



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 31, 2023 – 01:07 PM JST

PDB ID : 5ECI  
Title : Crystal Structure of FIN219-FIP1 complex with JA, ATP and Mg  
Authors : Chen, C.Y.; Cheng, Y.S.  
Deposited on : 2015-10-20  
Resolution : 1.56 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

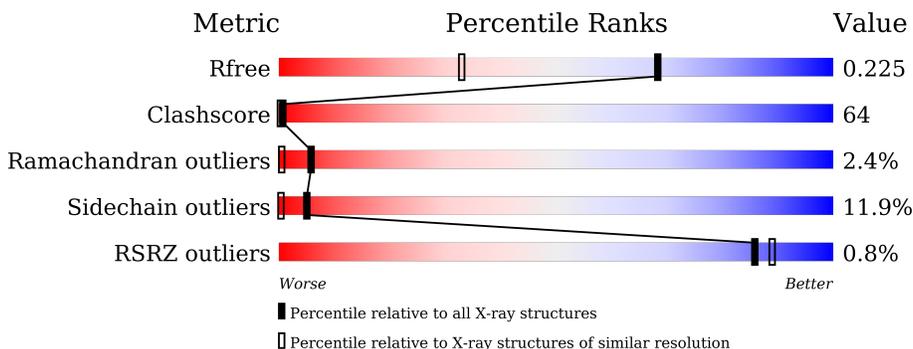
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.56 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1483 (1.56-1.56)
Clashscore	141614	1529 (1.56-1.56)
Ramachandran outliers	138981	1498 (1.56-1.56)
Sidechain outliers	138945	1495 (1.56-1.56)
RSRZ outliers	127900	1465 (1.56-1.56)

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

Mol	Chain	Length	Quality of chain
1	A	575	 23% 64% 10% ..
1	D	575	 23% 65% 10% ..
2	B	223	 27% 60% 8% .
2	C	223	 30% 60% 6% .
2	E	223	 3% 20% 63% 13% .
2	F	223	 34% 55% 7% .

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:

<b>Mol</b>	<b>Type</b>	<b>Chain</b>	<b>Res</b>	<b>Chirality</b>	<b>Geometry</b>	<b>Clashes</b>	<b>Electron density</b>
4	ATP	A	602	-	-	X	-
4	ATP	D	602	-	-	X	-
6	GSH	B	301	-	-	X	-
6	GSH	E	301	-	-	X	-

## 2 Entry composition i

There are 7 unique types of molecules in this entry. The entry contains 17930 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
			Total	C	N	O	S			
1	A	569	4479	2859	748	850	22	0	0	0
1	D	569	4479	2859	748	850	22	0	0	0

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

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

There are 24 discrepancies between the modelled and reference sequences:

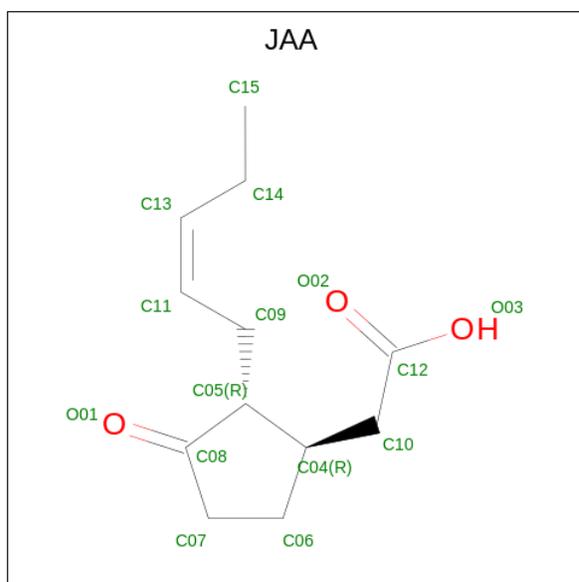
Chain	Residue	Modelled	Actual	Comment	Reference
B	-5	HIS	-	expression tag	UNP Q8L7C9
B	-4	HIS	-	expression tag	UNP Q8L7C9
B	-3	HIS	-	expression tag	UNP Q8L7C9
B	-2	HIS	-	expression tag	UNP Q8L7C9
B	-1	HIS	-	expression tag	UNP Q8L7C9
B	0	HIS	-	expression tag	UNP Q8L7C9
C	-5	HIS	-	expression tag	UNP Q8L7C9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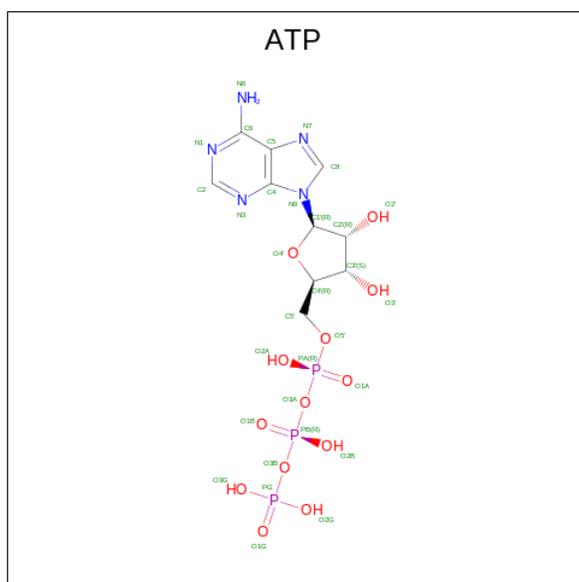
Chain	Residue	Modelled	Actual	Comment	Reference
E	-5	HIS	-	expression tag	UNP Q8L7C9
E	-4	HIS	-	expression tag	UNP Q8L7C9
E	-3	HIS	-	expression tag	UNP Q8L7C9
E	-2	HIS	-	expression tag	UNP Q8L7C9
E	-1	HIS	-	expression tag	UNP Q8L7C9
E	0	HIS	-	expression tag	UNP Q8L7C9
F	-5	HIS	-	expression tag	UNP Q8L7C9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

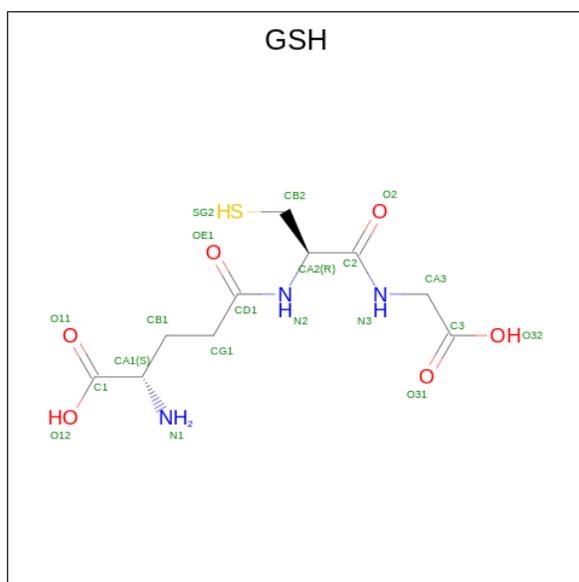


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
4	A	1	31	10	5	13	3	0	0
4	D	1	31	10	5	13	3	0	0

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

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

- 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
			Total	C	N	O	S		
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		

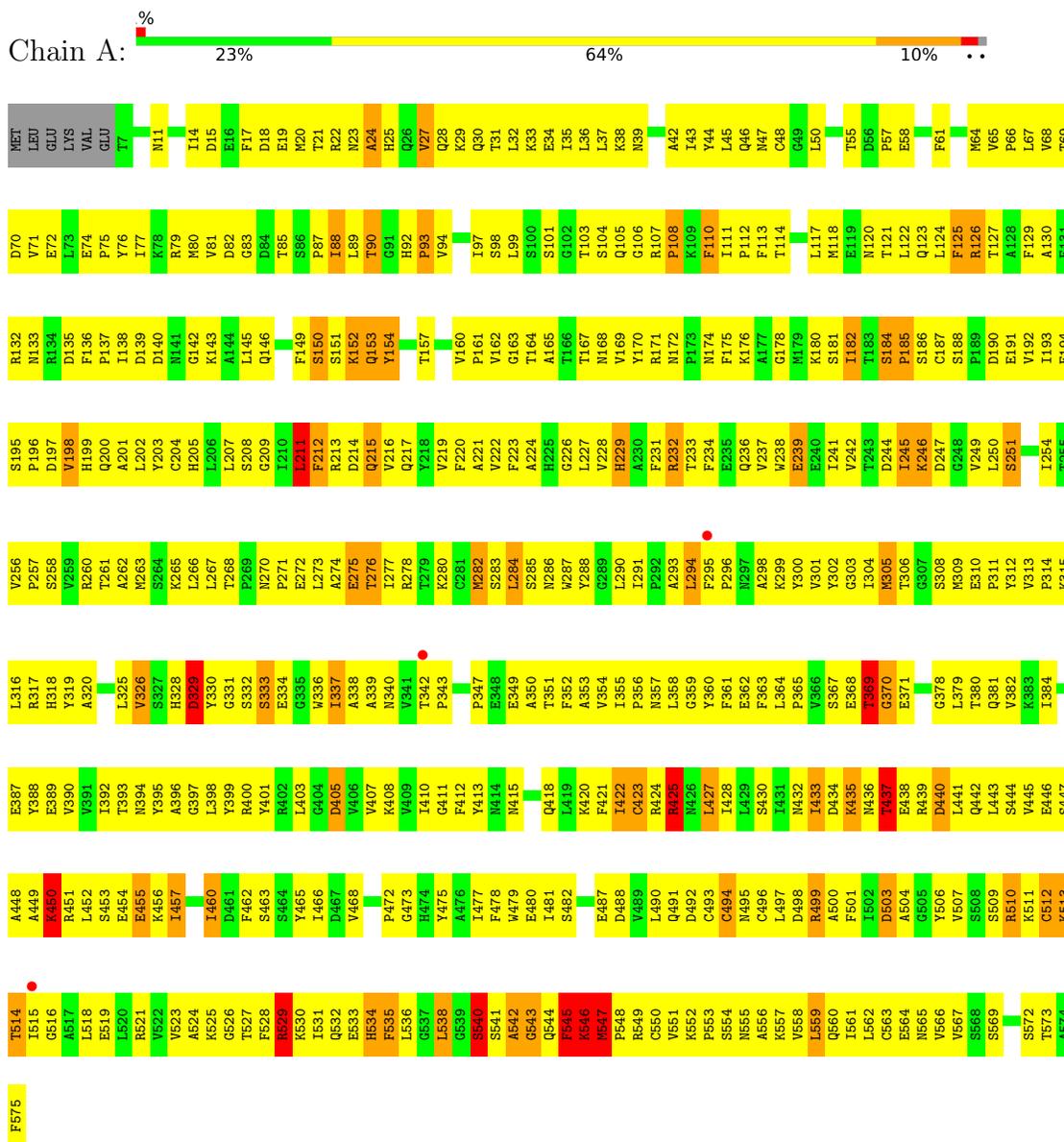
- Molecule 7 is water.

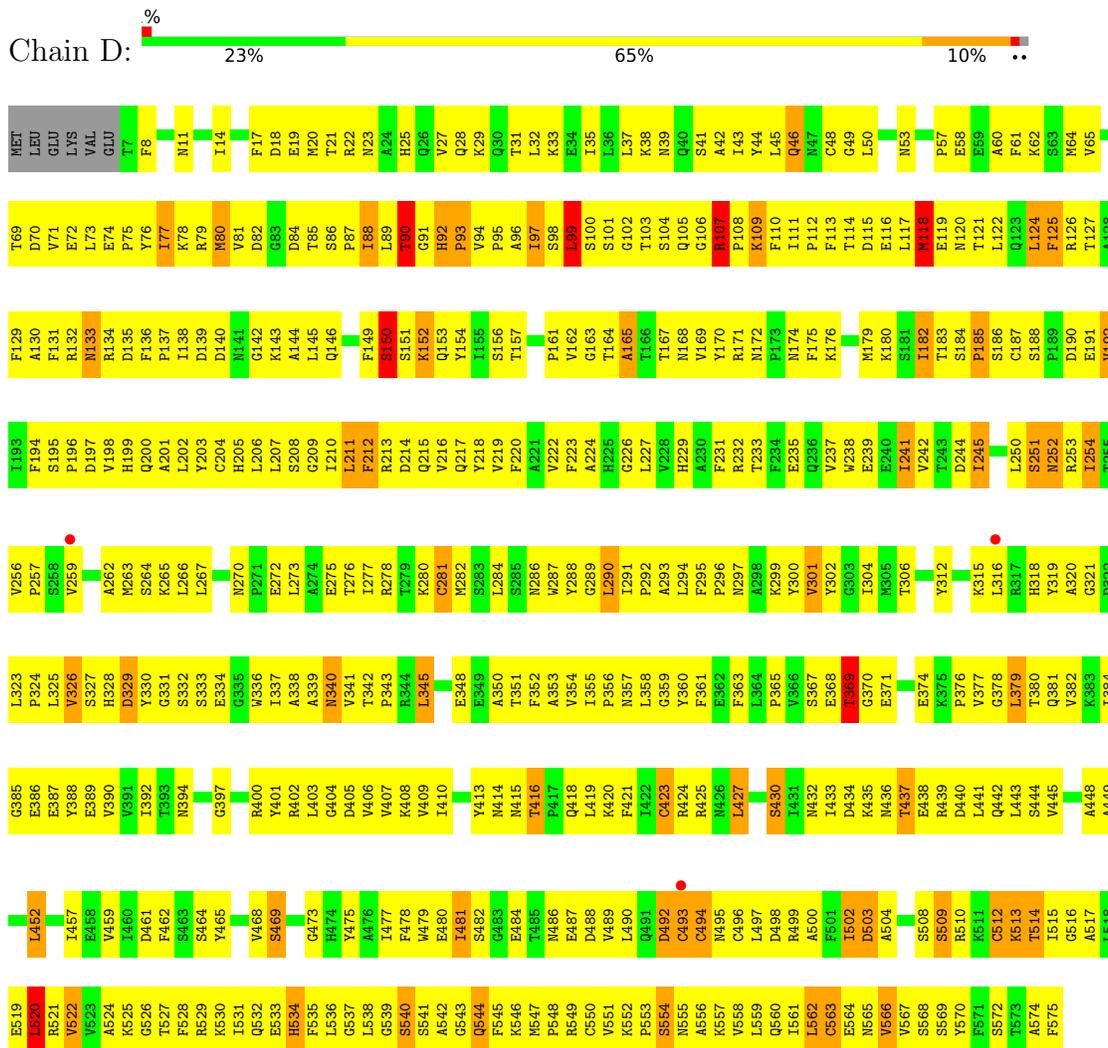
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	424	Total	O	0	0
			424	424		
7	B	219	Total	O	0	0
			219	219		
7	C	203	Total	O	0	0
			203	203		
7	D	474	Total	O	0	0
			474	474		
7	E	260	Total	O	0	0
			260	260		
7	F	226	Total	O	0	0
			226	226		

### 3 Residue-property plots

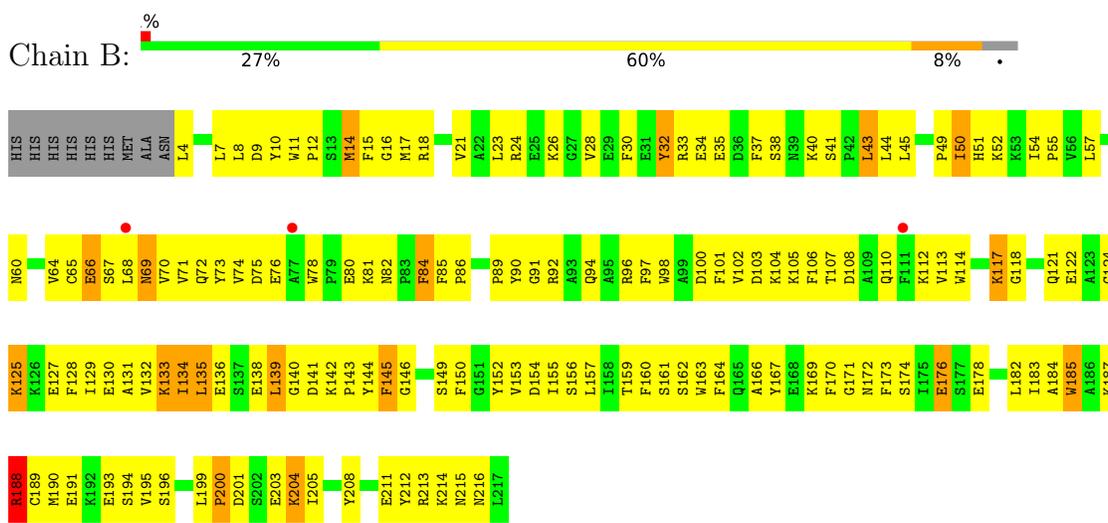
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: Jasmonic acid-amido synthetase JAR1





• Molecule 2: Glutathione S-transferase U20



• Molecule 2: Glutathione S-transferase U20





## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	53.89Å 53.86Å 195.40Å 92.52° 97.02° 113.58°	Depositor
Resolution (Å)	24.57 – 1.56 24.57 – 1.56	Depositor EDS
% Data completeness (in resolution range)	97.2 (24.57-1.56) 97.2 (24.57-1.56)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.51 (at 1.56Å)	Xtrriage
Refinement program	PHENIX 1.9_1692	Depositor
R, $R_{free}$	0.212 , 0.225 0.212 , 0.225	Depositor DCC
$R_{free}$ test set	27504 reflections (9.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	2.0	Xtrriage
Anisotropy	0.438	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.59 , 229.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.061 for k,h,-h-k-l 0.018 for -k,-h,-l 0.014 for -h,-k,h+k+l	Xtrriage
$F_o, F_c$ correlation	0.83	EDS
Total number of atoms	17930	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	3.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 36.49 % 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 4.9588e-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 [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.58	2/4581 (0.0%)	0.85	8/6219 (0.1%)
1	D	0.55	2/4581 (0.0%)	0.80	4/6219 (0.1%)
2	B	0.51	0/1799	0.70	2/2428 (0.1%)
2	C	0.50	0/1799	0.74	1/2428 (0.0%)
2	E	0.55	0/1799	0.75	0/2428
2	F	0.49	0/1799	0.68	0/2428
All	All	0.54	4/16358 (0.0%)	0.78	15/22150 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	D	0	1
2	C	0	1
All	All	0	5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	520	LEU	CG-CD2	-7.42	1.24	1.51
1	A	450	LYS	CD-CE	-6.33	1.35	1.51
1	A	546	LYS	CG-CD	-5.69	1.33	1.52
1	D	522	VAL	CB-CG2	-5.07	1.42	1.52

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	14	MET	CG-SD-CE	-19.82	68.49	100.20
1	A	425	ARG	NE-CZ-NH1	-11.86	114.37	120.30
1	A	546	LYS	CA-CB-CG	10.61	136.74	113.40
1	D	107	ARG	NE-CZ-NH2	-10.02	115.29	120.30
1	D	118	MET	CG-SD-CE	-8.45	86.68	100.20
1	A	559	LEU	CA-CB-CG	7.88	133.42	115.30
1	A	546	LYS	N-CA-CB	-6.80	98.35	110.60
2	B	188	ARG	NE-CZ-NH1	-6.08	117.26	120.30
1	A	547	MET	N-CA-CB	-5.57	100.57	110.60
2	B	188	ARG	NE-CZ-NH2	5.33	122.97	120.30
1	D	520	LEU	CA-CB-CG	5.33	127.56	115.30
1	A	529	ARG	NE-CZ-NH2	5.32	122.96	120.30
1	D	99	LEU	CA-CB-CG	5.16	127.18	115.30
1	A	545	PHE	N-CA-C	5.16	124.92	111.00
1	A	211	LEU	CA-CB-CG	5.09	127.00	115.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	427	LEU	Peptide
1	A	545	PHE	Peptide
1	A	546	LYS	Peptide
2	C	140	GLY	Peptide
1	D	427	LEU	Peptide

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4479	0	4434	668	2
1	D	4479	0	4434	634	5
2	B	1748	0	1704	225	1
2	C	1748	0	1704	191	1
2	E	1748	0	1704	257	2
2	F	1748	0	1704	174	2
3	A	15	0	0	3	0
3	D	15	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	31	0	7	12	0
4	D	31	0	8	14	0
5	A	1	0	0	0	0
5	D	1	0	0	0	0
6	B	20	0	15	8	0
6	C	20	0	15	0	0
6	E	20	0	15	12	0
6	F	20	0	15	2	0
7	A	424	0	0	115	2
7	B	219	0	0	40	2
7	C	203	0	0	47	4
7	D	474	0	0	107	10
7	E	260	0	0	55	6
7	F	226	0	0	48	5
All	All	17930	0	15759	2054	26

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 64.

