



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 24, 2016 – 05:57 PM EDT

PDB ID : 5ECQ  
Title : Crystal Structure of FIN219-FIP1 complex with JA, VAL and ATP  
Authors : Chen, C.Y.; Cheng, Y.S.  
Deposited on : 2015-10-20  
Resolution : 1.66 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

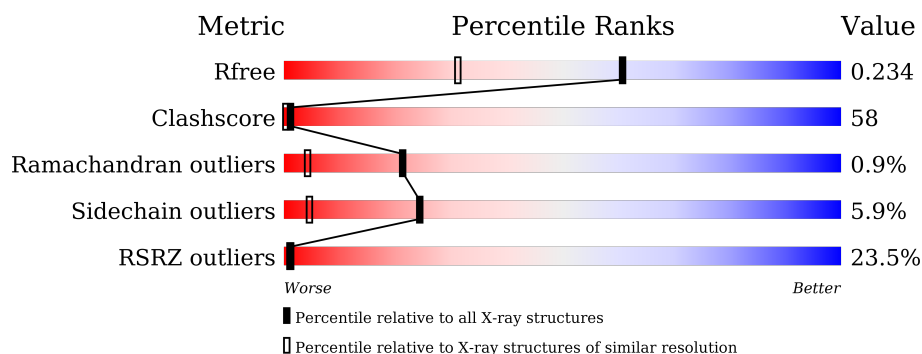
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.66 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	1226 (1.66-1.66)
Clashscore	102246	1323 (1.66-1.66)
Ramachandran outliers	100387	1295 (1.66-1.66)
Sidechain outliers	100360	1295 (1.66-1.66)
RSRZ outliers	91569	1227 (1.66-1.66)

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>27%</div> <div>31%</div> <div>62%</div> <div>6%</div> </div>
1	D	575	<div> <div>25%</div> <div>23%</div> <div>67%</div> <div>8%</div> </div>
2	B	223	<div> <div>22%</div> <div>33%</div> <div>57%</div> <div>6%</div> </div>
2	C	223	<div> <div>18%</div> <div>42%</div> <div>52%</div> <div>.</div> </div>
2	E	223	<div> <div>20%</div> <div>28%</div> <div>63%</div> <div>.</div> </div>
2	F	223	<div> <div>15%</div> <div>41%</div> <div>52%</div> <div>.</div> </div>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	JAA	A	601	-	-	X	-
3	JAA	D	601	-	-	-	X
4	VAL	A	602	-	-	X	-
4	VAL	D	602	-	-	X	-
5	ATP	A	603	-	-	X	-
5	ATP	D	603	-	-	X	-

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 17969 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:

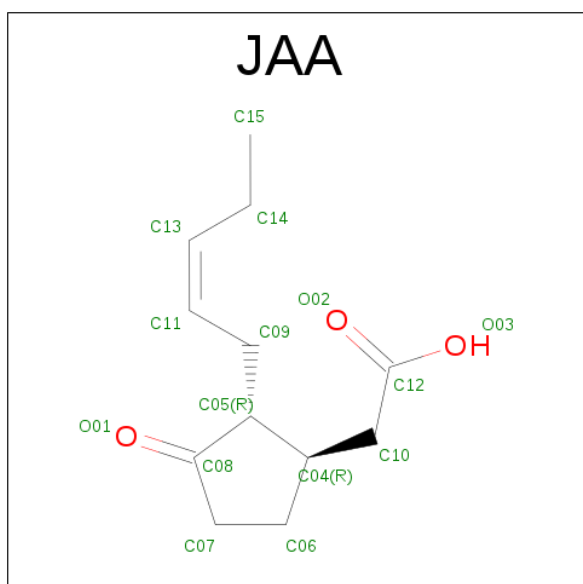
Chain	Residue	Modelled	Actual	Comment	Reference
B	-5	HIS	-	expression tag	UNP Q8L7C9
B	-4	HIS	-	expression tag	UNP Q8L7C9
B	-3	HIS	-	expression tag	UNP Q8L7C9
B	-2	HIS	-	expression tag	UNP Q8L7C9
B	-1	HIS	-	expression tag	UNP Q8L7C9
B	0	HIS	-	expression tag	UNP Q8L7C9
C	-5	HIS	-	expression tag	UNP Q8L7C9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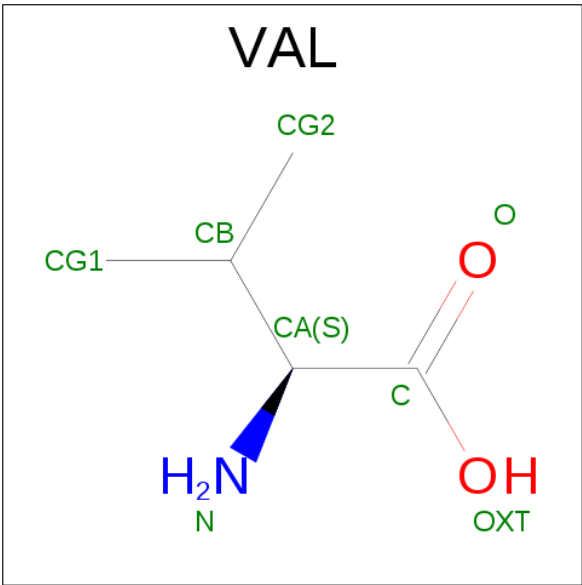
Chain	Residue	Modelled	Actual	Comment	Reference
E	-5	HIS	-	expression tag	UNP Q8L7C9
E	-4	HIS	-	expression tag	UNP Q8L7C9
E	-3	HIS	-	expression tag	UNP Q8L7C9
E	-2	HIS	-	expression tag	UNP Q8L7C9
E	-1	HIS	-	expression tag	UNP Q8L7C9
E	0	HIS	-	expression tag	UNP Q8L7C9
F	-5	HIS	-	expression tag	UNP Q8L7C9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



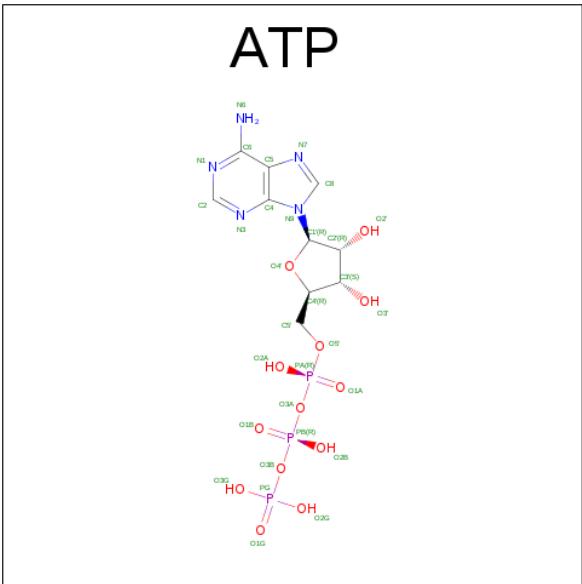
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			15	12	3		
3	D	1	Total	C	O	0	0
			15	12	3		

- Molecule 4 is VALINE (three-letter code: VAL) (formula: C<sub>5</sub>H<sub>11</sub>NO<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			8	5	1	2		
4	D	1	Total	C	N	O	0	0
			8	5	1	2		

- Molecule 5 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>).



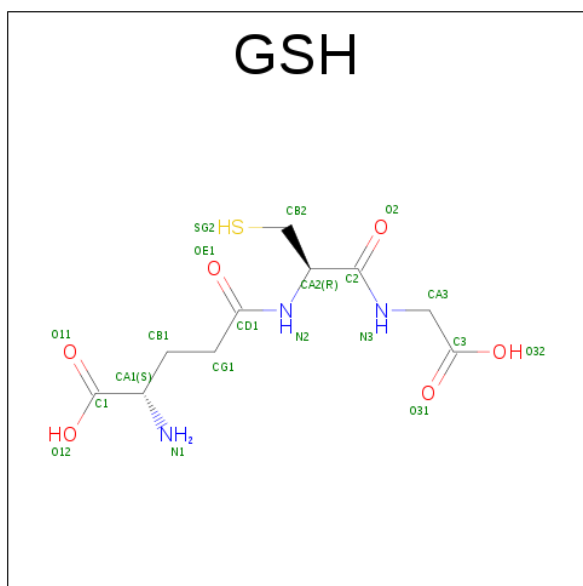
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	D	1	Total	C	N	O	P	0	0
			31	10	5	13	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	459	Total	O	0	0
			459	459		
7	B	252	Total	O	0	0
			252	252		
7	C	193	Total	O	0	0
			193	193		
7	D	506	Total	O	0	0
			506	506		

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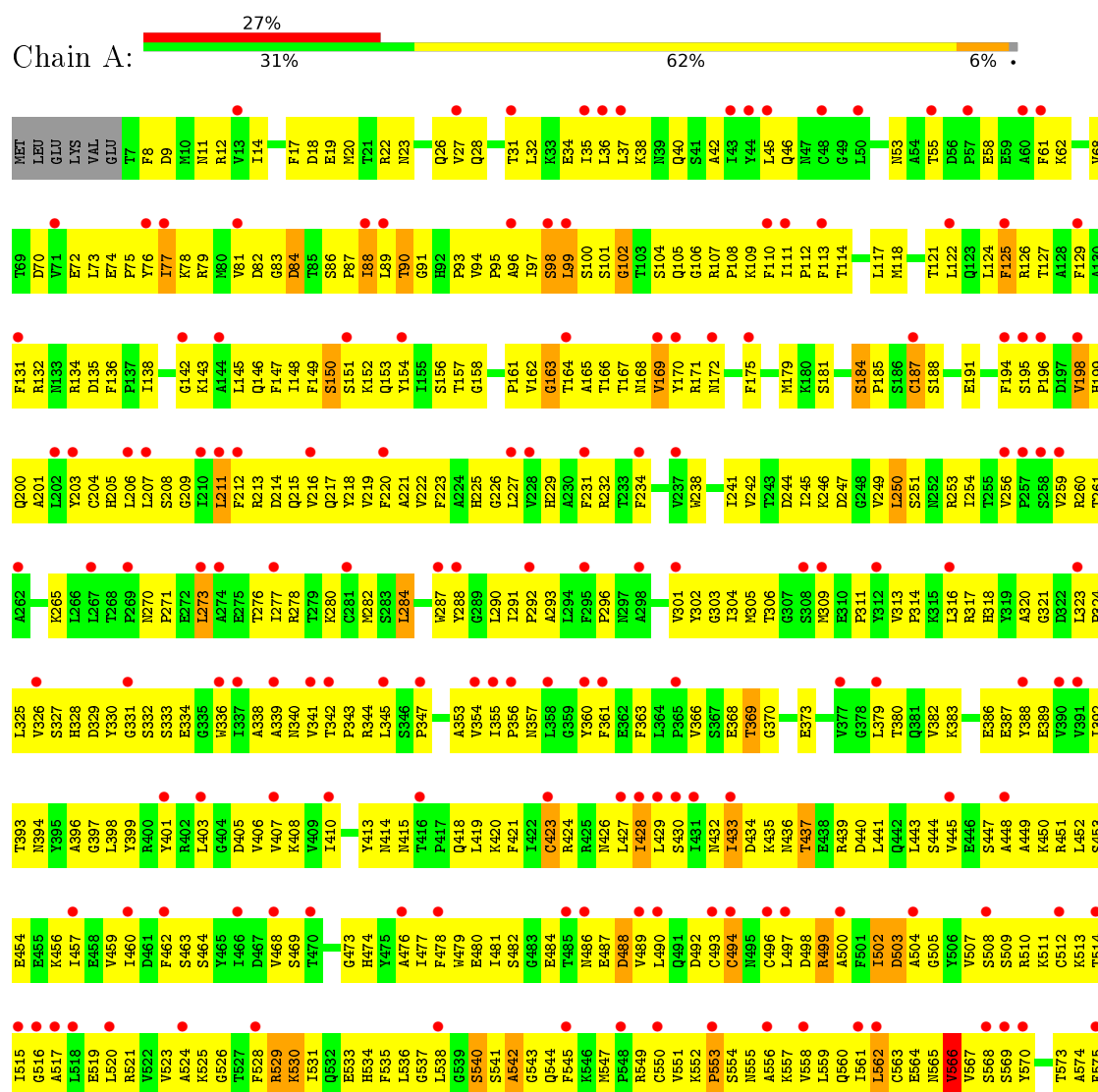
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	E	229	Total 229	O 229	0	0
7	F	192	Total 192	O 192	0	0

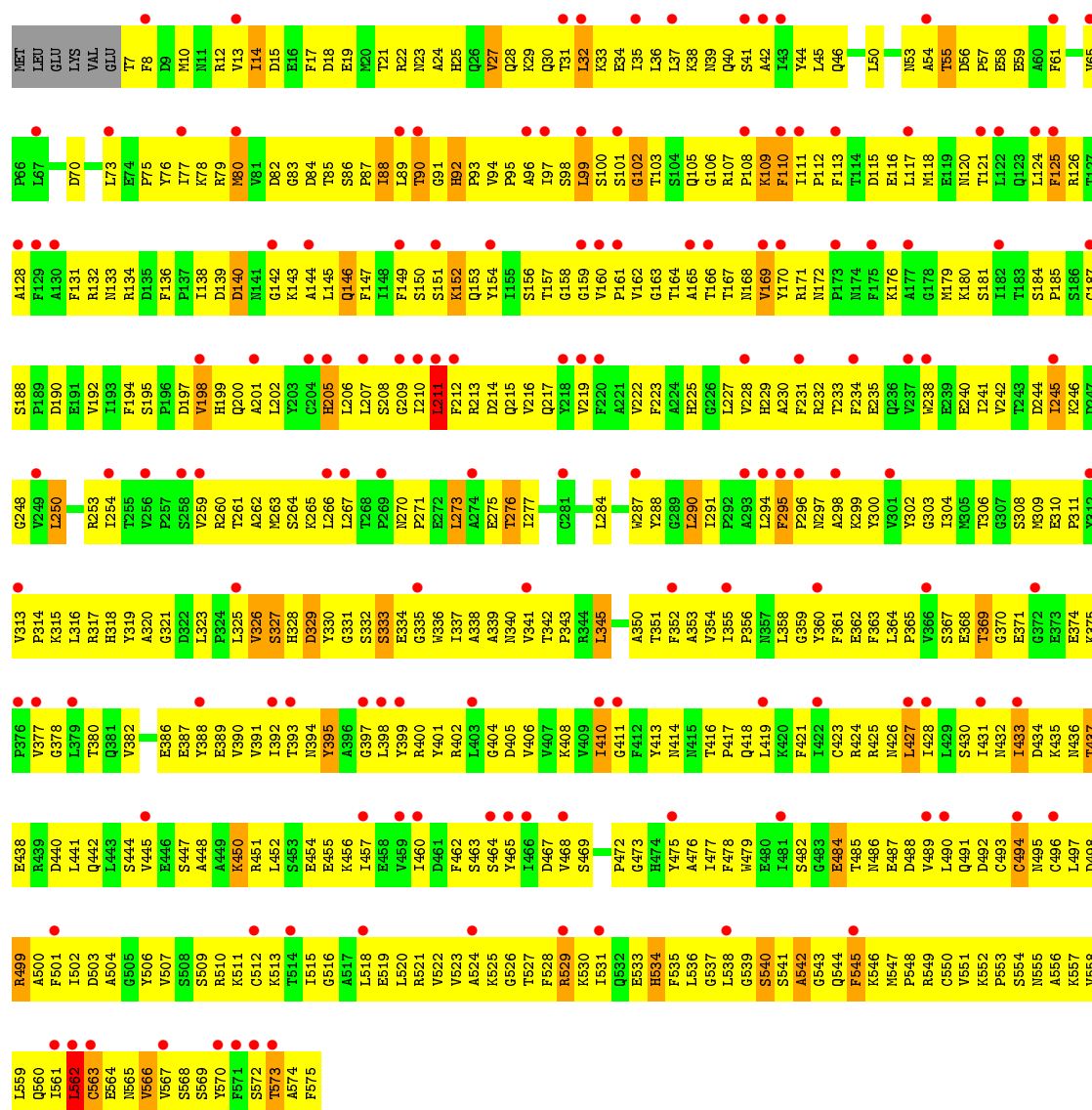


### 3 Residue-property plots

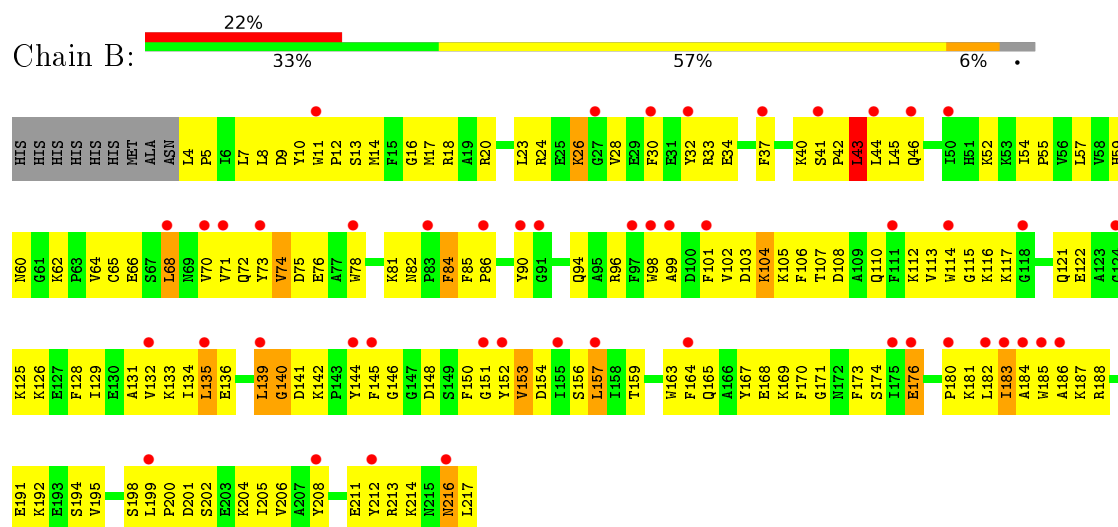
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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





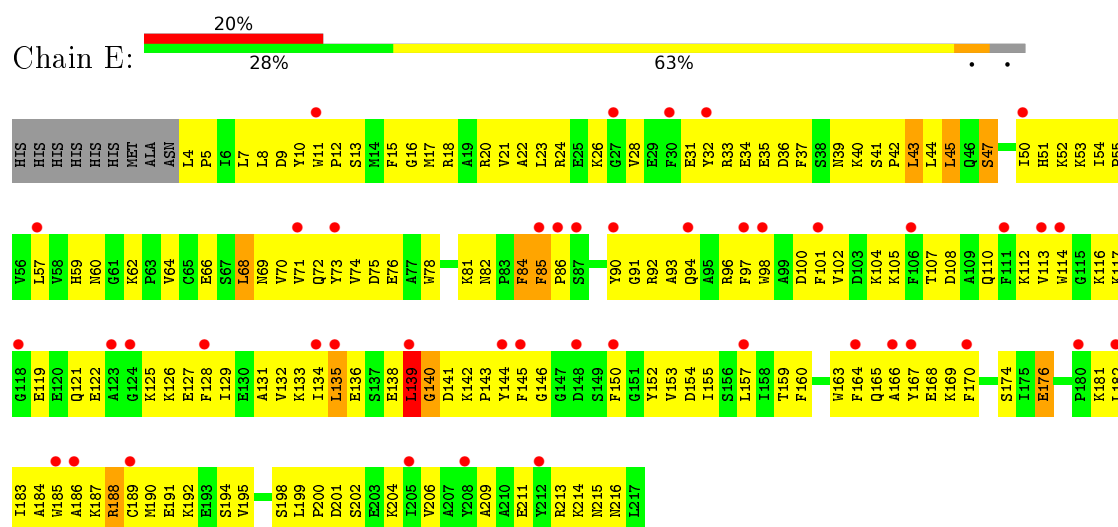
### • Molecule 2: Glutathione S-transferase U20



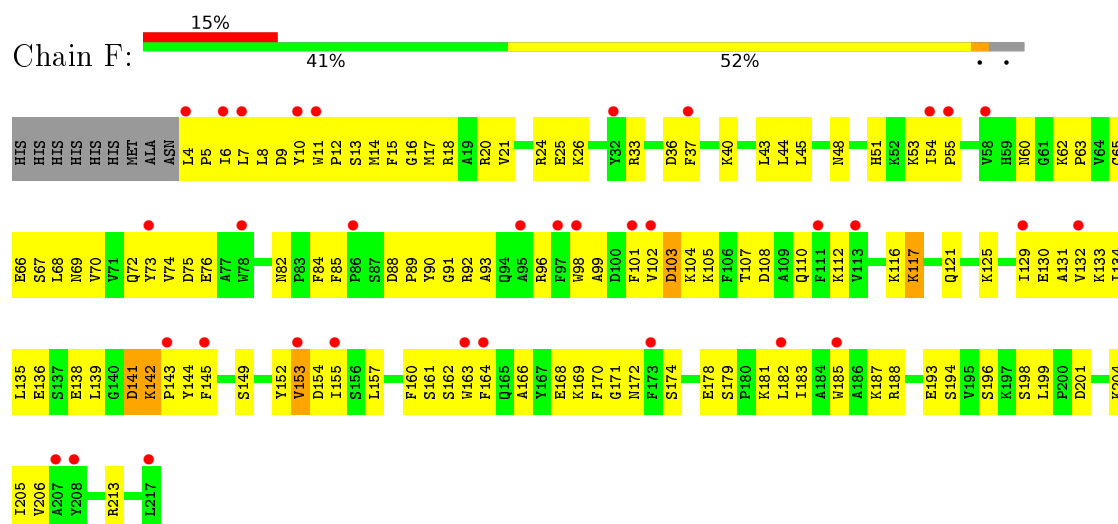
• Molecule 2: Glutathione S-transferase U20



• Molecule 2: Glutathione S-transferase U20



• Molecule 2: Glutathione S-transferase U20



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	53.84Å 53.87Å 196.27Å 92.25° 97.17° 113.72°	Depositor
Resolution (Å)	24.54 – 1.66 24.54 – 1.66	Depositor EDS
% Data completeness (in resolution range)	98.9 (24.54-1.66) 95.4 (24.54-1.66)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.70 (at 1.66Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692+SVN)	Depositor
R, $R_{free}$	0.228 , 0.234 0.228 , 0.234	Depositor DCC
$R_{free}$ test set	23271 reflections (9.99%)	DCC
Wilson B-factor (Å <sup>2</sup> )	-3.4	Xtriage
Anisotropy	-0.302	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.54 , 266.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.079 for k,h,-h-k-l 0.008 for -k,-h,l 0.008 for -h,-k,h+k+l	Xtriage
$F_o, F_c$ correlation	0.81	EDS
Total number of atoms	17969	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 47.18 % 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 1.0294e-04. 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, ATP, 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	0.49	0/4581	0.90	13/6219 (0.2%)
1	D	0.50	0/4581	0.93	13/6219 (0.2%)
2	B	0.45	0/1799	0.85	3/2428 (0.1%)
2	C	0.38	0/1799	0.70	1/2428 (0.0%)
2	E	0.46	0/1799	0.81	5/2428 (0.2%)
2	F	0.37	0/1799	0.69	0/2428
All	All	0.46	0/16358	0.85	35/22150 (0.2%)

There are no bond length outliers.

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	135	LEU	CB-CG-CD1	-9.66	94.58	111.00
1	D	211	LEU	CA-CB-CG	8.89	135.75	115.30
2	C	153	VAL	CA-CB-CG2	8.55	123.73	110.90
2	E	139	LEU	CB-CG-CD2	-7.73	97.86	111.00
1	D	563	CYS	N-CA-C	7.35	130.84	111.00
1	D	102	GLY	N-CA-C	-7.33	94.77	113.10
1	A	428	ILE	N-CA-C	-7.03	92.01	111.00
1	D	169	VAL	CA-CB-CG2	6.99	121.39	110.90
1	A	102	GLY	N-CA-C	-6.94	95.74	113.10
1	A	563	CYS	N-CA-C	6.77	129.27	111.00
1	D	562	LEU	CA-CB-CG	6.74	130.81	115.30
2	B	43	LEU	CA-CB-CG	6.72	130.76	115.30
1	A	566	VAL	N-CA-C	-6.48	93.51	111.00
1	D	427	LEU	N-CA-C	6.22	127.79	111.00
1	D	99	LEU	CA-CB-CG	6.20	129.56	115.30
1	A	163	GLY	N-CA-C	6.15	128.47	113.10
2	E	188	ARG	NE-CZ-NH1	-6.15	117.22	120.30
1	A	99	LEU	CA-CB-CG	6.10	129.34	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	427	LEU	N-CA-C	6.03	127.29	111.00
1	A	198	VAL	CA-CB-CG2	5.93	119.80	110.90
2	E	68	LEU	CA-CB-CG	5.93	128.94	115.30
1	A	169	VAL	CB-CA-C	-5.88	100.24	111.40
1	D	32	LEU	CA-CB-CG	5.88	128.81	115.30
2	B	68	LEU	CA-CB-CG	5.75	128.53	115.30
1	D	428	ILE	N-CA-C	-5.70	95.60	111.00
1	A	562	LEU	CA-CB-CG	5.68	128.37	115.30
1	A	211	LEU	CB-CG-CD1	-5.24	102.09	111.00
1	A	90	THR	N-CA-C	-5.24	96.86	111.00
1	A	84	ASP	N-CA-C	-5.20	96.96	111.00
1	D	198	VAL	CA-CB-CG2	5.18	118.67	110.90
1	D	395	TYR	CA-CB-CG	5.16	123.20	113.40
2	E	36	ASP	N-CA-C	-5.10	97.22	111.00
1	D	566	VAL	N-CA-C	-5.07	97.32	111.00
1	D	88	ILE	N-CA-C	5.06	124.66	111.00
2	E	45	LEU	CA-CB-CG	5.04	126.90	115.30

There are no chirality outliers.

There are no planarity outliers.

## 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	543	2
1	D	4479	0	4434	652	1
2	B	1748	0	1704	226	0
2	C	1748	0	1704	138	0
2	E	1748	0	1704	232	0
2	F	1748	0	1704	135	1
3	A	15	0	0	7	0
3	D	15	0	0	2	0
4	A	8	0	8	8	0
4	D	8	0	8	5	0
5	A	31	0	8	22	0
5	D	31	0	8	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	20	0	15	0	0
6	C	20	0	15	2	0
6	E	20	0	15	5	0
6	F	20	0	15	5	0
7	A	459	0	0	97	2
7	B	252	0	0	44	1
7	C	193	0	0	15	1
7	D	506	0	0	112	3
7	E	229	0	0	47	1
7	F	192	0	0	34	1
All	All	17969	0	15776	1835	9

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 58.

