465:TYR:CG	1:A:466:ILE:N	2.89	0.40
1:A:547:MET:HA	1:A:548:PRO:HD3	1.76	0.40
2:B:167:TYR:N	2:B:167:TYR:CD1	2.83	0.40
1:D:132:ARG:HE	1:D:326:VAL:HG21	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:228:VAL:CG1	1:D:315:LYS:HD3	2.47	0.40
1:D:452:LEU:CG	1:D:457:ILE:HD11	2.52	0.40
1:D:465:TYR:CD1	1:D:551:VAL:HG23	2.53	0.40
2:E:101:PHE:CE2	2:E:135:LEU:HD11	2.56	0.40
2:E:151:GLY:N	2:E:154:ASP:OD2	2.49	0.40
1:D:87:PRO:HD2	2:E:188:ARG:HB3	2.02	0.40
1:A:164:THR:HA	1:A:557:LYS:HG3	2.04	0.40
1:A:329:ASP:HA	1:A:352:PHE:CD1	2.57	0.40
2:B:129:ILE:HA	2:B:129:ILE:HD13	1.89	0.40
2:B:35:GLU:HG3	2:B:44:LEU:CD2	2.52	0.40
2:C:33:ARG:HE	2:C:33:ARG:HB3	1.75	0.40
1:D:43:ILE:H	1:D:43:ILE:HG23	1.64	0.40
1:D:43:ILE:HG13	1:D:44:TYR:N	2.36	0.40
1:D:496:CYS:HA	1:D:499:ARG:CZ	2.50	0.40
1:D:81:VAL:HG21	1:D:110:PHE:HE2	1.77	0.40
2:F:166:ALA:HB2	7:F:453:HOH:O	2.21	0.40
2:F:43:LEU:H	2:F:43:LEU:HG	1.45	0.40

All (8) 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:A:234:PHE:O	2:F:177:SER:OG[1_554]	1.77	0.43
1:A:214:ASP:OD2	1:A:475:TYR:OH[1_545]	1.90	0.30
7:D:897:HOH:O	7:D:961:HOH:O[1_455]	2.06	0.14
7:A:831:HOH:O	7:A:847:HOH:O[1_565]	2.15	0.05
2:E:61:GLY:N	2:F:211:GLU:OE2[1_565]	2.16	0.04
7:B:411:HOH:O	7:C:456:HOH:O[1_565]	2.17	0.03
7:A:822:HOH:O	7:F:486:HOH:O[1_554]	2.17	0.03
7:D:918:HOH:O	7:D:930: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%)	531 (94%)	27 (5%)	9 (2%)	12	3
1	D	567/575 (99%)	544 (96%)	16 (3%)	7 (1%)	16	4
2	B	212/223 (95%)	198 (93%)	13 (6%)	1 (0%)	34	17
2	C	212/223 (95%)	200 (94%)	9 (4%)	3 (1%)	14	3
2	E	212/223 (95%)	200 (94%)	10 (5%)	2 (1%)	21	7
2	F	212/223 (95%)	198 (93%)	11 (5%)	3 (1%)	14	3
All	All	1982/2042 (97%)	1871 (94%)	86 (4%)	25 (1%)	15	3

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	286	ASN
1	A	513	LYS
1	A	540	SER
1	D	180	LYS
1	D	540	SER
1	D	542	ALA
2	E	141	ASP
1	A	287	TRP
2	C	140	GLY
1	D	437	THR
2	F	140	GLY
1	A	552	LYS
1	D	88	ILE
2	F	80	GLU
2	F	180	PRO
1	A	88	ILE
1	A	369	THR
2	C	66	GLU
1	A	574	ALA
1	D	368	GLU
1	D	552	LYS
2	B	82	ASN
2	E	66	GLU
2	C	83	PRO
1	A	523	VAL

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	499/505 (99%)	420 (84%)	79 (16%)	3	0
1	D	499/505 (99%)	424 (85%)	75 (15%)	3	0
2	B	187/195 (96%)	168 (90%)	19 (10%)	9	1
2	C	187/195 (96%)	167 (89%)	20 (11%)	8	1
2	E	187/195 (96%)	169 (90%)	18 (10%)	10	1
2	F	187/195 (96%)	159 (85%)	28 (15%)	3	0
All	All	1746/1790 (98%)	1507 (86%)	239 (14%)	4	0

All (239) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	MET
1	A	13	VAL
1	A	14	ILE
1	A	15	ASP
1	A	16	GLU
1	A	18	ASP
1	A	26	GLN
1	A	29	LYS
1	A	40	GLN
1	A	41	SER
1	A	61	PHE
1	A	65	VAL
1	A	71	VAL
1	A	72	GLU
1	A	73	LEU
1	A	78	LYS
1	A	84	ASP
1	A	88	ILE
1	A	90	THR
1	A	92	HIS
1	A	99	LEU
1	A	100	SER