All (2054) 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:A:529:ARG:NH1	1:A:533:GLU:OE2	1.81	1.14
1:A:101:SER:HA	1:A:546:LYS:HD3	1.27	1.14
2:B:26:LYS:NZ	2:B:82:ASN:O	1.83	1.12
1:D:176:LYS:NZ	1:D:190:ASP:OD2	1.84	1.11
1:A:437:THR:HG22	1:A:440:ASP:H	1.18	1.06
1:A:425:ARG:HH22	1:A:546:LYS:HA	1.21	1.06
1:D:90:THR:OG1	1:D:91:GLY:N	1.85	1.05
1:D:143:LYS:HD3	1:D:212:PHE:HB2	1.41	1.03
1:D:496:CYS:HA	2:E:188:ARG:NH2	1.76	1.01
1:A:546:LYS:HD2	1:A:547:MET:HA	1.39	1.00
1:A:425:ARG:HH12	1:A:546:LYS:N	1.60	0.99
2:F:145:PHE:HB3	2:F:153:VAL:HG13	1.43	0.98
2:C:167:TYR:OH	7:C:401:HOH:O	1.80	0.97
1:D:108:PRO:HG2	1:D:552:LYS:H	1.30	0.96
1:D:90:THR:HG22	1:D:397:GLY:HA2	1.47	0.96
2:E:183:ILE:O	2:E:187:LYS:NZ	1.98	0.96
1:A:500:ALA:HA	2:B:188:ARG:HH12	1.29	0.94
2:E:183:ILE:HG12	2:E:187:LYS:HD3	1.49	0.94
1:A:425:ARG:HH12	1:A:546:LYS:CA	1.79	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:499:ARG:O	2:B:188:ARG:NH1	2.00	0.93
1:D:219:VAL:HB	1:D:295:PHE:HZ	1.32	0.93
1:D:143:LYS:NZ	7:D:710:HOH:O	2.01	0.93
2:C:26:LYS:NZ	2:C:82:ASN:O	2.02	0.92
1:D:145:LEU:HD13	1:D:209:GLY:HA3	1.50	0.92
1:A:546:LYS:HZ3	1:A:548:PRO:HG2	1.32	0.92
1:A:176:LYS:NZ	1:A:190:ASP:OD2	2.01	0.92
2:B:157:LEU:O	7:B:401:HOH:O	1.86	0.92
1:D:329:ASP:OD2	7:D:701:HOH:O	1.88	0.92
1:D:98:SER:O	7:D:702:HOH:O	1.88	0.92
2:E:88:ASP:OD2	7:E:401:HOH:O	1.88	0.92
2:E:132:VAL:HG23	2:E:182:LEU:HD13	1.52	0.92
1:D:499:ARG:HB2	2:E:188:ARG:NH2	1.83	0.92
2:E:55:PRO:HD2	6:E:301:GSH:HB12	1.49	0.91
1:D:494:CYS:HB3	1:D:520:LEU:HD23	1.53	0.90
1:A:425:ARG:NH1	1:A:546:LYS:N	2.19	0.90
1:A:126:ARG:HA	1:A:182:ILE:HG21	1.53	0.90
2:F:15:PHE:HB3	2:F:67:SER:HB3	1.54	0.90
1:A:480:GLU:OE2	1:A:526:GLY:N	2.05	0.89
1:A:546:LYS:CD	1:A:548:PRO:HD2	2.02	0.89
1:D:107:ARG:HH22	1:D:552:LYS:HB2	1.36	0.89
1:A:546:LYS:HD2	1:A:548:PRO:HD2	1.52	0.89
1:A:226:GLY:HA3	1:A:529:ARG:NH1	1.86	0.89
1:A:432:ASN:ND2	7:A:712:HOH:O	2.06	0.88
1:A:425:ARG:NH2	1:A:546:LYS:HA	1.88	0.88
2:F:116:LYS:O	2:F:213:ARG:NH1	2.06	0.88
2:E:31:GLU:OE2	7:E:402:HOH:O	1.91	0.88
1:A:410:ILE:HB	1:A:418:GLN:HE21	1.39	0.88
1:D:487:GLU:OE2	7:D:703:HOH:O	1.91	0.88
1:A:219:VAL:HB	1:A:295:PHE:HZ	1.37	0.88
1:A:310:GLU:OE2	7:A:701:HOH:O	1.91	0.87
1:D:74:GLU:HA	1:D:77:ILE:HD11	1.54	0.87
1:A:450:LYS:HZ2	2:B:191:GLU:HA	1.40	0.87
1:A:487:GLU:OE2	7:A:702:HOH:O	1.92	0.86
2:B:80:GLU:OE2	7:B:402:HOH:O	1.91	0.86
1:A:145:LEU:HD13	1:A:209:GLY:HA3	1.58	0.86
1:D:297:ASN:OD1	7:D:704:HOH:O	1.94	0.86
1:A:121:THR:OG1	4:A:602:ATP:O2'	1.92	0.85
1:A:463:SER:HB2	1:A:528:PHE:HE2	1.40	0.85
2:E:109:ALA:N	7:E:403:HOH:O	2.03	0.85
1:A:369:THR:HG22	1:A:370:GLY:N	1.92	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:66:GLU:OE2	7:C:402:HOH:O	1.94	0.85
1:A:546:LYS:CD	1:A:547:MET:HA	2.06	0.85
1:D:19:GLU:O	1:D:23:ASN:ND2	2.09	0.85
1:D:519:GLU:OE2	1:D:569:SER:OG	1.95	0.84
1:D:90:THR:HG22	1:D:397:GLY:CA	2.07	0.84
2:E:105:LYS:O	7:E:403:HOH:O	1.95	0.84
2:F:145:PHE:N	2:F:154:ASP:OD2	2.11	0.84
1:D:405:ASP:HB2	1:D:541:SER:HB3	1.60	0.84
2:B:125:LYS:O	7:B:403:HOH:O	1.95	0.83
1:A:101:SER:CA	1:A:546:LYS:HD3	2.07	0.83
1:D:529:ARG:NH2	7:D:722:HOH:O	2.12	0.82
2:C:142:LYS:HD2	1:D:41:SER:HB2	1.61	0.82
2:B:26:LYS:HG2	2:B:81:LYS:HZ3	1.44	0.82
1:D:87:PRO:HD3	1:D:93:PRO:HG3	1.60	0.82
1:A:22:ARG:HA	1:A:415:ASN:HB2	1.61	0.82
2:E:67:SER:H	6:E:301:GSH:HN11	1.26	0.82
1:A:332:SER:HB2	1:A:538:LEU:HA	1.62	0.82
2:F:190:MET:SD	7:F:462:HOH:O	2.38	0.82
1:D:171:ARG:HH21	1:D:194:PHE:HB3	1.44	0.82
2:F:201:ASP:HB2	2:F:204:LYS:HG3	1.60	0.82
1:D:90:THR:HG1	1:D:91:GLY:H	1.24	0.82
2:E:206:VAL:O	7:E:404:HOH:O	1.97	0.82
1:A:498:ASP:O	1:A:510:ARG:NH2	2.11	0.81
1:D:18:ASP:OD2	7:D:705:HOH:O	1.96	0.81
1:D:198:VAL:HA	1:D:201:ALA:HB3	1.60	0.81
1:A:546:LYS:O	7:A:703:HOH:O	1.98	0.81
1:A:35:ILE:O	7:A:704:HOH:O	1.99	0.81
1:A:456:LYS:NZ	2:B:201:ASP:OD2	2.13	0.81
1:D:496:CYS:HA	2:E:188:ARG:HH22	1.46	0.81
1:D:152:LYS:HA	1:D:564:GLU:HB2	1.62	0.81
1:D:126:ARG:NH2	7:D:726:HOH:O	2.14	0.81
1:A:64:MET:SD	7:A:1047:HOH:O	2.39	0.80
2:F:193:GLU:OE2	7:F:401:HOH:O	1.98	0.80
1:A:422:ILE:O	7:A:705:HOH:O	1.99	0.80
1:A:498:ASP:HA	1:A:510:ARG:HH12	1.46	0.80
2:B:35:GLU:OE1	7:B:404:HOH:O	1.99	0.80
1:A:82:ASP:OD2	7:A:707:HOH:O	1.99	0.80
2:E:53:LYS:HA	6:E:301:GSH:HA31	1.62	0.80
2:C:78:TRP:O	7:C:403:HOH:O	1.99	0.80
1:A:150:SER:HB2	1:A:167:THR:HA	1.63	0.80
1:A:167:THR:O	7:A:708:HOH:O	2.00	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:328:HIS:NE2	3:A:601:JAA:O02	2.14	0.80
2:E:201:ASP:HB2	2:E:204:LYS:HG3	1.63	0.80
1:D:88:ILE:O	7:D:706:HOH:O	1.99	0.79
1:A:101:SER:HA	1:A:546:LYS:CD	2.12	0.79
1:A:138:ILE:O	7:A:706:HOH:O	1.99	0.79
1:A:437:THR:HG22	1:A:440:ASP:N	1.95	0.79
1:A:98:SER:HB2	1:A:111:ILE:HB	1.65	0.78
1:A:149:PHE:HB2	1:A:530:LYS:HE3	1.63	0.78
2:C:188:ARG:HE	1:D:86:SER:HB2	1.48	0.78
2:C:201:ASP:O	7:C:405:HOH:O	2.01	0.78
1:D:180:LYS:NZ	7:D:733:HOH:O	2.16	0.78
2:F:98:TRP:HE1	2:F:138:GLU:HG2	1.46	0.78
1:A:19:GLU:O	1:A:23:ASN:ND2	2.11	0.78
1:D:124:LEU:HD21	1:D:355:ILE:HD13	1.63	0.78
1:A:495:ASN:ND2	1:A:572:SER:OG	2.16	0.78
2:E:97:PHE:O	2:F:51:HIS:NE2	2.17	0.78
1:A:87:PRO:HD3	1:A:93:PRO:HG3	1.63	0.78
2:B:176:GLU:OE1	7:B:405:HOH:O	2.02	0.78
2:E:184:ALA:HA	2:E:187:LYS:HZ1	1.48	0.78
6:E:301:GSH:N1	7:E:419:HOH:O	2.17	0.78
1:D:280:LYS:NZ	1:D:293:ALA:O	2.14	0.77
2:B:144:TYR:HB3	2:B:154:ASP:OD2	1.83	0.77
2:C:48:ASN:ND2	7:C:414:HOH:O	2.16	0.77
2:C:187:LYS:O	7:C:404:HOH:O	2.01	0.77
1:D:502:ILE:O	7:D:709:HOH:O	2.01	0.77
1:A:249:VAL:O	7:A:711:HOH:O	2.03	0.77
2:C:21:VAL:O	7:C:406:HOH:O	2.02	0.77
1:A:304:ILE:HG13	1:A:328:HIS:HB3	1.66	0.77
1:A:146:GLN:OE1	7:A:710:HOH:O	2.02	0.77
2:B:121:GLN:O	7:B:407:HOH:O	2.03	0.77
2:E:9:ASP:HA	2:E:54:ILE:HD13	1.67	0.77
2:E:93:ALA:HB1	2:F:65:CYS:H	1.49	0.77
1:A:500:ALA:HA	2:B:188:ARG:NH1	2.01	0.76
2:C:14:MET:HE2	2:C:160:PHE:HA	1.68	0.76
2:F:169:LYS:HE2	2:F:206:VAL:HG13	1.68	0.76
2:C:145:PHE:N	2:C:154:ASP:OD1	2.18	0.76
1:D:199:HIS:HB3	1:D:525:LYS:H	1.49	0.76
1:D:442:GLN:HG2	1:D:462:PHE:HZ	1.51	0.76
2:F:98:TRP:NE1	2:F:138:GLU:HG2	2.01	0.76
2:F:109:ALA:O	7:F:402:HOH:O	2.02	0.76
1:A:535:PHE:O	1:A:538:LEU:HB3	1.86	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:414:ASN:ND2	7:D:738:HOH:O	2.18	0.76
1:A:223:PHE:HE2	1:A:545:PHE:HZ	1.34	0.76
1:A:362:GLU:HG3	1:A:400:ARG:HH21	1.51	0.76
2:B:216:ASN:OD1	7:B:406:HOH:O	2.02	0.76
2:F:14:MET:SD	7:F:407:HOH:O	2.43	0.76
2:B:132:VAL:HG23	2:B:182:LEU:HD13	1.68	0.76
2:C:110:GLN:OE1	7:C:401:HOH:O	2.02	0.76
2:C:136:GLU:OE2	2:C:181:LYS:HE2	1.86	0.76
1:A:369:THR:HG22	1:A:370:GLY:H	1.46	0.75
1:A:535:PHE:CE2	1:A:546:LYS:HE2	2.21	0.75
1:A:541:SER:O	1:A:543:GLY:N	2.18	0.75
2:C:140:GLY:HA3	1:D:38:LYS:HB3	1.65	0.75
1:A:393:THR:HG23	1:A:399:TYR:HA	1.67	0.75
1:D:440:ASP:OD1	7:D:712:HOH:O	2.03	0.75
2:E:211:GLU:OE1	7:E:405:HOH:O	2.03	0.75
2:E:56:VAL:O	7:E:406:HOH:O	2.03	0.75
1:A:152:LYS:HA	1:A:564:GLU:HB2	1.69	0.75
1:A:219:VAL:HB	1:A:295:PHE:CZ	2.21	0.75
1:D:425:ARG:HB2	1:D:427:LEU:HB2	1.69	0.75
1:D:500:ALA:O	7:D:712:HOH:O	2.04	0.75
2:E:184:ALA:CA	2:E:187:LYS:HZ1	2.00	0.75
2:C:101:PHE:HE2	2:C:135:LEU:HG	1.50	0.75
1:D:94:VAL:HG11	1:D:112:PRO:HB3	1.68	0.75
1:A:559:LEU:HD23	1:A:562:LEU:HD12	1.69	0.74
2:F:110:GLN:NE2	7:F:407:HOH:O	2.10	0.74
1:A:399:TYR:OH	7:A:704:HOH:O	2.05	0.74
1:D:494:CYS:CB	1:D:520:LEU:HD23	2.17	0.74
2:C:26:LYS:HB3	2:C:28:VAL:HG23	1.66	0.74
1:D:102:GLY:N	1:D:546:LYS:O	2.16	0.74
1:D:219:VAL:HB	1:D:295:PHE:CZ	2.20	0.74
2:B:57:LEU:HB3	2:B:64:VAL:HG22	1.69	0.74
2:C:18:ARG:NH2	7:C:419:HOH:O	2.20	0.74
1:D:521:ARG:HB3	1:D:566:VAL:HG12	1.68	0.74
1:A:434:ASP:N	7:A:741:HOH:O	2.20	0.74
2:B:103:ASP:OD1	7:B:408:HOH:O	2.05	0.74
1:A:47:ASN:ND2	7:A:746:HOH:O	2.21	0.74
1:A:111:ILE:HG21	1:A:334:GLU:HG2	1.70	0.73
1:D:389:GLU:OE2	1:D:404:GLY:HA2	1.87	0.73
1:D:390:VAL:O	7:D:713:HOH:O	2.04	0.73
1:D:151:SER:OG	1:D:565:ASN:OD1	2.05	0.73
1:A:546:LYS:HD2	1:A:547:MET:CA	2.15	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:15:PHE:HB3	2:C:67:SER:HB3	1.70	0.73
1:A:98:SER:OG	4:A:602:ATP:O3B	2.02	0.73
1:D:106:GLY:O	1:D:432:ASN:ND2	2.19	0.73
2:E:22:ALA:HB2	2:E:71:VAL:HG12	1.69	0.73
1:A:546:LYS:HZ3	1:A:548:PRO:CG	2.01	0.73
2:C:166:ALA:HA	2:C:169:LYS:HG2	1.70	0.73
1:D:99:LEU:HB3	1:D:557:LYS:H	1.53	0.73
1:D:206:LEU:O	1:D:210:ILE:HG12	1.88	0.73
1:D:340:ASN:HB2	1:D:352:PHE:CD2	2.23	0.73
1:A:154:TYR:CZ	1:A:162:VAL:HG23	2.23	0.73
1:D:423:CYS:HB2	1:D:543:GLY:N	2.04	0.73
2:F:217:LEU:O	7:F:404:HOH:O	2.05	0.73
2:E:158:ILE:O	7:E:408:HOH:O	2.06	0.73
1:A:546:LYS:NZ	1:A:548:PRO:HG2	2.04	0.73
2:C:110:GLN:NE2	7:C:421:HOH:O	2.21	0.73
1:D:219:VAL:HG11	1:D:291:ILE:HG21	1.70	0.73
1:A:496:CYS:HB2	2:B:187:LYS:NZ	2.04	0.73
1:D:53:ASN:OD1	7:D:714:HOH:O	2.06	0.73
1:A:27:VAL:O	1:A:31:THR:OG1	2.03	0.72
1:D:440:ASP:O	7:D:712:HOH:O	2.06	0.72
2:E:54:ILE:O	6:E:301:GSH:N2	2.22	0.72
1:D:473:GLY:O	1:D:516:GLY:N	2.20	0.72
2:E:16:GLY:HA2	2:E:55:PRO:HG3	1.70	0.72
1:D:152:LYS:HD3	1:D:561:ILE:HG23	1.71	0.72
1:D:494:CYS:SG	1:D:495:ASN:N	2.62	0.72
2:E:54:ILE:N	6:E:301:GSH:O2	2.17	0.72
2:E:75:ASP:HB2	2:E:84:PHE:CE2	2.23	0.72
1:A:407:VAL:O	7:A:713:HOH:O	2.07	0.72
1:D:547:MET:SD	7:D:764:HOH:O	2.47	0.72
2:E:26:LYS:HD2	2:E:74:VAL:HG13	1.71	0.72
1:A:247:ASP:OD2	7:A:714:HOH:O	2.07	0.72
1:D:174:ASN:OD1	7:D:716:HOH:O	2.06	0.72
1:A:143:LYS:O	7:A:717:HOH:O	2.08	0.72
1:A:101:SER:HB2	1:A:546:LYS:HG2	1.70	0.72
1:A:48:CYS:SG	1:A:65:VAL:HG23	2.30	0.72
1:A:126:ARG:NH1	7:A:753:HOH:O	2.22	0.72
6:B:301:GSH:O11	7:B:410:HOH:O	2.08	0.72
2:E:141:ASP:OD1	7:E:410:HOH:O	2.08	0.72
1:D:151:SER:HB3	1:D:565:ASN:HD21	1.55	0.71
1:A:411:GLY:H	1:A:418:GLN:HG2	1.55	0.71
1:A:534:HIS:CG	1:A:557:LYS:HE2	2.24	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:110:PHE:O	7:D:718:HOH:O	2.08	0.71
1:D:528:PHE:HB3	1:D:547:MET:HE1	1.71	0.71
2:C:25:GLU:N	7:C:406:HOH:O	2.23	0.71
1:A:76:TYR:HB2	7:A:767:HOH:O	1.91	0.71
1:A:224:ALA:H	1:A:309:MET:HE1	1.55	0.71
1:D:223:PHE:HA	7:D:750:HOH:O	1.90	0.71
1:A:70:ASP:OD2	1:A:104:SER:HA	1.90	0.71
6:B:301:GSH:O12	7:B:409:HOH:O	2.08	0.71
2:C:120:GLU:O	7:C:407:HOH:O	2.09	0.71
1:A:521:ARG:HB3	1:A:566:VAL:HG12	1.73	0.71
1:D:115:ASP:HA	1:D:118:MET:HE1	1.71	0.71
1:D:22:ARG:NH1	7:D:749:HOH:O	2.21	0.71
1:D:432:ASN:OD1	1:D:434:ASP:N	2.23	0.71
1:A:66:PRO:O	7:A:719:HOH:O	2.09	0.71
1:A:506:TYR:OH	1:A:510:ARG:NH1	2.24	0.71
1:A:512:CYS:SG	1:A:514:THR:OG1	2.46	0.71
2:B:98:TRP:HE3	2:B:101:PHE:HB2	1.56	0.71
1:A:153:GLN:NE2	7:A:750:HOH:O	2.22	0.71
2:B:8:LEU:HD21	2:B:43:LEU:HD11	1.71	0.71
2:C:53:LYS:NZ	7:C:422:HOH:O	2.22	0.71
1:D:526:GLY:HA2	1:D:529:ARG:HB3	1.73	0.71
7:E:477:HOH:O	2:F:65:CYS:SG	2.39	0.71
1:A:425:ARG:HH22	1:A:546:LYS:CA	2.01	0.71
2:F:59:HIS:CD2	2:F:60:ASN:HD22	2.09	0.71
1:A:463:SER:HB2	1:A:528:PHE:CE2	2.26	0.70
1:A:490:LEU:O	7:A:715:HOH:O	2.08	0.70
2:B:7:LEU:HD21	2:B:23:LEU:HD12	1.71	0.70
1:D:387:GLU:HG3	1:D:408:LYS:HB2	1.73	0.70
2:F:142:LYS:HE2	2:F:145:PHE:HA	1.72	0.70
1:A:435:LYS:HG2	1:A:438:GLU:N	2.05	0.70
1:A:531:ILE:HA	1:A:534:HIS:NE2	2.05	0.70
1:D:340:ASN:HB2	1:D:352:PHE:CE2	2.26	0.70
2:B:159:THR:HA	2:B:199:LEU:HD21	1.73	0.70
1:D:312:TYR:OH	7:D:711:HOH:O	2.02	0.70
1:A:223:PHE:HE2	1:A:545:PHE:CZ	2.10	0.70
2:B:60:ASN:ND2	7:B:427:HOH:O	2.23	0.70
1:A:97:ILE:H	1:A:163:GLY:H	1.40	0.70
1:A:132:ARG:O	1:A:136:PHE:N	2.16	0.70
1:A:339:ALA:HB2	1:A:355:ILE:HD11	1.74	0.70
1:A:556:ALA:O	7:A:716:HOH:O	2.08	0.70
1:D:22:ARG:NH1	1:D:414:ASN:OD1	2.24	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:84:PHE:CD1	2:E:152:TYR:HB2	2.27	0.70
1:D:275:GLU:OE1	7:D:717:HOH:O	2.07	0.70
2:B:26:LYS:HE2	2:B:75:ASP:HA	1.73	0.70
1:A:425:ARG:NH1	1:A:546:LYS:CA	2.53	0.70
1:D:414:ASN:ND2	7:D:705:HOH:O	2.25	0.70
2:E:68:LEU:HD21	2:E:103:ASP:OD2	1.92	0.70
1:A:152:LYS:HE2	1:A:565:ASN:HD22	1.57	0.70
1:A:547:MET:HB3	7:A:780:HOH:O	1.91	0.70
2:F:86:PRO:O	7:F:405:HOH:O	2.09	0.70
1:A:104:SER:O	1:A:107:ARG:HB2	1.92	0.69
2:C:61:GLY:O	7:C:409:HOH:O	2.10	0.69
1:A:39:ASN:ND2	1:A:90:THR:O	2.26	0.69
2:B:10:TYR:OH	2:B:208:TYR:OH	2.08	0.69
1:D:265:LYS:NZ	7:D:747:HOH:O	2.21	0.69
1:D:437:THR:OG1	1:D:440:ASP:HB2	1.91	0.69
2:E:97:PHE:CZ	2:F:51:HIS:HB2	2.27	0.69
1:A:69:THR:OG1	1:A:72:GLU:OE1	2.07	0.69
1:A:387:GLU:HG2	1:A:408:LYS:HG2	1.73	0.69
1:A:447:SER:HA	1:A:450:LYS:CE	2.22	0.69
2:B:10:TYR:HH	2:B:208:TYR:HH	1.36	0.69
1:D:484:GLU:O	7:D:720:HOH:O	2.10	0.69
2:E:100:ASP:OD2	7:E:411:HOH:O	2.09	0.69
2:E:137:SER:OG	7:E:413:HOH:O	2.11	0.69
1:A:519:GLU:OE2	1:A:569:SER:OG	2.11	0.69
2:B:178:GLU:O	7:B:413:HOH:O	2.10	0.69
2:C:14:MET:SD	7:C:401:HOH:O	2.49	0.69
2:F:5:PRO:HB3	2:F:57:LEU:HD11	1.74	0.69
1:A:180:LYS:O	7:A:722:HOH:O	2.11	0.69
1:A:80:MET:HG2	1:A:88:ILE:HD12	1.75	0.69
1:A:154:TYR:HB3	1:A:563:CYS:HB2	1.74	0.69
2:B:69:ASN:HD22	2:C:97:PHE:HB3	1.58	0.69
1:A:89:LEU:HD11	7:A:767:HOH:O	1.93	0.69
1:A:163:GLY:HA2	1:A:560:GLN:HB2	1.74	0.69
2:B:127:GLU:OE2	7:B:411:HOH:O	2.08	0.69
2:F:168:GLU:OE2	7:F:406:HOH:O	2.10	0.69
1:A:143:LYS:O	1:A:216:VAL:HA	1.92	0.69
1:A:450:LYS:NZ	2:B:191:GLU:HA	2.08	0.69
1:D:185:PRO:O	7:D:721:HOH:O	2.11	0.69
1:D:242:VAL:HG12	1:D:277:ILE:HD13	1.75	0.69
2:F:113:VAL:O	7:F:408:HOH:O	2.10	0.69
1:A:263:MET:SD	7:A:894:HOH:O	2.52	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:491:GLN:HG2	2:B:176:GLU:OE2	1.93	0.69
1:D:45:LEU:O	1:D:49:GLY:N	2.25	0.69
1:D:329:ASP:OD1	1:D:329:ASP:N	2.24	0.69
6:B:301:GSH:O2	7:B:412:HOH:O	2.10	0.68
1:A:350:ALA:O	7:A:723:HOH:O	2.11	0.68
2:B:164:PHE:HD2	2:B:183:ILE:HD13	1.58	0.68
1:D:75:PRO:O	1:D:79:ARG:HG3	1.93	0.68
1:D:534:HIS:CG	1:D:557:LYS:HE2	2.28	0.68
2:E:121:GLN:O	2:E:125:LYS:HG3	1.94	0.68
2:C:125:LYS:HB3	2:C:173:PHE:CE2	2.27	0.68
2:C:212:TYR:OH	7:C:408:HOH:O	2.10	0.68
1:D:432:ASN:HD21	1:D:434:ASP:CG	1.96	0.68
2:E:139:LEU:O	2:E:141:ASP:N	2.26	0.68
1:A:137:PRO:O	1:A:299:LYS:NZ	2.23	0.68
1:A:152:LYS:NZ	1:A:561:ILE:O	2.14	0.68
1:A:415:ASN:OD1	7:A:725:HOH:O	2.12	0.68
1:D:384:ILE:HA	1:D:409:VAL:HG13	1.75	0.68
2:E:174:SER:O	7:E:412:HOH:O	2.10	0.68
2:F:213:ARG:NH1	7:F:416:HOH:O	2.27	0.68
2:B:98:TRP:CE3	2:B:101:PHE:HB2	2.27	0.68
1:D:132:ARG:HA	1:D:343:PRO:HG3	1.76	0.68
1:D:532:GLN:NE2	7:D:764:HOH:O	2.25	0.68
1:D:540:SER:OG	1:D:544:GLN:NE2	2.26	0.68
1:A:548:PRO:O	7:A:726:HOH:O	2.12	0.68
1:D:137:PRO:O	7:D:719:HOH:O	2.10	0.68
1:D:184:SER:O	7:D:721:HOH:O	2.12	0.68
2:F:8:LEU:HG	2:F:33:ARG:NH1	2.08	0.68
1:A:181:SER:OG	7:A:724:HOH:O	2.12	0.68
1:D:107:ARG:HE	1:D:433:ILE:HG13	1.59	0.68
2:E:26:LYS:NZ	2:E:82:ASN:O	2.27	0.68
1:D:99:LEU:HB3	1:D:557:LYS:HB2	1.75	0.68
2:E:122:GLU:HA	2:E:125:LYS:HE2	1.76	0.68
2:F:48:ASN:OD1	7:F:410:HOH:O	2.12	0.68
1:D:353:ALA:HB2	1:D:413:TYR:CD2	2.28	0.68
1:D:162:VAL:HG21	1:D:559:LEU:HD23	1.75	0.67
2:E:35:GLU:OE1	7:E:414:HOH:O	2.12	0.67
2:E:189:CYS:O	7:E:415:HOH:O	2.12	0.67
2:F:9:ASP:OD1	2:F:16:GLY:HA3	1.94	0.67
2:F:195:VAL:O	7:F:409:HOH:O	2.11	0.67
1:A:560:GLN:NE2	7:A:761:HOH:O	2.26	0.67
1:D:332:SER:HB2	1:D:538:LEU:HA	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:6:ILE:O	7:E:406:HOH:O	2.12	0.67
1:A:199:HIS:HB3	1:A:525:LYS:H	1.59	0.67
1:D:408:LYS:HD3	1:D:420:LYS:HE3	1.75	0.67
2:F:102:VAL:O	2:F:107:THR:OG1	2.09	0.67
1:A:99:LEU:HB3	1:A:557:LYS:HB3	1.76	0.67
2:C:20:ARG:NH2	7:C:412:HOH:O	2.27	0.67
1:A:229:HIS:HA	1:A:232:ARG:HE	1.59	0.67
1:A:200:GLN:NE2	1:A:204:CYS:SG	2.68	0.67
1:D:39:ASN:HD21	1:D:90:THR:C	1.98	0.67
1:D:430:SER:OG	7:D:708:HOH:O	2.00	0.67
2:E:197:LYS:NZ	7:E:430:HOH:O	2.27	0.67
1:A:146:GLN:NE2	1:A:186:SER:OG	2.28	0.67
1:A:193:ILE:HG12	1:A:205:HIS:HE1	1.60	0.67
2:B:170:PHE:CD2	2:B:213:ARG:HD2	2.30	0.67
1:D:192:VAL:HG23	1:D:259:VAL:HG23	1.77	0.67
2:F:9:ASP:OD2	2:F:20:ARG:NE	2.28	0.67
2:B:18:ARG:NH1	7:B:410:HOH:O	2.26	0.67
2:E:98:TRP:CD1	2:E:153:VAL:HG21	2.29	0.67
2:C:195:VAL:HG13	2:C:199:LEU:HD22	1.77	0.66
2:F:143:PRO:O	7:F:412:HOH:O	2.13	0.66
1:A:559:LEU:HA	1:A:562:LEU:HG	1.76	0.66
1:D:114:THR:OG1	7:D:723:HOH:O	2.13	0.66
2:E:150:PHE:HE2	2:E:189:CYS:HB3	1.60	0.66
1:A:229:HIS:O	1:A:233:THR:OG1	2.06	0.66
2:C:190:MET:SD	7:C:424:HOH:O	2.53	0.66
1:A:330:TYR:HE2	1:A:540:SER:H	1.42	0.66
1:D:461:ASP:O	7:D:727:HOH:O	2.14	0.66
2:F:174:SER:O	7:F:411:HOH:O	2.13	0.66
1:A:83:GLY:O	7:A:727:HOH:O	2.12	0.66
1:A:223:PHE:HZ	1:A:536:LEU:HB3	1.59	0.66
1:A:546:LYS:HG3	1:A:547:MET:HG3	1.77	0.66
1:D:143:LYS:HA	1:D:184:SER:HB2	1.78	0.66
1:A:438:GLU:OE2	7:A:730:HOH:O	2.12	0.66
1:D:198:VAL:HG22	1:D:524:ALA:HB3	1.76	0.66
3:D:601:JAA:O02	4:D:602:ATP:N6	2.29	0.66
1:A:339:ALA:CB	1:A:355:ILE:HD11	2.26	0.66
1:A:545:PHE:HA	1:A:546:LYS:HB3	1.76	0.66
1:A:545:PHE:CA	1:A:546:LYS:HB3	2.08	0.66
1:D:19:GLU:OE1	7:D:725:HOH:O	2.14	0.66
1:D:172:ASN:ND2	7:D:707:HOH:O	1.99	0.66
2:F:128:PHE:O	7:F:414:HOH:O	2.13	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:SER:HB3	1:A:170:TYR:CD2	2.31	0.66
1:A:254:ILE:O	7:A:729:HOH:O	2.12	0.66
1:A:381:GLN:NE2	7:A:773:HOH:O	2.28	0.66
2:C:45:LEU:O	7:C:411:HOH:O	2.14	0.66
1:D:187:CYS:SG	7:D:729:HOH:O	2.54	0.66
1:A:493:CYS:HA	2:B:187:LYS:HE3	1.78	0.65
2:E:184:ALA:C	2:E:187:LYS:HZ1	1.99	0.65
1:A:143:LYS:HB2	1:A:185:PRO:O	1.96	0.65
1:A:477:ILE:N	7:A:762:HOH:O	2.26	0.65
1:D:97:ILE:H	1:D:162:VAL:HA	1.61	0.65
1:D:109:LYS:O	7:D:702:HOH:O	2.13	0.65
1:D:191:GLU:OE1	7:D:724:HOH:O	2.13	0.65
1:D:445:VAL:HG21	1:D:462:PHE:CG	2.31	0.65
1:A:105:GLN:HA	1:A:430:SER:HB3	1.78	0.65
2:B:102:VAL:O	2:B:107:THR:HG23	1.95	0.65
2:E:98:TRP:CZ2	2:E:135:LEU:HD21	2.31	0.65
1:A:452:LEU:HD23	1:A:481:ILE:HG21	1.77	0.65
2:E:67:SER:O	2:E:71:VAL:HG22	1.96	0.65
1:A:405:ASP:OD1	1:A:405:ASP:N	2.30	0.65
1:D:119:GLU:OE2	7:D:730:HOH:O	2.15	0.65
1:D:162:VAL:O	1:D:560:GLN:HB2	1.96	0.65
2:E:122:GLU:OE1	7:E:416:HOH:O	2.13	0.65
1:A:46:GLN:NE2	7:A:777:HOH:O	2.29	0.65
2:C:139:LEU:HB3	2:C:142:LYS:H	1.62	0.65
1:A:197:ASP:HB2	1:A:256:VAL:HG21	1.77	0.65
2:C:113:VAL:O	7:C:410:HOH:O	2.13	0.65
1:D:332:SER:OG	1:D:333:SER:N	2.30	0.65
1:A:165:ALA:O	1:A:169:VAL:HG23	1.97	0.65
1:A:549:ARG:NH1	7:A:780:HOH:O	2.30	0.65
1:D:146:GLN:O	7:D:729:HOH:O	2.15	0.65
1:D:546:LYS:NZ	7:D:778:HOH:O	2.29	0.65
2:E:9:ASP:HB2	2:E:20:ARG:HH21	1.60	0.65
2:E:93:ALA:O	2:E:97:PHE:HB2	1.96	0.65
2:E:114:TRP:CD1	2:E:167:TYR:HE1	2.15	0.65
1:A:499:ARG:CZ	2:B:184:ALA:HB1	2.27	0.65
2:C:15:PHE:HA	2:C:18:ARG:HD2	1.79	0.65
1:D:143:LYS:HD3	1:D:212:PHE:CB	2.22	0.65
2:F:158:ILE:O	2:F:161:SER:OG	2.06	0.65
1:A:331:GLY:O	4:A:602:ATP:N6	2.30	0.65
1:A:513:LYS:NZ	1:A:575:PHE:HB3	2.11	0.65
2:B:114:TRP:CD1	2:B:167:TYR:HE1	2.15	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:188:ARG:NE	1:D:86:SER:HB2	2.12	0.65
1:A:332:SER:OG	1:A:333:SER:N	2.28	0.64
1:A:546:LYS:CE	1:A:547:MET:HA	2.26	0.64
2:E:139:LEU:HG	2:E:145:PHE:CZ	2.32	0.64
2:F:86:PRO:O	7:F:413:HOH:O	2.13	0.64
2:F:139:LEU:HA	2:F:142:LYS:HD3	1.78	0.64
1:A:164:THR:HG21	1:A:561:ILE:HD11	1.79	0.64
1:A:308:SER:HB3	1:A:424:ARG:HA	1.79	0.64
2:C:142:LYS:HA	1:D:91:GLY:HA3	1.79	0.64
1:D:135:ASP:OD2	7:D:728:HOH:O	2.15	0.64
1:A:342:THR:OG1	1:A:413:TYR:OH	2.09	0.64
1:D:163:GLY:HA3	1:D:168:ASN:HD21	1.60	0.64
1:D:241:ILE:O	1:D:245:ILE:HG12	1.96	0.64
2:F:138:GLU:OE1	7:F:415:HOH:O	2.14	0.64
1:A:425:ARG:NH1	1:A:546:LYS:H	1.93	0.64
2:B:40:LYS:H	2:B:40:LYS:HZ3	1.45	0.64
2:C:14:MET:CE	7:C:401:HOH:O	2.45	0.64
1:D:535:PHE:CZ	1:D:545:PHE:HB3	2.32	0.64
1:D:231:PHE:CZ	1:D:291:ILE:HG12	2.33	0.64
2:E:183:ILE:C	2:E:187:LYS:HZ2	1.98	0.64
2:F:18:ARG:O	7:F:417:HOH:O	2.14	0.64
1:D:535:PHE:O	1:D:538:LEU:HB3	1.97	0.64
1:A:143:LYS:HD2	1:A:212:PHE:HB2	1.79	0.64
1:A:165:ALA:H	1:A:557:LYS:HE3	1.62	0.64
1:A:192:VAL:HA	1:A:195:SER:HB2	1.80	0.64
1:A:556:ALA:O	1:A:559:LEU:HB2	1.97	0.64
1:D:98:SER:HB2	1:D:111:ILE:HB	1.80	0.64
1:D:342:THR:O	1:D:345:LEU:HG	1.98	0.64
2:E:33:ARG:O	7:E:414:HOH:O	2.14	0.64
2:E:172:ASN:ND2	7:E:433:HOH:O	2.30	0.64
1:A:34:GLU:OE2	7:A:732:HOH:O	2.15	0.64
1:A:150:SER:O	1:A:150:SER:OG	2.15	0.64
2:C:130:GLU:O	7:C:413:HOH:O	2.15	0.64
1:D:23:ASN:ND2	7:D:783:HOH:O	2.30	0.64
2:E:54:ILE:HG13	6:E:301:GSH:O2	1.98	0.64
1:A:94:VAL:HG11	1:A:112:PRO:HB3	1.80	0.63
2:C:193:GLU:HB3	2:C:197:LYS:HD3	1.79	0.63
1:D:144:ALA:N	7:D:721:HOH:O	2.31	0.63
1:D:306:THR:OG1	1:D:330:TYR:OH	2.15	0.63
1:D:513:LYS:NZ	1:D:575:PHE:HB3	2.13	0.63
2:E:195:VAL:HG13	2:E:199:LEU:HD13	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:499:ARG:NH1	2:B:184:ALA:HB1	2.13	0.63
1:A:108:PRO:HG2	1:A:552:LYS:CB	2.29	0.63
1:A:536:LEU:HB2	1:A:545:PHE:CE2	2.33	0.63
2:B:17:MET:HE2	2:B:200:PRO:HD2	1.80	0.63
1:D:435:LYS:HZ2	1:D:438:GLU:HA	1.64	0.63
2:B:150:PHE:HE1	2:B:155:ILE:HG13	1.64	0.63
2:E:210:ALA:N	7:E:404:HOH:O	2.11	0.63
2:B:145:PHE:HB3	2:B:153:VAL:HG13	1.79	0.63
2:F:8:LEU:HD12	2:F:56:VAL:HB	1.80	0.63
1:A:340:ASN:HB2	1:A:352:PHE:HD1	1.64	0.63
2:C:33:ARG:NE	7:C:433:HOH:O	2.28	0.63
1:D:32:LEU:HD21	1:D:61:PHE:HD2	1.64	0.63
1:D:99:LEU:HD13	1:D:558:VAL:H	1.63	0.63
1:D:386:GLU:O	7:D:731:HOH:O	2.16	0.63
2:E:33:ARG:HH12	2:E:41:SER:CB	2.11	0.63
2:E:89:PRO:HB3	2:F:73:TYR:CE1	2.34	0.63
2:F:143:PRO:O	2:F:185:TRP:HD1	1.82	0.63
1:A:80:MET:SD	7:A:768:HOH:O	2.56	0.63
1:A:153:GLN:HG3	1:A:171:ARG:HD2	1.79	0.63
1:A:191:GLU:OE2	7:A:733:HOH:O	2.15	0.63
2:B:157:LEU:O	7:B:415:HOH:O	2.15	0.63
1:D:153:GLN:H	1:D:564:GLU:HB2	1.63	0.63
1:D:242:VAL:HG21	1:D:278:ARG:HH21	1.63	0.63
1:D:437:THR:O	1:D:440:ASP:N	2.31	0.63
1:A:106:GLY:O	1:A:432:ASN:ND2	2.32	0.63
1:A:512:CYS:O	1:A:513:LYS:HB2	1.97	0.63
1:D:22:ARG:HA	1:D:415:ASN:HB2	1.81	0.63
2:E:50:ILE:HG13	2:E:51:HIS:H	1.64	0.63
1:A:97:ILE:HD13	1:A:112:PRO:HA	1.81	0.63
1:A:151:SER:OG	1:A:195:SER:O	2.17	0.63
1:A:171:ARG:N	7:A:708:HOH:O	2.31	0.63
2:B:9:ASP:HA	2:B:54:ILE:HD13	1.80	0.63
2:B:143:PRO:HB2	2:B:144:TYR:CD2	2.34	0.63
2:E:33:ARG:HH12	2:E:41:SER:HB2	1.62	0.63
1:A:515:ILE:O	7:A:734:HOH:O	2.16	0.62
2:C:14:MET:HE3	2:C:163:TRP:CD1	2.34	0.62
1:D:157:THR:HG22	1:D:469:SER:HB3	1.81	0.62
1:A:101:SER:CB	1:A:546:LYS:HG2	2.29	0.62
1:A:108:PRO:HG2	1:A:552:LYS:HB3	1.81	0.62
1:A:451:ARG:NH2	7:A:738:HOH:O	2.19	0.62
2:E:54:ILE:HG22	2:E:56:VAL:HG23	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:THR:OG1	1:A:557:LYS:O	2.15	0.62
1:D:35:ILE:HD11	1:D:359:GLY:HA2	1.80	0.62
2:E:7:LEU:HD11	2:E:23:LEU:HD21	1.81	0.62