All (1835) 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:500:ALA:HA	2:E:188:ARG:HH12	1.14	1.11
1:D:456:LYS:NZ	2:E:201:ASP:OD2	1.86	1.09
1:A:499:ARG:O	2:B:188:ARG:NH1	1.88	1.07
1:A:500:ALA:HA	2:B:188:ARG:HH12	1.02	1.06
1:D:491:GLN:O	7:D:701:HOH:O	1.73	1.05
2:B:40:LYS:NZ	7:B:402:HOH:O	1.91	1.03
1:A:99:LEU:HG	1:A:557:LYS:HB2	1.39	1.02
2:F:66:GLU:OE2	7:F:401:HOH:O	1.78	1.02
1:D:88:ILE:HD12	1:D:89:LEU:H	1.26	0.98
1:A:492:ASP:OD2	7:A:701:HOH:O	1.79	0.98
2:E:165:GLN:O	7:E:401:HOH:O	1.81	0.98
1:A:187:CYS:SG	7:A:736:HOH:O	2.13	0.98
5:D:603:ATP:O2B	7:D:702:HOH:O	1.82	0.97
1:D:499:ARG:O	2:E:188:ARG:NH1	1.98	0.96
1:A:163:GLY:HA2	1:A:560:GLN:HB2	1.47	0.95
1:A:500:ALA:HA	2:B:188:ARG:NH1	1.81	0.95
1:D:70:ASP:OD2	1:D:109:LYS:NZ	1.99	0.95
1:D:452:LEU:HB3	1:D:457:ILE:HD11	1.49	0.95
1:A:226:GLY:HA3	1:A:529:ARG:HH11	1.31	0.94
1:A:105:GLN:HA	1:A:430:SER:HB3	1.47	0.94
1:A:199:HIS:HB3	1:A:525:LYS:H	1.35	0.92
1:D:500:ALA:CA	2:E:188:ARG:HH12	1.81	0.91
2:C:181:LYS:HE3	1:D:95:PRO:HD3	1.53	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:392:ILE:HB	1:D:398:LEU:HD11	1.51	0.90
2:B:66:GLU:OE2	7:B:401:HOH:O	1.86	0.90
1:D:176:LYS:NZ	1:D:190:ASP:OD2	2.05	0.90
1:A:77:ILE:HD13	1:A:110:PHE:HB2	1.53	0.90
1:D:462:PHE:O	1:D:549:ARG:NH1	2.04	0.89
1:A:573:THR:OG1	2:B:176:GLU:OE2	1.90	0.88
1:D:477:ILE:HG12	1:D:518:LEU:HD11	1.56	0.87
1:A:199:HIS:H	1:A:524:ALA:HB1	1.39	0.86
1:A:98:SER:HB3	5:A:603:ATP:PG	2.14	0.86
1:A:152:LYS:HA	1:A:564:GLU:HB2	1.56	0.86
1:A:143:LYS:HD2	1:A:212:PHE:HB2	1.56	0.86
1:D:198:VAL:HA	1:D:201:ALA:HB3	1.55	0.86
1:D:521:ARG:HB3	1:D:566:VAL:HG12	1.57	0.86
1:A:541:SER:O	1:A:543:GLY:N	2.08	0.86
1:D:152:LYS:NZ	1:D:565:ASN:HB2	1.90	0.86
1:A:152:LYS:HE3	1:A:565:ASN:HB2	1.56	0.86
1:D:152:LYS:HA	1:D:564:GLU:HB2	1.58	0.86
1:D:495:ASN:ND2	1:D:572:SER:OG	2.08	0.86
1:A:226:GLY:HA3	1:A:529:ARG:NH1	1.90	0.85
2:B:98:TRP:CH2	2:B:135:LEU:HD11	2.10	0.85
1:D:424:ARG:HD2	1:D:425:ARG:HH11	1.42	0.85
1:A:487:GLU:OE2	7:A:702:HOH:O	1.95	0.84
1:A:28:GLN:HE21	1:A:379:LEU:HD22	1.42	0.84
1:A:28:GLN:NE2	7:A:706:HOH:O	2.06	0.84
2:E:188:ARG:NH2	7:E:409:HOH:O	2.10	0.84
1:D:208:SER:HA	1:D:211:LEU:HG	1.59	0.84
1:D:519:GLU:OE2	1:D:569:SER:OG	1.95	0.84
1:D:541:SER:O	1:D:543:GLY:N	2.11	0.84
1:A:229:HIS:HA	1:A:232:ARG:HE	1.40	0.83
1:D:291:ILE:O	7:D:703:HOH:O	1.94	0.83
1:A:529:ARG:NH1	1:A:533:GLU:OE2	2.11	0.83
1:D:500:ALA:HA	2:E:188:ARG:NH1	1.94	0.83
2:B:74:VAL:O	7:B:403:HOH:O	1.95	0.83
1:D:88:ILE:O	7:D:704:HOH:O	1.95	0.83
1:A:557:LYS:NZ	5:A:603:ATP:O2G	2.12	0.83
2:E:190:MET:SD	7:E:558:HOH:O	2.38	0.82
1:A:142:GLY:HA2	1:A:215:GLN:HB2	1.61	0.82
2:E:132:VAL:HG23	2:E:182:LEU:HD13	1.62	0.82
1:A:198:VAL:HA	1:A:201:ALA:HB3	1.61	0.82
1:A:19:GLU:O	1:A:23:ASN:ND2	2.11	0.82
1:A:493:CYS:SG	7:A:711:HOH:O	2.37	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:534:HIS:CD2	1:A:557:LYS:HZ3	1.98	0.81
1:A:97:ILE:H	1:A:163:GLY:H	1.26	0.81
2:E:76:GLU:OE2	7:E:402:HOH:O	1.95	0.81
1:A:521:ARG:HH11	1:A:562:LEU:HD21	1.44	0.81
1:D:106:GLY:O	1:D:432:ASN:ND2	2.13	0.81
5:D:603:ATP:N6	7:D:720:HOH:O	2.14	0.81
1:A:150:SER:HB2	1:A:167:THR:HA	1.62	0.81
2:B:76:GLU:HG3	2:C:89:PRO:HB3	1.61	0.81
1:D:499:ARG:CZ	2:E:184:ALA:HB1	2.09	0.81
1:A:223:PHE:CZ	1:A:536:LEU:HB3	2.16	0.80
2:B:125:LYS:NZ	7:B:412:HOH:O	2.14	0.80
1:D:164:THR:OG1	1:D:557:LYS:O	1.99	0.80
1:A:145:LEU:HD13	1:A:209:GLY:HA3	1.63	0.80
1:D:143:LYS:HD2	1:D:212:PHE:HB2	1.62	0.80
1:D:499:ARG:NH1	2:E:184:ALA:HB1	1.96	0.80
2:F:15:PHE:HA	2:F:18:ARG:HD2	1.62	0.80
2:B:62:LYS:NZ	7:B:409:HOH:O	2.12	0.80
1:D:108:PRO:HG2	1:D:552:LYS:H	1.47	0.80
1:A:166:THR:HG21	1:A:530:LYS:HD2	1.63	0.79
1:A:222:VAL:HG21	4:A:602:VAL:HG22	1.63	0.79
1:D:89:LEU:O	7:D:707:HOH:O	2.00	0.79
1:D:354:VAL:O	7:D:706:HOH:O	2.00	0.79
1:D:138:ILE:HB	1:D:217:GLN:HG3	1.63	0.79
1:D:107:ARG:HH22	1:D:552:LYS:HD3	1.48	0.79
1:A:164:THR:OG1	1:A:557:LYS:O	2.00	0.79
1:D:400:ARG:NH1	7:D:723:HOH:O	2.15	0.79
1:D:509:SER:O	1:D:513:LYS:N	2.17	0.78
2:F:48:ASN:ND2	7:F:411:HOH:O	2.17	0.78
2:E:144:TYR:HB3	2:E:154:ASP:OD2	1.84	0.78
1:D:338:ALA:HA	1:D:354:VAL:HA	1.65	0.78
2:C:145:PHE:N	2:C:154:ASP:OD2	2.17	0.78
2:B:217:LEU:O	7:B:404:HOH:O	2.02	0.77
1:A:153:GLN:HG2	1:A:167:THR:HG21	1.67	0.77
5:A:603:ATP:O1B	7:A:703:HOH:O	2.03	0.77
1:D:199:HIS:HB3	1:D:525:LYS:H	1.49	0.77
1:D:345:LEU:HD13	1:D:350:ALA:HA	1.65	0.77
1:D:132:ARG:O	1:D:136:PHE:N	2.17	0.77
2:E:98:TRP:CD1	2:E:153:VAL:HG11	2.20	0.77
1:D:495:ASN:ND2	1:D:574:ALA:H	1.82	0.77
2:F:145:PHE:HB3	2:F:153:VAL:HG13	1.65	0.77
1:A:451:ARG:O	1:A:454:GLU:HG2	1.85	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:8:LEU:HD22	2:B:33:ARG:HH21	1.50	0.76
1:D:432:ASN:OD1	1:D:434:ASP:N	2.16	0.76
1:A:152:LYS:HG2	1:A:565:ASN:H	1.50	0.76
2:F:101:PHE:HZ	2:F:131:ALA:HB1	1.49	0.76
1:D:492:ASP:O	2:E:187:LYS:HE3	1.85	0.76
2:E:8:LEU:HD22	2:E:33:ARG:HH21	1.49	0.76
1:A:98:SER:HB3	5:A:603:ATP:O2G	1.85	0.76
2:E:11:TRP:CD1	2:E:12:PRO:HD3	2.20	0.76
1:A:162:VAL:O	7:A:704:HOH:O	2.03	0.76
1:A:540:SER:OG	1:A:544:GLN:NE2	2.18	0.76
1:A:151:SER:HB3	1:A:565:ASN:HD21	1.49	0.76
1:A:526:GLY:HA2	1:A:529:ARG:HB3	1.68	0.75
2:E:54:ILE:O	7:E:403:HOH:O	2.02	0.75
2:F:166:ALA:O	7:F:402:HOH:O	2.03	0.75
1:A:278:ARG:NH1	7:A:727:HOH:O	2.20	0.75
2:E:215:ASN:OD1	7:E:405:HOH:O	2.05	0.75
1:A:219:VAL:HG11	1:A:291:ILE:HG21	1.67	0.75
1:A:164:THR:HG21	1:A:561:ILE:HD11	1.69	0.75
1:D:150:SER:HB2	1:D:167:THR:HA	1.68	0.75
1:D:498:ASP:HB3	1:D:510:ARG:HH22	1.50	0.75
2:B:117:LYS:O	7:B:405:HOH:O	2.04	0.75
2:E:64:VAL:HG23	2:E:70:VAL:HG22	1.68	0.75
1:A:150:SER:HB3	1:A:170:TYR:CD2	2.22	0.75
1:D:105:GLN:HA	1:D:430:SER:HB3	1.68	0.75
1:D:351:THR:HG21	1:D:410:ILE:HG12	1.68	0.74
1:A:108:PRO:O	7:A:705:HOH:O	2.04	0.74
2:B:98:TRP:CD1	2:B:153:VAL:HG21	2.22	0.74
1:D:199:HIS:H	1:D:524:ALA:HB1	1.52	0.74
1:A:432:ASN:OD1	1:A:434:ASP:N	2.20	0.74
1:D:306:THR:O	7:D:709:HOH:O	2.05	0.74
2:F:162:SER:HB3	2:F:199:LEU:HD23	1.67	0.74
1:A:329:ASP:HB3	1:A:339:ALA:HA	1.70	0.74
1:A:500:ALA:CA	2:B:188:ARG:HH12	1.92	0.74
1:D:230:ALA:O	7:D:708:HOH:O	2.03	0.74
1:A:353:ALA:HB2	1:A:413:TYR:HD2	1.53	0.74
2:C:85:PHE:HB3	2:C:92:ARG:HG2	1.70	0.74
1:A:199:HIS:N	1:A:524:ALA:HB1	2.02	0.73
1:D:19:GLU:O	1:D:23:ASN:ND2	2.14	0.73
1:A:165:ALA:H	1:A:557:LYS:HE3	1.53	0.73
1:D:559:LEU:O	1:D:562:LEU:HB3	1.87	0.73
2:F:136:GLU:HG3	2:F:181:LYS:HD3	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:163:GLY:HA2	1:D:560:GLN:HB2	1.69	0.73
1:A:221:ALA:HB3	1:A:227:LEU:HG	1.71	0.73
1:A:106:GLY:O	1:A:432:ASN:ND2	2.22	0.73
2:C:117:LYS:HD2	2:C:213:ARG:HH11	1.54	0.73
1:D:492:ASP:OD2	7:D:710:HOH:O	2.07	0.73
1:A:204:CYS:SG	7:A:1054:HOH:O	2.47	0.73
1:A:486:ASN:ND2	7:A:732:HOH:O	2.22	0.73
1:D:35:ILE:HB	7:D:811:HOH:O	1.88	0.73
2:F:84:PHE:O	7:F:404:HOH:O	2.07	0.73
2:E:66:GLU:OE2	7:E:407:HOH:O	2.07	0.73
1:A:516:GLY:O	7:A:707:HOH:O	2.06	0.73
1:D:45:LEU:HG	1:D:50:LEU:HD22	1.69	0.73
1:D:495:ASN:HD21	1:D:574:ALA:H	1.33	0.73
2:F:139:LEU:O	2:F:141:ASP:N	2.21	0.72
2:B:26:LYS:NZ	2:B:82:ASN:O	2.21	0.72
1:D:529:ARG:NH1	1:D:533:GLU:OE2	2.22	0.72
2:E:206:VAL:HA	7:E:495:HOH:O	1.88	0.72
1:D:125:PHE:HE2	1:D:328:HIS:HE1	1.37	0.72
1:D:330:TYR:HE2	1:D:540:SER:H	1.36	0.72
1:D:107:ARG:HH21	1:D:434:ASP:HB3	1.53	0.72
2:C:139:LEU:HD23	2:C:142:LYS:HB3	1.71	0.72
1:D:297:ASN:O	7:D:711:HOH:O	2.08	0.72
1:A:305:MET:HB2	1:A:347:PRO:HB3	1.72	0.71
1:D:35:ILE:HD13	1:D:394:ASN:HA	1.71	0.71
1:D:490:LEU:HD22	1:D:522:VAL:HG21	1.69	0.71
1:A:12:ARG:NH2	7:A:739:HOH:O	2.23	0.71
1:A:82:ASP:OD1	7:A:708:HOH:O	2.08	0.71
2:B:99:ALA:HA	7:B:510:HOH:O	1.90	0.71
1:D:493:CYS:SG	7:D:732:HOH:O	2.44	0.71
1:D:573:THR:HG21	2:E:176:GLU:OE2	1.90	0.71
2:B:98:TRP:NE1	2:B:153:VAL:HG21	2.05	0.71
1:D:423:CYS:SG	1:D:541:SER:OG	2.48	0.71
2:F:26:LYS:NZ	2:F:82:ASN:O	2.22	0.71
1:A:94:VAL:HG11	1:A:112:PRO:HB3	1.73	0.71
1:A:383:LYS:O	7:A:709:HOH:O	2.09	0.70
1:D:100:SER:HB3	1:D:109:LYS:HG3	1.74	0.70
2:E:26:LYS:HG2	2:E:81:LYS:NZ	2.06	0.70
2:E:114:TRP:HA	2:E:170:PHE:HD2	1.54	0.70
2:B:188:ARG:NH2	7:B:425:HOH:O	2.23	0.70
2:B:26:LYS:HD2	2:B:74:VAL:HG13	1.73	0.70
1:A:99:LEU:HA	1:A:109:LYS:O	1.92	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:23:LEU:HD22	2:B:28:VAL:HG11	1.74	0.70
1:D:107:ARG:NH1	1:D:433:ILE:HG13	2.06	0.70
1:D:491:GLN:NE2	7:D:756:HOH:O	2.23	0.70
2:B:201:ASP:HB2	2:B:204:LYS:HG3	1.72	0.70
1:A:568:SER:HB2	1:A:570:TYR:HE1	1.55	0.70
1:D:331:GLY:HA3	1:D:336:TRP:CE3	2.26	0.70
1:D:431:ILE:O	7:D:712:HOH:O	2.08	0.70
1:A:99:LEU:HB2	1:A:555:ASN:OD1	1.92	0.70
1:A:99:LEU:HB3	1:A:556:ALA:H	1.56	0.70
2:E:23:LEU:HD22	2:E:28:VAL:HG11	1.72	0.70
1:D:162:VAL:HG21	1:D:559:LEU:HD23	1.72	0.70
1:A:451:ARG:NH2	7:A:701:HOH:O	2.24	0.69
1:A:493:CYS:SG	7:A:813:HOH:O	2.47	0.69
2:E:10:TYR:O	2:E:20:ARG:NH2	2.25	0.69
1:A:552:LYS:O	1:A:554:SER:N	2.25	0.69
1:D:442:GLN:HG2	1:D:462:PHE:HZ	1.57	0.69
1:A:493:CYS:SG	7:A:902:HOH:O	2.37	0.69
2:B:184:ALA:HA	2:B:187:LYS:NZ	2.07	0.69
1:A:221:ALA:HB1	1:A:529:ARG:HH12	1.56	0.69
2:B:135:LEU:HD23	2:B:182:LEU:HD11	1.74	0.69
2:C:149:SER:OG	1:D:46:GLN:OE1	2.11	0.69
1:A:98:SER:O	1:A:110:PHE:HA	1.92	0.69
1:D:199:HIS:N	1:D:524:ALA:HB1	2.08	0.69
1:D:73:LEU:HD22	1:D:89:LEU:HD13	1.73	0.69
1:A:70:ASP:HB3	1:A:109:LYS:HD2	1.75	0.69
1:D:105:GLN:NE2	7:D:764:HOH:O	2.25	0.69
1:D:332:SER:OG	1:D:333:SER:N	2.24	0.69
1:A:166:THR:HG22	4:A:602:VAL:HB	1.74	0.69
2:E:34:GLU:OE1	7:E:408:HOH:O	2.10	0.69
1:A:331:GLY:N	1:A:537:GLY:O	2.26	0.69
2:B:151:GLY:N	2:B:154:ASP:OD2	2.24	0.69
1:A:338:ALA:HA	1:A:354:VAL:HA	1.74	0.68
2:C:193:GLU:O	7:C:402:HOH:O	2.10	0.68
1:A:200:GLN:NE2	7:A:745:HOH:O	2.25	0.68
1:A:90:THR:OG1	1:A:91:GLY:N	2.26	0.68
1:D:133:ASN:ND2	7:D:746:HOH:O	2.20	0.68
1:D:152:LYS:HZ3	1:D:565:ASN:HB2	1.56	0.68
1:D:97:ILE:N	7:D:702:HOH:O	2.25	0.68
2:F:170:PHE:N	7:F:402:HOH:O	2.25	0.68
1:A:521:ARG:NH1	1:A:562:LEU:HD21	2.08	0.68
1:D:146:GLN:NE2	7:D:766:HOH:O	2.26	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:557:LYS:HE3	5:D:603:ATP:O2G	1.93	0.68
2:E:11:TRP:CG	2:E:12:PRO:HD3	2.29	0.68
2:B:10:TYR:O	2:B:20:ARG:NH2	2.22	0.68
1:D:524:ALA:O	7:D:713:HOH:O	2.11	0.68
1:A:331:GLY:HA3	1:A:336:TRP:CE3	2.28	0.68
2:B:121:GLN:NE2	7:B:432:HOH:O	2.26	0.68
2:B:198:SER:O	7:B:407:HOH:O	2.11	0.68
1:D:98:SER:HB2	1:D:111:ILE:HB	1.74	0.68
1:D:342:THR:OG1	1:D:413:TYR:OH	2.05	0.68
1:A:448:ALA:O	7:A:711:HOH:O	2.12	0.68
1:A:9:ASP:O	7:A:710:HOH:O	2.11	0.68
1:A:287:TRP:HB3	1:A:290:LEU:HD11	1.76	0.68
2:F:168:GLU:OE1	7:F:405:HOH:O	2.11	0.68
2:B:131:ALA:O	2:B:135:LEU:HB2	1.94	0.67
2:F:152:TYR:O	7:F:406:HOH:O	2.12	0.67
1:A:534:HIS:CE1	1:A:557:LYS:HZ3	2.13	0.67
1:A:223:PHE:HE2	1:A:545:PHE:HZ	1.42	0.67
1:D:475:TYR:HE1	1:D:515:ILE:HG21	1.60	0.67
1:A:196:PRO:HD2	1:A:256:VAL:HG11	1.76	0.67
2:B:46:GLN:O	7:B:410:HOH:O	2.13	0.67
2:B:60:ASN:OD1	7:B:408:HOH:O	2.11	0.67
1:A:511:LYS:O	7:A:712:HOH:O	2.12	0.67
5:D:603:ATP:O3'	7:D:715:HOH:O	2.12	0.67
1:D:94:VAL:HG11	1:D:112:PRO:HB3	1.76	0.67
1:D:76:TYR:HA	1:D:79:ARG:HG3	1.76	0.67
1:A:172:ASN:ND2	7:A:748:HOH:O	2.26	0.67
1:A:313:VAL:O	1:A:317:ARG:N	2.25	0.67
1:A:536:LEU:HB2	1:A:545:PHE:CZ	2.29	0.67
1:A:20:MET:SD	7:A:1064:HOH:O	2.52	0.67
1:A:432:ASN:OD1	1:A:433:ILE:N	2.27	0.67
1:D:138:ILE:HG22	1:D:217:GLN:HE21	1.59	0.67
1:D:531:ILE:HG13	1:D:558:VAL:HG22	1.76	0.67
2:F:16:GLY:HA2	2:F:55:PRO:HB3	1.76	0.67
1:A:557:LYS:HG2	5:A:603:ATP:O3G	1.94	0.67
2:C:181:LYS:HA	1:D:93:PRO:HG2	1.77	0.67
2:F:121:GLN:NE2	7:F:423:HOH:O	2.27	0.67
2:F:17:MET:O	7:F:408:HOH:O	2.12	0.67
1:A:109:LYS:HE3	1:A:111:ILE:HD11	1.77	0.66
1:A:121:THR:OG1	5:A:603:ATP:O2'	2.06	0.66
1:A:132:ARG:O	1:A:136:PHE:N	2.22	0.66
1:D:355:ILE:O	7:D:718:HOH:O	2.13	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:432:ASN:O	1:D:433:ILE:HG23	1.95	0.66
1:A:184:SER:O	7:A:716:HOH:O	2.14	0.66
1:A:242:VAL:HG22	1:A:277:ILE:HD13	1.77	0.66
1:A:334:GLU:OE2	7:A:713:HOH:O	2.12	0.66
1:A:456:LYS:NZ	2:B:201:ASP:OD2	2.28	0.66
1:A:496:CYS:HA	1:A:499:ARG:NH1	2.11	0.66
1:A:53:ASN:O	7:A:715:HOH:O	2.13	0.66
1:A:556:ALA:HA	1:A:559:LEU:HB2	1.77	0.66
2:C:26:LYS:NZ	2:C:82:ASN:O	2.28	0.66
1:D:495:ASN:HB3	1:D:499:ARG:HH11	1.60	0.66
1:D:8:PHE:CD1	1:D:181:SER:HB3	2.28	0.66
2:E:26:LYS:HG2	2:E:81:LYS:HZ3	1.58	0.66
1:D:125:PHE:HE2	1:D:328:HIS:CE1	2.13	0.66
1:D:198:VAL:HG22	1:D:524:ALA:HB3	1.77	0.66
1:D:472:PRO:O	7:D:716:HOH:O	2.12	0.66
1:D:562:LEU:O	7:D:714:HOH:O	2.12	0.66
1:A:261:THR:HG22	1:A:265:LYS:HE3	1.75	0.66
1:A:42:ALA:HB3	1:A:45:LEU:HD13	1.78	0.66
1:D:233:THR:OG1	7:D:719:HOH:O	2.13	0.66
2:B:28:VAL:O	7:B:411:HOH:O	2.13	0.66
2:F:145:PHE:N	2:F:154:ASP:OD2	2.25	0.66
2:E:42:PRO:HA	2:E:45:LEU:HG	1.77	0.66
2:C:114:TRP:O	2:C:213:ARG:NH2	2.29	0.66
1:A:451:ARG:HD3	2:B:187:LYS:HG2	1.76	0.66
1:A:496:CYS:HB2	2:B:187:LYS:HE2	1.78	0.66
1:A:223:PHE:HE1	1:A:304:ILE:HD12	1.60	0.66
1:D:140:ASP:N	1:D:140:ASP:OD1	2.29	0.66
1:D:228:VAL:O	7:D:721:HOH:O	2.14	0.66
1:A:187:CYS:HB2	1:A:208:SER:HB3	1.78	0.66
2:B:194:SER:O	2:B:198:SER:OG	2.13	0.66
1:D:473:GLY:O	1:D:516:GLY:N	2.22	0.66
2:C:125:LYS:HE2	2:C:171:GLY:HA2	1.77	0.65
2:C:188:ARG:HB2	1:D:86:SER:HB2	1.79	0.65
2:B:76:GLU:CG	2:C:89:PRO:HB3	2.26	0.65
2:F:110:GLN:NE2	7:F:426:HOH:O	2.29	0.65
1:D:121:THR:HB	7:D:788:HOH:O	1.97	0.65
2:E:73:TYR:HE1	2:F:96:ARG:HH11	1.43	0.65
1:A:332:SER:OG	1:A:333:SER:N	2.29	0.65
2:F:179:SER:O	7:F:409:HOH:O	2.13	0.65
1:A:553:PRO:O	7:A:708:HOH:O	2.14	0.65
2:B:24:ARG:HB3	2:B:194:SER:HA	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:178:GLU:O	7:F:410:HOH:O	2.14	0.65
1:A:276:THR:OG1	1:A:277:ILE:N	2.28	0.65
1:D:32:LEU:HD13	1:D:61:PHE:HE2	1.62	0.65
1:D:442:GLN:HG2	1:D:462:PHE:CZ	2.31	0.65
2:E:139:LEU:O	2:E:141:ASP:N	2.29	0.65
1:A:146:GLN:NE2	7:A:716:HOH:O	2.29	0.65
1:A:152:LYS:HZ1	1:A:523:VAL:HB	1.62	0.65
1:A:150:SER:HB3	1:A:170:TYR:HD2	1.62	0.65
1:A:353:ALA:HB2	1:A:413:TYR:CD2	2.31	0.65
1:A:492:ASP:HB3	2:B:187:LYS:HD3	1.79	0.65
2:F:116:LYS:O	2:F:213:ARG:NH1	2.30	0.65
2:F:117:LYS:HG3	2:F:213:ARG:HH11	1.60	0.65
1:D:116:GLU:OE2	1:D:395:TYR:HB2	1.96	0.65
1:D:316:LEU:O	1:D:320:ALA:N	2.30	0.65
2:E:98:TRP:HZ2	2:E:157:LEU:HD22	1.60	0.65
1:A:393:THR:HG23	1:A:399:TYR:HD1	1.61	0.65
2:B:98:TRP:HE3	2:B:101:PHE:HB2	1.62	0.65
1:A:499:ARG:CZ	2:B:184:ALA:HB1	2.27	0.65
1:D:261:THR:HG22	1:D:265:LYS:HE3	1.79	0.65
2:E:8:LEU:HD21	2:E:43:LEU:HD11	1.77	0.65
1:A:206:LEU:HB3	7:A:1060:HOH:O	1.96	0.65
1:A:499:ARG:NH1	2:B:184:ALA:HB1	2.12	0.65
1:D:253:ARG:NH2	7:D:781:HOH:O	2.30	0.65
1:D:504:ALA:O	1:D:507:VAL:HB	1.96	0.65
1:A:330:TYR:OH	1:A:542:ALA:N	2.30	0.64
1:D:559:LEU:HD12	1:D:562:LEU:HD13	1.80	0.64
2:B:148:ASP:OD2	7:B:413:HOH:O	2.15	0.64
1:D:273:LEU:HA	1:D:276:THR:HG23	1.79	0.64
2:E:100:ASP:HB3	7:F:401:HOH:O	1.97	0.64
2:E:135:LEU:HD13	2:E:182:LEU:HD11	1.78	0.64
2:E:18:ARG:NH2	7:E:422:HOH:O	2.29	0.64
2:B:64:VAL:HB	2:B:73:TYR:CD2	2.32	0.64
1:D:152:LYS:HD2	1:D:565:ASN:ND2	2.13	0.64
2:F:161:SER:OG	7:F:403:HOH:O	2.05	0.64
1:D:244:ASP:OD1	1:D:250:LEU:HA	1.98	0.64
1:D:58:GLU:OE2	1:D:360:TYR:OH	2.09	0.64
1:D:78:LYS:HA	1:D:110:PHE:HD2	1.63	0.64
1:A:463:SER:HB2	1:A:528:PHE:HE2	1.62	0.64
1:A:121:THR:HG23	3:A:601:JAA:C13	2.27	0.64
1:A:111:ILE:HG23	1:A:396:ALA:O	1.98	0.64
2:B:75:ASP:HB2	2:B:84:PHE:CE2	2.32	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:GLU:HA	1:A:77:ILE:HD11	1.78	0.64
2:B:121:GLN:O	2:B:125:LYS:HG3	1.97	0.64
2:B:16:GLY:HA2	2:B:55:PRO:HB3	1.78	0.64
1:D:499:ARG:C	2:E:188:ARG:NH1	2.52	0.64
1:A:435:LYS:HB3	1:A:436:ASN:C	2.19	0.63
1:D:535:PHE:O	1:D:538:LEU:HB3	1.97	0.63
2:E:54:ILE:HB	2:E:55:PRO:HA	1.79	0.63
2:F:15:PHE:HB3	2:F:67:SER:HB3	1.79	0.63
1:A:113:PHE:HB2	5:A:603:ATP:PB	2.38	0.63
1:A:476:ALA:HA	1:A:519:GLU:O	1.98	0.63
2:B:26:LYS:HG2	2:B:81:LYS:NZ	2.14	0.63
2:B:33:ARG:NH2	7:B:440:HOH:O	2.31	0.63
2:C:117:LYS:CD	2:C:213:ARG:HH11	2.12	0.63
1:D:456:LYS:HZ1	2:E:204:LYS:HE2	1.63	0.63
2:F:169:LYS:NZ	2:F:206:VAL:HG13	2.14	0.63
1:A:145:LEU:HA	7:A:736:HOH:O	1.99	0.63
1:A:568:SER:HB2	1:A:570:TYR:CE1	2.33	0.63
1:D:238:TRP:O	1:D:242:VAL:HG23	1.97	0.63
1:D:494:CYS:SG	1:D:520:LEU:HB3	2.38	0.63
1:D:456:LYS:NZ	2:E:204:LYS:HE2	2.13	0.63
1:A:280:LYS:HE2	1:A:293:ALA:HB1	1.79	0.63
1:A:162:VAL:HG21	1:A:559:LEU:HD23	1.80	0.63
1:A:478:PHE:CZ	1:A:562:LEU:HG	2.33	0.63
1:D:143:LYS:HA	1:D:184:SER:HB2	1.79	0.63
1:D:145:LEU:HD13	1:D:209:GLY:HA3	1.81	0.63
1:A:74:GLU:HB2	7:A:820:HOH:O	1.99	0.63
1:A:386:GLU:N	7:A:746:HOH:O	2.30	0.63
2:C:52:LYS:NZ	7:C:421:HOH:O	2.30	0.63
1:D:40:GLN:NE2	7:D:717:HOH:O	2.13	0.63
2:E:98:TRP:CE3	2:E:101:PHE:HB2	2.33	0.63
1:A:151:SER:OG	1:A:195:SER:O	2.16	0.62
2:B:114:TRP:HA	2:B:170:PHE:HD2	1.63	0.62
1:D:213:ARG:HG3	1:D:214:ASP:N	2.13	0.62
1:D:29:LYS:O	1:D:32:LEU:HG	1.99	0.62
1:D:164:THR:HG23	1:D:557:LYS:HG3	1.81	0.62
2:E:84:PHE:HD1	2:E:85:PHE:N	1.97	0.62
1:A:131:PHE:O	1:A:134:ARG:HB3	1.99	0.62
1:A:223:PHE:HZ	1:A:536:LEU:HB3	1.63	0.62
1:D:499:ARG:NH2	2:E:184:ALA:O	2.32	0.62
1:A:143:LYS:HD3	1:A:187:CYS:SG	2.39	0.62
2:C:143:PRO:HG2	1:D:42:ALA:HA	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:98:SER:HA	5:D:603:ATP:O3G	1.99	0.62
2:E:71:VAL:O	2:E:74:VAL:HB	2.00	0.62
1:A:451:ARG:NH1	1:A:454:GLU:OE2	2.32	0.62
2:E:188:ARG:NE	7:E:411:HOH:O	2.17	0.62
2:E:73:TYR:HA	2:E:76:GLU:OE2	2.00	0.62
1:A:554:SER:HB2	7:A:948:HOH:O	1.98	0.62
2:B:33:ARG:HH22	2:B:41:SER:HB3	1.65	0.62
2:C:184:ALA:HB1	1:D:85:THR:O	2.00	0.62
2:C:33:ARG:NH1	2:C:43:LEU:HD12	2.15	0.62
1:D:107:ARG:HH11	1:D:107:ARG:HG3	1.64	0.62
2:E:72:GLN:HE21	2:F:96:ARG:HD2	1.65	0.62
1:A:519:GLU:OE2	1:A:569:SER:OG	2.17	0.62
2:B:144:TYR:HB3	2:B:154:ASP:OD2	2.00	0.62
1:D:231:PHE:O	1:D:235:GLU:HG3	2.00	0.62
1:D:465:TYR:HB2	1:D:551:VAL:HG22	1.82	0.62
2:E:57:LEU:HB3	2:E:64:VAL:HG22	1.81	0.62
1:A:108:PRO:HB3	1:A:555:ASN:CG	2.20	0.62
1:D:83:GLY:H	1:D:158:GLY:HA3	1.64	0.62
2:C:110:GLN:HG3	2:C:111:PHE:N	2.15	0.61
1:D:17:PHE:HE1	1:D:355:ILE:HG12	1.64	0.61
2:E:98:TRP:HE3	2:E:101:PHE:HB2	1.64	0.61
1:A:138:ILE:HA	1:A:217:GLN:HE21	1.65	0.61
2:B:13:SER:O	2:B:17:MET:HG3	2.00	0.61
1:D:314:PRO:HB3	1:D:317:ARG:HH12	1.65	0.61
1:D:361:PHE:HE1	1:D:392:ILE:HG23	1.65	0.61
1:D:424:ARG:HD2	1:D:425:ARG:NH1	2.14	0.61
2:B:17:MET:HG2	7:B:407:HOH:O	2.01	0.61
1:A:451:ARG:HE	2:B:183:ILE:HD11	1.64	0.61
2:B:11:TRP:CD1	2:B:12:PRO:HD3	2.36	0.61
1:A:149:PHE:CZ	1:A:205:HIS:HD2	2.18	0.61
2:B:141:ASP:OD1	2:B:141:ASP:N	2.32	0.61
2:B:7:LEU:HD21	2:B:23:LEU:HD12	1.81	0.61
1:D:362:GLU:OE2	7:D:725:HOH:O	2.16	0.61
1:D:552:LYS:O	1:D:554:SER:N	2.32	0.61
1:A:498:ASP:CG	1:A:510:ARG:HH22	2.04	0.61
1:A:58:GLU:HG2	1:A:62:LYS:HE2	1.82	0.61
2:B:139:LEU:HG	2:B:145:PHE:CZ	2.36	0.61
1:A:99:LEU:HB3	1:A:556:ALA:N	2.14	0.61
2:C:17:MET:O	2:C:21:VAL:HG23	2.01	0.61
1:D:25:HIS:NE2	1:D:380:THR:OG1	2.33	0.61
1:D:394:ASN:N	7:D:749:HOH:O	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:534:HIS:HE1	1:D:535:PHE:CE1	2.18	0.61
2:E:24:ARG:HB3	2:E:194:SER:HA	1.83	0.61
2:E:64:VAL:HB	2:E:73:TYR:CD2	2.35	0.61
2:F:10:TYR:O	2:F:20:ARG:NH2	2.34	0.61
1:A:165:ALA:O	1:A:169:VAL:HG23	2.01	0.61
2:C:142:LYS:HG2	1:D:41:SER:HB2	1.82	0.61
1:D:206:LEU:O	1:D:210:ILE:HG12	2.01	0.61
1:D:242:VAL:HG22	1:D:277:ILE:HD13	1.83	0.61
1:D:229:HIS:NE2	1:D:525:LYS:HD3	2.15	0.61
1:D:96:ALA:HB3	1:D:113:PHE:CD2	2.36	0.61
2:E:7:LEU:HD21	2:E:23:LEU:HD12	1.83	0.61
2:F:101:PHE:HE1	2:F:105:LYS:HE3	1.66	0.61
1:A:147:PHE:O	1:A:529:ARG:NH2	2.33	0.60
1:A:451:ARG:O	7:A:718:HOH:O	2.16	0.60
1:D:200:GLN:HB3	1:D:254:ILE:HD12	1.83	0.60
1:D:152:LYS:HB2	1:D:561:ILE:HA	1.83	0.60
2:E:26:LYS:NZ	2:E:82:ASN:O	2.34	0.60
2:F:48:ASN:HB2	7:F:520:HOH:O	2.00	0.60
1:A:18:ASP:OD1	1:A:414:ASN:ND2	2.34	0.60
1:A:445:VAL:HG21	1:A:462:PHE:CG	2.35	0.60
1:A:496:CYS:HB2	2:B:187:LYS:CE	2.31	0.60
1:A:164:THR:HG23	1:A:557:LYS:HD3	1.83	0.60
1:A:165:ALA:HA	5:A:603:ATP:O5'	2.01	0.60
1:D:248:GLY:HA2	1:D:267:LEU:HD22	1.82	0.60
1:D:334:GLU:O	1:D:392:ILE:HG21	2.00	0.60
