



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 19, 2020 – 08:02 pm BST

PDB ID : 5ECP
Title : Crystal Structure of FIN219-FIP1 complex with JA, MET and ATP
Authors : Chen, C.Y.; Cheng, Y.S.
Deposited on : 2015-10-20
Resolution : 2.25 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

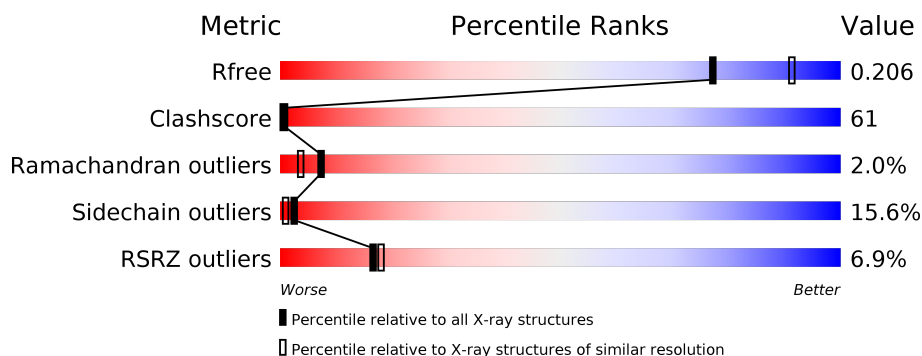
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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

Mol	Chain	Length	Quality of chain
1	A	575	<div> <div>9%</div> <div>23% 61% 13%</div> <div>..</div> </div>
1	D	575	<div> <div>10%</div> <div>23% 60% 15%</div> <div>..</div> </div>
2	B	223	<div> <div>4%</div> <div>35% 54% 6%</div> <div>..</div> </div>
2	C	223	<div> <div>%</div> <div>30% 56% 9%</div> <div>.</div> </div>
2	E	223	<div> <div>6%</div> <div>35% 53% 8%</div> <div>.</div> </div>
2	F	223	<div> <div>%</div> <div>25% 58% 13%</div> <div>.</div> </div>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	ATP	A	603	-	-	X	-
5	ATP	D	603	-	-	X	-

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 17707 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Jasmonic acid-amido synthetase JAR1.

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

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

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

There are 24 discrepancies between the modelled and reference sequences:

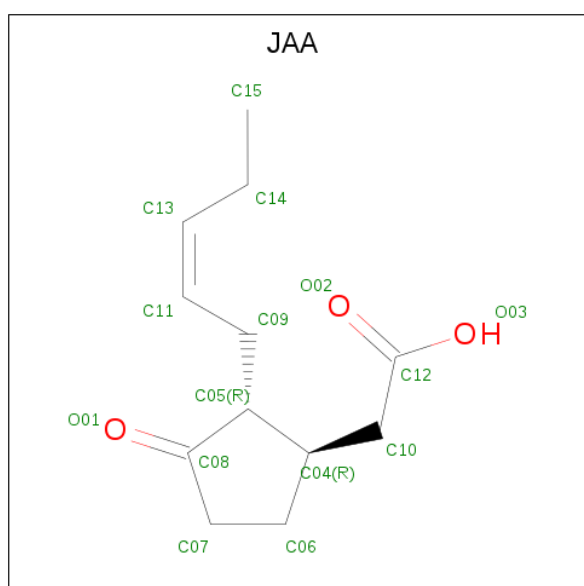
Chain	Residue	Modelled	Actual	Comment	Reference
B	-5	HIS	-	expression tag	UNP Q8L7C9
B	-4	HIS	-	expression tag	UNP Q8L7C9
B	-3	HIS	-	expression tag	UNP Q8L7C9
B	-2	HIS	-	expression tag	UNP Q8L7C9
B	-1	HIS	-	expression tag	UNP Q8L7C9
B	0	HIS	-	expression tag	UNP Q8L7C9
C	-5	HIS	-	expression tag	UNP Q8L7C9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

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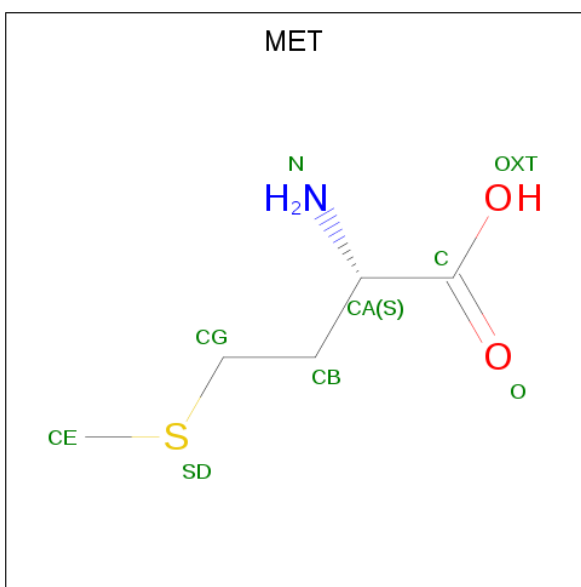
Chain	Residue	Modelled	Actual	Comment	Reference
E	-5	HIS	-	expression tag	UNP Q8L7C9
E	-4	HIS	-	expression tag	UNP Q8L7C9
E	-3	HIS	-	expression tag	UNP Q8L7C9
E	-2	HIS	-	expression tag	UNP Q8L7C9
E	-1	HIS	-	expression tag	UNP Q8L7C9
E	0	HIS	-	expression tag	UNP Q8L7C9
F	-5	HIS	-	expression tag	UNP Q8L7C9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

- Molecule 3 is {(1R,2R)-3-oxo-2-[(2Z)-pent-2-en-1-yl]cyclopentyl}acetic acid (three-letter code: JAA) (formula: C₁₂H₁₈O₃).



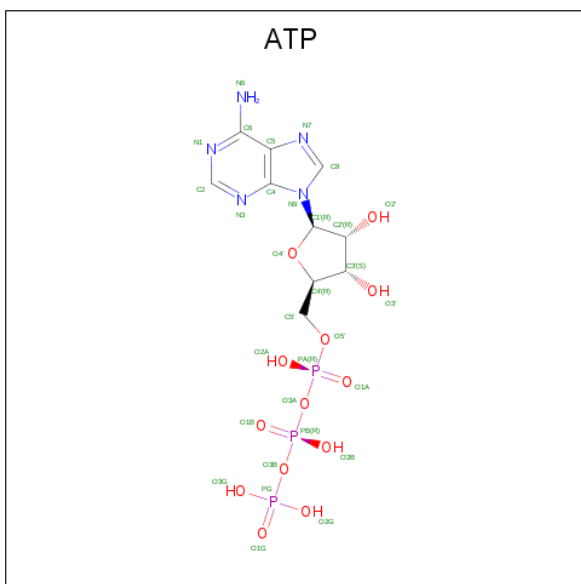
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			15	12	3		
3	D	1	Total	C	O	0	0
			15	12	3		

- Molecule 4 is METHIONINE (three-letter code: MET) (formula: C₅H₁₁NO₂S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 9	C 5	N 1	O 2	S 1	0	0
4	D	1	Total 9	C 5	N 1	O 2	S 1	0	0

- Molecule 5 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $\text{C}_{10}\text{H}_{16}\text{N}_5\text{O}_{13}\text{P}_3$).



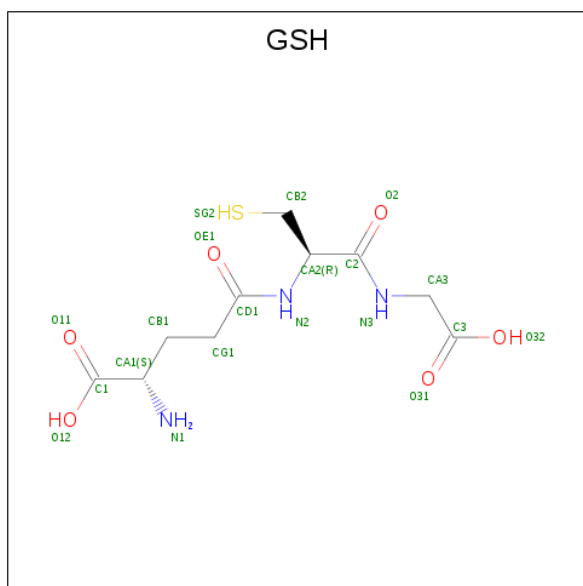
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total 31	C 10	N 5	O 13	P 3	0	0

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

- Molecule 6 is GLUTATHIONE (three-letter code: GSH) (formula: C₁₀H₁₇N₃O₆S).



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

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	357	Total	O	0	0
			357	357		
7	B	193	Total	O	0	0
			193	193		
7	C	214	Total	O	0	0
			214	214		
7	D	403	Total	O	0	0
			403	403		

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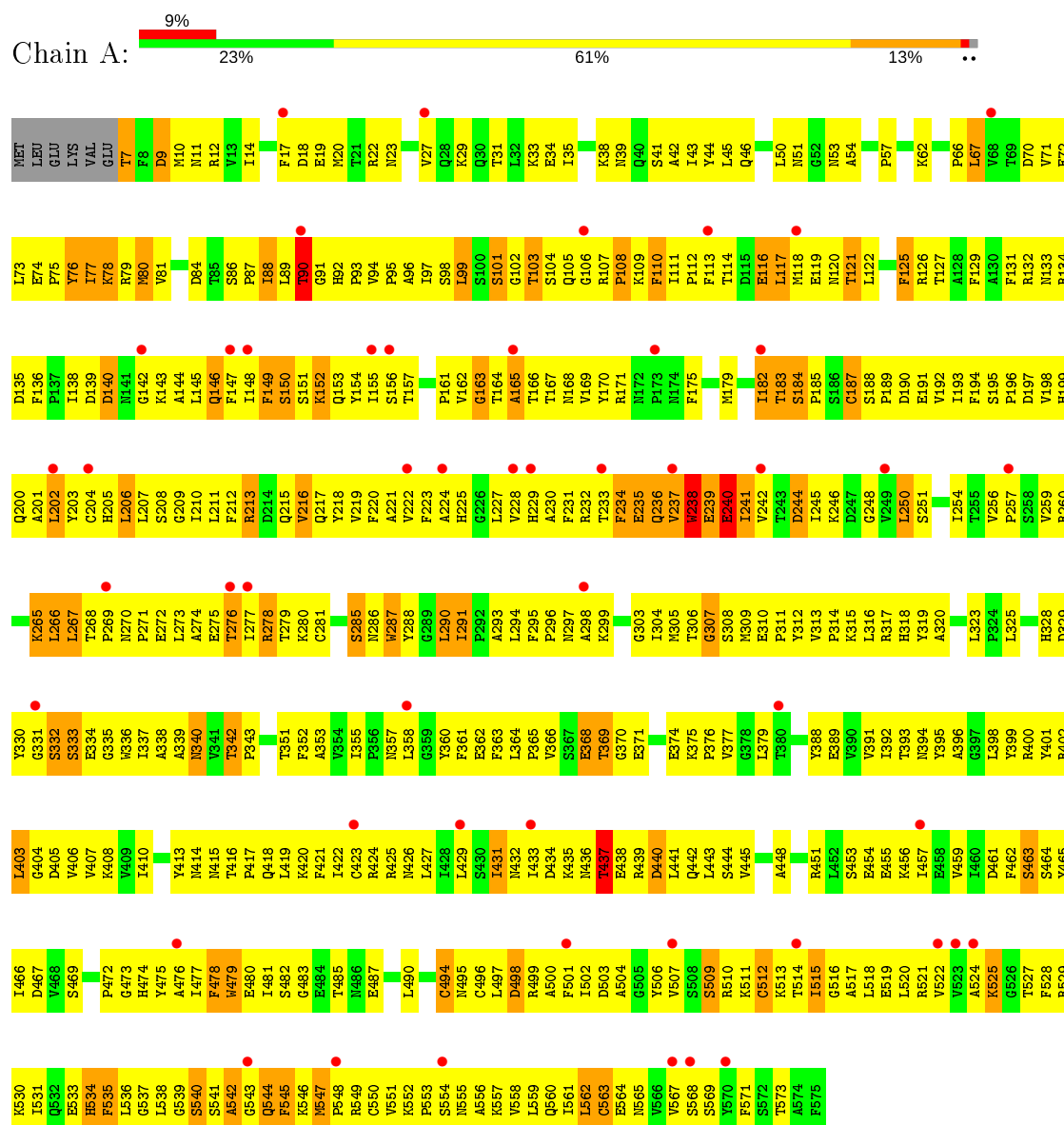
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	E	201	Total 201	O 201	0	0
7	F	199	Total 199	O 199	0	0

3 Residue-property plots

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

- Molecule 1: Jasmonic acid-amido synthetase JAR1



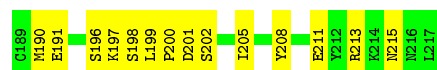
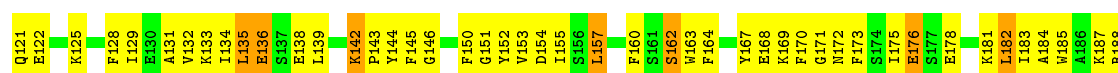
- Molecule 1: Jasmonic acid-amido synthetase JAR1



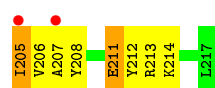
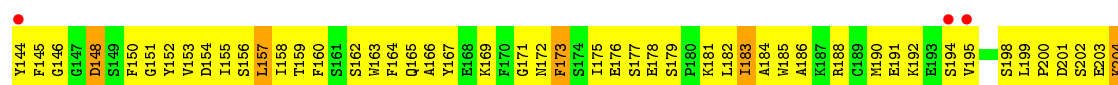




• Molecule 2: Glutathione S-transferase U20

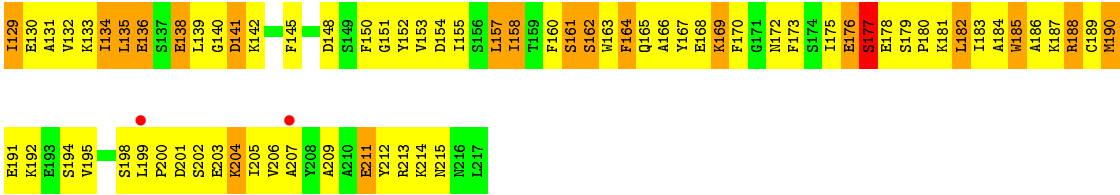


• Molecule 2: Glutathione S-transferase U20



• Molecule 2: Glutathione S-transferase U20





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	53.71Å 53.70Å 192.03Å 89.96° 90.16° 113.24°	Depositor
Resolution (Å)	23.35 – 2.25 23.35 – 2.25	Depositor EDS
% Data completeness (in resolution range)	95.5 (23.35-2.25) 95.1 (23.35-2.25)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.65 (at 2.24Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.185 , 0.208 0.184 , 0.206	Depositor DCC
R_{free} test set	2254 reflections (2.53%)	wwPDB-VP
Wilson B-factor (Å ²)	11.4	Xtriage
Anisotropy	0.085	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.20 , 249.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.053 for -h,-k,l 0.076 for -k,-h,-l 0.076 for k,h,-l	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	17707	wwPDB-VP
Average B, all atoms (Å ²)	11.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 27.70 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.1005e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.67	1/4581 (0.0%)	0.82	6/6219 (0.1%)
1	D	0.66	0/4581	0.80	7/6219 (0.1%)
2	B	0.72	0/1799	0.70	1/2428 (0.0%)
2	C	0.84	0/1799	0.72	0/2428
2	E	0.73	0/1799	0.69	1/2428 (0.0%)
2	F	0.90	0/1799	0.85	1/2428 (0.0%)
All	All	0.73	1/16358 (0.0%)	0.78	16/22150 (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	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	238	TRP	CB-CG	-5.44	1.40	1.50

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	99	LEU	CA-CB-CG	7.91	133.50	115.30
1	A	99	LEU	CB-CG-CD2	6.70	122.38	111.00
1	A	290	LEU	CB-CG-CD1	-6.05	100.72	111.00
1	A	99	LEU	CB-CG-CD1	-5.92	100.94	111.00
1	D	536	LEU	CA-CB-CG	5.85	128.76	115.30
2	B	139	LEU	CA-CB-CG	5.68	128.35	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	250	LEU	CA-CB-CG	5.66	128.31	115.30
1	D	475	TYR	CA-CB-CG	-5.59	102.78	113.40
1	A	163	GLY	N-CA-C	5.57	127.03	113.10
1	D	211	LEU	CA-CB-CG	5.37	127.66	115.30
1	D	86	SER	C-N-CD	-5.36	108.82	120.60
2	E	11	TRP	C-N-CD	5.34	139.62	128.40
2	F	177	SER	N-CA-CB	-5.30	102.55	110.50
1	D	419	LEU	CA-CB-CG	5.24	127.34	115.30
1	D	536	LEU	CB-CG-CD2	5.11	119.69	111.00
1	D	284	LEU	CA-CB-CG	5.02	126.84	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	234	PHE	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4479	0	4434	615	6
1	D	4479	0	4434	639	5
2	B	1748	0	1704	187	1
2	C	1748	0	1704	197	1
2	E	1748	0	1704	180	1
2	F	1748	0	1704	211	1
3	A	15	0	0	0	0
3	D	15	0	0	3	0
4	A	9	0	8	2	0
4	D	9	0	8	5	0
5	A	31	0	8	17	0
5	D	31	0	8	26	0
6	B	20	0	15	1	0
6	C	20	0	15	0	0
6	E	20	0	15	3	0
6	F	20	0	15	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	357	0	0	75	7
7	B	193	0	0	28	2
7	C	214	0	0	30	1
7	D	403	0	0	74	4
7	E	201	0	0	28	1
7	F	199	0	0	35	3
All	All	17707	0	15776	1939	22

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 61.