1:A:437:THR:HG22	1:A:440:ASP:HB2	1.81	0.62
1:A:110:PHE:CE1	1:A:556:ALA:HB2	2.34	0.62
1:A:442:GLN:HG2	1:A:462:PHE:CE1	2.35	0.62
1:A:503:ASP:OD1	1:A:504:ALA:N	2.33	0.62
2:B:44:LEU:N	7:B:433:HOH:O	2.30	0.62
1:D:132:ARG:O	1:D:136:PHE:N	2.27	0.62
1:D:280:LYS:HE2	1:D:293:ALA:HB1	1.80	0.62
1:D:441:LEU:HD23	1:D:549:ARG:HB3	1.81	0.62
2:C:85:PHE:HB3	2:C:92:ARG:HG2	1.80	0.62
1:D:99:LEU:HB3	1:D:557:LYS:CB	2.30	0.62
1:D:425:ARG:HD3	1:D:427:LEU:HD13	1.81	0.62
1:A:226:GLY:O	1:A:229:HIS:CD2	2.53	0.62
1:A:355:ILE:HG22	7:A:721:HOH:O	1.99	0.62
2:B:32:TYR:HD2	2:B:32:TYR:H	1.44	0.62
2:C:5:PRO:HB3	2:C:57:LEU:HD21	1.80	0.62
2:C:8:LEU:HB2	2:C:56:VAL:HG13	1.81	0.62
1:D:76:TYR:CD1	1:D:88:ILE:HD13	2.35	0.62
2:E:8:LEU:HD22	2:E:33:ARG:NH2	2.14	0.62
1:A:546:LYS:HZ2	1:A:547:MET:HA	1.64	0.62
1:D:77:ILE:HD13	1:D:110:PHE:O	2.00	0.62
1:A:214:ASP:HB2	1:A:215:GLN:HE21	1.65	0.61
2:B:129:ILE:HA	2:B:132:VAL:HG12	1.81	0.61
1:D:126:ARG:HA	1:D:182:ILE:HD13	1.82	0.61
1:D:152:LYS:NZ	1:D:527:THR:CG2	2.63	0.61
1:A:154:TYR:HE1	1:A:559:LEU:HD13	1.63	0.61
1:A:392:ILE:HG12	1:A:401:TYR:HB3	1.82	0.61
1:A:452:LEU:HD21	7:A:1090:HOH:O	1.99	0.61
2:B:195:VAL:HG23	2:B:199:LEU:HD13	1.81	0.61
2:C:14:MET:HE1	7:C:401:HOH:O	1.99	0.61
2:C:154:ASP:OD2	2:C:185:TRP:NE1	2.30	0.61
1:D:413:TYR:CD2	1:D:418:GLN:HG2	2.35	0.61
1:A:449:ALA:O	1:A:452:LEU:N	2.33	0.61
1:D:144:ALA:HA	1:D:216:VAL:HG13	1.82	0.61
2:E:66:GLU:HB2	2:E:69:ASN:HB2	1.81	0.61
1:A:168:ASN:ND2	4:A:602:ATP:O2A	2.33	0.61
2:B:75:ASP:HB2	2:B:84:PHE:CE2	2.35	0.61
1:A:198:VAL:HA	1:A:201:ALA:HB3	1.83	0.61
2:E:37:PHE:O	2:E:40:LYS:HE3	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:ARG:HA	7:A:712:HOH:O	2.00	0.61
2:E:8:LEU:HD13	2:E:44:LEU:HB2	1.83	0.61
1:A:226:GLY:O	1:A:229:HIS:HD2	1.83	0.61
2:C:169:LYS:HG3	2:C:170:PHE:N	2.16	0.61
2:E:161:SER:HB3	7:E:408:HOH:O	2.01	0.61
2:F:117:LYS:HD3	2:F:213:ARG:HH11	1.66	0.61
1:A:363:PHE:HD2	1:A:382:VAL:HG21	1.66	0.61
1:D:87:PRO:HB3	1:D:93:PRO:HD3	1.83	0.61
2:E:53:LYS:NZ	7:E:407:HOH:O	2.04	0.61
1:A:154:TYR:H	1:A:154:TYR:HD2	1.47	0.61
2:C:45:LEU:HG	7:C:447:HOH:O	2.00	0.61
2:B:69:ASN:ND2	2:B:73:TYR:OH	2.33	0.60
1:D:302:TYR:HD1	1:D:326:VAL:HG13	1.66	0.60
2:E:9:ASP:HA	2:E:54:ILE:CD1	2.31	0.60
2:E:11:TRP:CD1	2:E:12:PRO:HD3	2.35	0.60
1:A:223:PHE:HE1	1:A:304:ILE:HD12	1.66	0.60
1:D:48:CYS:SG	7:D:960:HOH:O	2.56	0.60
2:E:184:ALA:HA	2:E:187:LYS:NZ	2.16	0.60
1:D:98:SER:N	1:D:111:ILE:O	2.33	0.60
1:D:168:ASN:O	1:D:172:ASN:HB2	2.02	0.60
2:B:57:LEU:HB3	2:B:64:VAL:CG2	2.31	0.60
1:D:113:PHE:HB2	4:D:602:ATP:PB	2.42	0.60
1:A:369:THR:CG2	1:A:370:GLY:N	2.62	0.60
2:C:142:LYS:HE3	2:C:145:PHE:HA	1.83	0.60
1:D:46:GLN:O	7:D:734:HOH:O	2.17	0.60
1:D:376:PRO:O	7:D:735:HOH:O	2.17	0.60
2:E:17:MET:O	2:E:21:VAL:HG23	2.02	0.60
2:F:98:TRP:HB3	2:F:153:VAL:HG21	1.83	0.60
1:A:118:MET:SD	7:A:755:HOH:O	2.56	0.60
2:E:201:ASP:OD2	2:E:204:LYS:HE2	2.02	0.60
2:F:8:LEU:N	2:F:33:ARG:HH11	1.99	0.60
2:B:114:TRP:HD1	2:B:167:TYR:HE1	1.49	0.60
1:A:154:TYR:CE1	1:A:559:LEU:HB3	2.37	0.60
1:A:223:PHE:CE2	1:A:545:PHE:HZ	2.17	0.60
1:A:496:CYS:HB2	2:B:187:LYS:HZ3	1.64	0.60
1:A:501:PHE:HB2	1:A:506:TYR:CD2	2.36	0.60
2:B:8:LEU:HD22	2:B:33:ARG:HE	1.67	0.60
2:C:14:MET:HE1	2:C:163:TRP:HB2	1.84	0.60
1:D:238:TRP:HZ3	1:D:278:ARG:HA	1.67	0.60
2:B:166:ALA:HA	2:B:169:LYS:HG2	1.84	0.59
1:D:512:CYS:O	1:D:513:LYS:HB2	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4:LEU:O	7:B:416:HOH:O	2.15	0.59
2:B:34:GLU:OE2	7:B:417:HOH:O	2.16	0.59
6:B:301:GSH:N2	7:B:412:HOH:O	2.32	0.59
1:D:557:LYS:NZ	4:D:602:ATP:O1G	2.34	0.59
2:E:144:TYR:HE1	2:E:189:CYS:SG	2.25	0.59
2:B:64:VAL:HB	2:B:73:TYR:CD2	2.38	0.59
2:F:110:GLN:OE1	2:F:167:TYR:OH	2.10	0.59
1:A:132:ARG:HA	1:A:343:PRO:HG3	1.85	0.59
1:A:199:HIS:N	1:A:524:ALA:HB1	2.17	0.59
1:A:246:LYS:HD2	1:A:274:ALA:HB2	1.85	0.59
1:A:363:PHE:CD1	1:A:390:VAL:HA	2.38	0.59
2:F:56:VAL:HA	2:F:64:VAL:O	2.03	0.59
1:A:221:ALA:HB3	1:A:227:LEU:HG	1.84	0.59
1:A:451:ARG:NH1	1:A:454:GLU:OE2	2.36	0.59
1:D:498:ASP:OD2	1:D:510:ARG:NH1	2.34	0.59
1:A:199:HIS:H	1:A:524:ALA:HB1	1.67	0.59
1:A:363:PHE:HB3	1:A:388:TYR:HB3	1.84	0.59
1:A:25:HIS:NE2	1:A:380:THR:OG1	2.23	0.59
1:A:280:LYS:HE2	1:A:293:ALA:HB1	1.82	0.59
1:A:392:ILE:HD11	1:A:398:LEU:HD13	1.85	0.59
2:C:7:LEU:HD21	2:C:9:ASP:OD2	2.03	0.59
1:D:231:PHE:O	1:D:235:GLU:HG3	2.03	0.59
2:F:66:GLU:OE1	7:F:418:HOH:O	2.17	0.59
1:A:137:PRO:O	7:A:735:HOH:O	2.17	0.59
1:A:139:ASP:N	1:A:217:GLN:HE21	2.01	0.59
1:A:250:LEU:HD11	1:A:260:ARG:NH1	2.18	0.59
1:A:305:MET:HB3	1:A:347:PRO:HB3	1.85	0.59
2:C:144:TYR:HB2	1:D:41:SER:HB3	1.85	0.59
1:D:80:MET:HG3	1:D:88:ILE:HD11	1.85	0.59
1:D:107:ARG:NE	1:D:433:ILE:HG13	2.18	0.59
1:D:115:ASP:HA	1:D:118:MET:CE	2.33	0.59
2:F:159:THR:HA	2:F:199:LEU:HD21	1.85	0.59
2:B:204:LYS:NZ	7:B:419:HOH:O	2.19	0.58
2:E:9:ASP:HB2	2:E:20:ARG:NH2	2.18	0.58
2:E:114:TRP:O	7:E:420:HOH:O	2.17	0.58
2:F:21:VAL:HG13	2:F:194:SER:HB2	1.84	0.58
2:B:107:THR:HG22	2:B:160:PHE:CZ	2.38	0.58
1:A:223:PHE:CZ	1:A:536:LEU:HB3	2.39	0.58
1:A:448:ALA:HB2	1:A:496:CYS:HB3	1.86	0.58
1:D:465:TYR:HD1	1:D:551:VAL:HG23	1.68	0.58
2:E:69:ASN:ND2	2:E:73:TYR:OH	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:125:LYS:HA	2:E:128:PHE:CD2	2.39	0.58
2:F:139:LEU:HD22	2:F:142:LYS:HD3	1.85	0.58
1:A:35:ILE:HA	1:A:395:TYR:CE1	2.38	0.58
1:A:250:LEU:HD11	1:A:260:ARG:CZ	2.34	0.58
1:A:456:LYS:HG3	2:B:201:ASP:OD2	2.03	0.58
1:D:99:LEU:HB2	1:D:556:ALA:H	1.68	0.58
1:D:138:ILE:HD13	1:D:217:GLN:HE22	1.68	0.58
1:A:154:TYR:CE2	1:A:560:GLN:HA	2.38	0.58
1:A:425:ARG:HD2	1:A:427:LEU:HB2	1.84	0.58
1:D:339:ALA:N	1:D:353:ALA:O	2.25	0.58
1:D:489:VAL:HA	1:D:492:ASP:OD2	2.04	0.58
1:D:499:ARG:HD2	2:E:188:ARG:CZ	2.34	0.58
2:E:48:ASN:HB2	7:E:440:HOH:O	2.03	0.58
2:E:143:PRO:HB2	7:E:451:HOH:O	2.03	0.58
2:F:125:LYS:NZ	7:F:420:HOH:O	2.18	0.58
2:E:130:GLU:O	2:E:134:ILE:HG22	2.03	0.58
1:A:154:TYR:CZ	1:A:559:LEU:HB3	2.39	0.58
1:A:246:LYS:NZ	1:A:271:PRO:HA	2.18	0.58
1:D:98:SER:OG	4:D:602:ATP:O3B	2.08	0.58
1:D:110:PHE:CE1	1:D:556:ALA:HB2	2.39	0.58
1:D:449:ALA:HB1	1:D:459:VAL:HG21	1.86	0.58
1:D:532:GLN:HA	1:D:535:PHE:CD2	2.39	0.58
1:A:434:ASP:OD2	7:A:712:HOH:O	2.17	0.58
1:D:109:LYS:HG3	7:D:718:HOH:O	2.04	0.58
2:B:37:PHE:O	2:B:40:LYS:NZ	2.34	0.58
2:C:14:MET:HE1	2:C:163:TRP:CG	2.38	0.58
1:D:124:LEU:HD23	1:D:336:TRP:CE3	2.39	0.58
1:D:154:TYR:HB2	1:D:563:CYS:HB2	1.86	0.58
1:D:267:LEU:HG	7:D:883:HOH:O	2.03	0.58
1:D:532:GLN:HA	1:D:535:PHE:HD2	1.68	0.58
2:E:64:VAL:HG23	2:E:70:VAL:HG22	1.85	0.58
2:E:89:PRO:HB3	2:F:73:TYR:CD1	2.38	0.58
2:E:191:GLU:O	7:E:418:HOH:O	2.17	0.58
1:A:143:LYS:HA	1:A:184:SER:HB3	1.86	0.58
1:A:164:THR:HA	1:A:557:LYS:HG3	1.85	0.58
1:A:450:LYS:HZ1	2:B:191:GLU:CB	2.17	0.58
2:C:40:LYS:HE3	2:C:52:LYS:HD3	1.86	0.58
2:C:191:GLU:HG2	7:C:404:HOH:O	2.03	0.58
1:A:364:LEU:HB2	1:A:389:GLU:HG2	1.86	0.57
1:D:31:THR:OG1	1:D:357:ASN:OD1	2.22	0.57
1:D:108:PRO:HG2	1:D:552:LYS:N	2.10	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:SER:HB3	1:A:170:TYR:HD2	1.68	0.57
1:A:165:ALA:HB1	4:A:602:ATP:C2	2.39	0.57
1:A:223:PHE:CG	1:A:533:GLU:HG2	2.38	0.57
2:E:145:PHE:HB3	2:E:153:VAL:HG13	1.86	0.57
2:E:215:ASN:O	7:E:421:HOH:O	2.17	0.57
1:A:473:GLY:O	1:A:516:GLY:N	2.29	0.57
1:D:531:ILE:HA	1:D:534:HIS:ND1	2.19	0.57
1:D:535:PHE:HE1	1:D:536:LEU:HD13	1.68	0.57
2:E:69:ASN:ND2	2:F:100:ASP:OD2	2.37	0.57
1:D:212:PHE:O	1:D:216:VAL:HG23	2.04	0.57
1:D:224:ALA:HA	1:D:227:LEU:HD12	1.85	0.57
1:D:363:PHE:HD1	1:D:390:VAL:HA	1.69	0.57
1:D:559:LEU:HA	1:D:562:LEU:HD23	1.86	0.57
2:E:37:PHE:CE1	6:E:301:GSH:HA32	2.38	0.57
2:E:184:ALA:CA	2:E:187:LYS:NZ	2.68	0.57
1:A:446:GLU:O	1:A:450:LYS:HE2	2.04	0.57
1:D:152:LYS:HB2	1:D:561:ILE:HA	1.86	0.57
2:E:90:TYR:HB2	2:F:62:LYS:HB3	1.86	0.57
2:F:110:GLN:HB2	2:F:167:TYR:CZ	2.40	0.57
1:A:101:SER:HB2	1:A:546:LYS:CG	2.34	0.57
1:A:142:GLY:O	1:A:185:PRO:HD2	2.05	0.57
1:A:236:GLN:NE2	7:A:791:HOH:O	2.36	0.57
1:A:411:GLY:N	1:A:418:GLN:HG2	2.20	0.57
2:B:163:TRP:HB3	2:B:167:TYR:CZ	2.39	0.57
2:C:94:GLN:OE1	7:C:415:HOH:O	2.16	0.57
1:D:514:THR:O	7:D:736:HOH:O	2.17	0.57
2:E:125:LYS:HA	2:E:128:PHE:CE2	2.40	0.57
1:A:302:TYR:O	7:A:736:HOH:O	2.17	0.57
1:A:439:ARG:O	1:A:443:LEU:HB2	2.04	0.57
1:D:499:ARG:HH11	2:E:143:PRO:HA	1.70	0.57
1:A:521:ARG:HA	1:A:569:SER:HA	1.87	0.57
1:D:150:SER:O	1:D:150:SER:OG	2.16	0.57
1:D:462:PHE:CE1	1:D:549:ARG:HD2	2.40	0.57
2:F:8:LEU:HB2	2:F:56:VAL:HB	1.86	0.57
1:A:132:ARG:NH1	1:A:300:TYR:OH	2.38	0.57
2:C:124:GLY:HA2	2:C:127:GLU:OE1	2.05	0.57
1:A:149:PHE:HD2	1:A:198:VAL:HG22	1.70	0.56
2:B:18:ARG:NH2	7:B:408:HOH:O	2.37	0.56
2:B:131:ALA:HB2	7:B:478:HOH:O	2.04	0.56
2:B:171:GLY:O	2:B:173:PHE:HD1	1.88	0.56
1:D:179:MET:O	1:D:183:THR:OG1	2.23	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:199:HIS:N	1:D:524:ALA:HB1	2.20	0.56
1:A:133:ASN:OD1	1:A:138:ILE:N	2.36	0.56
1:A:403:LEU:HD21	1:A:538:LEU:HD11	1.86	0.56
2:B:161:SER:N	7:B:401:HOH:O	2.37	0.56
1:D:212:PHE:N	1:D:212:PHE:HD1	2.03	0.56
1:D:299:LYS:HG2	7:D:832:HOH:O	2.03	0.56
2:F:7:LEU:O	2:F:33:ARG:HG3	2.05	0.56
1:A:107:ARG:HG2	7:A:741:HOH:O	2.05	0.56
1:A:117:LEU:HD11	1:A:396:ALA:HB2	1.88	0.56
1:A:139:ASP:H	1:A:217:GLN:HE21	1.51	0.56
1:A:152:LYS:HE2	1:A:565:ASN:ND2	2.19	0.56
1:A:169:VAL:HG22	4:A:602:ATP:H2'	1.87	0.56
1:A:242:VAL:HG22	1:A:277:ILE:HD13	1.86	0.56
1:A:379:LEU:HD12	1:A:380:THR:HG23	1.85	0.56
1:A:451:ARG:HD3	2:B:187:LYS:HG2	1.86	0.56
1:A:557:LYS:HZ2	4:A:602:ATP:PG	2.27	0.56
1:D:415:ASN:ND2	7:D:732:HOH:O	2.16	0.56
1:D:464:SER:O	1:D:551:VAL:N	2.37	0.56
1:D:526:GLY:O	1:D:530:LYS:HG3	2.03	0.56
2:E:10:TYR:CD2	2:E:12:PRO:HD2	2.40	0.56
2:F:64:VAL:HG21	2:F:73:TYR:CD2	2.40	0.56
1:A:140:ASP:O	7:A:737:HOH:O	2.17	0.56
1:A:360:TYR:N	1:A:393:THR:O	2.30	0.56
2:C:14:MET:CE	2:C:163:TRP:CD1	2.88	0.56
2:C:139:LEU:HD22	1:D:92:HIS:CE1	2.40	0.56
1:D:97:ILE:HG13	1:D:111:ILE:C	2.26	0.56
1:A:193:ILE:HG12	1:A:205:HIS:CE1	2.40	0.56
1:A:425:ARG:HE	1:A:427:LEU:HD12	1.70	0.56
2:E:67:SER:N	6:E:301:GSH:HN11	1.98	0.56
2:E:88:ASP:OD1	2:E:89:PRO:HD2	2.05	0.56
2:E:90:TYR:CE1	2:F:63:PRO:HG2	2.41	0.56
2:F:195:VAL:HG13	2:F:199:LEU:HD22	1.86	0.56
1:A:149:PHE:CE2	1:A:205:HIS:HD2	2.24	0.56
1:A:302:TYR:OH	1:A:328:HIS:ND1	2.21	0.56
2:C:163:TRP:CD1	2:C:205:ILE:HG21	2.40	0.56
1:D:339:ALA:HB2	1:D:355:ILE:HD11	1.87	0.56
2:F:51:HIS:HB3	2:F:53:LYS:HD2	1.87	0.56
1:A:152:LYS:HB2	1:A:561:ILE:HA	1.88	0.56
1:A:363:PHE:HD1	1:A:390:VAL:HA	1.71	0.56
1:A:425:ARG:CZ	1:A:546:LYS:HA	2.33	0.56
2:B:64:VAL:HB	2:B:73:TYR:CE2	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:444:SER:HA	1:D:500:ALA:CB	2.35	0.56
2:F:108:ASP:OD1	7:F:419:HOH:O	2.17	0.56
1:A:76:TYR:O	1:A:88:ILE:HD13	2.05	0.56
1:A:132:ARG:HD3	1:A:326:VAL:HG21	1.88	0.56
1:A:142:GLY:HA3	7:A:745:HOH:O	2.05	0.56
1:A:513:LYS:HZ2	1:A:575:PHE:HB3	1.71	0.56
1:A:529:ARG:NH1	1:A:533:GLU:CD	2.58	0.56
2:B:194:SER:N	7:B:431:HOH:O	2.28	0.56
1:D:104:SER:O	1:D:107:ARG:HB2	2.06	0.56
1:D:288:TYR:O	7:D:737:HOH:O	2.17	0.56
1:D:499:ARG:HD3	2:E:188:ARG:HD2	1.87	0.56
1:A:152:LYS:O	1:A:167:THR:HG21	2.06	0.56
1:A:226:GLY:HA3	1:A:529:ARG:HH11	1.71	0.56
1:A:498:ASP:C	1:A:510:ARG:HH22	2.06	0.56
1:D:220:PHE:HB3	7:D:936:HOH:O	2.05	0.56
1:D:421:PHE:CD2	1:D:541:SER:HA	2.41	0.56
1:A:99:LEU:H	1:A:557:LYS:HB2	1.70	0.56
1:A:499:ARG:NH2	2:B:184:ALA:O	2.39	0.56
2:E:9:ASP:OD2	2:E:34:GLU:OE2	2.24	0.56
2:C:188:ARG:HB2	1:D:86:SER:HB2	1.87	0.55
1:D:95:PRO:O	1:D:161:PRO:HB2	2.06	0.55
2:E:101:PHE:CZ	2:F:50:ILE:HG12	2.42	0.55
1:A:105:GLN:OE1	1:A:107:ARG:NH2	2.39	0.55
1:D:217:GLN:HG3	1:D:218:TYR:CD1	2.42	0.55
1:D:513:LYS:HG3	7:D:809:HOH:O	2.06	0.55
2:E:37:PHE:HE2	6:E:301:GSH:HSG	1.54	0.55
2:E:158:ILE:HD13	2:E:189:CYS:HB2	1.87	0.55
1:A:138:ILE:HB	1:A:217:GLN:HG3	1.89	0.55
1:A:526:GLY:O	1:A:530:LYS:HG3	2.06	0.55
1:D:331:GLY:N	1:D:537:GLY:O	2.40	0.55
2:E:97:PHE:HA	2:F:66:GLU:OE2	2.06	0.55
1:A:405:ASP:HB2	1:A:541:SER:HB3	1.89	0.55
2:C:121:GLN:O	2:C:125:LYS:HG3	2.06	0.55
1:D:101:SER:OG	1:D:544:GLN:O	2.24	0.55
1:D:369:THR:HG23	1:D:370:GLY:H	1.71	0.55
1:D:385:GLY:HA2	1:D:408:LYS:HE3	1.87	0.55
1:D:551:VAL:HG11	1:D:558:VAL:HG11	1.86	0.55
1:A:43:ILE:HD11	1:A:88:ILE:HG23	1.87	0.55
2:B:114:TRP:HA	2:B:170:PHE:HD2	1.71	0.55
1:D:76:TYR:O	1:D:79:ARG:HB2	2.06	0.55
1:A:447:SER:HA	1:A:450:LYS:HE2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:25:HIS:CE1	1:D:380:THR:HG1	2.25	0.55
1:D:152:LYS:NZ	1:D:527:THR:HG21	2.21	0.55
1:D:403:LEU:HD23	1:D:540:SER:OG	2.07	0.55
1:A:208:SER:HA	1:A:211:LEU:HG	1.88	0.55
2:B:43:LEU:HG	7:B:433:HOH:O	2.07	0.55
2:B:98:TRP:CZ2	2:B:135:LEU:HD21	2.41	0.55
2:B:107:THR:HG22	2:B:160:PHE:HZ	1.72	0.55
2:B:139:LEU:O	2:B:141:ASP:N	2.39	0.55
1:D:168:ASN:ND2	4:D:602:ATP:O2A	2.40	0.55
1:D:184:SER:HB3	1:D:217:GLN:NE2	2.22	0.55
1:D:492:ASP:OD1	1:D:492:ASP:N	2.38	0.55
2:E:170:PHE:CD2	2:E:213:ARG:HD2	2.42	0.55
1:D:99:LEU:CB	1:D:557:LYS:H	2.19	0.55
1:D:109:LYS:NZ	1:D:334:GLU:OE2	2.39	0.55
1:D:213:ARG:HH21	1:D:296:PRO:HD3	1.71	0.55
1:D:440:ASP:OD2	1:D:502:ILE:HG13	2.07	0.55
2:F:129:ILE:O	2:F:132:VAL:HG12	2.06	0.55
2:F:162:SER:HB2	2:F:205:ILE:HD13	1.89	0.55
2:F:169:LYS:HG3	2:F:170:PHE:N	2.22	0.55
1:A:363:PHE:O	1:A:365:PRO:HD3	2.07	0.55
1:A:425:ARG:HH12	1:A:546:LYS:CB	2.19	0.55
2:C:125:LYS:HB3	2:C:173:PHE:HE2	1.71	0.55
1:D:135:ASP:HB2	7:D:901:HOH:O	2.07	0.55
1:A:61:PHE:O	1:A:65:VAL:HG12	2.07	0.55
1:D:25:HIS:NE2	1:D:380:THR:OG1	2.40	0.55
1:D:222:VAL:HB	1:D:533:GLU:HB3	1.89	0.55
2:E:185:TRP:O	2:E:188:ARG:HB3	2.07	0.55
2:F:102:VAL:HA	2:F:106:PHE:HB3	1.88	0.55
1:A:333:SER:HB3	4:A:602:ATP:O1A	2.06	0.54
1:D:111:ILE:HG12	7:D:718:HOH:O	2.06	0.54
2:E:117:LYS:N	7:E:442:HOH:O	2.39	0.54
2:F:139:LEU:HB3	2:F:142:LYS:HG2	1.89	0.54
2:F:200:PRO:O	7:F:421:HOH:O	2.18	0.54
1:A:68:VAL:HG13	1:A:401:TYR:HD1	1.72	0.54
1:A:337:ILE:HA	1:A:358:LEU:HD22	1.89	0.54
1:D:113:PHE:HD1	1:D:117:LEU:HD12	1.73	0.54
1:D:386:GLU:N	7:D:731:HOH:O	2.39	0.54
1:D:545:PHE:N	7:D:799:HOH:O	2.40	0.54
1:A:97:ILE:H	1:A:163:GLY:N	2.05	0.54
2:B:73:TYR:HA	2:B:76:GLU:OE2	2.07	0.54
2:C:49:PRO:HA	7:C:447:HOH:O	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:169:VAL:O	1:D:175:PHE:HB2	2.08	0.54
2:C:145:PHE:HB3	2:C:153:VAL:HB	1.90	0.54
1:D:520:LEU:CD1	1:D:522:VAL:HG23	2.37	0.54
2:E:71:VAL:HG23	2:E:152:TYR:CE1	2.42	0.54
2:F:123:ALA:HB3	7:F:440:HOH:O	2.07	0.54
2:F:142:LYS:HG3	2:F:144:TYR:O	2.07	0.54
1:A:365:PRO:HB2	7:A:774:HOH:O	2.08	0.54
2:B:138:GLU:HG3	2:B:145:PHE:HE1	1.71	0.54
1:D:212:PHE:N	1:D:212:PHE:CD1	2.75	0.54
1:D:290:LEU:O	1:D:294:LEU:HG	2.07	0.54
2:E:102:VAL:O	2:E:107:THR:HG23	2.08	0.54
2:F:6:ILE:HB	2:F:33:ARG:NH2	2.23	0.54
2:F:57:LEU:O	2:F:63:PRO:HA	2.08	0.54
2:B:108:ASP:O	2:B:112:LYS:HG2	2.08	0.54
1:D:29:LYS:O	1:D:33:LYS:HG2	2.06	0.54
1:D:143:LYS:O	1:D:216:VAL:HA	2.07	0.54
2:E:14:MET:H	2:E:14:MET:HE2	1.72	0.54
2:E:72:GLN:NE2	7:E:445:HOH:O	2.40	0.54
2:B:169:LYS:HG3	2:B:170:PHE:H	1.73	0.54
2:C:168:GLU:HA	2:C:173:PHE:O	2.08	0.54
2:E:88:ASP:O	2:E:92:ARG:HG3	2.08	0.54
1:A:136:PHE:CD2	1:A:300:TYR:HB3	2.41	0.54
2:B:75:ASP:OD2	7:B:418:HOH:O	2.18	0.54
2:C:142:LYS:HB2	1:D:39:ASN:HA	1.90	0.54
1:D:76:TYR:O	1:D:88:ILE:HG12	2.08	0.54
1:D:306:THR:OG1	7:D:740:HOH:O	2.19	0.54
1:D:552:LYS:C	1:D:554:SER:H	2.10	0.54
1:A:124:LEU:HD12	1:A:336:TRP:CE3	2.42	0.54
1:A:492:ASP:HB3	2:B:187:LYS:HD3	1.89	0.54
2:C:121:GLN:NE2	2:C:170:PHE:O	2.41	0.54
1:D:20:MET:CE	1:D:357:ASN:HB2	2.38	0.54
1:D:118:MET:CE	7:D:707:HOH:O	2.54	0.54
1:D:124:LEU:HD11	1:D:355:ILE:HG12	1.90	0.54
1:D:492:ASP:OD1	2:E:187:LYS:HD2	2.08	0.54
1:D:556:ALA:N	7:D:702:HOH:O	2.41	0.54
2:F:169:LYS:HG3	2:F:170:PHE:H	1.71	0.54
1:D:226:GLY:HA2	1:D:529:ARG:HD2	1.90	0.54
1:D:332:SER:CB	1:D:538:LEU:HA	2.37	0.54
1:D:361:PHE:CE2	1:D:392:ILE:HG23	2.42	0.54
1:A:32:LEU:HA	1:A:35:ILE:HG12	1.89	0.53
1:A:546:LYS:NZ	1:A:547:MET:HA	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:190:MET:O	2:B:196:SER:HB2	2.08	0.53
1:D:331:GLY:HA3	1:D:336:TRP:CE3	2.43	0.53
2:F:5:PRO:HA	2:F:58:VAL:O	2.08	0.53
2:F:122:GLU:HG3	2:F:123:ALA:N	2.23	0.53
1:A:534:HIS:CE1	1:A:557:LYS:HD3	2.43	0.53
2:B:169:LYS:HG3	2:B:170:PHE:N	2.23	0.53
1:D:207:LEU:O	1:D:211:LEU:HG	2.09	0.53
2:E:21:VAL:HG13	2:E:195:VAL:HG23	1.90	0.53
2:E:33:ARG:HH22	2:E:41:SER:HB2	1.73	0.53
2:E:36:ASP:O	2:E:39:ASN:N	2.32	0.53
2:F:144:TYR:HB3	2:F:154:ASP:OD2	2.08	0.53
1:A:77:ILE:HG13	1:A:89:LEU:HD12	1.89	0.53
1:A:122:LEU:HD11	1:A:174:ASN:HD22	1.73	0.53
1:A:172:ASN:ND2	7:A:795:HOH:O	2.38	0.53
2:B:64:VAL:HG23	2:B:70:VAL:HG22	1.89	0.53
2:B:122:GLU:HA	2:B:125:LYS:HE2	1.90	0.53
1:D:132:ARG:HA	1:D:343:PRO:CG	2.38	0.53
1:D:363:PHE:CD1	1:D:390:VAL:HA	2.43	0.53
1:A:360:TYR:HB3	1:A:393:THR:HB	1.91	0.53
1:A:549:ARG:NH2	7:A:799:HOH:O	2.40	0.53
1:A:566:VAL:CG1	1:A:569:SER:HB2	2.39	0.53
2:B:92:ARG:NH2	2:C:76:GLU:OE1	2.42	0.53
1:A:70:ASP:HB2	1:A:104:SER:HB2	1.91	0.53
1:A:223:PHE:CE2	1:A:533:GLU:HA	2.43	0.53
1:A:466:ILE:O	1:A:466:ILE:HG13	2.07	0.53
2:C:143:PRO:HG2	1:D:42:ALA:HA	1.90	0.53
2:E:112:LYS:HB2	2:E:124:GLY:HA3	1.89	0.53
2:F:119:GLU:HA	2:F:122:GLU:HG2	1.91	0.53
1:A:98:SER:OG	1:A:111:ILE:O	2.26	0.53
2:C:10:TYR:O	2:C:20:ARG:NH2	2.42	0.53
1:D:70:ASP:HA	1:D:73:LEU:HG	1.90	0.53
1:D:76:TYR:CE2	1:D:89:LEU:HD13	2.42	0.53
1:D:486:ASN:O	1:D:489:VAL:HG22	2.09	0.53
1:D:498:ASP:CG	1:D:510:ARG:HH22	2.12	0.53
2:E:21:VAL:HG22	2:E:195:VAL:HG22	1.91	0.53
2:E:96:ARG:HH12	2:F:68:LEU:HB2	1.74	0.53
1:A:226:GLY:CA	1:A:529:ARG:NH1	2.68	0.53
2:C:188:ARG:NH2	1:D:86:SER:OG	2.36	0.53
1:D:135:ASP:OD2	1:D:343:PRO:HD2	2.08	0.53
1:D:200:GLN:O	1:D:203:TYR:HB3	2.09	0.53
2:E:9:ASP:N	7:E:414:HOH:O	2.22	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:17:MET:SD	2:F:199:LEU:HG	2.49	0.53
1:A:472:PRO:HG2	1:A:516:GLY:HA2	1.91	0.53
2:B:76:GLU:O	7:B:420:HOH:O	2.19	0.53
1:D:462:PHE:HB3	7:D:727:HOH:O	2.09	0.53
2:E:102:VAL:O	2:E:106:PHE:HB3	2.09	0.53
2:B:92:ARG:O	2:B:96:ARG:HG3	2.09	0.53
1:D:81:VAL:HG21	1:D:97:ILE:HG21	1.90	0.53
1:D:134:ARG:O	7:D:741:HOH:O	2.19	0.53
1:D:152:LYS:HZ2	1:D:527:THR:CG2	2.21	0.53
1:D:153:GLN:HG3	1:D:171:ARG:HD2	1.91	0.53
1:D:165:ALA:O	1:D:169:VAL:HG23	2.09	0.53
1:D:266:LEU:HB2	7:D:883:HOH:O	2.09	0.53
2:F:93:ALA:HA	2:F:96:ARG:CZ	2.39	0.53
1:A:213:ARG:NH1	7:A:804:HOH:O	2.41	0.53
1:D:164:THR:HG21	1:D:561:ILE:HD12	1.91	0.53
2:E:150:PHE:CE2	2:E:189:CYS:HB3	2.44	0.53
1:A:305:MET:CB	1:A:347:PRO:HB3	2.38	0.52
1:A:432:ASN:HB2	7:A:935:HOH:O	2.08	0.52
1:A:477:ILE:HG21	1:A:497:LEU:HD22	1.89	0.52
1:D:115:ASP:O	1:D:118:MET:HE3	2.09	0.52
1:D:522:VAL:O	1:D:567:VAL:HG22	2.08	0.52
2:F:33:ARG:HH21	2:F:43:LEU:HD23	1.74	0.52
2:F:139:LEU:HD11	2:F:145:PHE:CZ	2.44	0.52
1:A:217:GLN:CD	1:A:299:LYS:HZ1	2.12	0.52
1:A:445:VAL:HG22	1:A:479:TRP:HE1	1.74	0.52
1:D:20:MET:HE3	1:D:357:ASN:HB2	1.89	0.52
1:D:282:MET:O	7:D:743:HOH:O	2.19	0.52
1:D:439:ARG:O	1:D:443:LEU:HB2	2.09	0.52
1:D:520:LEU:HD12	1:D:522:VAL:HG23	1.90	0.52
1:D:575:PHE:O	7:D:744:HOH:O	2.19	0.52
1:A:299:LYS:NZ	7:A:735:HOH:O	2.42	0.52
1:A:441:LEU:HG	7:A:947:HOH:O	2.09	0.52
2:B:68:LEU:HD12	2:B:72:GLN:HE21	1.75	0.52
1:D:88:ILE:CD1	1:D:89:LEU:H	2.22	0.52
1:D:329:ASP:HA	1:D:352:PHE:CD2	2.45	0.52
2:E:135:LEU:HB3	2:E:182:LEU:HD12	1.92	0.52
1:A:111:ILE:HG23	1:A:396:ALA:O	2.09	0.52
1:A:420:LYS:HA	7:A:723:HOH:O	2.09	0.52
1:A:452:LEU:HB3	1:A:457:ILE:HD11	1.90	0.52
1:A:523:VAL:HG12	1:A:565:ASN:O	2.09	0.52
2:B:23:LEU:HD11	2:B:57:LEU:HD13	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:184:ALA:HB1	1:D:85:THR:O	2.10	0.52
1:D:153:GLN:HA	1:D:560:GLN:HG3	1.92	0.52
1:D:300:TYR:HB2	1:D:326:VAL:HG12	1.91	0.52
2:F:158:ILE:HG12	2:F:195:VAL:HG21	1.92	0.52
1:A:35:ILE:HA	1:A:395:TYR:HE1	1.75	0.52
1:A:329:ASP:N	1:A:329:ASP:OD1	2.40	0.52
2:B:7:LEU:HD13	2:B:30:PHE:HD2	1.73	0.52
2:B:98:TRP:O	2:B:102:VAL:HG23	2.10	0.52
2:C:117:LYS:NZ	7:C:423:HOH:O	2.22	0.52
2:C:168:GLU:OE2	2:C:174:SER:HA	2.09	0.52
1:D:35:ILE:HD13	1:D:394:ASN:HA	1.91	0.52
1:D:217:GLN:HG3	1:D:218:TYR:HD1	1.72	0.52
1:D:437:THR:HG21	1:D:439:ARG:HH21	1.72	0.52
2:E:54:ILE:HD12	2:E:55:PRO:HD3	1.91	0.52
1:A:478:PHE:CE1	1:A:562:LEU:HD13	2.45	0.52
2:C:17:MET:HB2	2:C:159:THR:HB	1.92	0.52
2:E:84:PHE:HB2	2:E:152:TYR:N	2.25	0.52
2:E:114:TRP:HD1	2:E:167:TYR:HE1	1.55	0.52
2:F:139:LEU:HD21	2:F:145:PHE:CE2	2.44	0.52
1:A:25:HIS:HA	1:A:28:GLN:HG2	1.91	0.52
1:A:107:ARG:HD3	1:A:433:ILE:HG13	1.92	0.52
1:A:534:HIS:HE1	1:A:535:PHE:CE2	2.28	0.52
1:D:163:GLY:HA2	1:D:560:GLN:HB2	1.90	0.52
1:D:199:HIS:HB2	1:D:525:LYS:HE3	1.91	0.52
1:D:464:SER:HA	7:D:780:HOH:O	2.09	0.52
2:F:148:ASP:OD1	2:F:148:ASP:N	2.42	0.52
1:A:77:ILE:HA	1:A:80:MET:HG3	1.91	0.52
1:A:143:LYS:HD3	1:A:187:CYS:HB3	1.92	0.52
1:A:153:GLN:H	1:A:564:GLU:HB2	1.74	0.52
1:A:164:THR:N	1:A:560:GLN:OE1	2.42	0.52
1:A:296:PRO:HD2	7:A:804:HOH:O	2.10	0.52
1:A:531:ILE:HA	1:A:534:HIS:CE1	2.44	0.52
2:F:77:ALA:O	7:F:423:HOH:O	2.19	0.52
2:F:125:LYS:HB3	2:F:173:PHE:HE2	1.75	0.52
1:A:152:LYS:HD3	1:A:561:ILE:HA	1.90	0.52
1:A:329:ASP:HB3	1:A:338:ALA:O	2.10	0.52
2:B:124:GLY:HA2	2:B:127:GLU:HB2	1.91	0.52
2:C:90:TYR:O	2:C:93:ALA:HB3	2.10	0.52
1:D:143:LYS:O	1:D:217:GLN:HG2	2.10	0.52
1:D:435:LYS:NZ	1:D:549:ARG:HB2	2.25	0.52
1:D:529:ARG:NH1	1:D:533:GLU:OE2	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:54:ILE:HD12	2:E:55:PRO:CD	2.40	0.52
2:F:25:GLU:HG3	7:F:489:HOH:O	2.08	0.52
1:A:76:TYR:HD2	1:A:88:ILE:HG21	1.75	0.52
1:A:152:LYS:HD3	1:A:561:ILE:HG23	1.92	0.52
1:A:450:LYS:NZ	2:B:191:GLU:CB	2.73	0.52
2:B:129:ILE:O	2:B:133:LYS:HB2	2.10	0.52
2:C:142:LYS:CA	1:D:91:GLY:HA3	2.40	0.52
1:D:17:PHE:CD1	1:D:127:THR:HG21	2.45	0.52
1:D:301:VAL:HG13	1:D:325:LEU:HA	1.92	0.52
1:D:493:CYS:SG	1:D:520:LEU:HD22	2.50	0.52
1:D:535:PHE:CE1	1:D:536:LEU:HD13	2.44	0.52
1:A:169:VAL:O	1:A:175:PHE:HB2	2.10	0.51
2:B:106:PHE:HD2	2:B:131:ALA:HB1	1.75	0.51
2:C:148:ASP:N	2:C:148:ASP:OD1	2.43	0.51
1:D:98:SER:H	1:D:111:ILE:H	1.57	0.51
1:D:152:LYS:HA	1:D:564:GLU:CB	2.36	0.51
1:A:295:PHE:HD1	1:A:298:ALA:HB2	1.75	0.51
2:B:69:ASN:ND2	2:C:97:PHE:HB3	2.25	0.51
2:C:139:LEU:O	2:C:141:ASP:N	2.43	0.51
1:D:65:VAL:N	7:D:753:HOH:O	2.31	0.51
1:D:238:TRP:CZ3	1:D:278:ARG:HA	2.45	0.51
1:A:285:SER:HB3	7:A:817:HOH:O	2.09	0.51
1:A:450:LYS:NZ	2:B:191:GLU:CA	2.74	0.51
2:C:14:MET:CE	2:C:160:PHE:HA	2.38	0.51