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Mol	Chain	Res	Type
1	A	101	SER
1	A	103	THR
1	A	110	PHE
1	A	111	ILE
1	A	122	LEU
1	A	125	PHE
1	A	140	ASP
1	A	143	LYS
1	A	167	THR
1	A	180	LYS
1	A	184	SER
1	A	190	ASP
1	A	195	SER
1	A	197	ASP
1	A	205	HIS
1	A	208	SER
1	A	212	PHE
1	A	238	TRP
1	A	253	ARG
1	A	260	ARG
1	A	265	LYS
1	A	268	THR
1	A	276	THR
1	A	285	SER
1	A	288	TYR
1	A	294	LEU
1	A	305	MET
1	A	327	SER
1	A	333	SER
1	A	368	GLU
1	A	373	GLU
1	A	374	GLU
1	A	379	LEU
1	A	384	ILE
1	A	390	VAL
1	A	405	ASP
1	A	425	ARG
1	A	426	ASN
1	A	427	LEU
1	A	428	ILE
1	A	437	THR
1	A	443	LEU

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Mol	Chain	Res	Type
1	A	464	SER
1	A	468	VAL
1	A	477	ILE
1	A	494	CYS
1	A	507	VAL
1	A	511	LYS
1	A	514	THR
1	A	515	ILE
1	A	518	LEU
1	A	536	LEU
1	A	538	LEU
1	A	562	LEU
1	A	565	ASN
1	A	569	SER
1	A	573	THR
2	B	26	LYS
2	B	33	ARG
2	B	50	ILE
2	B	101	PHE
2	B	102	VAL
2	B	104	LYS
2	B	113	VAL
2	B	117	LYS
2	B	132	VAL
2	B	134	ILE
2	B	139	LEU
2	B	150	PHE
2	B	153	VAL
2	B	154	ASP
2	B	173	PHE
2	B	181	LYS
2	B	182	LEU
2	B	196	SER
2	B	208	TYR
2	C	14	MET
2	C	40	LYS
2	C	43	LEU
2	C	64	VAL
2	C	65	CYS
2	C	74	VAL
2	C	84	PHE
2	C	87	SER

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Mol	Chain	Res	Type
2	C	105	LYS
2	C	121	GLN
2	C	128	PHE
2	C	133	LYS
2	C	134	ILE
2	C	135	LEU
2	C	145	PHE
2	C	162	SER
2	C	173	PHE
2	C	176	GLU
2	C	188	ARG
2	C	198	SER
1	D	15	ASP
1	D	26	GLN
1	D	43	ILE
1	D	57	PRO
1	D	59	GLU
1	D	68	VAL
1	D	69	THR
1	D	79	ARG
1	D	87	PRO
1	D	90	THR
1	D	92	HIS
1	D	100	SER
1	D	104	SER
1	D	110	PHE
1	D	111	ILE
1	D	116	GLU
1	D	125	PHE
1	D	126	ARG
1	D	131	PHE
1	D	133	ASN
1	D	135	ASP
1	D	154	TYR
1	D	162	VAL
1	D	164	THR
1	D	176	LYS
1	D	188	SER
1	D	195	SER
1	D	198	VAL
1	D	202	LEU
1	D	204	CYS

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Mol	Chain	Res	Type
1	D	205	HIS
1	D	211	LEU
1	D	245	ILE
1	D	250	LEU
1	D	273	LEU
1	D	284	LEU
1	D	295	PHE
1	D	299	LYS
1	D	304	ILE
1	D	305	MET
1	D	318	HIS
1	D	323	LEU
1	D	326	VAL
1	D	329	ASP
1	D	333	SER
1	D	345	LEU
1	D	351	THR
1	D	364	LEU
1	D	379	LEU
1	D	406	VAL
1	D	416	THR
1	D	423	CYS
1	D	424	ARG
1	D	426	ASN
1	D	427	LEU
1	D	433	ILE
1	D	435	LYS
1	D	439	ARG
1	D	450	LYS
1	D	459	VAL
1	D	464	SER
1	D	482	SER
1	D	493	CYS
1	D	499	ARG
1	D	502	ILE
1	D	503	ASP
1	D	507	VAL
1	D	512	CYS
1	D	518	LEU
1	D	521	ARG
1	D	544	GLN
1	D	547	MET

