



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 15, 2020 – 11:57 pm BST

PDB ID : 5ECK
Title : Crystal Structure of FIN219-FIP1 complex with JA, Ile and ATP
Authors : Chen, C.Y.; Cheng, Y.S.
Deposited on : 2015-10-20
Resolution : 1.54 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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

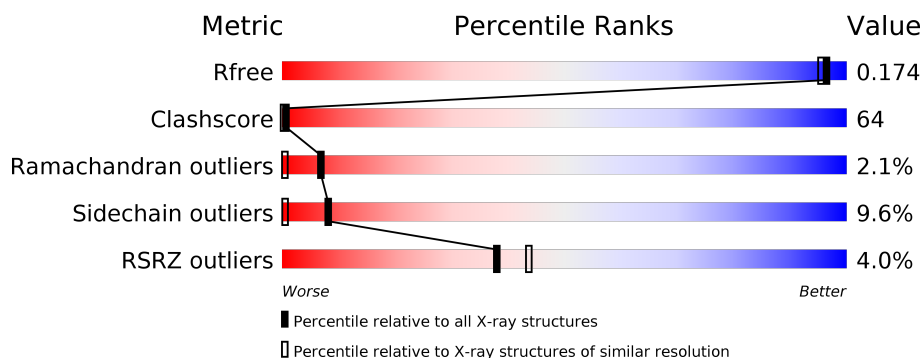
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.54 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	2556 (1.56-1.52)
Clashscore	141614	2634 (1.56-1.52)
Ramachandran outliers	138981	2580 (1.56-1.52)
Sidechain outliers	138945	2577 (1.56-1.52)
RSRZ outliers	127900	2524 (1.56-1.52)

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

Mol	Chain	Length	Quality of chain
1	A	575	<div> <div>4%</div> <div>26% 63% 9%</div> </div>
1	D	575	<div> <div>5%</div> <div>22% 66% 10%</div> </div>
2	B	223	<div> <div>4%</div> <div>27% 63% 5%</div> </div>
2	C	223	<div> <div>3%</div> <div>36% 53% 6%</div> </div>
2	E	223	<div> <div>%</div> <div>27% 63% 5%</div> </div>
2	F	223	<div> <div>4%</div> <div>35% 56%</div> </div>

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

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

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 18113 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:

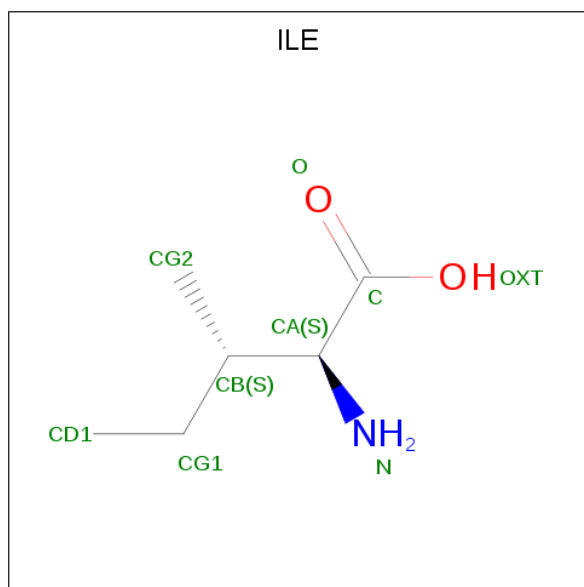
Chain	Residue	Modelled	Actual	Comment	Reference
B	-5	HIS	-	expression tag	UNP Q8L7C9
B	-4	HIS	-	expression tag	UNP Q8L7C9
B	-3	HIS	-	expression tag	UNP Q8L7C9
B	-2	HIS	-	expression tag	UNP Q8L7C9
B	-1	HIS	-	expression tag	UNP Q8L7C9
B	0	HIS	-	expression tag	UNP Q8L7C9
C	-5	HIS	-	expression tag	UNP Q8L7C9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

Continued on next page...

Continued from previous page...