All (1939) 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:121:THR:HG21	1:A:175:PHE:CE1	1.69	1.27
1:A:121:THR:CG2	1:A:175:PHE:HE1	1.56	1.18
1:A:120:ASN:HD21	1:A:358:LEU:HD22	1.17	1.10
1:A:121:THR:HG21	1:A:175:PHE:HE1	0.93	1.05
1:D:334:GLU:O	1:D:394:ASN:ND2	1.93	1.02
1:D:150:SER:HB2	1:D:170:TYR:HD2	1.19	1.02
1:A:233:THR:HA	1:A:236:GLN:HB2	1.38	1.01
2:C:201:ASP:OD2	1:D:456:LYS:NZ	1.92	1.01
1:A:547:MET:SD	7:A:966:HOH:O	2.17	1.01
1:A:437:THR:HG21	1:A:439:ARG:HH21	1.25	1.01
1:D:15:ASP:OD2	7:D:702:HOH:O	1.79	1.00
1:D:480:GLU:OE2	7:D:701:HOH:O	1.79	0.99
1:D:58:GLU:OE2	1:D:62:LYS:NZ	1.97	0.98
1:A:132:ARG:HA	1:A:343:PRO:HG3	1.46	0.97
1:A:152:LYS:HE2	1:A:565:ASN:HB2	1.47	0.96
1:A:169:VAL:HB	5:A:603:ATP:O3'	1.64	0.96
1:A:232:ARG:HA	1:A:235:GLU:HG3	1.46	0.96
1:D:235:GLU:OE2	7:D:703:HOH:O	1.83	0.95
1:A:477:ILE:HG12	1:A:518:LEU:HD11	1.47	0.95
1:A:426:ASN:ND2	1:A:543:GLY:O	2.01	0.94
1:D:465:TYR:H	1:D:476:ALA:HA	1.32	0.93
1:D:199:HIS:HB3	1:D:525:LYS:H	1.32	0.93
1:D:126:ARG:HA	1:D:182:ILE:HG21	1.51	0.93
1:A:199:HIS:HB3	1:A:525:LYS:H	1.33	0.93
1:D:20:MET:SD	1:D:357:ASN:ND2	2.42	0.93
1:A:213:ARG:NH1	7:A:704:HOH:O	1.97	0.93
1:D:143:LYS:HD3	1:D:212:PHE:HB2	1.48	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:439:ARG:NH1	7:A:705:HOH:O	2.02	0.92
1:D:150:SER:HB2	1:D:170:TYR:CD2	2.05	0.92
1:D:432:ASN:ND2	1:D:434:ASP:OD1	2.01	0.92
2:F:189:CYS:SG	7:F:445:HOH:O	2.27	0.92
2:F:139:LEU:HB3	2:F:181:LYS:HD2	1.51	0.92
2:F:139:LEU:HD13	2:F:181:LYS:HB3	1.50	0.92
2:B:18:ARG:HD2	2:B:156:SER:HA	1.52	0.91
1:D:135:ASP:OD2	7:D:704:HOH:O	1.87	0.91
2:F:26:LYS:NZ	2:F:82:ASN:O	2.04	0.91
1:A:99:LEU:HB3	1:A:557:LYS:HB3	1.51	0.91
1:A:152:LYS:HA	1:A:564:GLU:HB3	1.52	0.90
1:D:477:ILE:HD11	1:D:520:LEU:HA	1.53	0.90
2:B:88:ASP:OD2	2:B:91:GLY:N	2.04	0.90
1:A:199:HIS:H	1:A:524:ALA:HB1	1.35	0.90
2:B:165:GLN:NE2	7:B:403:HOH:O	2.04	0.90
1:D:432:ASN:HD22	1:D:434:ASP:H	1.19	0.89
2:C:80:GLU:OE2	7:C:401:HOH:O	1.91	0.89
1:A:332:SER:HB2	1:A:538:LEU:HA	1.53	0.89
1:A:92:HIS:CE1	2:B:139:LEU:HB3	2.08	0.88
1:A:228:VAL:O	1:A:232:ARG:N	2.07	0.88
2:B:166:ALA:HB2	2:B:206:VAL:HG12	1.56	0.88
1:D:87:PRO:HB3	1:D:92:HIS:HA	1.54	0.88
2:E:10:TYR:O	2:E:20:ARG:NH2	2.06	0.88
1:D:557:LYS:NZ	5:D:603:ATP:O2G	2.08	0.87
2:E:122:GLU:HA	2:E:125:LYS:HD2	1.55	0.87
1:D:475:TYR:OH	7:D:705:HOH:O	1.89	0.87
1:D:56:ASP:HB2	1:D:59:GLU:HB2	1.54	0.87
1:A:451:ARG:NH1	1:A:454:GLU:OE1	2.07	0.87
2:B:145:PHE:N	2:B:154:ASP:OD2	2.08	0.86
2:C:135:LEU:HD22	2:C:182:LEU:HD12	1.58	0.86
1:A:231:PHE:HA	1:A:234:PHE:HB2	1.57	0.86
1:D:87:PRO:HD2	2:E:188:ARG:HB2	1.55	0.86
1:A:442:GLN:NE2	7:A:710:HOH:O	2.07	0.86
1:D:9:ASP:HB3	1:D:12:ARG:HB3	1.57	0.86
2:E:41:SER:O	7:E:401:HOH:O	1.94	0.85
1:A:556:ALA:O	7:A:702:HOH:O	1.94	0.85
1:D:387:GLU:HG2	1:D:408:LYS:HB2	1.57	0.85
1:A:98:SER:HB3	1:A:111:ILE:HB	1.55	0.85
1:D:333:SER:OG	5:D:603:ATP:O1A	1.95	0.85
1:A:467:ASP:OD2	7:A:703:HOH:O	1.95	0.85
1:A:162:VAL:HB	1:A:556:ALA:HB1	1.56	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:66:GLU:OE2	2:B:69:ASN:ND2	2.10	0.85
1:D:245:ILE:O	7:D:706:HOH:O	1.94	0.85
1:D:464:SER:HA	1:D:477:ILE:H	1.41	0.85
1:A:457:ILE:HD13	1:A:483:GLY:HA3	1.58	0.84
1:A:241:ILE:O	1:A:245:ILE:HG12	1.77	0.84
4:D:602:MET:HA	5:D:603:ATP:H2	1.41	0.84
1:D:434:ASP:OD1	1:D:435:LYS:HD2	1.78	0.84
1:A:285:SER:O	7:A:701:HOH:O	1.93	0.83
1:A:42:ALA:HA	2:B:143:PRO:HG2	1.59	0.83
1:A:90:THR:OG1	1:A:91:GLY:N	2.08	0.83
2:C:188:ARG:NH1	1:D:499:ARG:O	2.11	0.83
2:E:155:ILE:O	7:E:403:HOH:O	1.97	0.83
1:D:477:ILE:HD12	1:D:518:LEU:HD21	1.59	0.82
2:E:145:PHE:N	2:E:154:ASP:OD2	2.12	0.82
2:E:89:PRO:O	7:E:402:HOH:O	1.96	0.82
1:A:482:SER:O	1:A:525:LYS:NZ	2.12	0.82
1:D:330:TYR:CZ	1:D:338:ALA:HB3	2.15	0.82
1:D:528:PHE:HB3	1:D:531:ILE:HD12	1.60	0.81
2:B:145:PHE:HB3	2:B:153:VAL:HG13	1.62	0.81
1:D:169:VAL:HB	5:D:603:ATP:H3'	1.63	0.81
1:D:284:LEU:HD21	1:D:290:LEU:HD12	1.61	0.81
1:A:167:THR:OG1	1:A:560:GLN:OE1	1.99	0.81
2:B:37:PHE:O	7:B:401:HOH:O	1.99	0.81
1:A:102:GLY:N	1:A:546:LYS:O	2.11	0.80
1:A:92:HIS:HE1	2:B:139:LEU:HB3	1.45	0.80
1:D:551:VAL:HG13	1:D:555:ASN:HB2	1.63	0.80
2:B:152:TYR:CD1	2:B:153:VAL:HG12	2.16	0.80
1:D:171:ARG:NH2	7:D:721:HOH:O	2.12	0.80
1:D:199:HIS:H	1:D:524:ALA:HB1	1.44	0.80
1:D:22:ARG:HA	1:D:415:ASN:HB2	1.63	0.80
2:B:142:LYS:HD3	2:B:145:PHE:HA	1.62	0.80
1:A:164:THR:OG1	1:A:557:LYS:O	2.00	0.80
1:D:236:GLN:OE1	1:D:482:SER:HB2	1.82	0.80
1:A:342:THR:HG1	1:A:413:TYR:HH	1.01	0.79
1:A:231:PHE:HB3	1:A:290:LEU:HD22	1.64	0.79
2:C:70:VAL:HA	2:C:73:TYR:CD2	2.16	0.79
4:D:602:MET:HA	5:D:603:ATP:C2	2.18	0.79
1:D:87:PRO:HD3	1:D:93:PRO:HD3	1.65	0.79
2:B:178:GLU:OE2	7:B:402:HOH:O	2.01	0.79
1:D:143:LYS:HE2	1:D:216:VAL:HG13	1.64	0.79
1:D:143:LYS:HG2	1:D:215:GLN:HB2	1.65	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:ASN:ND2	1:A:358:LEU:HD22	1.94	0.79
1:A:113:PHE:HB2	1:A:117:LEU:HD11	1.65	0.78
1:A:199:HIS:HE1	1:A:567:VAL:HG11	1.46	0.78
1:D:496:CYS:O	1:D:500:ALA:N	2.15	0.78
2:F:69:ASN:HA	2:F:72:GLN:HG3	1.65	0.78
1:D:425:ARG:HB2	1:D:427:LEU:HB2	1.65	0.78
2:F:136:GLU:HG3	2:F:180:PRO:HD2	1.63	0.78
2:F:75:ASP:OD1	7:F:401:HOH:O	2.00	0.78
1:A:512:CYS:SG	1:A:514:THR:OG1	2.40	0.78
2:C:8:LEU:HD21	2:C:43:LEU:HD11	1.66	0.78
2:F:161:SER:HA	2:F:164:PHE:CD2	2.19	0.78
1:A:233:THR:HG22	1:A:237:VAL:HG22	1.64	0.78
1:A:473:GLY:O	1:A:516:GLY:N	2.14	0.78
1:D:540:SER:O	7:D:709:HOH:O	2.02	0.78
2:F:26:LYS:HD3	2:F:78:TRP:HB2	1.63	0.77
1:D:480:GLU:HB2	1:D:528:PHE:CZ	2.19	0.77
2:B:6:ILE:HG12	2:B:31:GLU:OE2	1.85	0.77
1:D:361:PHE:N	7:D:717:HOH:O	2.13	0.77
2:F:184:ALA:HA	2:F:187:LYS:HB2	1.65	0.77
2:F:169:LYS:HD2	2:F:206:VAL:HG13	1.66	0.77
1:D:451:ARG:NH2	7:D:730:HOH:O	2.18	0.77
1:D:329:ASP:HB3	1:D:339:ALA:HA	1.65	0.77
1:D:287:TRP:CE3	1:D:290:LEU:HD13	2.19	0.77
1:D:551:VAL:HG11	1:D:559:LEU:HD13	1.66	0.77
1:D:345:LEU:HD13	1:D:350:ALA:HA	1.65	0.77
2:C:103:ASP:O	2:C:107:THR:OG1	2.02	0.77
1:D:141:ASN:OD1	7:D:707:HOH:O	2.01	0.77
2:E:96:ARG:HH21	2:F:73:TYR:HE1	1.33	0.76
1:A:79:ARG:HB2	1:A:88:ILE:HD11	1.64	0.76
2:B:178:GLU:N	7:B:409:HOH:O	2.16	0.76
1:D:39:ASN:ND2	2:E:141:ASP:O	2.18	0.76
2:E:35:GLU:OE2	7:E:405:HOH:O	2.03	0.76
1:A:143:LYS:HB2	1:A:185:PRO:O	1.85	0.76
1:A:418:GLN:NE2	7:A:733:HOH:O	2.18	0.76
1:A:560:GLN:NE2	7:A:738:HOH:O	2.19	0.76
2:E:41:SER:OG	7:E:405:HOH:O	2.02	0.76
1:A:121:THR:CG2	1:A:175:PHE:CE1	2.48	0.76
1:D:108:PRO:HG2	1:D:552:LYS:H	1.50	0.76
1:D:154:TYR:HD1	1:D:560:GLN:HA	1.50	0.76
1:D:120:ASN:HB3	1:D:358:LEU:HD23	1.68	0.76
1:D:437:THR:HB	1:D:439:ARG:HH21	1.51	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:184:ALA:O	2:F:188:ARG:N	2.19	0.76
1:A:511:LYS:O	7:A:708:HOH:O	2.05	0.75
1:A:319:TYR:OH	7:A:707:HOH:O	2.05	0.75
1:D:108:PRO:HD2	1:D:552:LYS:HE3	1.68	0.75
1:D:292:PRO:HB3	1:D:323:LEU:HD13	1.67	0.75
2:E:162:SER:HB3	2:E:199:LEU:HD23	1.66	0.75
2:E:50:ILE:HD12	2:E:51:HIS:H	1.50	0.75
1:A:405:ASP:HB2	1:A:541:SER:HB3	1.68	0.75
1:D:331:GLY:N	1:D:537:GLY:O	2.19	0.75
2:F:69:ASN:OD1	7:F:402:HOH:O	2.03	0.75
1:A:465:TYR:HB3	1:A:476:ALA:HB3	1.68	0.75
2:B:16:GLY:HA2	2:B:55:PRO:HG3	1.69	0.75
2:C:196:SER:O	7:C:402:HOH:O	2.04	0.75
2:C:15:PHE:HB3	2:C:67:SER:HB3	1.69	0.75
2:C:26:LYS:HD3	2:C:74:VAL:HG12	1.69	0.75
1:D:497:LEU:O	7:D:710:HOH:O	2.04	0.75
7:E:402:HOH:O	2:F:76:GLU:OE1	2.03	0.75
2:E:166:ALA:HB2	2:E:206:VAL:HG12	1.68	0.75
2:F:165:GLN:HA	2:F:168:GLU:HG3	1.68	0.74
1:A:190:ASP:O	1:A:194:PHE:N	2.19	0.74
1:A:287:TRP:HB3	1:A:290:LEU:HD11	1.68	0.74
1:A:433:ILE:O	1:A:552:LYS:NZ	2.20	0.74
1:D:322:ASP:OD2	7:D:711:HOH:O	2.05	0.74
2:F:9:ASP:HB2	2:F:20:ARG:HH21	1.52	0.74
1:A:234:PHE:CZ	1:A:294:LEU:HD21	2.22	0.74
1:D:363:PHE:HD2	1:D:382:VAL:HG21	1.52	0.74
2:F:176:GLU:HB2	2:F:183:ILE:HB	1.69	0.74
1:D:464:SER:HB3	1:D:476:ALA:HB1	1.68	0.74
1:D:154:TYR:CD1	1:D:560:GLN:HA	2.21	0.74
2:E:94:GLN:NE2	7:E:407:HOH:O	2.14	0.74
2:F:68:LEU:HD23	2:F:103:ASP:OD2	1.87	0.74
1:A:67:LEU:O	7:A:709:HOH:O	2.06	0.73
1:A:113:PHE:HB3	5:A:603:ATP:O2B	1.87	0.73
1:A:291:ILE:HG13	1:A:320:ALA:HA	1.70	0.73
2:B:130:GLU:OE2	7:B:404:HOH:O	2.05	0.73
1:A:234:PHE:HZ	1:A:294:LEU:HD21	1.53	0.73
1:A:355:ILE:O	7:A:711:HOH:O	2.07	0.73
1:D:229:HIS:NE2	7:D:701:HOH:O	2.00	0.73
1:D:239:GLU:OE2	1:D:278:ARG:NH2	2.21	0.73
2:B:7:LEU:O	7:B:405:HOH:O	2.06	0.73
2:F:57:LEU:N	7:F:405:HOH:O	2.11	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:408:LYS:NZ	7:A:727:HOH:O	2.16	0.73
1:D:490:LEU:HD13	1:D:522:VAL:HG21	1.68	0.73
2:C:16:GLY:HA2	2:C:55:PRO:HB3	1.71	0.73
2:C:108:ASP:OD2	7:C:405:HOH:O	2.06	0.72
2:E:92:ARG:HB2	7:E:402:HOH:O	1.88	0.72
1:D:223:PHE:CZ	1:D:536:LEU:HB3	2.24	0.72
1:D:330:TYR:OH	1:D:419:LEU:HB2	1.88	0.72
2:B:53:LYS:HD3	6:B:301:GSH:HB12	1.71	0.72
2:C:10:TYR:O	2:C:20:ARG:NH2	2.22	0.72
1:A:38:LYS:O	2:B:142:LYS:HB2	1.89	0.72
2:B:169:LYS:O	7:B:406:HOH:O	2.07	0.72
1:A:99:LEU:HB3	1:A:557:LYS:HE3	1.70	0.72
1:D:105:GLN:HA	1:D:430:SER:HB2	1.71	0.72
1:D:461:ASP:O	7:D:712:HOH:O	2.06	0.72
1:D:480:GLU:HB2	1:D:528:PHE:CE1	2.24	0.72
2:F:10:TYR:O	2:F:20:ARG:NH2	2.20	0.72
1:D:432:ASN:ND2	1:D:434:ASP:H	1.87	0.72
2:E:73:TYR:OH	7:E:404:HOH:O	2.00	0.72
1:D:482:SER:HA	1:D:525:LYS:HD2	1.72	0.72
1:A:221:ALA:HB3	1:A:227:LEU:HG	1.72	0.72
2:B:162:SER:O	2:B:165:GLN:NE2	2.19	0.72
1:D:73:LEU:HD22	1:D:89:LEU:HD22	1.70	0.72
1:A:290:LEU:N	1:A:319:TYR:O	2.23	0.72
1:A:93:PRO:HB2	2:B:181:LYS:HA	1.71	0.72
1:D:46:GLN:HB2	2:E:148:ASP:HB3	1.71	0.72
1:D:527:THR:HG23	1:D:561:ILE:HG21	1.70	0.72
1:A:375:LYS:NZ	7:A:728:HOH:O	2.17	0.72
2:B:172:ASN:ND2	7:B:413:HOH:O	2.22	0.72
1:D:213:ARG:NH1	1:D:214:ASP:OD1	2.23	0.72
1:A:316:LEU:O	1:A:320:ALA:N	2.22	0.71
1:A:39:ASN:ND2	1:A:399:TYR:OH	2.19	0.71
2:C:162:SER:OG	7:C:406:HOH:O	2.08	0.71
2:F:135:LEU:HB3	2:F:182:LEU:HD11	1.72	0.71
2:F:64:VAL:HB	2:F:73:TYR:CE2	2.25	0.71
1:D:99:LEU:HG	1:D:557:LYS:HB2	1.72	0.71
2:F:26:LYS:HE2	2:F:75:ASP:HA	1.72	0.71
2:F:92:ARG:NH2	7:F:415:HOH:O	2.21	0.71
1:A:219:VAL:HG21	1:A:231:PHE:CZ	2.25	0.71
2:B:190:MET:O	2:B:196:SER:OG	2.07	0.71
1:A:405:ASP:HB3	1:A:426:ASN:HD22	1.56	0.71
1:A:304:ILE:HG13	1:A:328:HIS:HB3	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:509:SER:O	1:A:513:LYS:N	2.22	0.71
1:A:375:LYS:O	7:A:714:HOH:O	2.09	0.71
1:D:22:ARG:O	7:D:714:HOH:O	2.09	0.71
1:D:306:THR:HA	1:D:310:GLU:HG3	1.73	0.71
1:A:98:SER:O	7:A:713:HOH:O	2.08	0.71
1:D:330:TYR:HE1	1:D:352:PHE:HB2	1.56	0.71
1:A:432:ASN:ND2	1:A:434:ASP:OD2	2.17	0.71
1:D:231:PHE:HA	1:D:234:PHE:HD2	1.56	0.71
2:C:117:LYS:HA	2:C:121:GLN:HB2	1.73	0.70
2:C:40:LYS:HZ3	2:C:40:LYS:H	1.35	0.70
1:D:99:LEU:HD21	1:D:558:VAL:HG23	1.73	0.70
2:F:201:ASP:OD2	7:F:403:HOH:O	2.07	0.70
2:C:188:ARG:HB2	1:D:499:ARG:HH21	1.56	0.70
1:D:330:TYR:HD1	1:D:352:PHE:HD2	1.39	0.70
1:D:394:ASN:N	1:D:398:LEU:O	2.24	0.70
2:C:114:TRP:CD1	2:C:167:TYR:HE1	2.09	0.70
1:D:444:SER:HA	1:D:500:ALA:HB1	1.72	0.70
1:A:162:VAL:O	7:A:702:HOH:O	2.09	0.70
1:A:239:GLU:O	1:A:241:ILE:N	2.24	0.70
1:A:199:HIS:N	1:A:524:ALA:HB1	2.07	0.70
1:D:519:GLU:O	7:D:708:HOH:O	2.10	0.70
1:D:87:PRO:O	2:E:188:ARG:NH1	2.25	0.70
2:E:9:ASP:OD1	2:E:10:TYR:N	2.23	0.70
2:C:84:PHE:CD1	2:C:152:TYR:HB2	2.27	0.70
1:A:210:ILE:HG22	1:A:294:LEU:HD13	1.74	0.70
1:A:136:PHE:HD1	1:A:299:LYS:HD2	1.56	0.70
1:A:521:ARG:HH11	1:A:562:LEU:HD11	1.56	0.70
1:A:87:PRO:HD3	1:A:93:PRO:HD3	1.74	0.70
1:D:212:PHE:HB3	1:D:215:GLN:HG3	1.71	0.70
1:D:27:VAL:HA	1:D:30:GLN:HB3	1.74	0.70
1:D:424:ARG:NH2	7:D:749:HOH:O	2.24	0.70
2:C:142:LYS:NZ	7:C:418:HOH:O	2.23	0.70
2:B:109:ALA:HB2	2:B:127:GLU:HG2	1.73	0.70
2:B:172:ASN:OD1	7:B:406:HOH:O	2.09	0.70
1:A:223:PHE:CZ	1:A:536:LEU:HB3	2.27	0.69
1:A:22:ARG:HA	1:A:415:ASN:HB2	1.74	0.69
1:A:271:PRO:O	7:A:716:HOH:O	2.10	0.69
2:C:92:ARG:HB3	2:C:96:ARG:NH2	2.07	0.69
1:D:96:ALA:HA	1:D:162:VAL:HA	1.75	0.69
1:D:229:HIS:O	1:D:233:THR:OG1	2.06	0.69
1:D:272:GLU:OE1	7:D:716:HOH:O	2.10	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:364:LEU:HB3	1:D:389:GLU:HG3	1.74	0.69
1:D:498:ASP:OD1	1:D:518:LEU:HD22	1.92	0.69
1:A:540:SER:OG	1:A:541:SER:N	2.24	0.69
2:B:136:GLU:HG3	2:B:181:LYS:HD3	1.74	0.69
1:A:240:GLU:O	1:A:244:ASP:N	2.19	0.69
1:D:85:THR:HB	2:E:184:ALA:HB1	1.73	0.69
2:F:40:LYS:NZ	7:F:420:HOH:O	2.26	0.69
2:F:88:ASP:O	7:F:404:HOH:O	2.10	0.69
2:E:26:LYS:HE2	2:E:78:TRP:HD1	1.57	0.69
1:A:290:LEU:HD13	1:A:319:TYR:CD1	2.28	0.69
2:E:132:VAL:HG13	2:E:182:LEU:HD13	1.74	0.69
1:A:213:ARG:HA	1:A:216:VAL:HG22	1.75	0.69
1:A:290:LEU:HD13	1:A:319:TYR:HD1	1.57	0.69
1:A:330:TYR:HE2	1:A:540:SER:H	1.40	0.69
1:A:490:LEU:HD22	1:A:522:VAL:HG21	1.72	0.69
1:A:74:GLU:O	1:A:78:LYS:HG2	1.93	0.69
1:A:46:GLN:HA	2:B:148:ASP:HB2	1.75	0.69
2:C:176:GLU:OE2	1:D:573:THR:OG1	2.07	0.69
1:D:470:THR:HG21	1:D:474:HIS:ND1	2.08	0.69
2:F:64:VAL:HG23	2:F:70:VAL:HG22	1.75	0.69
1:A:145:LEU:HD13	1:A:209:GLY:HA3	1.75	0.69
1:A:199:HIS:N	7:A:712:HOH:O	2.26	0.69
1:A:475:TYR:OH	1:A:515:ILE:HD12	1.91	0.69
1:A:534:HIS:CE1	1:A:557:LYS:HD2	2.28	0.69
1:D:425:ARG:HD3	1:D:427:LEU:HD13	1.75	0.69
1:D:89:LEU:HD12	1:D:90:THR:HG23	1.75	0.69
2:F:181:LYS:O	2:F:185:TRP:HB3	1.93	0.69
1:A:96:ALA:HB3	1:A:113:PHE:CE2	2.28	0.69
2:B:150:PHE:CE1	2:B:155:ILE:HG13	2.27	0.69
1:A:143:LYS:HG2	7:A:720:HOH:O	1.92	0.68
1:A:149:PHE:CZ	1:A:152:LYS:HD2	2.29	0.68
1:A:219:VAL:HG21	1:A:231:PHE:HZ	1.58	0.68
1:D:59:GLU:OE2	7:D:715:HOH:O	2.10	0.68
1:A:108:PRO:HB2	1:A:554:SER:HB2	1.74	0.68
2:B:150:PHE:HE1	2:B:155:ILE:HG13	1.59	0.68
2:E:139:LEU:HG	2:E:142:LYS:HG3	1.76	0.68
1:A:149:PHE:HZ	1:A:152:LYS:HD2	1.59	0.68
2:B:169:LYS:HZ1	2:B:206:VAL:HG11	1.59	0.68
1:D:305:MET:HA	7:D:756:HOH:O	1.92	0.68
1:D:147:PHE:O	1:D:529:ARG:NH2	2.25	0.68
1:A:108:PRO:HB3	1:A:555:ASN:CG	2.14	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:225:HIS:O	1:D:229:HIS:N	2.23	0.68
1:D:461:ASP:HB3	1:D:528:PHE:CD1	2.27	0.68
2:F:201:ASP:OD1	7:F:406:HOH:O	2.11	0.68
1:A:232:ARG:CA	1:A:235:GLU:HG3	2.23	0.68
2:E:18:ARG:NH1	7:E:415:HOH:O	2.26	0.68
1:D:152:LYS:HD3	1:D:561:ILE:HA	1.75	0.68
2:C:17:MET:HE2	2:C:200:PRO:HD2	1.75	0.68
2:C:24:ARG:HG3	2:C:30:PHE:HE1	1.57	0.68
2:F:135:LEU:HD13	2:F:182:LEU:HD21	1.76	0.68
1:A:163:GLY:HA3	1:A:168:ASN:HD21	1.59	0.68
1:A:223:PHE:CE1	1:A:304:ILE:HB	2.29	0.68
1:A:223:PHE:CE2	1:A:533:GLU:HA	2.28	0.68
1:D:28:GLN:OE1	7:D:717:HOH:O	2.10	0.68
2:F:15:PHE:HB3	2:F:67:SER:HB3	1.76	0.68
1:A:444:SER:HA	1:A:500:ALA:HB1	1.76	0.67
1:A:143:LYS:HD2	1:A:212:PHE:HB2	1.76	0.67
1:A:287:TRP:O	1:A:290:LEU:HD12	1.94	0.67
2:C:187:LYS:HD3	1:D:492:ASP:HB3	1.74	0.67
1:A:31:THR:HA	1:A:34:GLU:HG2	1.74	0.67
1:A:421:PHE:CE1	1:A:541:SER:HA	2.29	0.67
1:A:86:SER:HB2	2:B:188:ARG:NE	2.10	0.67
2:B:189:CYS:HB3	2:B:195:VAL:HG21	1.76	0.67
1:A:99:LEU:HD13	1:A:558:VAL:H	1.58	0.67
1:A:329:ASP:HB3	1:A:339:ALA:HA	1.75	0.67
2:F:188:ARG:HD3	2:F:191:GLU:OE2	1.95	0.67
1:A:179:MET:HA	1:A:182:ILE:HD11	1.77	0.67
1:A:525:LYS:O	7:A:718:HOH:O	2.12	0.67
2:E:139:LEU:HD23	2:E:142:LYS:HB2	1.75	0.67
1:A:238:TRP:CZ3	1:A:281:CYS:HB3	2.30	0.67
2:B:203:GLU:OE1	7:B:408:HOH:O	2.13	0.67
2:C:17:MET:SD	7:C:406:HOH:O	2.52	0.67
2:C:68:LEU:O	2:C:72:GLN:HG3	1.95	0.67
1:A:478:PHE:CZ	1:A:562:LEU:HD22	2.30	0.67
1:A:494:CYS:HA	1:A:497:LEU:HD12	1.76	0.67
1:A:154:TYR:CD2	1:A:563:CYS:HB2	2.30	0.67
1:A:71:VAL:HG13	1:A:107:ARG:HH22	1.60	0.67
2:C:171:GLY:N	7:C:407:HOH:O	2.13	0.67
1:D:149:PHE:HZ	1:D:202:LEU:HB2	1.59	0.67
1:A:235:GLU:OE1	7:A:719:HOH:O	2.13	0.67
2:C:110:GLN:HA	2:C:113:VAL:HG12	1.76	0.67
1:D:132:ARG:HA	1:D:343:PRO:HG2	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:603:ATP:O2'	5:D:603:ATP:N3	2.27	0.67
1:A:519:GLU:CD	1:A:521:ARG:HE	1.98	0.66
2:C:84:PHE:HB2	2:C:152:TYR:N	2.10	0.66
1:D:76:TYR:HB3	1:D:88:ILE:HG21	1.75	0.66
1:A:87:PRO:HD2	2:B:188:ARG:HB2	1.78	0.66
1:D:108:PRO:HG2	1:D:552:LYS:HB2	1.77	0.66
1:A:514:THR:OG1	7:A:721:HOH:O	2.13	0.66
1:A:509:SER:HB3	1:A:515:ILE:HD11	1.75	0.66
1:D:331:GLY:HA3	1:D:336:TRP:CE3	2.30	0.66
1:D:533:GLU:OE1	7:D:720:HOH:O	2.12	0.66
2:F:96:ARG:HD3	7:F:415:HOH:O	1.96	0.66
2:B:114:TRP:CD1	2:B:167:TYR:HE1	2.13	0.66
1:D:169:VAL:HB	5:D:603:ATP:C3'	2.24	0.66
2:B:161:SER:HA	2:B:164:PHE:CD2	2.30	0.66
1:D:331:GLY:O	5:D:603:ATP:N6	2.29	0.66
1:D:407:VAL:HG21	1:D:419:LEU:HB3	1.78	0.66
1:A:391:VAL:HG22	1:A:402:ARG:HG2	1.78	0.66
2:F:85:PHE:CD2	2:F:92:ARG:HG2	2.31	0.66
1:D:121:THR:CG2	1:D:336:TRP:CZ2	2.79	0.66
1:A:212:PHE:O	7:A:720:HOH:O	2.13	0.65
2:E:182:LEU:O	7:E:406:HOH:O	2.13	0.65
1:A:96:ALA:HB3	1:A:113:PHE:HE2	1.60	0.65
1:A:19:GLU:O	1:A:23:ASN:ND2	2.20	0.65
1:A:403:LEU:HB3	1:A:405:ASP:OD1	1.97	0.65
2:C:125:LYS:HE2	2:C:171:GLY:HA2	1.78	0.65
2:E:37:PHE:CZ	6:E:301:GSH:HA32	2.32	0.65
1:A:135:ASP:OD1	7:A:723:HOH:O	2.13	0.65
1:A:229:HIS:O	1:A:233:THR:N	2.30	0.65
2:E:151:GLY:H	2:E:154:ASP:HB2	1.62	0.65
1:A:494:CYS:HB2	1:A:520:LEU:HB3	1.78	0.65
1:A:395:TYR:HD1	2:B:141:ASP:OD2	1.79	0.65
2:C:34:GLU:O	7:C:408:HOH:O	2.13	0.65
1:D:76:TYR:HD2	1:D:88:ILE:HD13	1.60	0.65
2:F:48:ASN:HB2	7:F:414:HOH:O	1.95	0.65
2:C:70:VAL:HA	2:C:73:TYR:HD2	1.61	0.65
2:C:92:ARG:HB3	2:C:96:ARG:HH22	1.61	0.65
2:B:145:PHE:CD2	2:B:153:VAL:HG22	2.32	0.65
1:D:164:THR:OG1	1:D:557:LYS:O	2.11	0.65
1:D:570:TYR:O	7:D:723:HOH:O	2.14	0.65
2:E:26:LYS:HG3	2:E:78:TRP:HE1	1.61	0.65
1:A:432:ASN:OD1	1:A:434:ASP:N	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:603:ATP:O2A	5:A:603:ATP:O2B	2.12	0.65
1:A:98:SER:OG	5:A:603:ATP:O2G	2.15	0.65
2:C:164:PHE:HD2	2:C:183:ILE:HD13	1.61	0.65
1:D:36:LEU:HD11	1:D:50:LEU:HD11	1.79	0.65
1:D:38:LYS:O	2:E:142:LYS:HG2	1.96	0.65
1:D:473:GLY:O	1:D:516:GLY:N	2.29	0.65
2:E:192:LYS:NZ	7:E:420:HOH:O	2.30	0.65
1:A:77:ILE:HD13	1:A:112:PRO:HD3	1.78	0.64
2:B:7:LEU:HD11	2:B:55:PRO:HB2	1.78	0.64
1:D:110:PHE:CE1	1:D:556:ALA:HB2	2.31	0.64
1:A:465:TYR:HD1	1:A:551:VAL:HG23	1.61	0.64
1:A:152:LYS:NZ	1:A:561:ILE:HG22	2.11	0.64
1:D:445:VAL:HA	1:D:479:TRP:HZ2	1.62	0.64
1:D:98:SER:HB3	5:D:603:ATP:O2G	1.97	0.64
1:A:236:GLN:OE1	7:A:724:HOH:O	2.15	0.64
1:A:531:ILE:HD13	1:A:558:VAL:HG22	1.78	0.64
1:A:426:ASN:HD21	1:A:544:GLN:NE2	1.96	0.64
1:D:309:MET:HB3	7:D:756:HOH:O	1.96	0.64
2:F:16:GLY:HA2	2:F:55:PRO:HB3	1.78	0.64
1:A:77:ILE:HB	1:A:110:PHE:HD2	1.62	0.64
2:B:152:TYR:CE1	2:B:153:VAL:HG12	2.32	0.64
1:A:143:LYS:HD3	1:A:187:CYS:HB3	1.80	0.64
2:C:139:LEU:HB3	2:C:181:LYS:HZ1	1.60	0.64
2:F:170:PHE:CD2	2:F:213:ARG:HD2	2.32	0.64
1:D:229:HIS:HA	1:D:232:ARG:HE	1.63	0.64
1:D:535:PHE:O	1:D:538:LEU:HB3	1.97	0.64
1:A:152:LYS:HZ2	1:A:561:ILE:HG22	1.62	0.64
1:D:143:LYS:NZ	1:D:209:GLY:O	2.29	0.64
1:D:227:LEU:HD13	1:D:231:PHE:HE2	1.63	0.64
1:D:77:ILE:HG12	1:D:89:LEU:HD11	1.79	0.64
1:A:200:GLN:HA	1:A:203:TYR:CE2	2.32	0.64
2:B:26:LYS:HB2	2:B:81:LYS:HE3	1.78	0.64
1:A:464:SER:HB3	1:A:550:CYS:HB2	1.80	0.64
1:A:560:GLN:N	7:A:702:HOH:O	2.16	0.64
2:C:26:LYS:HB3	2:C:78:TRP:HE1	1.62	0.64
2:E:17:MET:HG2	2:E:20:ARG:NH1	2.13	0.64
2:F:165:GLN:HG2	2:F:206:VAL:HG21	1.80	0.64
1:A:462:PHE:N	7:A:752:HOH:O	2.29	0.63
2:C:172:ASN:OD1	7:C:409:HOH:O	2.15	0.63
1:D:330:TYR:CE1	1:D:352:PHE:HB2	2.32	0.63
1:D:476:ALA:O	7:D:708:HOH:O	2.15	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:65:CYS:O	2:F:69:ASN:ND2	2.25	0.63
1:D:316:LEU:O	1:D:320:ALA:N	2.31	0.63
1:D:38:LYS:HG2	1:D:395:TYR:HE2	1.63	0.63
2:C:201:ASP:OD2	1:D:456:LYS:HG3	1.97	0.63
2:F:199:LEU:O	7:F:408:HOH:O	2.15	0.63
2:E:85:PHE:O	7:E:409:HOH:O	2.15	0.63
2:C:24:ARG:HG3	2:C:30:PHE:CE1	2.34	0.63
2:E:183:ILE:HG13	2:E:184:ALA:N	2.14	0.63
1:A:150:SER:OG	1:A:150:SER:O	2.10	0.63
1:A:165:ALA:N	5:A:603:ATP:O3G	2.31	0.63
1:D:284:LEU:HD21	1:D:287:TRP:HA	1.80	0.63
1:A:98:SER:N	1:A:111:ILE:O	2.20	0.63
1:A:72:GLU:OE1	1:A:72:GLU:N	2.27	0.63
1:D:494:CYS:SG	1:D:495:ASN:N	2.71	0.63
1:A:295:PHE:HD2	1:A:298:ALA:HB2	1.62	0.63
1:A:136:PHE:CD1	1:A:299:LYS:HD2	2.34	0.63
1:A:405:ASP:OD1	1:A:540:SER:HB2	1.99	0.63
1:D:219:VAL:HB	1:D:295:PHE:CZ	2.34	0.63
2:F:84:PHE:CD1	2:F:152:TYR:HB2	2.34	0.63
2:B:145:PHE:CB	2:B:153:VAL:HG13	2.27	0.62
2:C:163:TRP:HB3	2:C:167:TYR:CZ	2.34	0.62
1:D:498:ASP:HB3	1:D:510:ARG:NH1	2.14	0.62
1:A:17:PHE:HA	1:A:20:MET:SD	2.39	0.62
1:D:203:TYR:HA	1:D:206:LEU:HD12	1.81	0.62
2:F:92:ARG:HG3	7:F:404:HOH:O	1.98	0.62
2:B:6:ILE:HG23	2:B:31:GLU:HG2	1.81	0.62
2:E:188:ARG:NE	2:E:191:GLU:OE2	2.33	0.62
2:F:153:VAL:O	2:F:157:LEU:HD23	1.99	0.62
1:A:423:CYS:HB2	1:A:542:ALA:HB3	1.81	0.62
1:D:498:ASP:HB3	1:D:510:ARG:CZ	2.30	0.62
1:D:88:ILE:HG22	1:D:89:LEU:N	2.14	0.62
2:C:114:TRP:HA	2:C:170:PHE:HD2	1.64	0.62
1:D:101:SER:HB3	1:D:535:PHE:CD2	2.35	0.62
2:E:36:ASP:HB3	2:E:39:ASN:OD1	2.00	0.62
1:A:276:THR:OG1	1:A:277:ILE:N	2.33	0.62
1:A:440:ASP:O	1:A:444:SER:N	2.33	0.62
1:A:92:HIS:CE1	2:B:142:LYS:HB3	2.34	0.62
2:C:110:GLN:HB3	2:C:167:TYR:CZ	2.35	0.62
1:D:330:TYR:CD1	1:D:352:PHE:HD2	2.18	0.62
1:A:274:ALA:O	1:A:278:ARG:HB2	2.00	0.62
1:D:12:ARG:C	1:D:14:ILE:H	2.03	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:146:GLN:HB2	1:D:220:PHE:HD2	1.65	0.62
1:D:81:VAL:HG22	1:D:97:ILE:HG13	1.80	0.62
1:D:41:SER:HB2	2:E:142:LYS:HD2	1.81	0.62
1:D:464:SER:O	1:D:551:VAL:N	2.31	0.62
2:F:84:PHE:CG	2:F:152:TYR:HB2	2.34	0.62
1:A:200:GLN:HA	1:A:203:TYR:CZ	2.35	0.62
1:A:238:TRP:CH2	1:A:287:TRP:HZ2	2.16	0.62
1:A:246:LYS:O	1:A:269:PRO:HA	2.00	0.62
2:C:64:VAL:HB	2:C:73:TYR:CE2	2.35	0.62
2:C:98:TRP:CE3	2:C:101:PHE:HB2	2.34	0.62
1:A:333:SER:HB3	5:A:603:ATP:PA	2.39	0.61
1:A:451:ARG:O	1:A:454:GLU:HG2	2.00	0.61
1:A:51:ASN:ND2	2:B:87:SER:OG	2.33	0.61
1:D:476:ALA:O	1:D:477:ILE:HD13	2.00	0.61
2:E:148:ASP:OD1	7:E:410:HOH:O	2.16	0.61
2:F:107:THR:HA	2:F:110:GLN:HE21	1.64	0.61
1:A:496:CYS:O	1:A:500:ALA:N	2.33	0.61
1:D:204:CYS:O	1:D:208:SER:N	2.24	0.61
2:E:202:SER:HA	2:E:205:ILE:HD11	1.82	0.61
2:F:132:VAL:O	2:F:179:SER:HB3	2.00	0.61
2:F:37:PHE:O	2:F:40:LYS:NZ	2.29	0.61
1:A:207:LEU:O	1:A:211:LEU:HG	1.99	0.61
1:D:377:VAL:O	7:D:725:HOH:O	2.16	0.61
1:D:62:LYS:O	1:D:400:ARG:NH2	2.33	0.61
1:A:287:TRP:HB3	1:A:290:LEU:CD1	2.31	0.61
1:A:140:ASP:OD1	1:A:140:ASP:N	2.31	0.61
1:D:121:THR:CG2	1:D:336:TRP:HZ2	2.14	0.61
1:D:434:ASP:OD2	1:D:550:CYS:HB3	2.00	0.61
2:E:145:PHE:H	2:E:154:ASP:CG	2.02	0.61
1:A:224:ALA:HA	1:A:227:LEU:HD12	1.83	0.61
2:B:6:ILE:HG21	2:B:33:ARG:HD2	1.82	0.61
1:D:344:ARG:N	7:D:704:HOH:O	2.33	0.61
2:E:50:ILE:HG21	2:F:134:ILE:HD12	1.81	0.61
2:F:211:GLU:HA	2:F:214:LYS:HE3	1.83	0.61
1:A:88:ILE:HG22	1:A:89:LEU:N	2.15	0.61
2:B:135:LEU:HD13	2:B:157:LEU:HD11	1.82	0.61
1:D:338:ALA:HB2	1:D:354:VAL:HG22	1.83	0.61
1:D:93:PRO:O	2:E:181:LYS:HG2	2.00	0.61
1:A:498:ASP:OD1	1:A:498:ASP:N	2.33	0.61
2:F:136:GLU:CG	2:F:180:PRO:HD2	2.30	0.61
1:A:154:TYR:O	7:A:726:HOH:O	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:445:VAL:HG21	1:A:462:PHE:CG	2.36	0.60
2:F:164:PHE:O	2:F:168:GLU:HG3	2.01	0.60
2:F:132:VAL:HG13	2:F:179:SER:OG	2.00	0.60
2:F:84:PHE:HB2	2:F:152:TYR:N	2.16	0.60
1:A:195:SER:OG	1:A:197:ASP:OD1	2.18	0.60
1:A:229:HIS:HB2	1:A:529:ARG:CZ	2.31	0.60
1:A:273:LEU:HA	1:A:276:THR:HG23	1.83	0.60
1:A:404:GLY:O	1:A:426:ASN:HB2	2.02	0.60
1:A:444:SER:HA	1:A:500:ALA:CB	2.31	0.60
1:A:41:SER:OG	2:B:144:TYR:O	2.12	0.60
1:D:39:ASN:HD21	2:E:143:PRO:HD3	1.65	0.60
1:A:225:HIS:O	1:A:229:HIS:N	2.29	0.60
1:D:285:SER:O	1:D:287:TRP:N	2.35	0.60
1:D:538:LEU:CD2	1:D:540:SER:HB2	2.31	0.60
1:D:202:LEU:O	1:D:206:LEU:HG	2.01	0.60
1:D:278:ARG:NH1	7:D:752:HOH:O	2.25	0.60
1:A:530:LYS:HA	1:A:533:GLU:HG3	1.83	0.60
1:A:86:SER:HB2	2:B:188:ARG:HE	1.65	0.60
2:C:184:ALA:HB1	1:D:499:ARG:HH11	1.65	0.60
1:A:245:ILE:HA	1:A:267:LEU:HD11	1.83	0.60
2:B:64:VAL:HG12	2:C:90:TYR:HD1	1.67	0.60
2:F:165:GLN:HG2	2:F:206:VAL:CG2	2.31	0.60
2:F:33:ARG:NH2	2:F:41:SER:OG	2.26	0.60
2:F:64:VAL:HB	2:F:73:TYR:CD2	2.36	0.60
2:C:168:GLU:OE2	1:D:488:ASP:OD2	2.19	0.60
1:D:92:HIS:HB2	1:D:93:PRO:HD2	1.83	0.60
2:F:114:TRP:HA	2:F:170:PHE:HD2	1.67	0.60
1:D:435:LYS:HE2	1:D:438:GLU:HB3	1.82	0.60
2:E:112:LYS:O	2:E:116:LYS:HB2	2.01	0.60
1:A:20:MET:HA	1:A:23:ASN:HB2	1.84	0.60
1:A:421:PHE:HB3	1:A:542:ALA:HB2	1.83	0.60
2:C:125:LYS:HA	2:C:128:PHE:CD2	2.36	0.60
1:D:461:ASP:HB3	1:D:528:PHE:CE1	2.36	0.60
1:A:213:ARG:HH21	1:A:296:PRO:HD2	1.66	0.59
2:B:169:LYS:NZ	2:B:206:VAL:HG11	2.17	0.59
2:C:4:LEU:O	7:C:411:HOH:O	2.17	0.59
2:C:52:LYS:HA	7:C:413:HOH:O	2.01	0.59
2:F:204:LYS:NZ	7:F:409:HOH:O	2.35	0.59
1:A:223:PHE:CD1	1:A:304:ILE:HB	2.37	0.59
1:A:510:ARG:HH21	1:A:517:ALA:HA	1.67	0.59
1:A:78:LYS:HE3	1:A:554:SER:HA	1.82	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:47:SER:OG	2:B:56:VAL:HG21	2.02	0.59
1:D:120:ASN:CB	1:D:358:LEU:HD23	2.32	0.59
1:A:151:SER:HB3	1:A:193:ILE:O	2.02	0.59
1:D:287:TRP:HE3	1:D:290:LEU:HD13	1.65	0.59
1:D:231:PHE:CZ	1:D:291:ILE:HG12	2.37	0.59
2:B:96:ARG:HD2	2:C:73:TYR:CE1	2.37	0.59
1:D:41:SER:HA	2:E:148:ASP:HA	1.85	0.59
1:D:523:VAL:HG12	1:D:565:ASN:HB3	1.83	0.59
1:D:99:LEU:H	1:D:557:LYS:H	1.50	0.59
1:D:82:ASP:O	1:D:84:ASP:N	2.34	0.59
1:D:8:PHE:CZ	1:D:130:ALA:HB2	2.37	0.59
2:E:30:PHE:O	7:E:411:HOH:O	2.16	0.59
1:A:42:ALA:HB3	1:A:45:LEU:HB2	1.84	0.59
1:A:435:LYS:HA	1:A:436:ASN:HB2	1.84	0.59
2:C:188:ARG:HB2	1:D:499:ARG:NH2	2.17	0.59
2:B:93:ALA:HA	2:C:73:TYR:HE1	1.66	0.59
1:D:431:ILE:O	7:D:728:HOH:O	2.17	0.59
2:F:169:LYS:NZ	7:F:424:HOH:O	2.35	0.59
1:A:198:VAL:O	1:A:202:LEU:N	2.31	0.59
1:D:14:ILE:HG22	1:D:16:GLU:HB2	1.83	0.59
1:D:504:ALA:O	1:D:507:VAL:HB	2.02	0.59
2:F:70:VAL:HG23	7:F:402:HOH:O	2.01	0.59
2:C:42:PRO:O	7:C:410:HOH:O	2.16	0.59
1:D:527:THR:O	1:D:530:LYS:HB2	2.02	0.59
2:F:110:GLN:HG2	2:F:167:TYR:HE2	1.67	0.59
1:A:116:GLU:O	1:A:119:GLU:HG2	2.02	0.59
1:A:31:THR:O	1:A:35:ILE:HG13	2.02	0.59
1:A:406:VAL:O	1:A:541:SER:OG	2.21	0.59
1:D:286:ASN:O	7:D:726:HOH:O	2.16	0.59
1:A:423:CYS:SG	1:A:541:SER:OG	2.61	0.59
2:C:10:TYR:HH	2:C:208:TYR:HH	1.48	0.59
2:E:116:LYS:O	2:E:213:ARG:NH1	2.36	0.59
2:F:141:ASP:N	2:F:141:ASP:OD1	2.33	0.59
2:F:157:LEU:HG	2:F:185:TRP:CH2	2.38	0.59
1:A:27:VAL:O	1:A:31:THR:OG1	2.13	0.59
2:B:145:PHE:H	2:B:154:ASP:CG	2.06	0.59
2:C:27:GLY:O	7:C:412:HOH:O	2.17	0.59
1:A:223:PHE:HE2	1:A:533:GLU:HA	1.67	0.58
1:D:65:VAL:HG21	1:D:399:TYR:HE2	1.66	0.58
1:D:470:THR:N	7:D:705:HOH:O	2.35	0.58
2:E:125:LYS:HD3	2:E:173:PHE:HZ	1.67	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:465:TYR:N	1:A:476:ALA:O	2.35	0.58
1:A:45:LEU:HG	1:A:50:LEU:HB2	1.85	0.58
1:D:15:ASP:OD1	7:D:727:HOH:O	2.17	0.58
2:F:23:LEU:HD23	2:F:74:VAL:HG22	1.85	0.58
1:A:197:ASP:OD1	1:A:197:ASP:N	2.37	0.58
1:A:331:GLY:HA3	1:A:336:TRP:HA	1.84	0.58
2:C:37:PHE:O	2:C:40:LYS:NZ	2.36	0.58
1:D:94:VAL:HG21	1:D:113:PHE:H	1.66	0.58
2:E:110:GLN:HB2	2:E:167:TYR:CZ	2.39	0.58
2:F:165:GLN:O	2:F:168:GLU:HB2	2.03	0.58
1:A:216:VAL:N	7:A:720:HOH:O	2.36	0.58
1:A:244:ASP:HB2	1:A:251:SER:N	2.18	0.58
1:D:424:ARG:C	1:D:543:GLY:HA2	2.23	0.58
1:D:478:PHE:CZ	1:D:562:LEU:HA	2.38	0.58
1:A:535:PHE:CZ	1:A:557:LYS:HE2	2.37	0.58
2:B:119:GLU:N	7:B:425:HOH:O	2.35	0.58
2:C:102:VAL:O	2:C:106:PHE:HB3	2.03	0.58
2:C:84:PHE:HD1	2:C:85:PHE:N	2.01	0.58
1:D:227:LEU:HD12	1:D:316:LEU:HD21	1.85	0.58
1:D:551:VAL:HG22	1:D:555:ASN:HD22	1.69	0.58
2:F:132:VAL:HG22	2:F:182:LEU:HD13	1.85	0.58
1:A:352:PHE:HA	7:A:856:HOH:O	2.04	0.58
1:A:353:ALA:HB2	1:A:413:TYR:CD2	2.39	0.58
1:A:441:LEU:HD23	1:A:549:ARG:HB3	1.86	0.58
2:C:114:TRP:HA	2:C:170:PHE:CD2	2.38	0.58
1:D:393:THR:HA	1:D:399:TYR:HA	1.85	0.58
1:D:466:ILE:HD12	1:D:552:LYS:HG3	1.84	0.58
2:E:172:ASN:OD1	7:E:412:HOH:O	2.16	0.58
2:E:183:ILE:O	2:E:186:ALA:HB3	2.03	0.58
2:F:22:ALA:HA	2:F:155:ILE:HD13	1.85	0.58
1:D:99:LEU:HG	1:D:557:LYS:CB	2.32	0.58
2:E:65:CYS:HB3	2:F:97:PHE:CZ	2.38	0.58
1:A:222:VAL:HG21	4:A:602:MET:N	2.19	0.58
1:A:233:THR:HA	1:A:236:GLN:CB	2.24	0.58
1:A:88:ILE:HG22	1:A:89:LEU:HG	1.85	0.58
2:B:165:GLN:O	2:B:169:LYS:HE3	2.03	0.58
2:B:188:ARG:NH1	7:B:426:HOH:O	2.37	0.58
2:B:163:TRP:CD2	2:B:205:ILE:HD13	2.39	0.58
1:D:169:VAL:O	1:D:172:ASN:HB2	2.04	0.58
2:F:85:PHE:CG	2:F:92:ARG:HG2	2.39	0.58
1:A:442:GLN:HG2	1:A:462:PHE:HZ	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:478:PHE:HB2	1:A:528:PHE:HZ	1.69	0.58
1:A:541:SER:O	1:A:543:GLY:N	2.37	0.58
