



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 01:26 PM BST

PDB ID : 5ECH  
Title : Crystal Structure of FIN219-FIP1 complex with JA and ATP  
Authors : Chen, C.Y.; Cheng, Y.S.  
Deposited on : 2015-10-20  
Resolution : 2.14 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
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) : 2.13.1

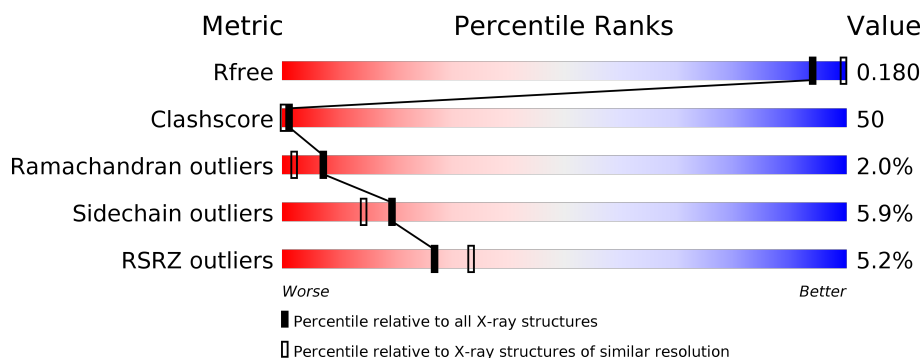
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.14 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	2523 (2.16-2.12)
Clashscore	141614	2653 (2.16-2.12)
Ramachandran outliers	138981	2618 (2.16-2.12)
Sidechain outliers	138945	2617 (2.16-2.12)
RSRZ outliers	127900	2485 (2.16-2.12)

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

Mol	Chain	Length	Quality of chain
1	A	575	<div> <div>7%</div> <div> <div></div> <div>35%</div> <div>58%</div> <div>6%</div> </div> </div>
1	D	575	<div> <div>6%</div> <div> <div></div> <div>30%</div> <div>61%</div> <div>8%</div> </div> </div>
2	B	223	<div> <div>4%</div> <div> <div></div> <div>37%</div> <div>54%</div> <div></div> </div> </div>
2	C	223	<div> <div>2%</div> <div> <div></div> <div>41%</div> <div>49%</div> <div>6%</div> </div> </div>
2	E	223	<div> <div>4%</div> <div> <div></div> <div>36%</div> <div>56%</div> <div></div> </div> </div>
2	F	223	<div> <div>3%</div> <div> <div></div> <div>39%</div> <div>52%</div> <div>5%</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
4	ATP	A	602	-	-	X	-
4	ATP	D	602	-	-	X	-

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 17375 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

There are 24 discrepancies between the modelled and reference sequences:

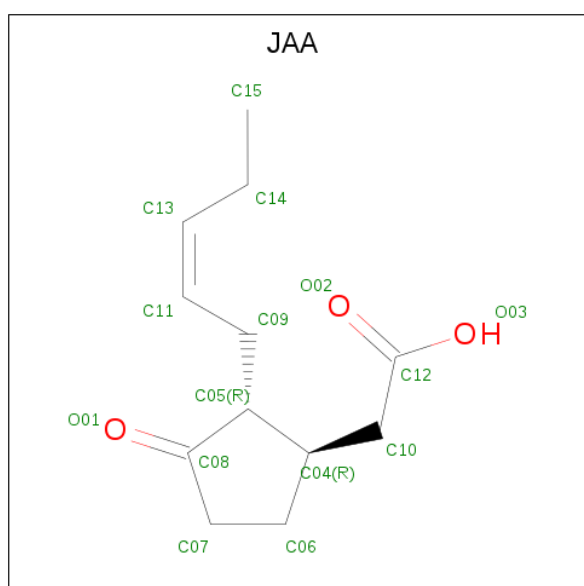
Chain	Residue	Modelled	Actual	Comment	Reference
B	-5	HIS	-	expression tag	UNP Q8L7C9
B	-4	HIS	-	expression tag	UNP Q8L7C9
B	-3	HIS	-	expression tag	UNP Q8L7C9
B	-2	HIS	-	expression tag	UNP Q8L7C9
B	-1	HIS	-	expression tag	UNP Q8L7C9
B	0	HIS	-	expression tag	UNP Q8L7C9
C	-5	HIS	-	expression tag	UNP Q8L7C9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

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

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



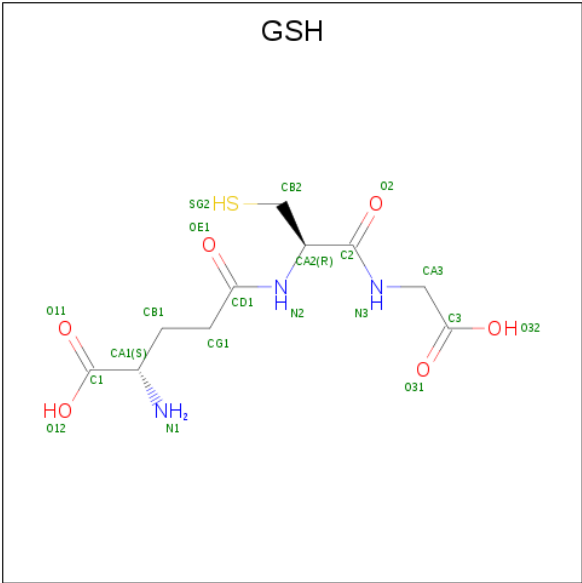
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			15	12	3		
3	D	1	Total	C	O	0	0
			15	12	3		

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>).



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

- Molecule 5 is GLUTATHIONE (three-letter code: GSH) (formula: C<sub>10</sub>H<sub>17</sub>N<sub>3</sub>O<sub>6</sub>S).



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

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

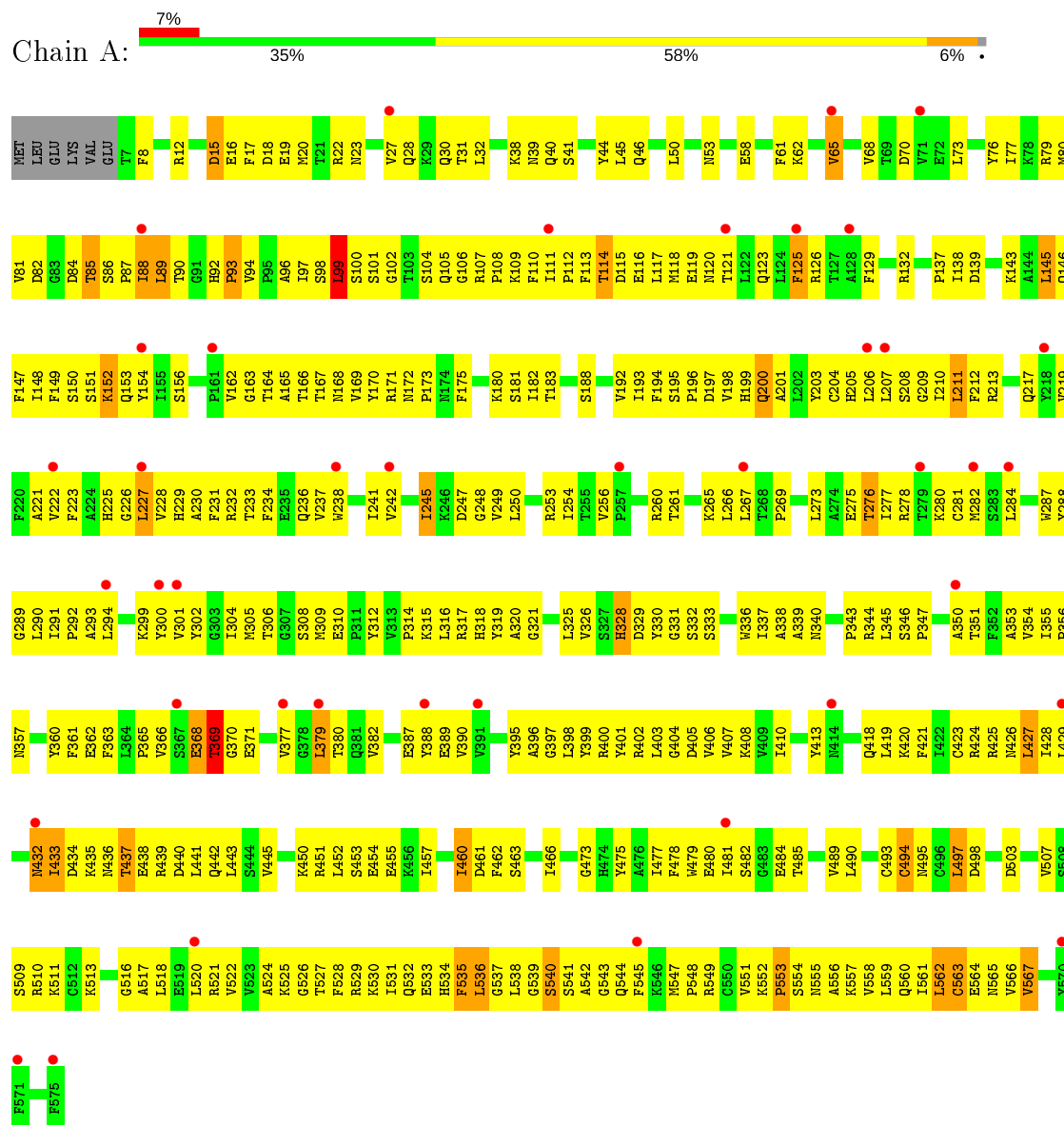
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	325	Total	O	0	0
			325	325		
6	B	142	Total	O	0	0
			142	142		
6	C	150	Total	O	0	0
			150	150		
6	D	362	Total	O	0	0
			362	362		
6	E	124	Total	O	0	0
			124	124		
6	F	150	Total	O	0	0
			150	150		

### 3 Residue-property plots

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

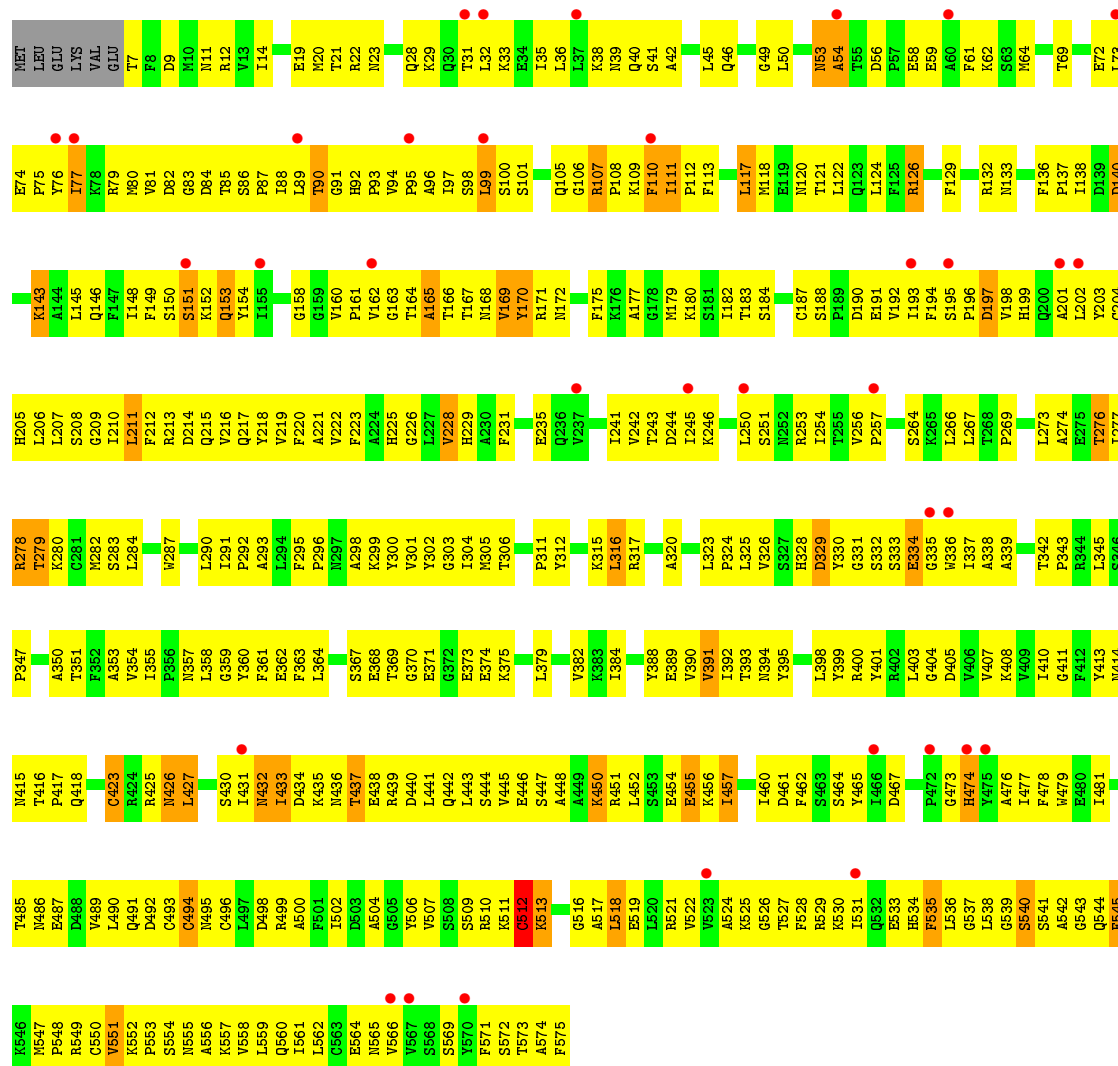
#### • Molecule 1: Jasmonic acid-amido synthetase JAR1



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







• Molecule 2: Glutathione S-transferase U20



• Molecule 2: Glutathione S-transferase U20



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	53.92Å 53.98Å 193.94Å 90.35° 90.00° 113.68°	Depositor
Resolution (Å)	25.27 – 2.14 25.27 – 2.14	Depositor EDS
% Data completeness (in resolution range)	98.6 (25.27-2.14) 98.6 (25.27-2.14)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.11 (at 2.13Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, $R_{free}$	0.160 , 0.180 0.160 , 0.180	Depositor DCC
$R_{free}$ test set	10846 reflections (9.96%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	-7.7	Xtriage
Anisotropy	-0.379	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 215.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.38$ , $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	0.096 for -h,-k,l 0.097 for k,h,-l 0.089 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	17375	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	5.0	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 37.15 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.4784e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

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

## 5 Model quality

### 5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.36	0/4581	0.67	4/6219 (0.1%)
1	D	0.37	0/4581	0.69	4/6219 (0.1%)
2	B	0.33	0/1799	0.54	0/2428
2	C	0.34	0/1799	0.54	0/2428
2	E	0.34	0/1799	0.56	0/2428
2	F	0.43	0/1799	0.63	0/2428
All	All	0.36	0/16358	0.63	8/22150 (0.0%)

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
1	D	0	2
2	B	0	1
All	All	0	4

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	107	ARG	NE-CZ-NH2	13.43	127.02	120.30
1	D	107	ARG	NE-CZ-NH1	-7.95	116.33	120.30
1	A	562	LEU	CA-CB-CG	7.39	132.31	115.30
1	A	278	ARG	CG-CD-NE	6.99	126.48	111.80
1	A	99	LEU	CA-CB-CG	6.25	129.68	115.30
1	A	278	ARG	CB-CG-CD	6.16	127.61	111.60
1	D	211	LEU	CA-CB-CG	6.12	129.37	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	99	LEU	CA-CB-CG	5.68	128.37	115.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	427	LEU	Peptide
2	B	173	PHE	Peptide
1	D	427	LEU	Peptide
1	D	432	ASN	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	481	2
1	D	4479	0	4434	580	2
2	B	1748	0	1704	158	1
2	C	1748	0	1704	165	0
2	E	1748	0	1704	177	1
2	F	1748	0	1704	141	1
3	A	15	0	0	0	0
3	D	15	0	0	3	0
4	A	31	0	10	17	0
4	D	31	0	10	15	0
5	B	20	0	15	2	0
5	C	20	0	15	0	0
5	E	20	0	15	0	0
5	F	20	0	15	1	0
6	A	325	0	0	49	1
6	B	142	0	0	14	1
6	C	150	0	0	25	0
6	D	362	0	0	61	0
6	E	124	0	0	27	1
6	F	150	0	0	23	1
All	All	17375	0	15764	1608	6

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 50.