2:C:54:ILE:HB	2:C:55:PRO:HA	1.92	0.51
2:C:101:PHE:CE2	2:C:135:LEU:HG	2.38	0.51
1:D:212:PHE:HB3	1:D:215:GLN:NE2	2.26	0.51
1:D:480:GLU:HB2	1:D:528:PHE:CD1	2.45	0.51
1:A:199:HIS:HA	1:A:525:LYS:HB2	1.92	0.51
1:D:99:LEU:HD22	1:D:557:LYS:HB3	1.92	0.51
1:D:342:THR:OG1	1:D:413:TYR:OH	2.14	0.51
2:F:8:LEU:HD22	2:F:44:LEU:HB2	1.93	0.51
1:A:108:PRO:HB3	1:A:555:ASN:N	2.25	0.51
1:A:169:VAL:HB	1:A:170:TYR:CD1	2.45	0.51
1:A:333:SER:OG	4:A:602:ATP:O1G	2.11	0.51
2:B:130:GLU:O	2:B:134:ILE:HG22	2.11	0.51
2:C:7:LEU:HD23	2:C:32:TYR:HD1	1.75	0.51
2:C:81:LYS:O	7:C:417:HOH:O	2.18	0.51
2:C:191:GLU:N	7:C:404:HOH:O	2.40	0.51
1:D:94:VAL:HG11	1:D:112:PRO:CB	2.39	0.51
1:A:71:VAL:HG21	1:A:105:GLN:HG3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:TYR:CE1	1:A:559:LEU:HD13	2.44	0.51
1:A:187:CYS:O	1:A:208:SER:HB3	2.11	0.51
1:D:96:ALA:HB1	1:D:163:GLY:N	2.24	0.51
1:D:336:TRP:CZ2	4:D:602:ATP:C8	2.99	0.51
1:D:365:PRO:HB2	7:D:839:HOH:O	2.11	0.51
2:E:32:TYR:CD1	2:E:34:GLU:OE2	2.63	0.51
2:F:101:PHE:HZ	2:F:131:ALA:HB1	1.76	0.51
1:A:104:SER:N	1:A:107:ARG:O	2.33	0.51
1:A:272:GLU:O	1:A:275:GLU:HG2	2.11	0.51
2:B:98:TRP:CD2	2:B:138:GLU:OE2	2.63	0.51
1:D:69:THR:OG1	1:D:72:GLU:OE1	2.25	0.51
1:D:76:TYR:HD1	1:D:88:ILE:HD13	1.75	0.51
2:E:97:PHE:CD2	2:F:51:HIS:HD2	2.29	0.51
7:E:401:HOH:O	2:F:62:LYS:NZ	2.40	0.51
1:A:98:SER:CB	1:A:111:ILE:HB	2.39	0.51
1:A:392:ILE:CD1	1:A:398:LEU:HD13	2.40	0.51
1:D:43:ILE:HG13	1:D:44:TYR:HD1	1.76	0.51
1:D:44:TYR:HB2	7:D:884:HOH:O	2.11	0.51
1:D:77:ILE:HB	1:D:110:PHE:HB3	1.93	0.51
1:D:150:SER:HB3	1:D:170:TYR:HD2	1.75	0.51
1:D:152:LYS:O	1:D:167:THR:HG21	2.10	0.51
1:D:244:ASP:OD2	1:D:251:SER:HB2	2.11	0.51
2:E:71:VAL:HB	7:E:540:HOH:O	2.11	0.51
1:A:17:PHE:CD1	1:A:127:THR:HG21	2.46	0.51
1:A:48:CYS:HB2	1:A:50:LEU:HD13	1.93	0.51
2:B:205:ILE:HG12	7:B:518:HOH:O	2.10	0.51
1:D:103:THR:HG22	1:D:548:PRO:HB3	1.93	0.51
1:D:143:LYS:HZ2	1:D:187:CYS:HA	1.76	0.51
1:D:163:GLY:CA	1:D:168:ASN:HD21	2.23	0.51
1:D:197:ASP:N	1:D:197:ASP:OD1	2.44	0.51
2:F:125:LYS:HB3	2:F:173:PHE:CE2	2.46	0.51
1:A:108:PRO:HB3	1:A:554:SER:C	2.31	0.51
2:B:85:PHE:HB3	2:B:92:ARG:HG2	1.93	0.51
2:B:122:GLU:HA	2:B:125:LYS:HB2	1.93	0.51
2:C:33:ARG:NH1	7:C:440:HOH:O	2.43	0.51
1:D:220:PHE:CD1	1:D:302:TYR:HD2	2.29	0.51
1:D:323:LEU:HB3	7:D:821:HOH:O	2.10	0.51
1:D:494:CYS:HA	1:D:497:LEU:HD12	1.93	0.51
2:F:20:ARG:HB3	2:F:198:SER:HB3	1.93	0.51
1:A:261:THR:O	1:A:265:LYS:HG3	2.11	0.50
1:A:351:THR:HG21	1:A:418:GLN:CD	2.32	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:116:GLU:OE2	7:D:745:HOH:O	2.19	0.50
1:D:164:THR:HG23	1:D:557:LYS:HG2	1.93	0.50
1:D:171:ARG:NH2	1:D:194:PHE:HB3	2.21	0.50
1:D:427:LEU:HD12	1:D:546:LYS:HD2	1.93	0.50
1:D:478:PHE:N	7:D:780:HOH:O	2.44	0.50
2:E:8:LEU:HG	7:E:406:HOH:O	2.10	0.50
2:F:82:ASN:HB2	7:F:489:HOH:O	2.11	0.50
2:F:152:TYR:O	7:F:422:HOH:O	2.19	0.50
1:A:239:GLU:HB2	7:A:784:HOH:O	2.11	0.50
1:A:381:GLN:OE1	1:A:381:GLN:N	2.44	0.50
1:A:425:ARG:CD	1:A:427:LEU:HB2	2.40	0.50
2:B:11:TRP:CD1	2:B:12:PRO:HD3	2.46	0.50
2:C:141:ASP:CA	1:D:92:HIS:HB2	2.40	0.50
1:D:165:ALA:HB2	4:D:602:ATP:C2	2.46	0.50
2:E:9:ASP:OD1	2:E:33:ARG:N	2.44	0.50
2:E:98:TRP:CZ2	2:E:157:LEU:HD22	2.46	0.50
1:A:425:ARG:HB3	1:A:427:LEU:HB2	1.94	0.50
2:B:162:SER:HB2	2:B:205:ILE:HD12	1.94	0.50
1:D:28:GLN:NE2	7:D:815:HOH:O	2.44	0.50
2:E:17:MET:HE2	2:E:200:PRO:HD2	1.93	0.50
2:E:204:LYS:NZ	7:E:436:HOH:O	2.32	0.50
2:F:91:GLY:N	7:F:403:HOH:O	2.05	0.50
1:A:154:TYR:OH	1:A:162:VAL:HG23	2.11	0.50
1:A:432:ASN:OD1	1:A:434:ASP:N	2.44	0.50
1:A:432:ASN:CG	1:A:435:LYS:HD2	2.32	0.50
2:B:90:TYR:CE1	2:C:62:LYS:HB3	2.45	0.50
2:C:163:TRP:CD1	2:C:205:ILE:HD13	2.47	0.50
1:D:286:ASN:HB3	7:D:847:HOH:O	2.10	0.50
1:D:377:VAL:HG11	7:D:1104:HOH:O	2.10	0.50
1:D:405:ASP:OD1	1:D:540:SER:HB2	2.11	0.50
1:D:495:ASN:O	2:E:188:ARG:NH1	2.42	0.50
1:A:224:ALA:HA	1:A:227:LEU:HD12	1.94	0.50
1:A:302:TYR:HD1	1:A:326:VAL:HG13	1.77	0.50
2:B:153:VAL:HA	2:B:156:SER:OG	2.12	0.50
2:B:157:LEU:HG	2:B:185:TRP:HH2	1.76	0.50
2:C:45:LEU:HB2	7:C:441:HOH:O	2.12	0.50
1:D:77:ILE:HB	1:D:110:PHE:CB	2.41	0.50
1:D:140:ASP:OD1	1:D:140:ASP:N	2.28	0.50
2:E:158:ILE:HA	7:E:501:HOH:O	2.11	0.50
2:E:180:PRO:HG2	7:E:504:HOH:O	2.12	0.50
1:A:107:ARG:HG2	7:A:712:HOH:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:TYR:HA	1:A:175:PHE:CD2	2.47	0.50
1:A:205:HIS:O	7:A:739:HOH:O	2.19	0.50
1:A:337:ILE:HG22	1:A:338:ALA:HB2	1.92	0.50
1:A:526:GLY:HA2	1:A:529:ARG:HB3	1.93	0.50
1:A:532:GLN:HB3	1:A:545:PHE:CZ	2.46	0.50
2:E:54:ILE:HB	2:E:56:VAL:H	1.76	0.50
2:C:65:CYS:O	2:C:66:GLU:HB2	2.12	0.50
1:D:11:ASN:O	1:D:14:ILE:HG13	2.11	0.50
1:D:62:LYS:HG2	1:D:400:ARG:NH2	2.26	0.50
1:D:262:ALA:O	1:D:266:LEU:HG	2.11	0.50
1:D:544:GLN:N	7:D:799:HOH:O	2.37	0.50
2:F:15:PHE:HB3	2:F:67:SER:CB	2.35	0.50
1:A:425:ARG:NH2	1:A:546:LYS:CA	2.68	0.50
2:B:157:LEU:HG	2:B:185:TRP:CH2	2.46	0.50
2:C:32:TYR:HB3	7:C:452:HOH:O	2.12	0.50
2:C:148:ASP:OD2	1:D:46:GLN:HA	2.11	0.50
1:D:149:PHE:HE2	1:D:202:LEU:HD13	1.77	0.50
1:D:499:ARG:HH21	2:E:188:ARG:NE	2.10	0.50
1:A:14:ILE:HG13	1:A:15:ASP:N	2.26	0.50
1:A:557:LYS:NZ	7:A:731:HOH:O	2.13	0.50
2:C:85:PHE:O	7:C:418:HOH:O	2.19	0.50
1:D:316:LEU:O	1:D:320:ALA:N	2.45	0.50
1:D:509:SER:O	1:D:513:LYS:N	2.38	0.50
2:E:18:ARG:NH1	2:E:68:LEU:CD2	2.74	0.50
2:F:135:LEU:O	2:F:139:LEU:HG	2.12	0.50
1:A:150:SER:CB	1:A:167:THR:HA	2.36	0.49
1:A:332:SER:H	1:A:336:TRP:HA	1.77	0.49
1:A:425:ARG:NH1	1:A:546:LYS:HA	2.27	0.49
1:D:198:VAL:HA	1:D:201:ALA:CB	2.39	0.49
1:D:423:CYS:HB2	1:D:543:GLY:H	1.73	0.49
1:D:423:CYS:H	1:D:542:ALA:HB3	1.77	0.49
1:D:440:ASP:O	1:D:444:SER:OG	2.28	0.49
2:F:8:LEU:N	2:F:33:ARG:NH1	2.60	0.49
2:F:10:TYR:O	2:F:20:ARG:NH2	2.44	0.49
1:A:77:ILE:HD13	1:A:110:PHE:O	2.12	0.49
1:A:143:LYS:CD	1:A:212:PHE:HB2	2.41	0.49
1:A:496:CYS:SG	1:A:499:ARG:NH2	2.85	0.49
2:B:33:ARG:HH22	2:B:41:SER:HB3	1.77	0.49
2:C:108:ASP:O	2:C:112:LYS:HG2	2.12	0.49
2:C:210:ALA:HA	2:C:213:ARG:HB2	1.93	0.49
1:D:238:TRP:O	1:D:242:VAL:HG13	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:LEU:HD21	1:A:61:PHE:HD2	1.77	0.49
1:A:488:ASP:OD2	2:B:174:SER:OG	2.26	0.49
2:B:84:PHE:CD1	2:B:152:TYR:HB2	2.46	0.49
2:B:141:ASP:N	2:B:141:ASP:OD1	2.45	0.49
1:A:164:THR:H	1:A:560:GLN:CB	2.25	0.49
1:A:316:LEU:HD12	1:A:319:TYR:HB2	1.93	0.49
1:A:361:PHE:HB2	7:A:983:HOH:O	2.11	0.49
1:A:371:GLU:OE2	7:A:740:HOH:O	2.19	0.49
1:A:423:CYS:HB2	7:A:770:HOH:O	2.12	0.49
1:A:499:ARG:NE	2:B:184:ALA:HB1	2.27	0.49
2:C:184:ALA:HB2	7:C:438:HOH:O	2.12	0.49
2:E:178:GLU:N	7:E:448:HOH:O	2.42	0.49
2:F:4:LEU:N	7:F:450:HOH:O	2.44	0.49
2:F:157:LEU:HD21	2:F:182:LEU:HD11	1.95	0.49
1:D:490:LEU:O	1:D:520:LEU:HD21	2.12	0.49
2:E:110:GLN:O	2:E:113:VAL:HG12	2.13	0.49
1:A:228:VAL:HG13	1:A:319:TYR:HE2	1.77	0.49
1:A:316:LEU:O	1:A:320:ALA:N	2.43	0.49
1:D:96:ALA:O	1:D:113:PHE:N	2.40	0.49
1:A:75:PRO:O	1:A:79:ARG:HG3	2.12	0.49
1:A:332:SER:HB2	1:A:538:LEU:CA	2.40	0.49
1:A:432:ASN:CB	1:A:435:LYS:HD2	2.43	0.49
2:B:11:TRP:O	2:B:200:PRO:HG2	2.13	0.49
2:B:34:GLU:HA	7:B:417:HOH:O	2.12	0.49
1:D:106:GLY:C	1:D:432:ASN:HD22	2.15	0.49
2:F:192:LYS:HB2	7:F:439:HOH:O	2.13	0.49
1:A:300:TYR:CD2	1:A:302:TYR:HB2	2.48	0.49
2:B:14:MET:HG3	2:B:163:TRP:CZ3	2.47	0.49
2:C:204:LYS:HB2	7:C:405:HOH:O	2.13	0.49
1:D:74:GLU:O	1:D:78:LYS:HB2	2.12	0.49
1:D:277:ILE:O	1:D:281:CYS:HB2	2.13	0.49
1:D:513:LYS:HZ1	1:D:575:PHE:HB3	1.77	0.49
2:F:165:GLN:O	2:F:169:LYS:HG2	2.13	0.49
1:A:450:LYS:HZ2	2:B:191:GLU:CA	2.21	0.49
2:B:125:LYS:HA	2:B:128:PHE:CE2	2.48	0.49
2:B:172:ASN:OD1	7:B:421:HOH:O	2.19	0.49
1:D:32:LEU:HD22	1:D:360:TYR:CE2	2.48	0.49
1:D:423:CYS:HG	1:D:541:SER:HG	1.59	0.49
2:F:37:PHE:CE1	6:F:301:GSH:HA32	2.48	0.49
2:F:67:SER:O	2:F:71:VAL:HG23	2.13	0.49
1:A:316:LEU:HD23	7:A:994:HOH:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:546:LYS:NZ	1:A:548:PRO:CD	2.76	0.49
2:C:107:THR:HA	2:C:110:GLN:HG2	1.95	0.49
1:D:478:PHE:CZ	1:D:562:LEU:HD13	2.48	0.49
1:D:534:HIS:C	1:D:534:HIS:CD2	2.85	0.49
2:F:74:VAL:HG12	7:F:431:HOH:O	2.12	0.49
1:A:217:GLN:HG2	7:A:745:HOH:O	2.12	0.48
1:A:256:VAL:HG22	7:A:1013:HOH:O	2.13	0.48
1:A:355:ILE:O	1:A:358:LEU:HD23	2.13	0.48
2:B:178:GLU:HB3	7:B:480:HOH:O	2.12	0.48
1:D:77:ILE:HG22	1:D:97:ILE:HD11	1.95	0.48
1:D:299:LYS:HB2	1:D:300:TYR:HD1	1.77	0.48
1:D:493:CYS:O	1:D:497:LEU:HG	2.13	0.48
1:D:551:VAL:HB	1:D:555:ASN:CB	2.42	0.48
2:E:54:ILE:HD12	2:E:55:PRO:N	2.28	0.48
2:E:76:GLU:OE2	2:F:96:ARG:NE	2.46	0.48
2:E:157:LEU:HG	2:E:185:TRP:CH2	2.47	0.48
1:A:313:VAL:O	1:A:317:ARG:N	2.40	0.48
1:A:340:ASN:HB2	1:A:352:PHE:CD1	2.46	0.48
1:A:424:ARG:HG3	1:A:425:ARG:H	1.78	0.48
2:B:89:PRO:HB2	2:C:73:TYR:CE1	2.48	0.48
1:D:73:LEU:HB2	1:D:76:TYR:CZ	2.48	0.48
1:D:478:PHE:CE2	1:D:562:LEU:HB2	2.47	0.48
2:E:24:ARG:HB3	2:E:194:SER:HA	1.94	0.48
2:E:90:TYR:O	2:E:94:GLN:HG3	2.13	0.48
2:E:194:SER:O	2:E:198:SER:OG	2.21	0.48
2:F:24:ARG:NH2	7:F:437:HOH:O	2.30	0.48
1:A:122:LEU:O	1:A:126:ARG:HG3	2.13	0.48
1:A:152:LYS:HD2	7:A:844:HOH:O	2.13	0.48
2:B:92:ARG:HB3	2:B:96:ARG:NH2	2.29	0.48
1:D:535:PHE:CD1	1:D:536:LEU:N	2.81	0.48
1:A:72:GLU:HG2	7:A:988:HOH:O	2.14	0.48
1:A:105:GLN:CA	1:A:430:SER:HB3	2.43	0.48
1:A:164:THR:OG1	1:A:560:GLN:HB3	2.13	0.48
1:A:222:VAL:HB	1:A:533:GLU:HB3	1.94	0.48
1:A:365:PRO:HD2	7:A:758:HOH:O	2.12	0.48
1:A:425:ARG:NE	1:A:427:LEU:HD12	2.28	0.48
2:C:181:LYS:HA	1:D:93:PRO:HB2	1.95	0.48
2:F:58:VAL:HG22	2:F:63:PRO:HB3	1.95	0.48
1:A:31:THR:O	1:A:35:ILE:HG23	2.13	0.48
1:A:118:MET:O	1:A:121:THR:HB	2.14	0.48
1:A:123:GLN:OE1	7:A:744:HOH:O	2.20	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:392:ILE:HG13	1:A:398:LEU:HB3	1.95	0.48
1:A:528:PHE:HB3	1:A:547:MET:HE3	1.95	0.48
2:B:21:VAL:HG22	2:B:195:VAL:HA	1.96	0.48
2:B:92:ARG:HB3	2:B:96:ARG:HH22	1.78	0.48
2:B:187:LYS:HE2	2:B:187:LYS:HB2	1.55	0.48
1:D:76:TYR:HB2	1:D:88:ILE:HG21	1.95	0.48
1:D:150:SER:HB3	1:D:170:TYR:CD2	2.49	0.48
1:D:186:SER:OG	7:D:739:HOH:O	2.18	0.48
1:D:527:THR:HG23	1:D:561:ILE:CG2	2.43	0.48
1:D:534:HIS:CE1	1:D:557:LYS:HD3	2.49	0.48
2:E:93:ALA:HA	2:F:69:ASN:ND2	2.29	0.48
2:E:181:LYS:HA	2:E:184:ALA:HB3	1.95	0.48
1:A:76:TYR:HB3	1:A:88:ILE:HG21	1.95	0.48
1:A:231:PHE:CZ	1:A:291:ILE:HG12	2.49	0.48
1:A:271:PRO:HG2	7:A:913:HOH:O	2.14	0.48
2:C:139:LEU:O	2:C:142:LYS:HB3	2.14	0.48
1:D:402:ARG:NH2	7:D:823:HOH:O	2.46	0.48
1:A:441:LEU:O	1:A:445:VAL:HG23	2.14	0.48
1:A:573:THR:HG21	2:B:176:GLU:OE2	2.14	0.48
2:B:49:PRO:O	2:B:52:LYS:NZ	2.31	0.48
2:C:142:LYS:HB2	1:D:39:ASN:OD1	2.14	0.48
2:F:18:ARG:N	2:F:159:THR:HG21	2.29	0.48
2:F:188:ARG:HG2	7:F:412:HOH:O	2.14	0.48
1:A:212:PHE:HB3	1:A:215:GLN:OE1	2.13	0.48
1:A:534:HIS:CD2	1:A:557:LYS:HE2	2.49	0.48
1:D:124:LEU:HD11	1:D:355:ILE:CD1	2.43	0.48
1:D:356:PRO:HA	7:D:815:HOH:O	2.14	0.48
1:D:482:SER:HB2	7:D:877:HOH:O	2.14	0.48
2:E:153:VAL:O	2:E:157:LEU:HD23	2.13	0.48
1:A:201:ALA:O	1:A:205:HIS:N	2.46	0.48
2:B:135:LEU:HD13	2:B:182:LEU:HD11	1.96	0.48
2:B:211:GLU:O	2:B:214:LYS:HG2	2.14	0.48
2:C:13:SER:O	2:C:17:MET:HG3	2.14	0.48
2:C:57:LEU:HD23	2:C:59:HIS:HD2	1.79	0.48
2:C:184:ALA:HB3	1:D:93:PRO:HG2	1.95	0.48
1:D:64:MET:N	7:D:753:HOH:O	2.46	0.48
1:D:164:THR:HG23	1:D:557:LYS:CG	2.43	0.48
1:D:170:TYR:HA	1:D:175:PHE:CD2	2.49	0.48
1:A:99:LEU:HB2	1:A:557:LYS:H	1.78	0.48
1:A:112:PRO:HD2	1:A:397:GLY:HA3	1.96	0.48
1:A:215:GLN:O	7:A:745:HOH:O	2.20	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:423:CYS:HB3	1:A:542:ALA:HB3	1.95	0.48
1:A:546:LYS:CD	1:A:547:MET:CA	2.86	0.48
2:B:37:PHE:HZ	2:B:54:ILE:HG12	1.79	0.48
2:B:66:GLU:OE1	2:C:100:ASP:OD2	2.30	0.48
2:B:125:LYS:HA	2:B:128:PHE:CD2	2.49	0.48
1:D:88:ILE:HD12	1:D:89:LEU:H	1.79	0.48
1:D:118:MET:HA	4:D:602:ATP:O3'	2.14	0.48
1:D:156:SER:OG	1:D:157:THR:N	2.46	0.48
1:D:223:PHE:HZ	1:D:536:LEU:HB2	1.79	0.48
2:E:57:LEU:HB3	2:E:64:VAL:HG22	1.94	0.48
1:A:340:ASN:ND2	1:A:343:PRO:HA	2.28	0.47
2:E:40:LYS:O	7:E:422:HOH:O	2.20	0.47
2:E:217:LEU:O	7:E:423:HOH:O	2.20	0.47
2:F:125:LYS:HE2	2:F:171:GLY:O	2.14	0.47
1:A:358:LEU:HD12	1:A:359:GLY:N	2.29	0.47
2:B:54:ILE:HB	2:B:55:PRO:HA	1.95	0.47
2:C:159:THR:HA	2:C:199:LEU:HD21	1.96	0.47
1:D:80:MET:SD	1:D:94:VAL:HG22	2.54	0.47
2:E:139:LEU:HD13	2:E:181:LYS:HE2	1.95	0.47
1:A:143:LYS:CA	1:A:184:SER:HB3	2.44	0.47
1:A:164:THR:O	1:A:168:ASN:ND2	2.47	0.47
1:A:168:ASN:O	1:A:172:ASN:HB2	2.15	0.47
1:A:245:ILE:HA	1:A:267:LEU:HD21	1.94	0.47
2:B:84:PHE:HB2	2:B:152:TYR:N	2.29	0.47
2:B:135:LEU:HD22	2:B:182:LEU:CD1	2.44	0.47
1:D:284:LEU:HD22	1:D:287:TRP:HA	1.95	0.47
2:E:98:TRP:O	2:E:98:TRP:CE3	2.67	0.47
2:B:66:GLU:HB3	7:B:457:HOH:O	2.14	0.47
2:B:101:PHE:CE1	2:C:51:HIS:CE1	3.02	0.47
2:B:135:LEU:HD22	2:B:182:LEU:HD12	1.97	0.47
2:B:201:ASP:HB2	2:B:204:LYS:HG3	1.97	0.47
2:C:128:PHE:HE2	2:C:175:ILE:HG12	1.79	0.47
1:D:122:LEU:O	1:D:126:ARG:HB2	2.14	0.47
1:D:125:PHE:HB3	7:D:863:HOH:O	2.15	0.47
1:D:407:VAL:HG21	1:D:419:LEU:HB3	1.97	0.47
1:D:465:TYR:CD1	1:D:551:VAL:HG23	2.50	0.47
1:D:551:VAL:HB	1:D:555:ASN:HB2	1.95	0.47
2:E:23:LEU:HG	7:E:590:HOH:O	2.14	0.47
2:E:114:TRP:HD1	2:E:167:TYR:CE1	2.31	0.47
1:A:34:GLU:O	1:A:38:LYS:HG2	2.14	0.47
2:B:7:LEU:HD13	2:B:30:PHE:CD2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:143:PRO:O	2:C:185:TRP:HD1	1.96	0.47
2:C:150:PHE:HE1	2:C:189:CYS:SG	2.37	0.47
2:C:188:ARG:CB	1:D:87:PRO:HD2	2.45	0.47
1:D:31:THR:OG1	1:D:357:ASN:HA	2.14	0.47
1:D:152:LYS:CE	1:D:565:ASN:HB2	2.44	0.47
1:D:462:PHE:O	1:D:549:ARG:NH1	2.47	0.47
1:D:508:SER:O	1:D:512:CYS:HB3	2.15	0.47
1:A:110:PHE:HE1	1:A:556:ALA:HB2	1.76	0.47
1:A:172:ASN:N	7:A:708:HOH:O	2.47	0.47
1:A:556:ALA:HA	1:A:559:LEU:HD12	1.97	0.47
2:B:67:SER:HB3	6:B:301:GSH:O12	2.15	0.47
2:B:153:VAL:HG23	2:B:156:SER:HB2	1.97	0.47
2:C:213:ARG:HH21	2:C:213:ARG:HA	1.78	0.47
1:D:233:THR:O	1:D:237:VAL:HG22	2.15	0.47
1:D:498:ASP:CB	1:D:510:ARG:HH22	2.28	0.47
1:D:552:LYS:O	1:D:554:SER:N	2.43	0.47
2:E:54:ILE:HG13	6:E:301:GSH:HB22	1.96	0.47
2:E:211:GLU:HG2	7:E:597:HOH:O	2.13	0.47
2:F:7:LEU:HD23	2:F:32:TYR:HD1	1.79	0.47
1:A:31:THR:OG1	1:A:357:ASN:HA	2.15	0.47
1:A:103:THR:HG22	1:A:548:PRO:HB3	1.96	0.47
1:A:151:SER:HA	1:A:194:PHE:HA	1.97	0.47
1:A:203:TYR:CE2	1:A:244:ASP:OD2	2.68	0.47
1:A:425:ARG:N	1:A:543:GLY:HA2	2.29	0.47
1:A:512:CYS:SG	1:A:513:LYS:N	2.88	0.47
2:B:17:MET:HE3	2:B:163:TRP:HH2	1.80	0.47
2:B:164:PHE:CD2	2:B:183:ILE:HD13	2.44	0.47
2:C:77:ALA:HB3	2:C:78:TRP:CE3	2.50	0.47
1:D:39:ASN:ND2	7:D:751:HOH:O	2.22	0.47
1:D:96:ALA:HB3	1:D:113:PHE:HB3	1.96	0.47
1:D:149:PHE:HZ	1:D:202:LEU:HA	1.80	0.47
1:D:294:LEU:O	1:D:296:PRO:HD3	2.15	0.47
2:E:9:ASP:O	2:E:35:GLU:HB2	2.15	0.47
2:E:26:LYS:HE2	2:E:75:ASP:HA	1.95	0.47
2:E:184:ALA:C	2:E:187:LYS:NZ	2.67	0.47
2:F:107:THR:O	2:F:110:GLN:HG3	2.14	0.47
1:A:506:TYR:CZ	1:A:510:ARG:NH1	2.83	0.47
2:B:128:PHE:N	7:B:403:HOH:O	2.47	0.47
6:B:301:GSH:N1	7:B:425:HOH:O	2.22	0.47
2:C:111:PHE:HA	2:C:114:TRP:NE1	2.30	0.47
1:D:133:ASN:OD1	1:D:138:ILE:HG13	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:88:ASP:OD2	2:F:62:LYS:NZ	2.33	0.47
2:F:90:TYR:N	7:F:403:HOH:O	2.48	0.47
1:A:278:ARG:HG2	1:A:282:MET:SD	2.55	0.47
1:A:370:GLY:HA2	1:A:371:GLU:HA	1.55	0.47
2:B:70:VAL:HA	2:B:73:TYR:CD2	2.50	0.47
1:D:90:THR:HG1	1:D:91:GLY:N	1.92	0.47
1:A:478:PHE:CD2	1:A:562:LEU:HD22	2.49	0.47
1:A:494:CYS:SG	1:A:495:ASN:N	2.88	0.47
2:B:97:PHE:CE1	2:C:65:CYS:HB2	2.50	0.47
2:C:128:PHE:HE2	2:C:175:ILE:CG1	2.27	0.47
1:D:304:ILE:N	7:D:750:HOH:O	2.48	0.47
1:D:315:LYS:O	1:D:318:HIS:HB3	2.15	0.47
2:F:26:LYS:HD3	7:F:489:HOH:O	2.14	0.47
1:A:213:ARG:HG3	1:A:214:ASP:N	2.30	0.46
1:A:478:PHE:HZ	1:A:521:ARG:NH1	2.13	0.46
1:D:76:TYR:OH	1:D:89:LEU:HD22	2.15	0.46
1:D:222:VAL:HB	1:D:533:GLU:CG	2.45	0.46
1:D:449:ALA:CB	1:D:459:VAL:HG21	2.44	0.46
1:D:531:ILE:HG23	1:D:534:HIS:CE1	2.50	0.46
2:E:76:GLU:H	2:E:76:GLU:HG2	1.46	0.46
2:F:54:ILE:HB	2:F:55:PRO:HA	1.96	0.46
1:A:304:ILE:HG22	7:A:749:HOH:O	2.14	0.46
1:A:392:ILE:HD13	1:A:403:LEU:HD22	1.97	0.46
2:B:14:MET:HG3	2:B:163:TRP:CH2	2.50	0.46
2:C:94:GLN:HA	2:C:97:PHE:CE2	2.50	0.46
2:C:148:ASP:HA	1:D:41:SER:HA	1.96	0.46
1:D:169:VAL:HG22	4:D:602:ATP:O2'	2.16	0.46
1:D:296:PRO:HB2	7:D:704:HOH:O	2.15	0.46
1:D:401:TYR:CE2	1:D:403:LEU:HD12	2.50	0.46
2:E:171:GLY:O	2:E:173:PHE:HD2	1.97	0.46
1:A:99:LEU:HD13	1:A:558:VAL:H	1.80	0.46
1:A:401:TYR:HA	7:A:775:HOH:O	2.15	0.46
2:C:112:LYS:HB3	7:C:407:HOH:O	2.15	0.46
2:C:112:LYS:O	2:C:116:LYS:HB2	2.16	0.46
2:C:142:LYS:C	1:D:91:GLY:HA3	2.36	0.46
1:D:76:TYR:CD1	1:D:77:ILE:N	2.83	0.46
1:D:327:SER:HB2	1:D:352:PHE:HZ	1.80	0.46
1:D:328:HIS:CG	1:D:329:ASP:N	2.83	0.46
2:E:72:GLN:O	2:E:76:GLU:HG2	2.15	0.46
2:E:181:LYS:HB2	2:E:181:LYS:HE3	1.73	0.46
2:E:195:VAL:HB	7:E:415:HOH:O	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:195:VAL:N	7:F:439:HOH:O	2.30	0.46
1:A:222:VAL:O	1:A:223:PHE:HD1	1.99	0.46
1:A:290:LEU:O	1:A:294:LEU:HG	2.15	0.46
1:A:491:GLN:HG2	2:B:176:GLU:CD	2.36	0.46
2:B:17:MET:HB3	2:B:199:LEU:HD11	1.98	0.46
2:B:121:GLN:O	2:B:125:LYS:HB2	2.16	0.46
2:C:188:ARG:HB2	1:D:87:PRO:HD2	1.97	0.46
1:D:409:VAL:HA	1:D:418:GLN:O	2.15	0.46
2:E:33:ARG:NH2	2:E:35:GLU:OE1	2.48	0.46
2:E:76:GLU:CD	2:F:96:ARG:CZ	2.83	0.46
1:A:450:LYS:HA	1:A:453:SER:HB3	1.98	0.46
2:B:118:GLY:N	2:B:121:GLN:HB2	2.30	0.46
2:C:11:TRP:CD1	2:C:12:PRO:HD3	2.50	0.46
1:D:42:ALA:HB1	7:D:884:HOH:O	2.15	0.46
1:D:289:GLY:HA2	1:D:321:GLY:CA	2.45	0.46
1:D:442:GLN:HG2	1:D:462:PHE:CZ	2.41	0.46
2:F:132:VAL:N	7:F:414:HOH:O	2.49	0.46
1:A:234:PHE:HE2	1:A:287:TRP:HZ3	1.64	0.46
1:A:303:GLY:O	1:A:328:HIS:N	2.49	0.46
2:B:131:ALA:O	2:B:135:LEU:HB2	2.15	0.46
1:D:229:HIS:HA	1:D:232:ARG:NE	2.30	0.46
2:E:139:LEU:HB3	2:E:181:LYS:HE2	1.97	0.46
2:F:93:ALA:HA	2:F:96:ARG:NH1	2.30	0.46
2:F:106:PHE:N	7:F:424:HOH:O	2.47	0.46
2:F:170:PHE:CE2	2:F:213:ARG:HD2	2.50	0.46
1:A:11:ASN:ND2	7:A:798:HOH:O	2.39	0.46
1:A:238:TRP:HB2	7:A:868:HOH:O	2.15	0.46
1:A:357:ASN:OD1	7:A:721:HOH:O	2.20	0.46
2:B:18:ARG:HH21	2:B:160:PHE:HE2	1.62	0.46
2:B:71:VAL:HG13	2:B:152:TYR:HE1	1.79	0.46
2:C:175:ILE:HB	2:C:183:ILE:HD11	1.96	0.46
1:A:316:LEU:HA	1:A:319:TYR:CD2	2.51	0.46
2:C:200:PRO:HB2	7:C:405:HOH:O	2.15	0.46
1:D:287:TRP:HE3	1:D:290:LEU:HD21	1.80	0.46
1:D:488:ASP:O	1:D:492:ASP:OD1	2.34	0.46
1:D:555:ASN:HA	7:D:702:HOH:O	2.15	0.46
2:F:92:ARG:HB3	2:F:96:ARG:HH22	1.81	0.46
1:A:113:PHE:HB2	4:A:602:ATP:PB	2.56	0.46
1:A:425:ARG:CZ	1:A:546:LYS:CA	2.94	0.46
1:A:460:ILE:HD11	1:A:480:GLU:CD	2.36	0.46
2:B:37:PHE:CZ	6:B:301:GSH:HA32	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:132:VAL:HG23	2:C:182:LEU:HD23	1.98	0.46
1:D:21:THR:HB	1:D:416:THR:HB	1.98	0.46
1:D:370:GLY:HA2	1:D:371:GLU:HA	1.57	0.46
4:D:602:ATP:C8	4:D:602:ATP:O2'	2.67	0.46
1:A:349:GLU:OE2	7:A:742:HOH:O	2.20	0.46
1:A:546:LYS:HD2	1:A:548:PRO:CD	2.37	0.46
2:C:99:ALA:O	2:C:103:ASP:HB2	2.16	0.46
1:D:100:SER:HB2	1:D:109:LYS:NZ	2.31	0.46
1:D:213:ARG:HG3	1:D:214:ASP:N	2.31	0.46
1:D:331:GLY:HA3	1:D:336:TRP:HA	1.98	0.46
2:E:148:ASP:N	2:E:148:ASP:OD1	2.48	0.46
2:F:18:ARG:NE	2:F:156:SER:HA	2.31	0.46
2:F:50:ILE:HG23	2:F:51:HIS:H	1.80	0.46
1:A:233:THR:O	1:A:237:VAL:HG22	2.16	0.45
1:A:405:ASP:CG	1:A:540:SER:HB2	2.35	0.45
1:A:444:SER:HA	1:A:500:ALA:CB	2.46	0.45
2:C:18:ARG:HG2	2:C:156:SER:HA	1.98	0.45
2:C:95:ALA:HB1	2:C:152:TYR:HD2	1.81	0.45
1:D:77:ILE:CD1	1:D:110:PHE:HB2	2.46	0.45
1:D:77:ILE:HD12	1:D:110:PHE:HB2	1.97	0.45
1:D:153:GLN:N	1:D:564:GLU:HB2	2.28	0.45
2:E:90:TYR:HA	2:F:63:PRO:O	2.16	0.45
2:E:163:TRP:HB3	2:E:167:TYR:CZ	2.51	0.45
2:E:187:LYS:H	2:E:187:LYS:HZ3	1.64	0.45
2:E:209:ALA:HA	2:E:212:TYR:HB2	1.98	0.45
1:A:37:LEU:HD23	1:A:37:LEU:HA	1.65	0.45
1:A:105:GLN:HA	1:A:430:SER:CB	2.46	0.45
1:A:421:PHE:CE1	1:A:541:SER:HA	2.51	0.45
1:A:558:VAL:O	1:A:562:LEU:HG	2.16	0.45
2:B:110:GLN:HA	2:B:113:VAL:HG12	1.98	0.45
2:C:141:ASP:CB	1:D:92:HIS:HB2	2.47	0.45
1:D:8:PHE:HE1	1:D:130:ALA:HB2	1.81	0.45
1:D:338:ALA:HA	1:D:354:VAL:HA	1.97	0.45
1:D:435:LYS:HB3	1:D:436:ASN:C	2.36	0.45
2:F:26:LYS:HD3	2:F:26:LYS:HA	1.72	0.45
2:F:101:PHE:CZ	2:F:131:ALA:HB1	2.51	0.45
1:A:98:SER:HG	4:A:602:ATP:PG	2.33	0.45
1:A:222:VAL:HG12	1:A:223:PHE:CD1	2.51	0.45
1:A:437:THR:HG23	1:A:439:ARG:HE	1.81	0.45
1:A:482:SER:O	1:A:525:LYS:HE2	2.16	0.45
2:C:36:ASP:OD2	2:C:38:SER:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:180:PRO:HD2	2:C:181:LYS:NZ	2.31	0.45
1:D:86:SER:HA	1:D:87:PRO:HD2	1.72	0.45
1:D:272:GLU:HG3	1:D:273:LEU:HD13	1.97	0.45
1:D:423:CYS:SG	1:D:541:SER:OG	2.69	0.45
2:E:169:LYS:HB2	2:E:169:LYS:HE3	1.72	0.45
2:F:133:LYS:HG2	7:F:454:HOH:O	2.17	0.45
1:A:11:ASN:HA	1:A:14:ILE:HG12	1.97	0.45
1:A:77:ILE:CG2	1:A:97:ILE:HD12	2.46	0.45
1:A:120:ASN:O	7:A:747:HOH:O	2.21	0.45
1:A:445:VAL:HG22	1:A:479:TRP:NE1	2.32	0.45
1:A:513:LYS:HZ1	1:A:575:PHE:HB3	1.80	0.45
1:A:535:PHE:CD2	1:A:546:LYS:HE2	2.52	0.45
1:D:37:LEU:HD23	1:D:37:LEU:HA	1.85	0.45
1:D:149:PHE:HB2	1:D:530:LYS:CE	2.47	0.45
1:D:392:ILE:CD1	1:D:403:LEU:HD22	2.47	0.45
2:E:110:GLN:HE21	2:E:167:TYR:HE2	1.63	0.45
1:A:122:LEU:HD11	1:A:174:ASN:ND2	2.32	0.45
2:B:26:LYS:HG2	2:B:81:LYS:NZ	2.24	0.45
2:C:10:TYR:HB3	2:C:13:SER:HB2	1.98	0.45
2:C:59:HIS:ND1	2:C:59:HIS:O	2.49	0.45
1:D:495:ASN:O	1:D:498:ASP:HB2	2.17	0.45
2:F:92:ARG:HB3	2:F:96:ARG:NH2	2.30	0.45
2:F:170:PHE:HD1	2:F:170:PHE:HA	1.66	0.45
1:A:401:TYR:HE2	1:A:403:LEU:HD13	1.82	0.45
2:B:23:LEU:HD11	2:B:57:LEU:CD1	2.47	0.45
2:B:26:LYS:HE3	2:B:78:TRP:O	2.17	0.45
1:D:219:VAL:O	1:D:219:VAL:HG13	2.17	0.45
1:D:382:VAL:HG11	1:D:388:TYR:CE1	2.51	0.45
2:E:152:TYR:O	2:E:155:ILE:HB	2.16	0.45
1:A:44:TYR:OH	1:A:68:VAL:HB	2.16	0.45
1:A:98:SER:H	1:A:111:ILE:H	1.65	0.45
2:B:98:TRP:CD1	2:B:153:VAL:HG11	2.51	0.45
2:C:5:PRO:O	2:C:30:PHE:HB2	2.16	0.45
2:C:154:ASP:HA	2:C:185:TRP:HZ2	1.82	0.45
1:D:490:LEU:HD21	7:D:1046:HOH:O	2.17	0.45
2:F:162:SER:HG	2:F:163:TRP:HD1	1.64	0.45
1:A:25:HIS:O	1:A:28:GLN:HG2	2.16	0.45
1:A:79:ARG:HB2	1:A:88:ILE:HD11	1.98	0.45
2:B:73:TYR:HA	2:B:76:GLU:HG2	1.99	0.45
2:C:14:MET:HE1	2:C:163:TRP:CB	2.47	0.45
2:C:142:LYS:CB	1:D:39:ASN:HA	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:107:ARG:NH2	1:D:552:LYS:HB2	2.18	0.45
1:D:251:SER:N	7:D:801:HOH:O	2.38	0.45
1:D:324:PRO:HD2	7:D:821:HOH:O	2.16	0.45
1:D:351:THR:HG21	1:D:410:ILE:HG12	1.99	0.45
1:D:487:GLU:OE1	1:D:568:SER:HB2	2.17	0.45