1:A:78:LYS:NZ	1:A:553:PRO:O	2.25	0.58
1:D:78:LYS:HA	1:D:110:PHE:HD2	1.68	0.58
1:D:98:SER:HB3	1:D:113:PHE:CE2	2.38	0.58
1:D:94:VAL:CG2	1:D:113:PHE:H	2.17	0.58
1:A:149:PHE:CE2	1:A:530:LYS:HD3	2.39	0.58
2:B:51:HIS:NE2	7:B:422:HOH:O	2.32	0.58
1:D:194:PHE:O	7:D:721:HOH:O	2.18	0.58
1:D:246:LYS:HB2	7:D:852:HOH:O	2.03	0.58
2:F:140:GLY:C	2:F:181:LYS:HE2	2.25	0.58
1:A:457:ILE:HG22	1:A:481:ILE:HG22	1.85	0.57
2:B:155:ILE:HD13	7:B:516:HOH:O	2.02	0.57
2:B:155:ILE:O	2:B:158:ILE:HG22	2.04	0.57
1:D:287:TRP:HA	1:D:290:LEU:HD12	1.85	0.57
1:A:233:THR:O	1:A:237:VAL:N	2.35	0.57
1:A:552:LYS:HB3	1:A:553:PRO:HD2	1.84	0.57
2:B:130:GLU:O	2:B:134:ILE:HG13	2.05	0.57
2:B:85:PHE:CE1	2:B:152:TYR:HB3	2.40	0.57
1:A:108:PRO:HB2	1:A:554:SER:CB	2.33	0.57
1:A:191:GLU:O	1:A:195:SER:N	2.37	0.57
1:A:223:PHE:HB3	1:A:309:MET:HG3	1.86	0.57
1:A:480:GLU:HB2	1:A:528:PHE:CD2	2.39	0.57
2:C:26:LYS:NZ	2:C:82:ASN:O	2.32	0.57
1:D:203:TYR:HE2	1:D:253:ARG:HD3	1.68	0.57
2:C:22:ALA:HA	2:C:155:ILE:HD13	1.85	0.57
1:D:121:THR:HG23	1:D:336:TRP:CZ2	2.39	0.57
1:D:199:HIS:N	1:D:524:ALA:HB1	2.17	0.57
2:E:14:MET:HB3	2:E:163:TRP:NE1	2.19	0.57
1:A:101:SER:OG	1:A:544:GLN:HB3	2.04	0.57
1:A:71:VAL:O	1:A:75:PRO:HD3	2.03	0.57
2:B:153:VAL:HA	2:B:156:SER:OG	2.04	0.57
2:C:187:LYS:HA	2:C:190:MET:HG3	1.87	0.57
1:D:199:HIS:H	1:D:524:ALA:CB	2.17	0.57
1:A:365:PRO:HG2	1:A:374:GLU:HG2	1.87	0.57
1:D:114:THR:HB	1:D:395:TYR:HE1	1.70	0.57
1:D:201:ALA:O	1:D:205:HIS:N	2.37	0.57
1:D:253:ARG:HG3	1:D:484:GLU:HB3	1.87	0.57
1:A:138:ILE:HB	1:A:217:GLN:HG3	1.87	0.57
1:A:187:CYS:SG	1:A:209:GLY:HA2	2.45	0.57
1:A:291:ILE:CG1	1:A:320:ALA:HA	2.33	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:339:ALA:HB3	1:A:355:ILE:HD11	1.87	0.57
2:C:131:ALA:O	2:C:135:LEU:HB2	2.03	0.57
2:E:208:TYR:O	2:E:212:TYR:N	2.26	0.57
2:E:26:LYS:HE2	2:E:78:TRP:CD1	2.40	0.57
2:C:169:LYS:HG3	2:C:170:PHE:N	2.19	0.57
1:A:332:SER:N	1:A:335:GLY:O	2.37	0.57
2:B:22:ALA:HA	7:B:496:HOH:O	2.05	0.57
1:D:219:VAL:HB	1:D:295:PHE:CE2	2.40	0.57
1:D:338:ALA:CB	1:D:354:VAL:HA	2.34	0.57
1:D:110:PHE:HE1	1:D:556:ALA:HB2	1.69	0.57
1:A:369:THR:N	7:A:739:HOH:O	2.38	0.56
2:B:175:ILE:HB	2:B:183:ILE:HD13	1.87	0.56
2:C:75:ASP:HB2	2:C:84:PHE:CE2	2.39	0.56
1:D:223:PHE:HD2	1:D:225:HIS:CE1	2.23	0.56
1:D:354:VAL:O	1:D:416:THR:HG21	2.05	0.56
1:D:47:ASN:OD1	1:D:47:ASN:N	2.33	0.56
1:D:80:MET:SD	1:D:88:ILE:N	2.78	0.56
2:F:68:LEU:HD12	2:F:69:ASN:N	2.20	0.56
1:A:18:ASP:OD1	7:A:729:HOH:O	2.17	0.56
1:A:551:VAL:HB	1:A:555:ASN:HB2	1.87	0.56
1:A:535:PHE:CE1	1:A:557:LYS:HE2	2.40	0.56
1:D:445:VAL:HA	1:D:479:TRP:CZ2	2.39	0.56
1:D:474:HIS:HB2	1:D:517:ALA:O	2.04	0.56
1:D:75:PRO:HA	1:D:78:LYS:HG2	1.87	0.56
2:E:92:ARG:O	2:E:96:ARG:HG2	2.05	0.56
1:A:97:ILE:HG21	1:A:110:PHE:CZ	2.41	0.56
1:A:463:SER:HB3	1:A:478:PHE:CD2	2.40	0.56
2:B:146:GLY:HA2	2:B:152:TYR:CZ	2.40	0.56
1:D:223:PHE:CE2	1:D:533:GLU:HA	2.40	0.56
1:D:463:SER:O	1:D:477:ILE:HA	2.05	0.56
1:D:557:LYS:HD2	5:D:603:ATP:O1G	2.05	0.56
1:A:107:ARG:HG3	1:A:108:PRO:HD2	1.87	0.56
1:D:304:ILE:HG12	1:D:328:HIS:O	2.06	0.56
2:E:192:LYS:HZ1	2:E:194:SER:HB3	1.70	0.56
2:B:31:GLU:OE1	2:B:31:GLU:N	2.38	0.56
2:B:51:HIS:O	2:B:52:LYS:HG2	2.05	0.56
1:D:169:VAL:HG13	1:D:170:TYR:CD1	2.40	0.56
2:F:23:LEU:HG	7:F:417:HOH:O	2.06	0.56
1:D:421:PHE:CD2	1:D:541:SER:HA	2.40	0.56
2:E:40:LYS:HB3	7:E:401:HOH:O	2.05	0.56
2:B:66:GLU:CD	2:B:69:ASN:HB2	2.26	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:162:SER:HB3	2:B:199:LEU:HG	1.86	0.56
2:B:114:TRP:CD1	2:B:167:TYR:CE1	2.94	0.56
1:D:149:PHE:CZ	1:D:198:VAL:HB	2.40	0.56
1:D:219:VAL:HG21	1:D:231:PHE:HZ	1.69	0.56
2:E:104:LYS:O	2:E:108:ASP:N	2.37	0.56
2:C:54:ILE:HB	2:C:55:PRO:HA	1.88	0.56
1:D:238:TRP:O	1:D:240:GLU:N	2.39	0.56
1:D:435:LYS:HG2	1:D:438:GLU:N	2.21	0.56
1:D:451:ARG:NH1	1:D:454:GLU:OE2	2.38	0.56
2:F:129:ILE:HA	2:F:132:VAL:HG12	1.87	0.56
2:F:214:LYS:NZ	7:F:428:HOH:O	2.39	0.56
1:A:309:MET:SD	1:A:312:TYR:HD2	2.29	0.56
2:C:125:LYS:HA	2:C:128:PHE:CE2	2.41	0.56
1:D:34:GLU:O	1:D:38:LYS:HB2	2.06	0.56
1:A:104:SER:O	1:A:107:ARG:HB3	2.06	0.56
1:A:152:LYS:HD3	1:A:561:ILE:HA	1.88	0.56
2:C:64:VAL:HG23	2:C:70:VAL:HG22	1.87	0.56
1:D:389:GLU:OE1	7:D:729:HOH:O	2.18	0.56
1:D:501:PHE:HD2	1:D:506:TYR:CZ	2.22	0.56
2:E:96:ARG:HD2	2:F:73:TYR:CE1	2.40	0.56
2:C:184:ALA:HB1	1:D:499:ARG:NH1	2.21	0.55
1:D:169:VAL:O	1:D:175:PHE:HB2	2.06	0.55
2:E:85:PHE:HE1	2:E:152:TYR:CG	2.24	0.55
1:A:92:HIS:CE1	2:B:142:LYS:H	2.25	0.55
1:D:197:ASP:OD2	1:D:200:GLN:NE2	2.40	0.55
1:D:233:THR:HG23	1:D:525:LYS:HZ3	1.71	0.55
1:D:36:LEU:O	1:D:40:GLN:N	2.39	0.55
1:D:532:GLN:HB3	1:D:545:PHE:CZ	2.41	0.55
2:E:175:ILE:H	2:E:175:ILE:HD12	1.70	0.55
1:D:92:HIS:CE1	2:E:181:LYS:HE3	2.40	0.55
2:E:176:GLU:HB2	2:E:183:ILE:HG12	1.87	0.55
1:A:126:ARG:HE	1:A:182:ILE:HG21	1.71	0.55
2:B:146:GLY:H	2:B:151:GLY:HA3	1.71	0.55
1:A:163:GLY:HA2	1:A:560:GLN:HB2	1.88	0.55
1:D:8:PHE:HZ	1:D:130:ALA:HB2	1.70	0.55
1:D:89:LEU:HD12	1:D:90:THR:CG2	2.36	0.55
1:A:256:VAL:O	1:A:260:ARG:HB2	2.06	0.55
2:B:32:TYR:OH	2:B:34:GLU:OE1	2.24	0.55
1:D:403:LEU:HD21	1:D:544:GLN:HE22	1.71	0.55
1:A:227:LEU:O	1:A:231:PHE:N	2.29	0.55
1:D:206:LEU:HD11	1:D:233:THR:HG22	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:165:GLN:CA	2:F:168:GLU:HG3	2.37	0.55
2:B:92:ARG:NH1	2:B:96:ARG:HH12	2.04	0.55
2:C:169:LYS:HG3	2:C:170:PHE:H	1.71	0.55
2:C:92:ARG:HD2	7:C:488:HOH:O	2.06	0.55
1:D:357:ASN:ND2	7:D:718:HOH:O	2.11	0.55
1:A:351:THR:N	7:A:774:HOH:O	2.39	0.55
2:B:96:ARG:NH2	2:C:76:GLU:OE1	2.40	0.55
1:D:107:ARG:HB2	1:D:552:LYS:CE	2.36	0.55
2:E:125:LYS:HD3	2:E:173:PHE:CZ	2.42	0.55
2:F:26:LYS:HG2	2:F:81:LYS:NZ	2.22	0.55
1:A:498:ASP:HB3	1:A:510:ARG:NH1	2.22	0.55
2:B:97:PHE:N	2:C:69:ASN:HD21	2.04	0.55
1:D:466:ILE:N	1:D:551:VAL:O	2.40	0.55
2:F:128:PHE:O	2:F:132:VAL:HG12	2.05	0.55
1:A:156:SER:HB2	1:A:162:VAL:HG13	1.89	0.55
2:B:114:TRP:HD1	2:B:167:TYR:CE1	2.24	0.55
2:C:14:MET:HE2	2:C:14:MET:H	1.72	0.55
1:D:97:ILE:HG23	1:D:111:ILE:H	1.70	0.55
1:D:271:PRO:HA	7:D:852:HOH:O	2.06	0.55
1:D:439:ARG:NH2	7:D:777:HOH:O	2.39	0.55
1:D:467:ASP:O	1:D:475:TYR:CZ	2.60	0.55
1:D:98:SER:HB2	1:D:557:LYS:HD3	1.89	0.55
1:A:117:LEU:HD13	5:A:603:ATP:N3	2.21	0.54
2:C:114:TRP:HD1	2:C:167:TYR:CE1	2.25	0.54
1:D:510:ARG:HB2	7:D:955:HOH:O	2.06	0.54
1:D:477:ILE:CD1	1:D:518:LEU:HD21	2.34	0.54
2:C:114:TRP:CD1	2:C:167:TYR:CE1	2.94	0.54
2:B:69:ASN:ND2	2:C:93:ALA:O	2.31	0.54
1:D:193:ILE:HG22	1:D:205:HIS:NE2	2.23	0.54
1:D:223:PHE:HZ	1:D:536:LEU:HB3	1.71	0.54
2:E:152:TYR:OH	7:E:408:HOH:O	2.14	0.54
2:F:183:ILE:O	2:F:186:ALA:HB3	2.06	0.54
1:A:405:ASP:HB3	1:A:426:ASN:ND2	2.20	0.54
1:A:440:ASP:OD1	1:A:502:ILE:HG13	2.08	0.54
2:B:202:SER:O	2:B:206:VAL:HG13	2.08	0.54
2:C:17:MET:CE	2:C:200:PRO:HD2	2.37	0.54
2:C:11:TRP:O	2:C:200:PRO:HG2	2.08	0.54
2:F:7:LEU:HA	2:F:56:VAL:O	2.08	0.54
1:A:287:TRP:CE3	1:A:287:TRP:HA	2.42	0.54
2:B:35:GLU:OE2	7:B:410:HOH:O	2.18	0.54
1:D:445:VAL:HG21	1:D:462:PHE:CD2	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:479:TRP:HB2	1:D:522:VAL:HG12	1.89	0.54
1:D:94:VAL:HG11	1:D:97:ILE:HG12	1.88	0.54
2:E:18:ARG:NH2	2:E:67:SER:OG	2.39	0.54
2:F:178:GLU:O	2:F:180:PRO:HD3	2.07	0.54
1:D:143:LYS:HB2	7:D:755:HOH:O	2.07	0.54
1:A:238:TRP:CH2	1:A:281:CYS:HB3	2.43	0.54
1:A:97:ILE:H	1:A:162:VAL:HA	1.70	0.54
2:C:138:GLU:HG3	2:C:145:PHE:HE1	1.72	0.54
1:D:113:PHE:CG	5:D:603:ATP:O1B	2.60	0.54
1:A:76:TYR:HB3	1:A:88:ILE:CG2	2.38	0.54
2:B:93:ALA:HA	2:C:73:TYR:CE1	2.43	0.54
1:D:498:ASP:O	1:D:510:ARG:NH2	2.41	0.54
1:D:99:LEU:HB3	1:D:556:ALA:H	1.71	0.54
2:E:201:ASP:HB3	2:E:203:GLU:HG2	1.90	0.54
2:F:110:GLN:O	2:F:113:VAL:HG12	2.08	0.54
1:A:97:ILE:HG21	1:A:110:PHE:CE2	2.43	0.54
2:C:26:LYS:HE3	2:C:78:TRP:NE1	2.23	0.54
2:C:98:TRP:CD1	2:C:153:VAL:HG11	2.42	0.54
1:D:191:GLU:OE1	1:D:191:GLU:N	2.41	0.54
1:D:332:SER:HA	5:D:603:ATP:N6	2.23	0.54
1:A:221:ALA:HA	7:A:751:HOH:O	2.07	0.54
1:D:290:LEU:O	1:D:293:ALA:N	2.41	0.54
1:A:234:PHE:CZ	1:A:294:LEU:HD11	2.43	0.53
1:A:535:PHE:O	1:A:538:LEU:HB3	2.07	0.53
1:A:536:LEU:HD23	1:A:542:ALA:HA	1.90	0.53
2:B:10:TYR:HB3	2:B:13:SER:HB3	1.90	0.53
2:C:139:LEU:HB3	2:C:181:LYS:NZ	2.23	0.53
1:D:130:ALA:HA	1:D:133:ASN:HB2	1.89	0.53
2:F:110:GLN:CG	2:F:167:TYR:HE2	2.21	0.53
1:A:242:VAL:O	1:A:246:LYS:HB2	2.09	0.53
1:A:286:ASN:O	7:A:735:HOH:O	2.19	0.53
1:D:116:GLU:HA	1:D:119:GLU:HG3	1.90	0.53
1:D:225:HIS:HA	1:D:228:VAL:HB	1.90	0.53
1:D:243:THR:HA	1:D:246:LYS:CD	2.38	0.53
1:D:290:LEU:N	7:D:753:HOH:O	2.34	0.53
1:D:413:TYR:N	1:D:418:GLN:OE1	2.39	0.53
1:D:409:VAL:HA	1:D:420:LYS:NZ	2.23	0.53
2:B:26:LYS:O	2:B:81:LYS:NZ	2.30	0.53
2:C:98:TRP:HD1	2:C:153:VAL:HG11	1.74	0.53
1:D:172:ASN:HB3	1:D:174:ASN:OD1	2.08	0.53
1:D:239:GLU:O	1:D:243:THR:N	2.30	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:192:LYS:NZ	2:E:194:SER:HB3	2.23	0.53
1:A:143:LYS:HD3	1:A:187:CYS:CB	2.39	0.53
1:A:9:ASP:OD2	1:A:12:ARG:HB3	2.09	0.53
2:B:154:ASP:OD1	2:B:185:TRP:NE1	2.38	0.53
2:B:90:TYR:O	2:B:93:ALA:HB3	2.09	0.53
2:F:169:LYS:HG3	2:F:170:PHE:N	2.24	0.53
1:A:22:ARG:HG2	1:A:414:ASN:HB3	1.89	0.53
2:C:10:TYR:CG	2:C:12:PRO:HD2	2.43	0.53
1:D:78:LYS:HA	1:D:110:PHE:CD2	2.43	0.53
2:F:9:ASP:HA	2:F:54:ILE:HD13	1.91	0.53
1:A:465:TYR:HB2	1:A:478:PHE:CZ	2.44	0.53
1:D:403:LEU:CD2	1:D:544:GLN:HE22	2.21	0.53
1:A:465:TYR:CD1	1:A:551:VAL:HG23	2.41	0.53
1:A:86:SER:HB2	2:B:188:ARG:HB2	1.90	0.53
2:C:170:PHE:CD2	2:C:213:ARG:HD2	2.43	0.53
2:C:84:PHE:CG	2:C:152:TYR:HB2	2.42	0.53
1:D:199:HIS:CD2	1:D:200:GLN:HG3	2.44	0.53
1:D:163:GLY:HA2	1:D:560:GLN:CD	2.29	0.53
2:F:110:GLN:HB3	2:F:167:TYR:OH	2.08	0.53
2:F:188:ARG:NE	2:F:188:ARG:HA	2.24	0.53
1:A:457:ILE:HG23	1:A:482:SER:OG	2.08	0.53
2:E:130:GLU:HG3	7:E:516:HOH:O	2.08	0.53
2:F:178:GLU:C	2:F:180:PRO:HD3	2.29	0.53
2:F:185:TRP:CE3	2:F:186:ALA:N	2.76	0.53
1:A:166:THR:HG21	1:A:530:LYS:HD2	1.91	0.53
1:A:106:GLY:O	1:A:432:ASN:ND2	2.41	0.53
1:A:465:TYR:HB2	1:A:478:PHE:HZ	1.74	0.53
2:B:152:TYR:HD1	2:B:153:VAL:HG12	1.72	0.53
1:D:152:LYS:HD3	1:D:560:GLN:O	2.09	0.53
1:D:336:TRP:HB2	1:D:358:LEU:HD22	1.90	0.53
2:F:188:ARG:NH1	7:F:432:HOH:O	2.41	0.53
1:A:139:ASP:OD1	7:A:736:HOH:O	2.19	0.53
2:C:48:ASN:O	7:C:413:HOH:O	2.19	0.53
2:C:4:LEU:HB3	2:C:31:GLU:OE1	2.08	0.53
2:C:69:ASN:HB3	2:C:73:TYR:CZ	2.44	0.53
1:D:338:ALA:HB2	1:D:354:VAL:HA	1.91	0.53
2:F:215:ASN:O	7:F:410:HOH:O	2.19	0.53
1:A:182:ILE:HD13	1:A:182:ILE:H	1.73	0.52
1:A:475:TYR:HE2	1:A:506:TYR:CE1	2.27	0.52
1:A:557:LYS:O	1:A:561:ILE:HG13	2.10	0.52
2:C:122:GLU:OE1	7:C:414:HOH:O	2.19	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:8:LEU:HB2	2:E:56:VAL:HG13	1.89	0.52
1:A:215:GLN:HB2	7:A:720:HOH:O	2.08	0.52
1:A:314:PRO:HA	1:A:317:ARG:NH1	2.24	0.52
1:A:329:ASP:OD1	1:A:340:ASN:N	2.27	0.52
2:B:6:ILE:CG2	2:B:33:ARG:HD2	2.39	0.52
1:D:410:ILE:H	1:D:420:LYS:HZ3	1.57	0.52
1:D:80:MET:HE1	1:D:88:ILE:HG13	1.90	0.52
1:D:90:THR:HG21	1:D:397:GLY:CA	2.39	0.52
2:E:45:LEU:N	7:E:401:HOH:O	2.43	0.52
2:F:26:LYS:NZ	7:F:401:HOH:O	2.17	0.52
1:A:363:PHE:HE2	1:A:419:LEU:HD11	1.74	0.52
1:A:442:GLN:HG2	1:A:462:PHE:CZ	2.44	0.52
1:A:94:VAL:HG22	1:A:96:ALA:H	1.72	0.52
1:D:336:TRP:CB	1:D:358:LEU:HD22	2.39	0.52
2:F:117:LYS:HA	2:F:121:GLN:HB2	1.91	0.52
2:F:181:LYS:N	7:F:411:HOH:O	2.40	0.52
2:F:32:TYR:HD1	2:F:32:TYR:H	1.57	0.52
1:A:152:LYS:HD3	1:A:561:ILE:O	2.09	0.52
1:A:424:ARG:HG2	1:A:425:ARG:HG3	1.91	0.52
2:B:10:TYR:CG	2:B:12:PRO:HD2	2.45	0.52
1:A:41:SER:HB2	2:B:143:PRO:HD2	1.91	0.52
5:D:603:ATP:C2'	5:D:603:ATP:N3	2.70	0.52
1:A:295:PHE:CD2	1:A:298:ALA:HB2	2.43	0.52
1:A:165:ALA:HA	5:A:603:ATP:O5'	2.09	0.52
1:A:94:VAL:HG11	1:A:97:ILE:HD11	1.92	0.52
2:C:198:SER:O	2:C:200:PRO:HD3	2.09	0.52
1:D:332:SER:HB2	1:D:539:GLY:H	1.74	0.52
1:D:335:GLY:O	1:D:539:GLY:HA3	2.10	0.52
1:A:122:LEU:HA	1:A:125:PHE:CZ	2.45	0.52
1:A:142:GLY:O	1:A:185:PRO:HD2	2.09	0.52
1:D:276:THR:OG1	1:D:277:ILE:N	2.43	0.52
1:D:480:GLU:HB2	1:D:528:PHE:HZ	1.69	0.52
1:D:77:ILE:O	1:D:81:VAL:HG23	2.09	0.52
2:E:12:PRO:HB2	2:E:208:TYR:CE2	2.45	0.52
2:F:24:ARG:HG3	2:F:30:PHE:CZ	2.45	0.52
1:A:241:ILE:HG22	1:A:242:VAL:N	2.25	0.52
1:D:248:GLY:O	1:D:267:LEU:HD13	2.10	0.52
2:F:132:VAL:HG13	2:F:179:SER:CB	2.39	0.52
2:B:162:SER:HG	2:B:163:TRP:HD1	1.57	0.52
2:B:18:ARG:HG2	2:B:159:THR:HB	1.92	0.52
2:C:199:LEU:O	7:C:402:HOH:O	2.19	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:354:VAL:HG11	1:D:379:LEU:HD11	1.90	0.52
1:D:465:TYR:HA	1:D:551:VAL:HB	1.91	0.52
1:D:513:LYS:NZ	1:D:575:PHE:HD2	2.07	0.52
2:E:10:TYR:HB3	2:E:13:SER:CB	2.40	0.52
1:A:213:ARG:HH21	1:A:296:PRO:CD	2.22	0.52
1:A:472:PRO:HD2	7:A:843:HOH:O	2.10	0.52
1:A:99:LEU:HG	1:A:555:ASN:OD1	2.09	0.52
1:D:241:ILE:O	1:D:245:ILE:HG23	2.10	0.52
1:D:452:LEU:HD11	1:D:490:LEU:HD23	1.91	0.52
2:E:139:LEU:O	2:E:141:ASP:N	2.43	0.52
1:A:328:HIS:CG	1:A:329:ASP:N	2.78	0.52
1:A:498:ASP:HB3	1:A:510:ARG:HH12	1.75	0.52
2:B:111:PHE:HA	2:B:114:TRP:NE1	2.25	0.52
1:D:262:ALA:HA	1:D:265:LYS:HE2	1.91	0.52
1:D:317:ARG:HA	1:D:320:ALA:HB3	1.92	0.52
1:D:75:PRO:O	1:D:79:ARG:HG2	2.10	0.52
2:E:13:SER:O	2:E:17:MET:HG3	2.10	0.52
1:A:143:LYS:C	1:A:184:SER:HB2	2.30	0.51
1:A:250:LEU:HD21	1:A:260:ARG:HA	1.91	0.51
1:A:39:ASN:OD1	2:B:143:PRO:HD3	2.10	0.51
2:C:8:LEU:HD13	2:C:44:LEU:HB2	1.92	0.51
2:F:84:PHE:HD1	2:F:85:PHE:N	2.08	0.51
1:A:366:VAL:O	7:A:739:HOH:O	2.19	0.51
1:A:164:THR:HG23	1:A:534:HIS:CE1	2.45	0.51
1:D:232:ARG:NH1	7:D:784:HOH:O	2.43	0.51
1:D:526:GLY:O	1:D:529:ARG:HG2	2.09	0.51
2:E:164:PHE:HE2	2:E:183:ILE:HA	1.76	0.51
2:F:26:LYS:HG2	2:F:81:LYS:HZ3	1.74	0.51
1:A:109:LYS:HG2	7:A:762:HOH:O	2.10	0.51
1:A:336:TRP:HD1	5:A:603:ATP:C5	2.28	0.51
2:C:144:TYR:HB3	2:C:154:ASP:OD2	2.10	0.51
1:D:10:MET:SD	7:D:931:HOH:O	2.59	0.51
1:D:384:ILE:HG13	7:D:841:HOH:O	2.11	0.51
2:F:163:TRP:O	2:F:166:ALA:N	2.42	0.51
1:A:29:LYS:NZ	7:A:732:HOH:O	2.17	0.51
2:C:26:LYS:HD3	2:C:74:VAL:CG1	2.39	0.51
1:D:368:GLU:O	7:D:731:HOH:O	2.19	0.51
1:D:48:CYS:O	7:D:732:HOH:O	2.19	0.51
2:F:70:VAL:HG21	7:F:405:HOH:O	2.09	0.51
1:A:407:VAL:CG2	1:A:419:LEU:HB3	2.40	0.51
2:C:153:VAL:O	2:C:157:LEU:HD23	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:197:ASP:HB2	1:D:256:VAL:HG21	1.93	0.51
1:D:223:PHE:HB3	1:D:309:MET:SD	2.51	0.51
1:D:328:HIS:CG	1:D:329:ASP:N	2.78	0.51
1:D:75:PRO:O	1:D:78:LYS:HG2	2.10	0.51
2:F:125:LYS:HA	2:F:128:PHE:CE2	2.45	0.51
2:F:203:GLU:OE2	7:F:409:HOH:O	2.18	0.51
1:A:495:ASN:HB3	1:A:499:ARG:HH11	1.76	0.51
2:C:20:ARG:HB3	2:C:198:SER:OG	2.11	0.51
1:D:208:SER:O	1:D:211:LEU:HB2	2.10	0.51
1:D:363:PHE:CD2	1:D:382:VAL:HG21	2.41	0.51
1:D:99:LEU:O	1:D:557:LYS:HD3	2.09	0.51
2:E:18:ARG:HH21	2:E:67:SER:HG	1.56	0.51
1:A:152:LYS:HE2	1:A:565:ASN:CB	2.31	0.51
1:A:197:ASP:OD2	1:A:200:GLN:HB2	2.10	0.51
1:A:224:ALA:O	1:A:228:VAL:HG23	2.11	0.51
1:A:45:LEU:HD11	1:A:50:LEU:HD22	1.93	0.51
2:B:135:LEU:O	2:B:139:LEU:HD22	2.11	0.51
2:B:86:PRO:HD3	2:B:152:TYR:HE2	1.75	0.51
2:C:26:LYS:HE2	2:C:75:ASP:HA	1.92	0.51
1:D:219:VAL:HG21	1:D:231:PHE:CZ	2.44	0.51
1:D:243:THR:HA	1:D:246:LYS:HD3	1.93	0.51
1:D:256:VAL:HB	1:D:259:VAL:HG12	1.92	0.51
1:D:93:PRO:HG2	2:E:184:ALA:HB3	1.92	0.51
2:E:85:PHE:HB3	2:E:92:ARG:HG2	1.93	0.51
1:A:330:TYR:CG	1:A:421:PHE:HE2	2.28	0.51
1:A:455:GLU:OE1	1:A:485:THR:HB	2.11	0.51
2:B:26:LYS:HG3	2:B:28:VAL:H	1.75	0.51
1:D:213:ARG:HG3	1:D:214:ASP:H	1.76	0.51
1:D:213:ARG:HG3	1:D:214:ASP:N	2.26	0.51
1:D:203:TYR:CE2	1:D:253:ARG:HD3	2.44	0.51
1:D:329:ASP:OD1	1:D:340:ASN:N	2.37	0.51
1:D:423:CYS:HB3	1:D:543:GLY:N	2.26	0.51
5:D:603:ATP:O2'	5:D:603:ATP:C4	2.62	0.51
2:F:23:LEU:HD22	2:F:28:VAL:HG11	1.92	0.51
1:A:277:ILE:HG23	1:A:278:ARG:N	2.25	0.51
1:A:62:LYS:HZ1	1:A:376:PRO:HB2	1.75	0.51
2:B:145:PHE:HD2	2:B:153:VAL:HG22	1.75	0.51
2:B:65:CYS:O	2:B:69:ASN:HB3	2.11	0.51
2:C:31:GLU:HB3	7:C:438:HOH:O	2.11	0.51
1:D:163:GLY:HA3	1:D:168:ASN:HD21	1.75	0.51
1:D:233:THR:HG23	1:D:525:LYS:NZ	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:229:HIS:ND1	1:D:529:ARG:HD3	2.25	0.51
1:A:90:THR:HG21	1:A:112:PRO:HG2	1.93	0.51
1:A:407:VAL:HB	1:A:541:SER:HB2	1.94	0.50
2:B:103:ASP:O	2:B:107:THR:OG1	2.20	0.50
1:D:103:THR:HB	1:D:106:GLY:CA	2.41	0.50
1:D:478:PHE:HZ	1:D:562:LEU:HA	1.76	0.50
2:E:98:TRP:NE1	2:E:138:GLU:HG2	2.26	0.50
2:F:190:MET:HA	2:F:195:VAL:CG1	2.41	0.50
1:A:201:ALA:O	1:A:205:HIS:N	2.45	0.50
1:A:330:TYR:HE1	1:A:536:LEU:O	1.95	0.50
1:A:521:ARG:HD2	1:A:562:LEU:HD11	1.94	0.50
1:A:87:PRO:HD2	2:B:188:ARG:CB	2.41	0.50
1:D:273:LEU:O	1:D:276:THR:HG23	2.10	0.50
2:F:114:TRP:CD1	2:F:167:TYR:CE1	2.99	0.50
1:A:199:HIS:CE1	1:A:567:VAL:HG11	2.36	0.50
2:B:79:PRO:HA	7:B:423:HOH:O	2.11	0.50
1:D:149:PHE:N	7:D:788:HOH:O	2.44	0.50
1:D:132:ARG:CA	1:D:343:PRO:HG2	2.41	0.50
1:D:334:GLU:HB3	1:D:398:LEU:HD12	1.93	0.50
1:D:509:SER:HA	1:D:512:CYS:SG	2.51	0.50
1:A:125:PHE:HD1	1:A:126:ARG:N	2.10	0.50
1:A:166:THR:HG23	4:A:602:MET:OXT	2.12	0.50
1:A:230:ALA:O	1:A:234:PHE:N	2.44	0.50
1:D:107:ARG:HB2	1:D:552:LYS:HE3	1.92	0.50
1:D:360:TYR:CE2	1:D:362:GLU:OE2	2.64	0.50
1:D:365:PRO:HA	1:D:388:TYR:CD1	2.46	0.50
2:F:183:ILE:O	2:F:187:LYS:HD2	2.11	0.50
2:F:68:LEU:O	2:F:72:GLN:HG2	2.11	0.50
1:A:240:GLU:HG3	1:A:251:SER:HB3	1.93	0.50
1:A:248:GLY:HA2	1:A:267:LEU:HG	1.94	0.50
1:A:479:TRP:HB3	1:A:481:ILE:HD11	1.93	0.50
1:A:552:LYS:C	1:A:554:SER:H	2.14	0.50
1:A:87:PRO:HG2	2:B:188:ARG:HG2	1.93	0.50
2:B:127:GLU:OE1	7:B:411:HOH:O	2.19	0.50
1:A:93:PRO:O	2:B:181:LYS:HG2	2.12	0.50
1:D:13:VAL:HG11	1:D:130:ALA:HB3	1.93	0.50
1:D:145:LEU:HD11	1:D:210:ILE:HD13	1.93	0.50
1:D:528:PHE:CB	1:D:531:ILE:HD12	2.36	0.50
6:E:301:GSH:O31	7:E:413:HOH:O	2.19	0.50
2:E:90:TYR:O	2:E:93:ALA:HB3	2.10	0.50
2:F:198:SER:N	7:F:436:HOH:O	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:8:LEU:HD22	2:F:33:ARG:HE	1.76	0.50
1:A:146:GLN:HB3	1:A:220:PHE:HD2	1.77	0.50
1:A:62:LYS:HA	1:A:400:ARG:CZ	2.41	0.50
2:B:92:ARG:O	2:B:95:ALA:HB3	2.12	0.50
1:D:10:MET:HA	1:D:13:VAL:CG2	2.42	0.50
1:D:445:VAL:HG21	1:D:462:PHE:CG	2.47	0.50
1:D:95:PRO:HD3	2:E:181:LYS:HZ2	1.76	0.50
2:E:204:LYS:O	2:E:207:ALA:HB3	2.10	0.50
2:F:150:PHE:CD1	2:F:192:LYS:HG3	2.47	0.50
2:F:162:SER:HB2	2:F:205:ILE:HD13	1.92	0.50
1:A:272:GLU:O	1:A:275:GLU:HB3	2.11	0.50
1:A:23:ASN:O	1:A:27:VAL:HG12	2.11	0.50
1:A:43:ILE:HG13	1:A:44:TYR:N	2.27	0.50
2:B:125:LYS:O	2:B:129:ILE:HG12	2.11	0.50
2:C:102:VAL:O	2:C:107:THR:HG23	2.11	0.50
2:C:98:TRP:CH2	2:C:135:LEU:HG	2.47	0.50
1:D:339:ALA:O	1:D:353:ALA:N	2.44	0.50
1:D:396:ALA:N	7:D:775:HOH:O	2.38	0.50
1:D:496:CYS:HA	1:D:499:ARG:CZ	2.42	0.50
1:D:528:PHE:O	1:D:532:GLN:HG3	2.12	0.50
2:E:11:TRP:CD1	2:E:12:PRO:HD3	2.47	0.50
1:D:91:GLY:HA2	2:E:142:LYS:C	2.31	0.50
1:A:480:GLU:HG2	1:A:525:LYS:HA	1.94	0.50
2:B:70:VAL:O	2:B:74:VAL:HB	2.11	0.50
1:D:174:ASN:N	1:D:174:ASN:OD1	2.33	0.50
1:D:440:ASP:O	1:D:444:SER:N	2.44	0.50
3:D:601:JAA:C08	4:D:602:MET:HE2	2.42	0.50
1:A:480:GLU:OE1	1:A:528:PHE:N	2.41	0.50
1:D:70:ASP:OD2	1:D:104:SER:HA	2.12	0.50
1:D:202:LEU:HA	1:D:205:HIS:HB2	1.94	0.50
1:D:291:ILE:HG21	1:D:301:VAL:HG22	1.94	0.50
1:D:121:THR:HG22	1:D:336:TRP:CZ2	2.45	0.50
1:D:473:GLY:HA3	1:D:475:TYR:CE2	2.46	0.50
1:A:104:SER:HB2	1:A:109:LYS:HG3	1.94	0.49
1:A:379:LEU:HG	1:A:417:PRO:HG3	1.94	0.49
1:A:364:LEU:O	1:A:389:GLU:N	2.45	0.49
1:A:78:LYS:CE	1:A:554:SER:HA	2.41	0.49
1:D:223:PHE:HD2	1:D:225:HIS:HE1	1.59	0.49
1:D:301:VAL:HB	1:D:325:LEU:HD23	1.94	0.49
2:E:166:ALA:O	2:E:169:LYS:HG2	2.11	0.49
2:E:18:ARG:NH2	7:E:425:HOH:O	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:26:LYS:HD2	2:F:74:VAL:HG12	1.94	0.49
1:A:194:PHE:O	7:A:737:HOH:O	2.19	0.49
2:B:66:GLU:HB2	2:B:69:ASN:HB2	1.94	0.49
2:B:69:ASN:OD1	2:C:96:ARG:NE	2.45	0.49
1:D:143:LYS:CD	1:D:212:PHE:HB2	2.32	0.49
1:D:494:CYS:HB2	1:D:520:LEU:HB2	1.95	0.49
2:E:121:GLN:HG2	2:E:125:LYS:HE3	1.93	0.49
2:E:166:ALA:HA	2:E:169:LYS:HG2	1.93	0.49
1:A:389:GLU:OE2	1:A:402:ARG:NH2	2.45	0.49
2:B:207:ALA:O	2:B:211:GLU:N	2.36	0.49
2:C:108:ASP:O	2:C:112:LYS:HG2	2.13	0.49
2:C:84:PHE:CD1	2:C:85:PHE:N	2.79	0.49
1:D:126:ARG:HE	1:D:182:ILE:HD11	1.76	0.49
1:D:39:ASN:OD1	1:D:90:THR:HA	2.12	0.49
2:F:129:ILE:HG13	2:F:130:GLU:N	2.28	0.49
1:A:96:ALA:HB1	1:A:163:GLY:N	2.28	0.49
2:B:23:LEU:HD23	2:B:30:PHE:HB3	1.94	0.49
2:C:143:PRO:HG2	7:C:424:HOH:O	2.12	0.49
1:D:233:THR:O	1:D:237:VAL:HG22	2.12	0.49
1:D:519:GLU:HG3	1:D:570:TYR:C	2.32	0.49
1:A:280:LYS:HE3	1:A:293:ALA:HB1	1.95	0.49
1:A:547:MET:HE2	1:A:549:ARG:HD3	1.95	0.49
1:A:333:SER:O	5:A:603:ATP:H2	1.96	0.49
1:A:407:VAL:HG21	1:A:419:LEU:HB3	1.94	0.49
2:B:195:VAL:HG11	7:B:414:HOH:O	2.13	0.49
2:B:65:CYS:HB3	7:B:437:HOH:O	2.12	0.49
1:D:224:ALA:HA	1:D:316:LEU:HD22	1.94	0.49
1:D:330:TYR:CE2	1:D:421:PHE:HZ	2.31	0.49
2:F:139:LEU:HB3	2:F:181:LYS:CD	2.32	0.49
2:F:39:ASN:OD1	7:F:413:HOH:O	2.20	0.49
1:A:445:VAL:HG13	1:A:479:TRP:NE1	2.27	0.49
2:C:146:GLY:HA3	2:C:151:GLY:HA3	1.95	0.49
2:C:60:ASN:O	2:C:60:ASN:ND2	2.44	0.49
2:C:57:LEU:O	2:C:64:VAL:HG22	2.12	0.49
1:A:148:ILE:HG12	1:A:170:TYR:OH	2.12	0.49
1:A:558:VAL:O	1:A:561:ILE:HB	2.13	0.49
2:B:15:PHE:HB3	2:B:67:SER:OG	2.13	0.49
2:B:135:LEU:HB2	2:B:182:LEU:HD11	1.95	0.49
2:B:26:LYS:CD	2:B:28:VAL:HB	2.43	0.49
1:D:103:THR:N	7:D:771:HOH:O	2.35	0.49
1:D:528:PHE:HA	1:D:531:ILE:CG1	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:165:GLN:HB3	2:F:202:SER:HB3	1.95	0.49
2:F:70:VAL:HA	2:F:73:TYR:CD2	2.47	0.49
1:A:305:MET:HB3	1:A:313:VAL:HG22	1.93	0.49
1:A:307:GLY:O	1:A:310:GLU:HB2	2.13	0.49
2:B:105:LYS:NZ	2:B:134:ILE:HD12	2.28	0.49
2:B:163:TRP:HA	2:B:205:ILE:HD11	1.95	0.49
2:F:108:ASP:O	2:F:112:LYS:HG2	2.13	0.49
1:A:10:MET:O	1:A:14:ILE:HG13	2.12	0.49
1:A:290:LEU:CD1	1:A:319:TYR:HD1	2.24	0.49
1:A:368:GLU:N	7:A:739:HOH:O	2.45	0.49
1:A:494:CYS:CB	1:A:520:LEU:HB3	2.40	0.49
1:A:33:LYS:HE3	1:A:57:PRO:HG3	1.95	0.49
1:A:91:GLY:HA2	2:B:143:PRO:HG3	1.93	0.49
1:A:95:PRO:HG3	7:A:851:HOH:O	2.13	0.49
1:D:388:TYR:OH	7:D:734:HOH:O	2.20	0.49
2:F:128:PHE:CE1	2:F:175:ILE:HB	2.48	0.49
1:A:153:GLN:HA	1:A:560:GLN:HG2	1.94	0.48
1:A:420:LYS:HG2	1:A:421:PHE:N	2.28	0.48
2:B:92:ARG:NE	7:B:434:HOH:O	2.46	0.48
2:C:70:VAL:O	2:C:74:VAL:HG23	2.12	0.48
2:C:99:ALA:HB2	2:C:152:TYR:CE2	2.48	0.48
1:D:13:VAL:C	1:D:14:ILE:HG13	2.33	0.48
1:D:405:ASP:CG	1:D:540:SER:HB3	2.33	0.48
2:E:10:TYR:HB3	2:E:13:SER:HB3	1.95	0.48
1:A:103:THR:HG22	1:A:548:PRO:HB3	1.93	0.48
1:A:475:TYR:CE2	1:A:506:TYR:CE1	3.01	0.48
1:D:304:ILE:HG13	1:D:328:HIS:HB3	1.93	0.48
2:F:7:LEU:HD13	2:F:30:PHE:HB2	1.94	0.48
1:A:203:TYR:HB3	1:A:237:VAL:HG21	1.95	0.48
1:D:121:THR:HG22	3:D:601:JAA:C13	2.44	0.48
1:D:10:MET:O	1:D:13:VAL:HG23	2.12	0.48
1:D:242:VAL:O	1:D:245:ILE:HG13	2.13	0.48
2:F:180:PRO:O	2:F:183:ILE:HG22	2.12	0.48
1:A:149:PHE:CZ	1:A:527:THR:HG22	2.48	0.48
1:A:421:PHE:CG	1:A:542:ALA:HB2	2.49	0.48
1:D:39:ASN:HD22	2:E:142:LYS:HA	1.78	0.48
1:D:538:LEU:HD23	1:D:540:SER:HB2	1.93	0.48
1:A:97:ILE:H	1:A:163:GLY:H	1.61	0.48
1:A:86:SER:CB	2:B:188:ARG:HE	2.26	0.48
2:C:40:LYS:N	2:C:40:LYS:HZ3	2.08	0.48
1:D:145:LEU:HG	1:D:209:GLY:HA3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:198:VAL:O	1:D:202:LEU:N	2.41	0.48
1:D:490:LEU:O	1:D:520:LEU:HD23	2.13	0.48
2:F:185:TRP:O	2:F:189:CYS:N	2.42	0.48
2:F:7:LEU:HD21	2:F:23:LEU:HD12	1.94	0.48
2:B:102:VAL:HG21	2:B:157:LEU:HG	1.94	0.48
2:B:135:LEU:C	2:B:139:LEU:HD22	2.34	0.48
2:C:113:VAL:HG23	2:C:125:LYS:HG2	1.96	0.48
2:C:64:VAL:HB	2:C:73:TYR:CD2	2.48	0.48
1:D:250:LEU:HD21	1:D:260:ARG:HG3	1.95	0.48
1:D:62:LYS:HE3	7:D:766:HOH:O	2.14	0.48
1:D:90:THR:HG21	1:D:397:GLY:HA3	1.94	0.48
2:E:26:LYS:HG3	2:E:78:TRP:NE1	2.29	0.48
2:F:192:LYS:HA	7:F:468:HOH:O	2.13	0.48
2:E:96:ARG:HD2	2:F:73:TYR:HE1	1.76	0.48
2:B:50:ILE:HG21	2:C:134:ILE:HG13	1.95	0.48
2:C:69:ASN:HB3	2:C:73:TYR:CE2	2.49	0.48
2:F:17:MET:HE3	2:F:163:TRP:HH2	1.79	0.48
2:F:18:ARG:NH2	2:F:102:VAL:HG12	2.28	0.48
1:A:351:THR:OG1	1:A:418:GLN:OE1	2.11	0.48
1:D:97:ILE:HD13	1:D:112:PRO:HA	1.96	0.48
1:D:168:ASN:HD22	5:D:603:ATP:PA	2.37	0.48
1:D:39:ASN:ND2	2:E:143:PRO:HD3	2.29	0.48
1:D:405:ASP:HB2	1:D:541:SER:HB2	1.96	0.48
2:F:166:ALA:HA	2:F:206:VAL:HG22	1.95	0.48
2:F:190:MET:HA	2:F:195:VAL:HG13	1.95	0.48
1:A:95:PRO:O	1:A:161:PRO:HG2	2.14	0.48
1:D:106:GLY:HA3	1:D:432:ASN:HB3	1.94	0.48
1:D:333:SER:HA	5:D:603:ATP:C8	2.48	0.48
2:E:145:PHE:CE2	2:E:157:LEU:HD13	2.48	0.48
2:F:21:VAL:HG12	2:F:155:ILE:HG12	1.96	0.48
2:F:163:TRP:CE3	2:F:163:TRP:N	2.81	0.48
2:F:40:LYS:H	2:F:40:LYS:HE2	1.79	0.48
1:A:233:THR:C	7:A:769:HOH:O	2.51	0.48
1:A:421:PHE:CZ	1:A:541:SER:HA	2.48	0.48
1:A:333:SER:HA	5:A:603:ATP:N3	2.29	0.48
2:B:11:TRP:CD1	2:B:12:PRO:HD3	2.49	0.48
2:B:205:ILE:HD11	7:B:403:HOH:O	2.14	0.48
1:D:377:VAL:HG13	1:D:378:GLY:O	2.14	0.48
1:D:513:LYS:HZ1	1:D:575:PHE:HD2	1.61	0.48
1:D:538:LEU:HD21	1:D:540:SER:HB2	1.94	0.48
1:D:108:PRO:CG	1:D:552:LYS:H	2.24	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:111:PHE:HA	2:E:114:TRP:NE1	2.28	0.48
2:F:161:SER:C	2:F:164:PHE:HB2	2.34	0.48
2:F:139:LEU:HD22	2:F:181:LYS:HD3	1.96	0.48
1:D:273:LEU:HA	1:D:276:THR:HG23	1.96	0.47
1:D:32:LEU:HB2	1:D:360:TYR:CD1	2.49	0.47
1:D:477:ILE:HG21	1:D:497:LEU:HD13	1.96	0.47
2:F:161:SER:HA	2:F:164:PHE:HD2	1.78	0.47
1:A:125:PHE:CD1	1:A:126:ARG:N	2.82	0.47
1:A:150:SER:HB3	1:A:170:TYR:HD2	1.78	0.47
2:C:178:GLU:HB3	7:C:468:HOH:O	2.14	0.47
1:D:164:THR:HA	5:D:603:ATP:O1G	2.14	0.47
1:D:223:PHE:CD2	1:D:533:GLU:HA	2.49	0.47
1:D:53:ASN:HB3	1:D:54:ALA:H	1.47	0.47
2:E:135:LEU:HD12	2:E:182:LEU:HD11	1.97	0.47
2:E:37:PHE:CE1	6:E:301:GSH:HA32	2.49	0.47
2:C:197:LYS:O	7:C:415:HOH:O	2.20	0.47
1:D:448:ALA:HB2	1:D:496:CYS:HB3	1.95	0.47
2:C:187:LYS:NZ	1:D:499:ARG:HH12	2.11	0.47
1:D:94:VAL:HG11	1:D:97:ILE:CD1	2.45	0.47
2:F:132:VAL:HG23	2:F:182:LEU:HD22	1.96	0.47
1:A:152:LYS:HG2	1:A:565:ASN:OD1	2.14	0.47
1:A:185:PRO:HA	7:A:886:HOH:O	2.13	0.47
1:A:435:LYS:HB3	1:A:437:THR:HA	1.97	0.47
1:A:478:PHE:CD1	1:A:478:PHE:N	2.82	0.47
2:B:63:PRO:O	2:C:90:TYR:HE1	1.97	0.47
1:D:303:GLY:O	1:D:327:SER:HA	2.14	0.47
2:F:91:GLY:HA2	2:F:94:GLN:OE1	2.14	0.47
1:A:310:GLU:N	1:A:311:PRO:HD2	2.29	0.47
1:A:445:VAL:HG22	1:A:479:TRP:HE1	1.79	0.47
1:A:70:ASP:OD1	1:A:71:VAL:HG23	2.14	0.47
2:C:176:GLU:HB2	2:C:183:ILE:HG21	1.97	0.47
2:C:14:MET:O	2:C:17:MET:HB2	2.14	0.47
2:C:187:LYS:CE	1:D:496:CYS:HB2	2.44	0.47
2:C:24:ARG:HD2	7:C:427:HOH:O	2.15	0.47
1:D:389:GLU:HA	1:D:405:ASP:O	2.14	0.47
1:D:412:PHE:N	7:D:791:HOH:O	2.47	0.47
1:D:410:ILE:H	1:D:420:LYS:NZ	2.12	0.47
1:D:465:TYR:O	1:D:475:TYR:HB3	2.14	0.47
1:A:330:TYR:CE1	1:A:536:LEU:O	2.68	0.47
1:A:135:ASP:OD2	1:A:343:PRO:HD2	2.15	0.47
2:B:154:ASP:O	2:B:158:ILE:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:143:LYS:HA	1:D:184:SER:HB2	1.96	0.47
2:E:120:GLU:HB2	7:E:468:HOH:O	2.15	0.47
2:E:205:ILE:HG22	2:E:208:TYR:HE2	1.80	0.47
2:F:154:ASP:HB3	7:F:445:HOH:O	2.14	0.47
1:A:7:THR:OG1	1:A:7:THR:O	2.31	0.47
1:A:81:VAL:CG1	1:A:97:ILE:HG13	2.43	0.47
1:D:77:ILE:CG1	1:D:89:LEU:HD11	2.44	0.47
2:E:171:GLY:O	2:E:172:ASN:HB2	2.15	0.47
2:E:65:CYS:O	2:E:66:GLU:HB2	2.15	0.47
2:F:75:ASP:HB2	2:F:84:PHE:CE2	2.49	0.47
1:A:527:THR:N	7:A:718:HOH:O	2.47	0.47
2:C:125:LYS:HD3	2:C:173:PHE:CE2	2.50	0.47
1:D:152:LYS:HD2	1:D:153:GLN:N	2.30	0.47
1:D:317:ARG:NH2	7:D:793:HOH:O	2.47	0.47
1:D:494:CYS:SG	1:D:495:ASN:ND2	2.88	0.47
2:E:10:TYR:CG	2:E:12:PRO:HD2	2.50	0.47
1:A:103:THR:CG2	1:A:548:PRO:HB3	2.45	0.47
1:A:105:GLN:NE2	7:A:722:HOH:O	2.13	0.47
1:A:164:THR:HA	1:A:557:LYS:HG3	1.97	0.47
1:A:200:GLN:N	7:A:712:HOH:O	2.07	0.47
1:A:236:GLN:O	7:A:724:HOH:O	2.20	0.47
1:A:547:MET:O	1:A:547:MET:HG3	2.13	0.47
1:A:90:THR:HG21	1:A:112:PRO:CG	2.45	0.47
1:A:90:THR:HG1	1:A:91:GLY:H	1.55	0.47
1:A:46:GLN:HB2	2:B:148:ASP:O	2.15	0.47
2:B:85:PHE:N	2:B:85:PHE:CD1	2.82	0.47
1:D:332:SER:C	5:D:603:ATP:N7	2.69	0.47
1:D:444:SER:HA	1:D:500:ALA:CB	2.43	0.47
1:D:470:THR:HG21	1:D:474:HIS:CE1	2.49	0.47
1:D:164:THR:N	1:D:560:GLN:OE1	2.40	0.47
1:D:87:PRO:HD2	2:E:188:ARG:CB	2.37	0.47
2:E:17:MET:SD	2:E:199:LEU:HG	2.55	0.47
2:F:44:LEU:HD13	2:F:56:VAL:HG21	1.96	0.47
1:A:232:ARG:O	1:A:232:ARG:HG2	2.15	0.47
1:A:552:LYS:O	1:A:554:SER:N	2.47	0.47