All (1608) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:107:ARG:NH1	1:D:433:ILE:HG13	1.61	1.14
1:A:284:LEU:HD13	1:A:287:TRP:H	1.19	1.06
2:E:24:ARG:NH1	2:E:24:ARG:O	1.92	1.01
2:C:26:LYS:NZ	2:C:82:ASN:O	1.92	1.01
1:A:529:ARG:NH1	1:A:533:GLU:OE2	1.94	1.00
1:D:138:ILE:HA	1:D:217:GLN:HE21	1.25	1.00
1:A:438:GLU:OE2	6:A:701:HOH:O	1.81	0.97
1:D:121:THR:HG21	4:D:602:ATP:H1'	1.46	0.96
1:D:92:HIS:HE1	2:E:185:TRP:HD1	1.10	0.95
1:A:521:ARG:HH12	1:A:562:LEU:HD13	1.31	0.95
1:A:99:LEU:HB3	1:A:556:ALA:H	1.27	0.94
1:A:58:GLU:OE2	6:A:702:HOH:O	1.85	0.94
1:D:108:PRO:HB2	1:D:554:SER:HG	1.29	0.94
2:C:26:LYS:HG2	2:C:81:LYS:NZ	1.83	0.93
2:B:112:LYS:HZ3	2:B:120:GLU:C	1.72	0.92
2:B:112:LYS:NZ	2:B:120:GLU:O	2.01	0.91
2:C:29:GLU:OE2	6:C:401:HOH:O	1.90	0.90
1:D:467:ASP:HB3	1:D:474:HIS:CD2	2.08	0.89
1:D:199:HIS:H	1:D:524:ALA:HB1	1.36	0.89
1:A:231:PHE:HA	1:A:234:PHE:HB2	1.51	0.89
1:A:540:SER:OG	1:A:544:GLN:NE2	2.07	0.88
1:A:557:LYS:NZ	4:A:602:ATP:O3G	2.07	0.88
1:D:152:LYS:HB2	1:D:561:ILE:HA	1.55	0.88
1:D:243:THR:HA	1:D:246:LYS:HE2	1.55	0.88
2:C:201:ASP:OD2	1:D:456:LYS:NZ	2.06	0.87
1:D:39:ASN:HA	2:E:142:LYS:HD3	1.56	0.87
2:F:26:LYS:HG2	2:F:81:LYS:HZ3	1.40	0.87
2:E:145:PHE:HB3	2:E:153:VAL:HG13	1.57	0.86
1:A:44:TYR:HB2	1:A:89:LEU:HD22	1.57	0.85
1:A:199:HIS:HB3	1:A:525:LYS:H	1.41	0.85
1:D:190:ASP:OD2	6:D:702:HOH:O	1.95	0.85
2:E:33:ARG:NH2	6:E:406:HOH:O	2.10	0.85
2:C:178:GLU:OE2	6:C:402:HOH:O	1.94	0.85
2:B:40:LYS:NZ	2:B:52:LYS:O	2.11	0.84
1:A:152:LYS:HZ3	1:A:564:GLU:H	1.24	0.84
1:D:495:ASN:ND2	1:D:572:SER:OG	2.10	0.84
1:D:512:CYS:SG	1:D:513:LYS:N	2.48	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:35:ILE:HD11	1:D:359:GLY:HA2	1.60	0.83
2:B:122:GLU:HA	2:B:125:LYS:HG2	1.59	0.83
2:C:33:ARG:HH22	2:C:41:SER:HB2	1.43	0.83
1:A:107:ARG:HD3	1:A:433:ILE:HG23	1.60	0.82
2:E:116:LYS:O	2:E:213:ARG:NH1	2.12	0.82
2:C:188:ARG:NH1	1:D:499:ARG:O	2.12	0.82
1:D:92:HIS:NE2	2:E:139:LEU:HD22	1.94	0.82
2:F:136:GLU:OE2	2:F:180:PRO:HD2	1.78	0.82
1:A:114:THR:OG1	2:B:141:ASP:OD2	1.96	0.82
1:D:88:ILE:HD12	1:D:89:LEU:H	1.44	0.81
1:D:250:LEU:HD21	1:D:254:ILE:HB	1.60	0.81
2:F:188:ARG:NH1	6:F:404:HOH:O	2.10	0.81
1:A:306:THR:HG1	1:A:330:TYR:HH	1.21	0.80
1:A:152:LYS:NZ	1:A:564:GLU:H	1.77	0.80
1:D:198:VAL:HG12	1:D:524:ALA:HB3	1.64	0.80
2:F:26:LYS:NZ	2:F:82:ASN:O	2.15	0.80
1:D:143:LYS:HD2	1:D:212:PHE:HB2	1.61	0.80
1:D:107:ARG:NH1	1:D:434:ASP:N	2.29	0.80
1:A:354:VAL:HG11	1:A:361:PHE:HZ	1.46	0.80
2:B:116:LYS:O	2:B:213:ARG:NH1	2.14	0.80
2:E:21:VAL:HG23	2:E:194:SER:HB2	1.63	0.79
1:A:152:LYS:HZ3	1:A:564:GLU:N	1.79	0.79
2:F:8:LEU:HD22	2:F:33:ARG:HH21	1.46	0.79
1:D:219:VAL:HB	1:D:295:PHE:HZ	1.47	0.79
1:D:169:VAL:HG22	4:D:602:ATP:H2'	1.64	0.79
1:D:165:ALA:H	1:D:557:LYS:HE3	1.44	0.79
2:B:10:TYR:OH	2:B:212:TYR:OH	2.01	0.78
1:D:552:LYS:O	1:D:554:SER:N	2.15	0.78
1:D:164:THR:HA	1:D:557:LYS:HG3	1.66	0.78
1:A:98:SER:HB2	1:A:111:ILE:HB	1.63	0.78
1:D:540:SER:OG	1:D:544:GLN:NE2	2.17	0.78
1:D:226:GLY:N	6:D:707:HOH:O	2.16	0.78
2:E:5:PRO:HB2	2:E:57:LEU:HD11	1.65	0.78
1:D:107:ARG:HD3	1:D:433:ILE:H	1.48	0.78
1:D:12:ARG:NH2	6:D:712:HOH:O	2.17	0.78
1:A:163:GLY:HA3	1:A:168:ASN:HD21	1.49	0.77
1:A:223:PHE:CZ	1:A:536:LEU:HB2	2.18	0.77
1:D:529:ARG:NH1	1:D:533:GLU:OE1	2.17	0.77
1:D:541:SER:O	1:D:543:GLY:N	2.17	0.77
1:D:162:VAL:O	1:D:560:GLN:NE2	2.16	0.77
1:A:162:VAL:O	6:A:704:HOH:O	2.01	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:371:GLU:O	6:A:703:HOH:O	2.00	0.77
1:A:281:CYS:HB3	1:A:287:TRP:CH2	2.20	0.77
2:B:112:LYS:NZ	2:B:120:GLU:OE2	2.17	0.77
1:A:238:TRP:HA	1:A:241:ILE:HG23	1.66	0.77
1:A:200:GLN:NE2	1:A:204:CYS:SG	2.58	0.77
1:D:425:ARG:HB2	1:D:427:LEU:HD23	1.68	0.77
2:E:75:ASP:OD2	6:E:401:HOH:O	2.03	0.77
1:A:147:PHE:O	1:A:529:ARG:NH2	2.19	0.76
2:C:191:GLU:HA	1:D:450:LYS:HE2	1.66	0.76
1:A:221:ALA:HB1	1:A:529:ARG:HH12	1.48	0.76
2:E:190:MET:SD	6:E:468:HOH:O	2.42	0.76
2:B:23:LEU:HD11	2:B:57:LEU:HD11	1.67	0.76
1:D:531:ILE:HA	1:D:534:HIS:CE1	2.21	0.76
1:D:113:PHE:HD1	1:D:117:LEU:HD11	1.49	0.76
1:D:442:GLN:HG2	1:D:462:PHE:HZ	1.49	0.76
1:A:151:SER:HA	1:A:194:PHE:HA	1.67	0.76
1:D:87:PRO:HB2	2:E:143:PRO:HA	1.68	0.76
1:A:198:VAL:HG12	1:A:524:ALA:HB3	1.68	0.75
2:E:72:GLN:HE22	2:E:85:PHE:HZ	1.34	0.75
2:C:122:GLU:HA	2:C:125:LYS:HE2	1.69	0.75
2:F:208:TYR:OH	6:F:401:HOH:O	2.03	0.75
1:A:152:LYS:HD2	1:A:564:GLU:HB2	1.67	0.75
2:C:26:LYS:HG2	2:C:81:LYS:HZ1	1.49	0.75
1:D:132:ARG:HA	1:D:343:PRO:HG3	1.68	0.75
1:D:301:VAL:HG11	1:D:316:LEU:HD21	1.68	0.75
1:A:149:PHE:HB2	1:A:530:LYS:NZ	2.02	0.74
1:D:329:ASP:O	6:D:703:HOH:O	2.04	0.74
2:B:205:ILE:HA	2:B:208:TYR:CD2	2.23	0.74
1:A:284:LEU:HD13	1:A:287:TRP:N	2.01	0.74
1:D:107:ARG:NH1	1:D:433:ILE:C	2.40	0.74
2:E:98:TRP:CE2	2:E:153:VAL:HG12	2.22	0.74
1:A:354:VAL:HG11	1:A:361:PHE:CZ	2.22	0.74
1:A:379:LEU:HD23	1:A:380:THR:HG23	1.69	0.74
2:C:55:PRO:O	6:C:403:HOH:O	2.04	0.74
1:D:132:ARG:O	1:D:136:PHE:N	2.16	0.74
1:D:219:VAL:HB	1:D:295:PHE:CZ	2.22	0.74
1:A:366:VAL:O	6:A:703:HOH:O	2.04	0.74
6:C:449:HOH:O	1:D:496:CYS:SG	2.46	0.73
2:F:26:LYS:HG2	2:F:81:LYS:NZ	2.03	0.73
1:D:86:SER:HB2	2:E:188:ARG:HE	1.52	0.73
2:B:129:ILE:HD12	2:B:178:GLU:OE2	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:521:ARG:NH1	1:A:562:LEU:HD13	2.03	0.73
1:A:137:PRO:O	1:A:299:LYS:NZ	2.16	0.73
1:A:82:ASP:OD2	6:A:705:HOH:O	2.06	0.73
1:A:552:LYS:O	1:A:554:SER:N	2.20	0.73
2:E:24:ARG:HE	2:E:193:GLU:HB3	1.53	0.73
1:A:106:GLY:HA3	1:A:432:ASN:HB2	1.70	0.73
2:C:64:VAL:HG23	2:C:70:VAL:HG22	1.71	0.73
1:A:58:GLU:HA	1:A:61:PHE:CE2	2.24	0.73
1:A:41:SER:HA	2:B:148:ASP:HA	1.70	0.72
2:F:16:GLY:HA2	2:F:55:PRO:HB3	1.70	0.72
1:D:360:TYR:OH	1:D:362:GLU:OE2	2.02	0.72
1:D:92:HIS:CE1	2:E:185:TRP:HD1	2.00	0.72
1:A:193:ILE:HG12	1:A:205:HIS:HE1	1.54	0.72
2:E:136:GLU:HA	2:E:139:LEU:HD21	1.70	0.72
2:F:68:LEU:HA	2:F:71:VAL:HG12	1.70	0.72
1:A:362:GLU:HG3	1:A:400:ARG:HH22	1.54	0.72
2:C:70:VAL:HA	2:C:73:TYR:CD2	2.25	0.72
2:F:40:LYS:HD2	2:F:52:LYS:HB3	1.72	0.72
1:D:41:SER:OG	6:D:701:HOH:O	1.86	0.72
1:D:42:ALA:HA	2:E:143:PRO:HG3	1.72	0.72
1:A:551:VAL:HG11	1:A:559:LEU:HD13	1.72	0.72
2:E:89:PRO:HB3	2:F:76:GLU:HG3	1.71	0.72
2:E:201:ASP:O	6:E:404:HOH:O	2.08	0.71
2:F:127:GLU:O	6:F:403:HOH:O	2.08	0.71
2:B:193:GLU:HA	2:B:196:SER:HB3	1.70	0.71
2:E:73:TYR:OH	6:E:403:HOH:O	2.07	0.71
1:A:331:GLY:N	1:A:537:GLY:O	2.23	0.71
1:A:90:THR:O	2:B:143:PRO:HD3	1.89	0.71
1:D:198:VAL:HA	1:D:201:ALA:HB3	1.70	0.71
2:F:151:GLY:N	2:F:154:ASP:OD2	2.23	0.71
1:A:339:ALA:N	1:A:353:ALA:O	2.20	0.71
1:A:557:LYS:HG2	4:A:602:ATP:O1G	1.90	0.71
2:E:53:LYS:O	6:E:405:HOH:O	2.09	0.71
1:D:87:PRO:HD2	2:E:188:ARG:HB2	1.73	0.71
1:A:96:ALA:O	1:A:113:PHE:N	2.23	0.71
1:A:534:HIS:ND1	6:A:726:HOH:O	2.24	0.71
1:D:353:ALA:HB2	1:D:413:TYR:CD2	2.26	0.71
2:B:104:LYS:NZ	6:B:409:HOH:O	2.24	0.70
2:C:188:ARG:HH12	1:D:500:ALA:HA	1.56	0.70
1:D:164:THR:OG1	1:D:557:LYS:O	2.08	0.70
1:D:462:PHE:O	1:D:549:ARG:NH1	2.24	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:291:ILE:HG13	1:A:292:PRO:HD3	1.73	0.70
1:A:108:PRO:O	6:A:708:HOH:O	2.10	0.70
1:A:116:GLU:OE1	6:A:707:HOH:O	2.09	0.70
1:A:208:SER:HA	1:A:211:LEU:HD23	1.72	0.70
2:B:212:TYR:O	6:B:402:HOH:O	2.09	0.70
1:D:107:ARG:HH21	1:D:552:LYS:HB3	1.55	0.70
1:D:92:HIS:HE1	2:E:185:TRP:CD1	2.01	0.70
1:D:170:TYR:OH	1:D:171:ARG:NH2	2.25	0.70
1:D:99:LEU:HB2	1:D:556:ALA:H	1.56	0.70
2:E:175:ILE:HB	2:E:183:ILE:HD11	1.73	0.70
1:A:200:GLN:OE1	6:A:706:HOH:O	2.09	0.70
1:A:210:ILE:HD11	1:A:234:PHE:HE2	1.55	0.70
1:D:329:ASP:HB3	1:D:339:ALA:HA	1.73	0.70
1:D:535:PHE:O	1:D:538:LEU:HB2	1.92	0.70
1:A:97:ILE:HD11	1:A:162:VAL:HG22	1.74	0.70
1:A:100:SER:HA	1:A:535:PHE:CZ	2.27	0.69
2:E:182:LEU:HA	2:E:185:TRP:CD1	2.27	0.69
1:D:107:ARG:HH12	1:D:433:ILE:HG13	1.56	0.69
1:D:447:SER:OG	6:D:704:HOH:O	2.10	0.69
1:A:238:TRP:HB2	1:A:241:ILE:HG12	1.74	0.69
1:A:261:THR:HG22	1:A:265:LYS:HE3	1.74	0.69
2:B:110:GLN:OE1	2:B:167:TYR:OH	2.07	0.69
2:E:169:LYS:NZ	2:E:206:VAL:HG11	2.08	0.69
2:E:98:TRP:CZ2	2:E:153:VAL:HG12	2.28	0.69
1:D:92:HIS:HE2	2:E:139:LEU:HD22	1.57	0.69
2:C:26:LYS:HG2	2:C:81:LYS:HZ3	1.53	0.69
2:E:88:ASP:O	6:E:407:HOH:O	2.11	0.69
2:C:96:ARG:NH1	6:C:413:HOH:O	2.25	0.69
1:A:121:THR:HG21	4:A:602:ATP:H1'	1.75	0.69
1:D:107:ARG:HH11	1:D:433:ILE:H	1.41	0.69
2:F:144:TYR:HA	2:F:185:TRP:HE1	1.57	0.69
1:A:229:HIS:HA	1:A:232:ARG:HE	1.58	0.68
1:A:27:VAL:O	1:A:31:THR:OG1	2.09	0.68
1:A:46:GLN:HB2	2:B:148:ASP:HB3	1.74	0.68
1:D:389:GLU:OE2	1:D:404:GLY:HA2	1.92	0.68
2:B:69:ASN:HA	2:B:72:GLN:HE21	1.58	0.68
1:D:152:LYS:HD3	1:D:561:ILE:HG22	1.74	0.68
1:A:363:PHE:HD2	1:A:382:VAL:HG11	1.57	0.68
1:A:451:ARG:NH1	1:A:454:GLU:OE1	2.27	0.68
2:C:139:LEU:O	2:C:141:ASP:N	2.24	0.68
1:A:329:ASP:OD1	1:A:340:ASN:N	2.20	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:353:ALA:HB2	1:A:413:TYR:CD2	2.29	0.68
1:A:84:ASP:O	1:A:86:SER:N	2.26	0.68
1:D:46:GLN:OE1	6:D:706:HOH:O	2.10	0.68
2:E:40:LYS:HZ1	2:E:52:LYS:HB2	1.58	0.68
2:B:26:LYS:NZ	2:B:78:TRP:O	2.23	0.68
1:D:45:LEU:HB3	1:D:50:LEU:HB2	1.74	0.68
2:E:145:PHE:CB	2:E:153:VAL:HG13	2.23	0.68
2:C:151:GLY:N	2:C:154:ASP:OD2	2.25	0.68
3:D:601:JAA:O03	4:D:602:ATP:N6	2.27	0.68
1:A:556:ALA:HA	1:A:559:LEU:HB2	1.75	0.68
2:C:144:TYR:HA	2:C:185:TRP:HE1	1.59	0.68
1:D:199:HIS:HB3	1:D:525:LYS:H	1.58	0.68
2:F:11:TRP:CD1	2:F:12:PRO:HD3	2.28	0.68
1:A:332:SER:OG	1:A:333:SER:N	2.26	0.67
1:D:569:SER:O	6:D:705:HOH:O	2.10	0.67
1:A:126:ARG:HA	1:A:182:ILE:HG21	1.76	0.67
1:D:280:LYS:O	6:D:709:HOH:O	2.12	0.67
1:D:22:ARG:HA	1:D:415:ASN:HB2	1.75	0.67
1:D:521:ARG:HB3	1:D:566:VAL:HG12	1.75	0.67
1:A:513:LYS:NZ	6:A:709:HOH:O	2.12	0.67
1:D:19:GLU:O	1:D:23:ASN:ND2	2.22	0.67
1:A:304:ILE:HG22	1:A:330:TYR:HE1	1.60	0.67
2:E:69:ASN:ND2	2:F:93:ALA:O	2.20	0.67
1:A:167:THR:OG1	1:A:560:GLN:OE1	2.12	0.67
6:D:701:HOH:O	2:E:144:TYR:N	2.25	0.67
1:A:38:LYS:HB3	2:B:140:GLY:HA3	1.75	0.67
1:A:39:ASN:HA	2:B:142:LYS:HG3	1.77	0.67
2:B:9:ASP:OD2	2:B:20:ARG:NE	2.27	0.67
2:E:142:LYS:O	6:E:408:HOH:O	2.11	0.67
1:A:210:ILE:HD11	1:A:234:PHE:CE2	2.29	0.67
1:A:162:VAL:HG11	1:A:559:LEU:HD23	1.76	0.67
1:A:165:ALA:HA	4:A:602:ATP:O5'	1.95	0.67
1:D:183:THR:O	6:D:708:HOH:O	2.12	0.67
1:D:64:MET:SD	6:D:838:HOH:O	2.52	0.67
2:E:8:LEU:HA	2:E:33:ARG:HG2	1.74	0.67
2:F:181:LYS:HA	2:F:184:ALA:HB3	1.77	0.67
1:D:80:MET:SD	6:D:859:HOH:O	2.53	0.67
1:A:241:ILE:O	1:A:245:ILE:HG13	1.95	0.66
1:A:302:TYR:CZ	1:A:328:HIS:HB2	2.29	0.66
1:A:340:ASN:ND2	6:A:716:HOH:O	2.18	0.66
1:D:31:THR:HG21	1:D:357:ASN:HA	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:LEU:HA	1:A:76:TYR:HE2	1.60	0.66
2:C:114:TRP:HA	2:C:170:PHE:HD2	1.59	0.66
2:E:145:PHE:HB3	2:E:153:VAL:CG1	2.24	0.66
1:D:330:TYR:OH	6:D:710:HOH:O	2.12	0.66
1:D:477:ILE:HG23	1:D:518:LEU:HD11	1.77	0.66
1:A:154:TYR:O	6:A:704:HOH:O	2.13	0.66
2:C:183:ILE:HD11	1:D:451:ARG:HE	1.61	0.66
2:F:66:GLU:OE1	6:F:405:HOH:O	2.11	0.66
1:A:219:VAL:HG22	1:A:227:LEU:HD11	1.78	0.66
1:D:113:PHE:CD1	1:D:117:LEU:HD11	2.30	0.66
2:F:84:PHE:O	6:F:406:HOH:O	2.13	0.66
1:D:465:TYR:HB2	1:D:551:VAL:HG13	1.78	0.66
1:D:280:LYS:HE2	1:D:293:ALA:HB1	1.76	0.66
1:A:250:LEU:HB2	1:A:254:ILE:HD13	1.76	0.66
1:D:473:GLY:O	1:D:516:GLY:N	2.20	0.66
1:D:74:GLU:OE1	6:D:711:HOH:O	2.12	0.66
2:E:15:PHE:HB3	2:E:67:SER:HB3	1.78	0.66
1:D:7:THR:OG1	6:D:712:HOH:O	2.13	0.66
1:A:241:ILE:HG13	1:A:242:VAL:N	2.09	0.66
2:B:125:LYS:HE2	2:B:171:GLY:HA2	1.78	0.66
2:B:25:GLU:OE1	6:B:404:HOH:O	2.12	0.66
2:E:11:TRP:CD1	2:E:12:PRO:HD3	2.31	0.66
1:A:316:LEU:O	1:A:320:ALA:N	2.29	0.65
1:A:304:ILE:HG23	1:A:328:HIS:CE1	2.30	0.65
2:B:176:GLU:OE1	6:B:405:HOH:O	2.14	0.65
1:D:100:SER:HB3	1:D:109:LYS:HD3	1.78	0.65
1:D:143:LYS:HD2	1:D:212:PHE:CB	2.25	0.65
1:D:445:VAL:HG22	1:D:479:TRP:HE1	1.60	0.65
2:E:96:ARG:NH1	6:F:405:HOH:O	2.19	0.65
1:D:506:TYR:OH	1:D:510:ARG:NH2	2.30	0.65
1:A:368:GLU:HG3	1:A:369:THR:HG22	1.77	0.65
1:D:332:SER:HB2	1:D:538:LEU:HA	1.79	0.65
1:D:535:PHE:HA	1:D:538:LEU:HD13	1.78	0.65
2:B:8:LEU:HA	2:B:33:ARG:HB2	1.78	0.65
1:A:73:LEU:HA	1:A:76:TYR:CE2	2.32	0.65
1:D:490:LEU:HD22	1:D:522:VAL:HG21	1.79	0.65
1:D:331:GLY:N	1:D:537:GLY:O	2.30	0.65
1:A:287:TRP:HE3	1:A:290:LEU:HD13	1.62	0.65
1:D:331:GLY:HA3	1:D:336:TRP:CG	2.31	0.65
1:A:118:MET:HA	4:A:602:ATP:O3'	1.97	0.65
1:D:529:ARG:HG3	1:D:529:ARG:HH11	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:GLN:OE1	6:A:710:HOH:O	2.15	0.64
1:A:226:GLY:HA3	1:A:529:ARG:HH11	1.62	0.64
2:B:211:GLU:OE2	2:B:214:LYS:HD2	1.97	0.64
1:D:162:VAL:HG21	1:D:559:LEU:HD23	1.78	0.64
2:E:145:PHE:N	2:E:154:ASP:OD2	2.31	0.64
2:F:188:ARG:NH2	6:F:413:HOH:O	2.29	0.64
2:B:216:ASN:OD1	6:B:402:HOH:O	2.15	0.64
2:E:146:GLY:H	2:E:151:GLY:HA3	1.61	0.64
1:A:387:GLU:HG2	1:A:408:LYS:HB2	1.80	0.64
2:B:175:ILE:HG23	2:B:183:ILE:HD11	1.78	0.64
1:D:197:ASP:OD1	1:D:197:ASP:N	2.30	0.64
1:A:132:ARG:NH1	6:A:724:HOH:O	2.29	0.64
2:B:8:LEU:HD13	2:B:44:LEU:HD22	1.80	0.64
2:C:33:ARG:NH1	2:C:41:SER:OG	2.24	0.64
1:D:363:PHE:HD2	1:D:382:VAL:HG21	1.62	0.64
1:D:84:ASP:OD1	6:D:713:HOH:O	2.15	0.64
1:D:88:ILE:HD12	1:D:89:LEU:N	2.12	0.64
2:C:132:VAL:HG22	2:C:182:LEU:HD22	1.77	0.64
1:A:41:SER:HB2	2:B:142:LYS:HG2	1.78	0.64
1:A:53:ASN:ND2	6:A:744:HOH:O	2.31	0.64
2:B:125:LYS:O	2:B:129:ILE:HG12	1.98	0.64
1:D:168:ASN:ND2	4:D:602:ATP:O1A	2.23	0.64
1:A:281:CYS:HB3	1:A:287:TRP:HH2	1.61	0.64
1:A:87:PRO:O	2:B:188:ARG:NH1	2.30	0.64
1:D:405:ASP:OD2	1:D:541:SER:N	2.30	0.64
1:A:164:THR:OG1	1:A:557:LYS:O	2.14	0.64
1:A:168:ASN:ND2	4:A:602:ATP:O1A	2.31	0.64
2:B:6:ILE:HG22	2:B:31:GLU:HB3	1.79	0.64
1:D:107:ARG:HH12	1:D:433:ILE:C	2.01	0.64
2:E:24:ARG:HH21	2:E:193:GLU:HB2	1.62	0.64
1:A:156:SER:HB2	1:A:162:VAL:HG23	1.79	0.63
1:D:225:HIS:HB3	1:D:312:TYR:CG	2.33	0.63
2:E:182:LEU:HG	2:E:185:TRP:HE1	1.63	0.63
1:A:152:LYS:HG3	1:A:560:GLN:O	1.97	0.63
1:D:110:PHE:CE1	1:D:556:ALA:HB2	2.33	0.63
2:F:57:LEU:O	2:F:64:VAL:HG22	1.98	0.63
2:F:60:ASN:O	6:F:407:HOH:O	2.15	0.63
1:D:97:ILE:HG13	1:D:162:VAL:HB	1.81	0.63
2:B:121:GLN:NE2	2:B:170:PHE:O	2.31	0.63
2:B:8:LEU:HD11	2:B:56:VAL:HG12	1.81	0.63
1:D:317:ARG:HA	1:D:320:ALA:HB3	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:187:LYS:HD3	1:D:492:ASP:HB3	1.81	0.63
1:D:76:TYR:O	1:D:88:ILE:HG21	1.98	0.63
2:F:21:VAL:HG12	2:F:155:ILE:HG12	1.80	0.63
1:D:73:LEU:HD11	1:D:109:LYS:HG3	1.81	0.63
2:E:187:LYS:O	6:E:410:HOH:O	2.16	0.63
1:A:164:THR:O	1:A:168:ASN:ND2	2.32	0.63
2:C:58:VAL:N	6:C:422:HOH:O	2.32	0.63
1:D:531:ILE:HD13	1:D:534:HIS:HE1	1.64	0.63
1:D:434:ASP:HB2	1:D:550:CYS:HB3	1.80	0.63
1:D:110:PHE:CE2	1:D:554:SER:HA	2.34	0.63
2:C:11:TRP:CD1	2:C:12:PRO:HD3	2.34	0.63
1:A:99:LEU:HD21	1:A:558:VAL:HG23	1.80	0.63
1:D:77:ILE:HD12	1:D:112:PRO:HD3	1.81	0.63
2:C:180:PRO:HG3	1:D:574:ALA:HA	1.81	0.63
2:E:20:ARG:NH2	6:E:409:HOH:O	2.13	0.62
2:F:17:MET:HE2	2:F:200:PRO:HD2	1.79	0.62
2:C:4:LEU:N	6:C:421:HOH:O	2.31	0.62
1:A:435:LYS:HZ2	1:A:549:ARG:HH12	1.47	0.62
2:E:24:ARG:NH2	6:E:422:HOH:O	2.32	0.62
1:D:9:ASP:OD2	6:D:712:HOH:O	2.16	0.62
2:E:82:ASN:ND2	6:E:423:HOH:O	2.33	0.62
2:C:188:ARG:NH2	6:C:423:HOH:O	2.32	0.62
1:A:226:GLY:HA2	1:A:529:ARG:HD2	1.82	0.62
1:A:559:LEU:O	1:A:562:LEU:HG	1.99	0.62
2:F:84:PHE:CD1	2:F:152:TYR:HB2	2.34	0.62
2:B:151:GLY:N	6:B:406:HOH:O	2.32	0.62
2:B:18:ARG:HH21	2:B:160:PHE:HE1	1.47	0.62
2:C:80:GLU:O	6:C:404:HOH:O	2.16	0.62
1:A:169:VAL:HG22	4:A:602:ATP:O2'	2.00	0.62
1:D:145:LEU:HD13	1:D:209:GLY:HA3	1.81	0.62
2:C:183:ILE:HG12	1:D:492:ASP:CG	2.20	0.62
1:D:92:HIS:CD2	2:E:139:LEU:HD22	2.34	0.62
2:F:168:GLU:HG2	2:F:175:ILE:HG23	1.82	0.62
2:F:98:TRP:CD1	2:F:153:VAL:HG11	2.34	0.62
2:B:101:PHE:CE2	2:B:135:LEU:HG	2.35	0.62
1:D:107:ARG:HH11	1:D:434:ASP:N	1.96	0.62
1:D:107:ARG:NH2	1:D:552:LYS:HB3	2.15	0.62
1:D:117:LEU:O	1:D:121:THR:HG23	2.00	0.62
2:B:112:LYS:NZ	2:B:120:GLU:C	2.46	0.62
2:C:136:GLU:HG3	2:C:181:LYS:HD3	1.81	0.62
1:D:217:GLN:HE22	1:D:299:LYS:HD3	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:266:LEU:HD12	1:D:267:LEU:HG	1.81	0.62
1:D:36:LEU:O	1:D:40:GLN:N	2.32	0.62
1:D:177:ALA:HA	1:D:180:LYS:HE3	1.82	0.61
1:A:344:ARG:NH2	6:A:748:HOH:O	2.32	0.61
1:D:95:PRO:HG3	2:E:181:LYS:NZ	2.15	0.61
2:C:23:LEU:HD11	2:C:57:LEU:HD13	1.82	0.61
2:C:184:ALA:HB1	1:D:499:ARG:NE	2.14	0.61
1:D:199:HIS:O	6:D:714:HOH:O	2.15	0.61
1:A:441:LEU:HD23	1:A:549:ARG:HG2	1.81	0.61
1:A:435:LYS:HZ2	1:A:549:ARG:NH1	1.98	0.61
1:A:96:ALA:HB1	1:A:163:GLY:HA3	1.82	0.61
1:D:150:SER:HB3	1:D:167:THR:HA	1.82	0.61
2:B:8:LEU:HD11	2:B:44:LEU:HD13	1.81	0.61
1:A:531:ILE:HA	1:A:534:HIS:CE1	2.36	0.61
2:C:188:ARG:NH1	1:D:500:ALA:HA	2.14	0.61
1:D:111:ILE:HD12	1:D:334:GLU:HG2	1.82	0.61
1:D:118:MET:SD	4:D:602:ATP:O3'	2.56	0.61
1:D:331:GLY:HA3	1:D:336:TRP:CD1	2.36	0.61
1:D:107:ARG:HH21	1:D:552:LYS:CB	2.13	0.61
1:D:86:SER:HB2	2:E:188:ARG:NE	2.15	0.61
1:D:92:HIS:CD2	2:E:142:LYS:H	2.19	0.61
1:A:94:VAL:HG11	1:A:112:PRO:HB2	1.82	0.61
2:B:149:SER:O	6:B:406:HOH:O	2.16	0.61
1:D:168:ASN:HB2	4:D:602:ATP:H5'2	1.82	0.61
1:D:407:VAL:HB	1:D:541:SER:HB2	1.82	0.60
1:D:331:GLY:HA3	1:D:336:TRP:HA	1.82	0.60
1:D:345:LEU:HD13	1:D:350:ALA:HA	1.82	0.60
1:D:445:VAL:HG21	1:D:462:PHE:CG	2.36	0.60
2:F:35:GLU:O	6:F:408:HOH:O	2.15	0.60
1:D:108:PRO:HG2	1:D:552:LYS:H	1.66	0.60
1:D:306:THR:OG1	1:D:330:TYR:OH	2.17	0.60
1:D:487:GLU:OE2	6:D:715:HOH:O	2.16	0.60
2:C:184:ALA:O	1:D:499:ARG:NH2	2.34	0.60
1:A:233:THR:HA	1:A:236:GLN:HB2	1.82	0.60
1:D:338:ALA:HA	1:D:354:VAL:HA	1.84	0.60
2:F:165:GLN:HG3	2:F:206:VAL:HG21	1.84	0.60