2:F:98:TRP:CE2	2:F:138:GLU:HG2	2.36	0.60
1:A:98:SER:OG	1:A:111:ILE:HB	2.02	0.60
1:D:495:ASN:CB	1:D:499:ARG:NH1	2.64	0.60
2:C:141:ASP:HA	1:D:92:HIS:HB2	1.82	0.60
1:D:261:THR:O	1:D:265:LYS:HG3	2.02	0.60
2:B:139:LEU:O	2:B:141:ASP:N	2.33	0.60
2:C:107:THR:HA	2:C:110:GLN:HG2	1.83	0.60
1:D:361:PHE:CE1	1:D:392:ILE:HG23	2.37	0.60
1:D:99:LEU:HD13	1:D:558:VAL:H	1.66	0.60
1:D:200:GLN:NE2	1:D:484:GLU:OE1	2.35	0.60
1:D:377:VAL:O	7:D:724:HOH:O	2.16	0.60
1:D:447:SER:OG	2:E:191:GLU:OE1	2.19	0.60
2:E:90:TYR:CD1	2:F:62:LYS:HB3	2.37	0.60
1:A:168:ASN:ND2	5:A:603:ATP:O2A	2.35	0.60
1:A:152:LYS:HB2	1:A:561:ILE:HA	1.83	0.60
2:E:47:SER:HB2	7:E:477:HOH:O	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:197:ASP:OD1	1:D:197:ASP:N	2.35	0.60
1:D:528:PHE:HB3	1:D:547:MET:HE1	1.83	0.60
1:D:441:LEU:HD23	1:D:549:ARG:HB3	1.82	0.60
4:A:602:VAL:HG12	5:A:603:ATP:H2	1.66	0.59
2:B:76:GLU:O	7:B:414:HOH:O	2.17	0.59
2:B:84:PHE:CD1	2:B:152:TYR:HB2	2.37	0.59
7:E:402:HOH:O	2:F:96:ARG:NH1	2.35	0.59
1:A:499:ARG:CZ	1:A:499:ARG:HB2	2.31	0.59
1:D:424:ARG:HG3	1:D:425:ARG:H	1.67	0.59
1:D:496:CYS:HB2	2:E:187:LYS:NZ	2.17	0.59
1:A:492:ASP:O	2:B:187:LYS:HE3	2.03	0.59
2:B:64:VAL:HB	2:B:73:TYR:CE2	2.37	0.59
1:D:314:PRO:HB3	1:D:317:ARG:NH1	2.17	0.59
1:A:107:ARG:HE	1:A:433:ILE:HG13	1.67	0.59
2:C:11:TRP:CG	2:C:12:PRO:HD3	2.38	0.59
1:D:149:PHE:HZ	1:D:202:LEU:HA	1.66	0.59
1:D:332:SER:HB2	1:D:538:LEU:HA	1.83	0.59
2:C:188:ARG:NE	1:D:86:SER:HB2	2.18	0.59
1:A:87:PRO:HB3	1:A:93:PRO:HD3	1.84	0.59
2:C:15:PHE:O	2:C:18:ARG:HB2	2.03	0.59
1:A:118:MET:HA	5:A:603:ATP:O3'	2.03	0.59
2:B:192:LYS:N	7:B:443:HOH:O	2.35	0.59
1:D:225:HIS:HB3	1:D:309:MET:SD	2.43	0.59
1:D:557:LYS:HD2	5:D:603:ATP:O3G	2.02	0.59
2:F:108:ASP:O	2:F:112:LYS:HG2	2.02	0.59
2:C:24:ARG:NH2	7:C:424:HOH:O	2.34	0.59
1:D:150:SER:HB2	1:D:167:THR:CA	2.32	0.59
1:D:284:LEU:HD13	1:D:287:TRP:HA	1.85	0.59
2:E:32:TYR:HD2	2:E:34:GLU:OE2	1.86	0.59
2:E:26:LYS:HE2	2:E:75:ASP:HA	1.83	0.59
2:C:125:LYS:HB3	2:C:173:PHE:HE2	1.68	0.59
2:E:10:TYR:HB3	2:E:13:SER:HB2	1.83	0.59
1:A:342:THR:HG1	1:A:413:TYR:HH	1.31	0.59
1:D:342:THR:O	1:D:345:LEU:HG	2.03	0.59
2:C:136:GLU:HG3	2:C:181:LYS:HD3	1.84	0.59
1:D:35:ILE:HA	1:D:395:TYR:CE2	2.38	0.59
2:E:125:LYS:HA	2:E:128:PHE:CE2	2.38	0.59
2:F:169:LYS:HG3	2:F:170:PHE:H	1.67	0.59
1:A:166:THR:CG2	4:A:602:VAL:HB	2.33	0.58
1:A:529:ARG:NH2	7:A:786:HOH:O	2.36	0.58
1:D:117:LEU:O	1:D:121:THR:OG1	2.20	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:363:PHE:CD2	1:D:382:VAL:HG21	2.38	0.58
1:A:435:LYS:HA	1:A:436:ASN:HB2	1.85	0.58
2:C:188:ARG:CB	1:D:87:PRO:HD2	2.32	0.58
1:D:367:SER:O	7:D:733:HOH:O	2.17	0.58
1:A:494:CYS:HA	1:A:497:LEU:HD12	1.85	0.58
2:B:191:GLU:HG2	7:B:443:HOH:O	2.02	0.58
1:D:162:VAL:HB	1:D:556:ALA:HB1	1.86	0.58
1:D:353:ALA:HB2	1:D:413:TYR:CD2	2.37	0.58
2:E:169:LYS:N	7:E:401:HOH:O	1.91	0.58
1:A:387:GLU:HG2	1:A:408:LYS:HB2	1.84	0.58
1:D:195:SER:OG	1:D:197:ASP:OD1	2.21	0.58
1:D:202:LEU:HA	1:D:205:HIS:HB2	1.85	0.58
1:D:496:CYS:HA	1:D:499:ARG:NH2	2.19	0.58
1:D:552:LYS:HD2	1:D:553:PRO:HD2	1.85	0.58
1:D:552:LYS:C	1:D:554:SER:H	2.06	0.58
1:D:88:ILE:HD12	1:D:89:LEU:N	2.08	0.58
2:E:75:ASP:HB2	2:E:84:PHE:CE2	2.39	0.58
1:A:107:ARG:HG3	7:A:705:HOH:O	2.04	0.58
1:A:213:ARG:HG3	1:A:214:ASP:N	2.18	0.58
1:A:448:ALA:HB2	1:A:496:CYS:HB3	1.86	0.58
1:A:223:PHE:CZ	1:A:533:GLU:HA	2.37	0.58
1:D:295:PHE:HD1	1:D:298:ALA:HB2	1.68	0.58
2:E:159:THR:HA	2:E:199:LEU:HD21	1.86	0.58
1:D:454:GLU:HB2	2:E:202:SER:OG	2.03	0.58
1:A:551:VAL:HG11	1:A:559:LEU:HD13	1.85	0.58
2:B:73:TYR:CZ	2:C:93:ALA:HB1	2.39	0.58
1:D:486:ASN:OD1	7:D:730:HOH:O	2.17	0.58
1:A:70:ASP:HB2	1:A:104:SER:HB2	1.84	0.58
1:D:438:GLU:O	1:D:442:GLN:HG3	2.04	0.58
1:D:152:LYS:HZ2	1:D:565:ASN:HB2	1.67	0.58
1:A:32:LEU:HD21	1:A:61:PHE:HD2	1.68	0.58
2:B:188:ARG:HD2	2:B:191:GLU:OE2	2.04	0.58
2:B:42:PRO:HA	2:B:45:LEU:HG	1.84	0.58
1:D:143:LYS:HZ2	1:D:187:CYS:HA	1.69	0.58
1:D:314:PRO:O	1:D:318:HIS:N	2.32	0.58
1:D:99:LEU:HB3	1:D:557:LYS:HB2	1.84	0.58
6:E:301:GSH:N2	7:E:403:HOH:O	2.29	0.58
2:E:92:ARG:NE	2:F:76:GLU:OE2	2.36	0.58
2:F:161:SER:HA	2:F:164:PHE:CD2	2.38	0.58
1:A:403:LEU:HD23	1:A:540:SER:HB3	1.84	0.58
2:B:86:PRO:HD3	2:B:146:GLY:O	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:17:MET:HG2	2:C:20:ARG:NH1	2.19	0.58
1:D:448:ALA:O	7:D:732:HOH:O	2.17	0.58
1:D:332:SER:HA	5:D:603:ATP:C6	2.39	0.58
1:D:29:LYS:O	1:D:33:LYS:HG2	2.04	0.58
2:E:39:ASN:ND2	7:E:432:HOH:O	2.37	0.58
1:A:253:ARG:NH2	7:A:784:HOH:O	2.36	0.57
3:A:601:JAA:C05	4:A:602:VAL:HG13	2.34	0.57
1:D:213:ARG:NH1	1:D:214:ASP:OD1	2.37	0.57
1:D:241:ILE:O	1:D:245:ILE:HG12	2.04	0.57
1:D:275:GLU:O	7:D:726:HOH:O	2.16	0.57
1:D:359:GLY:O	7:D:728:HOH:O	2.17	0.57
1:D:162:VAL:O	1:D:560:GLN:HB2	2.04	0.57
1:A:156:SER:HB3	1:A:162:VAL:HG13	1.85	0.57
2:B:164:PHE:HD2	2:B:183:ILE:HD12	1.69	0.57
1:D:17:PHE:CE2	1:D:341:VAL:HG11	2.39	0.57
1:D:387:GLU:HG3	1:D:408:LYS:HB2	1.86	0.57
1:D:448:ALA:HB2	1:D:496:CYS:HB3	1.85	0.57
2:B:195:VAL:HG23	2:B:199:LEU:HD13	1.86	0.57
2:E:138:GLU:HG3	2:E:145:PHE:HE1	1.68	0.57
2:F:8:LEU:O	7:F:412:HOH:O	2.17	0.57
1:A:437:THR:HG21	1:A:439:ARG:HH21	1.68	0.57
1:A:538:LEU:HD23	1:A:544:GLN:HG2	1.85	0.57
2:B:90:TYR:CD2	2:C:62:LYS:HD3	2.39	0.57
1:D:118:MET:SD	7:D:788:HOH:O	2.57	0.57
1:A:292:PRO:O	1:A:296:PRO:HA	2.04	0.57
1:A:473:GLY:O	1:A:516:GLY:N	2.34	0.57
2:B:68:LEU:HD23	2:B:103:ASP:OD2	2.04	0.57
2:E:86:PRO:HD3	2:E:146:GLY:O	2.04	0.57
1:A:361:PHE:CE1	1:A:392:ILE:HG23	2.40	0.57
1:D:310:GLU:O	1:D:313:VAL:HG12	2.05	0.57
1:D:465:TYR:CE2	1:D:467:ASP:HB2	2.40	0.57
1:D:488:ASP:OD2	2:E:168:GLU:OE2	2.22	0.57
1:D:534:HIS:CE1	1:D:557:LYS:HD3	2.39	0.57
2:F:25:GLU:OE1	7:F:407:HOH:O	2.17	0.57
1:A:454:GLU:OE2	2:B:202:SER:OG	2.14	0.57
2:C:176:GLU:HB2	2:C:183:ILE:HD12	1.85	0.57
1:D:165:ALA:O	1:D:169:VAL:HG23	2.05	0.57
1:D:328:HIS:CG	1:D:329:ASP:N	2.72	0.57
1:A:153:GLN:HG3	1:A:171:ARG:NH1	2.20	0.57
2:B:216:ASN:ND2	7:B:424:HOH:O	2.22	0.57
1:D:126:ARG:NH1	7:D:817:HOH:O	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:97:PHE:O	7:F:401:HOH:O	2.17	0.57
1:A:405:ASP:HB3	1:A:541:SER:HB3	1.87	0.57
1:A:424:ARG:C	1:A:543:GLY:HA2	2.24	0.57
1:A:551:VAL:HG13	1:A:555:ASN:HB2	1.87	0.57
2:C:193:GLU:HA	2:C:196:SER:HB3	1.85	0.57
1:D:108:PRO:HB2	1:D:554:SER:OG	2.04	0.57
1:D:208:SER:HA	1:D:211:LEU:CG	2.34	0.57
2:C:139:LEU:C	2:C:141:ASP:H	2.06	0.57
1:D:36:LEU:HD12	7:D:811:HOH:O	2.04	0.57
2:F:54:ILE:HB	2:F:55:PRO:HA	1.87	0.57
1:A:199:HIS:HA	1:A:525:LYS:HB2	1.87	0.56
1:A:83:GLY:H	1:A:158:GLY:HA3	1.70	0.56
1:A:76:TYR:HB3	1:A:88:ILE:HG21	1.86	0.56
1:D:498:ASP:CB	1:D:510:ARG:HH22	2.18	0.56
1:D:531:ILE:HA	1:D:534:HIS:CD2	2.39	0.56
2:E:114:TRP:HA	2:E:170:PHE:CD2	2.38	0.56
1:D:273:LEU:N	7:D:751:HOH:O	2.34	0.56
1:D:413:TYR:O	1:D:416:THR:HG22	2.06	0.56
2:E:26:LYS:HD2	2:E:74:VAL:HG13	1.87	0.56
2:F:11:TRP:CD1	2:F:12:PRO:HD3	2.39	0.56
1:A:229:HIS:CE1	1:A:525:LYS:HZ2	2.24	0.56
2:B:98:TRP:CZ3	2:B:135:LEU:HD11	2.39	0.56
1:A:499:ARG:NE	2:B:184:ALA:HB1	2.20	0.56
2:C:139:LEU:C	2:C:141:ASP:N	2.58	0.56
2:E:98:TRP:CZ2	2:E:157:LEU:HD22	2.40	0.56
2:B:54:ILE:HB	2:B:55:PRO:HA	1.86	0.56
2:C:108:ASP:O	2:C:112:LYS:HG2	2.06	0.56
2:C:188:ARG:HB2	1:D:87:PRO:HD2	1.86	0.56
1:D:168:ASN:O	1:D:172:ASN:HB2	2.05	0.56
2:E:125:LYS:HA	2:E:128:PHE:CD2	2.40	0.56
1:A:169:VAL:O	1:A:175:PHE:HB2	2.05	0.56
1:A:504:ALA:O	1:A:507:VAL:HB	2.05	0.56
2:B:82:ASN:ND2	7:B:447:HOH:O	2.38	0.56
1:D:215:GLN:O	7:D:731:HOH:O	2.17	0.56
1:A:114:THR:H	1:A:117:LEU:HD13	1.70	0.56
1:A:534:HIS:HB2	4:A:602:VAL:O	2.06	0.56
1:A:152:LYS:CE	1:A:565:ASN:HB2	2.31	0.56
2:B:10:TYR:HH	2:B:208:TYR:HH	1.53	0.56
1:D:124:LEU:HD12	1:D:355:ILE:HD12	1.87	0.56
1:A:223:PHE:CE2	1:A:545:PHE:HZ	2.21	0.56
1:A:444:SER:O	7:A:720:HOH:O	2.18	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:57:LEU:O	2:B:64:VAL:HG22	2.06	0.56
1:D:103:THR:HG22	1:D:548:PRO:HB3	1.86	0.56
1:D:566:VAL:HA	7:D:936:HOH:O	2.05	0.56
2:F:68:LEU:HD21	2:F:99:ALA:HB1	1.87	0.56
1:D:103:THR:O	7:D:735:HOH:O	2.18	0.56
1:D:394:ASN:ND2	7:D:749:HOH:O	2.38	0.56
1:D:169:VAL:HG22	5:D:603:ATP:H2'	1.88	0.56
2:E:53:LYS:HG2	6:E:301:GSH:HA31	1.87	0.56
2:B:136:GLU:HG3	2:B:181:LYS:HD3	1.88	0.56
2:C:15:PHE:HA	2:C:18:ARG:HD2	1.87	0.56
1:D:445:VAL:HG22	1:D:479:TRP:HE1	1.71	0.56
1:D:333:SER:OG	5:D:603:ATP:O1A	2.24	0.56
2:E:114:TRP:CD1	2:E:167:TYR:HE1	2.24	0.56
1:A:138:ILE:HB	1:A:217:GLN:HG3	1.88	0.56
2:B:17:MET:SD	2:B:199:LEU:HG	2.46	0.56
1:D:113:PHE:CD1	5:D:603:ATP:H5'1	2.41	0.56
1:A:242:VAL:O	1:A:246:LYS:HG3	2.06	0.55
1:A:535:PHE:O	1:A:538:LEU:HB3	2.06	0.55
1:A:403:LEU:HD21	1:A:538:LEU:HD21	1.87	0.55
2:B:23:LEU:HD11	2:B:57:LEU:HD22	1.88	0.55
1:D:299:LYS:HB2	1:D:300:TYR:HD1	1.71	0.55
1:D:566:VAL:HB	1:D:569:SER:HB2	1.88	0.55
2:E:163:TRP:HB3	2:E:167:TYR:CZ	2.41	0.55
2:E:201:ASP:HB2	2:E:204:LYS:HG3	1.88	0.55
1:A:169:VAL:HG12	1:A:175:PHE:CD1	2.41	0.55
2:C:141:ASP:O	1:D:91:GLY:HA3	2.05	0.55
1:D:23:ASN:O	1:D:27:VAL:HG12	2.05	0.55
1:D:18:ASP:OD1	1:D:414:ASN:ND2	2.39	0.55
1:D:7:THR:N	7:D:816:HOH:O	2.38	0.55
2:E:33:ARG:NH2	2:E:35:GLU:OE2	2.38	0.55
1:D:32:LEU:HD23	1:D:360:TYR:CE1	2.41	0.55
1:D:495:ASN:HD21	1:D:573:THR:N	2.04	0.55
2:E:97:PHE:HZ	2:F:48:ASN:HD21	1.54	0.55
1:A:557:LYS:NZ	5:A:603:ATP:PG	2.79	0.55
2:B:150:PHE:O	7:B:415:HOH:O	2.17	0.55
1:D:157:THR:HG22	1:D:469:SER:HB3	1.88	0.55
1:D:510:ARG:NH1	1:D:575:PHE:HE2	2.05	0.55
2:F:21:VAL:HG23	7:F:408:HOH:O	2.05	0.55
1:A:111:ILE:HG12	1:A:334:GLU:HG2	1.89	0.55
1:A:368:GLU:HG3	1:A:369:THR:HG22	1.88	0.55
1:A:342:THR:OG1	1:A:413:TYR:OH	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:139:LEU:HB3	2:C:142:LYS:H	1.71	0.55
1:D:77:ILE:HD13	1:D:112:PRO:HD3	1.87	0.55
1:D:152:LYS:HE3	1:D:561:ILE:O	2.07	0.55
2:E:209:ALA:HB3	7:E:495:HOH:O	2.06	0.55
2:E:76:GLU:HG3	2:F:89:PRO:HB3	1.88	0.55
1:D:187:CYS:HB2	1:D:208:SER:O	2.06	0.55
1:D:290:LEU:O	1:D:294:LEU:HG	2.06	0.55
2:E:53:LYS:HB3	7:E:403:HOH:O	2.05	0.55
1:A:479:TRP:HZ2	1:A:497:LEU:HD21	1.72	0.55
1:D:332:SER:CB	1:D:538:LEU:HA	2.37	0.55
2:E:8:LEU:HD13	2:E:44:LEU:HB2	1.89	0.55
1:D:448:ALA:HB3	1:D:479:TRP:CH2	2.42	0.55
2:B:18:ARG:NH2	7:B:421:HOH:O	2.40	0.55
1:A:447:SER:OG	2:B:191:GLU:OE1	2.18	0.55
2:C:117:LYS:HD2	2:C:213:ARG:NH1	2.21	0.55
1:D:10:MET:O	1:D:14:ILE:HG23	2.07	0.55
1:D:143:LYS:HB2	1:D:185:PRO:O	2.07	0.55
2:E:141:ASP:OD1	2:E:141:ASP:N	2.39	0.55
2:B:132:VAL:HG23	2:B:182:LEU:HD13	1.88	0.55
2:B:71:VAL:O	2:B:74:VAL:HB	2.07	0.55
2:C:174:SER:HB3	2:C:177:SER:HB2	1.89	0.55
1:A:328:HIS:CD2	3:A:601:JAA:O03	2.61	0.54
1:D:510:ARG:HH12	1:D:575:PHE:HE2	1.54	0.54
2:F:13:SER:O	2:F:17:MET:HG3	2.07	0.54
1:D:213:ARG:HH21	1:D:296:PRO:HD3	1.73	0.54
1:D:375:LYS:NZ	7:D:727:HOH:O	2.17	0.54
1:D:435:LYS:HB3	1:D:436:ASN:C	2.27	0.54
1:D:330:TYR:CE2	1:D:539:GLY:HA2	2.42	0.54
1:D:99:LEU:HB3	1:D:557:LYS:CB	2.37	0.54
1:A:247:ASP:HB2	1:A:249:VAL:HG12	1.89	0.54
1:A:35:ILE:HD13	1:A:394:ASN:HA	1.88	0.54
2:B:8:LEU:HD13	2:B:44:LEU:HB2	1.89	0.54
1:D:337:ILE:HG12	1:D:539:GLY:HA3	1.90	0.54
1:D:87:PRO:HD3	1:D:93:PRO:HD3	1.90	0.54
1:A:108:PRO:HB2	1:A:554:SER:C	2.28	0.54
2:B:104:LYS:HG3	2:B:105:LYS:N	2.22	0.54
2:C:135:LEU:O	2:C:139:LEU:HD12	2.07	0.54
2:E:119:GLU:OE1	7:E:412:HOH:O	2.17	0.54
2:E:187:LYS:NZ	2:E:187:LYS:HB2	2.23	0.54
2:F:60:ASN:O	7:F:414:HOH:O	2.18	0.54
1:A:150:SER:HB2	1:A:167:THR:CA	2.35	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:521:ARG:HA	1:A:569:SER:HA	1.89	0.54
1:A:332:SER:HA	5:A:603:ATP:N6	2.22	0.54
2:C:144:TYR:HB3	2:C:154:ASP:OD2	2.08	0.54
2:E:70:VAL:HA	2:E:73:TYR:CD2	2.42	0.54
1:A:150:SER:OG	1:A:150:SER:O	2.24	0.54
1:A:36:LEU:HD22	1:A:61:PHE:CZ	2.42	0.54
1:A:382:VAL:HG22	7:A:709:HOH:O	2.07	0.54
2:B:11:TRP:CG	2:B:12:PRO:HD3	2.43	0.54
1:A:134:ARG:NH2	7:A:793:HOH:O	2.39	0.54
1:A:153:GLN:HG3	1:A:171:ARG:HH11	1.73	0.54
1:A:303:GLY:HA2	7:A:887:HOH:O	2.06	0.54
1:A:88:ILE:HG22	1:A:89:LEU:N	2.21	0.54
1:A:99:LEU:HG	1:A:557:LYS:CB	2.27	0.54
1:D:484:GLU:HG3	1:D:485:THR:N	2.23	0.54
1:D:444:SER:HB3	1:D:497:LEU:HD23	1.89	0.54
2:C:139:LEU:HD22	1:D:92:HIS:CD2	2.41	0.54
2:E:43:LEU:O	2:E:47:SER:OG	2.25	0.54
1:A:99:LEU:HD12	1:A:535:PHE:HZ	1.72	0.54
1:D:113:PHE:HB2	5:D:603:ATP:PB	2.48	0.54
1:D:223:PHE:CZ	1:D:533:GLU:HA	2.42	0.54
1:D:311:PRO:O	7:D:734:HOH:O	2.18	0.54
1:D:125:PHE:CE2	1:D:328:HIS:HE1	2.22	0.54
2:C:142:LYS:HG3	1:D:39:ASN:HA	1.90	0.54
1:D:482:SER:HA	1:D:525:LYS:HE2	1.88	0.54
2:E:102:VAL:O	2:E:107:THR:HG23	2.07	0.54
1:A:328:HIS:CG	1:A:329:ASP:N	2.76	0.54
1:A:515:ILE:HG22	7:A:707:HOH:O	2.07	0.54
1:A:549:ARG:O	7:A:722:HOH:O	2.18	0.54
2:C:130:GLU:O	2:C:134:ILE:HG13	2.07	0.54
2:C:54:ILE:HG21	7:C:426:HOH:O	2.07	0.54
1:D:116:GLU:OE1	7:D:737:HOH:O	2.19	0.54
1:D:225:HIS:CE1	1:D:529:ARG:HG3	2.43	0.54
1:D:262:ALA:HA	1:D:265:LYS:HD2	1.90	0.54
1:D:495:ASN:HB3	1:D:499:ARG:NH1	2.21	0.54
1:D:99:LEU:HB2	1:D:557:LYS:H	1.72	0.54
1:D:113:PHE:HB2	5:D:603:ATP:O1B	2.07	0.54
2:E:5:PRO:HB3	2:E:59:HIS:NE2	2.23	0.54
1:A:288:TYR:HB2	1:A:318:HIS:CE1	2.43	0.54
1:A:329:ASP:OD1	1:A:340:ASN:N	2.31	0.54
2:B:144:TYR:HA	2:B:185:TRP:HE1	1.72	0.54
1:D:369:THR:OG1	7:D:736:HOH:O	2.19	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:121:GLN:O	2:E:125:LYS:HG3	2.08	0.54
2:F:37:PHE:CE1	6:F:301:GSH:HA32	2.43	0.54
1:A:317:ARG:O	1:A:321:GLY:N	2.40	0.53
1:A:107:ARG:HE	1:A:433:ILE:CG1	2.21	0.53
1:D:108:PRO:HB3	1:D:555:ASN:CG	2.28	0.53
1:D:250:LEU:HD11	1:D:260:ARG:CZ	2.38	0.53
1:D:313:VAL:HG23	1:D:325:LEU:HD12	1.89	0.53
1:D:329:ASP:HB3	1:D:339:ALA:HA	1.90	0.53
1:D:534:HIS:CG	1:D:557:LYS:HE2	2.43	0.53
1:A:107:ARG:HB2	1:A:108:PRO:HD2	1.89	0.53
1:A:222:VAL:HG12	1:A:223:PHE:CD1	2.43	0.53
2:B:163:TRP:HB3	2:B:167:TYR:CZ	2.43	0.53
2:B:64:VAL:HG23	2:B:70:VAL:HG22	1.89	0.53
2:E:32:TYR:CD2	2:E:34:GLU:OE2	2.61	0.53
2:F:9:ASP:OD1	2:F:10:TYR:N	2.34	0.53
1:A:241:ILE:O	1:A:245:ILE:HG13	2.08	0.53
1:A:459:VAL:HG22	1:A:481:ILE:HG22	1.89	0.53
2:C:70:VAL:O	2:C:74:VAL:HG23	2.08	0.53
2:C:90:TYR:O	2:C:93:ALA:HB3	2.08	0.53
1:D:163:GLY:HA2	1:D:560:GLN:CB	2.37	0.53
2:F:139:LEU:HG	2:F:142:LYS:HD2	1.89	0.53
1:A:131:PHE:HD1	1:A:134:ARG:NH1	2.05	0.53
2:B:184:ALA:HA	2:B:187:LYS:HZ2	1.73	0.53
2:C:169:LYS:HD3	2:C:206:VAL:HG13	1.91	0.53
2:E:40:LYS:HD2	2:E:52:LYS:HB3	1.89	0.53
2:E:60:ASN:ND2	2:E:60:ASN:O	2.41	0.53
2:C:169:LYS:HG3	2:C:170:PHE:N	2.23	0.53
1:D:437:THR:OG1	1:D:440:ASP:HB2	2.08	0.53
1:D:519:GLU:CD	1:D:521:ARG:HE	2.11	0.53
2:E:126:LYS:O	2:E:129:ILE:HG13	2.08	0.53
2:E:170:PHE:CD2	2:E:213:ARG:HD2	2.44	0.53
1:A:437:THR:O	1:A:440:ASP:N	2.41	0.53
2:B:10:TYR:HB3	2:B:13:SER:HB2	1.91	0.53
2:B:32:TYR:H	2:B:32:TYR:HD2	1.52	0.53
1:D:96:ALA:O	1:D:113:PHE:HB3	2.08	0.53
2:E:76:GLU:OE2	2:F:96:ARG:NH1	2.41	0.53
1:D:430:SER:O	7:D:740:HOH:O	2.19	0.53
2:E:108:ASP:O	2:E:112:LYS:HG2	2.08	0.53
1:A:151:SER:O	1:A:171:ARG:NH2	2.41	0.53
1:A:231:PHE:CZ	1:A:291:ILE:HG12	2.43	0.53
1:D:451:ARG:NE	2:E:183:ILE:HD11	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:522:VAL:O	1:D:567:VAL:HG22	2.08	0.53
2:C:188:ARG:HB2	1:D:86:SER:CB	2.39	0.53
2:E:23:LEU:HD11	2:E:57:LEU:HD22	1.91	0.53
2:E:57:LEU:HB3	2:E:64:VAL:CG2	2.39	0.53
1:A:512:CYS:O	1:A:513:LYS:HG2	2.09	0.53
2:C:194:SER:OG	7:C:405:HOH:O	2.18	0.53
1:D:100:SER:HB3	1:D:109:LYS:CG	2.37	0.53
1:D:180:LYS:NZ	7:D:826:HOH:O	2.40	0.53
1:A:521:ARG:NH1	7:A:806:HOH:O	2.42	0.53
1:D:142:GLY:HA2	1:D:215:GLN:HB2	1.90	0.53
2:E:119:GLU:N	7:E:425:HOH:O	2.42	0.53
2:E:188:ARG:HD2	2:E:191:GLU:OE2	2.08	0.53
1:A:219:VAL:HG13	1:A:301:VAL:HA	1.90	0.52
1:A:68:VAL:HG13	1:A:401:TYR:HD1	1.73	0.52
2:C:17:MET:HG2	2:C:20:ARG:HH12	1.72	0.52
1:A:567:VAL:O	7:A:725:HOH:O	2.19	0.52
2:C:18:ARG:NH1	2:C:103:ASP:OD1	2.40	0.52
2:C:11:TRP:O	2:C:200:PRO:HG3	2.08	0.52
1:D:314:PRO:HA	1:D:317:ARG:HB3	1.90	0.52
2:F:17:MET:HG2	2:F:20:ARG:NH1	2.24	0.52
2:C:139:LEU:O	2:C:141:ASP:N	2.28	0.52
1:D:126:ARG:NH2	7:D:783:HOH:O	2.42	0.52
1:D:387:GLU:N	1:D:387:GLU:OE1	2.42	0.52
2:C:144:TYR:HB2	1:D:41:SER:HB3	1.90	0.52
2:F:108:ASP:OD2	7:F:413:HOH:O	2.18	0.52
1:A:90:THR:HG23	1:A:397:GLY:HA2	1.89	0.52
1:D:363:PHE:HB3	1:D:388:TYR:HB3	1.91	0.52
1:D:574:ALA:O	1:D:575:PHE:HB2	2.09	0.52
2:E:68:LEU:HA	2:E:71:VAL:HG12	1.91	0.52
2:E:90:TYR:CG	2:F:62:LYS:HB3	2.45	0.52
2:B:98:TRP:CH2	2:B:102:VAL:HG22	2.43	0.52
2:B:73:TYR:HA	2:B:76:GLU:OE2	2.10	0.52
1:D:391:VAL:HG22	1:D:402:ARG:HA	1.91	0.52
1:D:392:ILE:HB	1:D:398:LEU:CD1	2.32	0.52
1:D:55:THR:C	1:D:57:PRO:HD3	2.28	0.52
1:A:17:PHE:CE2	1:A:341:VAL:HG11	2.45	0.52
1:A:464:SER:HB3	1:A:550:CYS:SG	2.49	0.52
2:C:127:GLU:OE1	7:C:406:HOH:O	2.19	0.52
1:A:168:ASN:O	1:A:172:ASN:HB2	2.09	0.52
1:A:55:THR:HG21	7:A:963:HOH:O	2.10	0.52
2:C:36:ASP:OD2	2:C:38:SER:HB2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:153:GLN:HA	1:D:560:GLN:HG2	1.91	0.52
1:D:534:HIS:CE1	1:D:535:PHE:CE1	2.98	0.52
1:D:556:ALA:HA	1:D:559:LEU:HB3	1.92	0.52
1:A:110:PHE:CE1	1:A:556:ALA:HB2	2.43	0.52
2:B:70:VAL:O	2:B:73:TYR:HB2	2.10	0.52
2:E:68:LEU:HB2	2:E:152:TYR:OH	2.09	0.52
2:B:62:LYS:HB3	2:C:90:TYR:CE1	2.45	0.52
1:D:464:SER:N	1:D:549:ARG:O	2.42	0.52
1:A:244:ASP:OD2	1:A:251:SER:HB2	2.10	0.52
2:B:150:PHE:CD1	2:B:192:LYS:HG3	2.45	0.52
1:D:475:TYR:CE1	1:D:515:ILE:HG21	2.44	0.52
2:F:163:TRP:CD1	2:F:205:ILE:HD13	2.45	0.52
1:A:217:GLN:HA	1:A:217:GLN:OE1	2.10	0.51
1:A:22:ARG:HA	1:A:415:ASN:HB2	1.92	0.51
1:A:393:THR:HG23	1:A:399:TYR:CD1	2.43	0.51
1:A:336:TRP:CZ2	5:A:603:ATP:C5	2.98	0.51
2:B:110:GLN:HG2	2:B:167:TYR:CE2	2.45	0.51
2:C:53:LYS:HG2	6:C:301:GSH:HA31	1.91	0.51
1:D:445:VAL:HA	1:D:479:TRP:CZ2	2.45	0.51
1:A:96:ALA:HB3	1:A:113:PHE:CD2	2.46	0.51
1:A:191:GLU:O	1:A:195:SER:N	2.43	0.51
1:A:81:VAL:HG21	1:A:110:PHE:CE2	2.45	0.51
1:D:544:GLN:HG3	7:D:744:HOH:O	2.09	0.51
2:E:117:LYS:HA	2:E:121:GLN:HB2	1.93	0.51
2:E:185:TRP:NE1	2:E:189:CYS:SG	2.84	0.51
1:A:557:LYS:HZ1	5:A:603:ATP:PG	2.34	0.51
2:B:121:GLN:HE21	2:B:125:LYS:HD3	1.76	0.51
2:C:172:ASN:ND2	7:C:411:HOH:O	2.23	0.51
1:D:115:ASP:O	1:D:118:MET:HB3	2.10	0.51
1:D:150:SER:CB	1:D:167:THR:HA	2.38	0.51
1:D:149:PHE:CZ	1:D:202:LEU:HA	2.45	0.51
1:D:96:ALA:HB1	7:D:702:HOH:O	2.09	0.51
2:B:72:GLN:NE2	7:B:448:HOH:O	2.42	0.51
2:B:84:PHE:HB2	2:B:152:TYR:N	2.25	0.51
2:E:17:MET:SD	2:E:199:LEU:HG	2.51	0.51
2:B:32:TYR:HD1	2:B:34:GLU:OE2	1.93	0.51
1:D:253:ARG:HH12	1:D:484:GLU:H	1.58	0.51
1:D:32:LEU:HA	7:D:811:HOH:O	2.10	0.51
1:D:34:GLU:O	1:D:38:LYS:HG2	2.11	0.51
2:C:142:LYS:HE2	1:D:41:SER:OG	2.10	0.51
2:E:96:ARG:NH1	2:F:69:ASN:OD1	2.39	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:121:GLN:NE2	2:F:170:PHE:O	2.44	0.51
1:A:311:PRO:O	1:A:314:PRO:HD2	2.11	0.51
2:C:141:ASP:OD2	2:C:181:LYS:NZ	2.42	0.51
1:D:405:ASP:HB2	1:D:541:SER:HB3	1.91	0.51
1:D:526:GLY:HA2	1:D:529:ARG:HB3	1.93	0.51
2:E:94:GLN:NE2	7:E:404:HOH:O	2.02	0.51
2:F:205:ILE:HG13	7:F:528:HOH:O	2.11	0.51
1:A:100:SER:HB3	1:A:109:LYS:HD3	1.92	0.51
1:A:34:GLU:O	1:A:38:LYS:HG2	2.10	0.51
2:B:24:ARG:HD2	2:B:198:SER:OG	2.11	0.51
1:D:107:ARG:NH2	1:D:552:LYS:HB2	2.25	0.51
1:D:143:LYS:NZ	1:D:187:CYS:HA	2.24	0.51
1:D:503:ASP:O	1:D:507:VAL:HG23	2.11	0.51
2:E:186:ALA:HB2	7:E:433:HOH:O	2.11	0.51
1:D:240:GLU:OE2	7:D:738:HOH:O	2.19	0.51
1:D:124:LEU:HD13	1:D:336:TRP:CE3	2.46	0.51
2:E:45:LEU:HA	7:E:424:HOH:O	2.11	0.51
2:E:98:TRP:O	2:E:101:PHE:HB2	2.10	0.51
1:A:108:PRO:CG	1:A:552:LYS:HB3	2.41	0.51
2:C:121:GLN:O	2:C:125:LYS:HG3	2.10	0.51
1:D:267:LEU:HD12	7:D:945:HOH:O	2.10	0.51
1:D:88:ILE:CD1	1:D:89:LEU:H	2.11	0.51
1:A:323:LEU:HB3	7:A:719:HOH:O	2.10	0.51
1:A:198:VAL:HG22	1:A:524:ALA:HB3	1.91	0.51
1:A:542:ALA:O	7:A:726:HOH:O	2.19	0.51
1:A:77:ILE:HG21	1:A:112:PRO:HD3	1.92	0.51
2:B:10:TYR:CG	2:B:12:PRO:HD2	2.45	0.51
2:B:98:TRP:CZ2	2:B:157:LEU:HD22	2.46	0.51
2:B:14:MET:HG3	2:B:163:TRP:CH2	2.46	0.51
1:D:563:CYS:O	1:D:566:VAL:HG22	2.11	0.51
1:A:150:SER:CB	1:A:167:THR:HA	2.38	0.50
1:A:261:THR:O	1:A:265:LYS:HG3	2.11	0.50