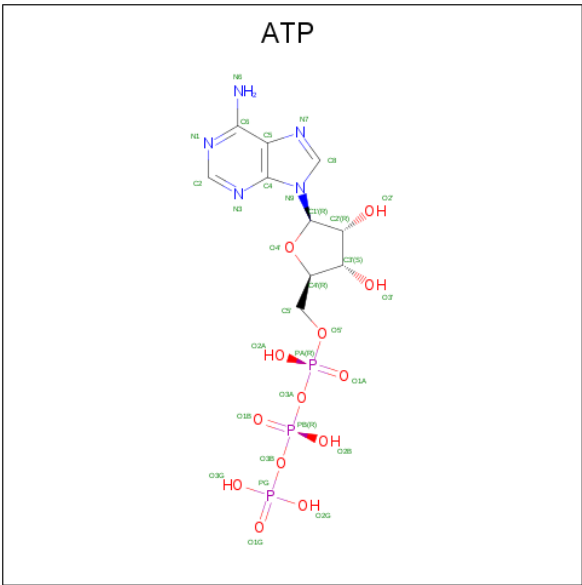
Chain	Residue	Modelled	Actual	Comment	Reference
E	-5	HIS	-	expression tag	UNP Q8L7C9
E	-4	HIS	-	expression tag	UNP Q8L7C9
E	-3	HIS	-	expression tag	UNP Q8L7C9
E	-2	HIS	-	expression tag	UNP Q8L7C9
E	-1	HIS	-	expression tag	UNP Q8L7C9
E	0	HIS	-	expression tag	UNP Q8L7C9
F	-5	HIS	-	expression tag	UNP Q8L7C9
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 ISOLEUCINE (three-letter code: ILE) (formula: $C_6H_{13}NO_2$).



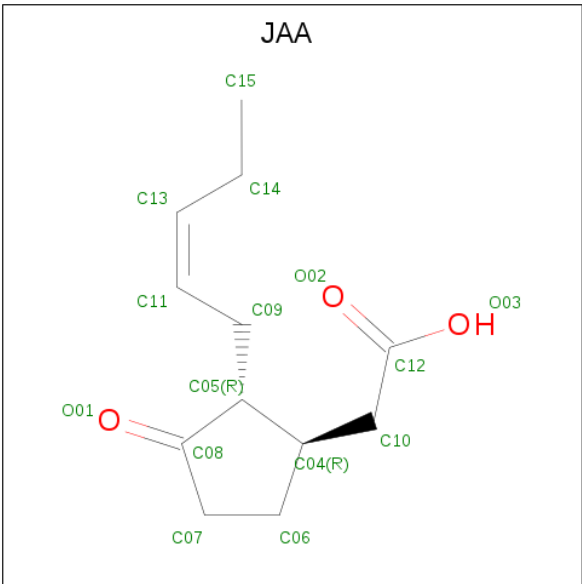
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			9	6	1	2		
3	D	1	Total	C	N	O	0	0
			9	6	1	2		

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



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



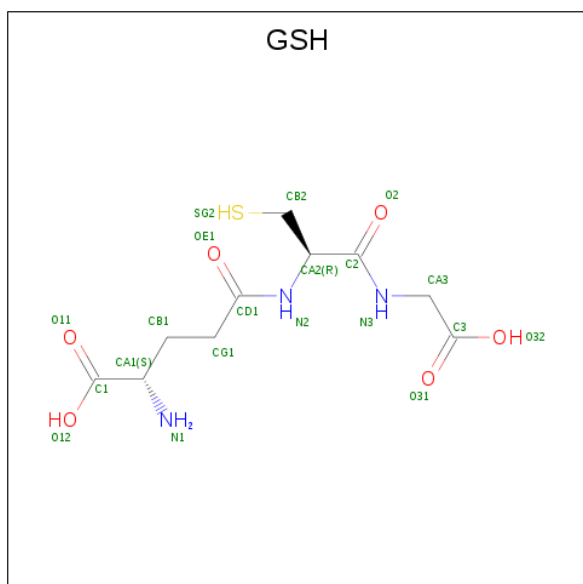
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			15	12	3		

Continued on next page...

Continued from previous page...

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

- Molecule 6 is GLUTATHIONE (three-letter code: GSH) (formula: $\text{C}_{10}\text{H}_{17}\text{N}_3\text{O}_6\text{S}$).