2:F:195:VAL:HG23	2:F:199:LEU:HD13	1.82	0.60
1:A:284:LEU:HD22	1:A:287:TRP:HA	1.82	0.60
2:C:176:GLU:OE2	1:D:491:GLN:HG2	2.01	0.60
1:D:29:LYS:O	1:D:32:LEU:HG	2.02	0.60
2:F:75:ASP:HB2	2:F:84:PHE:CE2	2.37	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:421:PHE:CD2	1:A:541:SER:HA	2.37	0.60
1:D:451:ARG:NH1	1:D:454:GLU:OE2	2.34	0.60
2:C:6:ILE:N	6:C:422:HOH:O	2.34	0.60
1:D:96:ALA:O	1:D:113:PHE:HB3	2.02	0.60
1:D:199:HIS:HA	1:D:525:LYS:HB2	1.84	0.60
1:A:198:VAL:HA	1:A:201:ALA:HB3	1.83	0.59
1:A:363:PHE:N	6:A:722:HOH:O	2.23	0.59
2:C:187:LYS:HE3	1:D:493:CYS:HA	1.81	0.59
1:D:560:GLN:N	6:D:742:HOH:O	2.35	0.59
2:F:139:LEU:HB3	2:F:181:LYS:HE2	1.83	0.59
1:A:149:PHE:HB2	1:A:530:LYS:HZ1	1.66	0.59
1:D:208:SER:HA	1:D:211:LEU:HG	1.84	0.59
1:D:22:ARG:HG2	1:D:414:ASN:HB3	1.84	0.59
1:D:231:PHE:O	1:D:235:GLU:HG3	2.03	0.59
1:D:510:ARG:HH21	1:D:518:LEU:HB2	1.67	0.59
2:F:132:VAL:HG23	2:F:182:LEU:HD13	1.83	0.59
1:A:101:SER:HA	1:A:548:PRO:HD3	1.84	0.59
1:A:230:ALA:O	1:A:234:PHE:N	2.29	0.59
1:A:40:GLN:HG2	2:B:142:LYS:HD3	1.84	0.59
1:D:291:ILE:HG13	1:D:292:PRO:HD3	1.83	0.59
1:D:332:SER:OG	1:D:333:SER:N	2.34	0.59
1:D:95:PRO:HG3	2:E:181:LYS:HZ1	1.66	0.59
1:A:150:SER:HA	1:A:167:THR:HG22	1.83	0.59
1:A:377:VAL:N	6:A:722:HOH:O	2.36	0.59
1:A:387:GLU:OE2	6:A:711:HOH:O	2.17	0.59
1:A:454:GLU:OE1	6:A:713:HOH:O	2.17	0.59
1:D:73:LEU:HD21	1:D:109:LYS:NZ	2.17	0.59
1:A:353:ALA:HB2	1:A:413:TYR:HD2	1.66	0.59
1:D:465:TYR:HD1	1:D:551:VAL:HG22	1.67	0.59
2:E:191:GLU:O	6:E:411:HOH:O	2.17	0.59
2:F:215:ASN:O	6:F:409:HOH:O	2.17	0.59
1:A:166:THR:HA	1:A:169:VAL:HG23	1.83	0.59
6:D:701:HOH:O	2:E:142:LYS:HD2	2.02	0.59
2:F:64:VAL:HB	2:F:73:TYR:CE2	2.37	0.59
1:A:250:LEU:HD13	1:A:254:ILE:HB	1.84	0.59
1:A:541:SER:O	1:A:543:GLY:N	2.36	0.59
1:D:81:VAL:HG21	1:D:110:PHE:CE2	2.38	0.59
2:F:10:TYR:HH	2:F:208:TYR:HH	1.50	0.59
1:A:70:ASP:HB3	1:A:109:LYS:HD2	1.85	0.58
1:D:226:GLY:HA2	1:D:229:HIS:HD1	1.67	0.58
1:D:46:GLN:OE1	2:E:149:SER:OG	2.21	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:LEU:HG	1:A:557:LYS:HG3	1.84	0.58
1:A:99:LEU:HB2	1:A:555:ASN:OD1	2.03	0.58
2:B:48:ASN:HD21	2:C:97:PHE:HZ	1.50	0.58
1:D:439:ARG:O	1:D:443:LEU:HB2	2.02	0.58
1:D:98:SER:OG	1:D:99:LEU:N	2.36	0.58
2:E:125:LYS:HE2	2:E:171:GLY:HA2	1.86	0.58
1:A:304:ILE:HG13	1:A:309:MET:HG2	1.84	0.58
2:B:51:HIS:HB3	2:B:53:LYS:HG3	1.83	0.58
1:D:191:GLU:HA	1:D:194:PHE:HB2	1.85	0.58
1:D:195:SER:HB3	1:D:201:ALA:HB2	1.86	0.58
1:D:426:ASN:N	1:D:426:ASN:OD1	2.33	0.58
1:D:457:ILE:HD13	1:D:481:ILE:HB	1.85	0.58
1:A:247:ASP:HB2	1:A:249:VAL:HG12	1.84	0.58
2:C:191:GLU:OE1	1:D:447:SER:OG	2.22	0.58
2:C:54:ILE:HB	2:C:55:PRO:HA	1.85	0.58
1:D:143:LYS:HD3	1:D:187:CYS:HB3	1.85	0.58
1:D:496:CYS:HA	1:D:499:ARG:CZ	2.34	0.58
1:A:46:GLN:O	6:A:712:HOH:O	2.17	0.58
2:B:154:ASP:OD2	6:B:406:HOH:O	2.17	0.58
1:D:274:ALA:O	1:D:277:ILE:HG13	2.03	0.58
1:D:336:TRP:HB3	1:D:358:LEU:HD22	1.85	0.58
4:D:602:ATP:N6	6:D:761:HOH:O	2.37	0.58
2:C:64:VAL:HB	2:C:73:TYR:CE2	2.39	0.58
1:D:219:VAL:HG13	1:D:301:VAL:HG13	1.84	0.58
1:D:536:LEU:HB2	1:D:545:PHE:CE1	2.39	0.58
2:F:181:LYS:O	2:F:185:TRP:N	2.34	0.58
1:A:86:SER:HB2	2:B:188:ARG:HB2	1.86	0.58
2:C:98:TRP:CD1	2:C:153:VAL:HG11	2.38	0.58
2:E:68:LEU:O	6:E:412:HOH:O	2.17	0.58
1:A:117:LEU:O	1:A:121:THR:HG23	2.04	0.58
1:A:165:ALA:HB1	4:A:602:ATP:C4	2.39	0.58
2:B:96:ARG:NH1	2:C:76:GLU:OE2	2.37	0.58
1:D:282:MET:O	6:D:716:HOH:O	2.17	0.58
2:E:166:ALA:HB2	2:E:206:VAL:HG22	1.85	0.58
2:F:139:LEU:O	2:F:141:ASP:N	2.36	0.58
2:B:10:TYR:HD2	2:B:13:SER:HB2	1.68	0.58
1:D:342:THR:O	1:D:345:LEU:HG	2.03	0.58
2:E:13:SER:O	6:E:409:HOH:O	2.17	0.58
2:F:165:GLN:HG3	2:F:206:VAL:CG2	2.34	0.58
1:A:110:PHE:CE1	1:A:556:ALA:HB2	2.38	0.57
1:D:441:LEU:HD23	1:D:549:ARG:HB3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:510:ARG:HD2	1:A:517:ALA:HA	1.86	0.57
1:A:99:LEU:HA	1:A:109:LYS:O	2.04	0.57
1:D:329:ASP:N	1:D:329:ASP:OD1	2.37	0.57
1:A:117:LEU:HD11	1:A:396:ALA:HB2	1.86	0.57
2:B:90:TYR:O	2:B:93:ALA:HB3	2.04	0.57
2:C:57:LEU:HB3	2:C:64:VAL:HG22	1.85	0.57
2:F:24:ARG:HB3	2:F:194:SER:HA	1.86	0.57
1:A:199:HIS:H	1:A:524:ALA:HB1	1.68	0.57
1:D:408:LYS:HZ2	1:D:410:ILE:HG22	1.69	0.57
1:D:152:LYS:HA	1:D:564:GLU:HB2	1.87	0.57
2:C:201:ASP:OD2	1:D:456:LYS:HG3	2.03	0.57
1:D:170:TYR:HA	1:D:175:PHE:CD2	2.39	0.57
1:A:19:GLU:OE1	6:A:715:HOH:O	2.18	0.57
1:A:94:VAL:HB	1:A:113:PHE:O	2.04	0.57
2:B:145:PHE:N	2:B:154:ASP:OD2	2.37	0.57
1:D:213:ARG:NH1	1:D:214:ASP:OD1	2.37	0.57
1:D:21:THR:HB	1:D:416:THR:HB	1.85	0.57
2:E:204:LYS:HB2	6:E:404:HOH:O	2.04	0.57
2:F:5:PRO:HB3	2:F:57:LEU:HD11	1.86	0.57
1:A:98:SER:N	1:A:111:ILE:O	2.38	0.57
1:A:172:ASN:ND2	6:A:755:HOH:O	2.36	0.57
1:A:77:ILE:HD12	1:A:112:PRO:HD3	1.85	0.57
1:D:167:THR:HG21	1:D:561:ILE:HG23	1.87	0.57
1:D:193:ILE:HG12	1:D:205:HIS:CE1	2.40	0.57
1:A:231:PHE:CE2	1:A:291:ILE:HG22	2.39	0.57
1:A:477:ILE:HD12	1:A:497:LEU:HD13	1.86	0.57
1:D:222:VAL:O	1:D:304:ILE:N	2.29	0.57
1:A:152:LYS:CD	1:A:564:GLU:H	2.18	0.57
2:C:114:TRP:HA	2:C:170:PHE:CD2	2.38	0.57
1:D:11:ASN:OD1	6:D:718:HOH:O	2.18	0.57
1:D:22:ARG:HH11	1:D:414:ASN:CG	2.07	0.57
1:D:231:PHE:HB3	1:D:290:LEU:HD23	1.85	0.57
1:D:521:ARG:HH11	1:D:562:LEU:CD1	2.17	0.57
1:D:526:GLY:HA2	1:D:529:ARG:HB3	1.86	0.57
1:A:116:GLU:OE1	1:A:395:TYR:HB3	2.05	0.56
1:A:23:ASN:O	1:A:27:VAL:HG12	2.05	0.56
1:A:479:TRP:CZ2	1:A:497:LEU:HD11	2.40	0.56
1:A:480:GLU:HG3	1:A:525:LYS:HA	1.87	0.56
1:A:560:GLN:NE2	6:A:757:HOH:O	2.38	0.56
2:B:105:LYS:HA	2:B:108:ASP:OD1	2.04	0.56
1:D:179:MET:O	1:D:183:THR:OG1	2.18	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:204:CYS:HA	1:D:207:LEU:HG	1.86	0.56
1:A:86:SER:HB2	2:B:188:ARG:NE	2.20	0.56
1:D:223:PHE:CE1	1:D:304:ILE:HD12	2.39	0.56
2:C:181:LYS:N	6:C:428:HOH:O	2.37	0.56
1:D:384:ILE:HD11	1:D:411:GLY:HA2	1.88	0.56
1:D:153:GLN:HA	1:D:560:GLN:HG3	1.88	0.56
2:F:163:TRP:HB3	2:F:167:TYR:CZ	2.40	0.56
1:A:102:GLY:HA3	1:A:426:ASN:HD21	1.71	0.56
2:B:205:ILE:HD12	2:B:208:TYR:CE2	2.40	0.56
1:D:99:LEU:HB2	1:D:557:LYS:H	1.69	0.56
2:F:125:LYS:HA	2:F:128:PHE:CE2	2.39	0.56
4:A:602:ATP:O2B	6:A:714:HOH:O	2.17	0.56
2:C:163:TRP:HB3	2:C:167:TYR:CZ	2.41	0.56
2:C:17:MET:SD	2:C:199:LEU:HG	2.44	0.56
1:D:534:HIS:CE1	1:D:557:LYS:HG2	2.40	0.56
1:A:17:PHE:HE1	1:A:355:ILE:HG12	1.69	0.56
1:A:535:PHE:O	1:A:538:LEU:HB3	2.04	0.56
1:A:555:ASN:ND2	6:A:740:HOH:O	2.29	0.56
1:D:334:GLU:OE2	1:D:538:LEU:HD21	2.05	0.56
1:D:58:GLU:HA	1:D:61:PHE:CE2	2.40	0.56
1:D:98:SER:CB	1:D:111:ILE:HG13	2.36	0.56
2:E:8:LEU:HD11	2:E:44:LEU:HD13	1.87	0.56
2:F:64:VAL:HB	2:F:73:TYR:CD2	2.41	0.56
1:A:149:PHE:HB2	1:A:530:LYS:HZ2	1.67	0.56
1:A:445:VAL:HG22	1:A:479:TRP:HE1	1.69	0.56
2:C:153:VAL:HA	2:C:156:SER:OG	2.06	0.56
1:D:363:PHE:HB3	1:D:388:TYR:HB3	1.87	0.56
2:E:40:LYS:NZ	2:E:52:LYS:HB2	2.21	0.56
2:F:23:LEU:HD22	2:F:28:VAL:HG11	1.86	0.56
2:F:114:TRP:HA	2:F:170:PHE:HD2	1.70	0.56
1:A:151:SER:OG	1:A:195:SER:O	2.23	0.56
1:A:31:THR:OG1	1:A:357:ASN:HA	2.06	0.56
1:D:474:HIS:H	1:D:474:HIS:HD2	1.52	0.56
1:A:92:HIS:CD2	2:B:142:LYS:O	2.59	0.56
2:B:121:GLN:HG2	2:B:125:LYS:HE3	1.88	0.56
2:B:12:PRO:HB3	2:B:208:TYR:CD2	2.41	0.56
1:D:242:VAL:HG11	1:D:277:ILE:HD13	1.87	0.56
1:D:291:ILE:HG12	1:D:320:ALA:HA	1.87	0.56
1:D:476:ALA:HB2	1:D:519:GLU:OE2	2.06	0.56
2:E:98:TRP:HH2	2:E:152:TYR:CG	2.24	0.56
2:F:135:LEU:HD13	2:F:182:LEU:HD11	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:LEU:HD13	1:A:209:GLY:HA3	1.88	0.55
1:A:39:ASN:HD21	1:A:90:THR:HA	1.71	0.55
1:A:41:SER:HB2	2:B:143:PRO:HD2	1.88	0.55
1:A:87:PRO:HD2	2:B:188:ARG:HB2	1.87	0.55
2:C:144:TYR:HB3	2:C:154:ASP:OD2	2.05	0.55
1:A:210:ILE:HG12	1:A:294:LEU:HD11	1.87	0.55
1:A:229:HIS:HA	1:A:232:ARG:NE	2.21	0.55
1:A:439:ARG:O	1:A:443:LEU:HB2	2.06	0.55
2:C:117:LYS:HA	2:C:121:GLN:HB2	1.89	0.55
2:C:33:ARG:NH2	2:C:35:GLU:OE1	2.40	0.55
1:D:194:PHE:O	6:D:717:HOH:O	2.17	0.55
1:D:199:HIS:N	1:D:524:ALA:HB1	2.13	0.55
1:D:526:GLY:O	1:D:530:LYS:HG3	2.06	0.55
1:D:521:ARG:HH11	1:D:562:LEU:HD13	1.71	0.55
1:D:85:THR:O	2:E:184:ALA:HB1	2.06	0.55
2:F:139:LEU:HG	2:F:145:PHE:CZ	2.41	0.55
1:A:227:LEU:HD23	1:A:316:LEU:HD11	1.88	0.55
1:A:61:PHE:CE1	1:A:62:LYS:HG3	2.41	0.55
2:C:21:VAL:HG12	2:C:155:ILE:HG12	1.88	0.55
2:C:26:LYS:HE2	2:C:75:ASP:HA	1.88	0.55
1:A:221:ALA:HB1	1:A:529:ARG:NH1	2.20	0.55
2:C:10:TYR:HB3	2:C:13:SER:HB2	1.88	0.55
1:D:101:SER:HB3	1:D:535:PHE:CE2	2.40	0.55
1:D:122:LEU:O	1:D:126:ARG:HB2	2.07	0.55
1:A:18:ASP:OD2	6:A:717:HOH:O	2.18	0.55
1:D:295:PHE:HD2	1:D:298:ALA:HB2	1.71	0.55
2:E:145:PHE:HB2	2:E:154:ASP:OD2	2.07	0.55
2:C:187:LYS:HG2	1:D:451:ARG:HD3	1.89	0.55
2:E:158:ILE:HA	2:E:185:TRP:HZ3	1.72	0.55
1:A:151:SER:HB3	1:A:565:ASN:HD21	1.71	0.55
2:C:169:LYS:NZ	2:C:206:VAL:HG11	2.22	0.55
2:C:73:TYR:HA	2:C:76:GLU:OE2	2.07	0.55
1:D:437:THR:O	1:D:440:ASP:N	2.40	0.55
1:D:461:ASP:HB3	1:D:528:PHE:CD2	2.41	0.55
2:C:184:ALA:HB1	1:D:499:ARG:CZ	2.37	0.55
1:A:188:SER:HB3	1:A:192:VAL:HG13	1.88	0.55
1:A:73:LEU:HD12	1:A:109:LYS:NZ	2.21	0.55
1:D:572:SER:HB3	1:D:575:PHE:CE2	2.42	0.55
2:B:169:LYS:HG3	2:B:170:PHE:H	1.71	0.55
2:B:7:LEU:HD23	2:B:57:LEU:HG	1.88	0.55
2:C:16:GLY:HA2	2:C:55:PRO:HB3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:403:LEU:HD23	1:D:540:SER:HB3	1.89	0.55
1:A:92:HIS:CD2	2:B:139:LEU:HD13	2.42	0.55
2:C:110:GLN:HA	2:C:113:VAL:HG12	1.89	0.55
1:D:165:ALA:N	4:D:602:ATP:O2G	2.40	0.55
1:D:535:PHE:HB3	1:D:544:GLN:O	2.07	0.55
1:D:98:SER:HB3	1:D:111:ILE:HG13	1.89	0.54
2:C:216:ASN:ND2	6:C:431:HOH:O	2.40	0.54
2:E:142:LYS:HE3	2:E:145:PHE:HA	1.89	0.54
1:A:147:PHE:HE1	1:A:206:LEU:HD12	1.72	0.54
2:B:24:ARG:NH1	2:B:30:PHE:HZ	2.05	0.54
2:C:70:VAL:HA	2:C:73:TYR:HD2	1.68	0.54
1:D:398:LEU:HA	1:D:401:TYR:CD1	2.41	0.54
1:A:153:GLN:HA	1:A:560:GLN:HG3	1.90	0.54
1:A:106:GLY:CA	1:A:432:ASN:HB2	2.37	0.54
1:A:93:PRO:HG2	2:B:184:ALA:HB3	1.88	0.54
1:D:235:GLU:HG2	1:D:287:TRP:CD2	2.42	0.54
1:A:314:PRO:HA	1:A:317:ARG:HG2	1.89	0.54
1:A:331:GLY:HA3	1:A:336:TRP:CE3	2.43	0.54
2:E:60:ASN:ND2	6:E:420:HOH:O	2.30	0.54
2:F:100:ASP:OD1	6:F:411:HOH:O	2.18	0.54
1:A:138:ILE:HA	1:A:217:GLN:HE21	1.73	0.54
1:A:288:TYR:CZ	1:A:321:GLY:HA2	2.43	0.54
1:D:73:LEU:HD23	1:D:401:TYR:CE2	2.42	0.54
2:F:108:ASP:O	2:F:112:LYS:HG2	2.07	0.54
2:B:169:LYS:HG3	2:B:170:PHE:N	2.23	0.54
2:C:70:VAL:O	2:C:73:TYR:HB2	2.08	0.54
2:C:80:GLU:OE2	6:C:407:HOH:O	2.19	0.54
1:D:353:ALA:HB2	1:D:413:TYR:HD2	1.72	0.54
2:F:98:TRP:HZ3	2:F:101:PHE:HD2	1.56	0.54
1:A:112:PRO:HG2	1:A:397:GLY:HA3	1.90	0.54
1:A:338:ALA:HA	1:A:354:VAL:HA	1.89	0.54
1:A:363:PHE:HB3	1:A:388:TYR:HB3	1.90	0.54
1:A:534:HIS:CD2	1:A:557:LYS:HE2	2.43	0.54
2:B:186:ALA:O	2:B:190:MET:N	2.40	0.54
2:B:204:LYS:HG3	2:B:208:TYR:CE1	2.43	0.54
1:D:138:ILE:HA	1:D:217:GLN:NE2	2.09	0.54
1:D:572:SER:HB3	1:D:575:PHE:HE2	1.72	0.54
1:D:87:PRO:CB	2:E:143:PRO:HA	2.36	0.54
1:A:105:GLN:NE2	6:A:758:HOH:O	2.38	0.54
1:A:325:LEU:HD23	1:A:347:PRO:HG2	1.89	0.54
1:D:164:THR:HB	1:D:167:THR:HG23	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:LEU:HD12	1:A:109:LYS:HZ1	1.73	0.54
1:A:87:PRO:HB3	1:A:92:HIS:HA	1.89	0.54
2:C:141:ASP:OD1	6:C:406:HOH:O	2.18	0.54
1:D:98:SER:OG	1:D:111:ILE:HG13	2.08	0.54
1:D:187:CYS:SG	6:D:813:HOH:O	2.59	0.54
1:D:222:VAL:HB	1:D:533:GLU:HB2	1.90	0.54
1:D:196:PRO:HG2	1:D:256:VAL:HG11	1.90	0.54
1:D:221:ALA:HB1	1:D:529:ARG:HH22	1.73	0.54
1:A:562:LEU:HD12	1:A:563:CYS:N	2.23	0.53
2:B:26:LYS:HA	2:B:81:LYS:NZ	2.23	0.53
1:D:154:TYR:HB3	1:D:560:GLN:HA	1.89	0.53
1:D:332:SER:HA	4:D:602:ATP:C6	2.43	0.53
1:D:39:ASN:O	6:D:719:HOH:O	2.18	0.53
2:E:88:ASP:OD2	2:E:91:GLY:HA3	2.07	0.53
1:A:123:GLN:HA	1:A:126:ARG:HB3	1.91	0.53
1:A:365:PRO:HA	1:A:388:TYR:CD1	2.42	0.53
1:A:85:THR:O	2:B:184:ALA:HB1	2.08	0.53
2:B:10:TYR:CZ	2:B:12:PRO:HG2	2.42	0.53
1:D:534:HIS:CG	1:D:557:LYS:HE2	2.43	0.53
1:D:98:SER:N	1:D:111:ILE:O	2.41	0.53
2:E:6:ILE:HB	2:E:58:VAL:HG13	1.89	0.53
1:D:316:LEU:O	1:D:320:ALA:N	2.38	0.53
1:D:437:THR:OG1	1:D:440:ASP:HB2	2.09	0.53
1:D:45:LEU:O	1:D:49:GLY:N	2.38	0.53
1:A:489:VAL:HG11	6:A:713:HOH:O	2.08	0.53
2:B:65:CYS:HB2	2:C:97:PHE:CE1	2.44	0.53
1:D:474:HIS:CD2	1:D:474:HIS:H	2.26	0.53
1:D:507:VAL:O	1:D:511:LYS:HB2	2.08	0.53
1:D:80:MET:HG3	1:D:88:ILE:HG12	1.90	0.53
1:D:117:LEU:HA	1:D:120:ASN:OD1	2.09	0.53
1:A:171:ARG:HG2	1:A:194:PHE:CE1	2.43	0.53
1:A:437:THR:OG1	1:A:440:ASP:HB2	2.09	0.53
2:C:201:ASP:OD2	2:C:204:LYS:HE2	2.09	0.53
1:D:493:CYS:SG	6:D:723:HOH:O	2.33	0.53
2:F:190:MET:O	2:F:196:SER:HB2	2.08	0.53
2:F:170:PHE:CD2	2:F:213:ARG:HD2	2.43	0.53
1:A:76:TYR:O	1:A:79:ARG:HB2	2.09	0.53
1:D:107:ARG:CZ	1:D:433:ILE:HG13	2.32	0.53
2:C:182:LEU:HD23	6:C:428:HOH:O	2.08	0.53
1:D:169:VAL:HA	4:D:602:ATP:O3'	2.09	0.53
1:D:206:LEU:O	1:D:210:ILE:HG12	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:253:ARG:NH2	6:D:772:HOH:O	2.41	0.53
1:D:77:ILE:O	1:D:80:MET:HB2	2.09	0.53
1:A:203:TYR:HD2	6:A:706:HOH:O	1.91	0.53
1:A:163:GLY:HA2	1:A:560:GLN:CD	2.29	0.53
2:B:109:ALA:O	2:B:113:VAL:HG23	2.09	0.53
2:B:71:VAL:HG21	2:B:155:ILE:HG21	1.90	0.53
2:E:93:ALA:HA	2:F:73:TYR:CE1	2.44	0.53
1:A:403:LEU:HD12	1:A:404:GLY:N	2.24	0.53
1:A:552:LYS:HE3	1:A:553:PRO:HD2	1.91	0.53
1:A:92:HIS:CD2	2:B:139:LEU:HB2	2.44	0.53
2:B:35:GLU:OE2	2:B:40:LYS:HA	2.09	0.53
2:C:108:ASP:O	2:C:112:LYS:HG2	2.08	0.53
2:C:180:PRO:CG	1:D:574:ALA:HA	2.38	0.53
6:D:701:HOH:O	2:E:142:LYS:HB3	2.08	0.53
2:B:112:LYS:HZ1	2:B:120:GLU:HB3	1.74	0.52
2:C:128:PHE:O	2:C:132:VAL:HB	2.07	0.52
2:C:75:ASP:HB2	2:C:84:PHE:CE2	2.44	0.52
1:D:113:PHE:HB2	4:D:602:ATP:PB	2.49	0.52
1:D:498:ASP:HB3	1:D:510:ARG:NH1	2.24	0.52
1:A:205:HIS:HA	1:A:208:SER:HB2	1.91	0.52
1:A:308:SER:OG	1:A:536:LEU:HD11	2.09	0.52
2:B:104:LYS:NZ	6:B:403:HOH:O	2.10	0.52
2:C:98:TRP:HE3	2:C:101:PHE:HB2	1.75	0.52
2:E:87:SER:N	6:E:418:HOH:O	2.29	0.52
2:E:95:ALA:HA	2:E:98:TRP:NE1	2.24	0.52
2:F:5:PRO:HG3	2:F:59:HIS:CE1	2.44	0.52
1:A:473:GLY:O	1:A:516:GLY:N	2.42	0.52
1:A:494:CYS:SG	1:A:495:ASN:N	2.82	0.52
1:D:197:ASP:O	1:D:201:ALA:N	2.43	0.52
2:F:114:TRP:CD1	2:F:167:TYR:HE1	2.27	0.52
1:A:455:GLU:HB2	6:A:871:HOH:O	2.10	0.52
2:B:154:ASP:OD1	2:B:185:TRP:NE1	2.41	0.52
2:B:5:PRO:HB2	2:B:57:LEU:HD22	1.92	0.52
2:E:182:LEU:HG	2:E:185:TRP:NE1	2.24	0.52
1:A:163:GLY:CA	1:A:168:ASN:HD21	2.21	0.52
1:A:99:LEU:H	1:A:557:LYS:HG3	1.74	0.52
1:D:325:LEU:N	6:D:771:HOH:O	2.40	0.52
1:D:334:GLU:O	1:D:392:ILE:HG21	2.10	0.52
1:A:150:SER:CB	1:A:167:THR:HA	2.39	0.52
1:A:201:ALA:O	1:A:205:HIS:N	2.43	0.52
2:B:15:PHE:HB3	2:B:67:SER:HB3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:452:LEU:HD23	1:D:481:ILE:HG21	1.91	0.52
2:E:176:GLU:HB2	2:E:183:ILE:HD12	1.92	0.52
2:E:95:ALA:HA	2:E:98:TRP:CE2	2.45	0.52
2:F:167:TYR:OH	6:F:402:HOH:O	2.04	0.52
2:F:128:PHE:CE1	2:F:175:ILE:HG22	2.45	0.52
1:A:117:LEU:N	6:A:707:HOH:O	2.27	0.52
1:D:101:SER:HB3	1:D:535:PHE:CD2	2.45	0.52
1:D:212:PHE:O	1:D:216:VAL:HG23	2.10	0.52
1:D:478:PHE:HE1	1:D:521:ARG:HD2	1.74	0.52
1:D:107:ARG:HE	1:D:108:PRO:HD2	1.75	0.52
1:D:140:ASP:N	1:D:140:ASP:OD1	2.27	0.52
1:D:246:LYS:O	1:D:269:PRO:HA	2.09	0.52
1:D:73:LEU:HB3	1:D:401:TYR:OH	2.10	0.52
1:D:440:ASP:OD2	6:D:720:HOH:O	2.18	0.52
2:E:161:SER:HA	2:E:164:PHE:CG	2.45	0.52
2:B:12:PRO:HB3	2:B:208:TYR:CE2	2.45	0.52
2:E:121:GLN:O	2:E:125:LYS:HG3	2.10	0.52
2:E:148:ASP:N	2:E:148:ASP:OD1	2.42	0.52
2:B:98:TRP:CE2	2:B:138:GLU:HG2	2.44	0.52
1:D:474:HIS:CD2	1:D:474:HIS:N	2.77	0.52
1:D:223:PHE:CZ	1:D:533:GLU:HA	2.44	0.52
1:D:92:HIS:H	2:E:142:LYS:N	2.08	0.52
1:D:46:GLN:HA	2:E:148:ASP:OD2	2.09	0.52
2:E:77:ALA:HB3	6:E:428:HOH:O	2.09	0.52
2:F:136:GLU:HG3	2:F:181:LYS:HD3	1.91	0.52
1:A:346:SER:N	6:A:770:HOH:O	2.43	0.51
2:C:24:ARG:HG3	2:C:30:PHE:CZ	2.45	0.51
1:D:81:VAL:HG21	1:D:110:PHE:CD2	2.45	0.51
1:D:223:PHE:CZ	1:D:536:LEU:HB3	2.45	0.51
1:D:494:CYS:SG	1:D:495:ASN:N	2.82	0.51
1:D:552:LYS:HZ3	1:D:554:SER:HG	1.54	0.51
2:F:150:PHE:CD1	2:F:192:LYS:HG3	2.45	0.51
2:F:54:ILE:HB	2:F:55:PRO:HA	1.92	0.51
1:A:291:ILE:HG13	1:A:292:PRO:CD	2.39	0.51
1:A:333:SER:OG	4:A:602:ATP:O3G	2.27	0.51
2:B:110:GLN:HB2	2:B:167:TYR:CZ	2.45	0.51
1:D:38:LYS:HD2	1:D:395:TYR:HE1	1.75	0.51
1:D:460:ILE:O	6:D:722:HOH:O	2.19	0.51
2:E:129:ILE:HA	2:E:132:VAL:HG12	1.92	0.51
2:E:7:LEU:HG	2:E:9:ASP:OD2	2.11	0.51
1:D:53:ASN:HB2	2:E:90:TYR:CE1	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:18:ARG:HH12	2:B:103:ASP:CG	2.14	0.51
1:D:223:PHE:HE1	1:D:304:ILE:HD12	1.75	0.51
2:E:98:TRP:HH2	2:E:152:TYR:CD2	2.29	0.51
1:A:180:LYS:O	6:A:718:HOH:O	2.19	0.51
1:A:98:SER:H	1:A:111:ILE:H	1.57	0.51
1:D:331:GLY:CA	1:D:336:TRP:HA	2.40	0.51
1:D:83:GLY:H	1:D:158:GLY:HA3	1.74	0.51
2:F:129:ILE:HA	2:F:132:VAL:HG12	1.92	0.51
1:D:361:PHE:HE1	1:D:379:LEU:HD22	1.75	0.51
2:F:102:VAL:O	2:F:107:THR:HG23	2.11	0.51
1:A:108:PRO:HG2	1:A:552:LYS:H	1.75	0.51
1:A:222:VAL:HG12	1:A:223:PHE:CD1	2.46	0.51
1:A:121:THR:CG2	4:A:602:ATP:H1'	2.40	0.51
2:C:68:LEU:O	2:C:72:GLN:HG3	2.10	0.51
1:D:143:LYS:O	1:D:216:VAL:HA	2.10	0.51
1:D:153:GLN:OE1	1:D:560:GLN:NE2	2.43	0.51
2:F:24:ARG:HG3	2:F:30:PHE:CZ	2.46	0.51
1:A:150:SER:HB2	1:A:167:THR:HA	1.93	0.51
2:B:136:GLU:HA	2:B:139:LEU:HD21	1.92	0.51
2:C:170:PHE:CD2	2:C:213:ARG:HD2	2.46	0.51
2:C:68:LEU:HA	2:C:71:VAL:HG12	1.92	0.51
1:D:333:SER:C	1:D:335:GLY:H	2.14	0.51
2:E:158:ILE:HA	2:E:185:TRP:CZ3	2.45	0.51
2:F:7:LEU:HD21	2:F:23:LEU:HD12	1.91	0.51
1:D:180:LYS:O	6:D:725:HOH:O	2.19	0.51
1:D:213:ARG:HG3	1:D:214:ASP:N	2.26	0.51
2:F:70:VAL:HA	2:F:73:TYR:CD2	2.45	0.51
1:A:362:GLU:HG3	1:A:400:ARG:NH2	2.25	0.51