2:E:14:MET:HE3	2:E:14:MET:HB2	1.93	0.45
2:E:86:PRO:HD3	2:E:146:GLY:O	2.17	0.45
2:E:101:PHE:CE2	2:F:50:ILE:HG12	2.51	0.45
2:E:187:LYS:HE2	2:E:187:LYS:HB2	1.78	0.45
1:A:87:PRO:HB3	1:A:93:PRO:HD3	1.99	0.45
1:A:140:ASP:HB3	7:A:951:HOH:O	2.16	0.45
1:A:455:GLU:HG2	2:B:203:GLU:OE1	2.17	0.45
1:A:475:TYR:HE2	1:A:477:ILE:HD11	1.82	0.45
1:A:559:LEU:HA	1:A:562:LEU:CG	2.44	0.45
2:C:135:LEU:O	2:C:139:LEU:HD12	2.16	0.45
2:C:142:LYS:N	1:D:92:HIS:H	2.15	0.45
1:D:403:LEU:HD23	1:D:540:SER:HG	1.82	0.45
2:F:4:LEU:O	2:F:6:ILE:HG13	2.17	0.45
1:A:306:THR:O	7:A:749:HOH:O	2.21	0.45
1:A:309:MET:O	1:A:312:TYR:N	2.35	0.45
1:A:496:CYS:HA	1:A:499:ARG:CZ	2.47	0.45
1:D:32:LEU:HD22	1:D:360:TYR:CD2	2.52	0.45
1:D:512:CYS:SG	1:D:513:LYS:N	2.89	0.45
1:A:85:THR:HG22	1:A:160:VAL:CG2	2.46	0.44
1:A:282:MET:HE2	1:A:282:MET:HB2	1.85	0.44
2:B:17:MET:HB2	2:B:159:THR:HB	1.98	0.44
1:D:154:TYR:CE2	1:D:156:SER:HA	2.51	0.44
1:D:363:PHE:HE2	1:D:379:LEU:HA	1.83	0.44
1:D:444:SER:HA	1:D:500:ALA:HB1	1.99	0.44
2:E:72:GLN:HA	2:E:84:PHE:CZ	2.52	0.44
2:E:187:LYS:NZ	2:E:187:LYS:H	2.15	0.44
1:A:384:ILE:O	7:A:748:HOH:O	2.21	0.44
1:A:506:TYR:CE2	1:A:510:ARG:CZ	3.00	0.44
2:C:14:MET:CE	2:C:163:TRP:CG	2.99	0.44
2:C:143:PRO:HD3	1:D:39:ASN:OD1	2.18	0.44
1:D:110:PHE:CE2	1:D:554:SER:HA	2.52	0.44
1:D:125:PHE:HD1	1:D:125:PHE:HA	1.58	0.44
1:D:163:GLY:C	1:D:168:ASN:HD21	2.20	0.44
1:D:301:VAL:HG11	1:D:325:LEU:HD23	2.00	0.44
1:D:464:SER:HB3	1:D:550:CYS:SG	2.57	0.44
1:D:494:CYS:CA	1:D:520:LEU:HD23	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:197:ASP:OD2	1:D:200:GLN:OE1	2.35	0.44
1:D:204:CYS:O	1:D:208:SER:N	2.50	0.44
1:D:278:ARG:O	1:D:282:MET:HE2	2.17	0.44
2:F:14:MET:HB3	2:F:159:THR:OG1	2.17	0.44
2:F:66:GLU:HA	6:F:301:GSH:O11	2.18	0.44
1:A:36:LEU:HD23	1:A:36:LEU:HA	1.75	0.44
2:B:10:TYR:CG	2:B:12:PRO:HD2	2.52	0.44
1:D:31:THR:O	1:D:35:ILE:HG13	2.17	0.44
1:D:401:TYR:HE2	1:D:403:LEU:HD12	1.81	0.44
1:A:58:GLU:OE2	1:A:360:TYR:OH	2.34	0.44
1:A:124:LEU:HD12	1:A:336:TRP:HE3	1.82	0.44
1:A:387:GLU:C	1:A:388:TYR:HD1	2.20	0.44
1:A:465:TYR:HD1	1:A:551:VAL:HG12	1.82	0.44
1:A:510:ARG:HB3	1:A:575:PHE:CE2	2.53	0.44
1:A:552:LYS:HG3	1:A:553:PRO:HD2	1.98	0.44
1:D:345:LEU:HD13	1:D:350:ALA:HA	2.00	0.44
1:D:378:GLY:O	1:D:382:VAL:HG23	2.17	0.44
2:E:14:MET:O	2:E:18:ARG:HG3	2.17	0.44
2:E:108:ASP:O	2:E:112:LYS:HG2	2.17	0.44
2:E:144:TYR:N	7:E:451:HOH:O	2.46	0.44
1:A:207:LEU:HD11	1:A:245:ILE:HD11	1.99	0.44
1:A:257:PRO:O	1:A:261:THR:HG23	2.17	0.44
1:A:273:LEU:HD23	1:A:276:THR:HG21	1.99	0.44
1:A:544:GLN:O	1:A:545:PHE:HD2	2.01	0.44
2:B:169:LYS:HE3	2:B:169:LYS:HB2	1.59	0.44
2:B:201:ASP:HB2	2:B:204:LYS:HD2	2.00	0.44
2:C:142:LYS:HD2	1:D:41:SER:CB	2.42	0.44
1:D:73:LEU:HB2	1:D:76:TYR:OH	2.17	0.44
1:D:196:PRO:HA	1:D:565:ASN:OD1	2.17	0.44
2:E:164:PHE:O	2:E:168:GLU:N	2.49	0.44
1:A:284:LEU:HD13	1:A:287:TRP:H	1.82	0.44
1:A:295:PHE:CD1	1:A:298:ALA:HB2	2.52	0.44
1:A:378:GLY:O	1:A:382:VAL:HG23	2.18	0.44
1:A:447:SER:CA	1:A:450:LYS:HE2	2.48	0.44
1:D:132:ARG:HG3	7:D:901:HOH:O	2.17	0.44
1:D:150:SER:HB2	1:D:167:THR:HA	2.00	0.44
1:D:337:ILE:O	1:D:355:ILE:HD12	2.17	0.44
1:A:151:SER:HB3	1:A:565:ASN:HD21	1.83	0.44
1:A:337:ILE:HG22	1:A:338:ALA:CB	2.47	0.44
2:B:169:LYS:NZ	7:B:414:HOH:O	2.13	0.44
1:D:133:ASN:OD1	1:D:138:ILE:N	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:11:TRP:O	2:E:200:PRO:HG3	2.17	0.44
2:E:11:TRP:CZ3	2:E:205:ILE:HG13	2.52	0.44
2:E:98:TRP:HH2	2:E:135:LEU:HD11	1.82	0.44
2:F:8:LEU:HD23	2:F:33:ARG:HD2	1.98	0.44
1:A:17:PHE:HA	1:A:20:MET:HB3	1.99	0.44
1:A:25:HIS:CD2	1:A:380:THR:HG1	2.26	0.44
1:A:98:SER:HG	4:A:602:ATP:PB	2.30	0.44
1:A:499:ARG:NH1	2:B:184:ALA:CB	2.80	0.44
1:A:507:VAL:O	1:A:511:LYS:HB2	2.17	0.44
1:A:546:LYS:NZ	1:A:548:PRO:CG	2.73	0.44
2:C:148:ASP:CG	1:D:46:GLN:HG2	2.39	0.44
1:D:164:THR:O	1:D:168:ASN:ND2	2.51	0.44
1:D:492:ASP:HB3	2:E:187:LYS:HB2	2.00	0.44
2:E:101:PHE:HE2	2:F:51:HIS:N	2.16	0.44
2:F:98:TRP:CE2	2:F:138:GLU:HG2	2.52	0.44
2:F:136:GLU:OE2	2:F:181:LYS:HD2	2.18	0.44
1:A:108:PRO:HG2	1:A:552:LYS:H	1.83	0.43
1:A:149:PHE:CZ	1:A:205:HIS:HD2	2.36	0.43
1:A:202:LEU:HD23	1:A:525:LYS:HD2	2.00	0.43
2:B:84:PHE:HD1	2:B:85:PHE:N	2.15	0.43
2:C:157:LEU:HB2	7:C:416:HOH:O	2.17	0.43
1:D:142:GLY:HA2	1:D:215:GLN:HB2	1.99	0.43
1:D:256:VAL:HA	1:D:257:PRO:HD3	1.75	0.43
1:D:330:TYR:HB3	7:D:813:HOH:O	2.18	0.43
1:D:409:VAL:HG12	7:D:731:HOH:O	2.17	0.43
2:E:17:MET:SD	2:E:199:LEU:HG	2.58	0.43
2:E:76:GLU:OE1	2:F:96:ARG:CZ	2.66	0.43
2:E:105:LYS:HB2	7:E:526:HOH:O	2.17	0.43
2:E:170:PHE:CE2	2:E:213:ARG:HD2	2.52	0.43
2:F:100:ASP:HA	7:F:427:HOH:O	2.17	0.43
1:A:98:SER:N	1:A:111:ILE:O	2.52	0.43
1:A:251:SER:O	1:A:254:ILE:HG12	2.19	0.43
2:B:17:MET:SD	2:B:199:LEU:HG	2.59	0.43
2:C:141:ASP:C	1:D:92:HIS:H	2.22	0.43
2:C:164:PHE:CD2	2:C:183:ILE:HG12	2.53	0.43
1:D:74:GLU:N	1:D:75:PRO:HD2	2.33	0.43
1:D:126:ARG:CZ	1:D:182:ILE:HD11	2.48	0.43
1:D:138:ILE:HG21	1:D:217:GLN:OE1	2.18	0.43
1:D:143:LYS:NZ	1:D:187:CYS:HA	2.32	0.43
1:D:235:GLU:HG2	1:D:287:TRP:CD2	2.52	0.43
1:D:459:VAL:HG22	1:D:481:ILE:HG22	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:132:VAL:HG13	7:F:434:HOH:O	2.18	0.43
1:A:32:LEU:HD21	1:A:61:PHE:CD2	2.53	0.43
1:A:68:VAL:N	7:A:775:HOH:O	2.47	0.43
2:B:73:TYR:HE1	2:C:96:ARG:HH11	1.61	0.43
2:C:6:ILE:O	2:C:57:LEU:HA	2.18	0.43
2:C:133:LYS:HB3	7:C:413:HOH:O	2.17	0.43
1:D:343:PRO:HD2	7:D:728:HOH:O	2.18	0.43
2:E:104:LYS:HG3	2:E:105:LYS:N	2.34	0.43
2:F:26:LYS:HD2	7:F:495:HOH:O	2.19	0.43
1:A:204:CYS:HA	1:A:207:LEU:HB2	2.01	0.43
1:A:337:ILE:HG23	1:A:354:VAL:HG22	2.00	0.43
1:A:436:ASN:O	1:A:440:ASP:HB3	2.19	0.43
2:C:170:PHE:HB3	7:C:410:HOH:O	2.17	0.43
1:D:58:GLU:OE2	1:D:360:TYR:OH	2.27	0.43
1:D:143:LYS:O	1:D:217:GLN:N	2.48	0.43
1:D:153:GLN:HG2	1:D:167:THR:HG21	2.00	0.43
1:D:445:VAL:HG13	1:D:479:TRP:CE2	2.53	0.43
1:A:27:VAL:HG13	1:A:356:PRO:HB2	2.00	0.43
1:A:87:PRO:C	1:A:88:ILE:HG13	2.39	0.43
1:A:213:ARG:HD2	7:A:804:HOH:O	2.18	0.43
1:A:262:ALA:O	1:A:266:LEU:HG	2.19	0.43
1:A:365:PRO:HG3	1:A:388:TYR:CE2	2.54	0.43
2:B:23:LEU:HD23	2:B:74:VAL:HG22	1.99	0.43
2:C:51:HIS:O	2:C:52:LYS:HG2	2.17	0.43
1:D:107:ARG:HH22	1:D:552:LYS:CB	2.19	0.43
1:D:149:PHE:HB2	1:D:530:LYS:HE3	2.00	0.43
1:D:315:LYS:HG2	1:D:319:TYR:CE2	2.53	0.43
1:D:329:ASP:HB3	1:D:338:ALA:O	2.19	0.43
2:E:10:TYR:H	2:E:20:ARG:NH2	2.16	0.43
2:E:26:LYS:HG2	2:E:81:LYS:HZ2	1.82	0.43
2:E:155:ILE:HG22	7:E:512:HOH:O	2.17	0.43
2:F:75:ASP:HA	7:F:431:HOH:O	2.18	0.43
2:F:138:GLU:C	2:F:140:GLY:H	2.22	0.43
1:A:77:ILE:CG2	1:A:110:PHE:HB3	2.48	0.43
1:A:130:ALA:HA	7:A:885:HOH:O	2.18	0.43
1:A:393:THR:OG1	1:A:400:ARG:N	2.50	0.43
1:A:527:THR:HG23	1:A:561:ILE:HG22	2.01	0.43
1:D:74:GLU:HA	1:D:77:ILE:CD1	2.37	0.43
1:D:120:ASN:O	1:D:124:LEU:HB2	2.18	0.43
1:D:124:LEU:HD23	1:D:336:TRP:CD2	2.52	0.43
1:D:495:ASN:C	2:E:188:ARG:NH1	2.72	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:13:SER:HB3	2:E:16:GLY:HA3	2.00	0.43
2:E:50:ILE:O	2:E:52:LYS:HG3	2.18	0.43
2:E:199:LEU:HA	2:E:200:PRO:HD2	1.74	0.43
1:A:161:PRO:HD3	7:A:812:HOH:O	2.18	0.43
1:A:268:THR:O	1:A:270:ASN:ND2	2.51	0.43
1:A:305:MET:SD	1:A:325:LEU:HB3	2.58	0.43
2:B:16:GLY:HA2	2:B:55:PRO:HB3	2.00	0.43
2:B:214:LYS:HE2	2:B:214:LYS:HB3	1.66	0.43
1:D:108:PRO:CG	1:D:552:LYS:H	2.16	0.43
1:D:113:PHE:CD1	4:D:602:ATP:H5'1	2.53	0.43
1:D:495:ASN:C	2:E:188:ARG:HH12	2.20	0.43
2:E:60:ASN:HB2	7:E:490:HOH:O	2.18	0.43
2:E:64:VAL:HB	2:E:73:TYR:CD2	2.53	0.43
2:E:133:LYS:HB3	2:E:133:LYS:HE2	1.82	0.43
2:E:135:LEU:HD22	2:E:182:LEU:CD1	2.49	0.43
2:F:73:TYR:CE1	2:F:77:ALA:HB2	2.54	0.43
2:F:112:LYS:HB2	7:F:402:HOH:O	2.18	0.43
1:A:30:GLN:NE2	7:A:819:HOH:O	2.52	0.43
1:A:70:ASP:OD1	1:A:71:VAL:HG23	2.19	0.43
1:A:135:ASP:OD2	1:A:343:PRO:HD2	2.18	0.43
1:A:353:ALA:HB3	7:A:765:HOH:O	2.19	0.43
2:B:10:TYR:CE2	2:B:12:PRO:HG2	2.54	0.43
2:B:91:GLY:HA2	2:B:94:GLN:OE1	2.19	0.43
2:B:133:LYS:HG3	7:B:480:HOH:O	2.19	0.43
2:B:157:LEU:HA	2:B:160:PHE:HD2	1.84	0.43
2:C:17:MET:HB3	2:C:199:LEU:HD12	2.01	0.43
2:C:162:SER:OG	2:C:163:TRP:HD1	2.02	0.43
1:D:118:MET:HE1	7:D:707:HOH:O	2.15	0.43
1:D:238:TRP:CE2	1:D:239:GLU:HG3	2.54	0.43
1:D:492:ASP:HA	2:E:187:LYS:HE2	2.01	0.43
2:E:35:GLU:HB3	2:E:37:PHE:CE1	2.53	0.43
1:A:154:TYR:CD2	1:A:560:GLN:HA	2.52	0.43
1:A:200:GLN:O	1:A:203:TYR:HB3	2.19	0.43
1:A:363:PHE:CE1	1:A:390:VAL:HG22	2.54	0.43
1:A:530:LYS:HE2	7:A:844:HOH:O	2.18	0.43
2:B:11:TRP:CG	2:B:12:PRO:HD3	2.54	0.43
2:B:78:TRP:HB3	2:B:81:LYS:NZ	2.34	0.43
1:D:487:GLU:HG2	1:D:570:TYR:CZ	2.54	0.43
2:E:166:ALA:O	7:E:424:HOH:O	2.22	0.43
2:E:187:LYS:HA	2:E:190:MET:CG	2.48	0.43
1:A:220:PHE:CD1	1:A:302:TYR:HD2	2.37	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:547:MET:HE1	1:A:549:ARG:HH22	1.82	0.43
2:B:24:ARG:HB3	2:B:194:SER:HA	2.01	0.43
2:B:33:ARG:NH2	2:B:41:SER:HB3	2.33	0.43
2:B:90:TYR:CD2	2:C:62:LYS:HD3	2.54	0.43
2:B:110:GLN:O	2:B:113:VAL:HG12	2.18	0.43
1:D:183:THR:O	7:D:748:HOH:O	2.21	0.43
2:E:33:ARG:NH1	2:E:41:SER:HB2	2.31	0.43
1:A:153:GLN:HB2	1:A:171:ARG:NH1	2.34	0.42
1:A:363:PHE:HE1	1:A:390:VAL:HG13	1.84	0.42
1:A:405:ASP:OD2	1:A:540:SER:HB2	2.18	0.42
2:C:170:PHE:CZ	2:C:213:ARG:HG3	2.54	0.42
1:D:253:ARG:HG3	1:D:484:GLU:HB3	2.01	0.42
1:D:424:ARG:HG3	1:D:425:ARG:H	1.84	0.42
1:D:464:SER:N	1:D:549:ARG:O	2.51	0.42
1:D:477:ILE:HB	1:D:497:LEU:HD13	2.00	0.42
1:D:503:ASP:OD1	1:D:504:ALA:N	2.52	0.42
2:E:71:VAL:HG23	2:E:152:TYR:HE1	1.84	0.42
2:F:33:ARG:NH2	2:F:43:LEU:HD23	2.32	0.42
1:A:32:LEU:HB2	1:A:360:TYR:CD1	2.54	0.42
1:A:94:VAL:HB	1:A:113:PHE:O	2.19	0.42
1:A:164:THR:OG1	1:A:561:ILE:HG13	2.20	0.42
1:A:338:ALA:HB1	1:A:352:PHE:C	2.40	0.42
2:B:33:ARG:NH2	2:B:35:GLU:OE2	2.52	0.42
1:D:94:VAL:HB	1:D:113:PHE:O	2.19	0.42
1:D:98:SER:HG	4:D:602:ATP:PG	2.36	0.42
1:D:129:PHE:O	1:D:133:ASN:HB2	2.19	0.42
1:D:237:VAL:HG23	7:D:941:HOH:O	2.18	0.42
1:D:363:PHE:HB3	1:D:388:TYR:CD2	2.54	0.42
1:D:435:LYS:HZ3	1:D:549:ARG:HB2	1.84	0.42
1:D:517:ALA:HB2	7:D:848:HOH:O	2.18	0.42
2:E:6:ILE:HG13	7:E:498:HOH:O	2.18	0.42
2:E:97:PHE:CD1	2:F:65:CYS:HB2	2.54	0.42
2:E:98:TRP:CE3	2:E:101:PHE:HB3	2.54	0.42
2:E:110:GLN:NE2	2:E:167:TYR:HE2	2.18	0.42
2:F:124:GLY:HA2	2:F:127:GLU:OE1	2.19	0.42
2:F:145:PHE:HB2	2:F:154:ASP:OD2	2.18	0.42
2:F:161:SER:O	2:F:164:PHE:CD2	2.72	0.42
1:A:142:GLY:HA2	1:A:215:GLN:HB3	2.01	0.42
1:A:549:ARG:HD3	1:A:549:ARG:HA	1.81	0.42
2:B:7:LEU:HD12	2:B:7:LEU:N	2.34	0.42
2:B:86:PRO:HD3	2:B:146:GLY:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:142:LYS:HB3	2:B:144:TYR:O	2.19	0.42
1:D:71:VAL:HG21	1:D:105:GLN:NE2	2.34	0.42
1:D:152:LYS:NZ	1:D:527:THR:OG1	2.50	0.42
1:D:403:LEU:HD21	1:D:538:LEU:HD11	2.01	0.42
1:D:480:GLU:OE2	1:D:526:GLY:N	2.41	0.42
1:D:481:ILE:O	1:D:525:LYS:HG3	2.19	0.42
2:E:7:LEU:HD11	2:E:23:LEU:CD2	2.47	0.42
1:A:223:PHE:CZ	1:A:533:GLU:HA	2.54	0.42
1:A:258:SER:OG	7:A:718:HOH:O	2.08	0.42
2:C:21:VAL:HG22	2:C:194:SER:O	2.18	0.42
2:C:22:ALA:HB1	2:C:74:VAL:HG11	2.00	0.42
1:D:111:ILE:HA	1:D:112:PRO:HD3	1.78	0.42
2:E:136:GLU:HG3	2:E:181:LYS:CD	2.49	0.42
2:F:70:VAL:O	2:F:74:VAL:HG23	2.19	0.42
1:A:315:LYS:HG3	1:A:319:TYR:CE2	2.54	0.42
1:A:424:ARG:C	1:A:543:GLY:HA2	2.39	0.42
1:A:573:THR:HG22	7:A:1001:HOH:O	2.19	0.42
2:B:193:GLU:N	7:B:431:HOH:O	2.53	0.42
2:B:215:ASN:O	7:B:423:HOH:O	2.21	0.42
1:D:23:ASN:O	1:D:27:VAL:HG12	2.20	0.42
1:D:358:LEU:HD21	7:D:924:HOH:O	2.20	0.42
1:D:378:GLY:N	1:D:381:GLN:HB2	2.35	0.42
2:E:41:SER:HB3	2:E:44:LEU:H	1.84	0.42
1:A:163:GLY:HA3	1:A:168:ASN:HD21	1.85	0.42
1:A:398:LEU:HD22	1:A:401:TYR:CD2	2.54	0.42
2:B:50:ILE:HG13	2:B:51:HIS:H	1.84	0.42
2:B:84:PHE:CD1	2:B:85:PHE:N	2.88	0.42
2:B:193:GLU:HA	2:B:196:SER:HB3	2.00	0.42
2:C:214:LYS:HG3	7:C:456:HOH:O	2.19	0.42
2:E:204:LYS:O	2:E:207:ALA:HB3	2.19	0.42
2:F:26:LYS:HE3	2:F:82:ASN:O	2.19	0.42
1:A:18:ASP:O	1:A:22:ARG:HG3	2.20	0.42
1:A:284:LEU:HD13	1:A:287:TRP:N	2.35	0.42
1:A:363:PHE:CD2	1:A:382:VAL:HG21	2.52	0.42
1:A:445:VAL:HA	1:A:479:TRP:CZ2	2.54	0.42
2:C:134:ILE:HG23	7:C:413:HOH:O	2.18	0.42
1:D:131:PHE:O	1:D:134:ARG:HB3	2.19	0.42
1:D:149:PHE:CZ	1:D:202:LEU:HA	2.55	0.42
1:D:280:LYS:HG3	7:D:992:HOH:O	2.20	0.42
1:D:300:TYR:HA	7:D:821:HOH:O	2.19	0.42
1:D:337:ILE:O	1:D:355:ILE:N	2.47	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:480:GLU:HB2	1:D:528:PHE:HD1	1.85	0.42
1:D:527:THR:O	1:D:530:LYS:HB2	2.20	0.42
1:A:331:GLY:CA	1:A:336:TRP:HA	2.50	0.42
2:B:76:GLU:OE2	2:C:96:ARG:NH1	2.52	0.42
2:B:132:VAL:HA	2:B:135:LEU:HB2	2.02	0.42
2:C:10:TYR:HA	2:C:34:GLU:OE2	2.20	0.42
1:D:82:ASP:O	1:D:84:ASP:N	2.47	0.42
1:D:108:PRO:HB3	1:D:555:ASN:CB	2.50	0.42
1:D:112:PRO:HD2	1:D:397:GLY:HA3	2.01	0.42
1:D:238:TRP:CD1	1:D:287:TRP:HH2	2.36	0.42
1:D:513:LYS:HZ2	1:D:575:PHE:HB3	1.83	0.42
1:D:556:ALA:HA	1:D:559:LEU:CB	2.50	0.42
2:E:5:PRO:HB3	2:E:59:HIS:NE2	2.35	0.42
2:E:15:PHE:HB3	6:E:301:GSH:HB13	2.02	0.42
2:E:103:ASP:O	2:E:107:THR:OG1	2.24	0.42
2:E:129:ILE:HG22	7:E:574:HOH:O	2.19	0.42
2:E:211:GLU:HA	2:E:214:LYS:HE3	2.02	0.42
1:A:101:SER:HB2	1:A:546:LYS:HB2	2.00	0.42
1:A:163:GLY:C	1:A:168:ASN:HD21	2.23	0.42
1:A:197:ASP:HB2	1:A:256:VAL:CG2	2.48	0.42
1:A:260:ARG:NE	7:A:814:HOH:O	2.49	0.42
1:A:498:ASP:CG	1:A:518:LEU:HB3	2.40	0.42
1:A:543:GLY:O	1:A:544:GLN:HG3	2.20	0.42
2:B:69:ASN:HD21	2:C:97:PHE:N	2.17	0.42
2:B:98:TRP:CH2	2:B:135:LEU:HG	2.55	0.42
2:C:4:LEU:HA	2:C:5:PRO:HD3	1.76	0.42
2:C:161:SER:HA	2:C:164:PHE:CG	2.55	0.42
1:D:28:GLN:CD	1:D:379:LEU:HD12	2.41	0.42
1:D:200:GLN:OE1	1:D:254:ILE:HA	2.20	0.42
1:D:239:GLU:O	1:D:242:VAL:HG22	2.20	0.42
1:D:448:ALA:CB	1:D:496:CYS:HB3	2.49	0.42
1:D:452:LEU:HB3	1:D:457:ILE:HD11	2.02	0.42
1:D:556:ALA:HA	1:D:559:LEU:HB2	2.01	0.42
1:D:565:ASN:O	1:D:567:VAL:N	2.53	0.42
2:E:68:LEU:HB3	7:E:438:HOH:O	2.20	0.42
1:A:29:LYS:O	1:A:33:LYS:HG2	2.19	0.42
1:A:33:LYS:NZ	1:A:57:PRO:HG2	2.34	0.42
1:A:81:VAL:HG13	1:A:162:VAL:HG11	2.00	0.42
1:A:133:ASN:OD1	1:A:138:ILE:HG23	2.20	0.42
1:A:196:PRO:HA	1:A:565:ASN:OD1	2.20	0.42
1:A:234:PHE:HE2	1:A:287:TRP:CZ3	2.38	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:511:LYS:HB2	1:A:511:LYS:HE2	1.78	0.42
2:B:17:MET:CE	2:B:200:PRO:HD2	2.48	0.42
2:C:26:LYS:HD3	2:C:26:LYS:HA	1.72	0.42
1:D:97:ILE:HG22	1:D:162:VAL:HB	2.01	0.42
2:E:24:ARG:CB	2:E:194:SER:HA	2.50	0.42
1:A:425:ARG:CG	1:A:427:LEU:HB2	2.50	0.41
1:A:448:ALA:HB3	1:A:479:TRP:CH2	2.55	0.41
1:A:527:THR:HG23	1:A:561:ILE:CG2	2.50	0.41
2:B:78:TRP:HB3	2:B:81:LYS:HZ2	1.85	0.41
2:B:97:PHE:CE2	2:B:101:PHE:CZ	3.08	0.41
2:C:40:LYS:HE2	2:C:40:LYS:HB2	1.77	0.41
1:D:143:LYS:HD3	1:D:212:PHE:CG	2.55	0.41
1:D:167:THR:HB	1:D:560:GLN:HE21	1.84	0.41
1:D:210:ILE:HD12	1:D:210:ILE:HG23	1.86	0.41
1:D:292:PRO:HD3	1:D:320:ALA:O	2.20	0.41
1:D:546:LYS:HE2	1:D:546:LYS:HB3	1.70	0.41
2:E:110:GLN:HE22	2:E:160:PHE:HB3	1.84	0.41
2:F:6:ILE:HD12	2:F:58:VAL:HB	2.01	0.41
2:F:131:ALA:HB3	7:F:414:HOH:O	2.20	0.41
1:A:21:THR:O	1:A:24:ALA:HB2	2.20	0.41
1:A:65:VAL:N	7:A:797:HOH:O	2.53	0.41
1:A:219:VAL:CG1	1:A:301:VAL:HG22	2.51	0.41
1:A:273:LEU:HA	1:A:276:THR:HG23	2.02	0.41
1:A:435:LYS:HG2	1:A:438:GLU:H	1.80	0.41
2:B:144:TYR:HB3	2:B:154:ASP:CG	2.40	0.41
1:D:94:VAL:CG1	1:D:112:PRO:HB3	2.43	0.41
1:D:132:ARG:CA	1:D:343:PRO:HG3	2.45	0.41
1:D:169:VAL:HG12	1:D:175:PHE:CD1	2.55	0.41
1:D:332:SER:HA	4:D:602:ATP:C5	2.56	0.41
1:D:387:GLU:HB3	1:D:406:VAL:CG1	2.50	0.41
1:D:479:TRP:HZ2	1:D:497:LEU:HD21	1.85	0.41
1:D:552:LYS:C	1:D:554:SER:N	2.73	0.41
2:E:110:GLN:HG2	2:E:167:TYR:CE2	2.55	0.41
2:F:182:LEU:O	2:F:185:TRP:HE3	2.02	0.41
1:A:44:TYR:HB2	7:A:939:HOH:O	2.18	0.41
1:A:157:THR:OG1	7:A:707:HOH:O	2.18	0.41
1:A:351:THR:HA	7:A:723:HOH:O	2.20	0.41
1:A:445:VAL:HG13	1:A:479:TRP:CE2	2.56	0.41
1:D:100:SER:CB	1:D:109:LYS:NZ	2.83	0.41
1:D:199:HIS:CD2	1:D:200:GLN:HG3	2.55	0.41
1:D:238:TRP:CD1	1:D:287:TRP:CH2	3.09	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:252:ASN:OD1	1:D:252:ASN:N	2.53	0.41
1:D:331:GLY:HA2	1:D:539:GLY:CA	2.51	0.41
1:D:449:ALA:HB3	7:D:865:HOH:O	2.20	0.41
1:D:520:LEU:CD1	1:D:522:VAL:CG2	2.97	0.41
1:A:90:THR:HG21	1:A:397:GLY:H	1.85	0.41
1:A:99:LEU:HG	1:A:555:ASN:OD1	2.21	0.41
1:A:212:PHE:N	1:A:212:PHE:CD1	2.88	0.41
2:B:73:TYR:HD1	2:B:76:GLU:OE2	2.02	0.41
2:C:8:LEU:O	2:C:55:PRO:HA	2.21	0.41
2:C:107:THR:HA	2:C:110:GLN:CG	2.51	0.41
2:C:123:ALA:HB3	7:C:450:HOH:O	2.19	0.41
2:C:158:ILE:O	2:C:161:SER:OG	2.12	0.41
2:C:163:TRP:CG	2:C:205:ILE:HG21	2.55	0.41
1:D:163:GLY:HA2	1:D:560:GLN:CB	2.50	0.41
2:E:4:LEU:HA	2:E:5:PRO:HD3	1.85	0.41
2:F:31:GLU:HB3	7:F:488:HOH:O	2.21	0.41
1:A:80:MET:SD	1:A:87:PRO:HA	2.60	0.41
1:A:145:LEU:O	1:A:220:PHE:N	2.51	0.41
2:B:15:PHE:HB3	6:B:301:GSH:O11	2.21	0.41
2:B:117:LYS:C	2:B:121:GLN:HB2	2.41	0.41
2:C:116:LYS:HD3	2:C:116:LYS:HA	1.87	0.41
1:D:475:TYR:HE1	1:D:515:ILE:HG21	1.86	0.41
2:E:120:GLU:O	2:E:123:ALA:HB3	2.21	0.41
2:E:144:TYR:CE1	2:E:189:CYS:SG	3.11	0.41
1:A:311:PRO:O	7:A:752:HOH:O	2.22	0.41
1:A:450:LYS:HD2	2:B:190:MET:C	2.41	0.41
2:B:89:PRO:HD2	7:B:492:HOH:O	2.20	0.41
2:B:98:TRP:CD1	2:B:153:VAL:HG21	2.56	0.41
2:B:150:PHE:CE1	2:B:155:ILE:HG13	2.49	0.41
2:C:18:ARG:N	2:C:159:THR:HG21	2.35	0.41
2:C:21:VAL:HG12	2:C:155:ILE:HG12	2.03	0.41
2:C:210:ALA:O	2:C:213:ARG:HB2	2.19	0.41
1:D:33:LYS:NZ	1:D:57:PRO:HG2	2.35	0.41
2:B:183:ILE:O	2:B:187:LYS:HG3	2.20	0.41
2:C:16:GLY:HA2	2:C:55:PRO:HG3	2.03	0.41
1:D:117:LEU:HB2	4:D:602:ATP:H4'	2.03	0.41
1:D:124:LEU:HA	1:D:124:LEU:HD12	1.42	0.41
1:D:245:ILE:HG12	1:D:245:ILE:H	1.53	0.41
1:D:527:THR:HG23	1:D:561:ILE:HG22	2.02	0.41
2:E:157:LEU:HA	2:E:160:PHE:HD2	1.86	0.41
2:F:177:SER:N	7:F:411:HOH:O	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:HIS:O	1:A:94:VAL:HG13	2.20	0.41
1:A:103:THR:HB	1:A:106:GLY:CA	2.51	0.41
1:A:203:TYR:HE2	1:A:244:ASP:OD2	2.03	0.41
1:A:203:TYR:OH	1:A:244:ASP:OD2	2.37	0.41
1:A:280:LYS:O	1:A:283:SER:OG	2.33	0.41
1:A:450:LYS:HZ1	2:B:191:GLU:HB3	1.84	0.41
1:A:496:CYS:HA	1:A:499:ARG:NH1	2.35	0.41
1:A:499:ARG:CZ	1:A:499:ARG:CB	2.97	0.41
1:A:538:LEU:O	1:A:544:GLN:NE2	2.48	0.41
2:B:114:TRP:CZ3	2:B:212:TYR:HD2	2.38	0.41
1:D:60:ALA:HB1	1:D:64:MET:SD	2.61	0.41
1:D:224:ALA:HB3	1:D:312:TYR:HB3	2.03	0.41
1:D:445:VAL:HG21	1:D:462:PHE:CD1	2.56	0.41
1:D:534:HIS:NE2	1:D:557:LYS:HD3	2.35	0.41
2:E:126:LYS:O	2:E:129:ILE:HG13	2.21	0.41
2:F:155:ILE:HG12	7:F:417:HOH:O	2.20	0.41
1:A:110:PHE:CZ	1:A:553:PRO:O	2.74	0.41
1:A:111:ILE:HD13	1:A:111:ILE:HA	1.84	0.41
1:A:153:GLN:HG2	1:A:167:THR:HG21	2.02	0.41
1:A:299:LYS:HB2	1:A:300:TYR:HD1	1.86	0.41
1:A:328:HIS:HE2	3:A:601:JAA:C04	2.33	0.41
1:A:491:GLN:CD	1:A:573:THR:HG23	2.41	0.41
1:A:542:ALA:O	1:A:544:GLN:N	2.52	0.41
1:A:550:CYS:O	7:A:751:HOH:O	2.22	0.41
2:B:12:PRO:O	2:B:163:TRP:HZ2	2.04	0.41
2:B:98:TRP:CE3	2:B:98:TRP:O	2.74	0.41
2:B:114:TRP:HD1	2:B:167:TYR:CE1	2.34	0.41
2:B:172:ASN:O	2:B:172:ASN:ND2	2.53	0.41
2:C:24:ARG:HD2	2:C:198:SER:OG	2.21	0.41
1:D:98:SER:O	1:D:110:PHE:HA	2.21	0.41
1:D:100:SER:CB	1:D:109:LYS:HZ2	2.34	0.41
1:D:162:VAL:CG2	1:D:559:LEU:HD23	2.48	0.41
1:D:363:PHE:O	1:D:365:PRO:HD3	2.21	0.41
1:D:494:CYS:SG	1:D:572:SER:HA	2.61	0.41
2:E:24:ARG:HG3	2:E:30:PHE:CZ	2.56	0.41
2:E:41:SER:OG	2:E:43:LEU:HD23	2.21	0.41
2:E:98:TRP:HE3	2:E:101:PHE:CB	2.34	0.41
2:F:48:ASN:ND2	2:F:65:CYS:SG	2.66	0.41
1:A:133:ASN:HB3	7:A:885:HOH:O	2.19	0.41
1:A:434:ASP:CG	1:A:550:CYS:HB3	2.41	0.41
2:C:23:LEU:HD22	2:C:30:PHE:CG	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:182:LEU:HD12	2:C:182:LEU:HA	1.82	0.41
1:D:22:ARG:HG2	1:D:415:ASN:OD1	2.21	0.41
1:D:45:LEU:HB3	1:D:50:LEU:HB2	2.03	0.41
1:D:96:ALA:HA	1:D:161:PRO:O	2.21	0.41
1:D:118:MET:O	1:D:121:THR:HB	2.21	0.41
1:D:330:TYR:CE2	1:D:352:PHE:CD1	3.09	0.41
1:D:413:TYR:N	1:D:416:THR:O	2.54	0.41
1:D:448:ALA:HB2	1:D:496:CYS:HB3	2.02	0.41
2:E:136:GLU:O	2:E:181:LYS:HD3	2.20	0.41
2:E:157:LEU:HG	2:E:185:TRP:HH2	1.84	0.41
1:A:76:TYR:CD2	1:A:88:ILE:HG21	2.55	0.40
1:A:97:ILE:HG22	1:A:98:SER:N	2.36	0.40
1:A:143:LYS:C	1:A:184:SER:HB3	2.41	0.40
1:A:246:LYS:HZ2	1:A:271:PRO:HA	1.86	0.40
1:A:265:LYS:NZ	7:A:823:HOH:O	2.54	0.40
1:A:278:ARG:HB2	7:A:771:HOH:O	2.21	0.40
1:A:295:PHE:CD2	1:A:295:PHE:N	2.89	0.40
2:C:73:TYR:OH	7:C:420:HOH:O	2.20	0.40
1:D:405:ASP:OD2	1:D:540:SER:HB2	2.21	0.40
1:D:480:GLU:HG3	1:D:525:LYS:HA	2.02	0.40
1:A:226:GLY:HA2	1:A:529:ARG:HD2	2.03	0.40
1:A:384:ILE:HG12	1:A:412:PHE:HE1	1.86	0.40
1:A:447:SER:HA	1:A:450:LYS:NZ	2.36	0.40
2:C:42:PRO:O	2:C:46:GLN:HB2	2.21	0.40
1:D:131:PHE:CE1	1:D:341:VAL:HB	2.55	0.40
1:D:212:PHE:HB3	1:D:215:GLN:HE21	1.86	0.40
2:E:26:LYS:HG2	2:E:81:LYS:NZ	2.36	0.40
2:E:64:VAL:HB	2:E:73:TYR:CE2	2.56	0.40
2:F:164:PHE:CD1	2:F:164:PHE:C	2.94	0.40
2:F:183:ILE:O	2:F:186:ALA:HB3	2.20	0.40
1:A:207:LEU:HA	1:A:207:LEU:HD12	1.69	0.40
1:A:224:ALA:H	1:A:309:MET:CE	2.28	0.40
1:A:330:TYR:HE1	1:A:536:LEU:O	2.05	0.40
2:B:100:ASP:HB3	7:C:402:HOH:O	2.20	0.40
2:C:199:LEU:HA	2:C:200:PRO:HD2	1.91	0.40
1:D:17:PHE:O	1:D:21:THR:HG23	2.22	0.40
1:D:116:GLU:O	1:D:119:GLU:HB2	2.20	0.40
1:D:263:MET:HE3	7:D:883:HOH:O	2.21	0.40
1:D:295:PHE:HA	1:D:296:PRO:HD3	1.87	0.40
2:E:12:PRO:O	2:E:163:TRP:HZ2	2.04	0.40
2:E:106:PHE:C	7:E:403:HOH:O	2.59	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:193:GLU:HA	2:F:196:SER:HB3	2.03	0.40
1:A:42:ALA:HB3	1:A:45:LEU:HD22	2.03	0.40
1:A:74:GLU:HG3	1:A:554:SER:HB2	2.03	0.40
1:A:125:PHE:O	1:A:129:PHE:HB2	2.22	0.40
1:A:178:GLY:N	7:A:783:HOH:O	2.55	0.40
1:A:313:VAL:N	1:A:314:PRO:HD2	2.37	0.40
2:B:104:LYS:HG3	2:B:105:LYS:N	2.35	0.40
2:C:129:ILE:O	2:C:132:VAL:HG12	2.22	0.40
2:C:181:LYS:H	2:C:181:LYS:HG2	1.48	0.40
1:D:108:PRO:HB2	1:D:554:SER:OG	2.22	0.40
1:D:149:PHE:CZ	1:D:205:HIS:CG	3.09	0.40
1:D:192:VAL:HA	1:D:195:SER:HB2	2.04	0.40
2:E:56:VAL:HG22	7:E:440:HOH:O	2.21	0.40
2:E:65:CYS:O	2:E:69:ASN:HB3	2.21	0.40
2:F:15:PHE:O	2:F:18:ARG:HB2	2.21	0.40
1:A:276:THR:OG1	1:A:277:ILE:N	2.54	0.40
1:A:288:TYR:CD1	1:A:318:HIS:HA	2.57	0.40
1:A:318:HIS:ND1	7:A:709:HOH:O	2.00	0.40
1:A:328:HIS:HE2	3:A:601:JAA:C12	2.26	0.40
1:D:43:ILE:HG13	1:D:44:TYR:CD1	2.56	0.40
1:D:235:GLU:HG2	1:D:287:TRP:CG	2.57	0.40
1:D:250:LEU:HD13	1:D:254:ILE:HG23	2.04	0.40
1:D:256:VAL:HB	1:D:259:VAL:HG12	2.03	0.40
1:D:566:VAL:CG1	1:D:569:SER:HB2	2.52	0.40
2:E:62:LYS:HA	2:E:63:PRO:HD2	1.88	0.40
2:E:79:PRO:HB3	7:E:466:HOH:O	2.20	0.40