1:A:71:VAL:HG11	1:A:105:GLN:NE2	2.30	0.47
2:B:168:GLU:CD	2:B:174:SER:HA	2.36	0.47
2:C:10:TYR:HB3	2:C:13:SER:HB2	1.97	0.47
2:E:188:ARG:HD3	2:E:188:ARG:O	2.14	0.47
1:A:363:PHE:CE2	1:A:419:LEU:HD11	2.50	0.47
1:A:475:TYR:CB	1:A:518:LEU:HD13	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:211:GLU:O	2:C:215:ASN:ND2	2.48	0.47
1:D:118:MET:HA	1:D:121:THR:OG1	2.15	0.47
1:D:301:VAL:HG11	1:D:316:LEU:HD21	1.97	0.47
1:D:361:PHE:HE1	1:D:392:ILE:HG23	1.79	0.47
1:D:467:ASP:O	1:D:475:TYR:CE2	2.68	0.47
2:E:99:ALA:O	2:E:103:ASP:HB2	2.15	0.47
2:F:155:ILE:O	2:F:158:ILE:HG22	2.15	0.47
1:A:131:PHE:HD1	1:A:134:ARG:HH22	1.62	0.46
1:A:498:ASP:OD2	1:A:510:ARG:NH2	2.48	0.46
1:A:519:GLU:HB2	1:A:571:PHE:CE1	2.50	0.46
2:B:129:ILE:HD12	7:B:453:HOH:O	2.14	0.46
1:D:314:PRO:O	1:D:318:HIS:N	2.38	0.46
1:D:527:THR:HA	1:D:530:LYS:HD3	1.97	0.46
1:D:98:SER:CB	5:D:603:ATP:O2G	2.62	0.46
1:D:76:TYR:O	1:D:80:MET:HG2	2.15	0.46
1:A:250:LEU:HD13	1:A:254:ILE:HB	1.97	0.46
1:A:353:ALA:HB2	1:A:413:TYR:CE2	2.49	0.46
1:D:362:GLU:HB2	1:D:391:VAL:HG13	1.96	0.46
1:D:409:VAL:HA	1:D:420:LYS:HZ1	1.80	0.46
1:D:543:GLY:C	1:D:544:GLN:HG2	2.34	0.46
1:D:9:ASP:O	1:D:13:VAL:HG22	2.15	0.46
2:E:17:MET:HB2	2:E:159:THR:HG22	1.96	0.46
2:E:16:GLY:HA2	2:E:55:PRO:HG3	1.96	0.46
2:F:151:GLY:O	2:F:154:ASP:HB2	2.14	0.46
2:F:24:ARG:HG3	2:F:30:PHE:CE1	2.50	0.46
1:A:169:VAL:CB	5:A:603:ATP:O3'	2.51	0.46
2:B:96:ARG:HB2	2:C:69:ASN:OD1	2.15	0.46
1:D:377:VAL:HB	7:D:782:HOH:O	2.14	0.46
1:D:496:CYS:HA	1:D:499:ARG:NH1	2.30	0.46
1:D:85:THR:CB	2:E:184:ALA:HB1	2.44	0.46
1:A:114:THR:HG21	2:B:141:ASP:HB3	1.97	0.46
1:A:35:ILE:HG12	1:A:395:TYR:CZ	2.49	0.46
1:A:225:HIS:HB2	1:A:529:ARG:HH21	1.80	0.46
1:A:527:THR:O	1:A:530:LYS:HB3	2.15	0.46
1:A:154:TYR:CB	1:A:560:GLN:HA	2.45	0.46
2:C:164:PHE:CZ	2:C:182:LEU:HD21	2.50	0.46
2:C:110:GLN:HE21	2:C:167:TYR:HE2	1.63	0.46
2:C:65:CYS:O	2:C:66:GLU:HB2	2.16	0.46
1:D:441:LEU:O	1:D:445:VAL:HG23	2.15	0.46
1:D:529:ARG:O	1:D:533:GLU:HG3	2.16	0.46
1:D:557:LYS:HD2	5:D:603:ATP:PG	2.56	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:152:LYS:CD	1:D:561:ILE:HA	2.45	0.46
2:F:167:TYR:HD1	2:F:167:TYR:N	2.13	0.46
1:A:72:GLU:O	1:A:76:TYR:CD2	2.69	0.46
2:B:66:GLU:O	2:B:70:VAL:HG23	2.15	0.46
1:D:402:ARG:NH2	7:D:729:HOH:O	2.43	0.46
1:D:461:ASP:OD2	1:D:547:MET:CE	2.63	0.46
2:E:48:ASN:HB2	7:E:446:HOH:O	2.15	0.46
1:A:104:SER:N	1:A:107:ARG:O	2.43	0.46
1:A:313:VAL:HA	7:A:940:HOH:O	2.15	0.46
1:A:465:TYR:O	1:A:476:ALA:N	2.46	0.46
1:D:97:ILE:HG22	1:D:98:SER:N	2.31	0.46
2:E:192:LYS:HZ2	2:E:194:SER:H	1.62	0.46
2:F:26:LYS:HE3	2:F:78:TRP:O	2.15	0.46
2:B:132:VAL:HG22	2:B:182:LEU:HD13	1.97	0.46
2:C:191:GLU:HA	1:D:450:LYS:HD2	1.98	0.46
1:D:477:ILE:O	1:D:477:ILE:HG12	2.15	0.46
2:F:185:TRP:O	2:F:188:ARG:N	2.49	0.46
1:A:303:GLY:O	1:A:328:HIS:N	2.49	0.46
1:A:544:GLN:NE2	7:A:730:HOH:O	2.17	0.46
2:C:10:TYR:HB3	2:C:13:SER:CB	2.46	0.46
1:D:165:ALA:HB1	5:D:603:ATP:C2	2.51	0.46
1:D:222:VAL:HG21	4:D:602:MET:N	2.30	0.46
1:D:467:ASP:OD2	1:D:475:TYR:HE1	1.99	0.46
2:E:135:LEU:HD13	2:E:157:LEU:HD11	1.96	0.46
2:E:51:HIS:O	2:E:53:LYS:HD2	2.16	0.46
2:F:22:ALA:O	2:F:74:VAL:HG11	2.16	0.46
1:A:157:THR:HG22	1:A:469:SER:HB3	1.98	0.46
1:A:97:ILE:N	1:A:163:GLY:H	2.14	0.46
2:C:38:SER:OG	7:C:403:HOH:O	2.05	0.46
1:D:124:LEU:HA	1:D:127:THR:HG22	1.97	0.46
1:D:152:LYS:HD3	1:D:561:ILE:CA	2.43	0.46
1:D:222:VAL:HB	1:D:533:GLU:HB3	1.97	0.46
1:D:398:LEU:HD23	1:D:398:LEU:HA	1.70	0.46
2:C:187:LYS:HG2	1:D:451:ARG:HD3	1.98	0.46
1:D:87:PRO:HB2	2:E:143:PRO:HB3	1.96	0.46
2:F:214:LYS:HE2	2:F:214:LYS:HB3	1.72	0.46
1:A:507:VAL:O	1:A:511:LYS:HB2	2.16	0.46
2:C:98:TRP:HE3	2:C:101:PHE:HB2	1.79	0.46
2:C:164:PHE:CD2	2:C:183:ILE:HD13	2.48	0.46
2:C:182:LEU:O	2:C:185:TRP:HE3	1.99	0.46
2:B:90:TYR:CZ	2:C:62:LYS:HB3	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:254:ILE:HD12	1:D:263:MET:SD	2.56	0.46
1:D:316:LEU:HD12	1:D:316:LEU:HA	1.63	0.46
2:E:102:VAL:HG21	2:E:157:LEU:HG	1.97	0.46
2:E:158:ILE:N	7:E:403:HOH:O	2.48	0.46
2:E:50:ILE:HD12	2:E:51:HIS:N	2.24	0.46
2:F:167:TYR:CD1	2:F:167:TYR:N	2.84	0.46
1:A:154:TYR:HD1	1:A:155:ILE:N	2.14	0.45
1:A:207:LEU:O	1:A:210:ILE:HG12	2.16	0.45
1:A:396:ALA:HA	7:A:768:HOH:O	2.16	0.45
2:B:9:ASP:OD1	2:B:16:GLY:HA3	2.15	0.45
2:C:146:GLY:O	7:C:417:HOH:O	2.21	0.45
1:D:98:SER:HB2	1:D:557:LYS:CD	2.46	0.45
1:A:41:SER:HB3	2:B:144:TYR:HB2	1.99	0.45
1:A:108:PRO:HB3	1:A:555:ASN:CB	2.46	0.45
1:A:76:TYR:HB3	1:A:88:ILE:HG21	1.98	0.45
2:C:72:GLN:NE2	7:C:425:HOH:O	2.35	0.45
1:D:437:THR:O	1:D:440:ASP:N	2.48	0.45
2:E:10:TYR:CD2	2:E:12:PRO:HD2	2.51	0.45
2:E:110:GLN:O	2:E:113:VAL:HG12	2.15	0.45
2:F:106:PHE:O	2:F:110:GLN:HG3	2.16	0.45
2:F:11:TRP:CD1	2:F:12:PRO:HD3	2.51	0.45
2:F:42:PRO:HA	2:F:45:LEU:HG	1.98	0.45
2:F:84:PHE:CD1	2:F:85:PHE:N	2.83	0.45
1:D:108:PRO:HG3	1:D:555:ASN:ND2	2.30	0.45
1:D:99:LEU:HA	1:D:109:LYS:O	2.16	0.45
1:D:24:ALA:HA	1:D:27:VAL:HG12	1.98	0.45
1:D:113:PHE:CE1	1:D:333:SER:HB3	2.52	0.45
1:D:393:THR:HG23	1:D:399:TYR:HA	1.97	0.45
1:D:330:TYR:CZ	1:D:421:PHE:HZ	2.34	0.45
2:C:187:LYS:HE3	1:D:493:CYS:HA	1.98	0.45
2:E:17:MET:HA	2:E:20:ARG:CD	2.47	0.45
2:F:21:VAL:O	2:F:194:SER:HB2	2.15	0.45
1:A:132:ARG:O	1:A:136:PHE:N	2.48	0.45
1:A:310:GLU:HA	1:A:313:VAL:HG23	1.97	0.45
2:B:4:LEU:HA	2:B:5:PRO:HD3	1.86	0.45
2:B:62:LYS:HB3	2:C:90:TYR:CE2	2.52	0.45
2:C:41:SER:O	7:C:416:HOH:O	2.21	0.45
2:E:11:TRP:O	2:E:200:PRO:HG3	2.15	0.45
2:F:10:TYR:CD2	2:F:12:PRO:HD2	2.52	0.45
2:F:135:LEU:HD22	2:F:182:LEU:HD11	1.97	0.45
1:A:150:SER:CB	1:A:167:THR:HA	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:240:GLU:O	1:A:241:ILE:C	2.54	0.45
1:A:398:LEU:HD13	1:A:401:TYR:CD1	2.52	0.45
1:A:426:ASN:ND2	7:A:730:HOH:O	2.50	0.45
2:B:176:GLU:HB2	2:B:183:ILE:HG21	1.98	0.45
2:C:23:LEU:HD23	2:C:78:TRP:HH2	1.81	0.45
1:D:253:ARG:NH2	7:D:796:HOH:O	2.49	0.45
1:D:42:ALA:HB3	1:D:45:LEU:HG	1.99	0.45
1:D:521:ARG:HB3	1:D:566:VAL:CG1	2.46	0.45
2:F:107:THR:O	2:F:110:GLN:HB2	2.16	0.45
2:F:114:TRP:HA	2:F:170:PHE:CD2	2.50	0.45
2:F:84:PHE:HE1	2:F:85:PHE:CD2	2.35	0.45
1:A:107:ARG:HG3	1:A:433:ILE:HD11	1.99	0.45
1:A:229:HIS:CE1	1:A:525:LYS:HD2	2.51	0.45
1:A:315:LYS:HD2	1:A:315:LYS:HA	1.58	0.45
2:B:66:GLU:OE2	2:B:69:ASN:CG	2.54	0.45
2:B:9:ASP:HB3	2:B:32:TYR:CE2	2.52	0.45
2:C:62:LYS:HA	2:C:63:PRO:HD3	1.81	0.45
1:D:17:PHE:CD1	1:D:18:ASP:N	2.85	0.45
1:D:198:VAL:HA	1:D:201:ALA:HB3	1.99	0.45
1:D:295:PHE:HA	1:D:296:PRO:HD2	1.73	0.45
1:D:428:ILE:O	7:D:735:HOH:O	2.21	0.45
1:D:80:MET:CE	1:D:88:ILE:HG13	2.46	0.45
1:D:80:MET:HA	1:D:80:MET:HE2	1.99	0.45
2:F:160:PHE:O	2:F:164:PHE:CG	2.70	0.45
2:F:24:ARG:HB3	2:F:194:SER:HA	1.99	0.45
1:A:121:THR:HG22	1:A:175:PHE:HE1	1.66	0.45
1:A:490:LEU:HD11	7:A:745:HOH:O	2.17	0.45
1:A:549:ARG:N	7:A:786:HOH:O	2.49	0.45
2:C:11:TRP:CZ2	2:C:208:TYR:HB2	2.52	0.45
1:D:461:ASP:OD1	1:D:462:PHE:N	2.43	0.45
2:E:102:VAL:HG22	2:E:160:PHE:HE2	1.82	0.45
2:F:207:ALA:O	2:F:211:GLU:N	2.37	0.45
1:A:94:VAL:HG23	1:A:113:PHE:O	2.17	0.45
1:A:125:PHE:O	1:A:129:PHE:HB2	2.17	0.45
1:A:162:VAL:HG23	7:A:702:HOH:O	2.16	0.45
1:A:501:PHE:HD2	1:A:506:TYR:CZ	2.35	0.45
1:A:73:LEU:HA	1:A:76:TYR:HD2	1.82	0.45
1:D:41:SER:OG	2:E:144:TYR:O	2.35	0.45
1:D:477:ILE:HB	1:D:479:TRP:HZ3	1.82	0.45
1:D:525:LYS:HG2	7:D:701:HOH:O	2.16	0.45
1:D:95:PRO:HD3	2:E:181:LYS:NZ	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:70:VAL:O	2:E:74:VAL:N	2.43	0.45
2:F:142:LYS:HE2	7:F:515:HOH:O	2.15	0.45
2:F:163:TRP:HB3	2:F:167:TYR:CE1	2.51	0.45
1:A:361:PHE:HD1	1:A:392:ILE:HG12	1.82	0.45
1:A:394:ASN:OD1	7:A:741:HOH:O	2.21	0.45
1:A:435:LYS:HD3	1:A:438:GLU:H	1.82	0.45
1:A:199:HIS:HB2	1:A:525:LYS:HE2	1.99	0.45
1:A:540:SER:HG	1:A:541:SER:N	2.14	0.45
1:A:466:ILE:CG1	1:A:552:LYS:HA	2.47	0.45
2:B:171:GLY:O	2:B:172:ASN:HB2	2.17	0.45
1:D:103:THR:HB	1:D:106:GLY:HA2	1.98	0.45
1:D:108:PRO:HB3	1:D:555:ASN:N	2.32	0.45
1:D:160:VAL:O	1:D:162:VAL:HG22	2.17	0.45
1:D:510:ARG:HH11	1:D:575:PHE:HZ	1.64	0.45
2:E:128:PHE:HE2	2:E:175:ILE:HG12	1.81	0.45
2:E:194:SER:OG	2:E:195:VAL:N	2.50	0.45
2:E:17:MET:HB3	2:E:199:LEU:HD12	1.98	0.45
2:F:157:LEU:HG	2:F:185:TRP:HH2	1.82	0.45
1:A:102:GLY:O	1:A:548:PRO:HD3	2.17	0.45
1:A:536:LEU:HD21	7:A:765:HOH:O	2.16	0.45
2:C:136:GLU:HG2	7:C:471:HOH:O	2.16	0.45
1:D:124:LEU:HD11	1:D:339:ALA:HB2	1.98	0.45
1:D:272:GLU:O	1:D:275:GLU:HB3	2.17	0.45
1:D:351:THR:HG22	1:D:420:LYS:HD2	1.98	0.45
1:D:361:PHE:CE1	1:D:392:ILE:HG23	2.51	0.45
1:D:503:ASP:O	1:D:507:VAL:HG23	2.17	0.45
1:D:509:SER:O	1:D:513:LYS:N	2.49	0.45
1:D:97:ILE:HG21	1:D:110:PHE:CD1	2.52	0.45
2:E:24:ARG:HD2	2:E:198:SER:OG	2.16	0.45
2:F:69:ASN:OD1	2:F:70:VAL:N	2.50	0.45
1:A:238:TRP:CH2	1:A:281:CYS:SG	3.10	0.44
1:A:437:THR:HG21	1:A:439:ARG:NH2	2.10	0.44
2:B:68:LEU:HD12	2:B:69:ASN:N	2.32	0.44
2:C:89:PRO:O	2:C:92:ARG:HB2	2.17	0.44
1:D:152:LYS:HG2	1:D:565:ASN:HB2	1.99	0.44
1:D:330:TYR:CE2	1:D:338:ALA:HB3	2.51	0.44
1:D:455:GLU:O	1:D:456:LYS:HB2	2.17	0.44
1:D:96:ALA:HB1	1:D:163:GLY:N	2.31	0.44
2:E:18:ARG:HD2	2:E:156:SER:HA	1.99	0.44
2:F:142:LYS:HE3	2:F:142:LYS:HB2	1.84	0.44
1:A:219:VAL:CG1	1:A:291:ILE:HG21	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:453:SER:C	1:A:456:LYS:H	2.20	0.44
1:A:464:SER:HB3	1:A:550:CYS:CB	2.46	0.44
1:A:480:GLU:HB2	1:A:528:PHE:CE2	2.51	0.44
1:D:113:PHE:HD1	1:D:117:LEU:CD1	2.30	0.44
1:D:132:ARG:O	1:D:136:PHE:N	2.47	0.44
1:D:193:ILE:H	1:D:193:ILE:HG12	1.54	0.44
1:D:97:ILE:CG2	1:D:111:ILE:H	2.31	0.44
2:F:172:ASN:ND2	2:F:172:ASN:O	2.50	0.44
1:A:494:CYS:SG	1:A:495:ASN:N	2.91	0.44
1:A:53:ASN:HB3	1:A:54:ALA:H	1.41	0.44
1:A:86:SER:CB	2:B:188:ARG:HB2	2.47	0.44
2:C:10:TYR:CD2	2:C:12:PRO:HD2	2.52	0.44
1:D:291:ILE:HG13	7:D:844:HOH:O	2.17	0.44
1:D:145:LEU:HD13	1:D:295:PHE:CD1	2.52	0.44
1:D:464:SER:HA	1:D:477:ILE:N	2.20	0.44
2:E:155:ILE:O	2:E:158:ILE:HG22	2.16	0.44
1:A:320:ALA:O	1:A:323:LEU:HB2	2.17	0.44
1:A:501:PHE:CD2	1:A:506:TYR:CZ	3.06	0.44
2:B:40:LYS:NZ	2:B:52:LYS:HB2	2.33	0.44
2:C:172:ASN:ND2	2:C:172:ASN:O	2.50	0.44
1:D:225:HIS:ND1	1:D:309:MET:SD	2.74	0.44
1:D:447:SER:HB2	1:D:496:CYS:SG	2.57	0.44
2:E:17:MET:HB2	2:E:159:THR:CG2	2.47	0.44
2:E:54:ILE:HB	2:E:55:PRO:HA	2.00	0.44
1:A:153:GLN:HG2	7:A:726:HOH:O	2.17	0.44
1:A:154:TYR:CD1	1:A:155:ILE:N	2.86	0.44
1:A:167:THR:O	1:A:171:ARG:HG2	2.17	0.44
1:A:195:SER:HA	1:A:196:PRO:HD3	1.90	0.44
1:A:204:CYS:SG	7:A:970:HOH:O	2.51	0.44
1:A:242:VAL:CG2	1:A:277:ILE:HD13	2.47	0.44
1:A:238:TRP:HH2	1:A:287:TRP:HZ2	1.63	0.44
1:A:353:ALA:HB2	1:A:413:TYR:HD2	1.81	0.44
2:B:4:LEU:HB3	2:B:31:GLU:OE1	2.17	0.44
2:C:128:PHE:HE1	2:C:175:ILE:HG22	1.83	0.44
2:C:150:PHE:HE2	2:C:155:ILE:HG12	1.82	0.44
1:D:138:ILE:HD12	1:D:139:ASP:O	2.17	0.44
1:D:442:GLN:HG2	1:D:462:PHE:CZ	2.53	0.44
1:D:528:PHE:HA	1:D:531:ILE:HG13	1.97	0.44
2:E:99:ALA:HB2	2:E:152:TYR:HE1	1.82	0.44
2:E:40:LYS:HB2	2:E:40:LYS:HE3	1.60	0.44
1:A:232:ARG:HA	1:A:235:GLU:CG	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:363:PHE:HB3	1:A:388:TYR:CB	2.48	0.44
1:A:434:ASP:OD1	1:A:435:LYS:HG3	2.18	0.44
1:A:439:ARG:O	1:A:443:LEU:HB2	2.16	0.44
1:A:463:SER:HB2	1:A:528:PHE:CE1	2.52	0.44
2:B:155:ILE:HG21	7:B:516:HOH:O	2.17	0.44
2:C:187:LYS:NZ	1:D:496:CYS:HB2	2.32	0.44
2:C:53:LYS:NZ	7:C:444:HOH:O	2.46	0.44
1:D:163:GLY:HA2	1:D:560:GLN:CG	2.47	0.44
2:E:116:LYS:HA	2:E:116:LYS:HD3	1.65	0.44
2:E:20:ARG:HB2	2:E:198:SER:HB3	2.00	0.44
1:A:351:THR:HB	1:A:410:ILE:HG12	1.98	0.44
1:A:73:LEU:HD13	1:A:89:LEU:HD13	1.99	0.44
2:C:169:LYS:HE3	2:C:169:LYS:HB2	1.77	0.44
1:D:473:GLY:C	1:D:516:GLY:H	2.21	0.44
2:F:8:LEU:HD22	2:F:33:ARG:HH21	1.83	0.44
1:A:143:LYS:NZ	1:A:187:CYS:HA	2.33	0.44
1:A:95:PRO:HD3	2:B:181:LYS:NZ	2.33	0.44
1:D:477:ILE:CD1	1:D:520:LEU:HA	2.37	0.44
1:D:433:ILE:CD1	1:D:552:LYS:HD2	2.48	0.44
2:E:98:TRP:O	2:E:102:VAL:HG12	2.18	0.44
2:F:132:VAL:C	2:F:179:SER:HB3	2.39	0.44
1:A:265:LYS:HG2	1:A:266:LEU:HG	2.00	0.44
1:A:330:TYR:CD1	1:A:421:PHE:HE2	2.36	0.44
1:A:337:ILE:HG13	1:A:338:ALA:H	1.83	0.44
1:A:358:LEU:N	1:A:358:LEU:HD23	2.33	0.44
1:A:79:ARG:O	1:A:84:ASP:O	2.36	0.44
2:C:129:ILE:HA	2:C:132:VAL:HG12	2.00	0.44
2:C:16:GLY:HA3	2:C:20:ARG:NH2	2.33	0.44
1:D:104:SER:O	1:D:107:ARG:HG2	2.18	0.44
1:D:81:VAL:HG12	1:D:156:SER:OG	2.18	0.44
1:D:332:SER:OG	1:D:333:SER:N	2.51	0.44
2:E:125:LYS:HB3	2:E:173:PHE:CE2	2.52	0.44
2:F:177:SER:O	2:F:180:PRO:HG3	2.18	0.44
2:F:72:GLN:O	2:F:76:GLU:HG2	2.17	0.44
1:A:108:PRO:HD2	1:A:433:ILE:HD11	2.00	0.43
1:A:244:ASP:HB2	1:A:250:LEU:HA	2.00	0.43
1:A:99:LEU:CD1	1:A:558:VAL:H	2.26	0.43
1:D:35:ILE:HG23	7:E:454:HOH:O	2.18	0.43
2:E:202:SER:O	2:E:206:VAL:HG22	2.18	0.43
2:E:65:CYS:O	2:E:69:ASN:ND2	2.42	0.43
2:F:163:TRP:HE3	2:F:163:TRP:H	1.64	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:VAL:HG23	1:A:524:ALA:HB3	1.99	0.43
2:C:163:TRP:HB3	2:C:167:TYR:CE1	2.53	0.43
1:D:227:LEU:HG	7:D:838:HOH:O	2.18	0.43
1:D:465:TYR:N	1:D:476:ALA:HA	2.15	0.43
1:D:531:ILE:HA	1:D:534:HIS:CE1	2.53	0.43
1:D:98:SER:CA	1:D:556:ALA:HB3	2.48	0.43
2:E:166:ALA:HA	2:E:169:LYS:CD	2.48	0.43
2:B:181:LYS:H	2:B:181:LYS:HG3	1.44	0.43
1:D:211:LEU:C	1:D:212:PHE:HD1	2.22	0.43
1:D:528:PHE:HA	1:D:531:ILE:HD12	2.00	0.43
2:F:98:TRP:CE3	2:F:138:GLU:OE2	2.72	0.43
2:F:203:GLU:HB2	7:F:454:HOH:O	2.18	0.43
1:A:481:ILE:N	1:A:481:ILE:HD12	2.33	0.43
1:A:66:PRO:HA	7:A:787:HOH:O	2.18	0.43
2:B:77:ALA:HB3	2:B:78:TRP:CZ3	2.54	0.43
1:D:13:VAL:HG21	1:D:130:ALA:CB	2.49	0.43
1:D:212:PHE:CD1	1:D:212:PHE:N	2.87	0.43
1:D:441:LEU:HB3	7:D:808:HOH:O	2.17	0.43
1:D:482:SER:CA	1:D:525:LYS:HD2	2.42	0.43
2:E:165:GLN:O	2:E:169:LYS:HE3	2.19	0.43
2:F:132:VAL:CG2	2:F:182:LEU:HD13	2.48	0.43
2:F:65:CYS:N	7:F:402:HOH:O	2.52	0.43
2:E:65:CYS:HB3	2:F:97:PHE:CE1	2.53	0.43
1:A:91:GLY:HA3	2:B:141:ASP:C	2.39	0.43
2:C:135:LEU:HD23	2:C:145:PHE:CZ	2.54	0.43
2:C:188:ARG:HH12	1:D:500:ALA:HA	1.84	0.43
1:D:117:LEU:O	1:D:120:ASN:HB2	2.18	0.43
1:D:176:LYS:HE3	1:D:176:LYS:HB2	1.84	0.43
1:D:126:ARG:HE	1:D:182:ILE:CD1	2.31	0.43
1:D:461:ASP:OD2	1:D:547:MET:SD	2.77	0.43
2:E:96:ARG:NH2	2:F:76:GLU:OE2	2.52	0.43
1:A:17:PHE:CE1	1:A:127:THR:HG21	2.54	0.43
1:A:147:PHE:HE1	1:A:206:LEU:HG	1.83	0.43
1:A:429:LEU:HD12	1:A:429:LEU:HA	1.71	0.43
1:A:504:ALA:O	1:A:507:VAL:HB	2.18	0.43
1:A:509:SER:HB3	1:A:515:ILE:CD1	2.47	0.43
1:A:421:PHE:CB	1:A:542:ALA:HB2	2.48	0.43
1:A:426:ASN:ND2	1:A:544:GLN:NE2	2.65	0.43
2:B:192:LYS:O	2:B:196:SER:OG	2.37	0.43
2:C:117:LYS:CA	2:C:121:GLN:HB2	2.45	0.43
2:C:14:MET:HA	2:C:17:MET:SD	2.58	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:81:VAL:HG13	1:D:162:VAL:HG11	2.01	0.43
1:D:364:LEU:HA	1:D:365:PRO:HD3	1.92	0.43
2:E:11:TRP:CG	2:E:12:PRO:HD3	2.54	0.43
1:A:182:ILE:HG12	1:A:183:THR:OG1	2.19	0.43
1:A:125:PHE:CD1	1:A:182:ILE:HG13	2.54	0.43
1:A:238:TRP:CH2	1:A:287:TRP:CZ2	3.03	0.43
1:A:360:TYR:CZ	1:A:362:GLU:OE2	2.71	0.43
2:C:84:PHE:HE1	2:C:85:PHE:CD2	2.36	0.43
1:D:124:LEU:HB3	3:D:601:JAA:C15	2.49	0.43
1:D:208:SER:HA	1:D:211:LEU:HG	2.01	0.43
1:D:460:ILE:HD12	7:D:701:HOH:O	2.17	0.43
1:A:242:VAL:HG22	1:A:277:ILE:HD13	2.00	0.43
1:A:510:ARG:HH21	1:A:518:LEU:H	1.67	0.43
1:A:94:VAL:HG22	1:A:96:ALA:N	2.34	0.43
2:C:18:ARG:HH21	2:C:160:PHE:HE1	1.62	0.43
1:D:13:VAL:HG21	1:D:130:ALA:HB1	2.01	0.43
1:D:534:HIS:HB3	4:D:602:MET:C	2.39	0.43
1:D:548:PRO:HG3	7:D:824:HOH:O	2.18	0.43
1:D:94:VAL:HG11	1:D:97:ILE:CG1	2.49	0.43
2:E:169:LYS:HZ1	2:E:206:VAL:HG11	1.84	0.43
1:A:155:ILE:HA	1:A:161:PRO:HA	1.99	0.43
1:A:117:LEU:HB2	5:A:603:ATP:C4	2.54	0.43
2:B:127:GLU:OE1	7:B:412:HOH:O	2.22	0.43
2:C:11:TRP:HZ2	2:C:208:TYR:HB2	1.83	0.43
1:D:217:GLN:O	7:D:738:HOH:O	2.21	0.43
1:D:198:VAL:HG22	1:D:524:ALA:HB3	2.01	0.43
1:D:98:SER:C	1:D:556:ALA:HB3	2.39	0.43
1:D:336:TRP:CZ2	5:D:603:ATP:N7	2.87	0.43
2:E:18:ARG:CD	2:E:156:SER:HA	2.49	0.43
2:F:135:LEU:HD12	7:F:426:HOH:O	2.17	0.43
1:A:187:CYS:HB2	1:A:208:SER:HB3	2.00	0.43
1:A:230:ALA:C	1:A:233:THR:H	2.23	0.43
1:A:273:LEU:O	1:A:277:ILE:HG22	2.18	0.43
2:C:23:LEU:O	2:C:28:VAL:HG12	2.19	0.43
2:C:95:ALA:HB1	7:C:461:HOH:O	2.18	0.43
1:D:231:PHE:HA	1:D:234:PHE:CD2	2.45	0.43
1:D:89:LEU:HG	1:D:89:LEU:H	1.54	0.43
2:E:18:ARG:N	2:E:159:THR:HG21	2.33	0.43
1:A:125:PHE:O	1:A:129:PHE:HD1	2.01	0.42
1:A:191:GLU:HA	1:A:194:PHE:HB2	2.01	0.42
1:A:336:TRP:HB2	5:A:603:ATP:N6	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:445:VAL:HG11	1:A:462:PHE:CD2	2.54	0.42
1:A:539:GLY:O	1:A:540:SER:HB3	2.18	0.42
1:A:531:ILE:CD1	1:A:558:VAL:HG22	2.45	0.42
2:B:33:ARG:N	7:B:405:HOH:O	2.33	0.42
2:C:66:GLU:HB2	2:C:69:ASN:HB2	2.01	0.42
2:C:6:ILE:HB	2:C:58:VAL:HB	2.00	0.42
1:D:197:ASP:CB	1:D:256:VAL:HG21	2.48	0.42
1:D:270:ASN:N	7:D:706:HOH:O	2.43	0.42
1:D:433:ILE:HD12	1:D:552:LYS:HD2	2.01	0.42
1:D:87:PRO:HB2	2:E:143:PRO:HA	2.00	0.42
2:E:146:GLY:HA3	2:E:151:GLY:HA3	2.00	0.42
1:A:295:PHE:HA	1:A:296:PRO:HD2	1.71	0.42
1:A:336:TRP:CD1	5:A:603:ATP:N7	2.87	0.42
1:D:143:LYS:HZ2	1:D:212:PHE:H	1.66	0.42
1:D:246:LYS:HG2	1:D:247:ASP:N	2.33	0.42
1:D:203:TYR:OH	1:D:482:SER:O	2.35	0.42
1:D:531:ILE:HD13	1:D:558:VAL:HG22	2.01	0.42
1:D:96:ALA:HB1	1:D:163:GLY:H	1.84	0.42
2:F:110:GLN:CB	2:F:167:TYR:HE2	2.32	0.42
1:A:213:ARG:HD3	7:A:704:HOH:O	2.18	0.42
1:A:286:ASN:O	1:A:318:HIS:NE2	2.51	0.42
2:B:11:TRP:CG	2:B:12:PRO:HD3	2.54	0.42
2:B:51:HIS:O	2:B:53:LYS:HG3	2.18	0.42
2:C:102:VAL:HG21	2:C:157:LEU:HB3	2.02	0.42
2:C:162:SER:HB2	2:C:205:ILE:HD13	2.00	0.42
1:D:143:LYS:O	7:D:740:HOH:O	2.22	0.42
1:D:168:ASN:ND2	5:D:603:ATP:O3A	2.40	0.42
1:A:133:ASN:HA	1:A:136:PHE:O	2.18	0.42
1:A:223:PHE:HB2	1:A:225:HIS:CE1	2.54	0.42
1:A:234:PHE:CE1	1:A:294:LEU:HD11	2.54	0.42
1:A:465:TYR:OH	7:A:734:HOH:O	2.18	0.42
1:A:91:GLY:HA3	2:B:142:LYS:N	2.34	0.42
2:C:97:PHE:CE2	2:C:101:PHE:CZ	3.07	0.42
1:D:222:VAL:HB	1:D:533:GLU:CD	2.39	0.42
1:D:314:PRO:HA	1:D:317:ARG:NH1	2.35	0.42
1:D:520:LEU:HD11	1:D:522:VAL:HG13	2.02	0.42
1:D:531:ILE:HD11	1:D:558:VAL:HG13	2.02	0.42
1:D:65:VAL:HA	1:D:66:PRO:HD2	1.82	0.42
1:D:86:SER:HB2	2:E:188:ARG:NE	2.34	0.42
2:F:118:GLY:HA2	7:F:513:HOH:O	2.18	0.42
2:F:166:ALA:HB1	2:F:209:ALA:CB	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:213:ARG:HG3	7:F:493:HOH:O	2.19	0.42
1:A:114:THR:O	1:A:117:LEU:HG	2.19	0.42
1:A:218:TYR:CD2	1:A:220:PHE:HB2	2.54	0.42
1:A:256:VAL:HB	1:A:259:VAL:HG12	2.00	0.42
1:A:273:LEU:HA	1:A:273:LEU:HD23	1.77	0.42
1:A:431:ILE:H	1:A:431:ILE:HG12	1.66	0.42
1:A:95:PRO:HD3	2:B:181:LYS:HZ3	1.84	0.42
2:B:13:SER:O	2:B:17:MET:HG3	2.20	0.42
1:D:113:PHE:CD2	5:D:603:ATP:O1B	2.72	0.42
1:D:14:ILE:HG22	1:D:16:GLU:CB	2.49	0.42
1:D:169:VAL:HG13	1:D:170:TYR:N	2.35	0.42
1:D:182:ILE:HG22	1:D:182:ILE:O	2.19	0.42
2:E:169:LYS:HE2	2:E:169:LYS:HB3	1.50	0.42
2:F:42:PRO:O	2:F:45:LEU:HG	2.19	0.42
1:A:208:SER:HA	1:A:211:LEU:CD1	2.49	0.42
1:A:286:ASN:ND2	1:A:288:TYR:CE2	2.85	0.42
1:A:98:SER:HB2	5:A:603:ATP:O3B	2.20	0.42
2:B:105:LYS:HE2	2:B:131:ALA:HB2	2.01	0.42
2:C:116:LYS:HA	2:C:116:LYS:HD3	1.86	0.42
1:D:333:SER:N	5:D:603:ATP:N7	2.68	0.42
2:F:131:ALA:O	2:F:135:LEU:HB2	2.20	0.42
1:A:169:VAL:HG23	1:A:175:PHE:CE1	2.55	0.42
1:A:38:LYS:HD3	1:A:395:TYR:CE1	2.55	0.42
2:B:142:LYS:HA	2:B:143:PRO:HD3	1.97	0.42
2:B:21:VAL:HG13	2:B:194:SER:HB2	2.01	0.42
2:C:17:MET:HE3	2:C:163:TRP:HH2	1.84	0.42
2:C:32:TYR:HD1	2:C:32:TYR:H	1.66	0.42
2:C:51:HIS:O	2:C:53:LYS:HG3	2.19	0.42
1:D:435:LYS:HA	1:D:436:ASN:HB2	2.00	0.42
1:D:538:LEU:HD22	1:D:544:GLN:CD	2.40	0.42
2:E:130:GLU:O	2:E:134:ILE:HG13	2.20	0.42
2:E:4:LEU:HA	2:E:5:PRO:HD3	1.91	0.42
2:F:136:GLU:HB2	2:F:179:SER:HA	2.02	0.42
1:A:200:GLN:HG3	7:A:712:HOH:O	2.19	0.42
1:A:143:LYS:O	1:A:216:VAL:HA	2.20	0.42
1:A:18:ASP:O	1:A:22:ARG:HG3	2.20	0.42
1:A:369:THR:HG23	1:A:370:GLY:H	1.84	0.42
1:A:99:LEU:HG	1:A:555:ASN:CG	2.40	0.42
1:A:80:MET:SD	1:A:94:VAL:HG12	2.60	0.42
2:C:125:LYS:CE	2:C:171:GLY:HA2	2.47	0.42
2:C:202:SER:OG	1:D:454:GLU:OE2	2.36	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:74:GLU:N	1:D:75:PRO:HD2	2.34	0.42
2:E:45:LEU:HB2	7:E:401:HOH:O	2.20	0.42
2:F:176:GLU:N	2:F:176:GLU:OE1	2.41	0.42
2:F:47:SER:HB2	2:F:63:PRO:HB2	2.02	0.42
2:F:54:ILE:HB	2:F:55:PRO:HA	2.00	0.42
1:A:219:VAL:HG11	1:A:291:ILE:HG21	2.01	0.42
1:A:221:ALA:CB	1:A:227:LEU:HG	2.43	0.42
1:A:360:TYR:N	1:A:393:THR:O	2.43	0.42
1:A:403:LEU:HD12	7:A:730:HOH:O	2.20	0.42
1:A:475:TYR:HB2	1:A:518:LEU:HD13	2.02	0.42
1:A:480:GLU:HB2	1:A:528:PHE:HD2	1.81	0.42
1:A:459:VAL:HA	1:A:481:ILE:HA	2.02	0.42
2:C:125:LYS:HD3	2:C:173:PHE:CD2	2.55	0.42
1:D:150:SER:OG	1:D:170:TYR:HB2	2.20	0.42
1:D:155:ILE:HD11	1:D:159:GLY:C	2.41	0.42
1:D:519:GLU:HG3	1:D:570:TYR:O	2.18	0.42
1:D:65:VAL:HG21	1:D:399:TYR:CE2	2.52	0.42
2:E:205:ILE:HG12	2:E:205:ILE:H	1.72	0.42
1:A:190:ASP:HA	1:A:193:ILE:HD12	2.02	0.42
1:A:29:LYS:HE2	1:A:33:LYS:HZ1	1.84	0.42
1:A:357:ASN:ND2	7:A:746:HOH:O	2.25	0.42
2:B:146:GLY:N	2:B:151:GLY:HA3	2.33	0.42
1:D:144:ALA:HB1	1:D:218:TYR:CE1	2.55	0.42
1:D:212:PHE:N	1:D:212:PHE:HD1	2.17	0.42
2:E:211:GLU:HA	2:E:214:LYS:HD2	2.02	0.42
2:E:68:LEU:HD21	2:E:99:ALA:HB1	2.02	0.42
2:F:154:ASP:O	2:F:158:ILE:HB	2.19	0.42
2:F:92:ARG:O	2:F:96:ARG:HG3	2.19	0.42
1:A:111:ILE:HD13	1:A:334:GLU:OE2	2.19	0.41
1:A:336:TRP:HB3	1:A:358:LEU:CD1	2.50	0.41
1:A:490:LEU:HA	1:A:490:LEU:HD23	1.86	0.41
1:A:474:HIS:NE2	1:A:521:ARG:NH2	2.68	0.41
1:A:98:SER:HB3	1:A:111:ILE:CB	2.40	0.41
1:D:106:GLY:C	1:D:432:ASN:HB3	2.40	0.41
1:D:14:ILE:C	1:D:16:GLU:N	2.72	0.41
1:D:530:LYS:HG3	7:D:769:HOH:O	2.19	0.41
1:D:561:ILE:HG12	1:D:561:ILE:H	1.48	0.41
1:A:152:LYS:HD3	1:A:561:ILE:CA	2.50	0.41
1:D:104:SER:HB3	1:D:107:ARG:O	2.20	0.41
1:D:106:GLY:CA	1:D:432:ASN:HB3	2.49	0.41
2:E:151:GLY:H	2:E:154:ASP:CB	2.31	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:124:GLY:HA2	2:F:127:GLU:CD	2.41	0.41
2:F:185:TRP:CE2	2:F:189:CYS:SG	3.13	0.41
1:A:306:THR:HA	1:A:310:GLU:HG3	2.02	0.41
2:C:12:PRO:O	2:C:163:TRP:CZ2	2.73	0.41
2:C:181:LYS:HE3	2:C:181:LYS:HB2	1.91	0.41
2:C:7:LEU:HB2	2:C:31:GLU:O	2.20	0.41
1:D:143:LYS:HG3	1:D:216:VAL:HG13	2.02	0.41
1:D:67:LEU:HA	1:D:400:ARG:O	2.20	0.41
1:D:470:THR:HG23	1:D:473:GLY:HA2	2.01	0.41
1:D:154:TYR:HA	1:D:563:CYS:HB3	2.01	0.41
1:D:70:ASP:OD1	1:D:71:VAL:N	2.54	0.41
1:D:82:ASP:OD1	7:D:742:HOH:O	2.22	0.41
2:E:142:LYS:HB3	2:E:144:TYR:O	2.20	0.41
2:E:5:PRO:HB2	2:E:57:LEU:HD11	2.02	0.41
1:A:421:PHE:HB3	1:A:542:ALA:CB	2.49	0.41
1:A:487:GLU:OE1	1:A:568:SER:HB3	2.20	0.41
1:D:117:LEU:HD11	1:D:396:ALA:HB2	2.01	0.41
1:D:287:TRP:CE3	1:D:290:LEU:CD1	2.96	0.41
1:D:308:SER:O	1:D:311:PRO:HD2	2.20	0.41
1:D:328:HIS:CE1	1:D:329:ASP:OD2	2.74	0.41
1:D:340:ASN:HA	1:D:352:PHE:HA	2.02	0.41
1:D:382:VAL:HG22	1:D:388:TYR:HD2	1.86	0.41
2:E:151:GLY:O	2:E:154:ASP:HB2	2.20	0.41
2:F:161:SER:O	2:F:164:PHE:HB2	2.19	0.41
2:E:96:ARG:NH2	2:F:73:TYR:CE1	2.86	0.41
1:A:205:HIS:NE2	7:A:755:HOH:O	2.37	0.41
1:A:312:TYR:HD1	7:A:914:HOH:O	2.01	0.41
1:A:313:VAL:HG13	1:A:325:LEU:HD13	2.03	0.41
2:B:18:ARG:CD	2:B:156:SER:HA	2.37	0.41
2:C:5:PRO:HB3	2:C:59:HIS:NE2	2.35	0.41
2:B:66:GLU:HG3	2:C:97:PHE:CD1	2.56	0.41
1:D:125:PHE:O	1:D:129:PHE:HB2	2.20	0.41
1:D:240:GLU:OE2	1:D:253:ARG:NH1	2.52	0.41
1:D:58:GLU:O	1:D:62:LYS:HD3	2.21	0.41
1:A:118:MET:SD	5:A:603:ATP:H4'	2.60	0.41
1:A:315:LYS:HB2	7:A:914:HOH:O	2.21	0.41
1:A:462:PHE:CE1	1:A:549:ARG:HD2	2.56	0.41
1:A:519:GLU:HB2	1:A:571:PHE:CD1	2.55	0.41
1:A:551:VAL:HG12	1:A:555:ASN:HD22	1.86	0.41
2:C:182:LEU:HD23	2:C:183:ILE:N	2.35	0.41
2:C:9:ASP:OD2	2:C:32:TYR:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:247:ASP:O	1:D:249:VAL:HG23	2.20	0.41
1:A:121:THR:HG22	1:A:122:LEU:N	2.35	0.41
1:A:150:SER:HB3	1:A:170:TYR:CD2	2.55	0.41
1:A:144:ALA:HB2	1:A:184:SER:OG	2.21	0.41
1:A:521:ARG:NH1	7:A:797:HOH:O	2.53	0.41
1:A:331:GLY:N	1:A:537:GLY:O	2.53	0.41
2:B:157:LEU:HA	2:B:157:LEU:HD23	1.89	0.41
2:C:17:MET:HA	2:C:20:ARG:HD2	2.03	0.41
2:C:49:PRO:O	2:C:52:LYS:HG3	2.20	0.41
1:D:130:ALA:O	1:D:134:ARG:N	2.48	0.41
1:D:31:THR:HG21	1:D:359:GLY:CA	2.50	0.41
1:D:40:GLN:OE1	7:D:737:HOH:O	2.21	0.41
1:D:474:HIS:CG	1:D:474:HIS:O	2.73	0.41
1:D:309:MET:HE3	1:D:545:PHE:CZ	2.56	0.41
2:E:98:TRP:HH2	2:E:134:ILE:HG22	1.85	0.41
2:F:145:PHE:HB3	2:F:153:VAL:CG1	2.51	0.41
2:F:102:VAL:CG1	2:F:160:PHE:HE2	2.33	0.41
2:F:4:LEU:HA	2:F:5:PRO:HD3	1.90	0.41
1:A:145:LEU:HB2	1:A:209:GLY:HA3	2.03	0.41
2:C:197:LYS:HB2	7:C:427:HOH:O	2.20	0.41
1:D:222:VAL:O	1:D:223:PHE:HD1	2.04	0.41
1:D:299:LYS:O	1:D:324:PRO:HD2	2.21	0.41
1:D:531:ILE:CD1	1:D:558:VAL:HG22	2.51	0.41
1:D:43:ILE:CG2	1:D:88:ILE:HG23	2.51	0.41
2:E:25:GLU:HG2	2:E:84:PHE:CE1	2.55	0.41
2:F:73:TYR:HE2	7:F:402:HOH:O	2.03	0.41
1:A:448:ALA:HB2	1:A:496:CYS:HB3	2.03	0.41
2:B:158:ILE:HD11	7:B:414:HOH:O	2.20	0.41
2:B:201:ASP:OD1	2:B:202:SER:N	2.53	0.41
2:B:163:TRP:CG	2:B:205:ILE:HD13	2.55	0.41
7:B:538:HOH:O	2:C:104:LYS:HG2	2.20	0.41
1:D:169:VAL:HG11	7:D:803:HOH:O	2.20	0.41
2:E:154:ASP:O	2:E:158:ILE:HB	2.20	0.41
2:F:203:GLU:O	2:F:206:VAL:HB	2.20	0.41
1:A:43:ILE:HA	1:A:46:GLN:HB3	2.02	0.41
1:A:548:PRO:O	7:A:742:HOH:O	2.22	0.41
1:D:370:GLY:HA2	1:D:371:GLU:HA	1.47	0.41
1:D:45:LEU:HD13	1:D:50:LEU:HD13	2.02	0.41
2:E:66:GLU:CD	2:F:100:ASP:OD2	2.59	0.41
1:A:110:PHE:O	1:A:111:ILE:HG13	2.21	0.41
1:A:11:ASN:HA	1:A:14:ILE:HD12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:464:SER:O	1:A:551:VAL:N	2.40	0.41
2:B:117:LYS:HA	2:B:121:GLN:NE2	2.36	0.41
1:A:93:PRO:HG2	2:B:184:ALA:HB3	2.03	0.41
2:B:163:TRP:HZ3	2:B:209:ALA:HB2	1.86	0.41
2:B:58:VAL:HA	2:B:63:PRO:HA	2.04	0.41
1:D:19:GLU:O	1:D:23:ASN:ND2	2.41	0.41
1:D:362:GLU:OE1	7:D:739:HOH:O	2.22	0.41
1:A:337:ILE:O	1:A:355:ILE:N	2.32	0.40
1:A:362:GLU:O	1:A:363:PHE:HD1	2.04	0.40
2:B:48:ASN:HA	2:B:49:PRO:HD2	1.81	0.40
2:B:86:PRO:HG2	2:B:92:ARG:HG3	2.03	0.40
2:C:57:LEU:HB3	2:C:64:VAL:CG2	2.51	0.40
2:B:96:ARG:C	2:C:69:ASN:HD21	2.24	0.40
1:D:441:LEU:O	1:D:441:LEU:HD12	2.22	0.40
1:D:445:VAL:HG13	1:D:479:TRP:CZ2	2.56	0.40
1:D:481:ILE:HD12	1:D:483:GLY:O	2.21	0.40
1:D:500:ALA:O	7:D:743:HOH:O	2.22	0.40
1:D:87:PRO:HB2	2:E:143:PRO:CB	2.51	0.40
2:E:98:TRP:CE2	2:E:138:GLU:HG2	2.56	0.40
1:A:122:LEU:HD23	1:A:125:PHE:CZ	2.56	0.40
1:A:204:CYS:O	1:A:207:LEU:HB3	2.21	0.40
1:A:274:ALA:HB3	7:A:716:HOH:O	2.20	0.40
1:A:308:SER:HB2	1:A:545:PHE:CE2	2.55	0.40
1:A:559:LEU:O	1:A:562:LEU:N	2.43	0.40
2:B:153:VAL:O	2:B:157:LEU:HB2	2.21	0.40
1:D:139:ASP:OD1	1:D:141:ASN:N	2.53	0.40
1:D:155:ILE:HG22	7:D:831:HOH:O	2.21	0.40
1:D:295:PHE:CD1	1:D:295:PHE:N	2.89	0.40
1:D:366:VAL:HA	1:D:371:GLU:O	2.21	0.40
1:D:113:PHE:CD2	5:D:603:ATP:PB	3.14	0.40
2:E:156:SER:HB2	7:E:415:HOH:O	2.21	0.40
2:E:8:LEU:O	2:E:55:PRO:HA	2.22	0.40
2:F:17:MET:HE2	2:F:200:PRO:HD2	2.02	0.40
2:F:24:ARG:NH1	2:F:198:SER:OG	2.55	0.40
1:A:189:PRO:O	1:A:192:VAL:HG12	2.22	0.40
1:A:225:HIS:HD1	1:A:309:MET:CE	2.33	0.40
1:A:370:GLY:HA2	1:A:371:GLU:HA	1.85	0.40
1:A:330:TYR:CZ	1:A:538:LEU:O	2.74	0.40
1:D:116:GLU:HB2	1:D:395:TYR:CE1	2.56	0.40
1:D:144:ALA:HB2	1:D:184:SER:OG	2.21	0.40
1:D:167:THR:HB	1:D:560:GLN:OE1	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:210:ILE:O	1:D:213:ARG:N	2.53	0.40
1:D:246:LYS:HA	1:D:270:ASN:O	2.22	0.40
1:D:35:ILE:HD13	1:D:394:ASN:HA	2.04	0.40
1:D:308:SER:OG	1:D:536:LEU:HD12	2.21	0.40
1:D:76:TYR:CD2	1:D:88:ILE:HD13	2.49	0.40
2:E:128:PHE:CE2	2:E:175:ILE:HG12	2.56	0.40
2:E:66:GLU:O	2:E:70:VAL:HG13	2.22	0.40
2:C:128:PHE:CE1	2:C:175:ILE:HG22	2.55	0.40
1:D:187:CYS:SG	1:D:209:GLY:HA2	2.62	0.40
1:D:256:VAL:O	1:D:260:ARG:HB3	2.21	0.40
1:D:393:THR:HA	1:D:398:LEU:O	2.21	0.40
1:D:424:ARG:HG3	1:D:425:ARG:HD2	2.04	0.40
1:D:94:VAL:HG11	1:D:97:ILE:HD11	2.02	0.40
1:D:39:ASN:ND2	2:E:142:LYS:HA	2.36	0.40
2:F:176:GLU:O	2:F:177:SER:OG	2.32	0.40
1:A:256:VAL:HA	1:A:257:PRO:HD3	1.91	0.40
1:A:337:ILE:HG13	1:A:338:ALA:N	2.36	0.40
1:A:35:ILE:HA	1:A:395:TYR:CE1	2.56	0.40
1:A:552:LYS:C	1:A:554:SER:N	2.74	0.40
1:D:245:ILE:HD11	1:D:274:ALA:HB2	2.03	0.40
1:D:434:ASP:HB2	1:D:550:CYS:SG	2.61	0.40
2:E:10:TYR:HB3	2:E:13:SER:HB2	2.03	0.40
2:E:205:ILE:HA	2:E:208:TYR:CD2	2.57	0.40
2:F:123:ALA:O	2:F:127:GLU:HG3	2.21	0.40
2:F:11:TRP:CZ3	2:F:205:ILE:HG13	2.57	0.40
2:F:47:SER:HB2	2:F:63:PRO:CB	2.52	0.40