1:D:150:SER:HB2	1:D:170:TYR:CZ	2.46	0.51
1:D:448:ALA:O	6:D:723:HOH:O	2.19	0.51
1:D:529:ARG:HG3	1:D:529:ARG:NH1	2.25	0.51
2:F:10:TYR:O	2:F:20:ARG:NH2	2.37	0.51
2:C:188:ARG:HD2	2:C:191:GLU:OE2	2.10	0.51
1:D:188:SER:HB3	1:D:192:VAL:HG13	1.93	0.51
1:D:77:ILE:HA	1:D:88:ILE:HG12	1.93	0.51
2:E:33:ARG:CZ	2:E:43:LEU:HD21	2.41	0.51
2:E:90:TYR:O	2:E:93:ALA:HB3	2.11	0.51
2:F:159:THR:HA	2:F:199:LEU:HD21	1.93	0.51
1:A:236:GLN:O	6:A:719:HOH:O	2.19	0.50
1:A:92:HIS:CD2	2:B:139:LEU:HD22	2.45	0.50
1:D:96:ALA:HA	1:D:161:PRO:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:41:SER:HB3	2:E:142:LYS:NZ	2.26	0.50
2:E:37:PHE:HA	2:E:40:LYS:HG2	1.92	0.50
2:E:64:VAL:HG13	2:E:70:VAL:HG22	1.93	0.50
2:F:11:TRP:CG	2:F:12:PRO:HD3	2.45	0.50
2:C:153:VAL:O	2:C:157:LEU:HD23	2.11	0.50
1:D:153:GLN:NE2	6:D:775:HOH:O	2.44	0.50
1:D:519:GLU:HB3	1:D:571:PHE:CE2	2.46	0.50
2:E:71:VAL:HG21	2:E:155:ILE:HD13	1.93	0.50
2:F:110:GLN:O	2:F:113:VAL:HG12	2.10	0.50
1:A:98:SER:O	1:A:110:PHE:HA	2.11	0.50
1:A:291:ILE:HG12	1:A:320:ALA:HA	1.93	0.50
1:A:433:ILE:HD11	1:A:552:LYS:HD3	1.93	0.50
1:D:438:GLU:O	1:D:442:GLN:HG3	2.12	0.50
1:D:496:CYS:HA	1:D:499:ARG:NH1	2.26	0.50
2:E:94:GLN:N	2:E:94:GLN:OE1	2.44	0.50
1:A:455:GLU:OE1	1:A:485:THR:HB	2.12	0.50
2:B:145:PHE:HB3	2:B:153:VAL:HG23	1.91	0.50
2:B:144:TYR:HB3	2:B:154:ASP:OD2	2.10	0.50
1:D:149:PHE:HB2	1:D:530:LYS:NZ	2.27	0.50
1:D:448:ALA:HB2	1:D:496:CYS:HB3	1.92	0.50
1:D:512:CYS:O	1:D:513:LYS:HB3	2.10	0.50
3:D:601:JAA:O03	6:D:724:HOH:O	2.19	0.50
1:A:463:SER:HB2	1:A:528:PHE:HE2	1.76	0.50
1:A:110:PHE:CE2	1:A:554:SER:HA	2.47	0.50
1:D:444:SER:HA	1:D:500:ALA:CB	2.42	0.50
1:D:110:PHE:HE1	1:D:556:ALA:HB2	1.77	0.50
2:C:69:ASN:OD1	6:C:408:HOH:O	2.20	0.50
2:C:26:LYS:HE3	2:C:78:TRP:O	2.11	0.50
1:D:148:ILE:HD11	1:D:193:ILE:HD13	1.94	0.50
1:D:106:GLY:HA3	1:D:432:ASN:HB3	1.93	0.50
2:F:10:TYR:HB3	2:F:13:SER:HB2	1.92	0.50
2:F:194:SER:O	2:F:198:SER:OG	2.19	0.50
1:A:261:THR:O	1:A:265:LYS:HG3	2.12	0.50
1:D:166:THR:HA	1:D:169:VAL:HG23	1.93	0.50
1:D:241:ILE:O	1:D:245:ILE:HG12	2.12	0.50
1:D:75:PRO:O	1:D:79:ARG:HG3	2.11	0.50
2:F:122:GLU:HA	2:F:125:LYS:HE2	1.94	0.50
1:A:281:CYS:HB3	1:A:287:TRP:CZ3	2.45	0.50
2:B:164:PHE:CD2	2:B:183:ILE:HG12	2.46	0.50
2:B:26:LYS:HA	2:B:81:LYS:HZ3	1.76	0.50
2:B:7:LEU:O	2:B:33:ARG:N	2.43	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:304:ILE:HG21	1:D:536:LEU:HD23	1.94	0.50
1:D:302:TYR:OH	1:D:328:HIS:ND1	2.24	0.50
1:A:273:LEU:HA	1:A:276:THR:HB	1.94	0.50
2:C:114:TRP:CD1	2:C:167:TYR:HE1	2.30	0.50
2:E:101:PHE:CE1	2:E:134:ILE:HD11	2.47	0.50
2:E:96:ARG:CZ	2:F:68:LEU:HD11	2.42	0.50
2:F:140:GLY:C	2:F:181:LYS:HZ1	2.15	0.50
2:F:18:ARG:NH2	6:F:423:HOH:O	2.45	0.50
1:A:61:PHE:CE1	1:A:400:ARG:NH1	2.80	0.49
1:A:445:VAL:HG21	1:A:462:PHE:CG	2.47	0.49
1:A:164:THR:OG1	1:A:560:GLN:HB3	2.11	0.49
1:A:121:THR:HG21	4:A:602:ATP:O2'	2.11	0.49
2:B:130:GLU:O	2:B:134:ILE:HG13	2.12	0.49
1:D:250:LEU:O	6:D:727:HOH:O	2.20	0.49
2:F:178:GLU:HG3	6:F:420:HOH:O	2.11	0.49
1:A:8:PHE:CD1	1:A:181:SER:HB2	2.46	0.49
1:D:107:ARG:HH11	1:D:433:ILE:N	2.08	0.49
1:D:29:LYS:O	1:D:33:LYS:HG2	2.12	0.49
4:D:602:ATP:N6	6:D:724:HOH:O	2.44	0.49
1:A:432:ASN:CG	1:A:433:ILE:N	2.65	0.49
1:D:145:LEU:O	1:D:220:PHE:N	2.43	0.49
1:D:223:PHE:H	1:D:529:ARG:NH2	2.10	0.49
1:A:281:CYS:O	1:A:284:LEU:HD11	2.13	0.49
1:D:264:SER:O	6:D:726:HOH:O	2.20	0.49
1:D:81:VAL:CG2	1:D:97:ILE:HD13	2.42	0.49
1:D:80:MET:HG2	1:D:86:SER:O	2.13	0.49
2:F:154:ASP:OD1	2:F:185:TRP:HZ2	1.95	0.49
1:A:152:LYS:HE3	1:A:560:GLN:O	2.11	0.49
1:A:183:THR:O	6:A:718:HOH:O	2.20	0.49
2:B:167:TYR:HA	6:B:411:HOH:O	2.12	0.49
2:C:10:TYR:CD2	2:C:12:PRO:HD2	2.48	0.49
1:D:225:HIS:HB3	1:D:312:TYR:CD2	2.47	0.49
2:E:98:TRP:CH2	2:E:152:TYR:CD2	3.01	0.49
1:A:148:ILE:HD11	1:A:193:ILE:HD13	1.95	0.49
1:A:150:SER:OG	1:A:150:SER:O	2.25	0.49
1:A:188:SER:HB3	1:A:192:VAL:CG1	2.43	0.49
1:A:238:TRP:CZ3	1:A:277:ILE:HG12	2.47	0.49
1:A:463:SER:HB2	1:A:528:PHE:CE2	2.48	0.49
2:B:162:SER:O	2:B:205:ILE:HG21	2.12	0.49
1:D:452:LEU:HB3	1:D:457:ILE:HD11	1.95	0.49
2:F:217:LEU:N	6:F:425:HOH:O	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:PHE:CE1	1:A:533:GLU:HA	2.48	0.49
2:B:111:PHE:HA	2:B:114:TRP:NE1	2.28	0.49
2:B:37:PHE:CE1	5:B:301:GSH:HA32	2.48	0.49
2:C:84:PHE:HB2	2:C:152:TYR:N	2.27	0.49
1:D:198:VAL:HA	1:D:201:ALA:CB	2.41	0.49
1:A:104:SER:N	1:A:107:ARG:O	2.38	0.49
1:A:113:PHE:HB2	4:A:602:ATP:O2A	2.13	0.49
1:A:300:TYR:HB2	1:A:326:VAL:HG12	1.95	0.49
1:A:113:PHE:HB2	4:A:602:ATP:O2B	2.13	0.49
1:D:45:LEU:HD22	6:D:719:HOH:O	2.11	0.49
1:A:120:ASN:ND2	6:A:776:HOH:O	2.46	0.49
2:C:23:LEU:HD22	2:C:28:VAL:HG11	1.95	0.49
2:C:98:TRP:CE3	2:C:101:PHE:HB2	2.47	0.49
2:F:132:VAL:HG22	2:F:179:SER:HB2	1.95	0.49
1:A:199:HIS:N	1:A:524:ALA:HB1	2.27	0.49
1:D:80:MET:SD	1:D:93:PRO:HA	2.53	0.49
2:E:101:PHE:CZ	2:E:134:ILE:HD11	2.47	0.49
2:E:132:VAL:HG21	2:E:175:ILE:HG23	1.95	0.49
1:A:266:LEU:HD12	1:A:267:LEU:HG	1.94	0.48
1:A:339:ALA:O	1:A:353:ALA:N	2.42	0.48
1:A:534:HIS:NE2	1:A:557:LYS:HD3	2.28	0.48
2:C:24:ARG:HB3	2:C:194:SER:HA	1.95	0.48
2:C:57:LEU:HB3	2:C:64:VAL:CG2	2.43	0.48
1:D:151:SER:OG	1:D:151:SER:O	2.30	0.48
1:D:153:GLN:HA	1:D:560:GLN:CG	2.43	0.48
1:D:98:SER:HB3	1:D:111:ILE:O	2.12	0.48
2:E:43:LEU:O	2:E:47:SER:OG	2.18	0.48
2:F:188:ARG:HB2	6:F:443:HOH:O	2.12	0.48
2:F:32:TYR:HD2	2:F:32:TYR:H	1.61	0.48
1:A:152:LYS:NZ	1:A:563:CYS:HB3	2.29	0.48
1:A:280:LYS:HE2	1:A:293:ALA:HB1	1.95	0.48
1:A:400:ARG:HG2	1:A:400:ARG:HH11	1.78	0.48
1:A:535:PHE:CZ	1:A:557:LYS:HD2	2.48	0.48
1:A:147:PHE:CZ	1:A:234:PHE:HE1	2.30	0.48
1:D:32:LEU:O	1:D:36:LEU:HD12	2.14	0.48
1:D:80:MET:HG3	1:D:88:ILE:CG1	2.43	0.48
1:D:82:ASP:HA	6:D:763:HOH:O	2.12	0.48
1:D:98:SER:HB2	4:D:602:ATP:O3B	2.11	0.48
1:A:490:LEU:HD22	1:A:522:VAL:HG21	1.94	0.48
2:B:139:LEU:O	2:B:141:ASP:N	2.45	0.48
2:C:4:LEU:N	6:C:438:HOH:O	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:99:ALA:CB	2:C:152:TYR:HE2	2.27	0.48
1:D:291:ILE:HG13	1:D:292:PRO:CD	2.43	0.48
1:A:108:PRO:HG2	1:A:552:LYS:N	2.29	0.48
1:A:98:SER:C	1:A:556:ALA:HB3	2.33	0.48
2:B:18:ARG:NH1	2:B:103:ASP:OD2	2.42	0.48
1:A:86:SER:HB2	2:B:188:ARG:HE	1.79	0.48
2:B:205:ILE:HD12	2:B:208:TYR:HE2	1.76	0.48
2:C:64:VAL:HB	2:C:73:TYR:CD2	2.49	0.48
1:D:223:PHE:HE2	1:D:545:PHE:CZ	2.31	0.48
1:D:81:VAL:HG22	1:D:97:ILE:HD13	1.95	0.48
2:E:8:LEU:HD12	2:E:54:ILE:HG22	1.93	0.48
2:F:11:TRP:O	2:F:200:PRO:HG2	2.14	0.48
1:A:100:SER:HA	1:A:535:PHE:HZ	1.75	0.48
1:A:18:ASP:O	1:A:22:ARG:HG2	2.13	0.48
1:A:231:PHE:CA	1:A:234:PHE:HB2	2.35	0.48
1:A:289:GLY:C	1:A:292:PRO:HD2	2.34	0.48
1:A:45:LEU:HG	1:A:50:LEU:HD12	1.95	0.48
1:A:478:PHE:CZ	1:A:562:LEU:HB2	2.48	0.48
1:A:521:ARG:HB3	1:A:566:VAL:HG12	1.95	0.48
1:D:108:PRO:HB2	1:D:554:SER:OG	2.04	0.48
1:D:300:TYR:CE1	1:D:302:TYR:HB2	2.48	0.48
2:E:213:ARG:NE	6:E:431:HOH:O	2.45	0.48
1:A:156:SER:HB2	1:A:162:VAL:CG2	2.43	0.48
1:A:432:ASN:HD21	1:A:435:LYS:N	2.12	0.48
1:A:526:GLY:HA2	1:A:529:ARG:HB3	1.95	0.48
1:A:435:LYS:CD	1:A:549:ARG:HH12	2.27	0.48
2:C:182:LEU:HG	2:C:183:ILE:H	1.77	0.48
2:C:71:VAL:O	2:C:74:VAL:HB	2.13	0.48
1:D:138:ILE:HB	1:D:217:GLN:HG3	1.94	0.48
1:D:170:TYR:HH	1:D:171:ARG:NH2	2.09	0.48
1:D:351:THR:HG21	1:D:410:ILE:HD11	1.96	0.48
2:E:205:ILE:HG23	6:E:404:HOH:O	2.13	0.48
1:A:12:ARG:HA	1:A:15:ASP:OD1	2.14	0.48
1:A:524:ALA:HB2	1:A:567:VAL:HG11	1.95	0.48
1:A:551:VAL:HG13	1:A:555:ASN:HB2	1.96	0.48
1:A:70:ASP:HB2	1:A:104:SER:HB2	1.94	0.48
2:C:184:ALA:HA	2:C:187:LYS:NZ	2.28	0.48
1:D:107:ARG:HH21	1:D:552:LYS:CD	2.27	0.48
1:D:465:TYR:CD1	1:D:551:VAL:HG22	2.49	0.48
2:F:100:ASP:HA	6:F:449:HOH:O	2.13	0.48
1:A:532:GLN:NE2	6:A:725:HOH:O	2.24	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:421:PHE:HE2	1:A:540:SER:O	1.97	0.48
2:B:104:LYS:HE2	2:B:104:LYS:HB3	1.66	0.48
2:C:40:LYS:HD2	2:C:52:LYS:HB3	1.96	0.48
1:D:169:VAL:HG12	1:D:175:PHE:CD1	2.48	0.48
2:E:40:LYS:HD2	2:E:44:LEU:HD23	1.94	0.48
2:F:131:ALA:O	2:F:135:LEU:HB2	2.13	0.48
2:F:164:PHE:HD2	2:F:183:ILE:HD12	1.79	0.48
2:F:187:LYS:HA	2:F:190:MET:HB2	1.96	0.48
1:A:558:VAL:HA	1:A:561:ILE:HB	1.96	0.48
1:A:152:LYS:HZ3	1:A:563:CYS:CA	2.26	0.48
2:B:106:PHE:HZ	2:B:132:VAL:HG23	1.78	0.48
2:C:125:LYS:HA	2:C:128:PHE:CE2	2.49	0.48
1:D:222:VAL:C	1:D:223:PHE:HD1	2.18	0.48
1:D:336:TRP:HD1	1:D:337:ILE:H	1.61	0.48
1:D:35:ILE:HA	1:D:395:TYR:CE1	2.49	0.48
1:D:405:ASP:OD2	1:D:540:SER:OG	2.27	0.48
1:D:413:TYR:O	1:D:416:THR:HG22	2.13	0.48
1:D:92:HIS:CG	2:E:181:LYS:HB3	2.49	0.48
2:F:98:TRP:HZ2	2:F:157:LEU:HD22	1.78	0.48
2:F:135:LEU:HD22	2:F:182:LEU:HD12	1.96	0.48
1:A:331:GLY:HA3	1:A:336:TRP:HA	1.96	0.47
1:A:531:ILE:HA	1:A:534:HIS:NE2	2.30	0.47
1:D:39:ASN:HD21	1:D:90:THR:C	2.17	0.47
1:D:22:ARG:NH1	1:D:414:ASN:OD1	2.47	0.47
1:D:223:PHE:CE2	1:D:533:GLU:HA	2.49	0.47
2:F:8:LEU:HD13	2:F:44:LEU:HB2	1.96	0.47
1:A:305:MET:CB	1:A:347:PRO:HB3	2.44	0.47
1:D:333:SER:C	1:D:335:GLY:N	2.67	0.47
1:D:221:ALA:HB1	1:D:529:ARG:NH2	2.29	0.47
1:A:152:LYS:NZ	1:A:564:GLU:N	2.50	0.47
1:A:164:THR:HB	1:A:167:THR:OG1	2.15	0.47
2:B:161:SER:HA	2:B:164:PHE:CD2	2.49	0.47
1:A:92:HIS:ND1	2:B:185:TRP:HB2	2.29	0.47
1:D:91:GLY:HA2	2:E:143:PRO:HD3	1.95	0.47
1:A:241:ILE:HD12	1:A:245:ILE:HD11	1.97	0.47
1:A:424:ARG:HG3	1:A:425:ARG:H	1.80	0.47
1:A:332:SER:HB3	1:A:538:LEU:HD13	1.95	0.47
2:B:171:GLY:N	6:B:411:HOH:O	2.42	0.47
2:C:73:TYR:HD1	2:C:76:GLU:OE2	1.98	0.47
1:D:110:PHE:CD2	1:D:554:SER:HA	2.49	0.47
1:D:97:ILE:HD12	1:D:110:PHE:CE1	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:362:GLU:HG3	1:D:400:ARG:HH12	1.80	0.47
2:F:33:ARG:HG3	6:F:508:HOH:O	2.15	0.47
2:F:71:VAL:HG13	2:F:152:TYR:HE1	1.80	0.47
2:F:26:LYS:HE3	2:F:78:TRP:O	2.14	0.47
1:D:509:SER:O	1:D:513:LYS:N	2.48	0.47
1:A:132:ARG:HA	1:A:343:PRO:HG3	1.96	0.47
1:A:108:PRO:HB2	1:A:554:SER:OG	2.15	0.47
1:A:152:LYS:CE	1:A:564:GLU:H	2.28	0.47
2:C:92:ARG:HE	2:C:96:ARG:HH22	1.63	0.47
1:D:150:SER:HB3	1:D:167:THR:HG22	1.96	0.47
1:D:77:ILE:HD13	1:D:110:PHE:HB3	1.95	0.47
1:D:99:LEU:HA	1:D:109:LYS:O	2.15	0.47
2:E:133:LYS:O	2:E:136:GLU:HB3	2.15	0.47
2:E:139:LEU:O	2:E:141:ASP:N	2.47	0.47
2:F:68:LEU:HD13	2:F:152:TYR:OH	2.15	0.47
1:A:169:VAL:HG22	4:A:602:ATP:C2'	2.44	0.47
1:A:435:LYS:HB3	1:A:436:ASN:C	2.34	0.47
2:B:170:PHE:CE2	2:B:213:ARG:HD2	2.49	0.47
1:D:279:THR:O	1:D:283:SER:HB2	2.14	0.47
1:D:107:ARG:HH21	1:D:552:LYS:HD3	1.80	0.47
1:D:53:ASN:HB2	2:E:90:TYR:CZ	2.49	0.47
2:F:56:VAL:HG13	6:F:434:HOH:O	2.14	0.47
1:A:44:TYR:CG	1:A:89:LEU:HD13	2.49	0.47
2:B:11:TRP:CG	2:B:12:PRO:HD3	2.49	0.47
1:D:195:SER:OG	1:D:197:ASP:OD1	2.32	0.47
1:D:413:TYR:CD2	1:D:418:GLN:HG2	2.50	0.47
1:D:87:PRO:HB3	1:D:93:PRO:HD3	1.97	0.47
2:E:183:ILE:O	2:E:187:LYS:HG3	2.15	0.47
2:E:72:GLN:HB3	2:F:96:ARG:NH1	2.30	0.47
2:E:59:HIS:CE1	2:E:73:TYR:CZ	3.03	0.47
2:F:169:LYS:HG3	2:F:170:PHE:N	2.28	0.47
1:A:217:GLN:HA	1:A:217:GLN:OE1	2.15	0.47
1:A:466:ILE:O	1:A:466:ILE:HG13	2.14	0.47
1:A:41:SER:H	2:B:142:LYS:HG2	1.79	0.47
2:C:193:GLU:HA	2:C:196:SER:HB3	1.96	0.47
1:D:170:TYR:CD2	1:D:171:ARG:N	2.83	0.47
1:D:474:HIS:ND1	1:D:571:PHE:HE2	2.12	0.47
1:D:518:LEU:HD12	1:D:519:GLU:N	2.30	0.47
2:E:200:PRO:HB2	6:E:404:HOH:O	2.14	0.47
2:E:9:ASP:HA	2:E:54:ILE:HB	1.97	0.47
1:A:225:HIS:HB3	1:A:309:MET:SD	2.55	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:TRP:HZ3	1:A:277:ILE:HG12	1.79	0.47
1:A:337:ILE:O	1:A:354:VAL:HA	2.15	0.47
2:B:10:TYR:CD2	2:B:13:SER:HB2	2.49	0.47
2:B:62:LYS:HZ2	2:C:90:TYR:HE2	1.61	0.47
2:C:159:THR:HA	2:C:199:LEU:HD21	1.96	0.47
1:D:95:PRO:HD2	1:D:113:PHE:O	2.14	0.47
1:D:203:TYR:C	1:D:203:TYR:CD1	2.88	0.47
1:A:223:PHE:CZ	1:A:533:GLU:HA	2.50	0.47
2:B:112:LYS:HZ1	2:B:120:GLU:CB	2.27	0.47
2:C:33:ARG:HH22	2:C:41:SER:CB	2.21	0.47
1:D:339:ALA:N	1:D:353:ALA:O	2.32	0.47
1:D:393:THR:HG23	1:D:399:TYR:HA	1.97	0.47
1:D:478:PHE:CE1	1:D:521:ARG:HB2	2.49	0.47
1:D:95:PRO:HD3	2:E:181:LYS:NZ	2.30	0.47
1:A:530:LYS:NZ	1:A:530:LYS:HB2	2.30	0.46
2:B:101:PHE:HE2	2:B:135:LEU:HG	1.80	0.46
1:D:451:ARG:CZ	1:D:489:VAL:HG12	2.45	0.46
2:F:144:TYR:HB3	2:F:154:ASP:OD2	2.16	0.46
1:A:413:TYR:CD2	1:A:418:GLN:HG2	2.50	0.46
1:A:451:ARG:NH2	6:A:779:HOH:O	2.48	0.46
1:D:223:PHE:HE2	1:D:545:PHE:HZ	1.62	0.46
1:D:435:LYS:HB3	1:D:436:ASN:C	2.36	0.46
1:D:559:LEU:HA	1:D:562:LEU:HD23	1.96	0.46
1:A:406:VAL:O	1:A:541:SER:OG	2.28	0.46
1:D:100:SER:CB	1:D:109:LYS:HD3	2.46	0.46
2:E:98:TRP:CE3	2:E:153:VAL:HB	2.49	0.46
1:A:192:VAL:HA	1:A:195:SER:HB2	1.96	0.46
1:A:27:VAL:HG13	1:A:356:PRO:HB2	1.97	0.46
1:A:525:LYS:HG2	6:A:804:HOH:O	2.15	0.46
2:B:95:ALA:HB1	2:B:152:TYR:HD2	1.80	0.46
1:D:132:ARG:CA	1:D:343:PRO:HG3	2.44	0.46
1:D:363:PHE:CD1	1:D:390:VAL:HA	2.50	0.46
2:F:5:PRO:HG2	2:F:28:VAL:HG21	1.96	0.46
1:A:108:PRO:HB3	1:A:555:ASN:CB	2.44	0.46
1:A:152:LYS:HG3	1:A:561:ILE:HA	1.96	0.46
1:A:493:CYS:O	1:A:497:LEU:HD12	2.15	0.46
1:A:85:THR:HB	2:B:184:ALA:HB1	1.97	0.46
1:A:38:LYS:HD2	2:B:138:GLU:O	2.16	0.46
1:D:244:ASP:OD1	1:D:251:SER:HB2	2.15	0.46
1:D:339:ALA:O	1:D:353:ALA:N	2.42	0.46
1:D:451:ARG:NH1	1:D:454:GLU:CD	2.69	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:555:ASN:ND2	6:D:777:HOH:O	2.47	0.46
2:E:13:SER:O	2:E:17:MET:HG3	2.15	0.46
1:A:310:GLU:O	1:A:314:PRO:HD3	2.15	0.46
2:C:32:TYR:HD2	2:C:32:TYR:H	1.63	0.46
1:D:117:LEU:HG	6:D:782:HOH:O	2.15	0.46
1:D:53:ASN:HB3	1:D:54:ALA:H	1.30	0.46
1:D:559:LEU:O	1:D:562:LEU:HG	2.16	0.46
2:E:163:TRP:CZ3	2:E:209:ALA:HB2	2.51	0.46
1:A:152:LYS:HZ3	1:A:563:CYS:CB	2.29	0.46
2:B:96:ARG:HH11	2:C:73:TYR:HE1	1.63	0.46
2:C:201:ASP:HB2	2:C:204:LYS:HG3	1.98	0.46
2:C:26:LYS:HD2	2:C:74:VAL:HG12	1.97	0.46
2:C:92:ARG:HB3	2:C:96:ARG:NH2	2.31	0.46
1:D:363:PHE:HD1	1:D:390:VAL:HA	1.80	0.46
1:D:398:LEU:HD22	1:D:401:TYR:CG	2.51	0.46
2:F:128:PHE:HE1	2:F:175:ILE:HG22	1.80	0.46
2:F:4:LEU:HA	2:F:5:PRO:HD3	1.78	0.46
1:A:76:TYR:CZ	1:A:89:LEU:HG	2.51	0.46
2:B:127:GLU:HA	2:B:130:GLU:OE2	2.15	0.46
2:B:169:LYS:NZ	2:B:210:ALA:HB2	2.31	0.46
2:B:24:ARG:HB3	2:B:194:SER:HA	1.96	0.46
2:C:187:LYS:HB2	2:C:187:LYS:HE2	1.55	0.46
2:C:33:ARG:NH2	6:C:405:HOH:O	2.16	0.46
1:A:193:ILE:HG12	1:A:205:HIS:CE1	2.43	0.46
1:A:309:MET:SD	1:A:312:TYR:HB2	2.56	0.46
1:A:527:THR:O	1:A:531:ILE:HG23	2.16	0.46
1:D:170:TYR:HA	1:D:175:PHE:CG	2.51	0.46
1:D:496:CYS:O	1:D:500:ALA:N	2.48	0.46
2:E:169:LYS:HZ1	2:E:206:VAL:HG11	1.77	0.46
2:E:40:LYS:HZ2	2:E:44:LEU:HG	1.80	0.46
1:A:27:VAL:HA	1:A:30:GLN:HB2	1.98	0.46
1:A:199:HIS:HB3	1:A:524:ALA:HB1	1.98	0.46
2:C:24:ARG:HD2	2:C:198:SER:OG	2.16	0.46
2:C:184:ALA:HA	1:D:499:ARG:NH1	2.30	0.46
1:D:512:CYS:HG	1:D:513:LYS:H	1.54	0.46
1:D:107:ARG:HE	1:D:552:LYS:HD3	1.81	0.46
2:E:108:ASP:O	2:E:112:LYS:HG2	2.16	0.46
1:A:108:PRO:HD3	1:A:434:ASP:OD2	2.16	0.45
1:A:507:VAL:O	1:A:511:LYS:HB2	2.16	0.45
1:A:68:VAL:HG13	1:A:401:TYR:HD1	1.81	0.45
2:C:57:LEU:O	2:C:64:VAL:HG22	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:325:LEU:O	1:D:347:PRO:HD3	2.16	0.45
1:D:541:SER:C	1:D:543:GLY:H	2.15	0.45
1:D:99:LEU:CB	1:D:557:LYS:H	2.29	0.45
2:F:17:MET:SD	2:F:199:LEU:HG	2.56	0.45
2:F:86:PRO:HD3	2:F:146:GLY:O	2.15	0.45
1:A:466:ILE:HG22	1:A:475:TYR:CD1	2.51	0.45
4:A:602:ATP:O2B	4:A:602:ATP:O2A	2.35	0.45
1:D:150:SER:O	1:D:152:LYS:N	2.49	0.45
1:D:569:SER:O	6:D:728:HOH:O	2.21	0.45
1:A:147:PHE:HZ	1:A:234:PHE:HE1	1.63	0.45
1:A:248:GLY:O	1:A:267:LEU:HB3	2.17	0.45
1:A:369:THR:HG23	1:A:370:GLY:H	1.81	0.45
2:B:182:LEU:O	2:B:185:TRP:HB3	2.16	0.45
1:D:22:ARG:HH11	1:D:414:ASN:CB	2.29	0.45
1:D:370:GLY:HA2	1:D:371:GLU:HA	1.66	0.45
1:A:92:HIS:CE1	2:B:185:TRP:HB2	2.51	0.45
2:B:7:LEU:HD12	2:B:30:PHE:CE2	2.51	0.45
2:C:71:VAL:O	2:C:84:PHE:HE2	2.00	0.45
6:B:429:HOH:O	2:C:92:ARG:NH2	2.49	0.45
1:D:277:ILE:HD12	1:D:278:ARG:N	2.31	0.45
1:D:99:LEU:HG	1:D:555:ASN:OD1	2.16	0.45
2:E:98:TRP:CE3	2:E:99:ALA:N	2.84	0.45
1:A:314:PRO:O	1:A:317:ARG:HG2	2.17	0.45
1:A:427:LEU:HD12	1:A:427:LEU:O	2.17	0.45
1:A:530:LYS:HZ3	1:A:530:LYS:HB2	1.82	0.45
2:C:184:ALA:HB1	1:D:499:ARG:NH1	2.31	0.45
1:D:394:ASN:OD1	1:D:398:LEU:HB2	2.16	0.45
1:D:446:GLU:O	1:D:450:LYS:HD3	2.17	0.45
1:D:510:ARG:NH2	1:D:518:LEU:HB2	2.30	0.45
1:A:228:VAL:O	1:A:232:ARG:HB3	2.17	0.45
1:A:269:PRO:O	6:A:720:HOH:O	2.21	0.45
1:A:113:PHE:CD1	4:A:602:ATP:H5'1	2.52	0.45
2:B:125:LYS:HA	2:B:173:PHE:HZ	1.81	0.45
2:B:6:ILE:HD13	2:B:33:ARG:NE	2.32	0.45
2:C:20:ARG:HB3	2:C:198:SER:HB3	1.97	0.45
1:D:11:ASN:O	1:D:14:ILE:HG13	2.17	0.45
2:E:183:ILE:O	2:E:186:ALA:HB3	2.17	0.45
1:D:358:LEU:HD12	1:D:359:GLY:N	2.32	0.45
1:D:92:HIS:ND1	2:E:181:LYS:HB3	2.31	0.45
2:E:14:MET:HA	2:E:17:MET:SD	2.57	0.45
2:E:51:HIS:O	2:E:52:LYS:HG2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:195:VAL:HG23	2:B:199:LEU:HD13	1.98	0.45
1:D:347:PRO:HG2	6:D:957:HOH:O	2.16	0.45
1:D:443:LEU:HG	6:D:704:HOH:O	2.16	0.45
1:D:152:LYS:NZ	1:D:530:LYS:HE2	2.31	0.45
1:D:557:LYS:HE3	4:D:602:ATP:O2G	2.16	0.45
2:E:6:ILE:HG21	2:E:33:ARG:HH11	1.82	0.45
1:A:291:ILE:CG1	1:A:320:ALA:HA	2.47	0.45
1:A:556:ALA:HA	1:A:559:LEU:CB	2.44	0.45
1:A:92:HIS:NE2	2:B:139:LEU:HD22	2.32	0.45
2:B:8:LEU:CD1	2:B:56:VAL:HG12	2.46	0.45
2:C:183:ILE:O	2:C:187:LYS:HG3	2.17	0.45
2:C:199:LEU:HA	2:C:200:PRO:HD2	1.86	0.45
1:D:399:TYR:N	1:D:401:TYR:HD1	2.15	0.45
1:D:517:ALA:HB2	1:D:575:PHE:CZ	2.52	0.45
1:D:108:PRO:HG2	1:D:552:LYS:HG2	1.99	0.45
2:F:117:LYS:HA	2:F:121:GLN:HB2	1.98	0.45
1:A:169:VAL:HB	1:A:170:TYR:CD1	2.52	0.45
1:A:208:SER:O	1:A:211:LEU:HG	2.17	0.45
1:A:211:LEU:HD12	1:A:212:PHE:CD1	2.52	0.45
1:A:510:ARG:HH11	1:A:510:ARG:HG2	1.81	0.45
1:D:218:TYR:HA	1:D:298:ALA:HB1	1.98	0.45