1:A:309:MET:HG2	1:A:536:LEU:CD2	2.42	0.50
1:D:128:ALA:HB2	1:D:329:ASP:OD2	2.11	0.50
2:F:44:LEU:HD12	7:F:445:HOH:O	2.11	0.50
1:A:361:PHE:HE1	1:A:392:ILE:HG23	1.75	0.50
1:A:492:ASP:C	2:B:187:LYS:HE3	2.32	0.50
1:A:332:SER:HB3	1:A:538:LEU:CD1	2.41	0.50
2:B:106:PHE:HB2	7:B:453:HOH:O	2.10	0.50
2:B:98:TRP:HZ2	2:B:157:LEU:HD22	1.76	0.50
2:C:23:LEU:HG	2:C:28:VAL:HB	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:215:GLN:N	1:D:215:GLN:OE1	2.45	0.50
2:E:50:ILE:HG13	2:E:51:HIS:H	1.77	0.50
2:F:7:LEU:O	2:F:33:ARG:HB2	2.12	0.50
1:A:101:SER:HB3	1:A:535:PHE:CD2	2.46	0.50
1:A:209:GLY:HA2	7:A:736:HOH:O	2.11	0.50
1:A:479:TRP:CH2	1:A:493:CYS:HB3	2.46	0.50
2:B:185:TRP:O	2:B:188:ARG:HB3	2.12	0.50
1:D:463:SER:HB2	1:D:528:PHE:HE2	1.75	0.50
1:D:477:ILE:HG21	1:D:497:LEU:HD22	1.92	0.50
1:D:101:SER:N	1:D:535:PHE:CZ	2.78	0.50
2:F:125:LYS:HE2	2:F:171:GLY:HA2	1.92	0.50
1:A:503:ASP:OD1	1:A:504:ALA:N	2.44	0.50
2:B:121:GLN:NE2	2:B:125:LYS:HD3	2.26	0.50
2:B:40:LYS:O	7:B:417:HOH:O	2.20	0.50
2:B:45:LEU:O	7:B:416:HOH:O	2.19	0.50
2:C:142:LYS:HA	1:D:39:ASN:OD1	2.12	0.50
2:E:33:ARG:NH1	2:E:41:SER:OG	2.43	0.50
1:A:366:VAL:HG22	1:A:387:GLU:O	2.12	0.50
2:C:73:TYR:OH	7:C:404:HOH:O	2.17	0.50
1:D:131:PHE:O	1:D:134:ARG:HB3	2.12	0.50
1:D:451:ARG:O	1:D:454:GLU:HG2	2.12	0.50
2:E:117:LYS:HE3	2:E:213:ARG:HH11	1.76	0.50
2:F:152:TYR:HA	2:F:155:ILE:HD12	1.92	0.50
1:A:424:ARG:O	7:A:726:HOH:O	2.20	0.50
1:A:74:GLU:OE2	7:A:723:HOH:O	2.19	0.50
1:A:76:TYR:O	1:A:79:ARG:HB2	2.11	0.50
1:A:84:ASP:C	1:A:86:SER:H	2.14	0.50
1:A:99:LEU:CD2	1:A:558:VAL:H	2.24	0.50
2:B:37:PHE:HZ	2:B:54:ILE:HG12	1.76	0.50
2:B:84:PHE:HD1	2:B:85:PHE:N	2.09	0.50
1:D:208:SER:CA	1:D:211:LEU:HG	2.36	0.50
1:D:425:ARG:NE	7:D:822:HOH:O	2.39	0.50
1:D:437:THR:O	1:D:440:ASP:N	2.45	0.50
2:F:101:PHE:HE2	2:F:135:LEU:HG	1.76	0.50
2:F:188:ARG:HG2	7:F:458:HOH:O	2.10	0.50
2:F:65:CYS:O	2:F:69:ASN:HB3	2.12	0.50
1:A:152:LYS:NZ	1:A:523:VAL:HB	2.25	0.50
1:D:238:TRP:O	1:D:241:ILE:HG22	2.12	0.50
1:D:535:PHE:HB3	1:D:544:GLN:O	2.12	0.50
1:D:90:THR:HA	1:D:399:TYR:HE2	1.77	0.50
1:A:213:ARG:HH21	1:A:296:PRO:HG3	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:ILE:O	1:A:81:VAL:HG23	2.11	0.50
2:B:5:PRO:HB3	2:B:57:LEU:HD11	1.93	0.50
1:D:8:PHE:O	7:D:743:HOH:O	2.20	0.50
1:D:171:ARG:NH1	7:D:729:HOH:O	2.17	0.50
1:D:451:ARG:HE	2:E:183:ILE:HD11	1.77	0.50
2:E:144:TYR:HB3	2:E:154:ASP:CG	2.32	0.50
2:E:163:TRP:O	2:E:166:ALA:HB3	2.12	0.50
1:A:324:PRO:O	7:A:719:HOH:O	2.17	0.49
2:C:33:ARG:HH12	2:C:43:LEU:HD12	1.77	0.49
1:D:288:TYR:CZ	1:D:321:GLY:HA2	2.47	0.49
2:C:138:GLU:O	1:D:38:LYS:HE3	2.12	0.49
1:D:435:LYS:HA	1:D:436:ASN:HB2	1.94	0.49
2:E:117:LYS:HE3	2:E:213:ARG:NH1	2.27	0.49
2:E:60:ASN:ND2	7:E:414:HOH:O	2.18	0.49
2:F:145:PHE:CB	2:F:153:VAL:HG13	2.40	0.49
1:A:445:VAL:HG22	1:A:479:TRP:HE1	1.77	0.49
1:A:517:ALA:HA	7:A:731:HOH:O	2.12	0.49
1:A:74:GLU:O	1:A:77:ILE:HD12	2.12	0.49
2:B:12:PRO:O	2:B:163:TRP:HZ2	1.95	0.49
1:D:425:ARG:CZ	1:D:545:PHE:HZ	2.25	0.49
1:D:328:HIS:CD2	3:D:601:JAA:O03	2.65	0.49
1:A:218:TYR:CE1	1:A:220:PHE:HB2	2.47	0.49
1:A:314:PRO:HB3	1:A:317:ARG:HH12	1.76	0.49
2:B:33:ARG:HH12	2:B:41:SER:HB2	1.78	0.49
2:C:139:LEU:HD22	1:D:92:HIS:NE2	2.27	0.49
2:C:13:SER:O	2:C:17:MET:HG3	2.12	0.49
1:D:153:GLN:HG2	1:D:167:THR:HG21	1.95	0.49
1:D:229:HIS:HA	1:D:232:ARG:HH11	1.78	0.49
2:F:53:LYS:HG2	6:F:301:GSH:HA31	1.95	0.49
1:A:94:VAL:HB	1:A:113:PHE:O	2.13	0.49
2:B:125:LYS:HD2	2:B:173:PHE:CE1	2.47	0.49
1:D:101:SER:HB3	1:D:535:PHE:CD2	2.48	0.49
1:D:362:GLU:HG3	1:D:400:ARG:NH2	2.27	0.49
1:D:531:ILE:HA	1:D:534:HIS:HD2	1.77	0.49
2:E:26:LYS:HE3	2:E:78:TRP:O	2.11	0.49
1:A:8:PHE:HB3	1:A:181:SER:OG	2.12	0.49
1:A:31:THR:O	1:A:35:ILE:HG13	2.13	0.49
1:A:164:THR:OG1	1:A:561:ILE:HG13	2.12	0.49
2:B:145:PHE:HB3	2:B:153:VAL:HG13	1.94	0.49
2:C:9:ASP:OD1	2:C:10:TYR:N	2.44	0.49
1:D:112:PRO:HG2	1:D:397:GLY:HA3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:219:VAL:HB	1:D:295:PHE:CZ	2.47	0.49
1:D:330:TYR:OH	1:D:542:ALA:N	2.45	0.49
1:D:479:TRP:CZ2	1:D:497:LEU:HD11	2.48	0.49
2:B:40:LYS:HD2	2:B:52:LYS:HB3	1.95	0.49
1:D:223:PHE:CE1	1:D:533:GLU:HA	2.48	0.49
1:D:386:GLU:O	7:D:739:HOH:O	2.19	0.49
1:D:153:GLN:HA	1:D:560:GLN:CG	2.43	0.49
2:E:73:TYR:HD1	2:E:76:GLU:OE2	1.95	0.49
1:A:222:VAL:C	1:A:223:PHE:HD1	2.16	0.49
2:C:85:PHE:CE1	2:C:152:TYR:HB2	2.48	0.49
2:F:183:ILE:O	2:F:187:LYS:HG3	2.12	0.49
1:A:490:LEU:HA	1:A:493:CYS:SG	2.53	0.49
1:D:17:PHE:O	1:D:21:THR:HG23	2.13	0.49
1:A:445:VAL:HG21	1:A:462:PHE:CD1	2.48	0.49
1:A:498:ASP:CB	1:A:510:ARG:HH22	2.25	0.49
2:F:182:LEU:O	7:F:415:HOH:O	2.20	0.49
1:A:27:VAL:O	1:A:31:THR:OG1	2.28	0.49
1:A:58:GLU:OE2	1:A:360:TYR:OH	2.31	0.49
1:A:437:THR:OG1	1:A:440:ASP:HB2	2.13	0.49
1:A:423:CYS:HB3	1:A:542:ALA:HB3	1.95	0.49
2:C:143:PRO:HA	1:D:87:PRO:HB2	1.94	0.49
1:D:147:PHE:O	1:D:529:ARG:NH2	2.45	0.49
1:D:492:ASP:HB3	2:E:187:LYS:HD3	1.94	0.49
1:A:405:ASP:OD1	1:A:426:ASN:HB3	2.13	0.48
2:C:111:PHE:HA	2:C:114:TRP:NE1	2.28	0.48
2:E:5:PRO:HB3	2:E:57:LEU:HD11	1.95	0.48
2:B:104:LYS:CG	2:B:105:LYS:N	2.77	0.48
1:D:543:GLY:O	7:D:744:HOH:O	2.20	0.48
2:E:97:PHE:CE1	2:E:101:PHE:HE1	2.30	0.48
1:A:171:ARG:HG2	1:A:194:PHE:CE2	2.48	0.48
1:A:213:ARG:NH2	1:A:296:PRO:HG3	2.28	0.48
2:C:201:ASP:HB2	2:C:204:LYS:HG3	1.94	0.48
1:D:331:GLY:N	1:D:537:GLY:O	2.46	0.48
1:D:333:SER:C	1:D:335:GLY:H	2.17	0.48
1:D:389:GLU:HA	1:D:405:ASP:O	2.13	0.48
1:D:417:PRO:O	7:D:745:HOH:O	2.20	0.48
1:D:107:ARG:NH2	1:D:434:ASP:HB3	2.25	0.48
1:D:451:ARG:HD3	2:E:187:LYS:HG2	1.95	0.48
1:A:95:PRO:O	1:A:161:PRO:HB2	2.13	0.48
2:B:191:GLU:OE2	7:B:418:HOH:O	2.20	0.48
2:B:23:LEU:O	2:B:28:VAL:HG12	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:201:ASP:HB3	2:C:203:GLU:HG2	1.95	0.48
1:D:139:ASP:OD2	1:D:142:GLY:HA3	2.13	0.48
1:D:302:TYR:HD1	1:D:326:VAL:HG13	1.79	0.48
1:D:413:TYR:CD2	1:D:418:GLN:HG2	2.48	0.48
1:D:419:LEU:O	7:D:741:HOH:O	2.19	0.48
1:A:223:PHE:HE2	1:A:545:PHE:CZ	2.27	0.48
1:A:549:ARG:NE	7:A:797:HOH:O	2.40	0.48
1:A:74:GLU:HG3	7:A:948:HOH:O	2.14	0.48
2:B:8:LEU:HD21	2:B:43:LEU:HD11	1.95	0.48
1:D:106:GLY:C	1:D:107:ARG:HD2	2.34	0.48
1:D:222:VAL:HB	1:D:533:GLU:HB3	1.96	0.48
1:D:27:VAL:O	1:D:31:THR:OG1	2.20	0.48
1:D:448:ALA:HB3	1:D:479:TRP:HH2	1.78	0.48
1:D:465:TYR:HD1	1:D:551:VAL:HG23	1.79	0.48
2:E:96:ARG:NH1	7:E:417:HOH:O	2.22	0.48
2:F:201:ASP:HB2	2:F:204:LYS:HG3	1.96	0.48
1:A:222:VAL:HG12	1:A:223:PHE:CE1	2.48	0.48
2:C:146:GLY:CA	2:C:151:GLY:HA3	2.44	0.48
2:C:92:ARG:NH1	2:C:96:ARG:HH22	2.12	0.48
1:D:96:ALA:HA	1:D:161:PRO:O	2.13	0.48
1:D:143:LYS:O	1:D:216:VAL:HA	2.12	0.48
2:F:90:TYR:O	2:F:93:ALA:HB3	2.13	0.48
1:A:203:TYR:HA	1:A:206:LEU:HD12	1.96	0.48
1:A:413:TYR:CD2	1:A:418:GLN:HG2	2.48	0.48
1:A:73:LEU:HD22	1:A:89:LEU:HD13	1.96	0.48
2:B:26:LYS:HE2	2:B:75:ASP:HA	1.96	0.48
2:C:119:GLU:OE2	7:C:407:HOH:O	2.20	0.48
2:E:146:GLY:HA3	7:E:478:HOH:O	2.14	0.48
2:E:195:VAL:HG23	2:E:199:LEU:HD13	1.95	0.48
2:F:104:LYS:NZ	7:F:448:HOH:O	2.46	0.48
2:F:24:ARG:HD2	2:F:198:SER:OG	2.13	0.48
2:B:140:GLY:C	2:B:181:LYS:NZ	2.66	0.48
2:B:117:LYS:HE3	2:B:213:ARG:HH11	1.78	0.48
1:D:77:ILE:HG22	1:D:110:PHE:HB3	1.96	0.48
1:D:95:PRO:HG2	1:D:113:PHE:CE2	2.49	0.48
1:D:207:LEU:HD11	1:D:245:ILE:HG23	1.94	0.48
1:D:223:PHE:CG	1:D:533:GLU:HG2	2.48	0.48
2:E:72:GLN:HG3	7:E:402:HOH:O	2.14	0.48
2:F:139:LEU:HB3	2:F:142:LYS:HB2	1.96	0.48
2:F:139:LEU:HD21	2:F:145:PHE:CD1	2.48	0.48
1:A:74:GLU:O	1:A:78:LYS:HB2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:26:LYS:HG2	2:B:81:LYS:HZ3	1.76	0.48
2:C:192:LYS:O	2:C:196:SER:N	2.39	0.48
1:D:518:LEU:HD12	1:D:519:GLU:N	2.28	0.48
1:A:175:PHE:CE1	1:A:179:MET:HG3	2.48	0.48
1:A:207:LEU:HD23	7:A:1054:HOH:O	2.13	0.48
1:A:479:TRP:CZ2	1:A:497:LEU:HD21	2.48	0.48
2:B:11:TRP:HB2	7:B:527:HOH:O	2.13	0.48
2:B:57:LEU:HB3	2:B:64:VAL:CG2	2.44	0.48
1:D:100:SER:OG	7:D:722:HOH:O	2.15	0.48
1:D:432:ASN:OD1	1:D:433:ILE:N	2.47	0.48
1:D:154:TYR:HB3	1:D:560:GLN:HA	1.96	0.48
1:D:75:PRO:O	1:D:79:ARG:HG3	2.14	0.48
1:D:496:CYS:HB2	2:E:187:LYS:CE	2.43	0.48
1:A:101:SER:HB3	1:A:535:PHE:CG	2.49	0.47
2:B:129:ILE:HA	2:B:132:VAL:HG12	1.96	0.47
2:C:37:PHE:HA	2:C:40:LYS:HG3	1.95	0.47
1:D:138:ILE:HG21	7:D:705:HOH:O	2.13	0.47
1:D:169:VAL:HG22	5:D:603:ATP:C2'	2.44	0.47
1:D:105:GLN:CA	1:D:430:SER:HB3	2.41	0.47
1:D:440:ASP:OD1	1:D:501:PHE:HA	2.14	0.47
1:D:534:HIS:CE1	1:D:535:PHE:CD1	3.02	0.47
1:A:143:LYS:HB2	1:A:185:PRO:O	2.14	0.47
1:A:246:LYS:NZ	1:A:271:PRO:HA	2.29	0.47
1:A:303:GLY:O	1:A:327:SER:HA	2.14	0.47
2:B:170:PHE:CD2	2:B:213:ARG:HD2	2.49	0.47
1:D:156:SER:HB2	1:D:160:VAL:O	2.14	0.47
1:D:234:PHE:N	7:D:708:HOH:O	2.47	0.47
1:D:287:TRP:O	1:D:290:LEU:HG	2.14	0.47
1:D:451:ARG:NH1	1:D:454:GLU:OE1	2.47	0.47
2:E:18:ARG:NH1	7:E:442:HOH:O	2.46	0.47
1:A:58:GLU:O	1:A:62:LYS:HG3	2.13	0.47
1:D:343:PRO:O	7:D:750:HOH:O	2.20	0.47
1:D:370:GLY:HA2	1:D:371:GLU:HA	1.74	0.47
2:E:185:TRP:O	2:E:188:ARG:HB3	2.14	0.47
2:F:68:LEU:HD22	2:F:152:TYR:OH	2.14	0.47
2:B:122:GLU:HA	2:B:125:LYS:HE2	1.96	0.47
2:B:136:GLU:HG3	2:B:181:LYS:CD	2.44	0.47
1:D:97:ILE:HG21	1:D:110:PHE:CD1	2.50	0.47
1:D:188:SER:HB3	1:D:192:VAL:HG13	1.95	0.47
1:D:110:PHE:CE2	1:D:554:SER:HA	2.50	0.47
1:D:77:ILE:HG13	1:D:89:LEU:HD12	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:104:LYS:HG3	2:E:105:LYS:N	2.29	0.47
2:E:93:ALA:O	2:F:69:ASN:ND2	2.38	0.47
2:F:164:PHE:HE2	7:F:415:HOH:O	1.96	0.47
1:A:287:TRP:O	1:A:290:LEU:HG	2.15	0.47
1:A:486:ASN:ND2	7:A:823:HOH:O	2.48	0.47
1:A:499:ARG:C	2:B:188:ARG:NH1	2.64	0.47
2:B:211:GLU:HA	2:B:214:LYS:HG2	1.96	0.47
1:D:198:VAL:HG13	1:D:565:ASN:HD21	1.79	0.47
2:E:90:TYR:HE1	2:F:63:PRO:O	1.97	0.47
2:F:18:ARG:NH1	2:F:103:ASP:OD1	2.46	0.47
2:F:142:LYS:HB3	2:F:144:TYR:O	2.15	0.47
1:A:556:ALA:HA	1:A:559:LEU:CB	2.44	0.47
2:B:9:ASP:HB2	2:B:20:ARG:HH21	1.80	0.47
6:C:301:GSH:HG12	6:C:301:GSH:O11	2.03	0.47
1:D:363:PHE:N	7:D:724:HOH:O	2.41	0.47
1:D:501:PHE:HD2	1:D:506:TYR:CE2	2.32	0.47
2:F:65:CYS:HB3	7:F:411:HOH:O	2.15	0.47
1:A:535:PHE:HB3	1:A:544:GLN:O	2.15	0.47
1:D:95:PRO:HD2	1:D:113:PHE:O	2.14	0.47
1:D:150:SER:HB3	1:D:170:TYR:HD2	1.80	0.47
6:F:301:GSH:O31	7:F:416:HOH:O	2.20	0.47
1:A:223:PHE:CE1	1:A:304:ILE:HD12	2.45	0.47
1:A:398:LEU:HD13	7:A:1023:HOH:O	2.15	0.47
1:A:45:LEU:HB2	7:A:747:HOH:O	2.15	0.47
1:A:474:HIS:HA	7:A:707:HOH:O	2.13	0.47
2:C:9:ASP:OD1	2:C:16:GLY:HA3	2.14	0.47
1:D:28:GLN:NE2	1:D:356:PRO:O	2.47	0.47
1:D:398:LEU:O	7:D:749:HOH:O	2.20	0.47
1:D:402:ARG:HG3	7:D:823:HOH:O	2.14	0.47
1:D:560:GLN:C	1:D:562:LEU:H	2.18	0.47
2:E:181:LYS:HA	2:E:184:ALA:HB3	1.97	0.47
1:A:36:LEU:HD11	7:A:1078:HOH:O	2.14	0.47
1:A:157:THR:HG22	1:A:469:SER:HB3	1.97	0.47
2:B:44:LEU:N	7:B:440:HOH:O	2.45	0.47
2:C:40:LYS:HG2	2:C:44:LEU:HD23	1.97	0.47
1:D:170:TYR:HB3	1:D:194:PHE:CZ	2.50	0.47
2:E:92:ARG:HE	2:E:96:ARG:HH22	1.61	0.47
1:A:306:THR:O	7:A:729:HOH:O	2.21	0.47
1:A:534:HIS:CG	1:A:557:LYS:HE2	2.50	0.47
2:B:102:VAL:O	2:B:107:THR:HG23	2.14	0.47
2:C:99:ALA:O	2:C:103:ASP:HB2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:TYR:O	7:A:704:HOH:O	2.20	0.47
1:A:219:VAL:HG11	1:A:301:VAL:HG22	1.97	0.47
1:A:32:LEU:HD21	1:A:61:PHE:CD2	2.49	0.47
1:A:452:LEU:HD11	7:A:873:HOH:O	2.15	0.47
1:A:444:SER:HA	1:A:500:ALA:HB1	1.97	0.47
1:A:108:PRO:HB3	1:A:555:ASN:CB	2.45	0.47
2:B:57:LEU:HB3	2:B:64:VAL:HG22	1.96	0.47
1:D:156:SER:HB3	7:D:813:HOH:O	2.14	0.47
1:D:76:TYR:HB3	1:D:88:ILE:HB	1.97	0.47
2:E:17:MET:HE2	2:E:200:PRO:HD2	1.97	0.47
2:E:62:LYS:HD3	2:F:90:TYR:CZ	2.50	0.47
2:E:84:PHE:CD1	2:E:152:TYR:HB2	2.50	0.47
2:E:90:TYR:CD2	2:F:62:LYS:HD3	2.50	0.47
2:F:101:PHE:CZ	2:F:131:ALA:HB1	2.40	0.47
2:F:169:LYS:HG3	2:F:170:PHE:N	2.28	0.47
1:A:496:CYS:CA	1:A:499:ARG:NH1	2.77	0.46
2:B:135:LEU:HD12	2:B:135:LEU:HA	1.38	0.46
2:B:17:MET:HE2	2:B:200:PRO:HD2	1.97	0.46
1:D:21:THR:HG22	7:D:706:HOH:O	2.15	0.46
1:D:363:PHE:CE1	1:D:390:VAL:HG22	2.50	0.46
1:D:78:LYS:HA	1:D:110:PHE:CD2	2.47	0.46
1:A:273:LEU:HD12	1:A:276:THR:HG21	1.96	0.46
2:B:126:LYS:HE3	7:B:561:HOH:O	2.15	0.46
2:C:161:SER:HB2	2:C:186:ALA:HB1	1.97	0.46
2:C:42:PRO:O	2:C:46:GLN:HB2	2.15	0.46
1:D:108:PRO:HB3	1:D:555:ASN:CB	2.45	0.46
1:D:507:VAL:HG13	1:D:511:LYS:HE2	1.97	0.46
2:E:143:PRO:HD2	7:E:443:HOH:O	2.14	0.46
2:E:183:ILE:O	2:E:187:LYS:HG3	2.15	0.46
1:A:150:SER:OG	1:A:170:TYR:HB2	2.16	0.46
1:A:188:SER:HG	1:A:205:HIS:CE1	2.33	0.46
1:A:360:TYR:N	7:A:763:HOH:O	2.48	0.46
1:A:534:HIS:CD2	1:A:557:LYS:NZ	2.77	0.46
2:C:95:ALA:HB1	2:C:152:TYR:HD2	1.81	0.46
2:C:65:CYS:O	2:C:66:GLU:HB2	2.15	0.46
1:D:166:THR:HG22	4:D:602:VAL:HB	1.98	0.46
2:E:98:TRP:CD1	2:E:153:VAL:HG21	2.50	0.46
2:E:187:LYS:HZ3	2:E:187:LYS:HB2	1.80	0.46
6:E:301:GSH:O2	7:E:403:HOH:O	2.20	0.46
2:F:40:LYS:HB3	2:F:44:LEU:HD23	1.96	0.46
1:A:387:GLU:C	1:A:388:TYR:HD1	2.18	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:452:LEU:HD13	7:A:711:HOH:O	2.15	0.46
2:B:73:TYR:HD1	2:B:76:GLU:OE2	1.98	0.46
2:C:125:LYS:HB3	2:C:173:PHE:CE2	2.50	0.46
2:C:169:LYS:NZ	2:C:206:VAL:HG13	2.30	0.46
1:D:168:ASN:HB3	5:D:603:ATP:H5'2	1.97	0.46
1:D:223:PHE:O	1:D:227:LEU:HD12	2.16	0.46
1:D:538:LEU:HG	1:D:544:GLN:NE2	2.30	0.46
1:D:39:ASN:ND2	1:D:90:THR:HG22	2.31	0.46
2:E:33:ARG:HH12	2:E:41:SER:CB	2.28	0.46
1:A:153:GLN:HG3	1:A:171:ARG:HD2	1.98	0.46
1:A:212:PHE:O	1:A:216:VAL:HG23	2.14	0.46
1:A:143:LYS:O	1:A:216:VAL:HA	2.16	0.46
1:A:90:THR:CG2	1:A:397:GLY:H	2.28	0.46
1:A:450:LYS:HE2	1:A:450:LYS:HB3	1.59	0.46
1:A:223:PHE:CE2	1:A:533:GLU:HA	2.51	0.46
1:D:107:ARG:HG3	1:D:107:ARG:NH1	2.30	0.46
1:D:246:LYS:HB3	1:D:246:LYS:HE3	1.53	0.46
1:D:527:THR:HG23	1:D:561:ILE:CG2	2.45	0.46
2:E:145:PHE:HB3	2:E:153:VAL:CG1	2.46	0.46
2:F:72:GLN:OE1	2:F:152:TYR:OH	2.15	0.46
1:A:361:PHE:HD2	7:A:706:HOH:O	1.99	0.46
1:A:519:GLU:CD	1:A:521:ARG:HE	2.18	0.46
2:B:126:LYS:O	2:B:129:ILE:HG13	2.16	0.46
2:B:75:ASP:OD1	7:B:419:HOH:O	2.20	0.46
2:B:90:TYR:CE2	2:C:62:LYS:HD3	2.50	0.46
1:D:374:GLU:N	7:D:754:HOH:O	2.48	0.46
1:D:378:GLY:O	1:D:382:VAL:HG23	2.15	0.46
1:D:478:PHE:O	1:D:479:TRP:HD1	1.98	0.46
2:E:64:VAL:HB	2:E:73:TYR:CE2	2.50	0.46
2:E:97:PHE:HD1	2:F:66:GLU:CD	2.18	0.46
1:A:166:THR:HG21	1:A:530:LYS:CD	2.40	0.46
1:A:199:HIS:CD2	1:A:200:GLN:HG3	2.51	0.46
2:B:114:TRP:HA	2:B:170:PHE:CD2	2.49	0.46
2:C:43:LEU:HD23	2:C:43:LEU:HA	1.62	0.46
1:D:164:THR:HG22	1:D:165:ALA:N	2.30	0.46
1:D:222:VAL:HG21	4:D:602:VAL:N	2.31	0.46
1:D:315:LYS:HG3	1:D:319:TYR:CE2	2.51	0.46
1:D:107:ARG:NH2	1:D:552:LYS:HD3	2.26	0.46
2:F:102:VAL:HG22	2:F:157:LEU:HD13	1.97	0.46
2:F:125:LYS:O	2:F:129:ILE:HG12	2.16	0.46
1:A:17:PHE:CD1	1:A:127:THR:HG21	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:292:PRO:HD3	1:A:323:LEU:HD12	1.97	0.46
1:A:406:VAL:O	1:A:541:SER:OG	2.30	0.46
1:A:490:LEU:HD23	7:A:873:HOH:O	2.16	0.46
2:B:108:ASP:O	2:B:112:LYS:HG2	2.16	0.46
2:B:171:GLY:O	2:B:173:PHE:HD1	1.97	0.46
2:B:43:LEU:HG	7:B:440:HOH:O	2.15	0.46
2:B:98:TRP:O	2:B:101:PHE:HB2	2.15	0.46
1:D:475:TYR:HB2	1:D:518:LEU:HB2	1.97	0.46
2:F:193:GLU:HA	2:F:196:SER:HB3	1.97	0.46
1:A:27:VAL:HB	1:A:356:PRO:HB2	1.96	0.46
1:D:328:HIS:CG	1:D:329:ASP:H	2.33	0.46
1:D:339:ALA:N	1:D:353:ALA:O	2.34	0.46
1:D:418:GLN:NE2	7:D:852:HOH:O	2.49	0.46
1:D:490:LEU:HD23	1:D:490:LEU:HA	1.81	0.46
1:D:223:PHE:CZ	1:D:536:LEU:HB2	2.51	0.46
5:D:603:ATP:O3A	5:D:603:ATP:O2G	2.34	0.46
1:D:82:ASP:HA	7:D:813:HOH:O	2.15	0.46
1:A:344:ARG:NH1	7:A:825:HOH:O	2.48	0.46
1:A:568:SER:HB3	7:A:725:HOH:O	2.16	0.46
2:B:173:PHE:O	7:B:420:HOH:O	2.21	0.46
2:B:205:ILE:HG23	7:B:477:HOH:O	2.15	0.46
2:B:9:ASP:HB2	2:B:20:ARG:NH2	2.30	0.46
1:D:42:ALA:HB3	1:D:45:LEU:HD13	1.98	0.46
1:D:499:ARG:HB2	1:D:499:ARG:CZ	2.45	0.46
1:D:495:ASN:HB2	1:D:499:ARG:NH1	2.31	0.46
1:D:101:SER:HB3	1:D:535:PHE:CE2	2.51	0.46
2:F:145:PHE:HB2	2:F:154:ASP:OD2	2.16	0.46
1:A:104:SER:O	1:A:107:ARG:HG2	2.17	0.45
1:A:166:THR:HG23	4:A:602:VAL:O	2.17	0.45
1:A:110:PHE:CE2	1:A:554:SER:HA	2.51	0.45
3:A:601:JAA:O02	5:A:603:ATP:N6	2.49	0.45
2:B:153:VAL:HG23	7:B:510:HOH:O	2.16	0.45
2:B:211:GLU:O	2:B:214:LYS:HG2	2.16	0.45
2:B:41:SER:HB3	7:B:440:HOH:O	2.16	0.45
2:C:75:ASP:OD2	7:C:408:HOH:O	2.21	0.45
1:D:105:GLN:HA	1:D:430:SER:CB	2.43	0.45
1:D:33:LYS:O	1:D:37:LEU:HB2	2.16	0.45
2:C:142:LYS:O	1:D:92:HIS:CD2	2.69	0.45
2:E:199:LEU:HA	2:E:200:PRO:HD2	1.80	0.45
2:E:44:LEU:HD12	7:E:477:HOH:O	2.15	0.45
1:A:145:LEU:O	1:A:220:PHE:N	2.41	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:380:THR:HG21	7:A:810:HOH:O	2.16	0.45
1:A:165:ALA:N	1:A:557:LYS:HE3	2.27	0.45
2:C:148:ASP:HB2	1:D:46:GLN:HB2	1.97	0.45
1:D:223:PHE:HZ	1:D:536:LEU:CB	2.29	0.45
1:D:263:MET:SD	1:D:266:LEU:HD12	2.56	0.45
1:D:35:ILE:HG12	1:D:395:TYR:CD1	2.51	0.45
1:D:45:LEU:HB3	1:D:50:LEU:HB2	1.98	0.45
2:F:75:ASP:OD2	2:F:85:PHE:HD1	2.00	0.45
1:A:18:ASP:O	1:A:22:ARG:HG3	2.16	0.45
1:A:253:ARG:HG3	1:A:484:GLU:OE1	2.15	0.45
1:A:449:ALA:O	1:A:452:LEU:HB2	2.16	0.45
2:B:165:GLN:HA	2:B:168:GLU:OE1	2.16	0.45
1:D:108:PRO:HA	7:D:855:HOH:O	2.14	0.45
1:D:270:ASN:O	7:D:751:HOH:O	2.21	0.45
2:E:34:GLU:HG2	7:E:548:HOH:O	2.15	0.45
2:E:91:GLY:HA2	7:E:404:HOH:O	2.15	0.45
1:A:328:HIS:CG	1:A:329:ASP:H	2.35	0.45
1:A:439:ARG:O	1:A:443:LEU:HB2	2.16	0.45
2:C:165:GLN:N	7:C:442:HOH:O	2.49	0.45
1:D:151:SER:HB3	1:D:565:ASN:HD21	1.80	0.45
1:D:167:THR:HB	1:D:560:GLN:OE1	2.17	0.45
1:D:320:ALA:O	1:D:323:LEU:HB2	2.15	0.45
1:D:491:GLN:HE21	1:D:570:TYR:HD2	1.63	0.45
2:F:24:ARG:HB3	2:F:194:SER:HA	1.99	0.45
1:A:110:PHE:CZ	1:A:554:SER:HA	2.52	0.45
2:B:125:LYS:HA	2:B:128:PHE:CE2	2.51	0.45
2:B:133:LYS:HE2	2:B:133:LYS:HB3	1.73	0.45
2:B:183:ILE:O	2:B:183:ILE:HG13	2.16	0.45
2:B:23:LEU:HB3	2:B:28:VAL:HG11	1.98	0.45
2:C:98:TRP:CE2	2:C:138:GLU:HG2	2.52	0.45
2:E:128:PHE:O	2:E:132:VAL:HG12	2.17	0.45
2:F:8:LEU:HD21	2:F:43:LEU:HD23	1.98	0.45
1:A:113:PHE:HB2	5:A:603:ATP:O1B	2.17	0.45
1:A:151:SER:HB2	1:A:194:PHE:HA	1.98	0.45
1:A:284:LEU:HG	1:A:284:LEU:H	1.60	0.45
2:B:117:LYS:HA	2:B:121:GLN:HB2	1.99	0.45
1:D:149:PHE:HB2	1:D:530:LYS:HE3	1.99	0.45
1:D:308:SER:O	1:D:311:PRO:HD2	2.17	0.45
1:D:329:ASP:HB3	1:D:338:ALA:O	2.17	0.45
2:E:139:LEU:HB3	2:E:181:LYS:HE2	1.99	0.45
2:F:51:HIS:O	2:F:53:LYS:HG3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:433:ILE:C	1:A:435:LYS:H	2.19	0.45
1:A:482:SER:HA	1:A:525:LYS:HE2	1.99	0.45
1:A:547:MET:SD	7:A:753:HOH:O	2.61	0.45
1:A:152:LYS:CG	1:A:565:ASN:H	2.27	0.45
2:B:98:TRP:O	2:B:98:TRP:CE3	2.70	0.45
1:D:230:ALA:O	1:D:233:THR:OG1	2.33	0.45
1:D:452:LEU:HD13	1:D:493:CYS:SG	2.57	0.45
1:D:492:ASP:C	7:D:701:HOH:O	2.55	0.45
2:E:122:GLU:HA	2:E:125:LYS:HE2	1.97	0.45
2:F:74:VAL:HG22	7:F:565:HOH:O	2.17	0.45
1:A:167:THR:HB	1:A:560:GLN:OE1	2.16	0.45
1:A:288:TYR:CZ	1:A:321:GLY:HA2	2.52	0.45
1:A:305:MET:CB	1:A:347:PRO:HB3	2.44	0.45
2:B:23:LEU:HB3	2:B:28:VAL:CG1	2.46	0.45
2:B:68:LEU:HA	2:B:71:VAL:HG12	1.99	0.45
1:D:143:LYS:HG3	1:D:144:ALA:N	2.32	0.45
1:D:138:ILE:HA	1:D:217:GLN:NE2	2.32	0.45
1:D:398:LEU:HD13	1:D:401:TYR:HB3	1.98	0.45
2:E:135:LEU:HD23	2:E:145:PHE:HZ	1.82	0.45
2:E:68:LEU:O	2:E:72:GLN:HG2	2.16	0.45
2:F:15:PHE:HB3	2:F:67:SER:CB	2.44	0.45
1:A:142:GLY:N	7:A:742:HOH:O	2.36	0.45
1:A:332:SER:HG	1:A:534:HIS:CD2	2.27	0.45
1:A:488:ASP:OD2	2:B:168:GLU:OE2	2.34	0.45
2:B:104:LYS:HG3	2:B:105:LYS:H	1.80	0.45
2:C:51:HIS:O	7:C:409:HOH:O	2.21	0.45
1:D:30:GLN:OE1	1:D:33:LYS:HG3	2.17	0.45
1:D:534:HIS:CE1	1:D:535:PHE:CZ	3.05	0.45
1:D:543:GLY:O	1:D:544:GLN:HG3	2.17	0.45
2:E:127:GLU:HG3	7:E:475:HOH:O	2.17	0.45
2:E:8:LEU:HD22	2:E:33:ARG:NH2	2.25	0.45
1:A:135:ASP:OD2	1:A:343:PRO:HD2	2.17	0.45
1:A:460:ILE:HD11	1:A:480:GLU:CD	2.36	0.45
1:A:552:LYS:HD2	1:A:553:PRO:HD2	1.99	0.45
2:B:23:LEU:CD2	2:B:28:VAL:HG11	2.45	0.45
1:D:330:TYR:CD2	1:D:539:GLY:HA2	2.51	0.45
1:A:11:ASN:O	1:A:14:ILE:HG13	2.17	0.44
1:A:520:LEU:HD21	7:A:984:HOH:O	2.17	0.44
1:A:519:GLU:HG3	1:A:570:TYR:O	2.17	0.44
1:A:451:ARG:NE	2:B:183:ILE:HD11	2.32	0.44