All (22) 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:297:ASN:ND2	1:D:435:LYS:O[1_655]	1.96	0.24
7:F:552:HOH:O	7:F:577:HOH:O[1_665]	2.00	0.20
1:A:239:GLU:OE1	2:F:178:GLU:N[1_554]	2.01	0.19
7:D:989:HOH:O	7:D:1008:HOH:O[1_665]	2.04	0.16
7:D:936:HOH:O	7:D:988:HOH:O[1_655]	2.04	0.16
7:A:953:HOH:O	7:F:463:HOH:O[1_454]	2.05	0.15
1:D:207:LEU:O	7:D:713:HOH:O[1_655]	2.08	0.12
1:A:268:THR:OG1	7:A:708:HOH:O[1_655]	2.08	0.12
1:A:503:ASP:O	7:A:706:HOH:O[1_455]	2.09	0.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:33:ARG:NH2	2:C:215:ASN:O[1_455]	2.09	0.11
7:A:1006:HOH:O	7:A:1015:HOH:O[1_665]	2.11	0.09
7:B:457:HOH:O	7:C:517:HOH:O[1_565]	2.11	0.09
7:A:719:HOH:O	7:F:432:HOH:O[1_554]	2.13	0.07
1:A:297:ASN:ND2	1:A:435:LYS:O[1_655]	2.14	0.06
7:D:773:HOH:O	7:E:507:HOH:O[1_545]	2.14	0.06
1:D:26:GLN:NE2	2:E:211:GLU:OE1[1_545]	2.17	0.03
7:B:590:HOH:O	7:B:591:HOH:O[1_655]	2.17	0.03
1:D:213:ARG:NE	1:D:503:ASP:OD2[1_655]	2.18	0.02
1:A:270:ASN:ND2	1:A:510:ARG:O[1_655]	2.18	0.02
7:A:1049:HOH:O	7:A:1056:HOH:O[1_665]	2.18	0.02
1:D:139:ASP:OD2	1:D:552:LYS:NZ[1_655]	2.18	0.02
1:A:436:ASN:ND2	7:A:704:HOH:O[1_455]	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%)	514 (91%)	38 (7%)	15 (3%)	5	2
1	D	567/575 (99%)	516 (91%)	36 (6%)	15 (3%)	5	2
2	B	212/223 (95%)	200 (94%)	10 (5%)	2 (1%)	17	14
2	C	212/223 (95%)	198 (93%)	12 (6%)	2 (1%)	17	14
2	E	212/223 (95%)	199 (94%)	12 (6%)	1 (0%)	29	29
2	F	212/223 (95%)	196 (92%)	11 (5%)	5 (2%)	6	3
All	All	1982/2042 (97%)	1823 (92%)	119 (6%)	40 (2%)	7	4