1:D:40:GLN:HG2	2:E:142:LYS:HZ3	1.82	0.45
2:F:98:TRP:O	2:F:102:VAL:HG23	2.17	0.45
1:A:98:SER:O	1:A:110:PHE:HD1	1.99	0.44
1:A:8:PHE:HD1	1:A:181:SER:HB2	1.82	0.44
1:A:351:THR:HG22	1:A:420:LYS:HB2	1.99	0.44
1:A:41:SER:HB3	2:B:144:TYR:HB2	1.99	0.44
2:B:203:GLU:O	2:B:206:VAL:HG12	2.17	0.44
2:B:8:LEU:HD12	2:B:8:LEU:O	2.17	0.44
2:C:139:LEU:HB3	2:C:181:LYS:HE2	1.98	0.44
1:D:133:ASN:ND2	6:D:781:HOH:O	2.50	0.44
2:E:62:LYS:HD3	2:F:90:TYR:CD2	2.52	0.44
2:F:33:ARG:HH12	2:F:41:SER:HB2	1.82	0.44
1:A:228:VAL:O	1:A:232:ARG:N	2.47	0.44
1:A:287:TRP:CE3	1:A:290:LEU:HD13	2.45	0.44
1:D:168:ASN:O	1:D:172:ASN:HB2	2.17	0.44
1:D:284:LEU:HD13	1:D:287:TRP:H	1.83	0.44
1:D:361:PHE:CE1	1:D:379:LEU:HD22	2.53	0.44
1:D:464:SER:HA	1:D:477:ILE:HA	1.99	0.44
1:D:476:ALA:HA	1:D:519:GLU:HG3	1.98	0.44
2:E:153:VAL:O	2:E:157:LEU:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:169:LYS:HZ2	2:E:206:VAL:HG11	1.79	0.44
2:E:36:ASP:OD2	2:E:38:SER:HB2	2.17	0.44
2:E:92:ARG:NH2	6:E:401:HOH:O	2.25	0.44
2:F:9:ASP:HA	2:F:54:ILE:HD13	1.99	0.44
1:A:151:SER:CA	1:A:194:PHE:HA	2.43	0.44
1:A:145:LEU:HB2	1:A:209:GLY:HA3	1.98	0.44
1:A:281:CYS:O	1:A:287:TRP:CZ3	2.71	0.44
1:A:162:VAL:O	1:A:560:GLN:HB2	2.18	0.44
1:A:152:LYS:CG	1:A:561:ILE:HA	2.47	0.44
2:C:185:TRP:CE2	2:C:189:CYS:SG	3.10	0.44
2:C:55:PRO:HG2	6:C:403:HOH:O	2.17	0.44
1:D:98:SER:O	1:D:110:PHE:HA	2.17	0.44
1:D:160:VAL:HG23	6:D:780:HOH:O	2.16	0.44
1:D:169:VAL:O	1:D:175:PHE:HB2	2.17	0.44
1:D:451:ARG:NH1	1:D:454:GLU:OE1	2.49	0.44
1:D:84:ASP:OD2	1:D:86:SER:OG	2.29	0.44
1:D:87:PRO:HD2	2:E:188:ARG:CB	2.46	0.44
2:E:135:LEU:HD23	2:E:135:LEU:HA	1.85	0.44
1:A:149:PHE:HE1	1:A:205:HIS:CD2	2.35	0.44
1:A:223:PHE:CD1	1:A:304:ILE:HG12	2.52	0.44
2:C:195:VAL:HG23	2:C:199:LEU:HD13	2.00	0.44
2:C:209:ALA:HB2	6:C:417:HOH:O	2.16	0.44
1:D:124:LEU:HD12	1:D:355:ILE:HD12	1.99	0.44
1:D:364:LEU:N	6:D:749:HOH:O	2.49	0.44
2:F:64:VAL:HG23	2:F:70:VAL:HG22	1.99	0.44
1:A:32:LEU:HB2	1:A:360:TYR:CG	2.53	0.44
1:A:362:GLU:HB3	6:A:722:HOH:O	2.18	0.44
1:A:494:CYS:HB2	1:A:520:LEU:HB3	2.00	0.44
1:A:76:TYR:CE2	1:A:89:LEU:HG	2.53	0.44
2:C:102:VAL:O	2:C:107:THR:HG23	2.18	0.44
2:C:65:CYS:O	2:C:69:ASN:HB3	2.17	0.44
1:D:304:ILE:HA	6:D:801:HOH:O	2.17	0.44
1:D:358:LEU:H	1:D:358:LEU:HG	1.63	0.44
1:D:442:GLN:HG2	1:D:462:PHE:CZ	2.40	0.44
1:D:445:VAL:HG13	1:D:479:TRP:NE1	2.33	0.44
2:E:17:MET:O	2:E:21:VAL:HG12	2.18	0.44
2:B:175:ILE:O	2:B:175:ILE:HG12	2.17	0.44
2:B:190:MET:HA	2:B:195:VAL:CG1	2.48	0.44
2:C:26:LYS:HD2	2:C:74:VAL:CG1	2.48	0.44
1:D:223:PHE:CD1	1:D:304:ILE:HB	2.53	0.44
1:D:329:ASP:HB3	1:D:338:ALA:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:342:THR:OG1	1:D:413:TYR:OH	2.16	0.44
1:D:437:THR:HG21	1:D:439:ARG:HH21	1.82	0.44
2:E:111:PHE:HA	2:E:114:TRP:NE1	2.33	0.44
2:E:18:ARG:NH2	6:E:432:HOH:O	2.46	0.44
2:E:24:ARG:HG2	2:E:194:SER:HA	1.99	0.44
2:F:8:LEU:HD22	2:F:33:ARG:NH2	2.25	0.44
1:A:77:ILE:HG12	1:A:110:PHE:HB3	2.00	0.44
1:A:16:GLU:O	1:A:20:MET:HB2	2.18	0.44
1:A:407:VAL:HG21	1:A:419:LEU:HB3	2.00	0.44
1:A:407:VAL:HG21	1:A:419:LEU:HD23	1.98	0.44
1:A:97:ILE:HD12	1:A:556:ALA:HB2	1.98	0.44
2:B:100:ASP:O	2:B:104:LYS:HB2	2.18	0.44
1:A:197:ASP:OD1	1:A:200:GLN:HB3	2.17	0.44
2:B:163:TRP:HB3	2:B:167:TYR:CZ	2.52	0.44
1:D:96:ALA:HA	1:D:162:VAL:HA	1.99	0.44
1:A:114:THR:HB	1:A:116:GLU:OE1	2.17	0.44
2:C:4:LEU:HA	2:C:5:PRO:HD3	1.73	0.44
1:D:120:ASN:O	1:D:124:LEU:N	2.44	0.44
1:D:304:ILE:HG23	1:D:330:TYR:OH	2.17	0.44
2:F:114:TRP:CZ3	2:F:212:TYR:HD2	2.36	0.44
2:F:168:GLU:CD	2:F:175:ILE:HG12	2.38	0.44
1:A:233:THR:C	1:A:236:GLN:H	2.21	0.43
1:A:445:VAL:HA	1:A:479:TRP:HZ2	1.82	0.43
1:A:450:LYS:HA	1:A:453:SER:HB3	2.00	0.43
1:A:461:ASP:OD2	1:A:547:MET:SD	2.76	0.43
2:C:15:PHE:O	2:C:55:PRO:HG3	2.18	0.43
2:E:121:GLN:NE2	2:E:170:PHE:O	2.51	0.43
2:E:135:LEU:HB3	2:E:182:LEU:HD21	2.00	0.43
2:F:185:TRP:O	2:F:188:ARG:HB3	2.18	0.43
2:F:26:LYS:HD2	2:F:74:VAL:CG1	2.48	0.43
1:A:117:LEU:HA	1:A:120:ASN:OD1	2.19	0.43
1:A:146:GLN:OE1	1:A:148:ILE:HG12	2.18	0.43
2:B:135:LEU:HD23	2:B:135:LEU:HA	1.81	0.43
2:B:142:LYS:HB3	2:B:144:TYR:O	2.17	0.43
2:B:202:SER:O	2:B:205:ILE:HG22	2.18	0.43
1:D:203:TYR:O	1:D:206:LEU:HB2	2.18	0.43
1:D:311:PRO:O	1:D:315:LYS:HE2	2.18	0.43
1:D:423:CYS:SG	1:D:541:SER:OG	2.75	0.43
1:D:521:ARG:NH1	1:D:562:LEU:CD1	2.80	0.43
1:D:53:ASN:HB2	2:E:90:TYR:OH	2.17	0.43
2:F:98:TRP:CZ2	2:F:157:LEU:HD22	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:LEU:HG	1:A:557:LYS:CG	2.46	0.43
2:C:98:TRP:HD1	2:C:153:VAL:HG11	1.81	0.43
1:D:133:ASN:OD1	1:D:138:ILE:N	2.51	0.43
1:D:256:VAL:HA	1:D:257:PRO:HD3	1.89	0.43
1:D:536:LEU:HB2	1:D:545:PHE:HE1	1.81	0.43
6:D:701:HOH:O	2:E:144:TYR:C	2.56	0.43
2:F:70:VAL:O	2:F:73:TYR:HB2	2.18	0.43
1:A:148:ILE:HB	1:A:170:TYR:CE2	2.54	0.43
1:A:317:ARG:O	1:A:321:GLY:N	2.49	0.43
2:C:11:TRP:CG	2:C:12:PRO:HD3	2.53	0.43
1:D:211:LEU:HD12	1:D:212:PHE:HD1	1.83	0.43
1:D:254:ILE:N	1:D:254:ILE:HD13	2.33	0.43
1:D:303:GLY:HA3	6:D:733:HOH:O	2.17	0.43
1:D:38:LYS:HD2	1:D:395:TYR:CE1	2.52	0.43
1:D:496:CYS:CA	1:D:499:ARG:NH1	2.81	0.43
1:D:163:GLY:HA2	1:D:560:GLN:CB	2.48	0.43
6:D:713:HOH:O	2:E:188:ARG:HA	2.17	0.43
1:A:96:ALA:HB3	1:A:113:PHE:HB3	1.99	0.43
1:A:435:LYS:HG2	1:A:549:ARG:HH12	1.82	0.43
1:A:99:LEU:HB2	1:A:555:ASN:CG	2.39	0.43
2:B:133:LYS:HE2	2:B:133:LYS:HB3	1.77	0.43
1:D:99:LEU:HD13	1:D:558:VAL:H	1.84	0.43
1:A:304:ILE:HG13	1:A:304:ILE:O	2.19	0.43
1:A:226:GLY:CA	1:A:529:ARG:HH11	2.29	0.43
2:B:37:PHE:CD1	2:B:40:LYS:HE3	2.54	0.43
1:D:301:VAL:HB	1:D:325:LEU:HD22	2.01	0.43
1:D:62:LYS:HG2	1:D:400:ARG:NH2	2.34	0.43
2:F:8:LEU:HB2	2:F:56:VAL:HB	2.01	0.43
1:A:65:VAL:HG11	1:A:399:TYR:CE2	2.53	0.43
1:D:363:PHE:HE1	1:D:390:VAL:HG13	1.84	0.43
2:C:187:LYS:CE	1:D:496:CYS:HB2	2.49	0.43
1:D:519:GLU:OE1	1:D:521:ARG:NE	2.51	0.43
1:D:529:ARG:O	1:D:529:ARG:HD2	2.18	0.43
1:D:94:VAL:HG11	1:D:112:PRO:HB2	1.99	0.43
2:E:85:PHE:CZ	2:E:152:TYR:CD2	3.07	0.43
2:E:169:LYS:HZ1	2:E:206:VAL:HG21	1.83	0.43
2:E:86:PRO:HB2	2:E:88:ASP:OD1	2.19	0.43
2:F:10:TYR:CG	2:F:12:PRO:HD2	2.54	0.43
1:A:105:GLN:OE1	1:A:107:ARG:NH2	2.52	0.43
2:C:150:PHE:N	6:C:436:HOH:O	2.43	0.43
2:C:154:ASP:OD1	2:C:185:TRP:HZ2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:290:LEU:O	1:D:293:ALA:HB3	2.19	0.43
1:D:41:SER:HB3	2:E:142:LYS:HZ1	1.83	0.43
1:D:73:LEU:HD12	1:D:74:GLU:N	2.33	0.43
1:A:222:VAL:C	1:A:223:PHE:HD1	2.22	0.43
1:A:466:ILE:HD11	1:A:552:LYS:HD2	1.99	0.43
1:A:80:MET:SD	1:A:88:ILE:HD11	2.59	0.43
2:B:202:SER:OG	6:B:407:HOH:O	2.22	0.43
2:C:125:LYS:HA	2:C:128:PHE:CD2	2.52	0.43
1:D:152:LYS:HE3	1:D:565:ASN:HB2	2.00	0.43
1:D:158:GLY:O	6:D:729:HOH:O	2.22	0.43
2:F:26:LYS:HE2	2:F:75:ASP:HA	2.00	0.43
2:C:17:MET:HE3	2:C:163:TRP:HH2	1.84	0.42
2:C:8:LEU:O	6:C:410:HOH:O	2.22	0.42
1:D:107:ARG:HD2	1:D:107:ARG:HA	1.78	0.42
1:D:277:ILE:CD1	1:D:278:ARG:HG2	2.49	0.42
1:D:82:ASP:O	1:D:84:ASP:N	2.47	0.42
1:A:143:LYS:HE3	1:A:212:PHE:CD2	2.54	0.42
1:A:424:ARG:O	1:A:545:PHE:HB2	2.19	0.42
2:C:170:PHE:CE2	2:C:213:ARG:HD2	2.54	0.42
2:C:92:ARG:HB3	2:C:96:ARG:HH22	1.84	0.42
1:D:28:GLN:O	1:D:31:THR:OG1	2.34	0.42
1:D:305:MET:CB	1:D:347:PRO:HB3	2.49	0.42
2:E:193:GLU:O	2:E:197:LYS:HB2	2.19	0.42
1:A:477:ILE:CD1	1:A:518:LEU:HD21	2.49	0.42
1:A:477:ILE:HD11	1:A:520:LEU:HB2	2.02	0.42
1:A:524:ALA:HB2	1:A:567:VAL:CG1	2.49	0.42
2:C:98:TRP:CD1	2:C:153:VAL:HG21	2.55	0.42
2:C:184:ALA:HB1	1:D:499:ARG:HE	1.82	0.42
1:D:145:LEU:HD23	1:D:295:PHE:CE1	2.54	0.42
1:D:556:ALA:HA	1:D:559:LEU:HB3	2.00	0.42
1:D:69:THR:N	1:D:72:GLU:OE2	2.49	0.42
2:E:20:ARG:NH2	6:E:439:HOH:O	2.53	0.42
1:A:125:PHE:O	1:A:129:PHE:HB2	2.19	0.42
1:A:315:LYS:O	1:A:318:HIS:HB3	2.19	0.42
1:A:442:GLN:HG2	1:A:462:PHE:HZ	1.83	0.42
1:A:152:LYS:HD3	1:A:565:ASN:H	1.84	0.42
1:D:225:HIS:O	1:D:228:VAL:HG12	2.20	0.42
1:D:337:ILE:O	1:D:354:VAL:HA	2.19	0.42
1:D:335:GLY:O	1:D:539:GLY:HA3	2.18	0.42
1:D:547:MET:HB3	1:D:547:MET:HE2	1.90	0.42
1:D:152:LYS:HE2	1:D:561:ILE:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:165:GLN:HA	2:E:168:GLU:HB2	2.01	0.42
2:F:179:SER:HA	2:F:180:PRO:HD2	1.49	0.42
2:E:93:ALA:HB1	2:F:73:TYR:CZ	2.54	0.42
2:F:9:ASP:OD1	2:F:9:ASP:N	2.53	0.42
1:A:363:PHE:CD2	1:A:382:VAL:HG11	2.45	0.42
1:A:73:LEU:HD22	1:A:76:TYR:CE2	2.54	0.42
2:B:162:SER:HB3	2:B:199:LEU:HD21	2.01	0.42
2:B:53:LYS:HD3	5:B:301:GSH:CD1	2.49	0.42
1:D:143:LYS:HA	1:D:184:SER:HB2	2.00	0.42
1:D:331:GLY:HA2	1:D:539:GLY:CA	2.49	0.42
2:F:15:PHE:O	2:F:18:ARG:HB2	2.19	0.42
1:A:108:PRO:HB3	1:A:555:ASN:CG	2.40	0.42
1:A:173:PRO:HG3	6:A:961:HOH:O	2.19	0.42
1:A:276:THR:HG22	1:A:277:ILE:N	2.33	0.42
1:A:99:LEU:O	1:A:535:PHE:HZ	2.02	0.42
1:A:101:SER:OG	1:A:544:GLN:O	2.35	0.42
2:C:36:ASP:O	2:C:39:ASN:N	2.41	0.42
1:D:129:PHE:HZ	1:D:218:TYR:CZ	2.37	0.42
1:D:464:SER:HA	1:D:476:ALA:O	2.20	0.42
2:E:74:VAL:HA	6:E:428:HOH:O	2.20	0.42
2:F:146:GLY:HA3	6:F:428:HOH:O	2.19	0.42
2:F:168:GLU:OE1	2:F:175:ILE:HG12	2.19	0.42
1:A:288:TYR:HA	1:A:318:HIS:O	2.19	0.42
1:A:81:VAL:HG21	1:A:110:PHE:CE2	2.54	0.42
2:C:24:ARG:HG3	2:C:30:PHE:CE1	2.54	0.42
2:C:72:GLN:HG2	2:C:152:TYR:HE1	1.84	0.42
1:D:19:GLU:O	1:D:23:ASN:N	2.50	0.42
1:D:433:ILE:C	1:D:435:LYS:H	2.22	0.42
1:D:450:LYS:HG2	1:D:450:LYS:H	1.54	0.42
1:D:113:PHE:HB2	4:D:602:ATP:O2A	2.19	0.42
2:E:50:ILE:HG23	2:E:51:HIS:H	1.85	0.42
2:E:69:ASN:OD1	2:F:96:ARG:NE	2.53	0.42
2:F:126:LYS:HB3	2:F:126:LYS:HE3	1.87	0.42
1:A:146:GLN:HB2	1:A:148:ILE:HG23	2.01	0.42
1:A:28:GLN:NE2	1:A:356:PRO:O	2.53	0.42
1:A:253:ARG:HG3	1:A:484:GLU:HB3	2.02	0.42
1:A:498:ASP:OD1	1:A:518:LEU:HD22	2.20	0.42
1:A:76:TYR:HD1	1:A:88:ILE:HG12	1.85	0.42
1:D:363:PHE:HB2	1:D:388:TYR:HD2	1.84	0.42
1:D:154:TYR:CD2	1:D:559:LEU:HG	2.55	0.42
1:D:93:PRO:HG2	2:E:184:ALA:CB	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:71:VAL:HG13	2:F:152:TYR:CE1	2.55	0.42
1:A:317:ARG:HA	1:A:320:ALA:HB3	2.02	0.42
2:B:169:LYS:NZ	6:B:401:HOH:O	2.04	0.42
1:D:213:ARG:HH21	1:D:296:PRO:HD3	1.85	0.42
1:D:451:ARG:HH11	1:D:454:GLU:CD	2.23	0.42
1:D:531:ILE:HD11	1:D:561:ILE:HD11	2.01	0.42
1:D:92:HIS:CE1	2:E:185:TRP:CD1	2.89	0.42
2:E:207:ALA:O	2:E:211:GLU:HB2	2.20	0.42
2:C:98:TRP:O	2:C:98:TRP:CE3	2.73	0.42
1:D:150:SER:HB3	1:D:167:THR:CA	2.50	0.42
1:D:273:LEU:HA	1:D:276:THR:HG23	2.02	0.42
1:D:548:PRO:HB2	6:D:829:HOH:O	2.20	0.42
1:A:207:LEU:HD22	6:A:876:HOH:O	2.20	0.41
1:A:139:ASP:H	1:A:217:GLN:HE21	1.66	0.41
1:A:290:LEU:N	1:A:319:TYR:O	2.53	0.41
1:A:400:ARG:NH1	1:A:400:ARG:HG2	2.34	0.41
1:A:427:LEU:O	1:A:428:ILE:HG12	2.20	0.41
1:A:451:ARG:NH1	1:A:454:GLU:CD	2.73	0.41
1:A:110:PHE:HE1	1:A:556:ALA:HB2	1.85	0.41
1:D:333:SER:O	1:D:335:GLY:N	2.53	0.41
1:D:362:GLU:HB2	1:D:391:VAL:HG12	2.02	0.41
1:D:496:CYS:N	1:D:499:ARG:NH1	2.68	0.41
1:D:56:ASP:HB2	1:D:59:GLU:OE1	2.20	0.41
2:E:132:VAL:HG21	2:E:175:ILE:CG2	2.49	0.41
1:A:111:ILE:HD12	1:A:398:LEU:HG	2.02	0.41
1:D:111:ILE:HG21	1:D:398:LEU:HD21	2.02	0.41
1:D:146:GLN:OE1	1:D:148:ILE:HG12	2.20	0.41
1:D:158:GLY:N	6:D:763:HOH:O	2.46	0.41
1:D:175:PHE:O	1:D:179:MET:HB2	2.20	0.41
1:D:192:VAL:HG21	1:D:204:CYS:HB3	2.02	0.41
2:E:139:LEU:H	2:E:139:LEU:HG	1.61	0.41
2:E:17:MET:SD	2:E:199:LEU:HD22	2.60	0.41
2:E:98:TRP:C	2:E:98:TRP:HE3	2.23	0.41
2:F:121:GLN:O	2:F:125:LYS:N	2.52	0.41
1:A:204:CYS:O	1:A:207:LEU:HB3	2.19	0.41
2:B:11:TRP:CD1	2:B:11:TRP:N	2.88	0.41
2:B:11:TRP:HZ3	2:B:204:LYS:HZ2	1.67	0.41
2:C:144:TYR:HB3	2:C:154:ASP:CG	2.41	0.41
1:D:167:THR:O	1:D:171:ARG:HG2	2.20	0.41
1:D:20:MET:HA	1:D:23:ASN:HB2	2.02	0.41
1:D:558:VAL:O	1:D:561:ILE:HG13	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:331:GLY:HA2	1:A:539:GLY:CA	2.51	0.41
2:B:56:VAL:HA	2:B:64:VAL:O	2.20	0.41
2:C:179:SER:HB3	2:C:182:LEU:CD2	2.51	0.41
2:C:98:TRP:O	2:C:102:VAL:HG23	2.19	0.41
1:D:107:ARG:NE	1:D:108:PRO:HD2	2.34	0.41
1:D:504:ALA:O	1:D:507:VAL:HB	2.20	0.41
1:D:32:LEU:HD13	1:D:61:PHE:HE2	1.85	0.41
1:D:41:SER:HB2	2:E:147:GLY:O	2.20	0.41
2:E:26:LYS:HZ3	2:E:82:ASN:C	2.24	0.41
2:E:66:GLU:HG2	2:E:69:ASN:HB3	2.02	0.41
2:F:98:TRP:O	2:F:98:TRP:CE3	2.73	0.41
1:A:199:HIS:NE2	1:A:484:GLU:HB2	2.35	0.41
1:A:503:ASP:O	1:A:507:VAL:HG23	2.20	0.41
2:B:14:MET:HG2	2:B:159:THR:O	2.21	0.41
2:C:169:LYS:HZ1	2:C:206:VAL:HG11	1.86	0.41
1:D:150:SER:HB2	1:D:170:TYR:CE1	2.56	0.41
1:D:190:ASP:O	1:D:194:PHE:N	2.45	0.41
1:D:379:LEU:HD11	1:D:417:PRO:HG3	2.02	0.41
1:D:440:ASP:OD2	1:D:502:ILE:HG13	2.21	0.41
1:D:121:THR:HB	3:D:601:JAA:C13	2.50	0.41
2:F:132:VAL:HG23	2:F:182:LEU:HD22	2.01	0.41
1:A:232:ARG:HD2	6:A:910:HOH:O	2.21	0.41
1:A:275:GLU:O	6:A:721:HOH:O	2.21	0.41
1:A:77:ILE:HA	1:A:80:MET:HG3	2.01	0.41
2:B:133:LYS:O	2:B:136:GLU:HB3	2.21	0.41
2:C:214:LYS:HB3	2:C:214:LYS:HE2	1.93	0.41
1:D:187:CYS:HB2	1:D:208:SER:O	2.19	0.41
1:D:432:ASN:H	1:D:432:ASN:ND2	2.19	0.41
1:D:565:ASN:ND2	6:D:791:HOH:O	2.53	0.41
2:F:141:ASP:N	2:F:141:ASP:OD1	2.53	0.41
1:A:115:ASP:O	1:A:119:GLU:HG2	2.21	0.41
1:A:250:LEU:HD11	1:A:260:ARG:NE	2.35	0.41
1:A:460:ILE:HD11	1:A:480:GLU:CD	2.41	0.41
2:C:62:LYS:NZ	6:C:425:HOH:O	2.36	0.41
1:D:9:ASP:OD2	1:D:12:ARG:NH2	2.54	0.41
1:D:133:ASN:CG	1:D:137:PRO:HA	2.41	0.41
1:D:175:PHE:N	6:D:769:HOH:O	2.54	0.41
1:D:215:GLN:HB2	6:D:822:HOH:O	2.20	0.41
1:D:105:GLN:HA	1:D:430:SER:HB3	2.02	0.41
1:D:225:HIS:NE2	1:D:529:ARG:HD3	2.35	0.41
1:D:538:LEU:HD22	1:D:544:GLN:HG2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:544:GLN:O	1:D:545:PHE:HD1	2.03	0.41
1:A:170:TYR:HA	1:A:175:PHE:CD2	2.56	0.41
1:A:233:THR:O	1:A:237:VAL:HG22	2.21	0.41
1:A:284:LEU:HG	1:A:284:LEU:H	1.59	0.41
1:A:363:PHE:CE1	1:A:390:VAL:HG22	2.55	0.41
1:A:410:ILE:HD11	1:A:420:LYS:HE2	2.03	0.41
1:A:452:LEU:HD23	1:A:481:ILE:HG21	2.02	0.41
1:A:99:LEU:HD13	1:A:548:PRO:HG3	2.02	0.41
2:B:62:LYS:HD3	2:C:90:TYR:CD2	2.56	0.41
2:B:81:LYS:HG3	2:B:82:ASN:H	1.85	0.41
1:D:360:TYR:CZ	1:D:362:GLU:OE2	2.73	0.41
1:D:399:TYR:H	1:D:401:TYR:HD1	1.67	0.41
1:D:485:THR:OG1	1:D:486:ASN:N	2.53	0.41
1:D:93:PRO:HG2	2:E:184:ALA:HB3	2.02	0.41
2:F:211:GLU:HB3	6:F:490:HOH:O	2.20	0.41
1:A:196:PRO:HD2	1:A:256:VAL:HG11	2.03	0.41
1:A:536:LEU:HD23	1:A:536:LEU:HA	1.91	0.41
2:B:136:GLU:HB2	2:B:182:LEU:HD21	2.03	0.41
2:B:22:ALA:HB2	2:B:71:VAL:HG23	2.02	0.41
2:C:90:TYR:OH	6:C:409:HOH:O	2.21	0.41
1:D:226:GLY:O	1:D:229:HIS:ND1	2.54	0.41
1:D:495:ASN:C	1:D:499:ARG:NH1	2.74	0.41
1:D:478:PHE:CD1	1:D:521:ARG:HB2	2.56	0.41
2:F:68:LEU:HD23	2:F:103:ASP:OD2	2.21	0.41
1:A:100:SER:HB3	1:A:109:LYS:HD3	2.03	0.41
1:A:28:GLN:O	1:A:360:TYR:HD1	2.04	0.41
1:A:90:THR:CG2	1:A:397:GLY:HA2	2.51	0.41
1:A:403:LEU:H	1:A:403:LEU:HG	1.68	0.41
2:C:18:ARG:NH2	2:C:103:ASP:OD1	2.46	0.41
2:C:187:LYS:H	2:C:187:LYS:HG3	1.75	0.41
1:D:368:GLU:HB2	1:D:374:GLU:OE2	2.21	0.41
1:D:444:SER:HA	1:D:500:ALA:HB1	2.03	0.41
1:D:549:ARG:HD3	1:D:549:ARG:HA	1.64	0.41
1:D:77:ILE:CD1	1:D:110:PHE:HB3	2.51	0.41
2:E:166:ALA:O	2:E:169:LYS:HG2	2.21	0.41
2:E:202:SER:O	2:E:206:VAL:HG23	2.21	0.41
2:E:37:PHE:HA	2:E:40:LYS:CG	2.51	0.41
2:F:14:MET:SD	6:F:402:HOH:O	2.62	0.41
1:A:301:VAL:HB	1:A:325:LEU:HD12	2.03	0.41
1:A:442:GLN:HG2	1:A:462:PHE:CZ	2.56	0.41
1:A:76:TYR:HB2	1:A:88:ILE:HG21	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:103:ASP:O	2:C:107:THR:OG1	2.32	0.41
1:D:323:LEU:HA	1:D:324:PRO:HD3	1.89	0.41
1:D:124:LEU:HD22	1:D:336:TRP:CZ2	2.56	0.41
1:D:367:SER:O	1:D:367:SER:OG	2.36	0.41
1:D:552:LYS:C	1:D:554:SER:H	2.16	0.41
2:E:11:TRP:HH2	2:E:204:LYS:HB3	1.86	0.41
2:E:26:LYS:HE3	2:E:78:TRP:O	2.21	0.41
2:F:180:PRO:HG2	2:F:181:LYS:HG2	2.03	0.41
2:F:211:GLU:HA	2:F:214:LYS:HG2	2.02	0.41
2:B:88:ASP:HA	2:B:89:PRO:HD3	1.97	0.40
2:C:98:TRP:CH2	2:C:135:LEU:HG	2.56	0.40
2:C:181:LYS:HA	2:C:184:ALA:HB3	2.03	0.40
1:D:143:LYS:CA	1:D:184:SER:HB2	2.51	0.40
1:D:328:HIS:CG	1:D:329:ASP:N	2.89	0.40
2:F:98:TRP:CZ3	2:F:101:PHE:HD2	2.39	0.40
1:A:305:MET:HB3	1:A:347:PRO:HB3	2.03	0.40
1:A:389:GLU:HG3	1:A:405:ASP:O	2.22	0.40
1:A:538:LEU:HD23	1:A:544:GLN:HG2	2.02	0.40
2:C:102:VAL:O	2:C:106:PHE:HB3	2.20	0.40
1:D:300:TYR:HE1	1:D:302:TYR:HB2	1.86	0.40
1:A:169:VAL:O	1:A:175:PHE:HB2	2.21	0.40
1:A:199:HIS:HD2	6:A:840:HOH:O	2.04	0.40
1:A:203:TYR:CE1	1:A:237:VAL:HB	2.57	0.40
1:A:211:LEU:O	1:A:212:PHE:HD1	2.05	0.40
1:A:238:TRP:CA	1:A:241:ILE:HG12	2.52	0.40
1:A:345:LEU:HD13	1:A:350:ALA:HA	2.02	0.40
1:A:457:ILE:HG23	1:A:482:SER:OG	2.20	0.40
1:A:87:PRO:HD2	2:B:188:ARG:CB	2.49	0.40
2:B:149:SER:HB3	2:B:150:PHE:H	1.58	0.40
1:D:222:VAL:HG12	1:D:223:PHE:CD1	2.56	0.40
1:D:455:GLU:OE1	1:D:485:THR:HB	2.21	0.40
1:D:164:THR:HG23	1:D:557:LYS:HG2	2.03	0.40
1:D:519:GLU:HB3	1:D:571:PHE:CD2	2.56	0.40
1:A:460:ILE:HG12	6:A:804:HOH:O	2.22	0.40
1:A:435:LYS:CE	1:A:549:ARG:HH22	2.35	0.40
1:A:93:PRO:HG2	2:B:184:ALA:CB	2.51	0.40
2:C:166:ALA:HA	2:C:206:VAL:HG22	2.03	0.40
1:D:164:THR:HB	1:D:167:THR:CG2	2.51	0.40
1:D:295:PHE:CD1	1:D:295:PHE:N	2.89	0.40
1:D:527:THR:HA	1:D:530:LYS:HE2	2.02	0.40
2:E:150:PHE:HE2	2:E:189:CYS:SG	2.44	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:40:LYS:HG3	6:E:459:HOH:O	2.20	0.40
2:F:15:PHE:CE1	5:F:301:GSH:HB12	2.57	0.40
1:A:114:THR:HB	1:A:116:GLU:CD	2.42	0.40
1:A:340:ASN:ND2	1:A:343:PRO:HA	2.36	0.40
2:B:186:ALA:O	2:B:190:MET:HG2	2.22	0.40
2:C:116:LYS:HE3	6:C:448:HOH:O	2.21	0.40
2:C:60:ASN:ND2	2:C:60:ASN:O	2.55	0.40
1:D:107:ARG:HH11	1:D:107:ARG:HD3	1.47	0.40
1:D:202:LEU:HD21	1:D:229:HIS:NE2	2.35	0.40
1:D:22:ARG:HH11	1:D:414:ASN:HB3	1.87	0.40
1:D:375:LYS:H	1:D:375:LYS:HG2	1.71	0.40
2:F:98:TRP:CD2	2:F:138:GLU:OE2	2.74	0.40
2:F:214:LYS:NZ	6:F:416:HOH:O	2.33	0.40