2:C:162:SER:HB3	2:C:199:LEU:HD23	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:33:ARG:CZ	2:C:43:LEU:HD12	2.46	0.44
1:D:421:PHE:CD1	1:D:541:SER:HA	2.52	0.44
1:D:526:GLY:O	1:D:530:LYS:HG3	2.16	0.44
1:D:170:TYR:OH	4:D:602:VAL:HG11	2.17	0.44
2:E:131:ALA:O	2:E:135:LEU:HB2	2.17	0.44
2:E:15:PHE:O	2:E:18:ARG:HB2	2.17	0.44
2:E:166:ALA:C	7:E:401:HOH:O	2.54	0.44
1:A:463:SER:HB2	1:A:528:PHE:CE2	2.48	0.44
2:B:98:TRP:CE3	2:B:101:PHE:HB2	2.48	0.44
1:D:169:VAL:HG21	4:D:602:VAL:HG12	1.98	0.44
1:D:29:LYS:HG2	1:D:33:LYS:HE2	1.99	0.44
1:D:398:LEU:CD1	1:D:401:TYR:HB3	2.47	0.44
1:D:494:CYS:SG	7:D:844:HOH:O	2.61	0.44
1:A:143:LYS:NZ	1:A:187:CYS:HA	2.32	0.44
1:A:164:THR:N	1:A:560:GLN:OE1	2.50	0.44
1:A:37:LEU:HD12	1:A:37:LEU:HA	1.91	0.44
1:A:407:VAL:HG21	1:A:419:LEU:HB3	1.98	0.44
2:C:169:LYS:HG3	2:C:170:PHE:H	1.83	0.44
1:D:510:ARG:NH1	1:D:575:PHE:CE2	2.85	0.44
1:A:314:PRO:HA	1:A:317:ARG:HB3	1.98	0.44
1:A:393:THR:HA	1:A:398:LEU:O	2.17	0.44
1:A:499:ARG:CZ	1:A:499:ARG:CB	2.95	0.44
1:A:521:ARG:HB2	7:A:803:HOH:O	2.17	0.44
2:C:146:GLY:HA3	2:C:151:GLY:HA3	1.99	0.44
1:D:28:GLN:NE2	7:D:728:HOH:O	2.17	0.44
1:D:29:LYS:NZ	1:D:33:LYS:HZ3	2.14	0.44
1:D:450:LYS:HD3	2:E:190:MET:HB3	1.98	0.44
2:F:132:VAL:HG22	2:F:182:LEU:HD23	1.99	0.44
1:D:159:GLY:HA3	7:D:892:HOH:O	2.18	0.44
1:D:369:THR:HG23	1:D:370:GLY:H	1.81	0.44
1:D:363:PHE:HD2	1:D:382:VAL:HG21	1.82	0.44
2:E:164:PHE:HB3	7:E:418:HOH:O	2.16	0.44
1:D:500:ALA:N	2:E:188:ARG:HH12	2.15	0.44
2:E:54:ILE:N	7:E:403:HOH:O	2.51	0.44
1:A:250:LEU:CD1	1:A:254:ILE:HB	2.48	0.44
2:B:159:THR:HA	2:B:199:LEU:HD21	2.00	0.44
2:C:163:TRP:HB3	2:C:167:TYR:CZ	2.53	0.44
1:D:32:LEU:HD13	1:D:61:PHE:CE2	2.48	0.44
1:D:465:TYR:CD1	1:D:551:VAL:HG23	2.53	0.44
2:E:70:VAL:O	2:E:73:TYR:HB2	2.18	0.44
2:F:18:ARG:HH12	2:F:103:ASP:CG	2.20	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:GLN:C	1:A:148:ILE:H	2.21	0.44
1:A:26:GLN:OE1	7:A:728:HOH:O	2.20	0.44
1:A:325:LEU:HD23	7:A:719:HOH:O	2.18	0.44
1:A:109:LYS:HE2	1:A:401:TYR:CZ	2.53	0.44
2:B:10:TYR:CD2	2:B:12:PRO:HD2	2.52	0.44
1:D:303:GLY:O	1:D:327:SER:HA	2.18	0.44
1:D:44:TYR:HB3	7:D:707:HOH:O	2.17	0.44
1:D:534:HIS:HA	7:D:720:HOH:O	2.17	0.44
1:D:223:PHE:CZ	1:D:536:LEU:CB	3.00	0.44
1:D:36:LEU:HD22	1:D:61:PHE:CE1	2.53	0.44
1:D:83:GLY:HA3	7:D:857:HOH:O	2.17	0.44
2:E:75:ASP:OD2	7:E:416:HOH:O	2.21	0.44
1:A:17:PHE:CZ	1:A:341:VAL:HG11	2.53	0.44
1:A:234:PHE:HD1	7:A:1060:HOH:O	2.01	0.44
1:A:434:ASP:HB2	1:A:550:CYS:HB3	2.00	0.44
2:B:81:LYS:HG3	2:B:82:ASN:H	1.83	0.44
1:D:212:PHE:O	1:D:216:VAL:HG23	2.18	0.44
1:D:337:ILE:O	1:D:354:VAL:HA	2.18	0.44
2:C:143:PRO:HD3	1:D:39:ASN:OD1	2.17	0.44
1:D:389:GLU:HG3	1:D:405:ASP:H	1.82	0.44
1:D:450:LYS:HD3	2:E:190:MET:C	2.37	0.44
2:E:187:LYS:HG3	2:E:187:LYS:H	1.64	0.44
2:E:84:PHE:CD1	2:E:85:PHE:N	2.82	0.44
2:F:168:GLU:OE2	2:F:174:SER:HA	2.18	0.44
2:F:170:PHE:HB3	7:F:423:HOH:O	2.17	0.44
1:A:102:GLY:HA3	1:A:426:ASN:HD21	1.83	0.44
1:A:164:THR:O	1:A:168:ASN:ND2	2.51	0.44
1:A:320:ALA:O	1:A:323:LEU:HB2	2.17	0.44
1:A:451:ARG:NH1	1:A:454:GLU:CD	2.71	0.44
1:A:559:LEU:HD12	1:A:562:LEU:HD12	1.99	0.44
1:A:81:VAL:HG21	1:A:110:PHE:CD2	2.53	0.44
1:A:90:THR:HG23	1:A:397:GLY:CA	2.47	0.44
2:B:183:ILE:O	2:B:186:ALA:HB3	2.17	0.44
2:C:21:VAL:HG12	2:C:155:ILE:HG12	2.00	0.44
1:D:405:ASP:HA	7:D:821:HOH:O	2.18	0.44
1:D:444:SER:HA	1:D:500:ALA:CB	2.48	0.44
1:D:557:LYS:HD2	5:D:603:ATP:PG	2.58	0.44
1:D:99:LEU:CB	1:D:557:LYS:H	2.31	0.44
1:D:162:VAL:CG2	1:D:559:LEU:HD23	2.46	0.44
2:E:17:MET:HB3	2:E:199:LEU:HD11	2.00	0.44
1:A:70:ASP:CB	1:A:109:LYS:HD2	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:208:SER:HA	1:A:211:LEU:HB2	1.99	0.43
1:A:256:VAL:O	1:A:260:ARG:HB2	2.18	0.43
1:A:574:ALA:O	1:A:575:PHE:HB2	2.17	0.43
1:A:500:ALA:CA	2:B:188:ARG:NH1	2.66	0.43
1:D:108:PRO:HG2	1:D:552:LYS:N	2.23	0.43
1:D:187:CYS:HB2	1:D:208:SER:C	2.39	0.43
1:D:219:VAL:HG22	1:D:227:LEU:HD23	2.00	0.43
1:D:405:ASP:OD1	1:D:540:SER:HB2	2.18	0.43
2:E:21:VAL:HG12	2:E:155:ILE:HG12	2.00	0.43
2:F:4:LEU:HA	2:F:5:PRO:HD3	1.86	0.43
2:F:6:ILE:HD12	2:F:6:ILE:N	2.33	0.43
1:A:138:ILE:CA	1:A:217:GLN:HE21	2.31	0.43
1:A:477:ILE:O	1:A:520:LEU:HD12	2.18	0.43
1:A:99:LEU:HD22	1:A:555:ASN:HB3	1.99	0.43
2:C:16:GLY:O	2:C:20:ARG:HG3	2.18	0.43
1:D:150:SER:OG	1:D:170:TYR:HB2	2.18	0.43
1:D:223:PHE:HZ	1:D:536:LEU:HB2	1.81	0.43
1:D:262:ALA:O	1:D:266:LEU:HG	2.18	0.43
1:D:387:GLU:HB3	1:D:406:VAL:HG13	1.99	0.43
1:D:406:VAL:O	1:D:541:SER:OG	2.33	0.43
1:D:56:ASP:N	1:D:57:PRO:HD3	2.33	0.43
2:E:13:SER:O	2:E:17:MET:HG3	2.18	0.43
2:F:15:PHE:O	2:F:18:ARG:HB2	2.19	0.43
1:A:302:TYR:OH	7:A:717:HOH:O	2.19	0.43
1:A:302:TYR:HD1	1:A:326:VAL:HG13	1.83	0.43
2:B:156:SER:O	7:B:421:HOH:O	2.21	0.43
2:B:17:MET:HE3	2:B:163:TRP:HH2	1.83	0.43
1:D:108:PRO:HG2	1:D:552:LYS:HB3	2.00	0.43
1:D:132:ARG:HD3	1:D:326:VAL:HG21	2.00	0.43
1:D:526:GLY:O	1:D:529:ARG:HB3	2.18	0.43
1:D:547:MET:HA	1:D:548:PRO:HD2	1.90	0.43
1:A:355:ILE:HG23	7:A:1064:HOH:O	2.17	0.43
1:A:403:LEU:HA	1:A:403:LEU:HD12	1.79	0.43
1:A:403:LEU:HD13	7:A:949:HOH:O	2.18	0.43
1:A:502:ILE:H	1:A:502:ILE:HG13	1.38	0.43
1:A:531:ILE:HG13	1:A:558:VAL:HG22	2.00	0.43
1:A:534:HIS:HB2	4:A:602:VAL:C	2.39	0.43
2:B:70:VAL:HA	2:B:73:TYR:CD2	2.53	0.43
2:B:78:TRP:N	7:B:403:HOH:O	2.09	0.43
1:D:445:VAL:HG22	1:D:479:TRP:NE1	2.32	0.43
1:D:473:GLY:N	7:D:856:HOH:O	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:489:VAL:O	1:D:492:ASP:HB2	2.18	0.43
1:D:549:ARG:HD3	1:D:549:ARG:HA	1.66	0.43
1:D:561:ILE:O	1:D:561:ILE:HG22	2.17	0.43
1:D:7:THR:N	7:D:817:HOH:O	2.51	0.43
2:E:40:LYS:HB3	2:E:44:LEU:HD23	2.01	0.43
2:E:84:PHE:HD1	2:E:84:PHE:C	2.21	0.43
1:A:198:VAL:HG13	1:A:565:ASN:ND2	2.34	0.43
2:B:114:TRP:CD1	2:B:167:TYR:HE1	2.35	0.43
2:B:26:LYS:HG2	2:B:81:LYS:HZ1	1.80	0.43
2:B:96:ARG:O	7:B:422:HOH:O	2.21	0.43
2:C:150:PHE:HE2	2:C:155:ILE:HG13	1.83	0.43
2:C:20:ARG:NH1	2:C:198:SER:O	2.50	0.43
1:D:330:TYR:HE2	1:D:540:SER:N	2.11	0.43
1:D:337:ILE:HG22	1:D:354:VAL:HG22	2.01	0.43
1:D:433:ILE:C	1:D:435:LYS:H	2.20	0.43
1:D:445:VAL:HG21	1:D:462:PHE:CG	2.54	0.43
1:D:551:VAL:HB	1:D:555:ASN:HB2	2.01	0.43
2:E:16:GLY:HA2	2:E:55:PRO:HB3	2.00	0.43
2:F:157:LEU:O	2:F:160:PHE:HB2	2.19	0.43
1:A:165:ALA:HB1	5:A:603:ATP:N3	2.34	0.43
2:B:125:LYS:HA	2:B:128:PHE:CD2	2.53	0.43
2:C:129:ILE:HA	2:C:132:VAL:HG22	2.01	0.43
2:C:141:ASP:C	1:D:92:HIS:H	2.21	0.43
2:C:149:SER:HB3	2:C:150:PHE:H	1.67	0.43
1:D:142:GLY:O	1:D:185:PRO:HD2	2.18	0.43
1:D:14:ILE:HG13	1:D:15:ASP:N	2.33	0.43
1:D:97:ILE:HB	1:D:162:VAL:HG12	2.01	0.43
1:D:25:HIS:CE1	1:D:380:THR:HG21	2.54	0.43
1:D:497:LEU:HB2	7:D:991:HOH:O	2.19	0.43
1:D:84:ASP:OD1	1:D:86:SER:HB3	2.19	0.43
2:F:107:THR:O	2:F:110:GLN:HG3	2.19	0.43
1:A:496:CYS:HA	1:A:499:ARG:CZ	2.48	0.43
2:B:199:LEU:HA	2:B:200:PRO:HD2	1.73	0.43
1:D:115:ASP:OD1	7:D:753:HOH:O	2.21	0.43
1:D:157:THR:HG23	7:D:946:HOH:O	2.17	0.43
1:D:552:LYS:C	1:D:554:SER:N	2.71	0.43
2:F:11:TRP:CG	2:F:12:PRO:HD3	2.53	0.43
1:A:316:LEU:O	1:A:320:ALA:N	2.46	0.43
1:A:31:THR:OG1	1:A:357:ASN:HA	2.19	0.43
1:A:42:ALA:N	7:A:747:HOH:O	2.52	0.43
1:D:464:SER:HA	1:D:476:ALA:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:165:ALA:N	5:D:603:ATP:O2G	2.52	0.43
2:C:188:ARG:HH22	1:D:88:ILE:HG22	1.83	0.43
2:E:10:TYR:CG	2:E:12:PRO:HD2	2.53	0.43
1:A:510:ARG:HD2	7:A:731:HOH:O	2.19	0.43
1:A:72:GLU:O	1:A:75:PRO:HD2	2.19	0.43
2:B:9:ASP:HA	2:B:54:ILE:HD13	2.00	0.43
2:C:54:ILE:HB	2:C:55:PRO:HA	2.01	0.43
1:D:465:TYR:HB3	1:D:476:ALA:HB3	2.00	0.43
2:E:129:ILE:HA	2:E:132:VAL:HG12	1.99	0.43
2:F:132:VAL:CG2	2:F:182:LEU:HD23	2.49	0.43
2:F:164:PHE:CD2	2:F:183:ILE:HD13	2.54	0.43
2:F:91:GLY:HA2	7:F:490:HOH:O	2.18	0.43
1:A:124:LEU:HB3	3:A:601:JAA:C15	2.48	0.43
1:A:149:PHE:CE1	1:A:205:HIS:HD2	2.37	0.43
1:A:282:MET:HB2	1:A:282:MET:HE2	1.78	0.43
1:A:330:TYR:HE2	1:A:540:SER:H	1.67	0.43
2:B:110:GLN:O	2:B:113:VAL:HG12	2.18	0.43
1:A:456:LYS:HZ3	2:B:204:LYS:HE2	1.83	0.43
2:B:65:CYS:HB3	7:B:436:HOH:O	2.19	0.43
2:C:150:PHE:CE2	2:C:155:ILE:HG13	2.54	0.43
1:D:145:LEU:HD23	1:D:219:VAL:HG23	2.01	0.43
1:D:232:ARG:HB3	7:D:721:HOH:O	2.19	0.43
1:D:423:CYS:HB2	1:D:542:ALA:HB3	2.00	0.43
1:A:146:GLN:HB3	1:A:148:ILE:HG23	2.01	0.42
1:A:444:SER:HA	1:A:500:ALA:CB	2.49	0.42
1:A:441:LEU:CD2	1:A:549:ARG:HB3	2.49	0.42
1:A:552:LYS:C	1:A:554:SER:H	2.16	0.42
1:A:93:PRO:HA	7:A:779:HOH:O	2.19	0.42
1:D:164:THR:HA	1:D:557:LYS:HG3	2.01	0.42
1:D:164:THR:HG23	1:D:557:LYS:CG	2.47	0.42
1:D:424:ARG:HB2	1:D:425:ARG:NH1	2.34	0.42
1:D:495:ASN:HB2	1:D:499:ARG:HH12	1.84	0.42
1:D:507:VAL:O	1:D:511:LYS:HB2	2.18	0.42
2:E:140:GLY:N	2:E:181:LYS:NZ	2.67	0.42
1:D:492:ASP:C	2:E:187:LYS:HE3	2.39	0.42
2:E:33:ARG:HH22	2:E:41:SER:HB2	1.84	0.42
2:B:76:GLU:OE2	2:C:96:ARG:NH1	2.52	0.42
2:B:90:TYR:O	2:B:94:GLN:HG3	2.18	0.42
2:C:11:TRP:CD2	2:C:12:PRO:HD3	2.54	0.42
1:D:398:LEU:HG	7:D:749:HOH:O	2.18	0.42
1:D:410:ILE:HG13	1:D:411:GLY:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:142:LYS:HG2	2:E:144:TYR:H	1.83	0.42
1:A:204:CYS:SG	7:A:767:HOH:O	2.39	0.42
1:A:369:THR:HG23	1:A:370:GLY:H	1.85	0.42
1:A:389:GLU:HA	1:A:405:ASP:O	2.19	0.42
1:A:198:VAL:CG2	1:A:524:ALA:HB3	2.50	0.42
1:A:529:ARG:O	1:A:533:GLU:HG3	2.19	0.42
1:D:369:THR:HG23	1:D:370:GLY:N	2.34	0.42
1:D:423:CYS:HB2	1:D:542:ALA:C	2.39	0.42
1:D:478:PHE:HZ	1:D:562:LEU:HG	1.84	0.42
1:D:80:MET:HG2	1:D:86:SER:O	2.19	0.42
2:E:37:PHE:HE2	6:E:301:GSH:HB22	1.84	0.42
2:F:152:TYR:O	2:F:155:ILE:HB	2.19	0.42
2:F:157:LEU:HA	2:F:160:PHE:CD1	2.55	0.42
2:F:170:PHE:CE2	2:F:213:ARG:HD2	2.54	0.42
1:A:302:TYR:OH	1:A:328:HIS:ND1	2.26	0.42
1:A:121:THR:HA	3:A:601:JAA:C15	2.49	0.42
2:B:4:LEU:HA	2:B:5:PRO:HD3	1.89	0.42
2:C:164:PHE:CD2	2:C:183:ILE:HG12	2.55	0.42
1:D:22:ARG:HH11	1:D:414:ASN:CG	2.22	0.42
1:D:294:LEU:O	1:D:296:PRO:HD3	2.19	0.42
1:D:107:ARG:HD3	1:D:432:ASN:HA	2.02	0.42
2:E:22:ALA:HA	2:E:155:ILE:HD13	2.02	0.42
1:A:238:TRP:HB2	7:A:1087:HOH:O	2.19	0.42
1:A:313:VAL:HB	1:A:314:PRO:HD3	2.01	0.42
1:A:407:VAL:CG2	1:A:419:LEU:HB3	2.50	0.42
1:A:108:PRO:HG3	1:A:552:LYS:HB3	2.02	0.42
1:A:169:VAL:HG22	5:A:603:ATP:O2'	2.19	0.42
2:B:7:LEU:HD13	2:B:30:PHE:CD2	2.55	0.42
2:B:84:PHE:CD1	2:B:85:PHE:N	2.88	0.42
2:C:17:MET:SD	2:C:199:LEU:HG	2.60	0.42
1:D:276:THR:HA	7:D:989:HOH:O	2.19	0.42
1:D:42:ALA:O	1:D:45:LEU:HB2	2.20	0.42
1:D:168:ASN:ND2	5:D:603:ATP:O2A	2.52	0.42
2:F:129:ILE:O	2:F:132:VAL:HG12	2.19	0.42
1:A:108:PRO:HG2	1:A:554:SER:OG	2.19	0.42
2:B:142:LYS:HB2	2:B:142:LYS:HE3	1.72	0.42
1:D:121:THR:HG21	5:D:603:ATP:O2'	2.19	0.42
1:D:13:VAL:HG23	7:D:952:HOH:O	2.18	0.42
1:D:36:LEU:O	1:D:40:GLN:N	2.52	0.42
1:D:434:ASP:HB2	1:D:550:CYS:HB3	2.01	0.42
2:E:107:THR:HG22	2:E:160:PHE:CZ	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:116:LYS:HE3	2:E:116:LYS:HB3	1.72	0.42
2:E:150:PHE:CD1	2:E:192:LYS:HG3	2.54	0.42
2:E:33:ARG:HH22	2:E:41:SER:CB	2.32	0.42
2:E:92:ARG:HE	2:E:92:ARG:HB3	1.73	0.42
2:F:161:SER:HA	2:F:164:PHE:CG	2.54	0.42
1:A:138:ILE:HA	1:A:217:GLN:NE2	2.32	0.42
1:A:219:VAL:CG1	1:A:301:VAL:HG22	2.50	0.42
1:A:86:SER:OG	7:A:714:HOH:O	2.13	0.42
2:C:159:THR:HA	2:C:199:LEU:HD21	2.02	0.42
1:D:198:VAL:HA	1:D:201:ALA:CB	2.39	0.42
1:D:399:TYR:HB3	7:D:1054:HOH:O	2.18	0.42
1:D:502:ILE:HG12	1:D:502:ILE:H	1.51	0.42
2:E:165:GLN:HA	2:E:168:GLU:OE1	2.20	0.42
2:F:143:PRO:O	2:F:185:TRP:HD1	2.02	0.42
2:F:66:GLU:HG2	6:F:301:GSH:N1	2.34	0.42
1:A:132:ARG:HA	1:A:343:PRO:HG3	2.02	0.42
1:A:218:TYR:CD1	1:A:220:PHE:HB2	2.54	0.42
1:A:253:ARG:O	1:A:484:GLU:HG3	2.20	0.42
1:A:492:ASP:CG	2:B:183:ILE:HG12	2.39	0.42
2:B:200:PRO:HG3	7:B:527:HOH:O	2.20	0.42
2:B:66:GLU:O	2:B:70:VAL:HG23	2.19	0.42
2:B:73:TYR:CE1	2:C:93:ALA:HB1	2.55	0.42
1:D:447:SER:O	1:D:450:LYS:HG3	2.19	0.42
1:D:534:HIS:CD2	1:D:557:LYS:HG2	2.55	0.42
2:E:4:LEU:HA	2:E:5:PRO:HD3	1.77	0.42
2:F:92:ARG:HB3	2:F:96:ARG:NH2	2.35	0.42
1:A:429:LEU:HD12	7:A:721:HOH:O	2.20	0.42
1:A:479:TRP:CZ2	1:A:497:LEU:HD11	2.55	0.42
1:D:387:GLU:C	1:D:388:TYR:HD1	2.23	0.42
1:D:334:GLU:HB3	1:D:398:LEU:HD21	2.02	0.42
1:D:352:PHE:CD2	1:D:421:PHE:HE2	2.38	0.42
1:D:425:ARG:HB3	1:D:427:LEU:HB2	2.01	0.42
1:D:45:LEU:HD23	7:D:960:HOH:O	2.19	0.42
1:D:491:GLN:NE2	1:D:570:TYR:HD2	2.17	0.42
2:E:110:GLN:HA	2:E:113:VAL:HG12	2.02	0.42
2:E:98:TRP:HD1	2:E:153:VAL:HG11	1.77	0.42
2:E:211:GLU:O	2:E:214:LYS:HG2	2.20	0.42
2:E:66:GLU:HB2	2:E:69:ASN:HB2	2.01	0.42
2:F:121:GLN:O	2:F:125:LYS:HG3	2.20	0.42
1:A:326:VAL:HG23	1:A:343:PRO:O	2.20	0.42
1:A:309:MET:HG2	1:A:536:LEU:HD23	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:332:SER:C	5:A:603:ATP:N7	2.74	0.42
2:B:115:GLY:O	2:B:116:LYS:HD2	2.19	0.42
2:C:162:SER:HA	7:C:487:HOH:O	2.20	0.42
1:D:333:SER:C	1:D:335:GLY:N	2.73	0.42
2:E:50:ILE:HG13	2:E:51:HIS:N	2.34	0.42
2:F:16:GLY:O	2:F:20:ARG:HG3	2.20	0.42
1:A:200:GLN:HB3	1:A:254:ILE:HD12	2.02	0.41
1:A:480:GLU:HB2	1:A:528:PHE:HD1	1.85	0.41
1:A:503:ASP:CG	1:A:505:GLY:H	2.23	0.41
1:A:509:SER:HB2	1:A:515:ILE:HB	2.02	0.41
2:B:180:PRO:HD2	2:B:181:LYS:H	1.85	0.41
2:E:101:PHE:HD1	7:F:401:HOH:O	2.03	0.41
1:A:96:ALA:HA	1:A:161:PRO:O	2.20	0.41
1:A:407:VAL:HB	1:A:541:SER:HB2	2.02	0.41
1:A:451:ARG:CZ	1:A:489:VAL:HG12	2.49	0.41
2:B:169:LYS:HG3	2:B:170:PHE:N	2.34	0.41
2:C:142:LYS:O	1:D:92:HIS:HD2	2.03	0.41
1:D:83:GLY:N	1:D:158:GLY:HA3	2.34	0.41
1:D:21:THR:O	1:D:24:ALA:HB2	2.20	0.41
1:D:264:SER:OG	7:D:752:HOH:O	2.21	0.41
1:D:426:ASN:HB3	1:D:543:GLY:O	2.19	0.41
1:D:451:ARG:HB2	2:E:187:LYS:HD2	2.02	0.41
1:D:523:VAL:HG23	7:D:713:HOH:O	2.20	0.41
1:D:566:VAL:CB	1:D:569:SER:HB2	2.49	0.41
2:E:107:THR:HG21	7:E:440:HOH:O	2.19	0.41
2:E:52:LYS:HG2	7:E:424:HOH:O	2.20	0.41
2:F:130:GLU:O	2:F:133:LYS:HB3	2.19	0.41
2:E:73:TYR:HE1	2:F:93:ALA:HA	1.85	0.41
1:A:213:ARG:NH1	7:A:841:HOH:O	2.54	0.41
1:A:332:SER:HB3	1:A:538:LEU:HD13	2.01	0.41
1:A:152:LYS:NZ	1:A:523:VAL:CG1	2.84	0.41
2:B:173:PHE:HB3	2:B:174:SER:H	1.67	0.41
1:D:125:PHE:CE2	1:D:328:HIS:CE1	3.01	0.41
1:D:389:GLU:OE2	1:D:404:GLY:HA2	2.20	0.41
1:D:495:ASN:C	1:D:499:ARG:NH1	2.72	0.41
1:D:53:ASN:HB3	1:D:54:ALA:H	1.51	0.41
1:D:487:GLU:CD	1:D:570:TYR:CE1	2.94	0.41
2:E:107:THR:HG21	7:E:422:HOH:O	2.19	0.41
2:E:181:LYS:HE3	2:E:181:LYS:HB2	1.84	0.41
2:F:45:LEU:HD23	2:F:45:LEU:HA	1.82	0.41
2:F:7:LEU:HG	2:F:9:ASP:HB2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:435:LYS:HB3	1:A:436:ASN:O	2.21	0.41
1:A:453:SER:HA	1:A:457:ILE:O	2.21	0.41
1:A:97:ILE:HB	1:A:162:VAL:HG12	2.02	0.41
2:B:132:VAL:HG23	2:B:182:LEU:HD22	2.02	0.41
1:D:450:LYS:HE3	1:D:450:LYS:HB3	1.89	0.41
1:D:101:SER:N	1:D:535:PHE:CE1	2.88	0.41
1:D:84:ASP:C	1:D:86:SER:H	2.24	0.41
2:E:12:PRO:O	2:E:163:TRP:CZ2	2.73	0.41
2:E:4:LEU:HA	2:E:4:LEU:HD23	1.80	0.41
1:A:229:HIS:CE1	1:A:525:LYS:NZ	2.88	0.41
1:A:360:TYR:O	1:A:393:THR:HB	2.19	0.41
1:A:464:SER:HA	1:A:476:ALA:O	2.19	0.41
2:C:122:GLU:HG2	7:C:437:HOH:O	2.21	0.41
2:C:211:GLU:O	2:C:214:LYS:HB2	2.21	0.41
1:D:107:ARG:HB3	7:D:966:HOH:O	2.20	0.41
1:D:150:SER:HB3	1:D:170:TYR:CD2	2.55	0.41
1:D:217:GLN:HG2	7:D:731:HOH:O	2.19	0.41
1:D:287:TRP:HB3	1:D:290:LEU:HD23	2.01	0.41
1:D:339:ALA:HB2	1:D:355:ILE:HD11	2.01	0.41
1:D:65:VAL:O	7:D:755:HOH:O	2.22	0.41
2:E:17:MET:HE3	2:E:163:TRP:HH2	1.85	0.41
2:E:194:SER:O	2:E:198:SER:OG	2.20	0.41
2:E:66:GLU:O	2:E:70:VAL:HG23	2.20	0.41
2:F:169:LYS:HZ3	2:F:206:VAL:HG13	1.85	0.41
1:A:118:MET:O	1:A:121:THR:HB	2.20	0.41
1:A:200:GLN:OE1	1:A:254:ILE:HA	2.20	0.41
1:A:36:LEU:O	1:A:40:GLN:N	2.53	0.41
1:A:526:GLY:O	1:A:530:LYS:HB2	2.20	0.41
1:A:165:ALA:HB1	5:A:603:ATP:C2	2.56	0.41
1:D:15:ASP:OD2	7:D:748:HOH:O	2.20	0.41
1:D:165:ALA:HB3	4:D:602:VAL:O	2.21	0.41
1:D:300:TYR:CD2	1:D:326:VAL:HG11	2.56	0.41
1:D:434:ASP:O	1:D:550:CYS:HB3	2.20	0.41
1:D:336:TRP:CZ2	5:D:603:ATP:N7	2.89	0.41
2:E:98:TRP:CE3	2:E:98:TRP:O	2.74	0.41
2:E:9:ASP:HB2	2:E:20:ARG:HH21	1.85	0.41
2:F:53:LYS:HD3	6:F:301:GSH:OE1	2.20	0.41
1:A:363:PHE:HB3	1:A:388:TYR:HD2	1.84	0.41
1:A:392:ILE:HD12	7:A:1023:HOH:O	2.19	0.41
2:B:214:LYS:HB3	2:B:214:LYS:HE2	1.89	0.41
2:B:73:TYR:CE1	2:C:93:ALA:CB	3.04	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:26:LYS:CG	2:B:81:LYS:HZ3	2.32	0.41
2:B:98:TRP:HE3	2:B:101:PHE:CB	2.33	0.41
1:D:126:ARG:HB2	1:D:126:ARG:HE	1.59	0.41
1:D:299:LYS:HB3	1:D:299:LYS:HE3	1.92	0.41
1:D:451:ARG:HH11	1:D:454:GLU:CD	2.23	0.41
2:E:31:GLU:HA	7:E:468:HOH:O	2.20	0.41
2:E:41:SER:O	2:E:45:LEU:N	2.42	0.41
1:A:164:THR:HG22	1:A:165:ALA:N	2.36	0.41
2:B:187:LYS:HE2	2:B:187:LYS:HB2	1.74	0.41
2:C:105:LYS:HB3	2:C:105:LYS:HE2	1.89	0.41
1:D:140:ASP:N	7:D:843:HOH:O	2.53	0.41
1:D:219:VAL:HB	1:D:295:PHE:CE1	2.56	0.41
1:D:336:TRP:CH2	3:D:601:JAA:C12	3.03	0.41
1:D:363:PHE:HB3	1:D:388:TYR:CB	2.49	0.41
1:D:477:ILE:HG12	1:D:518:LEU:CD1	2.38	0.41
1:A:23:ASN:O	1:A:27:VAL:HG23	2.20	0.41
1:A:287:TRP:HA	1:A:290:LEU:HD21	2.02	0.41
1:A:328:HIS:NE2	3:A:601:JAA:O03	2.54	0.41
2:B:169:LYS:HE3	2:B:169:LYS:HB2	1.88	0.41
2:B:216:ASN:HD22	2:B:216:ASN:HA	1.65	0.41
2:B:5:PRO:HB3	2:B:59:HIS:NE2	2.36	0.41
1:D:12:ARG:NH1	7:D:862:HOH:O	2.53	0.41
1:D:151:SER:HA	1:D:171:ARG:HH21	1.86	0.41
1:D:340:ASN:ND2	1:D:343:PRO:HA	2.36	0.41
1:D:494:CYS:HB3	7:D:784:HOH:O	2.19	0.41
1:A:132:ARG:NH1	7:A:717:HOH:O	2.14	0.41
1:A:560:GLN:C	1:A:562:LEU:H	2.23	0.41
1:A:566:VAL:C	1:A:568:SER:N	2.73	0.41
1:A:76:TYR:HD2	1:A:88:ILE:CG2	2.34	0.41
1:D:115:ASP:N	7:D:850:HOH:O	2.54	0.41
1:D:284:LEU:HD13	1:D:287:TRP:CA	2.50	0.41
6:E:301:GSH:OE1	7:E:415:HOH:O	2.21	0.41
2:F:73:TYR:HD1	7:F:533:HOH:O	2.03	0.41
1:A:125:PHE:O	1:A:129:PHE:HB2	2.20	0.41
1:A:184:SER:O	7:A:733:HOH:O	2.22	0.41
1:A:421:PHE:CD1	1:A:541:SER:HA	2.55	0.41
1:D:423:CYS:HB2	1:D:543:GLY:N	2.36	0.41
1:D:59:GLU:HG2	7:D:849:HOH:O	2.20	0.41
2:F:14:MET:O	2:F:17:MET:HB2	2.20	0.41
1:A:345:LEU:HD23	7:A:980:HOH:O	2.21	0.40
1:A:487:GLU:OE2	1:A:490:LEU:HB2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:521:ARG:HB3	1:A:566:VAL:HG12	2.01	0.40
1:A:169:VAL:HG22	5:A:603:ATP:C2'	2.51	0.40
2:C:142:LYS:HB2	1:D:38:LYS:O	2.21	0.40
1:D:270:ASN:HA	1:D:271:PRO:HD2	1.87	0.40
1:D:235:GLU:HG2	1:D:287:TRP:CD2	2.57	0.40
1:D:223:PHE:HE1	1:D:304:ILE:HD12	1.86	0.40
1:D:451:ARG:CZ	1:D:489:VAL:HG12	2.51	0.40
2:E:84:PHE:CD1	2:E:84:PHE:C	2.93	0.40
2:F:130:GLU:O	2:F:134:ILE:HG13	2.21	0.40
2:F:139:LEU:HD21	2:F:145:PHE:CE1	2.56	0.40
1:A:122:LEU:O	1:A:126:ARG:HB2	2.21	0.40
1:A:273:LEU:HA	1:A:276:THR:HG23	2.03	0.40
1:A:410:ILE:HG12	1:A:420:LYS:HB2	2.04	0.40
1:A:559:LEU:O	1:A:562:LEU:HB3	2.22	0.40
1:A:68:VAL:HG12	7:A:785:HOH:O	2.21	0.40
2:B:72:GLN:HA	2:B:84:PHE:CE2	2.56	0.40
2:C:40:LYS:NZ	7:C:429:HOH:O	2.37	0.40
1:D:234:PHE:HA	7:D:798:HOH:O	2.21	0.40
1:D:393:THR:HG23	1:D:399:TYR:HD1	1.86	0.40
1:D:441:LEU:O	1:D:445:VAL:HG23	2.21	0.40
1:D:570:TYR:HB3	7:D:844:HOH:O	2.20	0.40
2:E:114:TRP:HD1	2:E:167:TYR:HE1	1.66	0.40
2:E:110:GLN:HE21	2:E:167:TYR:HE2	1.68	0.40
2:E:37:PHE:HE1	7:E:436:HOH:O	2.05	0.40
2:E:72:GLN:NE2	2:F:96:ARG:HD2	2.32	0.40
1:A:108:PRO:HG3	1:A:552:LYS:H	1.87	0.40
1:A:334:GLU:HB3	7:A:949:HOH:O	2.22	0.40
2:C:121:GLN:NE2	2:C:170:PHE:O	2.54	0.40
1:D:165:ALA:H	1:D:557:LYS:HE3	1.86	0.40
1:D:566:VAL:C	1:D:568:SER:N	2.74	0.40
2:E:174:SER:HB2	7:E:483:HOH:O	2.22	0.40
2:F:139:LEU:C	2:F:141:ASP:N	2.74	0.40
1:A:508:SER:HB2	7:A:757:HOH:O	2.21	0.40
2:B:156:SER:HB2	7:B:510:HOH:O	2.21	0.40
2:C:81:LYS:O	2:C:83:PRO:HD3	2.22	0.40
2:E:16:GLY:O	2:E:20:ARG:HG3	2.21	0.40
2:E:42:PRO:HA	2:E:45:LEU:CG	2.47	0.40
2:E:44:LEU:HD11	7:E:436:HOH:O	2.22	0.40
1:A:480:GLU:HB2	1:A:528:PHE:CD1	2.57	0.40
1:A:540:SER:OG	1:A:541:SER:N	2.52	0.40
2:B:32:TYR:CD2	2:B:32:TYR:N	2.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:30:PHE:N	2:C:30:PHE:CD2	2.90	0.40
1:D:120:ASN:CG	1:D:358:LEU:HD22	2.42	0.40
1:D:364:LEU:HA	1:D:365:PRO:HD3	1.84	0.40
1:D:432:ASN:HD21	1:D:434:ASP:CG	2.25	0.40
1:D:102:GLY:N	1:D:546:LYS:O	2.38	0.40
1:D:121:THR:HG23	5:D:603:ATP:H8	1.86	0.40
2:E:204:LYS:NZ	7:E:410:HOH:O	2.15	0.40
2:E:9:ASP:HB2	2:E:20:ARG:NH2	2.37	0.40