All (40) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	238	TRP
1	A	241	ILE

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Mol	Chain	Res	Type
1	A	368	GLU
1	A	540	SER
1	A	542	ALA
2	B	66	GLU
1	D	286	ASN
1	D	368	GLU
1	D	476	ALA
1	D	540	SER
2	F	12	PRO
1	A	76	TYR
1	A	88	ILE
1	A	165	ALA
1	A	235	GLU
1	A	437	THR
2	C	104	LYS
1	D	83	GLY
1	D	239	GLU
1	D	477	ILE
1	D	561	ILE
2	F	177	SER
1	A	544	GLN
1	D	211	LEU
1	D	271	PRO
2	E	140	GLY
1	A	90	THR
1	A	307	GLY
1	D	14	ILE
1	D	369	THR
1	D	437	THR
2	F	141	ASP
1	A	236	GLN
1	D	13	VAL
1	A	240	GLU
2	F	66	GLU
2	B	140	GLY
2	C	12	PRO
2	F	83	PRO
1	D	88	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	499/505 (99%)	425 (85%)	74 (15%)	3	1
1	D	499/505 (99%)	402 (81%)	97 (19%)	1	0
2	B	187/195 (96%)	171 (91%)	16 (9%)	10	9
2	C	187/195 (96%)	164 (88%)	23 (12%)	4	3
2	E	187/195 (96%)	161 (86%)	26 (14%)	3	2
2	F	187/195 (96%)	150 (80%)	37 (20%)	1	0
All	All	1746/1790 (98%)	1473 (84%)	273 (16%)	2	1