All (26) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:107:ARG:NH1	1:D:139:ASP:OD2[1_545]	1.73	0.47
1:A:114:THR:OG1	2:F:141:ASP:OD2[1_454]	1.79	0.41
2:E:38:SER:O	2:F:29:GLU:N[1_565]	1.98	0.22
7:D:717:HOH:O	7:E:427:HOH:O[1_565]	2.04	0.16
7:E:605:HOH:O	7:F:538:HOH:O[1_565]	2.04	0.16
7:C:551:HOH:O	7:D:1021:HOH:O[1_655]	2.05	0.15
7:D:985:HOH:O	7:D:1015:HOH:O[1_565]	2.05	0.15
7:E:576:HOH:O	7:F:541:HOH:O[1_565]	2.06	0.14
1:A:213:ARG:NH2	1:A:436:ASN:OD1[1_565]	2.07	0.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:987:HOH:O	7:F:522:HOH:O[1_354]	2.07	0.13
7:D:733:HOH:O	7:D:785:HOH:O[1_665]	2.07	0.13
1:D:270:ASN:ND2	1:D:510:ARG:O[1_565]	2.09	0.11
7:D:1072:HOH:O	7:E:557:HOH:O[1_455]	2.09	0.11
1:D:213:ARG:NH1	1:D:436:ASN:OD1[1_565]	2.12	0.08
7:D:1172:HOH:O	7:E:659:HOH:O[1_565]	2.13	0.07
7:F:621:HOH:O	7:F:624:HOH:O[1_545]	2.14	0.06
1:D:272:GLU:OE1	2:E:188:ARG:NH1[1_565]	2.15	0.05
7:B:490:HOH:O	7:C:498:HOH:O[1_565]	2.16	0.04
7:E:566:HOH:O	7:F:538:HOH:O[1_565]	2.16	0.04
2:B:215:ASN:O	2:C:33:ARG:NH2[1_565]	2.17	0.03
7:B:572:HOH:O	7:B:591:HOH:O[1_665]	2.17	0.03
7:A:1034:HOH:O	7:A:1054:HOH:O[1_665]	2.18	0.02
7:C:456:HOH:O	7:D:948:HOH:O[1_655]	2.18	0.02
7:C:499:HOH:O	7:D:915:HOH:O[1_655]	2.18	0.02
1:D:276:THR:O	7:D:709:HOH:O[1_565]	2.19	0.01
7:D:724:HOH:O	7:D:873:HOH:O[1_665]	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%)	511 (90%)	36 (6%)	20 (4%)	<b>3</b> <b>0</b>
1	D	567/575 (99%)	512 (90%)	39 (7%)	16 (3%)	<b>5</b> <b>0</b>
2	B	212/223 (95%)	193 (91%)	17 (8%)	2 (1%)	<b>17</b> <b>3</b>
2	C	212/223 (95%)	196 (92%)	16 (8%)	0	<b>100</b> <b>100</b>
2	E	212/223 (95%)	192 (91%)	14 (7%)	6 (3%)	<b>5</b> <b>0</b>
2	F	212/223 (95%)	191 (90%)	18 (8%)	3 (1%)	<b>11</b> <b>1</b>
All	All	1982/2042 (97%)	1795 (91%)	140 (7%)	47 (2%)	<b>6</b> <b>0</b>