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Mol	Chain	Res	Type
1	D	562	LEU
1	D	568	SER
1	D	575	PHE
2	E	11	TRP
2	E	47	SER
2	E	70	VAL
2	E	106	PHE
2	E	113	VAL
2	E	117	LYS
2	E	132	VAL
2	E	137	SER
2	E	142	LYS
2	E	148	ASP
2	E	150	PHE
2	E	152	TYR
2	E	153	VAL
2	E	155	ILE
2	E	173	PHE
2	E	183	ILE
2	E	187	LYS
2	E	204	LYS
2	F	8	LEU
2	F	28	VAL
2	F	30	PHE
2	F	41	SER
2	F	43	LEU
2	F	57	LEU
2	F	59	HIS
2	F	64	VAL
2	F	85	PHE
2	F	88	ASP
2	F	98	TRP
2	F	101	PHE
2	F	128	PHE
2	F	136	GLU
2	F	148	ASP
2	F	153	VAL
2	F	168	GLU
2	F	170	PHE
2	F	172	ASN
2	F	175	ILE
2	F	176	GLU

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Mol	Chain	Res	Type
2	F	178	GLU
2	F	181	LYS
2	F	182	LEU
2	F	195	VAL
2	F	202	SER
2	F	203	GLU
2	F	216	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	ASN
1	A	40	GLN
1	A	92	HIS
1	A	153	GLN
1	A	200	GLN
1	A	215	GLN
1	A	426	ASN
1	A	534	HIS
2	B	110	GLN
2	C	121	GLN
1	D	46	GLN
1	D	133	ASN
1	D	153	GLN
1	D	172	ASN
1	D	217	GLN
1	D	270	ASN
1	D	418	GLN
1	D	491	GLN
1	D	544	GLN
2	E	60	ASN
2	E	82	ASN
2	E	94	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.



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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 12 ligands modelled in this entry, 4 are 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	A	601	-	12,15,15	5.37	6 (50%)	12,19,19	2.46	6 (50%)
4	ILE	A	602	-	5,8,8	0.90	0	5,10,10	0.62	0
6	GSH	B	301	-	13,19,19	1.73	2 (15%)	15,24,24	1.39	3 (20%)
6	GSH	C	301	-	13,19,19	1.67	2 (15%)	15,24,24	1.92	4 (26%)
3	JAA	D	601	-	12,15,15	5.66	6 (50%)	12,19,19	2.91	8 (66%)
4	ILE	D	602	-	5,8,8	1.03	1 (20%)	5,10,10	0.68	0
6	GSH	E	301	-	13,19,19	1.65	2 (15%)	15,24,24	1.94	2 (13%)
6	GSH	F	301	-	13,19,19	1.67	2 (15%)	15,24,24	1.57	3 (20%)

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	A	601	-	-	0/7/22/22	0/1/1/1
4	ILE	A	602	-	-	0/6/10/10	0/0/0/0
6	GSH	B	301	-	-	0/18/24/24	0/0/0/0
6	GSH	C	301	-	-	0/18/24/24	0/0/0/0
3	JAA	D	601	-	-	0/7/22/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ILE	D	602	-	-	0/6/10/10	0/0/0/0
6	GSH	E	301	-	-	0/18/24/24	0/0/0/0
6	GSH	F	301	-	-	0/18/24/24	0/0/0/0

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	601	JAA	C05-C08	-13.91	1.29	1.52
3	A	601	JAA	C05-C08	-12.73	1.31	1.52
3	A	601	JAA	C06-C04	-9.81	1.27	1.53
3	D	601	JAA	C06-C04	-9.68	1.27	1.53
3	D	601	JAA	C10-C04	-3.99	1.47	1.53
3	A	601	JAA	C10-C04	-3.60	1.48	1.53
4	D	602	ILE	CG2-CB	-2.01	1.47	1.53
3	D	601	JAA	C06-C07	2.68	1.59	1.53
3	A	601	JAA	C06-C07	2.72	1.59	1.53
6	E	301	GSH	C2-N3	3.28	1.40	1.33
6	E	301	GSH	CD1-N2	3.33	1.40	1.34
6	C	301	GSH	C2-N3	3.41	1.40	1.33
6	C	301	GSH	CD1-N2	3.48	1.41	1.34
6	F	301	GSH	CD1-N2	3.52	1.41	1.34
6	F	301	GSH	C2-N3	3.55	1.41	1.33
6	B	301	GSH	CD1-N2	3.73	1.41	1.34
6	B	301	GSH	C2-N3	3.82	1.41	1.33
3	D	601	JAA	C05-C04	4.99	1.67	1.55
3	A	601	JAA	C05-C04	5.08	1.67	1.55
3	A	601	JAA	C07-C08	6.34	1.62	1.50
3	D	601	JAA	C07-C08	6.86	1.63	1.50