All (9) 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:270:ASN:ND2	1:A:510:ARG:O[1_565]	2.11	0.09
7:D:712:HOH:O	7:D:765:HOH:O[1_545]	2.11	0.09
1:A:46:GLN:OE1	2:F:149:SER:OG[1_454]	2.12	0.08
7:C:410:HOH:O	7:D:848:HOH:O[1_655]	2.14	0.06
7:E:517:HOH:O	7:F:420:HOH:O[1_455]	2.16	0.04
7:D:1162:HOH:O	7:D:1177:HOH:O[1_565]	2.17	0.03
7:A:1105:HOH:O	7:A:1107:HOH:O[1_655]	2.18	0.02
7:A:1089:HOH:O	7:B:541:HOH:O[1_565]	2.18	0.02
1:D:270:ASN:ND2	1:D:510:ARG:O[1_565]	2.19	0.01

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	567/575 (99%)	534 (94%)	25 (4%)	8 (1%)	14	1
1	D	567/575 (99%)	534 (94%)	27 (5%)	6 (1%)	17	3
2	B	212/223 (95%)	194 (92%)	17 (8%)	1 (0%)	34	12
2	C	212/223 (95%)	201 (95%)	10 (5%)	1 (0%)	34	12

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	E	212/223 (95%)	196 (92%)	15 (7%)	1 (0%)	34 12
2	F	212/223 (95%)	201 (95%)	10 (5%)	1 (0%)	34 12
All	All	1982/2042 (97%)	1860 (94%)	104 (5%)	18 (1%)	21 4