All (47) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	368	GLU
1	A	437	THR
1	A	513	LYS
1	A	540	SER
1	A	542	ALA
1	A	546	LYS
1	D	90	THR
1	D	437	THR
1	D	513	LYS
1	D	544	GLN
2	E	140	GLY
1	A	286	ASN
2	B	140	GLY
1	D	368	GLU
1	D	369	THR
1	D	540	SER
1	A	211	LEU
1	D	211	LEU
1	D	566	VAL
1	A	24	ALA
1	A	329	ASP
1	A	367	SER
1	A	369	THR
1	A	433	ILE
1	D	93	PRO
1	D	150	SER
1	D	165	ALA
2	E	55	PRO
2	E	66	GLU
2	E	172	ASN
2	F	140	GLY
1	A	88	ILE
1	A	93	PRO
1	A	294	LEU
2	B	66	GLU
1	D	509	SER
1	D	574	ALA
1	A	547	MET
2	F	66	GLU
2	E	12	PRO
2	F	86	PRO
1	D	553	PRO
2	E	27	GLY

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Mol	Chain	Res	Type
1	A	185	PRO
1	D	185	PRO
1	A	543	GLY
1	A	370	GLY

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

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	499/505 (99%)	435 (87%)	64 (13%)	4	0
1	D	499/505 (99%)	442 (89%)	57 (11%)	5	0
2	B	187/195 (96%)	162 (87%)	25 (13%)	4	0
2	C	187/195 (96%)	174 (93%)	13 (7%)	15	1
2	E	187/195 (96%)	157 (84%)	30 (16%)	2	0
2	F	187/195 (96%)	169 (90%)	18 (10%)	8	0
All	All	1746/1790 (98%)	1539 (88%)	207 (12%)	5	0

All (207) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	VAL
1	A	55	THR
1	A	67	LEU
1	A	90	THR
1	A	108	PRO
1	A	110	PHE
1	A	125	PHE
1	A	126	ARG
1	A	150	SER
1	A	152	LYS
1	A	153	GLN
1	A	154	TYR
1	A	182	ILE
1	A	184	SER

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	188	SER
1	A	198	VAL
1	A	212	PHE
1	A	215	GLN
1	A	229	HIS
1	A	232	ARG
1	A	239	GLU
1	A	241	ILE
1	A	245	ILE
1	A	246	LYS
1	A	251	SER
1	A	275	GLU
1	A	276	THR
1	A	282	MET
1	A	284	LEU
1	A	305	MET
1	A	326	VAL
1	A	329	ASP
1	A	333	SER
1	A	337	ILE
1	A	369	THR
1	A	394	ASN
1	A	405	ASP
1	A	422	ILE
1	A	423	CYS
1	A	425	ARG
1	A	428	ILE
1	A	435	LYS
1	A	437	THR
1	A	440	ASP
1	A	450	LYS
1	A	455	GLU
1	A	457	ILE
1	A	460	ILE
1	A	468	VAL
1	A	494	CYS
1	A	499	ARG
1	A	503	ASP
1	A	509	SER
1	A	510	ARG
1	A	512	CYS
1	A	514	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	529	ARG
1	A	534	HIS
1	A	535	PHE
1	A	538	LEU
1	A	540	SER
1	A	545	PHE
1	A	547	MET
1	A	567	VAL
2	B	14	MET
2	B	28	VAL
2	B	32	TYR
2	B	38	SER
2	B	43	LEU
2	B	45	LEU
2	B	50	ILE
2	B	65	CYS
2	B	69	ASN
2	B	84	PHE
2	B	117	LYS
2	B	125	LYS
2	B	133	LYS
2	B	134	ILE
2	B	135	LEU
2	B	136	GLU
2	B	139	LEU
2	B	145	PHE
2	B	149	SER
2	B	176	GLU
2	B	185	TRP
2	B	188	ARG
2	B	189	CYS
2	B	200	PRO
2	B	204	LYS
2	C	23	LEU
2	C	26	LYS
2	C	33	ARG
2	C	57	LEU
2	C	80	GLU
2	C	103	ASP
2	C	110	GLN
2	C	122	GLU
2	C	145	PHE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	C	168	GLU
2	C	173	PHE
2	C	181	LYS
2	C	213	ARG
1	D	46	GLN
1	D	77	ILE
1	D	80	MET
1	D	88	ILE
1	D	90	THR
1	D	92	HIS
1	D	97	ILE
1	D	99	LEU
1	D	107	ARG
1	D	109	LYS
1	D	118	MET
1	D	124	LEU
1	D	125	PHE
1	D	133	ASN
1	D	150	SER
1	D	152	LYS
1	D	182	ILE
1	D	188	SER
1	D	192	VAL
1	D	212	PHE
1	D	241	ILE
1	D	245	ILE
1	D	251	SER
1	D	252	ASN
1	D	254	ILE
1	D	264	SER
1	D	281	CYS
1	D	290	LEU
1	D	301	VAL
1	D	326	VAL
1	D	329	ASP
1	D	340	ASN
1	D	345	LEU
1	D	348	GLU
1	D	367	SER
1	D	369	THR
1	D	374	GLU
1	D	379	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	D	416	THR
1	D	423	CYS
1	D	430	SER
1	D	452	LEU
1	D	468	VAL
1	D	469	SER
1	D	481	ILE
1	D	492	ASP
1	D	493	CYS
1	D	494	CYS
1	D	502	ILE
1	D	503	ASP
1	D	512	CYS
1	D	514	THR
1	D	520	LEU
1	D	534	HIS
1	D	554	SER
1	D	562	LEU
1	D	563	CYS
2	E	6	ILE
2	E	14	MET
2	E	35	GLU
2	E	43	LEU
2	E	48	ASN
2	E	64	VAL
2	E	68	LEU
2	E	74	VAL
2	E	76	GLU
2	E	84	PHE
2	E	96	ARG
2	E	101	PHE
2	E	134	ILE
2	E	135	LEU
2	E	137	SER
2	E	139	LEU
2	E	145	PHE
2	E	148	ASP
2	E	149	SER
2	E	157	LEU
2	E	161	SER
2	E	162	SER
2	E	173	PHE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	E	175	ILE
2	E	176	GLU
2	E	187	LYS
2	E	189	CYS
2	E	206	VAL
2	E	212	TYR
2	E	216	ASN
2	F	10	TYR
2	F	28	VAL
2	F	29	GLU
2	F	33	ARG
2	F	41	SER
2	F	65	CYS
2	F	103	ASP
2	F	110	GLN
2	F	132	VAL
2	F	148	ASP
2	F	150	PHE
2	F	153	VAL
2	F	170	PHE
2	F	173	PHE
2	F	183	ILE
2	F	185	TRP
2	F	211	GLU
2	F	213	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	30	GLN
1	A	123	GLN
1	A	146	GLN
1	A	200	GLN
1	A	215	GLN
1	A	229	HIS
1	A	357	ASN
1	A	394	ASN
1	A	418	GLN
1	A	491	GLN
1	A	495	ASN
1	A	565	ASN
2	B	60	ASN

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Mol	Chain	Res	Type
2	B	69	ASN
2	B	72	GLN
2	C	51	HIS
1	D	28	GLN
1	D	168	ASN
1	D	174	ASN
1	D	217	GLN
1	D	534	HIS
1	D	544	GLN
1	D	560	GLN
2	E	60	ASN
2	E	69	ASN
2	E	110	GLN
2	E	172	ASN
2	F	60	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 2 are monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	GSH	F	301	-	18,19,19	1.57	3 (16%)	23,24,24	2.55	6 (26%)
4	ATP	D	602	5	26,33,33	4.04	16 (61%)	31,52,52	3.15	13 (41%)
4	ATP	A	602	5	26,33,33	4.23	15 (57%)	31,52,52	3.18	15 (48%)
3	JAA	D	601	-	15,15,15	5.08	7 (46%)	15,19,19	3.17	8 (53%)
6	GSH	E	301	-	18,19,19	1.58	4 (22%)	23,24,24	3.19	7 (30%)
6	GSH	C	301	-	18,19,19	1.47	3 (16%)	23,24,24	2.93	6 (26%)
6	GSH	B	301	-	18,19,19	1.54	5 (27%)	23,24,24	2.64	7 (30%)
3	JAA	A	601	-	15,15,15	5.19	7 (46%)	15,19,19	3.21	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
6	GSH	F	301	-	-	6/24/24/24	-
4	ATP	D	602	5	-	5/18/38/38	0/3/3/3
4	ATP	A	602	5	-	6/18/38/38	0/3/3/3
3	JAA	D	601	-	-	6/9/22/22	0/1/1/1
6	GSH	E	301	-	-	9/24/24/24	-
6	GSH	C	301	-	-	7/24/24/24	-
6	GSH	B	301	-	-	3/24/24/24	-
3	JAA	A	601	-	-	6/9/22/22	0/1/1/1

All (60) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	601	JAA	C05-C08	-12.57	1.31	1.52
3	A	601	JAA	C05-C08	-12.31	1.31	1.52
3	A	601	JAA	C06-C04	-11.53	1.23	1.53
4	A	602	ATP	C4-N3	11.14	1.51	1.35
3	D	601	JAA	C06-C04	-11.01	1.25	1.53
4	A	602	ATP	C3'-C4'	-9.91	1.27	1.53
4	D	602	ATP	C4-N3	9.83	1.49	1.35
4	D	602	ATP	C3'-C4'	-8.53	1.31	1.53
3	A	601	JAA	C07-C08	7.06	1.62	1.51
4	D	602	ATP	C2'-C3'	-6.92	1.34	1.53
4	A	602	ATP	C2'-C3'	-6.85	1.34	1.53
4	D	602	ATP	C2'-C1'	-6.38	1.44	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	601	JAA	C07-C08	6.16	1.61	1.51
4	A	602	ATP	C2'-C1'	-5.85	1.44	1.53
4	A	602	ATP	C6-N6	-5.70	1.13	1.34
4	D	602	ATP	C2-N1	5.56	1.44	1.33
4	D	602	ATP	C6-N6	-5.42	1.14	1.34
4	A	602	ATP	C2-N1	5.08	1.43	1.33
3	D	601	JAA	C05-C04	5.05	1.67	1.54
4	D	602	ATP	O4'-C1'	4.86	1.47	1.41
3	A	601	JAA	C10-C04	-4.82	1.45	1.53
3	A	601	JAA	C05-C04	4.39	1.65	1.54
3	D	601	JAA	C09-C05	-4.18	1.48	1.54
4	A	602	ATP	C5-C4	-4.05	1.30	1.40
4	A	602	ATP	O4'-C1'	4.01	1.46	1.41
3	D	601	JAA	C10-C04	-3.93	1.47	1.53
3	A	601	JAA	C09-C05	-3.67	1.49	1.54
4	D	602	ATP	C5-C4	-3.53	1.31	1.40
6	F	301	GSH	C2-N3	3.39	1.41	1.33
4	D	602	ATP	PG-O1G	3.32	1.61	1.50
4	D	602	ATP	C5-N7	-3.24	1.28	1.39
4	A	602	ATP	C5-N7	-3.24	1.28	1.39
4	A	602	ATP	O3'-C3'	-3.21	1.35	1.43
6	C	301	GSH	CA2-N2	-3.11	1.39	1.45
4	A	602	ATP	O2'-C2'	-3.03	1.35	1.43
6	C	301	GSH	C2-N3	3.02	1.40	1.33
6	F	301	GSH	CA2-N2	-3.01	1.39	1.45
4	D	602	ATP	O2'-C2'	-3.00	1.35	1.43
4	A	602	ATP	O4'-C4'	-2.83	1.38	1.45
4	A	602	ATP	C2-N3	-2.80	1.27	1.32
6	F	301	GSH	CD1-N2	2.73	1.39	1.34
6	B	301	GSH	CA2-N2	-2.72	1.40	1.45
3	A	601	JAA	O03-C12	-2.66	1.21	1.30
4	A	602	ATP	PG-O3G	-2.62	1.44	1.54
6	E	301	GSH	O2-C2	-2.60	1.18	1.23
6	C	301	GSH	CD1-N2	2.54	1.39	1.34
6	E	301	GSH	CA2-N2	-2.54	1.40	1.45
4	D	602	ATP	PG-O3G	-2.52	1.45	1.54
6	B	301	GSH	C2-N3	2.50	1.39	1.33
4	A	602	ATP	O5'-C5'	-2.43	1.35	1.44
4	D	602	ATP	O3'-C3'	-2.35	1.37	1.43
6	B	301	GSH	CB2-CA2	-2.33	1.50	1.53
4	D	602	ATP	O4'-C4'	-2.30	1.39	1.45
6	B	301	GSH	CD1-N2	2.24	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	E	301	GSH	CD1-N2	2.20	1.38	1.34
4	D	602	ATP	O5'-C5'	-2.15	1.36	1.44
6	E	301	GSH	C2-N3	2.12	1.38	1.33
4	D	602	ATP	PG-O2G	-2.11	1.46	1.54
3	D	601	JAA	C06-C07	2.08	1.57	1.53
6	B	301	GSH	O12-C1	-2.05	1.23	1.30

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	E	301	GSH	CA2-CB2-SG2	-12.60	100.03	114.19
6	C	301	GSH	CA2-CB2-SG2	-9.68	103.31	114.19
6	B	301	GSH	CA2-CB2-SG2	-9.37	103.66	114.19
3	A	601	JAA	C07-C06-C04	-8.29	95.75	104.41
4	A	602	ATP	C4-C5-N7	-8.08	100.97	109.40
4	D	602	ATP	C4-C5-N7	-7.93	101.13	109.40
6	F	301	GSH	CA2-CB2-SG2	-7.61	105.64	114.19
4	D	602	ATP	C1'-N9-C4	6.86	138.70	126.64
4	A	602	ATP	PA-O3A-PB	-6.85	109.33	132.83
4	A	602	ATP	C5'-C4'-C3'	-6.53	90.69	115.18
4	D	602	ATP	PA-O3A-PB	-6.08	111.96	132.83
3	D	601	JAA	C07-C06-C04	-6.02	98.13	104.41
4	D	602	ATP	O2G-PG-O3B	5.46	122.96	104.64
3	A	601	JAA	C09-C11-C13	-5.31	106.69	126.40
3	D	601	JAA	C09-C11-C13	-5.28	106.79	126.40
6	C	301	GSH	CG1-CD1-N2	-5.23	106.76	115.83
4	D	602	ATP	C5'-C4'-C3'	-5.19	95.71	115.18
6	B	301	GSH	CB2-CA2-N2	-5.18	103.89	111.28
3	D	601	JAA	C06-C07-C08	-5.09	100.31	105.42
6	C	301	GSH	CB1-CG1-CD1	4.87	123.92	113.04
4	A	602	ATP	N3-C2-N1	-4.86	121.08	128.68
4	A	602	ATP	C2'-C3'-C4'	4.67	111.71	102.64
6	F	301	GSH	CB2-CA2-N2	-4.57	104.77	111.28
4	A	602	ATP	C1'-N9-C4	4.42	134.41	126.64
4	D	602	ATP	C2'-C3'-C4'	4.29	110.97	102.64
6	F	301	GSH	CG1-CD1-N2	-4.03	108.84	115.83
3	D	601	JAA	O03-C12-C10	3.97	126.78	114.07
6	C	301	GSH	OE1-CD1-CG1	3.95	129.25	122.02
6	F	301	GSH	CB1-CG1-CD1	3.92	121.80	113.04
6	C	301	GSH	CG1-CB1-CA1	-3.89	104.76	113.84
4	A	602	ATP	O4'-C4'-C3'	3.86	112.76	105.11
4	D	602	ATP	O4'-C4'-C3'	3.76	112.55	105.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	601	JAA	C06-C07-C08	-3.71	101.69	105.42
3	A	601	JAA	C06-C04-C10	-3.71	106.52	113.41
6	E	301	GSH	CB1-CG1-CD1	3.64	121.17	113.04
4	D	602	ATP	N3-C2-N1	-3.60	123.05	128.68
3	A	601	JAA	C07-C08-C05	-3.38	103.33	109.05
3	D	601	JAA	C07-C08-C05	-3.38	103.33	109.05
6	F	301	GSH	CG1-CB1-CA1	-3.36	106.01	113.84
4	A	602	ATP	C2-N1-C6	3.35	124.48	118.75
3	D	601	JAA	O01-C08-C05	3.29	129.82	125.58
4	A	602	ATP	O2'-C2'-C3'	3.26	122.36	111.82
4	A	602	ATP	N6-C6-N1	3.22	125.25	118.57
4	A	602	ATP	O3'-C3'-C2'	3.21	122.21	111.82
6	E	301	GSH	CG1-CB1-CA1	-3.19	106.39	113.84
3	A	601	JAA	O01-C08-C05	3.13	129.62	125.58
4	D	602	ATP	C5-C6-N1	-3.13	113.26	120.35
3	D	601	JAA	C06-C04-C10	-2.96	107.91	113.41
4	A	602	ATP	C5-C6-N1	-2.94	113.68	120.35
4	D	602	ATP	PA-O5'-C5'	-2.91	104.64	121.68
6	B	301	GSH	C3-CA3-N3	-2.88	104.17	113.06
6	E	301	GSH	C2-CA2-N2	-2.78	103.58	111.16
4	A	602	ATP	PA-O5'-C5'	-2.78	105.38	121.68
4	D	602	ATP	N6-C6-N1	2.76	124.30	118.57
3	D	601	JAA	O02-C12-C10	-2.71	114.10	122.80
6	E	301	GSH	CA2-N2-CD1	-2.60	114.97	121.65
4	D	602	ATP	C2-N1-C6	2.54	123.09	118.75
6	B	301	GSH	CG1-CB1-CA1	-2.51	107.98	113.84
6	F	301	GSH	CB2-CA2-C2	-2.46	104.69	109.76
6	B	301	GSH	CG1-CD1-N2	-2.44	111.61	115.83
6	E	301	GSH	CA3-N3-C2	-2.41	115.41	121.37
6	B	301	GSH	O11-C1-CA1	-2.38	113.73	122.14
6	C	301	GSH	CB2-CA2-N2	-2.37	107.90	111.28
6	E	301	GSH	OE1-CD1-CG1	2.19	126.02	122.02
4	A	602	ATP	O5'-PA-O1A	-2.08	100.94	109.07
6	B	301	GSH	C2-CA2-N2	-2.02	105.67	111.16
4	D	602	ATP	O3'-C3'-C4'	2.01	116.86	111.05
4	A	602	ATP	O3B-PG-O1G	2.01	122.33	111.19

There are no chirality outliers.