All (6) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:ARG:NH1	2:B:168:GLU:OE2[1_565]	1.86	0.34
1:D:19:GLU:OE2	2:E:172:ASN:ND2[1_565]	1.98	0.22
6:E:406:HOH:O	6:F:425:HOH:O[1_655]	2.07	0.13
1:A:234:PHE:O	2:F:177:SER:OG[1_554]	2.12	0.08
1:D:299:LYS:NZ	1:D:431:ILE:O[1_455]	2.15	0.05
6:A:882:HOH:O	6:B:509:HOH:O[1_565]	2.17	0.03

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	567/575 (99%)	518 (91%)	39 (7%)	10 (2%)	8 2
1	D	567/575 (99%)	509 (90%)	45 (8%)	13 (2%)	6 1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	212/223 (95%)	195 (92%)	13 (6%)	4 (2%)	8	2
2	C	212/223 (95%)	191 (90%)	17 (8%)	4 (2%)	8	2
2	E	212/223 (95%)	190 (90%)	20 (9%)	2 (1%)	17	10
2	F	212/223 (95%)	191 (90%)	15 (7%)	6 (3%)	5	1
All	All	1982/2042 (97%)	1794 (90%)	149 (8%)	39 (2%)	7	2

All (39) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	85	THR
1	A	540	SER
2	C	140	GLY
1	D	53	ASN
1	D	54	ALA
1	D	151	SER
1	D	513	LYS
1	D	542	ALA
2	F	140	GLY
2	F	174	SER
1	A	88	ILE
1	A	368	GLU
1	A	542	ALA
2	B	26	LYS
2	B	140	GLY
1	D	437	THR
1	D	540	SER
2	E	136	GLU
2	F	180	PRO
1	A	369	THR
1	A	437	THR
1	A	509	SER
2	C	66	GLU
1	D	165	ALA
1	D	334	GLU
2	E	66	GLU
2	F	66	GLU
1	A	93	PRO
2	B	27	GLY
2	B	79	PRO
1	D	369	THR
1	D	553	PRO