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	E	301	GSH	CA2-CB2-SG2	-6.12	107.26	113.99
6	C	301	GSH	CA3-N3-C2	-4.64	115.80	122.36
3	D	601	JAA	C07-C06-C04	-4.47	100.06	104.57
3	D	601	JAA	C09-C11-C13	-3.72	113.30	126.48
3	D	601	JAA	C14-C13-C11	-3.64	110.18	127.15
3	A	601	JAA	C07-C08-C05	-3.45	106.06	109.04
6	C	301	GSH	O2-C2-N3	-3.15	116.78	123.04
6	C	301	GSH	CA2-CB2-SG2	-3.02	110.67	113.99
6	F	301	GSH	CA3-N3-C2	-2.99	118.14	122.36
3	A	601	JAA	C09-C11-C13	-2.84	116.44	126.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	E	301	GSH	CA2-N2-CD1	-2.78	115.67	121.72
6	F	301	GSH	O2-C2-N3	-2.75	117.56	123.04
6	B	301	GSH	CA2-CB2-SG2	-2.71	111.01	113.99
3	A	601	JAA	C14-C13-C11	-2.59	115.06	127.15
6	B	301	GSH	O2-C2-N3	-2.57	117.94	123.04
6	F	301	GSH	CA2-CB2-SG2	-2.56	111.17	113.99
3	D	601	JAA	C07-C08-C05	-2.26	107.08	109.04
3	D	601	JAA	C06-C07-C08	-2.25	103.12	105.47
6	B	301	GSH	CA3-N3-C2	-2.04	119.48	122.36
3	A	601	JAA	C04-C05-C08	2.61	107.91	103.85
3	D	601	JAA	O01-C08-C05	2.69	128.88	125.41
6	C	301	GSH	CA2-C2-N3	2.76	122.30	116.66
3	A	601	JAA	C07-C06-C04	3.46	108.07	104.57
3	D	601	JAA	C06-C04-C05	3.67	108.75	103.44
3	D	601	JAA	C05-C09-C11	4.36	119.61	113.22
3	A	601	JAA	C06-C04-C05	4.63	110.12	103.44

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	601	JAA	1	0
4	A	602	ILE	4	0
6	B	301	GSH	3	0
6	C	301	GSH	1	0
3	D	601	JAA	1	0
4	D	602	ILE	1	0
6	E	301	GSH	2	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<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%)	0.43	16 (2%) 56 54	2, 5, 9, 13	0
1	D	569/575 (98%)	0.28	4 (0%) 89 88	2, 4, 7, 13	0
2	B	214/223 (95%)	0.15	0 100 100	2, 3, 6, 11	0
2	C	214/223 (95%)	0.16	4 (1%) 70 69	2, 3, 5, 9	0
2	E	214/223 (95%)	0.26	4 (1%) 70 69	2, 5, 8, 13	0
2	F	214/223 (95%)	0.19	1 (0%) 91 91	2, 4, 9, 22	0
All	All	1994/2042 (97%)	0.29	29 (1%) 76 76	2, 4, 8, 22	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	212	PHE	7.7
2	E	150	PHE	4.5
1	A	247	ASP	4.4
1	A	288	TYR	4.2
1	A	213	ARG	3.8
1	A	210	ILE	3.3
2	E	152	TYR	3.3
1	A	295	PHE	3.2
2	C	212	TYR	3.2
2	E	98	TRP	3.2
1	A	151	SER	3.1
2	C	32	TYR	2.8
1	D	370	GLY	2.7
2	F	86	PRO	2.6
1	A	305	MET	2.5
1	D	433	ILE	2.5
1	A	426	ASN	2.4
1	A	143	LYS	2.4
1	A	559	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	234	PHE	2.3
2	C	209	ALA	2.3
1	A	494	CYS	2.2
2	C	157	LEU	2.2
1	A	103	THR	2.1
1	A	209	GLY	2.1
1	D	285	SER	2.1
1	D	125	PHE	2.1
1	A	382	VAL	2.0
2	E	217	LEU	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	JAA	D	601	15/15	0.92	0.16	1.25	2,4,7,9	0
4	ILE	D	602	9/9	0.86	0.15	1.15	2,2,4,6	0
3	JAA	A	601	15/15	0.93	0.14	0.03	2,2,6,7	0
4	ILE	A	602	9/9	0.91	0.13	-0.14	2,2,4,5	0
6	GSH	F	301	20/20	0.97	0.08	-1.34	2,2,2,3	0
6	GSH	B	301	20/20	0.97	0.09	-1.36	2,2,3,5	0
6	GSH	E	301	20/20	0.96	0.09	-1.60	2,2,6,9	0
6	GSH	C	301	20/20	0.95	0.09	-1.62	2,2,4,8	0
5	MG	D	603	1/1	0.98	0.09	-2.42	9,9,9,9	0
5	MG	D	605	1/1	0.99	0.04	-3.13	9,9,9,9	0
5	MG	A	603	1/1	0.96	0.07	-6.04	10,10,10,10	0
5	MG	D	604	1/1	0.98	0.05	-	10,10,10,10	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.