All (273) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	THR
1	A	9	ASP
1	A	67	LEU
1	A	77	ILE
1	A	78	LYS
1	A	80	MET
1	A	90	THR
1	A	101	SER
1	A	103	THR
1	A	108	PRO
1	A	110	PHE
1	A	116	GLU
1	A	117	LEU
1	A	121	THR
1	A	125	PHE
1	A	140	ASP
1	A	146	GLN
1	A	149	PHE
1	A	150	SER
1	A	152	LYS
1	A	182	ILE
1	A	183	THR

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Mol	Chain	Res	Type
1	A	184	SER
1	A	187	CYS
1	A	188	SER
1	A	202	LEU
1	A	206	LEU
1	A	213	ARG
1	A	216	VAL
1	A	237	VAL
1	A	238	TRP
1	A	239	GLU
1	A	240	GLU
1	A	244	ASP
1	A	265	LYS
1	A	266	LEU
1	A	267	LEU
1	A	276	THR
1	A	278	ARG
1	A	279	THR
1	A	285	SER
1	A	287	TRP
1	A	291	ILE
1	A	332	SER
1	A	333	SER
1	A	340	ASN
1	A	342	THR
1	A	369	THR
1	A	377	VAL
1	A	403	LEU
1	A	416	THR
1	A	422	ILE
1	A	427	LEU
1	A	431	ILE
1	A	437	THR
1	A	440	ASP
1	A	461	ASP
1	A	463	SER
1	A	478	PHE
1	A	479	TRP
1	A	494	CYS
1	A	498	ASP
1	A	509	SER
1	A	512	CYS

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Mol	Chain	Res	Type
1	A	515	ILE
1	A	525	LYS
1	A	534	HIS
1	A	535	PHE
1	A	545	PHE
1	A	547	MET
1	A	562	LEU
1	A	563	CYS
1	A	569	SER
1	A	573	THR
2	B	4	LEU
2	B	40	LYS
2	B	48	ASN
2	B	52	LYS
2	B	66	GLU
2	B	74	VAL
2	B	81	LYS
2	B	132	VAL
2	B	138	GLU
2	B	139	LEU
2	B	153	VAL
2	B	157	LEU
2	B	168	GLU
2	B	181	LYS
2	B	182	LEU
2	B	199	LEU
2	C	4	LEU
2	C	9	ASP
2	C	14	MET
2	C	32	TYR
2	C	34	GLU
2	C	37	PHE
2	C	38	SER
2	C	43	LEU
2	C	65	CYS
2	C	68	LEU
2	C	80	GLU
2	C	81	LYS
2	C	84	PHE
2	C	85	PHE
2	C	104	LYS
2	C	133	LYS

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Mol	Chain	Res	Type
2	C	135	LEU
2	C	136	GLU
2	C	142	LYS
2	C	157	LEU
2	C	162	SER
2	C	176	GLU
2	C	182	LEU
1	D	13	VAL
1	D	17	PHE
1	D	33	LYS
1	D	44	TYR
1	D	47	ASN
1	D	55	THR
1	D	62	LYS
1	D	63	SER
1	D	69	THR
1	D	85	THR
1	D	89	LEU
1	D	90	THR
1	D	92	HIS
1	D	94	VAL
1	D	107	ARG
1	D	109	LYS
1	D	110	PHE
1	D	114	THR
1	D	121	THR
1	D	124	LEU
1	D	129	PHE
1	D	145	LEU
1	D	151	SER
1	D	152	LYS
1	D	154	TYR
1	D	162	VAL
1	D	174	ASN
1	D	186	SER
1	D	187	CYS
1	D	188	SER
1	D	190	ASP
1	D	193	ILE
1	D	212	PHE
1	D	213	ARG
1	D	216	VAL

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Mol	Chain	Res	Type
1	D	236	GLN
1	D	240	GLU
1	D	246	LYS
1	D	250	LEU
1	D	251	SER
1	D	254	ILE
1	D	259	VAL
1	D	264	SER
1	D	265	LYS
1	D	276	THR
1	D	284	LEU
1	D	290	LEU
1	D	295	PHE
1	D	299	LYS
1	D	306	THR
1	D	329	ASP
1	D	333	SER
1	D	342	THR
1	D	345	LEU
1	D	349	GLU
1	D	369	THR
1	D	377	VAL
1	D	379	LEU
1	D	380	THR
1	D	391	VAL
1	D	400	ARG
1	D	403	LEU
1	D	420	LYS
1	D	421	PHE
1	D	423	CYS
1	D	424	ARG
1	D	425	ARG
1	D	427	LEU
1	D	428	ILE
1	D	443	LEU
1	D	447	SER
1	D	450	LYS
1	D	452	LEU
1	D	463	SER
1	D	467	ASP
1	D	477	ILE
1	D	478	PHE

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Mol	Chain	Res	Type
1	D	481	ILE
1	D	484	GLU
1	D	494	CYS
1	D	499	ARG
1	D	502	ILE
1	D	512	CYS
1	D	522	VAL
1	D	523	VAL
1	D	528	PHE
1	D	536	LEU
1	D	538	LEU
1	D	545	PHE
1	D	547	MET
1	D	552	LYS
1	D	554	SER
1	D	561	ILE
1	D	562	LEU
1	D	563	CYS
1	D	565	ASN
1	D	573	THR
2	E	45	LEU
2	E	48	ASN
2	E	51	HIS
2	E	56	VAL
2	E	66	GLU
2	E	101	PHE
2	E	103	ASP
2	E	116	LYS
2	E	119	GLU
2	E	120	GLU
2	E	133	LYS
2	E	142	LYS
2	E	148	ASP
2	E	150	PHE
2	E	153	VAL
2	E	157	LEU
2	E	173	PHE
2	E	177	SER
2	E	178	GLU
2	E	179	SER
2	E	183	ILE
2	E	185	TRP

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Mol	Chain	Res	Type
2	E	190	MET
2	E	204	LYS
2	E	205	ILE
2	E	211	GLU
2	F	10	TYR
2	F	15	PHE
2	F	32	TYR
2	F	34	GLU
2	F	35	GLU
2	F	36	ASP
2	F	41	SER
2	F	43	LEU
2	F	71	VAL
2	F	72	GLN
2	F	75	ASP
2	F	84	PHE
2	F	105	LYS
2	F	111	PHE
2	F	128	PHE
2	F	129	ILE
2	F	133	LYS
2	F	134	ILE
2	F	135	LEU
2	F	136	GLU
2	F	138	GLU
2	F	148	ASP
2	F	157	LEU
2	F	158	ILE
2	F	161	SER
2	F	162	SER
2	F	164	PHE
2	F	169	LYS
2	F	173	PHE
2	F	176	GLU
2	F	182	LEU
2	F	185	TRP
2	F	188	ARG
2	F	190	MET
2	F	204	LYS
2	F	211	GLU
2	F	212	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	ASN
1	A	51	ASN
1	A	120	ASN
1	A	426	ASN
1	A	544	GLN
2	C	69	ASN
2	C	110	GLN
1	D	28	GLN
1	D	39	ASN
1	D	432	ASN
1	D	495	ASN
1	D	532	GLN
1	D	534	HIS
1	D	544	GLN
2	E	60	ASN
2	E	121	GLN
2	E	172	ASN
2	F	72	GLN
2	F	172	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

10 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	JAA	A	601	-	12,15,15	5.93	6 (50%)	12,19,19	2.42	5 (41%)
6	GSH	E	301	-	12,19,19	1.79	4 (33%)	15,24,24	3.21	7 (46%)
5	ATP	A	603	-	26,33,33	4.74	14 (53%)	31,52,52	3.16	9 (29%)
3	JAA	D	601	-	12,15,15	5.87	6 (50%)	12,19,19	2.59	5 (41%)
5	ATP	D	603	-	26,33,33	5.02	14 (53%)	31,52,52	2.91	12 (38%)
6	GSH	B	301	-	12,19,19	2.04	5 (41%)	15,24,24	3.27	7 (46%)
6	GSH	F	301	-	12,19,19	1.76	4 (33%)	15,24,24	4.11	7 (46%)
6	GSH	C	301	-	12,19,19	1.76	4 (33%)	15,24,24	3.18	6 (40%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	JAA	A	601	-	-	4/7/22/22	0/1/1/1
6	GSH	E	301	-	-	1/18/24/24	-
5	ATP	A	603	-	-	5/18/38/38	0/3/3/3
3	JAA	D	601	-	-	5/7/22/22	0/1/1/1
5	ATP	D	603	-	-	3/18/38/38	0/3/3/3
6	GSH	B	301	-	-	3/18/24/24	-
6	GSH	F	301	-	-	3/18/24/24	-
6	GSH	C	301	-	-	2/18/24/24	-

All (57) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	603	ATP	O4'-C1'	13.97	1.60	1.41
5	D	603	ATP	O4'-C1'	13.94	1.60	1.41
3	A	601	JAA	C05-C08	-13.50	1.29	1.52
3	D	601	JAA	C05-C08	-13.25	1.30	1.52
5	D	603	ATP	C2'-C1'	-11.14	1.36	1.53
3	D	601	JAA	C06-C04	-10.95	1.25	1.53
5	A	603	ATP	C2'-C1'	-10.69	1.37	1.53
3	A	601	JAA	C06-C04	-10.58	1.26	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	603	ATP	O4'-C4'	-9.44	1.23	1.45
5	D	603	ATP	O4'-C4'	-8.91	1.25	1.45
5	D	603	ATP	C4-N3	7.57	1.46	1.35
3	D	601	JAA	C10-C04	-6.95	1.44	1.53
5	A	603	ATP	C6-N6	-6.72	1.09	1.34
3	A	601	JAA	C07-C08	6.55	1.61	1.51
5	D	603	ATP	O3'-C3'	-6.38	1.27	1.43
3	A	601	JAA	C10-C04	-6.26	1.45	1.53
3	D	601	JAA	C07-C08	5.55	1.60	1.51
5	D	603	ATP	C6-N6	-5.43	1.14	1.34
5	D	603	ATP	C2-N1	5.36	1.43	1.33
5	A	603	ATP	C2-N1	5.27	1.43	1.33
5	A	603	ATP	O3'-C3'	-4.79	1.31	1.43
3	A	601	JAA	C05-C04	4.56	1.66	1.54
5	D	603	ATP	C3'-C4'	4.32	1.64	1.53
3	A	601	JAA	C09-C05	-4.28	1.48	1.54
3	D	601	JAA	C05-C04	4.25	1.65	1.54
5	D	603	ATP	C2'-C3'	-4.20	1.41	1.53
5	A	603	ATP	C2'-C3'	-4.06	1.42	1.53
5	D	603	ATP	C5'-C4'	-4.00	1.39	1.51
5	A	603	ATP	C3'-C4'	3.89	1.62	1.53
6	B	301	GSH	CD1-N2	3.84	1.42	1.34
3	D	601	JAA	C09-C05	-3.83	1.48	1.54
5	D	603	ATP	C2-N3	-3.73	1.26	1.32
6	E	301	GSH	C2-N3	3.67	1.41	1.33
6	F	301	GSH	CA2-N2	-3.48	1.38	1.45
6	B	301	GSH	C2-N3	3.31	1.40	1.33
5	A	603	ATP	C6-C5	-3.13	1.31	1.43
5	D	603	ATP	C5-C4	-3.10	1.32	1.40
6	F	301	GSH	C2-N3	2.99	1.40	1.33
6	C	301	GSH	CB2-CA2	-2.94	1.49	1.53
5	A	603	ATP	PG-O1G	-2.91	1.41	1.50
6	B	301	GSH	CB2-CA2	-2.80	1.50	1.53
6	C	301	GSH	C2-N3	2.79	1.39	1.33
6	C	301	GSH	CA2-N2	-2.71	1.40	1.45
5	D	603	ATP	C5-N7	-2.62	1.30	1.39
5	A	603	ATP	C5'-C4'	-2.41	1.44	1.51
5	A	603	ATP	O5'-C5'	-2.40	1.35	1.44
6	E	301	GSH	CD1-N2	2.35	1.39	1.34
6	E	301	GSH	CA2-N2	-2.33	1.41	1.45
5	A	603	ATP	C5-C4	2.24	1.46	1.40
5	D	603	ATP	PG-O1G	-2.24	1.43	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	301	GSH	CB2-CA2	-2.18	1.50	1.53
6	F	301	GSH	CB2-SG2	-2.17	1.77	1.81
5	A	603	ATP	C8-N7	-2.14	1.30	1.34
6	B	301	GSH	CB2-SG2	-2.08	1.77	1.81
6	B	301	GSH	CA3-N3	-2.06	1.42	1.46
6	C	301	GSH	CD1-N2	2.01	1.38	1.34
6	E	301	GSH	CB2-CA2	-2.00	1.50	1.53

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	301	GSH	CA2-CB2-SG2	-13.85	98.63	114.19
5	A	603	ATP	C4-C5-N7	-12.25	96.64	109.40
6	B	301	GSH	CA2-CB2-SG2	-10.39	102.51	114.19
6	E	301	GSH	CA2-CB2-SG2	-10.21	102.72	114.19
6	C	301	GSH	CA2-CB2-SG2	-9.74	103.25	114.19
5	D	603	ATP	PA-O3A-PB	-9.46	100.37	132.83
5	A	603	ATP	PA-O3A-PB	-6.70	109.83	132.83
5	A	603	ATP	O4'-C1'-C2'	-5.70	98.60	106.93
5	D	603	ATP	O4'-C1'-C2'	-5.55	98.82	106.93
3	A	601	JAA	C09-C11-C13	-4.89	108.23	126.40
3	D	601	JAA	C09-C11-C13	-4.71	108.93	126.40
5	D	603	ATP	N3-C2-N1	-4.69	121.35	128.68
5	D	603	ATP	C4-C5-N7	-4.53	104.68	109.40
5	A	603	ATP	O3G-PG-O3B	4.46	119.60	104.64
3	D	601	JAA	C07-C06-C04	-4.13	100.09	104.41
3	D	601	JAA	C06-C07-C08	-4.10	101.30	105.42
3	A	601	JAA	C06-C04-C10	-4.08	106.36	113.67
5	D	603	ATP	PB-O3B-PG	-3.99	119.15	132.83
3	D	601	JAA	C06-C04-C10	-3.97	106.56	113.67
6	F	301	GSH	CB2-CA2-N2	-3.96	105.64	111.28
6	B	301	GSH	CB2-CA2-C2	-3.90	101.72	109.76
6	C	301	GSH	C2-CA2-N2	-3.81	100.79	111.16
5	D	603	ATP	C2-N1-C6	3.79	125.24	118.75
6	C	301	GSH	CA3-N3-C2	-3.60	117.15	122.34
6	E	301	GSH	CG1-CD1-N2	-3.56	109.65	115.83
5	D	603	ATP	C5-C6-N1	-3.40	112.64	120.35
6	E	301	GSH	CB1-CG1-CD1	3.16	120.09	113.04
3	A	601	JAA	C06-C04-C05	3.13	107.85	103.34
6	B	301	GSH	CA3-N3-C2	-3.13	117.83	122.34
6	F	301	GSH	CG1-CD1-N2	-3.07	110.50	115.83
5	D	603	ATP	O3G-PG-O3B	3.06	114.88	104.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	301	GSH	OE1-CD1-CG1	2.98	127.46	122.02
6	F	301	GSH	C2-CA2-N2	-2.92	103.20	111.16
5	D	603	ATP	N6-C6-N1	2.86	124.52	118.57
6	C	301	GSH	CG1-CD1-N2	-2.81	110.95	115.83
6	F	301	GSH	CB1-CG1-CD1	2.79	119.26	113.04
6	C	301	GSH	CB1-CG1-CD1	2.70	119.08	113.04
5	A	603	ATP	O3'-C3'-C2'	2.70	120.55	111.82
5	A	603	ATP	PA-O5'-C5'	-2.67	106.05	121.68
5	A	603	ATP	C5'-C4'-C3'	-2.64	105.28	115.18
5	D	603	ATP	O2G-PG-O3B	2.52	113.09	104.64
3	A	601	JAA	O01-C08-C05	2.40	128.67	125.58
5	D	603	ATP	O4'-C4'-C5'	2.39	117.23	109.37
6	F	301	GSH	CG1-CB1-CA1	-2.38	108.28	113.84
6	E	301	GSH	C2-CA2-N2	-2.36	104.73	111.16
6	B	301	GSH	C2-CA2-N2	-2.35	104.77	111.16
6	C	301	GSH	OE1-CD1-CG1	2.34	126.29	122.02
5	A	603	ATP	N6-C6-N1	2.29	123.34	118.57
6	E	301	GSH	CG1-CB1-CA1	-2.29	108.49	113.84
6	E	301	GSH	CA3-N3-C2	-2.27	119.08	122.34
5	D	603	ATP	O2'-C2'-C1'	-2.26	102.52	110.85
3	A	601	JAA	C10-C04-C05	2.22	119.88	114.74
5	A	603	ATP	O5'-C5'-C4'	2.19	116.53	108.99
6	B	301	GSH	CG1-CD1-N2	-2.08	112.23	115.83
6	B	301	GSH	CB2-CA2-N2	-2.07	108.34	111.28
6	B	301	GSH	CG1-CB1-CA1	-2.02	109.13	113.84
3	D	601	JAA	O01-C08-C05	2.02	128.18	125.58
6	E	301	GSH	CB2-CA2-N2	-2.01	108.42	111.28

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	601	JAA	C08-C05-C09-C11
5	D	603	ATP	PB-O3B-PG-O3G
3	D	601	JAA	C11-C13-C14-C15
6	B	301	GSH	N2-CA2-CB2-SG2
6	B	301	GSH	C2-CA2-CB2-SG2
6	F	301	GSH	N2-CA2-CB2-SG2
6	F	301	GSH	C2-CA2-CB2-SG2
6	C	301	GSH	N2-CA2-CB2-SG2
6	C	301	GSH	C2-CA2-CB2-SG2
3	A	601	JAA	C09-C11-C13-C14

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Mol	Chain	Res	Type	Atoms
6	F	301	GSH	CA1-CB1-CG1-CD1
3	D	601	JAA	C09-C11-C13-C14
5	D	603	ATP	C4'-C5'-O5'-PA
3	A	601	JAA	C04-C05-C09-C11
3	D	601	JAA	C04-C05-C09-C11
5	A	603	ATP	C5'-O5'-PA-O2A
3	D	601	JAA	C08-C05-C09-C11
6	B	301	GSH	C1-CA1-CB1-CG1
5	A	603	ATP	PA-O3A-PB-O2B
5	A	603	ATP	PB-O3A-PA-O2A
3	D	601	JAA	C05-C09-C11-C13
5	D	603	ATP	PB-O3B-PG-O1G
6	E	301	GSH	CA1-CB1-CG1-CD1
3	A	601	JAA	C05-C09-C11-C13
5	A	603	ATP	C5'-O5'-PA-O3A
5	A	603	ATP	PB-O3A-PA-O1A

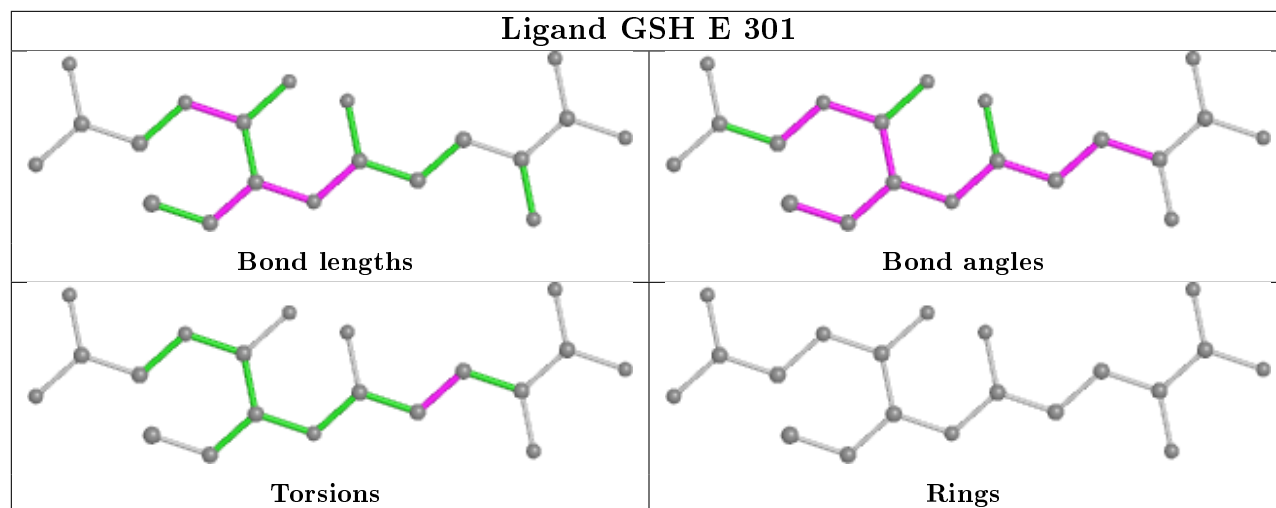
There are no ring outliers.