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Mol	Chain	Res	Type
2	C	141	ASP
1	D	512	CYS
1	A	553	PRO
2	C	180	PRO
2	F	27	GLY
2	F	12	PRO
1	D	433	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%)	469 (94%)	30 (6%)	19	14
1	D	499/505 (99%)	464 (93%)	35 (7%)	15	9
2	B	187/195 (96%)	180 (96%)	7 (4%)	34	31
2	C	187/195 (96%)	175 (94%)	12 (6%)	17	12
2	E	187/195 (96%)	178 (95%)	9 (5%)	25	21
2	F	187/195 (96%)	177 (95%)	10 (5%)	22	18
All	All	1746/1790 (98%)	1643 (94%)	103 (6%)	19	14

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

Mol	Chain	Res	Type
1	A	15	ASP
1	A	65	VAL
1	A	89	LEU
1	A	99	LEU
1	A	114	THR
1	A	125	PHE
1	A	145	LEU
1	A	152	LYS
1	A	200	GLN
1	A	211	LEU
1	A	213	ARG

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Mol	Chain	Res	Type
1	A	227	LEU
1	A	245	ILE
1	A	276	THR
1	A	282	MET
1	A	328	HIS
1	A	369	THR
1	A	379	LEU
1	A	402	ARG
1	A	423	CYS
1	A	429	LEU
1	A	432	ASN
1	A	433	ILE
1	A	460	ILE
1	A	494	CYS
1	A	497	LEU
1	A	535	PHE
1	A	536	LEU
1	A	563	CYS
1	A	567	VAL
2	B	11	TRP
2	B	40	LYS
2	B	108	ASP
2	B	110	GLN
2	B	132	VAL
2	B	153	VAL
2	B	206	VAL
2	C	33	ARG
2	C	80	GLU
2	C	81	LYS
2	C	84	PHE
2	C	87	SER
2	C	132	VAL
2	C	135	LEU
2	C	136	GLU
2	C	157	LEU
2	C	176	GLU
2	C	183	ILE
2	C	216	ASN
1	D	77	ILE
1	D	90	THR
1	D	110	PHE
1	D	111	ILE

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Mol	Chain	Res	Type
1	D	117	LEU
1	D	126	ARG
1	D	140	ASP
1	D	143	LYS
1	D	153	GLN
1	D	169	VAL
1	D	170	TYR
1	D	182	ILE
1	D	197	ASP
1	D	228	VAL
1	D	276	THR
1	D	278	ARG
1	D	279	THR
1	D	316	LEU
1	D	326	VAL
1	D	329	ASP
1	D	373	GLU
1	D	391	VAL
1	D	423	CYS
1	D	426	ASN
1	D	450	LYS
1	D	455	GLU
1	D	457	ILE
1	D	474	HIS
1	D	494	CYS
1	D	512	CYS
1	D	518	LEU
1	D	535	PHE
1	D	545	PHE
1	D	551	VAL
1	D	573	THR
2	E	9	ASP
2	E	45	LEU
2	E	66	GLU
2	E	98	TRP
2	E	139	LEU
2	E	153	VAL
2	E	164	PHE
2	E	168	GLU
2	E	203	GLU
2	F	32	TYR
2	F	43	LEU

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Mol	Chain	Res	Type
2	F	84	PHE
2	F	134	ILE
2	F	135	LEU
2	F	136	GLU
2	F	139	LEU
2	F	170	PHE
2	F	206	VAL
2	F	211	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	92	HIS
1	A	205	HIS
1	A	217	GLN
1	A	544	GLN
2	B	48	ASN
2	B	72	GLN
1	D	39	ASN
1	D	123	GLN
1	D	205	HIS
1	D	217	GLN
1	D	495	ASN
1	D	534	HIS
1	D	544	GLN
1	D	565	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry

8 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
4	ATP	D	602	-	26,33,33	4.95	14 (53%)	31,52,52	2.99	15 (48%)
4	ATP	A	602	-	26,33,33	5.03	15 (57%)	31,52,52	3.07	17 (54%)
3	JAA	D	601	-	12,15,15	5.83	6 (50%)	12,19,19	3.34	7 (58%)
5	GSH	E	301	-	12,19,19	1.78	4 (33%)	15,24,24	3.23	6 (40%)
5	GSH	C	301	-	12,19,19	1.67	3 (25%)	15,24,24	2.81	3 (20%)
5	GSH	F	301	-	12,19,19	1.65	3 (25%)	15,24,24	2.92	7 (46%)
3	JAA	A	601	-	12,15,15	5.75	6 (50%)	12,19,19	2.98	6 (50%)
5	GSH	B	301	-	12,19,19	1.69	3 (25%)	15,24,24	3.22	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
4	ATP	D	602	-	-	6/18/38/38	0/3/3/3
4	ATP	A	602	-	-	6/18/38/38	0/3/3/3
3	JAA	D	601	-	-	4/7/22/22	0/1/1/1
5	GSH	E	301	-	-	2/18/24/24	-
5	GSH	C	301	-	-	4/18/24/24	-
5	GSH	F	301	-	-	3/18/24/24	-
3	JAA	A	601	-	-	1/7/22/22	0/1/1/1
5	GSH	B	301	-	-	1/18/24/24	-

All (54) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	602	ATP	O4'-C1'	13.93	1.60	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	602	ATP	O4'-C1'	13.22	1.59	1.41
3	D	601	JAA	C05-C08	-12.52	1.31	1.52
3	A	601	JAA	C05-C08	-12.37	1.31	1.52
4	A	602	ATP	C2'-C1'	-12.26	1.35	1.53
3	D	601	JAA	C06-C04	-11.47	1.23	1.53
3	A	601	JAA	C06-C04	-11.29	1.24	1.53
4	D	602	ATP	C2'-C1'	-10.93	1.37	1.53
4	A	602	ATP	O4'-C4'	-10.08	1.22	1.45
4	D	602	ATP	O4'-C4'	-9.81	1.23	1.45
4	D	602	ATP	C4-N3	6.79	1.45	1.35
4	A	602	ATP	C4-N3	6.37	1.44	1.35
3	A	601	JAA	C07-C08	6.21	1.61	1.51
3	A	601	JAA	C10-C04	-6.01	1.46	1.53
3	D	601	JAA	C10-C04	-5.95	1.46	1.53
4	A	602	ATP	C2-N1	5.91	1.44	1.33
4	D	602	ATP	C2-N1	5.81	1.44	1.33
3	D	601	JAA	C07-C08	5.80	1.60	1.51
4	A	602	ATP	C6-N6	-5.63	1.13	1.34
4	A	602	ATP	C2'-C3'	-5.47	1.38	1.53
4	D	602	ATP	C6-N6	-5.44	1.14	1.34
4	D	602	ATP	O3'-C3'	5.28	1.55	1.43
3	D	601	JAA	C05-C04	4.84	1.66	1.54
3	A	601	JAA	C05-C04	4.79	1.66	1.54
3	D	601	JAA	C09-C05	-4.67	1.47	1.54
4	A	602	ATP	O3'-C3'	4.65	1.53	1.43
4	D	602	ATP	C2'-C3'	-4.53	1.40	1.53
3	A	601	JAA	C09-C05	-3.81	1.48	1.54
4	A	602	ATP	C5'-C4'	-3.40	1.41	1.51
4	D	602	ATP	O5'-C5'	-3.36	1.31	1.44
4	D	602	ATP	C5'-C4'	-3.30	1.41	1.51
4	A	602	ATP	C3'-C4'	3.27	1.61	1.53
4	D	602	ATP	C3'-C4'	3.26	1.61	1.53
4	A	602	ATP	C8-N7	-3.11	1.29	1.34
4	A	602	ATP	O5'-C5'	-3.10	1.32	1.44
5	C	301	GSH	C2-N3	3.09	1.40	1.33
5	B	301	GSH	C2-N3	3.07	1.40	1.33
5	F	301	GSH	C2-N3	3.06	1.40	1.33
5	B	301	GSH	CA2-N2	-2.98	1.39	1.45
5	E	301	GSH	CA2-N2	-2.97	1.39	1.45
5	E	301	GSH	C2-N3	2.96	1.40	1.33
5	C	301	GSH	CD1-N2	2.91	1.40	1.34
4	D	602	ATP	C8-N7	-2.91	1.29	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	301	GSH	CA2-N2	-2.90	1.39	1.45
4	A	602	ATP	PG-O1G	-2.64	1.42	1.50
5	E	301	GSH	CD1-N2	2.53	1.39	1.34
5	B	301	GSH	CD1-N2	2.50	1.39	1.34
5	F	301	GSH	CD1-N2	2.48	1.39	1.34
5	E	301	GSH	CB2-CA2	-2.43	1.50	1.53
4	D	602	ATP	PG-O1G	-2.41	1.42	1.50
5	C	301	GSH	CA2-N2	-2.40	1.40	1.45
4	D	602	ATP	PG-O2G	-2.23	1.46	1.54
4	A	602	ATP	PG-O2G	-2.21	1.46	1.54
4	A	602	ATP	C5-C4	-2.09	1.35	1.40

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	301	GSH	CA2-CB2-SG2	-9.67	103.32	114.19
5	B	301	GSH	CA2-CB2-SG2	-8.98	104.10	114.19
5	E	301	GSH	CA2-CB2-SG2	-8.72	104.40	114.19
5	F	301	GSH	CA2-CB2-SG2	-7.93	105.28	114.19
4	A	602	ATP	C4-C5-N7	-7.49	101.60	109.40
4	D	602	ATP	C3'-C2'-C1'	7.32	112.00	100.98
4	A	602	ATP	PA-O3A-PB	-7.25	107.94	132.83
4	D	602	ATP	C4-C5-N7	-6.68	102.44	109.40
4	D	602	ATP	O2G-PG-O3B	5.89	124.40	104.64
3	D	601	JAA	C07-C06-C04	-5.78	98.37	104.41
4	D	602	ATP	PA-O3A-PB	-5.75	113.09	132.83
3	D	601	JAA	C09-C11-C13	-5.57	105.71	126.40
4	A	602	ATP	O2G-PG-O3B	5.51	123.12	104.64
3	A	601	JAA	C07-C06-C04	-5.10	99.08	104.41
3	A	601	JAA	C06-C07-C08	-5.05	100.35	105.42
5	E	301	GSH	CB2-CA2-N2	-4.79	104.46	111.28
4	A	602	ATP	O4'-C1'-C2'	-4.71	100.04	106.93
5	B	301	GSH	CB2-CA2-N2	-4.53	104.83	111.28
5	F	301	GSH	CB2-CA2-N2	-4.35	105.08	111.28
3	D	601	JAA	C06-C04-C10	-4.35	105.88	113.67
3	D	601	JAA	O01-C08-C05	4.30	131.13	125.58
4	A	602	ATP	C5'-C4'-C3'	-4.24	99.30	115.18
3	A	601	JAA	C06-C04-C10	-4.23	106.09	113.67
5	B	301	GSH	CB1-CG1-CD1	4.09	122.17	113.04
3	D	601	JAA	C06-C07-C08	-4.08	101.33	105.42
5	E	301	GSH	CB1-CG1-CD1	3.96	121.89	113.04
5	E	301	GSH	CG1-CD1-N2	-3.89	109.08	115.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	602	ATP	O4'-C4'-C3'	3.73	112.49	105.11
3	A	601	JAA	C09-C11-C13	-3.71	112.63	126.40
5	B	301	GSH	CG1-CD1-N2	-3.66	109.49	115.83
4	A	602	ATP	N3-C2-N1	-3.63	123.01	128.68
3	A	601	JAA	O01-C08-C05	3.62	130.24	125.58
5	F	301	GSH	CG1-CD1-N2	-3.41	109.92	115.83
4	A	602	ATP	O4'-C4'-C3'	3.40	111.85	105.11
4	D	602	ATP	N3-C2-N1	-3.37	123.41	128.68
4	A	602	ATP	C5-C6-N1	-3.33	112.80	120.35
4	D	602	ATP	C5-C6-N1	-3.30	112.86	120.35
4	D	602	ATP	C5'-C4'-C3'	-3.22	103.11	115.18
3	D	601	JAA	C07-C08-C05	-3.22	103.60	109.05
4	A	602	ATP	C2'-C3'-C4'	-3.15	96.53	102.64
4	A	602	ATP	N6-C6-N1	3.12	125.04	118.57
5	F	301	GSH	CB1-CG1-CD1	3.11	119.97	113.04
5	E	301	GSH	OE1-CD1-CG1	2.88	127.28	122.02
4	D	602	ATP	N6-C6-N1	2.84	124.47	118.57
5	B	301	GSH	OE1-CD1-CG1	2.81	127.15	122.02
3	A	601	JAA	C07-C08-C05	-2.79	104.32	109.05
4	D	602	ATP	C2-N1-C6	2.79	123.52	118.75
4	A	602	ATP	PA-O5'-C5'	-2.72	105.73	121.68
4	D	602	ATP	O3'-C3'-C2'	2.65	120.38	111.82
4	A	602	ATP	C2-N1-C6	2.64	123.27	118.75
5	C	301	GSH	CB2-CA2-N2	-2.64	107.53	111.28
5	E	301	GSH	CA3-N3-C2	-2.62	118.57	122.34
4	D	602	ATP	C1'-N9-C4	2.60	131.21	126.64
5	F	301	GSH	OE1-CD1-CG1	2.58	126.73	122.02
4	D	602	ATP	O3B-PG-O1G	-2.57	96.91	111.19
4	A	602	ATP	O3'-C3'-C4'	2.51	118.31	111.05
5	B	301	GSH	CG1-CB1-CA1	-2.34	108.37	113.84
4	A	602	ATP	C3'-C2'-C1'	2.25	104.37	100.98
4	A	602	ATP	C1'-N9-C4	2.21	130.52	126.64
5	F	301	GSH	C2-CA2-N2	-2.19	105.20	111.16
4	D	602	ATP	PB-O3B-PG	-2.18	125.34	132.83
4	A	602	ATP	PB-O3B-PG	-2.18	125.34	132.83
4	A	602	ATP	O2'-C2'-C1'	-2.17	102.85	110.85
4	D	602	ATP	PA-O5'-C5'	-2.16	109.03	121.68
5	F	301	GSH	CA3-N3-C2	-2.09	119.33	122.34
5	C	301	GSH	CB1-CG1-CD1	2.04	117.59	113.04
3	D	601	JAA	C10-C04-C05	2.02	119.40	114.74

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	602	ATP	C5'-O5'-PA-O2A
4	D	602	ATP	C5'-O5'-PA-O3A
4	D	602	ATP	O4'-C4'-C5'-O5'
4	D	602	ATP	C3'-C4'-C5'-O5'
4	A	602	ATP	C5'-O5'-PA-O3A
4	A	602	ATP	O4'-C4'-C5'-O5'
4	A	602	ATP	C3'-C4'-C5'-O5'
5	C	301	GSH	N1-CA1-CB1-CG1
5	C	301	GSH	C1-CA1-CB1-CG1
5	C	301	GSH	N2-CA2-CB2-SG2
5	C	301	GSH	C2-CA2-CB2-SG2
5	F	301	GSH	N2-CA2-CB2-SG2
5	F	301	GSH	C2-CA2-CB2-SG2
5	B	301	GSH	C1-CA1-CB1-CG1
3	D	601	JAA	C09-C11-C13-C14
5	E	301	GSH	CA1-CB1-CG1-CD1
4	D	602	ATP	PG-O3B-PB-O3A
4	A	602	ATP	PG-O3B-PB-O3A
3	A	601	JAA	C11-C13-C14-C15
4	D	602	ATP	PB-O3B-PG-O1G
3	D	601	JAA	C04-C05-C09-C11
5	E	301	GSH	C1-CA1-CB1-CG1
4	A	602	ATP	C4'-C5'-O5'-PA
3	D	601	JAA	C05-C09-C11-C13
5	F	301	GSH	C3-CA3-N3-C2
4	A	602	ATP	PA-O3A-PB-O1B
3	D	601	JAA	C08-C05-C09-C11

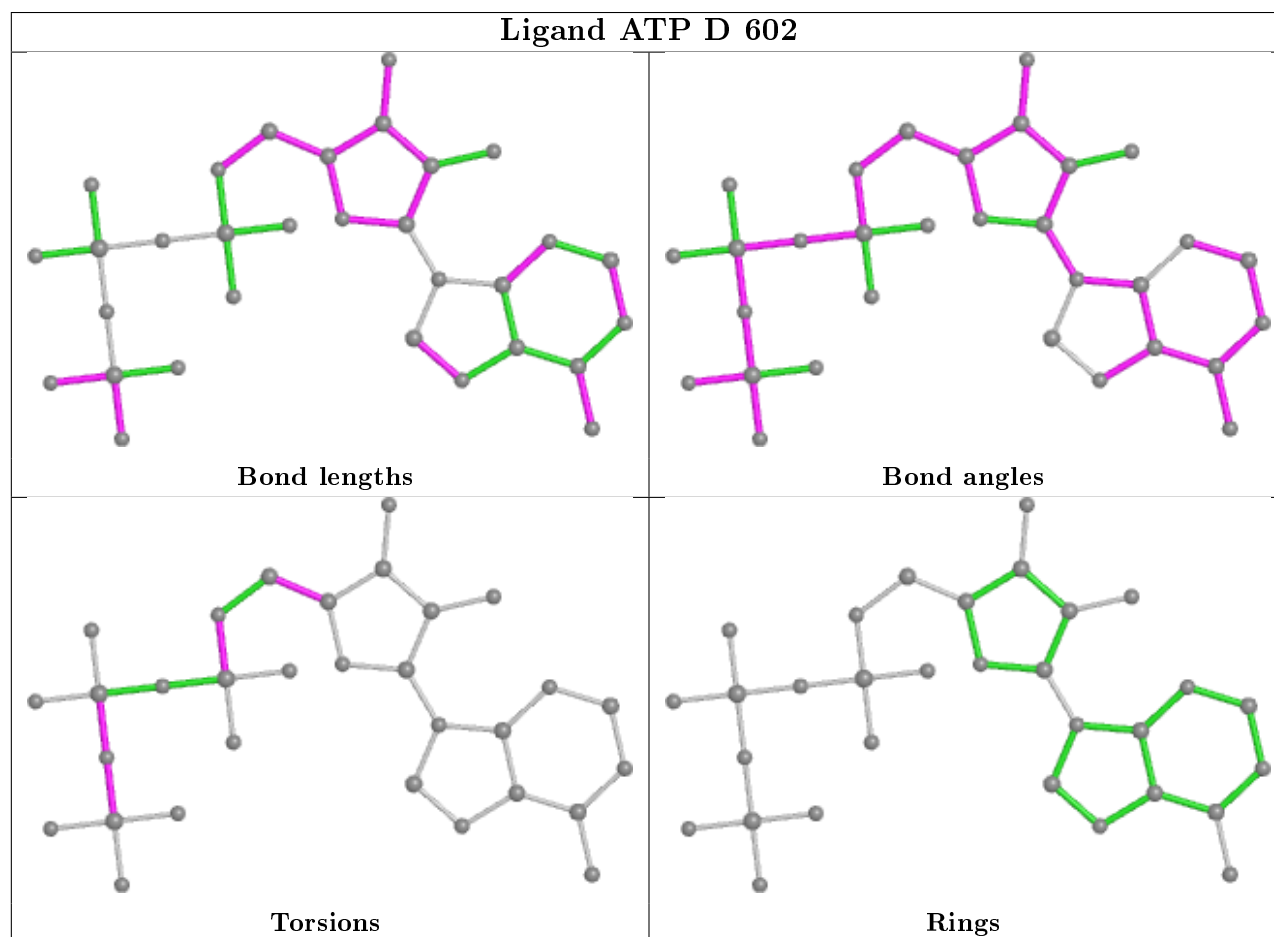
There are no ring outliers.

5 monomers are involved in 37 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	602	ATP	15	0
4	A	602	ATP	17	0
3	D	601	JAA	3	0
5	F	301	GSH	1	0
5	B	301	GSH	2	0

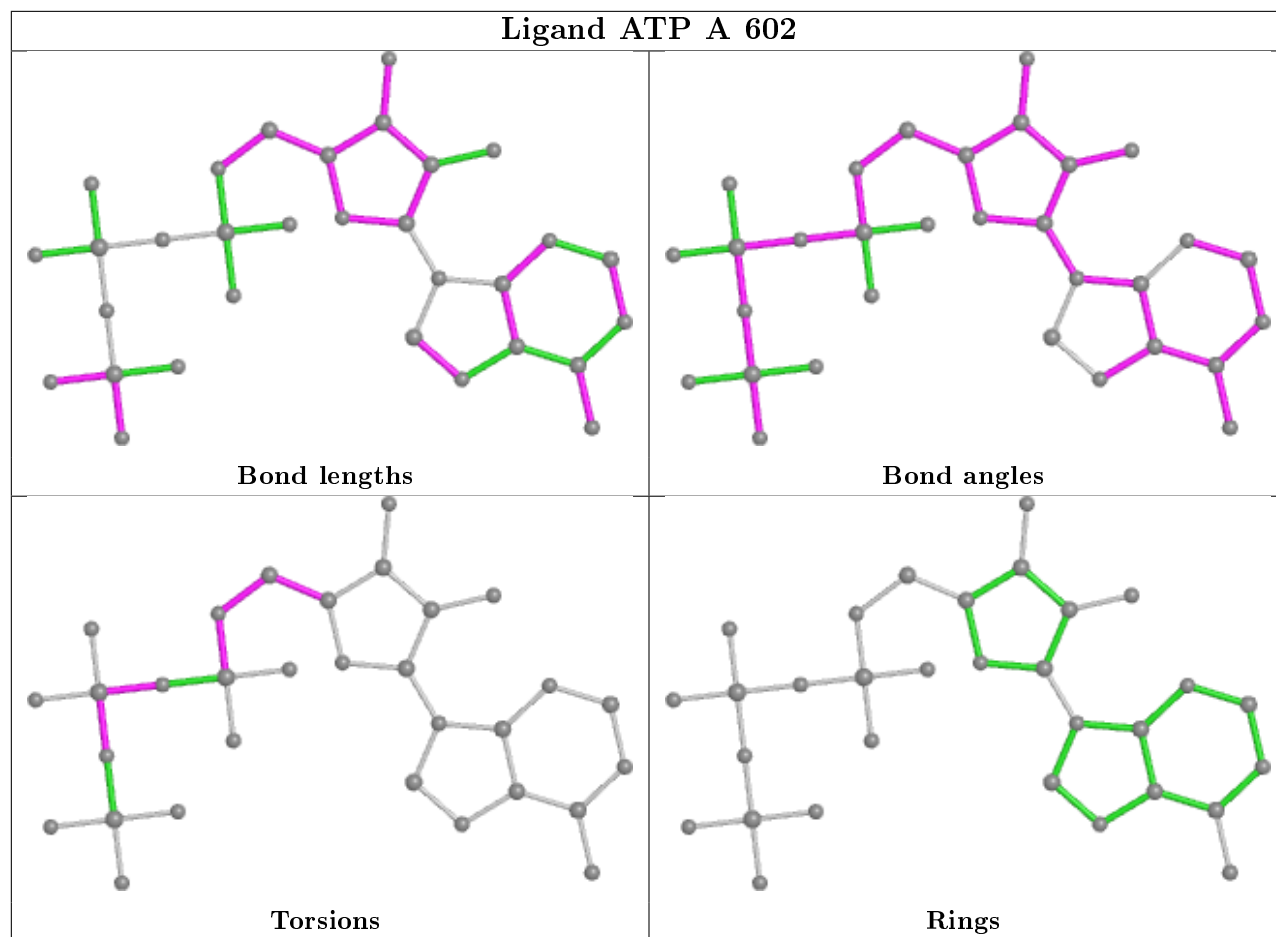
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

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.