All (48) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	601	JAA	C05-C04-C10-C12

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Mol	Chain	Res	Type	Atoms
3	A	601	JAA	C06-C04-C10-C12
3	A	601	JAA	C11-C13-C14-C15
3	D	601	JAA	C11-C13-C14-C15
4	A	602	ATP	C5'-O5'-PA-O1A
4	A	602	ATP	C5'-O5'-PA-O3A
4	A	602	ATP	O4'-C4'-C5'-O5'
4	A	602	ATP	C3'-C4'-C5'-O5'
4	D	602	ATP	C5'-O5'-PA-O3A
4	D	602	ATP	O4'-C4'-C5'-O5'
6	B	301	GSH	N2-CA2-CB2-SG2
6	B	301	GSH	C2-CA2-CB2-SG2
6	C	301	GSH	C1-CA1-CB1-CG1
6	C	301	GSH	N2-CA2-CB2-SG2
6	C	301	GSH	C2-CA2-CB2-SG2
6	E	301	GSH	C1-CA1-CB1-CG1
6	E	301	GSH	N2-CA2-CB2-SG2
6	E	301	GSH	C2-CA2-CB2-SG2
6	F	301	GSH	C1-CA1-CB1-CG1
6	F	301	GSH	C2-CA2-CB2-SG2
3	A	601	JAA	C09-C11-C13-C14
4	D	602	ATP	C3'-C4'-C5'-O5'
6	E	301	GSH	O12-C1-CA1-N1
6	E	301	GSH	O32-C3-CA3-N3
6	E	301	GSH	CA1-CB1-CG1-CD1
3	D	601	JAA	C09-C11-C13-C14
6	C	301	GSH	O31-C3-CA3-N3
6	C	301	GSH	O32-C3-CA3-N3
6	E	301	GSH	O31-C3-CA3-N3
6	F	301	GSH	O12-C1-CA1-N1
4	D	602	ATP	PG-O3B-PB-O3A
6	E	301	GSH	O11-C1-CA1-N1
6	F	301	GSH	O11-C1-CA1-N1
3	A	601	JAA	C04-C05-C09-C11
3	D	601	JAA	C04-C05-C09-C11
4	A	602	ATP	C4'-C5'-O5'-PA
6	F	301	GSH	N1-CA1-CB1-CG1
3	A	601	JAA	C08-C05-C09-C11
6	F	301	GSH	N2-CA2-CB2-SG2
4	A	602	ATP	PG-O3B-PB-O3A
3	D	601	JAA	C04-C10-C12-O03
6	B	301	GSH	O12-C1-CA1-N1
6	C	301	GSH	O11-C1-CA1-N1

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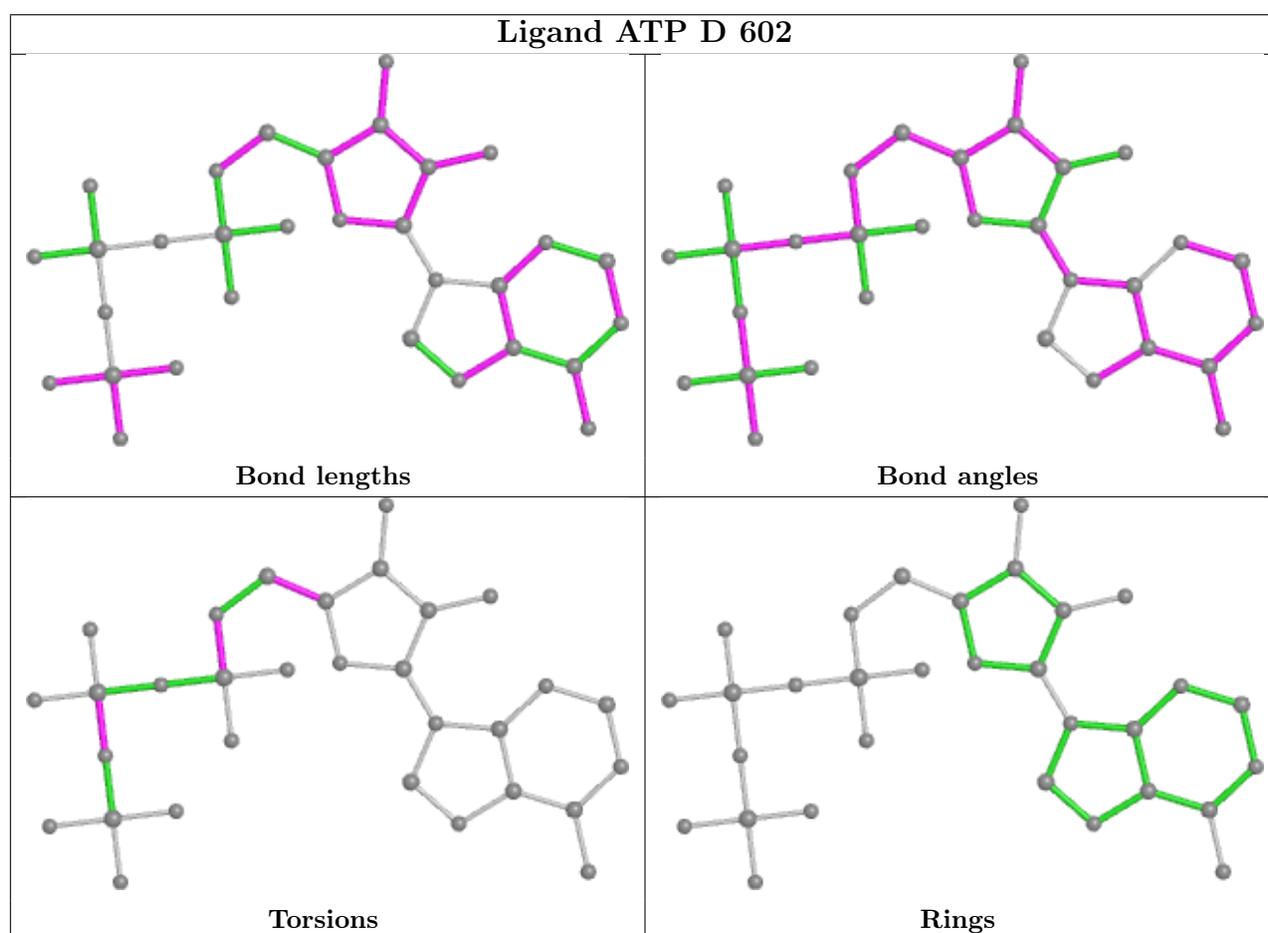
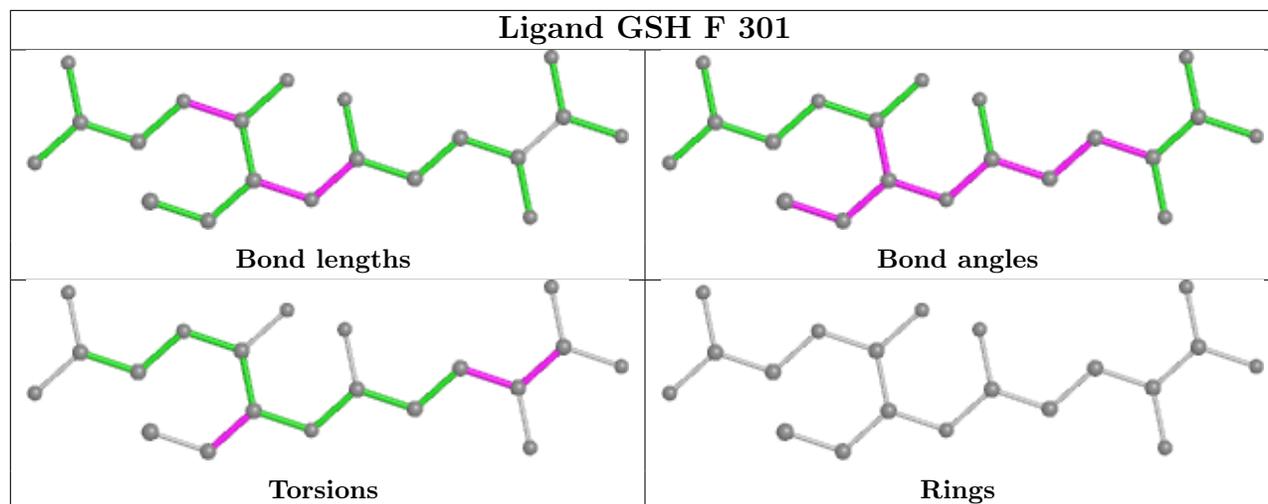
Mol	Chain	Res	Type	Atoms
3	D	601	JAA	C04-C10-C12-O02
6	C	301	GSH	O12-C1-CA1-N1
4	D	602	ATP	PG-O3B-PB-O1B
6	E	301	GSH	OE1-CD1-CG1-CB1
3	D	601	JAA	C08-C05-C09-C11

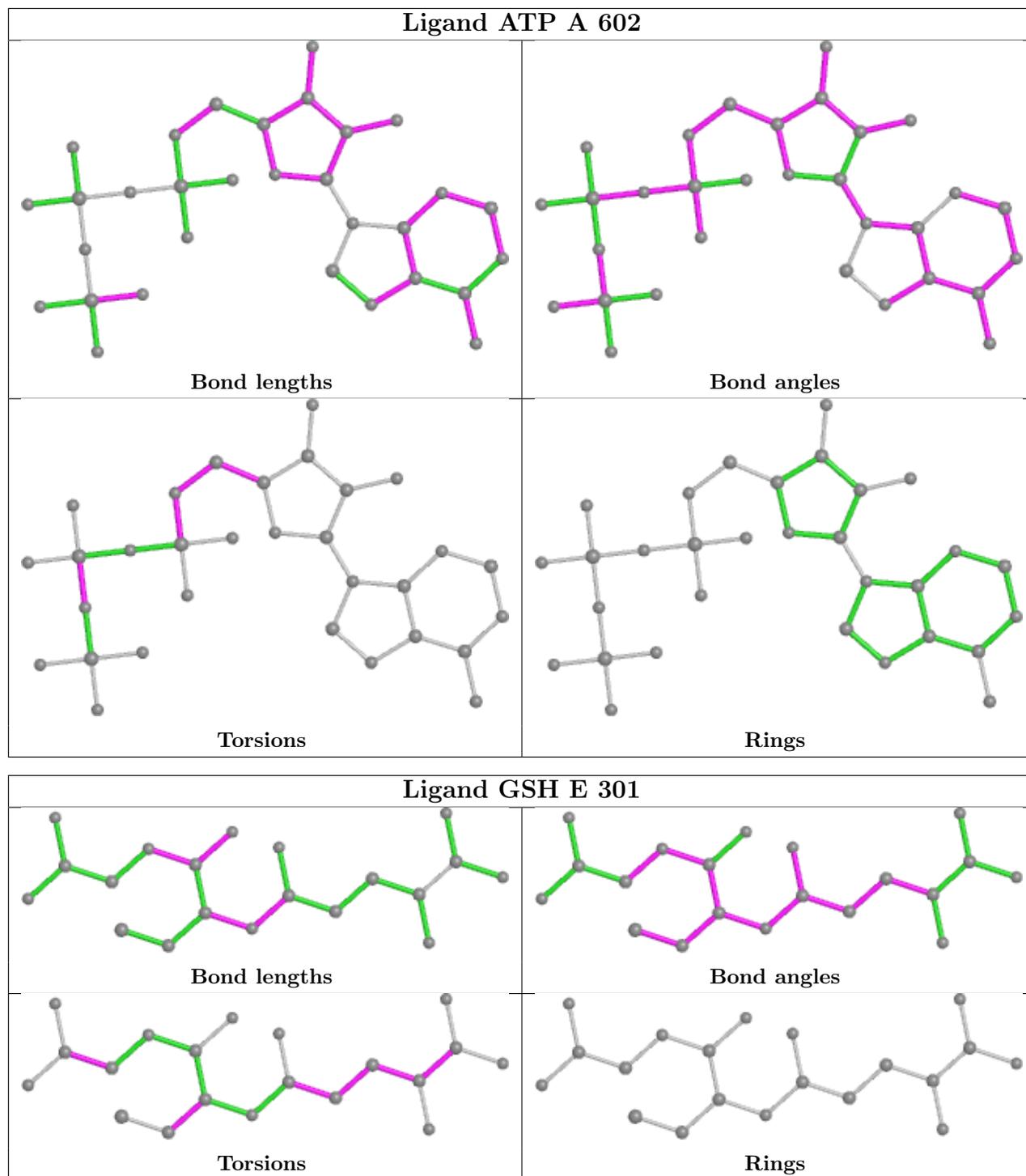
There are no ring outliers.

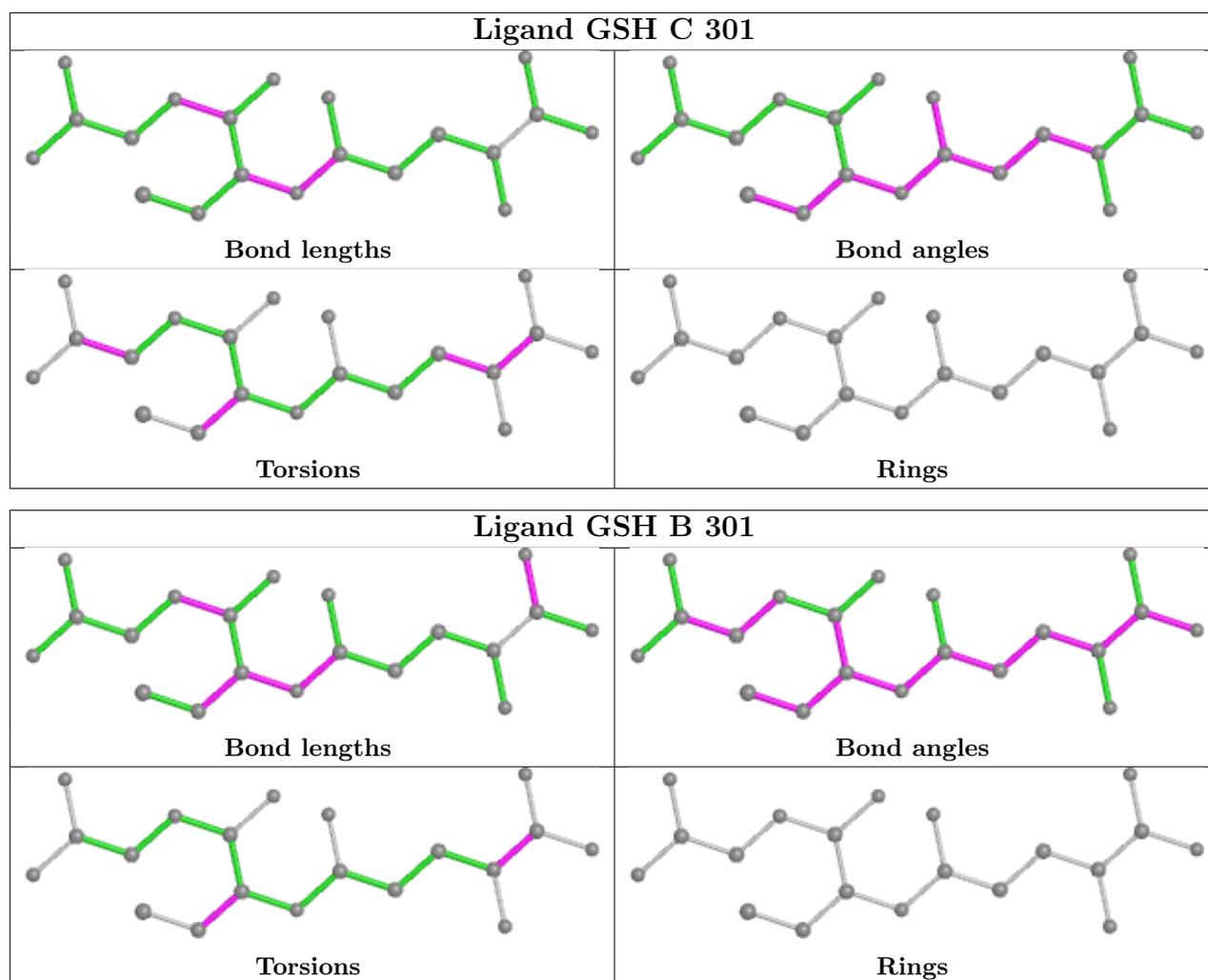
7 monomers are involved in 51 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	F	301	GSH	2	0
4	D	602	ATP	14	0
4	A	602	ATP	12	0
3	D	601	JAA	1	0
6	E	301	GSH	12	0
6	B	301	GSH	8	0
3	A	601	JAA	3	0

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







## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	569/575 (98%)	0.09	3 (0%) 91 93	3, 3, 3, 16	0
1	D	569/575 (98%)	0.08	3 (0%) 91 93	3, 3, 3, 16	0
2	B	214/223 (95%)	0.04	3 (1%) 75 80	2, 3, 7, 11	0
2	C	214/223 (95%)	-0.03	0 100 100	3, 3, 3, 4	0
2	E	214/223 (95%)	0.20	6 (2%) 53 60	2, 3, 7, 11	0
2	F	214/223 (95%)	-0.03	1 (0%) 91 93	3, 3, 3, 4	0
All	All	1994/2042 (97%)	0.07	16 (0%) 86 89	2, 3, 5, 16	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	77	ALA	4.3
1	D	493	CYS	3.0
2	E	186	ALA	2.9
2	E	32	TYR	2.9
2	E	13	SER	2.9
2	E	64	VAL	2.6
1	A	515	ILE	2.3
1	A	295	PHE	2.3
1	D	259	VAL	2.2
2	B	68	LEU	2.2
2	E	95	ALA	2.2
1	A	342	THR	2.1
2	E	78	TRP	2.1
2	F	158	ILE	2.0
2	B	111	PHE	2.0
1	D	316	LEU	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

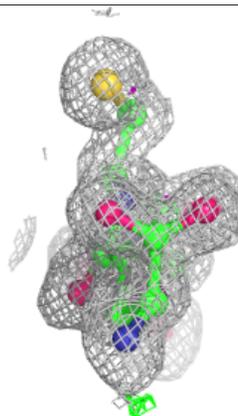
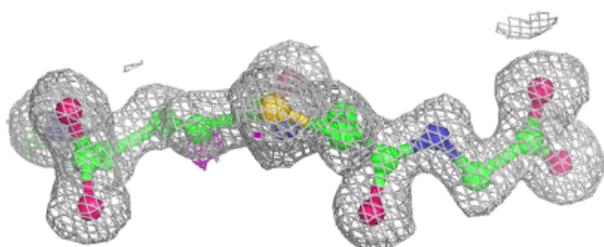
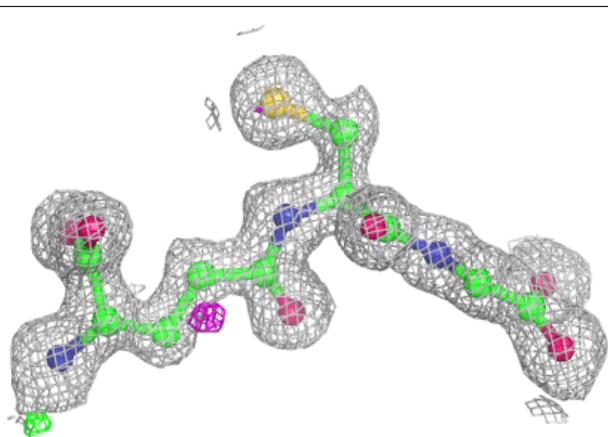
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	JAA	A	601	15/15	0.96	0.11	3,3,3,3	0
3	JAA	D	601	15/15	0.97	0.12	3,3,3,3	0
6	GSH	F	301	20/20	0.98	0.09	2,3,3,3	0
4	ATP	D	602	31/31	0.99	0.07	3,3,3,3	0
5	MG	D	603	1/1	0.99	0.06	3,3,3,3	0
6	GSH	B	301	20/20	0.99	0.08	2,2,3,3	0
6	GSH	C	301	20/20	0.99	0.08	2,3,3,3	0
6	GSH	E	301	20/20	0.99	0.07	2,2,3,3	0
4	ATP	A	602	31/31	0.99	0.07	3,3,3,3	0
5	MG	A	603	1/1	1.00	0.07	3,3,3,3	0

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

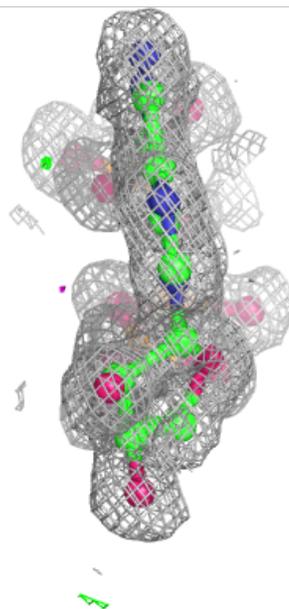
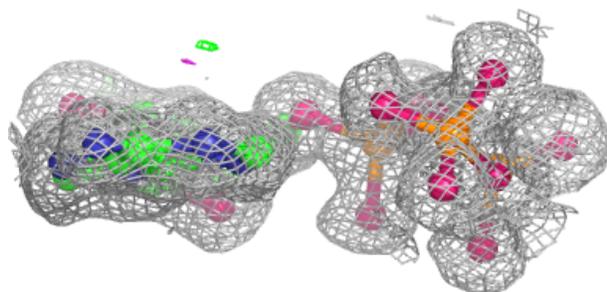
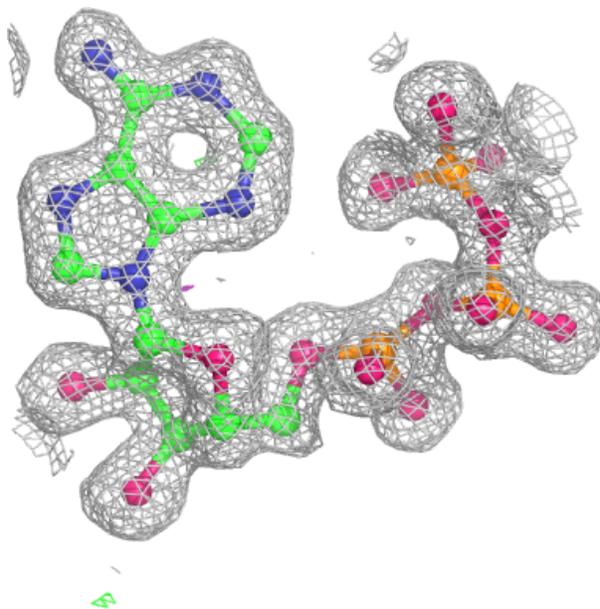
**Electron density around GSH F 301:**

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



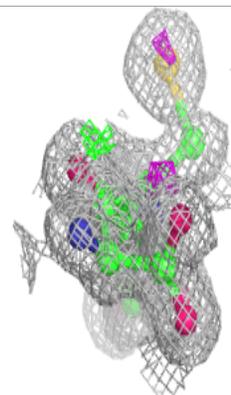
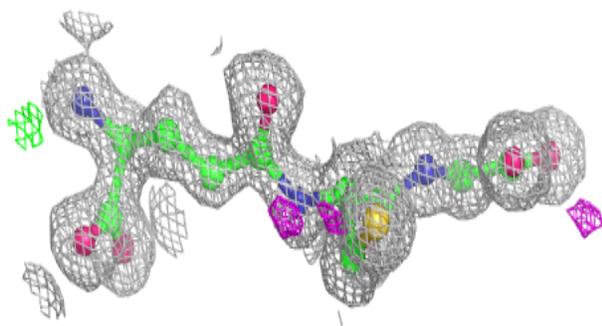
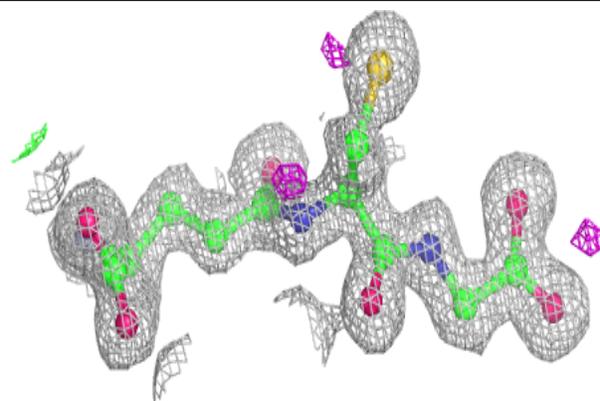
**Electron density around ATP D 602:**

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

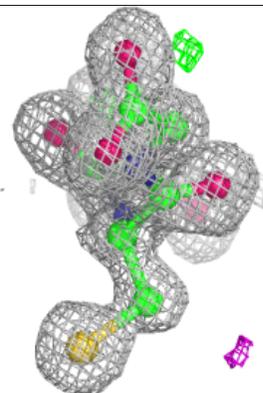
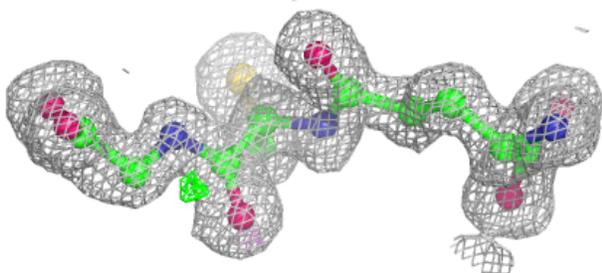
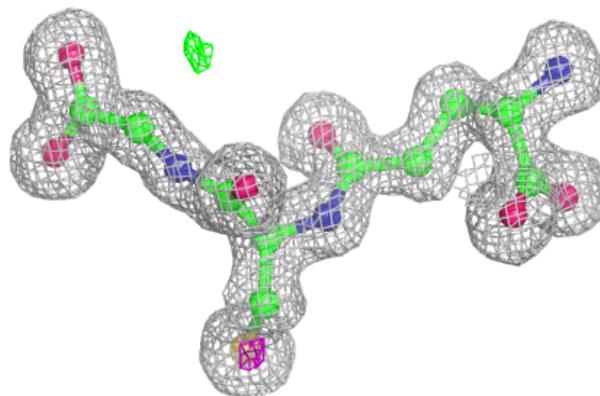


**Electron density around GSH B 301:**

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

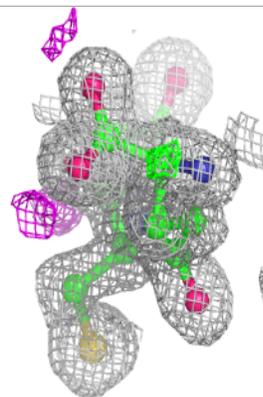
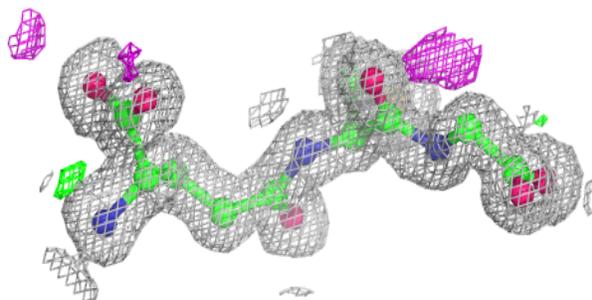
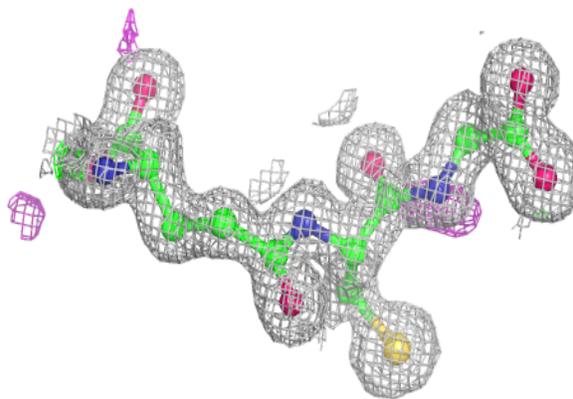
**Electron density around GSH C 301:**

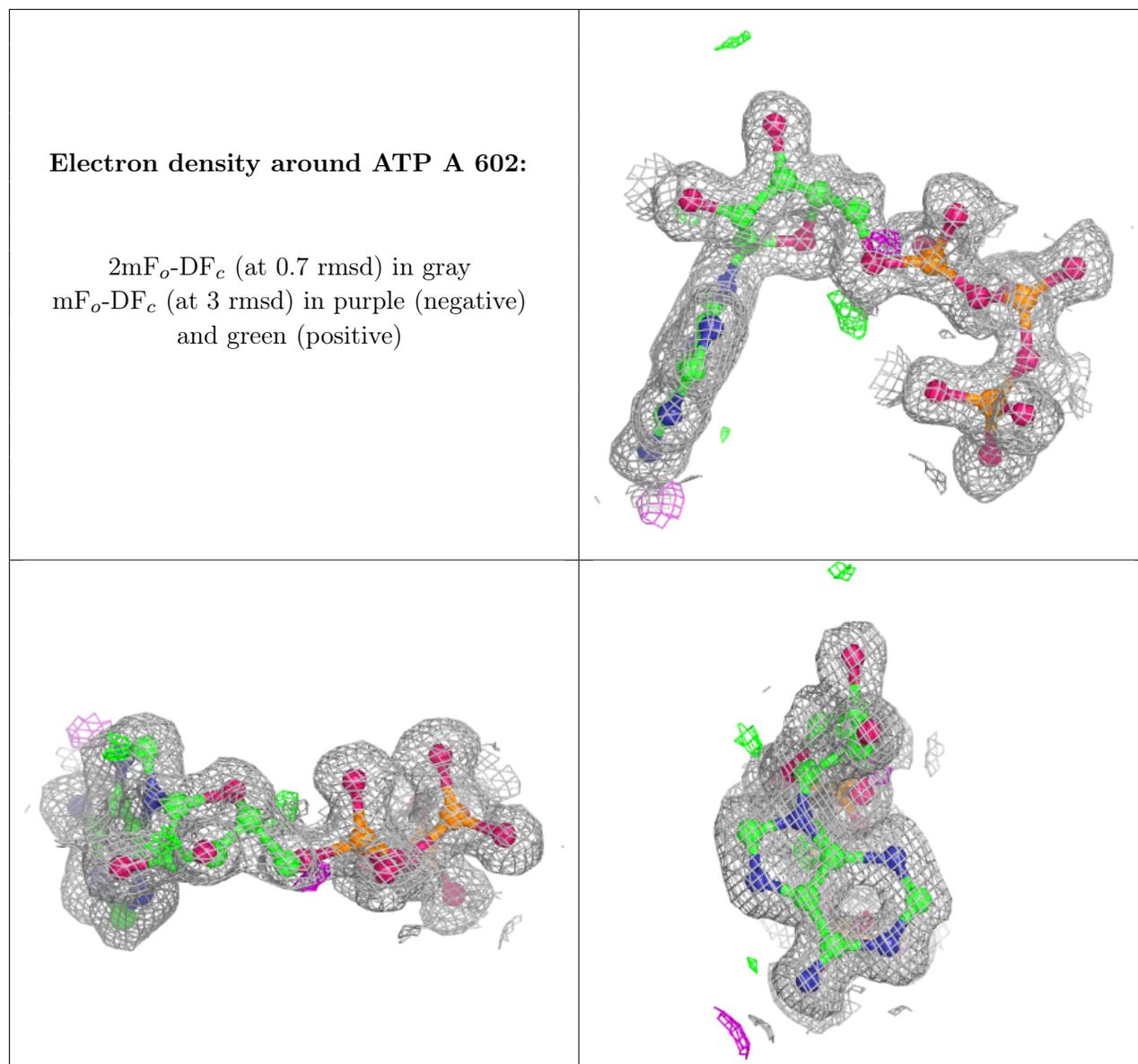
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around GSH E 301:**

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





## 6.5 Other polymers [i](#)

There are no such residues in this entry.