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	369	THR
1	A	540	SER
1	A	542	ALA
2	C	141	ASP
1	D	369	THR
1	D	433	ILE
1	D	437	THR
1	D	540	SER
1	D	542	ALA
2	F	141	ASP
1	A	437	THR
2	B	140	GLY
2	E	140	GLY
1	D	368	GLU
1	A	88	ILE
1	A	150	SER
1	A	433	ILE
1	A	553	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	499/505 (99%)	476 (95%)	23 (5%)	33 8
1	D	499/505 (99%)	458 (92%)	41 (8%)	14 2
2	B	187/195 (96%)	173 (92%)	14 (8%)	17 2
2	C	187/195 (96%)	181 (97%)	6 (3%)	46 16

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	E	187/195 (96%)	176 (94%)	11 (6%)	24	4
2	F	187/195 (96%)	179 (96%)	8 (4%)	35	9
All	All	1746/1790 (98%)	1643 (94%)	103 (6%)	24	4

All (103) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	77	ILE
1	A	98	SER
1	A	125	PHE
1	A	184	SER
1	A	187	CYS
1	A	225	HIS
1	A	250	LEU
1	A	259	VAL
1	A	273	LEU
1	A	284	LEU
1	A	373	GLU
1	A	423	CYS
1	A	428	ILE
1	A	468	VAL
1	A	488	ASP
1	A	494	CYS
1	A	499	ARG
1	A	502	ILE
1	A	503	ASP
1	A	514	THR
1	A	529	ARG
1	A	530	LYS
1	A	566	VAL
2	B	26	LYS
2	B	43	LEU
2	B	74	VAL
2	B	84	PHE
2	B	104	LYS
2	B	134	ILE
2	B	139	LEU
2	B	153	VAL
2	B	157	LEU
2	B	176	GLU
2	B	183	ILE

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Mol	Chain	Res	Type
2	B	206	VAL
2	B	212	TYR
2	B	216	ASN
2	C	30	PHE
2	C	69	ASN
2	C	103	ASP
2	C	145	PHE
2	C	149	SER
2	C	168	GLU
1	D	14	ILE
1	D	27	VAL
1	D	55	THR
1	D	80	MET
1	D	90	THR
1	D	92	HIS
1	D	109	LYS
1	D	110	PHE
1	D	125	PHE
1	D	140	ASP
1	D	146	GLN
1	D	152	LYS
1	D	179	MET
1	D	205	HIS
1	D	211	LEU
1	D	245	ILE
1	D	250	LEU
1	D	259	VAL
1	D	273	LEU
1	D	276	THR
1	D	290	LEU
1	D	295	PHE
1	D	326	VAL
1	D	327	SER
1	D	329	ASP
1	D	333	SER
1	D	345	LEU
1	D	410	ILE
1	D	450	LYS
1	D	455	GLU
1	D	460	ILE
1	D	468	VAL
1	D	484	GLU

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Mol	Chain	Res	Type
1	D	494	CYS
1	D	499	ARG
1	D	512	CYS
1	D	529	ARG
1	D	534	HIS
1	D	545	PHE
1	D	562	LEU
1	D	573	THR
2	E	43	LEU
2	E	47	SER
2	E	84	PHE
2	E	85	PHE
2	E	133	LYS
2	E	134	ILE
2	E	135	LEU
2	E	136	GLU
2	E	139	LEU
2	E	176	GLU
2	E	216	ASN
2	F	36	ASP
2	F	70	VAL
2	F	88	ASP
2	F	103	ASP
2	F	117	LYS
2	F	142	LYS
2	F	153	VAL
2	F	172	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	GLN
1	A	146	GLN
1	A	217	GLN
1	A	544	GLN
2	B	121	GLN
2	B	216	ASN
1	D	146	GLN
1	D	217	GLN
1	D	495	ASN
1	D	534	HIS



### 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 ⓘ

10 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	JAA	A	601	-	12,15,15	5.66	6 (50%)	12,19,19	3.57	6 (50%)
4	VAL	A	602	-	4,7,7	0.77	0	3,9,9	1.21	0
5	ATP	A	603	-	26,33,33	5.13	15 (57%)	26,52,52	3.01	14 (53%)
6	GSH	B	301	-	13,19,19	1.76	4 (30%)	15,24,24	3.16	5 (33%)
6	GSH	C	301	-	13,19,19	1.76	4 (30%)	15,24,24	3.29	7 (46%)
3	JAA	D	601	-	12,15,15	5.83	6 (50%)	12,19,19	3.19	7 (58%)
4	VAL	D	602	-	4,7,7	0.94	0	3,9,9	0.35	0
5	ATP	D	603	-	26,33,33	4.97	16 (61%)	26,52,52	2.86	11 (42%)
6	GSH	E	301	-	13,19,19	1.73	4 (30%)	15,24,24	3.50	8 (53%)
6	GSH	F	301	-	13,19,19	1.76	4 (30%)	15,24,24	3.32	6 (40%)