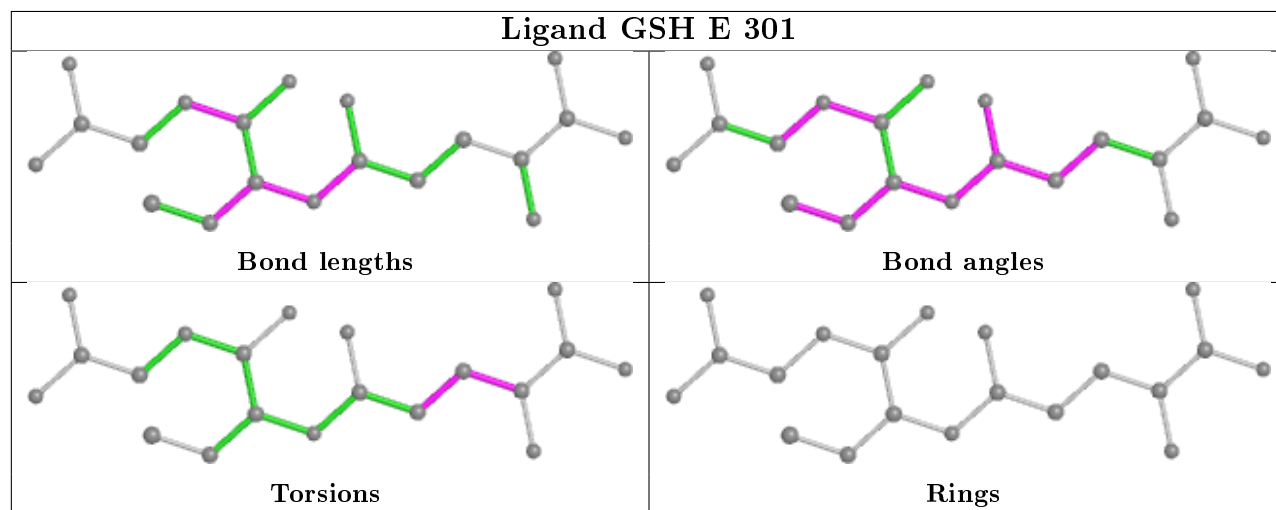


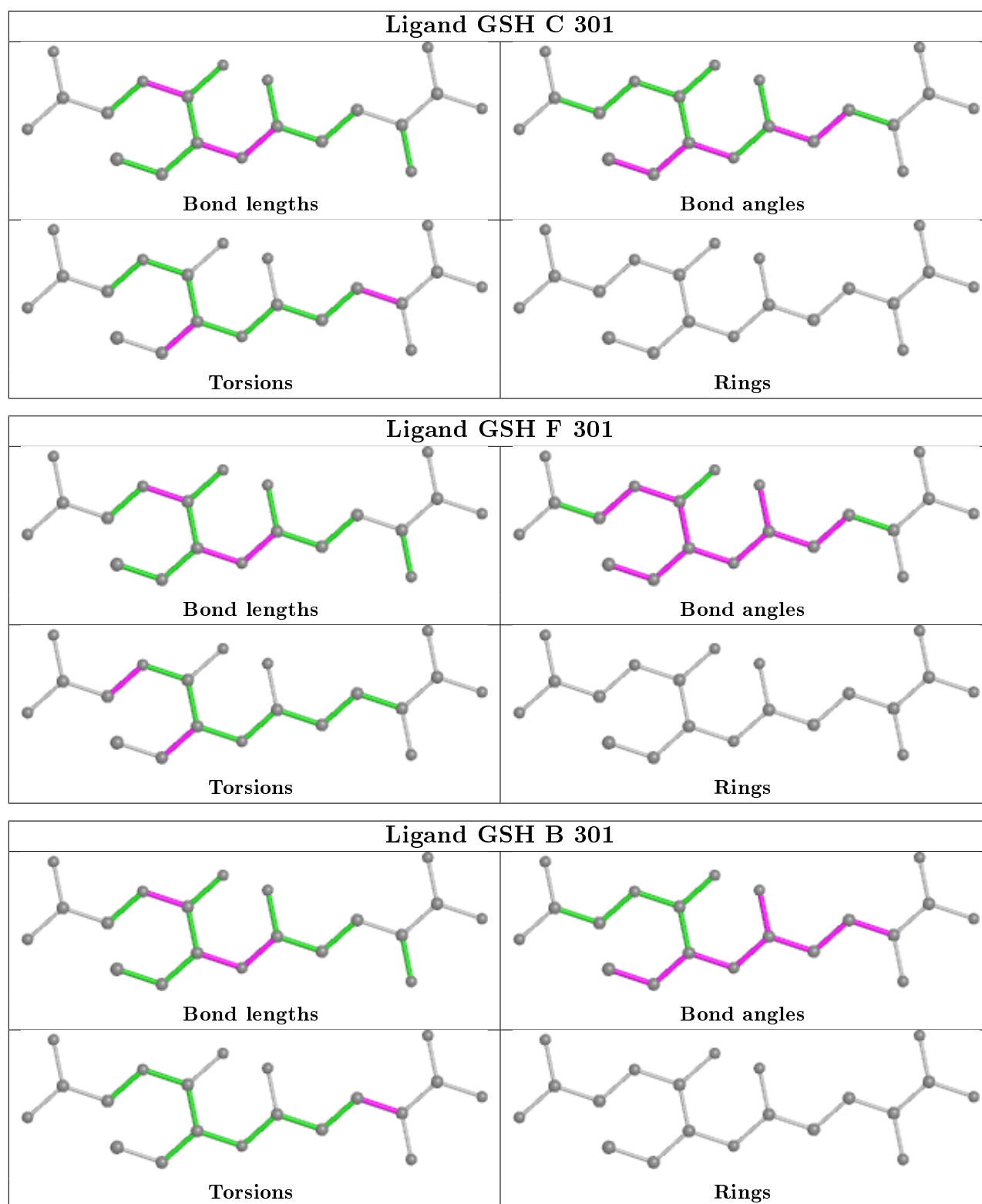


## Ligand ATP A 602



## Ligand GSH E 301





## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	569/575 (98%)	0.88	40 (7%) 16 21	3, 5, 9, 25	0
1	D	569/575 (98%)	0.85	35 (6%) 20 25	2, 5, 9, 24	0
2	B	214/223 (95%)	0.62	9 (4%) 36 44	2, 5, 8, 18	0
2	C	214/223 (95%)	0.55	5 (2%) 60 67	2, 3, 7, 11	0
2	E	214/223 (95%)	0.72	9 (4%) 36 44	3, 5, 8, 22	0
2	F	214/223 (95%)	0.57	6 (2%) 53 61	2, 3, 7, 11	0
All	All	1994/2042 (97%)	0.76	104 (5%) 27 33	2, 5, 8, 25	0

All (104) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	545	PHE	5.0
1	D	474	HIS	4.6
1	D	76	TYR	4.4
2	C	32	TYR	3.9
1	A	65	VAL	3.5
1	D	77	ILE	3.3
1	A	282	MET	3.2
2	B	123	ALA	3.1
2	C	83	PRO	3.1
1	D	195	SER	3.0
1	D	257	PRO	3.0
1	A	222	VAL	3.0
1	D	250	LEU	3.0
1	A	125	PHE	2.9
2	B	182	LEU	2.9
1	A	27	VAL	2.8
1	D	31	THR	2.8
2	E	90	TYR	2.8
1	D	193	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	431	ILE	2.8
1	D	60	ALA	2.8
1	A	238	TRP	2.8
1	D	523	VAL	2.7
2	E	6	ILE	2.7
1	D	245	ILE	2.6
1	D	73	LEU	2.6
1	D	335	GLY	2.6
1	A	257	PRO	2.6
1	A	350	ALA	2.6
2	F	143	PRO	2.6
1	D	162	VAL	2.5
2	F	86	PRO	2.5
2	C	166	ALA	2.5
1	A	301	VAL	2.5
1	A	294	LEU	2.5
2	E	201	ASP	2.5
1	D	531	ILE	2.4
2	B	32	TYR	2.4
1	D	202	LEU	2.4
1	A	570	TYR	2.4
1	A	377	VAL	2.4
2	B	180	PRO	2.4
1	A	88	ILE	2.4
1	A	284	LEU	2.3
1	D	32	LEU	2.3
1	A	154	TYR	2.3
1	A	207	LEU	2.3
1	A	391	VAL	2.3
2	C	42	PRO	2.3
1	D	151	SER	2.3
1	D	110	PHE	2.3
2	E	153	VAL	2.3
1	A	161	PRO	2.3
1	D	37	LEU	2.2
2	F	185	TRP	2.2
1	A	111	ILE	2.2
1	D	99	LEU	2.2
2	B	170	PHE	2.2
1	D	155	ILE	2.2
1	A	128	ALA	2.2
2	F	166	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	388	TYR	2.2
1	D	570	TYR	2.2
2	E	94	GLN	2.2
1	A	414	ASN	2.2
1	A	379	LEU	2.2
2	F	83	PRO	2.2
2	B	145	PHE	2.2
2	E	32	TYR	2.2
2	E	102	VAL	2.2
1	A	279	THR	2.2
1	A	429	LEU	2.2
1	A	300	TYR	2.2
1	A	121	THR	2.2
2	F	79	PRO	2.2
1	A	206	LEU	2.1
1	A	227	LEU	2.1
2	B	98	TRP	2.1
2	E	98	TRP	2.1
1	A	575	PHE	2.1
1	D	201	ALA	2.1
2	B	11	TRP	2.1
1	D	237	VAL	2.1
1	D	566	VAL	2.1
2	E	73	TYR	2.1
1	A	267	LEU	2.1
1	A	520	LEU	2.1
1	A	242	VAL	2.1
1	D	95	PRO	2.1
1	A	432	ASN	2.1
1	A	367	SER	2.1
1	D	89	LEU	2.1
1	D	472	PRO	2.1
1	D	567	VAL	2.1
1	A	71	VAL	2.0
1	D	54	ALA	2.0
1	A	218	TYR	2.0
1	D	336	TRP	2.0
2	C	185	TRP	2.0
1	A	571	PHE	2.0
1	D	475	TYR	2.0
1	A	481	ILE	2.0
1	D	466	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
2	B	153	VAL	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

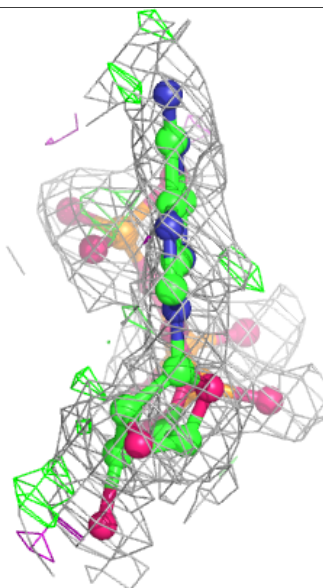
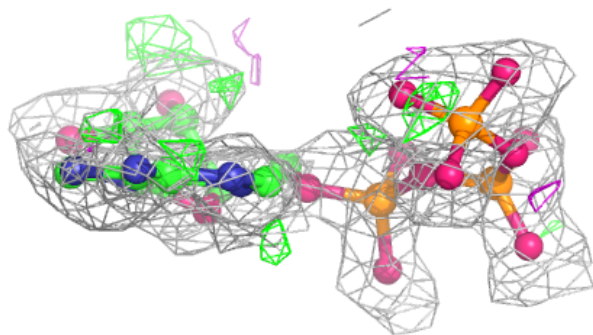
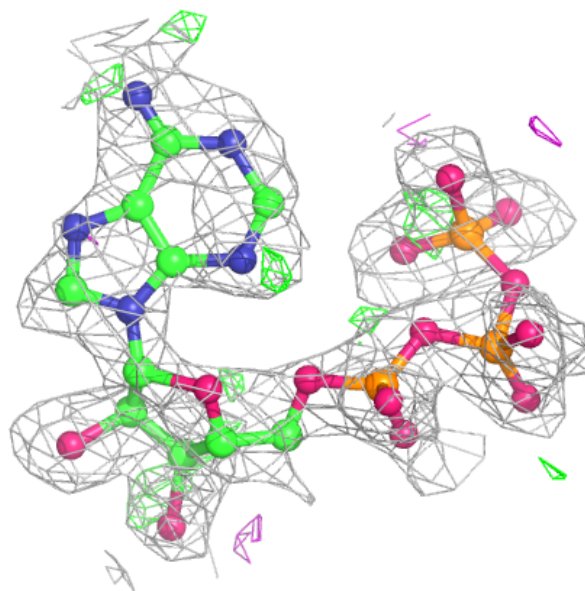
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	JAA	A	601	15/15	0.89	0.20	2,3,8,11	0
4	ATP	D	602	31/31	0.92	0.19	4,4,13,18	0
5	GSH	C	301	20/20	0.93	0.16	2,4,7,8	0
4	ATP	A	602	31/31	0.93	0.18	3,5,14,19	0
5	GSH	F	301	20/20	0.94	0.13	2,3,6,6	0
5	GSH	E	301	20/20	0.94	0.15	2,4,9,10	0
5	GSH	B	301	20/20	0.94	0.16	2,3,5,5	0
3	JAA	D	601	15/15	0.95	0.15	2,4,12,12	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 ATP D 602:**

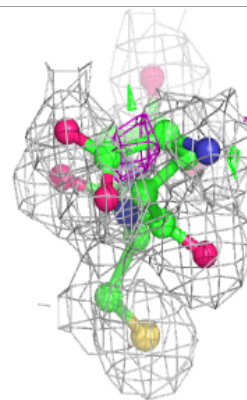
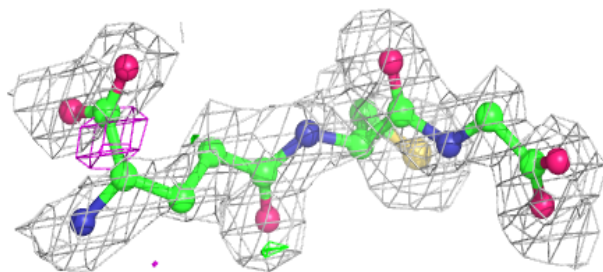
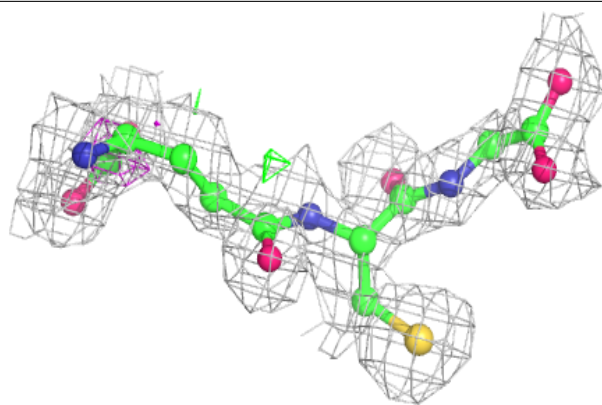
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





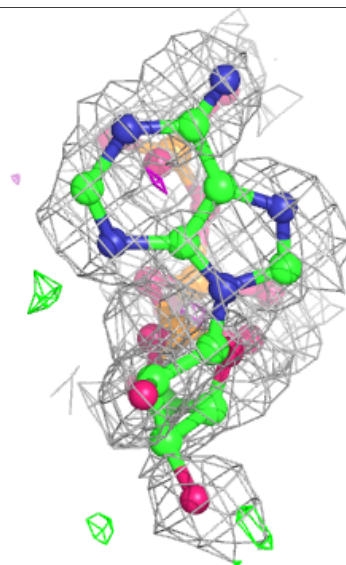
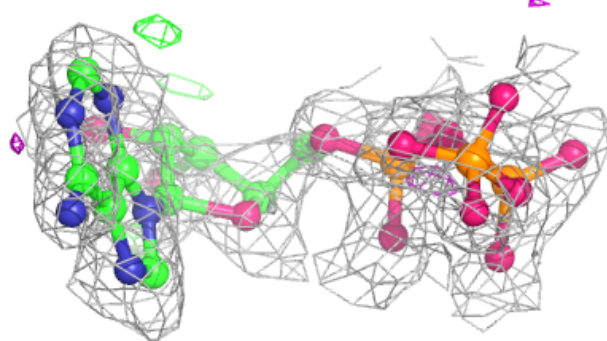
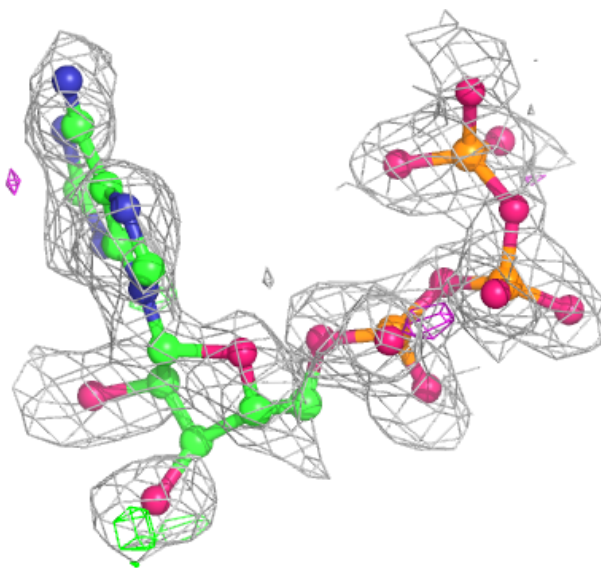
**Electron density around GSH C 301:**

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



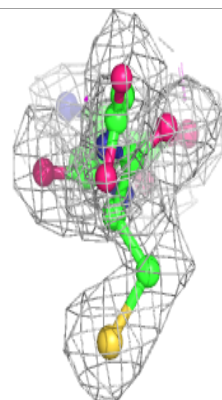
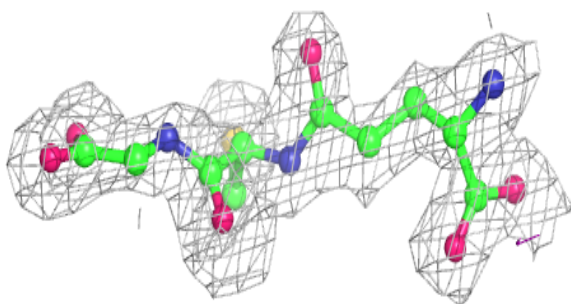
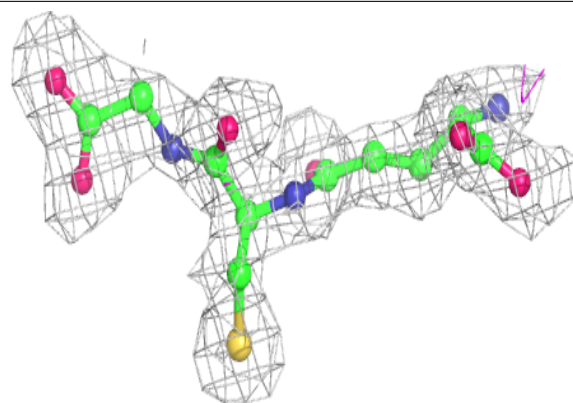
**Electron density around ATP A 602:**

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

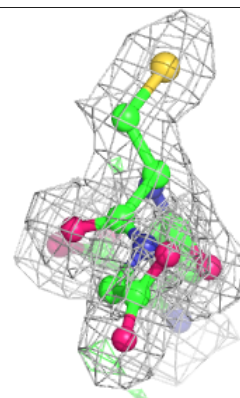
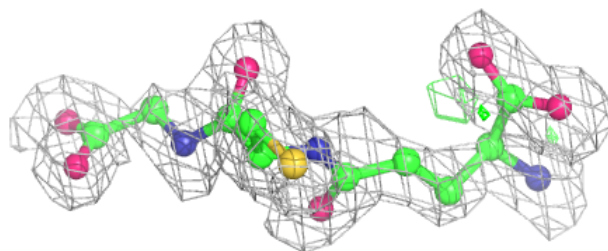
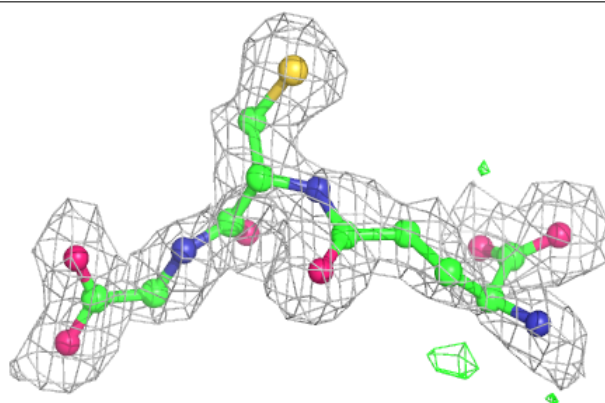


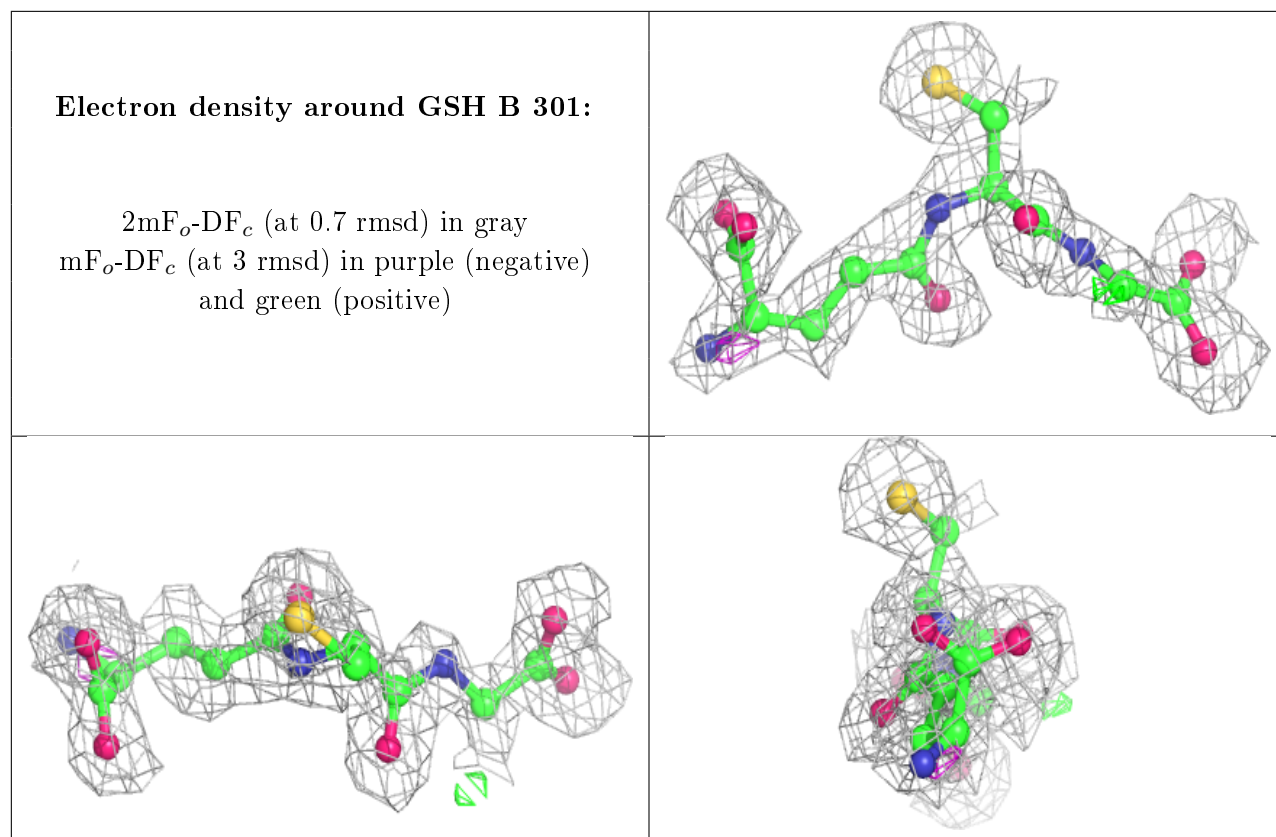
**Electron density around GSH F 301:**

$2mF_o-DF_c$  (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)





## 6.5 Other polymers [i](#)

There are no such residues in this entry.