5 monomers are involved in 50 short contacts:

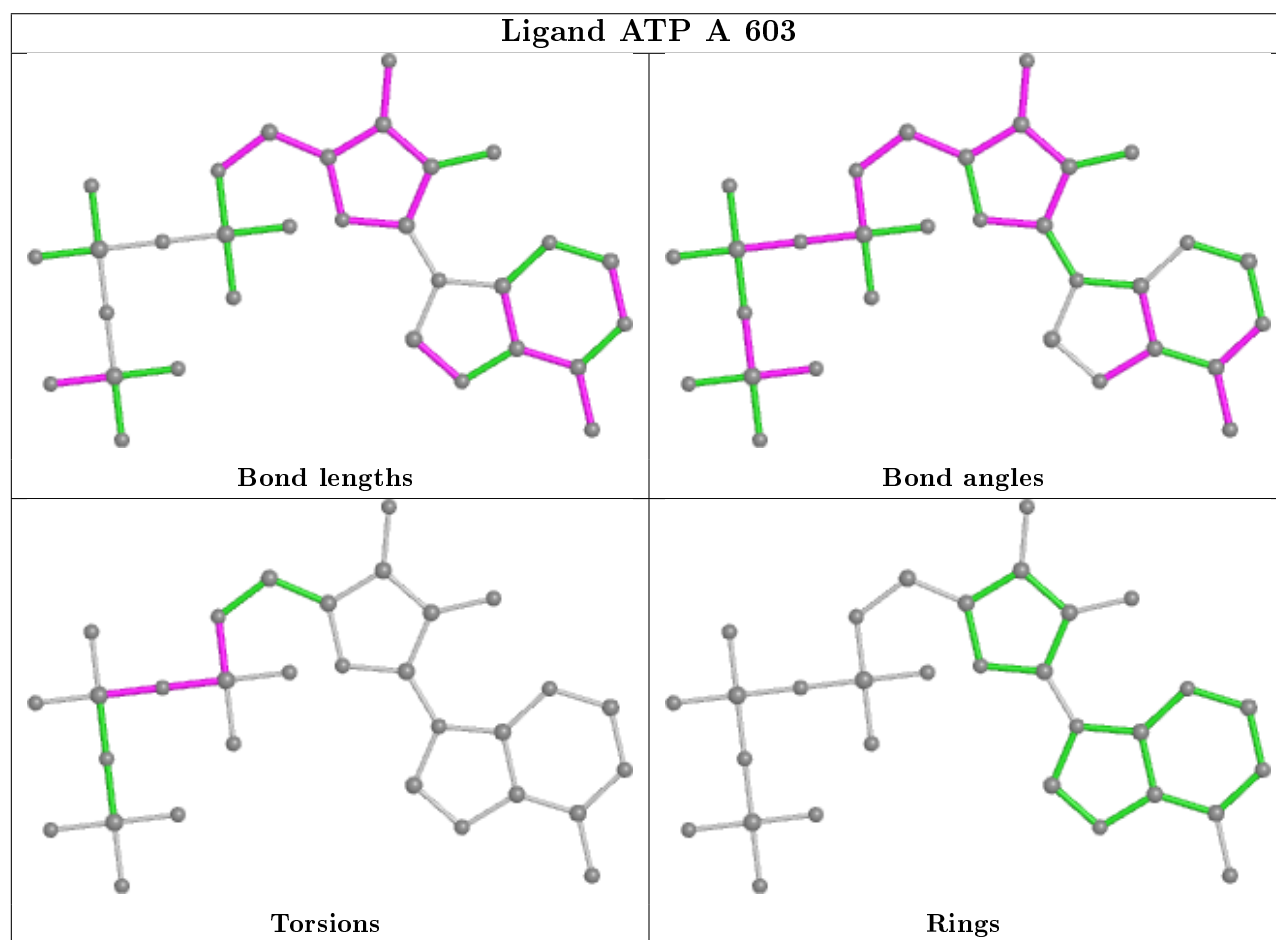
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	E	301	GSH	3	0
5	A	603	ATP	17	0
3	D	601	JAA	3	0
5	D	603	ATP	26	0
6	B	301	GSH	1	0

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

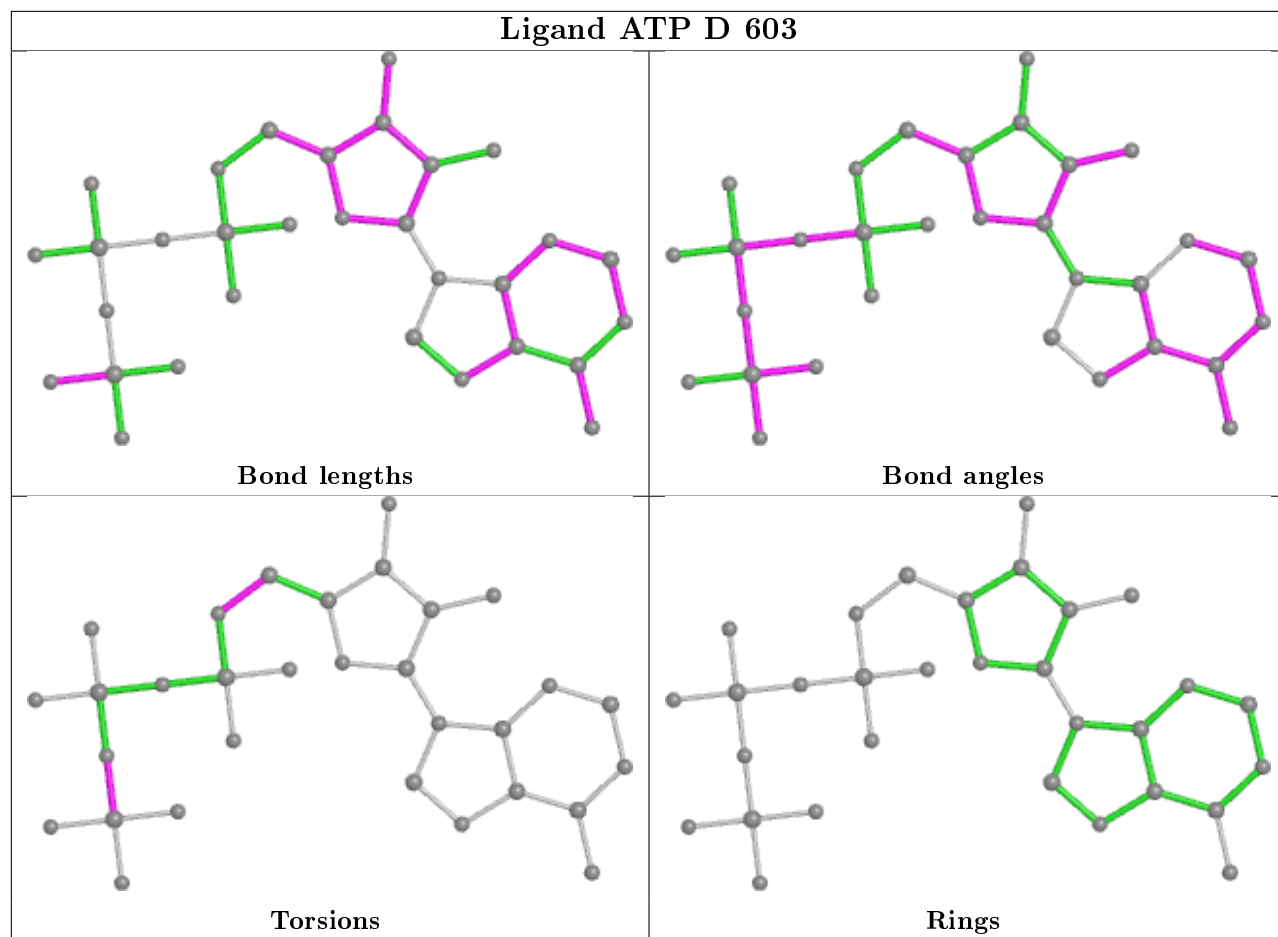
Ligand GSH E 301



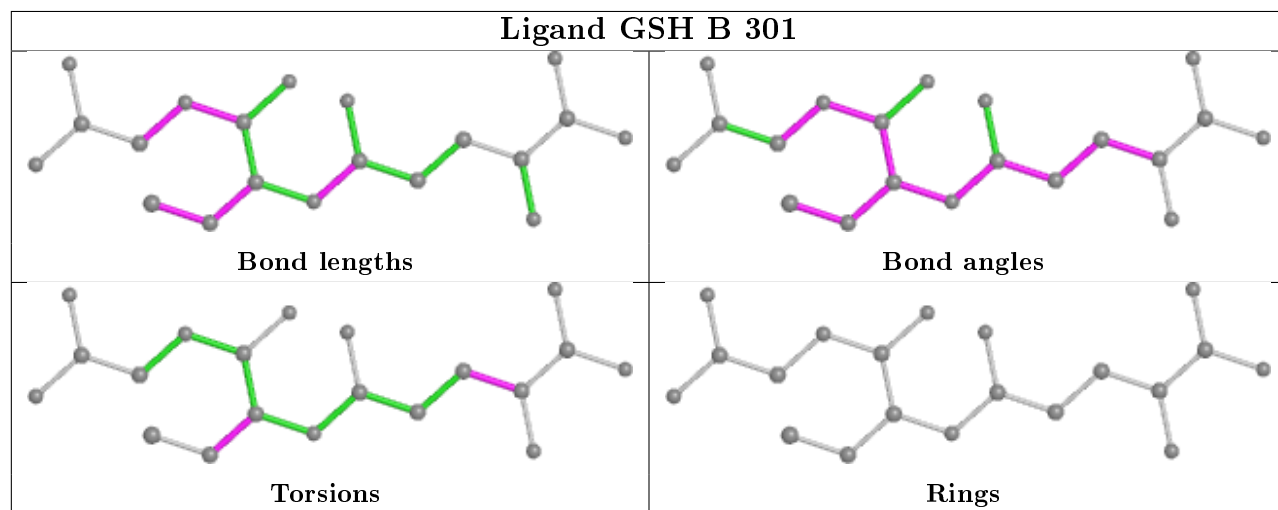
Ligand ATP A 603

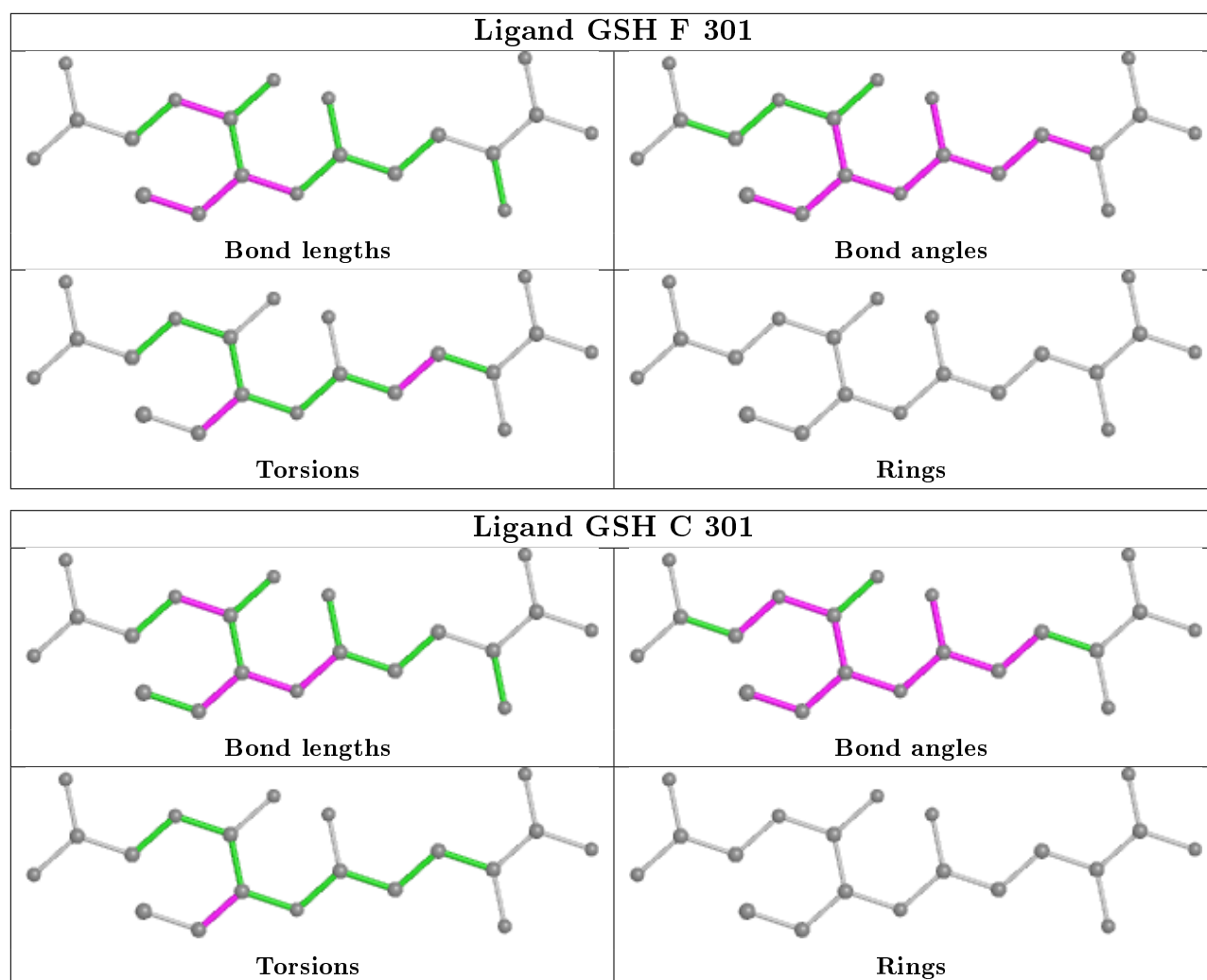


Ligand ATP D 603



Ligand GSH B 301





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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	569/575 (98%)	0.69	50 (8%) 10 11	3, 14, 22, 28	0
1	D	569/575 (98%)	0.79	59 (10%) 6 6	3, 15, 24, 31	0
2	B	214/223 (95%)	0.46	10 (4%) 31 34	4, 11, 20, 28	0
2	C	214/223 (95%)	0.20	3 (1%) 75 77	2, 3, 7, 11	0
2	E	214/223 (95%)	0.43	14 (6%) 18 20	4, 9, 16, 27	0
2	F	214/223 (95%)	0.16	2 (0%) 84 85	2, 3, 7, 11	0
All	All	1994/2042 (97%)	0.56	138 (6%) 16 18	2, 12, 22, 31	0

All (138) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	95	ALA	4.6
1	A	113	PHE	4.1
1	A	554	SER	3.9
2	B	205	ILE	3.6
1	D	111	ILE	3.5
1	D	380	THR	3.5
1	D	102	GLY	3.5
1	A	523	VAL	3.5
1	D	430	SER	3.4
1	A	429	LEU	3.3
2	E	101	PHE	3.3
1	A	507	VAL	3.3
2	B	61	GLY	3.2
1	A	277	ILE	3.2
1	A	269	PRO	3.2
1	A	358	LEU	3.2
2	B	153	VAL	3.2
1	D	186	SER	3.1
1	D	570	TYR	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	554	SER	3.1
1	D	71	VAL	3.0
1	A	257	PRO	3.0
1	D	31	THR	3.0
1	D	36	LEU	3.0
1	A	524	ALA	3.0
1	A	433	ILE	3.0
1	D	124	LEU	2.9
1	A	543	GLY	2.9
1	D	66	PRO	2.9
1	D	522	VAL	2.8
1	A	148	ILE	2.8
1	A	501	PHE	2.8
1	A	237	VAL	2.8
2	E	140	GLY	2.8
1	D	507	VAL	2.8
1	D	245	ILE	2.8
1	D	528	PHE	2.8
1	D	287	TRP	2.8
1	D	15	ASP	2.7
1	D	68	VAL	2.7
1	A	229	HIS	2.7
1	A	155	ILE	2.7
1	D	407	VAL	2.7
2	B	56	VAL	2.7
1	D	30	GLN	2.7
1	A	249	VAL	2.6
2	B	86	PRO	2.6
2	B	95	ALA	2.6
1	A	118	MET	2.6
1	D	238	TRP	2.5
1	D	518	LEU	2.5
1	D	110	PHE	2.5
1	A	27	VAL	2.5
1	A	233	THR	2.5
1	D	468	VAL	2.5
1	A	173	PRO	2.5
1	D	543	GLY	2.5
1	D	268	THR	2.5
1	A	224	ALA	2.4
1	A	90	THR	2.4
1	A	567	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	54	ALA	2.4
1	D	295	PHE	2.4
1	A	165	ALA	2.4
1	D	201	ALA	2.4
2	B	210	ALA	2.4
1	A	548	PRO	2.4
1	A	457	ILE	2.4
1	D	376	PRO	2.4
1	D	259	VAL	2.4
1	D	563	CYS	2.4
1	D	573	THR	2.4
2	C	113	VAL	2.3
1	D	288	TYR	2.3
2	E	63	PRO	2.3
1	A	380	THR	2.3
1	D	470	THR	2.3
2	E	205	ILE	2.3
1	D	75	PRO	2.3
1	A	570	TYR	2.3
1	D	338	ALA	2.3
1	A	476	ALA	2.3
1	D	345	LEU	2.3
1	D	242	VAL	2.3
1	A	276	THR	2.3
2	E	194	SER	2.3
2	B	57	LEU	2.2
1	D	572	SER	2.2
2	E	123	ALA	2.2
1	A	331	GLY	2.2
2	B	216	ASN	2.2
1	A	147	PHE	2.2
2	F	207	ALA	2.2
1	A	568	SER	2.2
1	A	106	GLY	2.2
2	C	8	LEU	2.2
2	F	199	LEU	2.2
1	D	469	SER	2.2
2	E	97	PHE	2.2
1	D	114	THR	2.2
1	D	14	ILE	2.2
1	A	204	CYS	2.2
1	A	242	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
2	E	207	ALA	2.1
1	D	32	LEU	2.1
1	D	237	VAL	2.1
1	D	500	ALA	2.1
1	D	273	LEU	2.1
1	D	429	LEU	2.1
2	C	118	GLY	2.1
1	A	514	THR	2.1
1	D	351	THR	2.1
2	E	195	VAL	2.1
1	D	241	ILE	2.1
1	A	202	LEU	2.1
1	D	553	PRO	2.1
1	A	423	CYS	2.1
1	A	522	VAL	2.1
2	E	64	VAL	2.1
1	A	156	SER	2.1
1	D	77	ILE	2.1
1	A	298	ALA	2.1
1	A	68	VAL	2.1
2	B	71	VAL	2.1
2	E	143	PRO	2.1
1	A	182	ILE	2.1
1	D	121	THR	2.1
1	A	142	GLY	2.1
1	D	226	GLY	2.1
1	D	335	GLY	2.1
2	E	11	TRP	2.1
1	A	17	PHE	2.1
1	D	271	PRO	2.1
1	D	567	VAL	2.0
2	E	144	TYR	2.0
1	D	64	MET	2.0
1	A	222	VAL	2.0
1	A	228	VAL	2.0

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

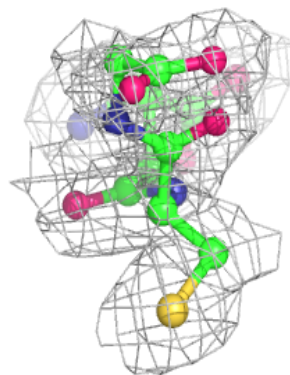
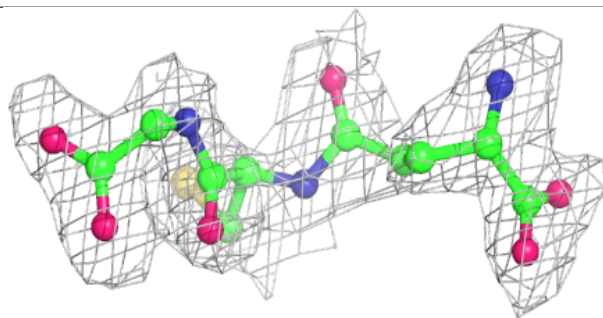
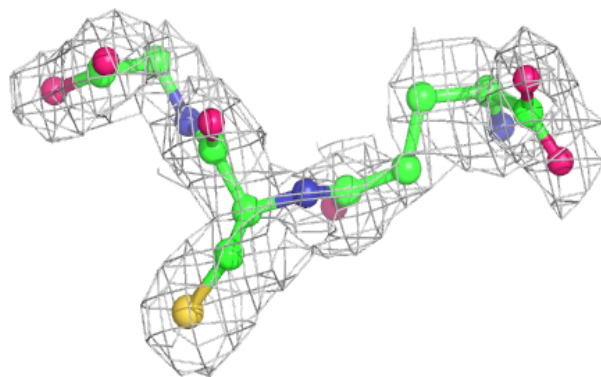
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	JAA	A	601	15/15	0.87	0.21	12,19,24,28	0
3	JAA	D	601	15/15	0.89	0.23	12,19,30,35	0
4	MET	D	602	9/9	0.90	0.19	14,20,29,39	0
6	GSH	F	301	20/20	0.90	0.19	9,16,23,25	0
6	GSH	E	301	20/20	0.92	0.15	6,13,21,22	0
5	ATP	D	603	31/31	0.92	0.18	13,20,30,32	0
4	MET	A	602	9/9	0.93	0.18	14,20,24,26	0
6	GSH	B	301	20/20	0.94	0.12	3,5,8,8	0
5	ATP	A	603	31/31	0.94	0.15	8,19,26,28	0
6	GSH	C	301	20/20	0.94	0.14	5,9,17,20	0

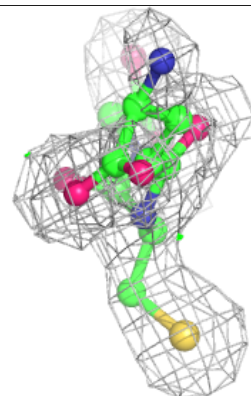
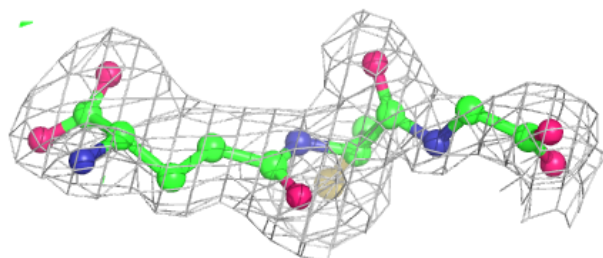
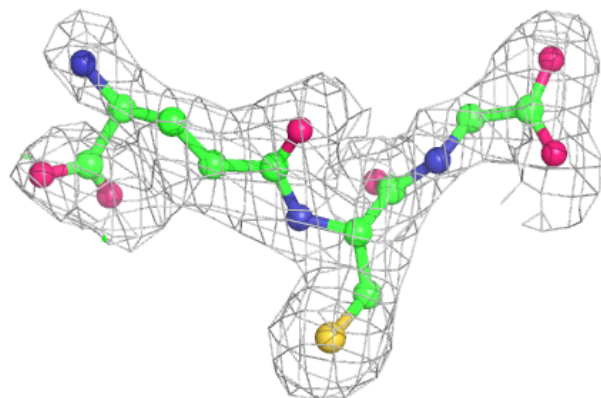
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

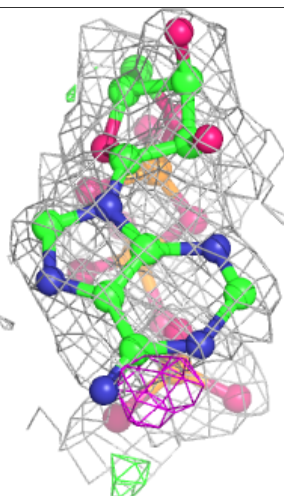
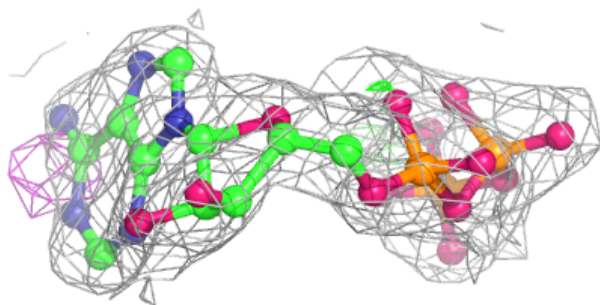
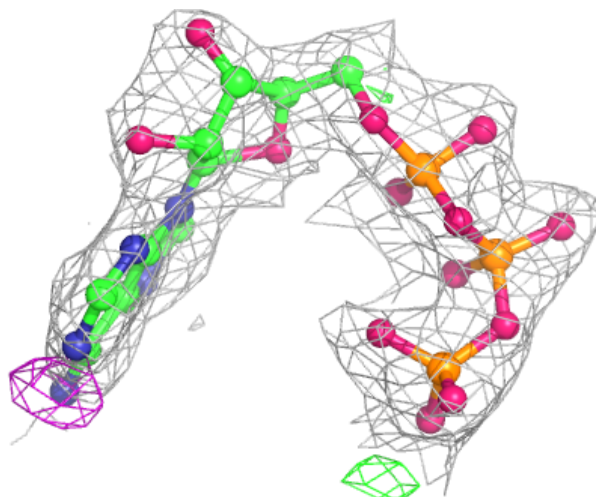
**Electron density around GSH E 301:**

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



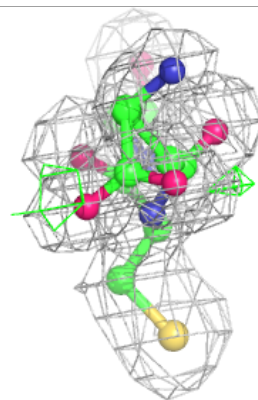
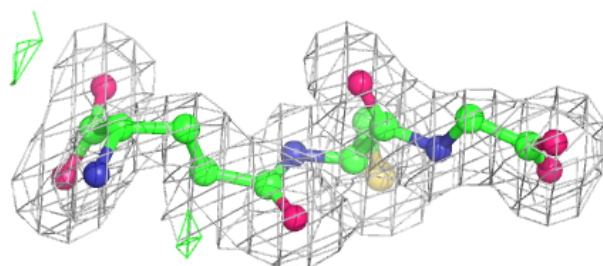
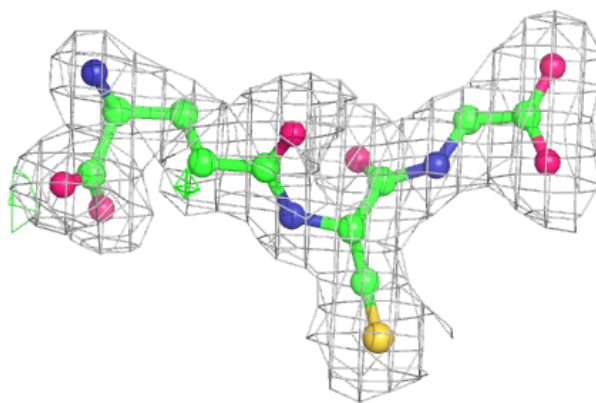
Electron density around ATP D 603:

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



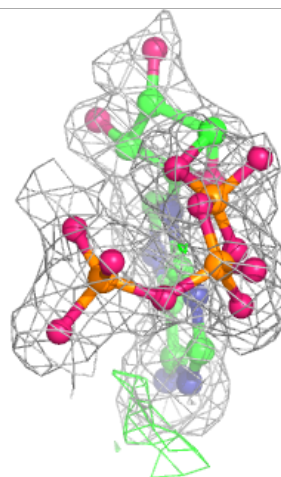
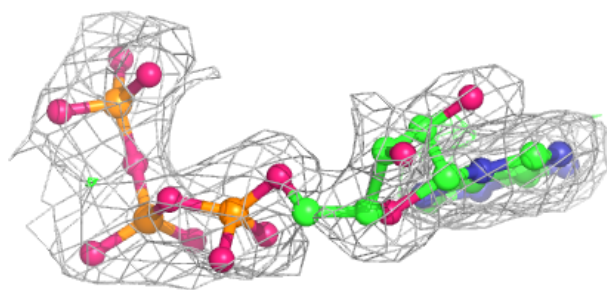
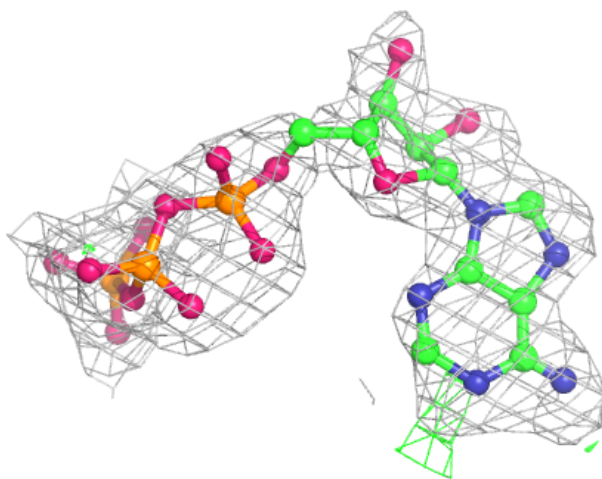
Electron density around GSH B 301:

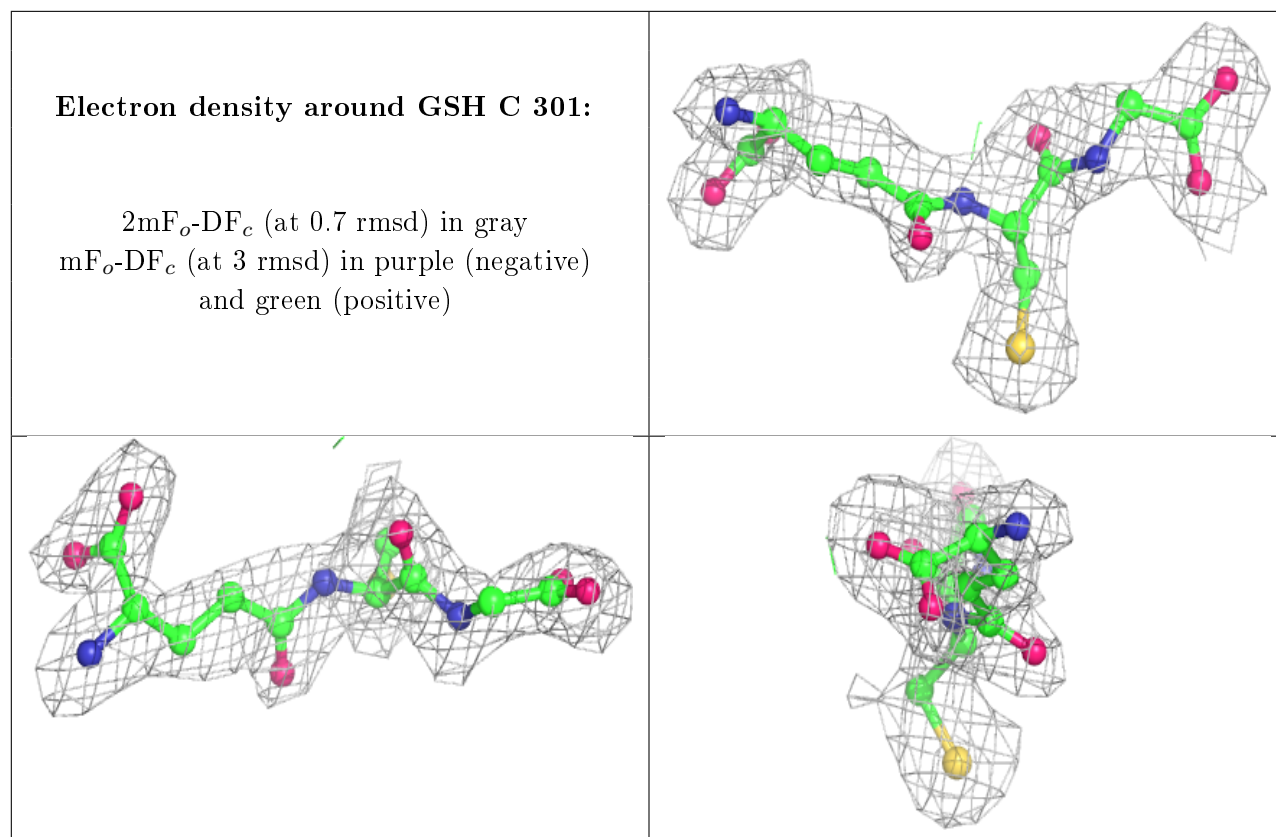
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around ATP A 603:

$2mF_o-DF_c$ (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.