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	VAL	A	602	-	-	0/4/8/8	0/0/0/0
5	ATP	A	603	-	-	0/18/38/38	0/3/3/3
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
4	VAL	D	602	-	-	0/4/8/8	0/0/0/0
5	ATP	D	603	-	-	0/18/38/38	0/3/3/3
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 (59) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	601	JAA	C05-C08	-13.20	1.30	1.52
3	A	601	JAA	C05-C08	-12.44	1.31	1.52
5	A	603	ATP	C2'-C1'	-12.40	1.33	1.53
3	A	601	JAA	C06-C04	-11.38	1.23	1.53
3	D	601	JAA	C06-C04	-11.32	1.23	1.53
5	D	603	ATP	C2'-C1'	-11.03	1.36	1.53
5	D	603	ATP	O4'-C4'	-9.62	1.23	1.45
5	A	603	ATP	O4'-C4'	-9.22	1.23	1.45
5	A	603	ATP	O3'-C3'	-6.18	1.28	1.43
3	D	601	JAA	C10-C04	-6.08	1.44	1.53
3	A	601	JAA	C10-C04	-6.04	1.44	1.53
5	A	603	ATP	C2'-C3'	-5.66	1.38	1.53
5	D	603	ATP	O3'-C3'	-5.26	1.30	1.43
5	D	603	ATP	C2'-C3'	-5.12	1.39	1.53
5	D	603	ATP	C6-N6	-4.97	1.13	1.34
5	A	603	ATP	C5-C4	-4.97	1.29	1.40
5	A	603	ATP	C6-N6	-4.97	1.13	1.34
5	D	603	ATP	C5-C4	-4.81	1.29	1.40
3	D	601	JAA	C09-C05	-4.49	1.48	1.54
3	A	601	JAA	C09-C05	-4.21	1.48	1.54
5	A	603	ATP	C5-N7	-3.09	1.28	1.39
5	D	603	ATP	PG-O3G	-2.96	1.44	1.54
5	D	603	ATP	C5-N7	-2.96	1.28	1.39
5	A	603	ATP	PG-O3G	-2.89	1.44	1.54
5	D	603	ATP	O5'-C5'	-2.87	1.33	1.44
6	F	301	GSH	CA2-N2	-2.84	1.39	1.45
5	A	603	ATP	O5'-C5'	-2.82	1.33	1.44
6	B	301	GSH	CA2-N2	-2.72	1.39	1.45
6	E	301	GSH	CA2-N2	-2.71	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	301	GSH	CA2-N2	-2.50	1.40	1.45
5	A	603	ATP	C2-N3	-2.49	1.27	1.32
6	C	301	GSH	CB2-CA2	-2.47	1.50	1.52
6	F	301	GSH	CB2-CA2	-2.44	1.50	1.52
6	E	301	GSH	CB2-CA2	-2.34	1.50	1.52
5	D	603	ATP	C2-N3	-2.30	1.28	1.32
6	B	301	GSH	CB2-CA2	-2.27	1.50	1.52
5	D	603	ATP	PG-O2G	-2.19	1.47	1.54
5	A	603	ATP	PG-O2G	2.05	1.61	1.54
6	E	301	GSH	CD1-N2	2.65	1.39	1.34
6	F	301	GSH	CD1-N2	2.70	1.39	1.34
6	B	301	GSH	CD1-N2	2.78	1.39	1.34
5	D	603	ATP	C3'-C4'	2.96	1.60	1.53
6	C	301	GSH	CD1-N2	2.97	1.40	1.34
5	A	603	ATP	C3'-C4'	3.07	1.61	1.53
6	F	301	GSH	C2-N3	3.09	1.40	1.33
6	E	301	GSH	C2-N3	3.21	1.40	1.33
6	B	301	GSH	C2-N3	3.30	1.40	1.33
6	C	301	GSH	C2-N3	3.34	1.40	1.33
5	D	603	ATP	PG-O1G	3.41	1.61	1.50
3	A	601	JAA	C05-C04	3.85	1.64	1.55
3	D	601	JAA	C05-C04	3.92	1.64	1.55
5	A	603	ATP	C2-N1	4.87	1.43	1.33
5	D	603	ATP	C2-N1	5.10	1.43	1.33
3	A	601	JAA	C07-C08	5.14	1.60	1.50
3	D	601	JAA	C07-C08	5.35	1.60	1.50
5	D	603	ATP	C4-N3	8.00	1.47	1.35
5	A	603	ATP	C4-N3	8.58	1.48	1.35
5	D	603	ATP	O4'-C1'	13.08	1.59	1.41
5	A	603	ATP	O4'-C1'	13.12	1.60	1.41

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	E	301	GSH	CA2-CB2-SG2	-11.47	101.39	113.99
6	F	301	GSH	CA2-CB2-SG2	-10.75	102.18	113.99
6	B	301	GSH	CA2-CB2-SG2	-10.53	102.42	113.99
6	C	301	GSH	CA2-CB2-SG2	-9.49	103.56	113.99
5	D	603	ATP	C5'-C4'-C3'	-7.42	86.50	115.20
3	A	601	JAA	C06-C07-C08	-7.13	98.03	105.47
3	A	601	JAA	C07-C08-C05	-6.15	103.72	109.04
3	D	601	JAA	C07-C08-C05	-5.75	104.07	109.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	603	ATP	C5'-C4'-C3'	-5.73	93.02	115.20
5	A	603	ATP	C4'-O4'-C1'	-5.70	103.60	109.64
3	D	601	JAA	C07-C06-C04	-5.52	98.99	104.57
5	A	603	ATP	N3-C2-N1	-5.47	124.57	128.87
6	C	301	GSH	CB2-CA2-N2	-5.22	104.40	111.43
5	D	603	ATP	N3-C2-N1	-4.98	124.96	128.87
3	A	601	JAA	C07-C06-C04	-4.87	99.65	104.57
5	D	603	ATP	C4'-O4'-C1'	-4.76	104.60	109.64
5	A	603	ATP	C2'-C3'-C4'	-4.19	94.06	102.64
3	D	601	JAA	C09-C11-C13	-4.15	111.80	126.48
5	D	603	ATP	O2A-PA-O3A	-4.05	87.92	105.27
5	A	603	ATP	O2A-PA-O3A	-3.94	88.37	105.27
3	A	601	JAA	C09-C11-C13	-3.93	112.58	126.48
3	D	601	JAA	C06-C07-C08	-3.80	101.51	105.47
6	B	301	GSH	CB2-CA2-N2	-3.80	106.32	111.43
5	A	603	ATP	O2G-PG-O1G	-3.66	98.68	110.63
6	F	301	GSH	CB2-CA2-N2	-3.58	106.62	111.43
6	E	301	GSH	CB2-CA2-N2	-3.36	106.91	111.43
6	C	301	GSH	CG1-CD1-N2	-3.34	110.23	115.85
5	A	603	ATP	O2'-C2'-C1'	-3.18	101.65	111.61
6	F	301	GSH	CG1-CD1-N2	-2.91	110.96	115.85
3	D	601	JAA	C14-C13-C11	-2.88	113.70	127.15
6	E	301	GSH	CG1-CD1-N2	-2.82	111.11	115.85
6	C	301	GSH	CA3-N3-C2	-2.75	118.48	122.36
6	E	301	GSH	CA3-N3-C2	-2.63	118.64	122.36
6	E	301	GSH	C2-CA2-N2	-2.53	104.13	111.28
6	C	301	GSH	CB2-CA2-C2	-2.41	104.17	109.72
5	D	603	ATP	C2'-C3'-C4'	-2.35	97.83	102.64
6	B	301	GSH	CG1-CD1-N2	-2.34	111.91	115.85
3	A	601	JAA	C14-C13-C11	-2.14	117.15	127.15
6	E	301	GSH	CG1-CB1-CA1	-2.12	109.17	114.18
6	B	301	GSH	CG1-CB1-CA1	-2.11	109.19	114.18
6	F	301	GSH	CA3-N3-C2	-2.05	119.47	122.36
3	D	601	JAA	C15-C14-C13	2.01	120.86	112.69
5	D	603	ATP	O2B-PB-O3A	2.10	114.25	105.27
6	C	301	GSH	OE1-CD1-CG1	2.10	125.61	121.97
6	B	301	GSH	CB1-CG1-CD1	2.15	118.17	113.26
6	E	301	GSH	OE1-CD1-CG1	2.16	125.73	121.97
5	D	603	ATP	C2'-C1'-N9	2.24	119.47	113.47
5	A	603	ATP	N6-C6-N1	2.29	122.36	118.52
6	F	301	GSH	OE1-CD1-CG1	2.41	126.16	121.97
5	A	603	ATP	O2B-PB-O3A	2.41	115.61	105.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	603	ATP	C1'-N9-C4	2.73	129.85	126.81
5	D	603	ATP	O3'-C3'-C4'	2.93	119.76	111.01
5	D	603	ATP	N6-C6-N1	2.95	123.47	118.52
6	E	301	GSH	CB1-CG1-CD1	2.96	120.02	113.26
6	F	301	GSH	CB1-CG1-CD1	3.00	120.11	113.26
5	A	603	ATP	C2'-C1'-N9	3.17	121.95	113.47
6	C	301	GSH	CB1-CG1-CD1	3.23	120.65	113.26
5	A	603	ATP	O3'-C3'-C4'	3.35	121.03	111.01
3	D	601	JAA	O01-C08-C05	3.38	129.78	125.41
5	A	603	ATP	O4'-C4'-C3'	3.43	112.11	105.16
5	D	603	ATP	O4'-C4'-C3'	3.81	112.88	105.16
3	A	601	JAA	O01-C08-C05	4.04	130.63	125.41
5	A	603	ATP	O4'-C1'-N9	4.74	117.07	108.11
5	D	603	ATP	O4'-C1'-N9	5.18	117.89	108.11

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 74 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	601	JAA	7	0
4	A	602	VAL	8	0
5	A	603	ATP	22	0
6	C	301	GSH	2	0
3	D	601	JAA	2	0
4	D	602	VAL	5	0
5	D	603	ATP	21	0
6	E	301	GSH	5	0
6	F	301	GSH	5	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%)	1.55	157 (27%)  	2, 4, 7, 16	0
1	D	569/575 (98%)	1.53	145 (25%)  	2, 4, 6, 16	0
2	B	214/223 (95%)	1.37	48 (22%)  	2, 3, 7, 11	0
2	C	214/223 (95%)	1.23	40 (18%)  	2, 3, 5, 7	0
2	E	214/223 (95%)	1.30	44 (20%)  	2, 3, 7, 11	0
2	F	214/223 (95%)	1.20	34 (15%)  	2, 4, 5, 7	0
All	All	1994/2042 (97%)	1.42	468 (23%)  	2, 4, 7, 16	0

All (468) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	561	ILE	5.7
2	B	185	TRP	5.7
1	A	125	PHE	5.3
2	E	134	ILE	5.0
1	D	428	ILE	5.0
1	D	427	LEU	5.0
2	B	32	TYR	4.9
1	A	187	CYS	4.7
1	D	13	VAL	4.6
1	A	428	ILE	4.5
1	D	433	ILE	4.5
1	D	545	PHE	4.5
1	D	377	VAL	4.4
2	B	101	PHE	4.4
1	A	429	LEU	4.3
1	D	468	VAL	4.3
1	A	570	TYR	4.2
1	D	65	VAL	4.2
1	D	149	PHE	4.2

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Mol	Chain	Res	Type	RSRZ
1	D	8	PHE	4.1
2	E	145	PHE	4.1
1	A	211	LEU	4.1
1	A	312	TYR	4.1
2	F	37	PHE	4.1
1	A	27	VAL	4.1
1	D	259	VAL	4.0
1	D	410	ILE	4.0
1	D	111	ILE	3.9
2	E	32	TYR	3.9
2	C	37	PHE	3.9
1	D	187	CYS	3.9
2	C	129	ILE	3.8
1	A	44	TYR	3.8
1	D	237	VAL	3.8
1	A	423	CYS	3.7
1	A	545	PHE	3.7
2	C	111	PHE	3.7
1	A	256	VAL	3.7
1	A	57	PRO	3.6
1	D	296	PRO	3.6
2	E	170	PHE	3.6
1	A	337	ILE	3.6
1	D	245	ILE	3.6
1	A	295	PHE	3.5
1	A	345	LEU	3.5
2	C	30	PHE	3.5
1	A	259	VAL	3.5
1	D	501	PHE	3.5
1	A	512	CYS	3.5
2	B	86	PRO	3.5
1	A	210	ILE	3.5
1	A	269	PRO	3.5
1	D	220	PHE	3.5
1	A	445	VAL	3.4
1	A	48	CYS	3.4
2	E	98	TRP	3.4
2	B	98	TRP	3.4
1	D	431	ILE	3.3
1	A	129	PHE	3.3
2	C	145	PHE	3.3
1	D	518	LEU	3.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	C	43	LEU	3.3
1	A	220	PHE	3.3
1	D	341	VAL	3.3
2	F	98	TRP	3.3
1	D	77	ILE	3.3
1	D	117	LEU	3.2
1	A	287	TRP	3.2
1	D	212	PHE	3.2
1	A	169	VAL	3.2
1	A	504	ALA	3.2
1	A	195	SER	3.2
1	D	154	TYR	3.2
1	A	569	SER	3.2
2	B	99	ALA	3.2
1	D	398	LEU	3.2
2	E	113	VAL	3.2
1	D	110	PHE	3.2
1	A	262	ALA	3.1
1	D	287	TRP	3.1
2	B	91	GLY	3.1
1	A	497	LEU	3.1
2	C	10	TYR	3.1
1	A	203	TYR	3.1
1	A	410	ILE	3.1
1	A	431	ILE	3.1
2	E	148	ASP	3.1
1	A	98	SER	3.1
1	D	113	PHE	3.0
2	E	94	GLN	3.0
1	A	342	THR	3.0
1	A	514	THR	3.0
2	B	83	PRO	3.0
1	A	88	ILE	3.0
1	D	570	TYR	3.0
1	D	205	HIS	3.0
1	A	427	LEU	3.0
1	D	198	VAL	3.0
1	A	494	CYS	3.0
1	D	182	ILE	3.0
1	D	231	PHE	3.0
1	A	273	LEU	3.0
1	A	391	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	388	TYR	3.0
1	D	475	TYR	3.0
2	C	173	PHE	3.0
1	A	202	LEU	3.0
1	D	166	THR	2.9
1	A	403	LEU	2.9
1	A	113	PHE	2.9
2	C	97	PHE	2.9
2	F	97	PHE	2.9
2	F	78	TRP	2.9
1	A	13	VAL	2.9
1	A	390	VAL	2.9
1	A	60	ALA	2.9
1	D	130	ALA	2.9
2	E	167	TYR	2.9
1	A	231	PHE	2.9
2	C	184	ALA	2.9
1	A	216	VAL	2.9
1	A	341	VAL	2.9
1	D	37	LEU	2.9
2	F	217	LEU	2.9
1	D	210	ILE	2.9
1	D	465	TYR	2.9
1	D	177	ALA	2.9
2	B	184	ALA	2.9
2	F	145	PHE	2.8
1	A	558	VAL	2.8
1	A	485	THR	2.8
2	E	182	LEU	2.8
1	A	274	ALA	2.8
1	A	45	LEU	2.8
2	B	132	VAL	2.8
1	A	194	PHE	2.8
2	E	157	LEU	2.8
1	A	111	ILE	2.8
2	F	143	PRO	2.8
2	E	208	TYR	2.8
1	A	227	LEU	2.8
1	A	267	LEU	2.8
1	D	32	LEU	2.8
2	F	102	VAL	2.8
2	B	111	PHE	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	257	PRO	2.8
1	A	347	PRO	2.8
2	B	216	ASN	2.8
1	D	392	ILE	2.7
1	D	388	TYR	2.7
1	A	55	THR	2.7
1	D	256	VAL	2.7
1	D	489	VAL	2.7
1	D	352	PHE	2.7
1	A	486	ASN	2.7
1	D	204	CYS	2.7
1	D	572	SER	2.7
2	E	205	ILE	2.7
1	A	377	VAL	2.7
1	D	567	VAL	2.7
2	B	139	LEU	2.7
1	D	295	PHE	2.7
2	B	145	PHE	2.7
1	D	494	CYS	2.7
1	D	563	CYS	2.7
1	D	35	ILE	2.7
1	D	312	TYR	2.7
2	E	11	TRP	2.7
2	E	114	TRP	2.7
1	A	316	LEU	2.7
2	E	139	LEU	2.7
2	C	170	PHE	2.7
2	F	173	PHE	2.7
1	A	35	ILE	2.7
1	A	508	SER	2.7
2	B	183	ILE	2.7
2	E	90	TYR	2.7
1	A	50	LEU	2.7
2	B	182	LEU	2.7
1	A	212	PHE	2.7
1	D	457	ILE	2.6
1	A	198	VAL	2.6
1	A	288	TYR	2.6
1	A	518	LEU	2.6
1	D	313	VAL	2.6
1	D	459	VAL	2.6
2	B	68	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
2	F	113	VAL	2.6
1	D	238	TRP	2.6
2	C	11	TRP	2.6
1	D	129	PHE	2.6
1	D	234	PHE	2.6
1	D	531	ILE	2.6
2	B	124	GLY	2.6
1	A	144	ALA	2.6
1	D	571	PHE	2.6
2	B	97	PHE	2.6
1	D	464	SER	2.6
1	D	422	ILE	2.6
2	F	155	ILE	2.6
2	C	153	VAL	2.6
1	A	562	LEU	2.6
1	D	267	LEU	2.6
2	E	212	TYR	2.6
1	A	433	ILE	2.6
2	B	71	VAL	2.6
1	A	89	LEU	2.6
2	C	123	ALA	2.6
2	B	73	TYR	2.6
2	F	208	TYR	2.6
1	A	416	THR	2.5
2	E	164	PHE	2.5
1	A	517	ALA	2.5
2	F	58	VAL	2.5
1	D	207	LEU	2.5
2	E	86	PRO	2.5
2	F	10	TYR	2.5
1	D	514	THR	2.5
1	D	96	ALA	2.5
2	C	164	PHE	2.5
1	A	365	PRO	2.5
1	A	561	ILE	2.5
1	D	219	VAL	2.5
1	D	89	LEU	2.5
2	C	199	LEU	2.5
1	A	172	ASN	2.5
1	D	170	TYR	2.5
1	A	258	SER	2.5
1	A	142	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	500	ALA	2.5
1	D	159	GLY	2.5
1	D	298	ALA	2.5
2	E	106	PHE	2.5
2	C	163	TRP	2.5
1	A	81	VAL	2.5
1	D	301	VAL	2.5
1	A	568	SER	2.5
1	A	170	TYR	2.5
1	D	335	GLY	2.5
1	D	372	GLY	2.5
1	A	476	ALA	2.5
2	B	186	ALA	2.5
1	A	493	CYS	2.5
1	A	131	PHE	2.5
1	A	478	PHE	2.5
2	C	101	PHE	2.5
1	D	445	VAL	2.5
2	C	8	LEU	2.5
2	C	98	TRP	2.5
1	D	173	PRO	2.4
2	B	180	PRO	2.4
1	D	393	THR	2.4
1	A	281	CYS	2.4
1	D	281	CYS	2.4
1	D	108	PRO	2.4
1	D	211	LEU	2.4
1	A	524	ALA	2.4
1	A	430	SER	2.4
2	B	90	TYR	2.4
2	F	86	PRO	2.4
1	A	110	PHE	2.4
1	A	206	LEU	2.4
1	A	207	LEU	2.4
1	A	575	PHE	2.4
1	D	99	LEU	2.4
2	E	97	PHE	2.4
2	E	111	PHE	2.4
2	F	7	LEU	2.4
1	A	516	GLY	2.4
2	B	78	TRP	2.4
1	A	71	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	43	ILE	2.4
1	D	122	LEU	2.4
1	D	125	PHE	2.4
1	D	411	GLY	2.4
2	B	118	GLY	2.4
1	A	196	PRO	2.4
2	B	176	GLU	2.4
2	E	73	TYR	2.4
1	A	448	ALA	2.4
2	F	95	ALA	2.4
1	D	31	THR	2.4
2	E	71	VAL	2.3
1	A	460	ILE	2.3
1	D	73	LEU	2.3
1	A	234	PHE	2.3
2	C	85	PHE	2.3
2	F	101	PHE	2.3
2	F	111	PHE	2.3
2	B	208	TYR	2.3
1	D	128	ALA	2.3
1	D	142	GLY	2.3
2	E	166	ALA	2.3
2	F	163	TRP	2.3
1	D	90	THR	2.3
1	A	308	SER	2.3
1	D	101	SER	2.3
1	D	151	SER	2.3
1	D	258	SER	2.3
2	F	132	VAL	2.3
1	A	490	LEU	2.3
1	D	403	LEU	2.3
1	A	466	ILE	2.3
1	D	355	ILE	2.3
2	F	129	ILE	2.3
1	D	512	CYS	2.3
2	F	164	PHE	2.3
1	A	154	TYR	2.3
2	B	144	TYR	2.3
2	C	185	TRP	2.3
1	A	358	LEU	2.3
1	A	379	LEU	2.3
1	D	209	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
2	C	158	ILE	2.3
2	C	175	ILE	2.3
2	E	124	GLY	2.3
1	A	175	PHE	2.3
2	E	85	PHE	2.3
2	F	207	ALA	2.3
2	C	32	TYR	2.3
2	C	115	GLY	2.3
1	D	67	LEU	2.3
1	D	124	LEU	2.3
1	D	379	LEU	2.3
2	B	135	LEU	2.3
1	A	355	ILE	2.3
2	E	180	PRO	2.3
2	B	30	PHE	2.3
1	A	228	VAL	2.2
1	A	237	VAL	2.2
1	A	356	PRO	2.2
1	A	407	VAL	2.2
1	A	468	VAL	2.2
2	B	157	LEU	2.2
1	D	460	ILE	2.2
2	B	50	ILE	2.2
2	B	155	ILE	2.2
2	E	27	GLY	2.2
2	E	128	PHE	2.2
2	E	150	PHE	2.2
1	A	401	TYR	2.2
1	A	550	CYS	2.2
2	E	87	SER	2.2
2	C	79	PRO	2.2
1	D	293	ALA	2.2
1	A	301	VAL	2.2
1	A	36	LEU	2.2
2	C	140	GLY	2.2
1	A	457	ILE	2.2
2	B	114	TRP	2.2
1	A	151	SER	2.2
2	B	212	TYR	2.2
2	B	46	GLN	2.2
1	A	96	ALA	2.2
2	B	27	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	489	VAL	2.2
1	A	122	LEU	2.2
1	A	309	MET	2.2
1	D	294	LEU	2.2
2	E	135	LEU	2.2
2	C	160	PHE	2.2
2	C	102	VAL	2.2
1	D	266	LEU	2.2
2	F	4	LEU	2.2
2	E	50	ILE	2.2
1	A	470	THR	2.2
2	E	186	ALA	2.2
2	F	185	TRP	2.2
1	A	76	TYR	2.1
1	A	462	PHE	2.1
1	D	61	PHE	2.1
2	E	144	TYR	2.1
1	D	269	PRO	2.1
1	A	323	LEU	2.1
1	A	538	LEU	2.1
1	D	419	LEU	2.1
1	D	490	LEU	2.1
2	C	57	LEU	2.1
2	F	182	LEU	2.1
1	A	164	THR	2.1
1	D	573	THR	2.1
2	B	175	ILE	2.1
1	D	144	ALA	2.1
1	D	201	ALA	2.1
1	D	399	TYR	2.1
2	C	90	TYR	2.1
2	F	32	TYR	2.1
1	A	361	PHE	2.1
1	A	528	PHE	2.1
2	E	118	GLY	2.1
1	A	326	VAL	2.1
1	A	496	CYS	2.1
2	B	70	VAL	2.1
1	A	37	LEU	2.1
2	C	209	ALA	2.1
1	D	43	ILE	2.1
1	D	254	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	553	PRO	2.1
2	F	55	PRO	2.1
1	D	397	GLY	2.1
2	B	152	TYR	2.1
2	F	73	TYR	2.1
1	A	61	PHE	2.1
2	C	15	PHE	2.1
1	D	228	VAL	2.1
1	D	42	ALA	2.1
1	D	54	ALA	2.1
1	D	165	ALA	2.1
1	D	274	ALA	2.1
2	B	44	LEU	2.1
1	D	496	CYS	2.1
2	E	123	ALA	2.1
1	D	529	ARG	2.1
1	A	515	ILE	2.1
1	D	97	ILE	2.1
2	C	6	ILE	2.1
2	F	6	ILE	2.1
1	A	360	TYR	2.1
1	D	175	PHE	2.1
2	E	30	PHE	2.1
1	A	298	ALA	2.1
1	A	336	TRP	2.1
1	A	548	PRO	2.1
1	D	160	VAL	2.1
1	D	161	PRO	2.1
1	D	169	VAL	2.1
1	D	524	ALA	2.1
2	C	99	ALA	2.1
2	C	166	ALA	2.1
2	F	11	TRP	2.1
2	F	153	VAL	2.1
1	A	520	LEU	2.1
1	D	325	LEU	2.1
1	A	77	ILE	2.1
1	D	376	PRO	2.0
1	A	339	ALA	2.0
1	D	218	TYR	2.0
1	D	360	TYR	2.0
2	C	95	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
2	B	37	PHE	2.0
2	B	164	PHE	2.0
2	E	101	PHE	2.0
2	B	199	LEU	2.0
2	E	57	LEU	2.0
2	B	11	TRP	2.0
2	E	185	TRP	2.0
1	A	31	THR	2.0
1	A	277	ILE	2.0
1	D	121	THR	2.0
1	D	466	ILE	2.0
1	D	481	ILE	2.0
2	E	189	CYS	2.0
2	F	54	ILE	2.0
1	A	292	PRO	2.0
1	A	331	GLY	2.0
1	D	80	MET	2.0
1	A	556	ALA	2.0
1	D	41	SER	2.0
2	B	41	SER	2.0
1	A	354	VAL	2.0
1	D	249	VAL	2.0
1	D	366	VAL	2.0
1	A	99	LEU	2.0
1	D	538	LEU	2.0
1	D	562	LEU	2.0
2	C	7	LEU	2.0
2	C	23	LEU	2.0
2	B	151	GLY	2.0

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

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

## 6.3 Carbohydrates ⓘ

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( $\text{\AA}^2$ )	Q<0.9
3	JAA	D	601	15/15	0.81	0.23	2.83	2,3,7,8	0
4	VAL	D	602	8/8	0.81	0.19	0.74	5,8,15,16	0
3	JAA	A	601	15/15	0.88	0.19	0.62	2,3,3,8	0
5	ATP	A	603	31/31	0.91	0.18	0.23	2,3,11,16	0
6	GSH	B	301	20/20	0.94	0.16	0.12	2,2,4,5	0
6	GSH	C	301	20/20	0.92	0.17	-0.13	2,3,9,20	0
4	VAL	A	602	8/8	0.88	0.17	-0.32	4,6,9,10	0
5	ATP	D	603	31/31	0.92	0.16	-0.39	2,5,10,11	0
6	GSH	F	301	20/20	0.93	0.14	-0.93	2,3,9,19	0
6	GSH	E	301	20/20	0.94	0.14	-0.96	2,2,4,5	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.