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

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	453	Total O 453 453	0	0
7	B	258	Total O 258 258	0	0
7	C	230	Total O 230 230	0	0
7	D	528	Total O 528 528	0	0

Continued on next page...

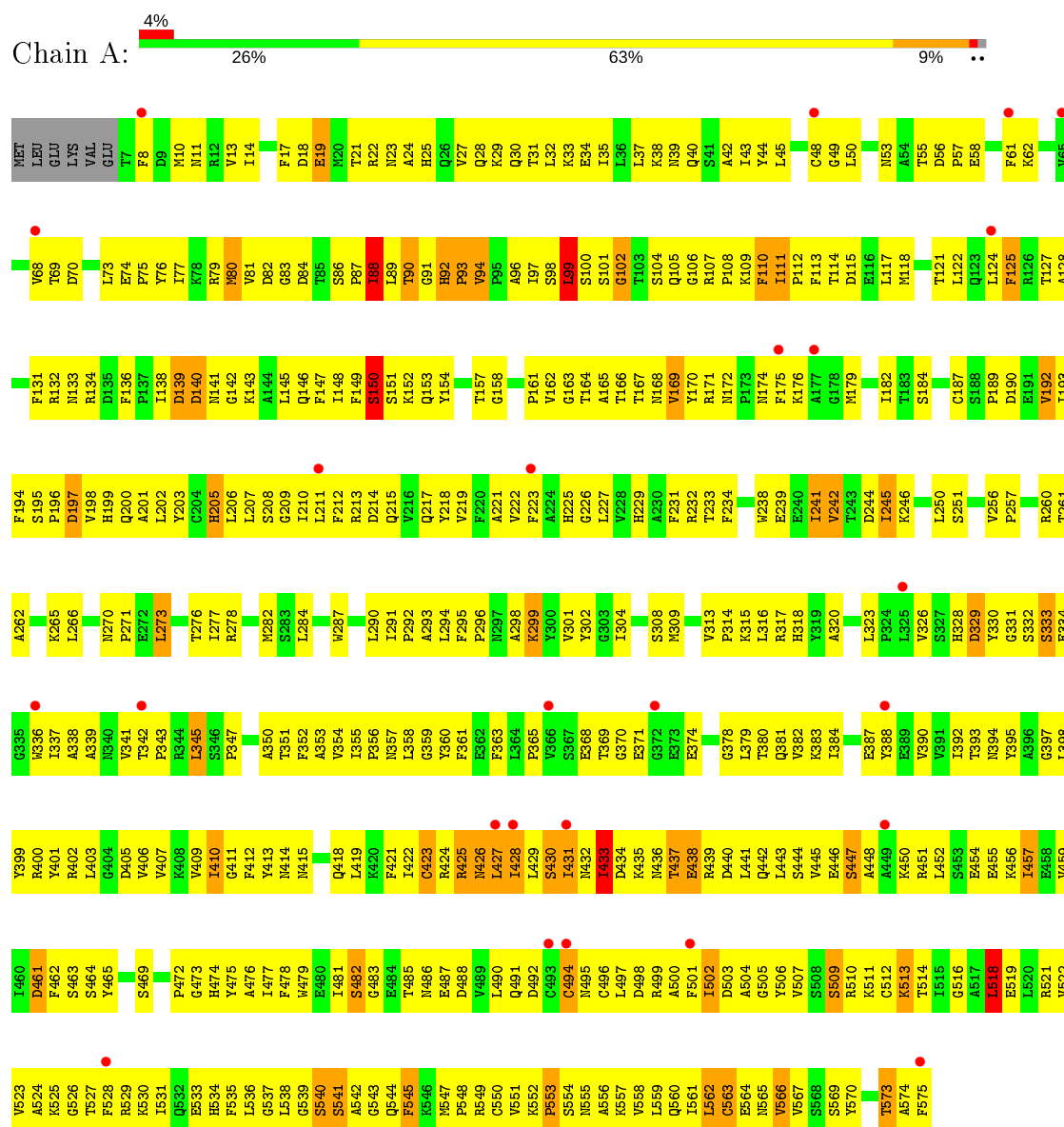
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	E	258	Total	O	0	0
			258	258		
7	F	246	Total	O	0	0
			246	246		

3 Residue-property plots

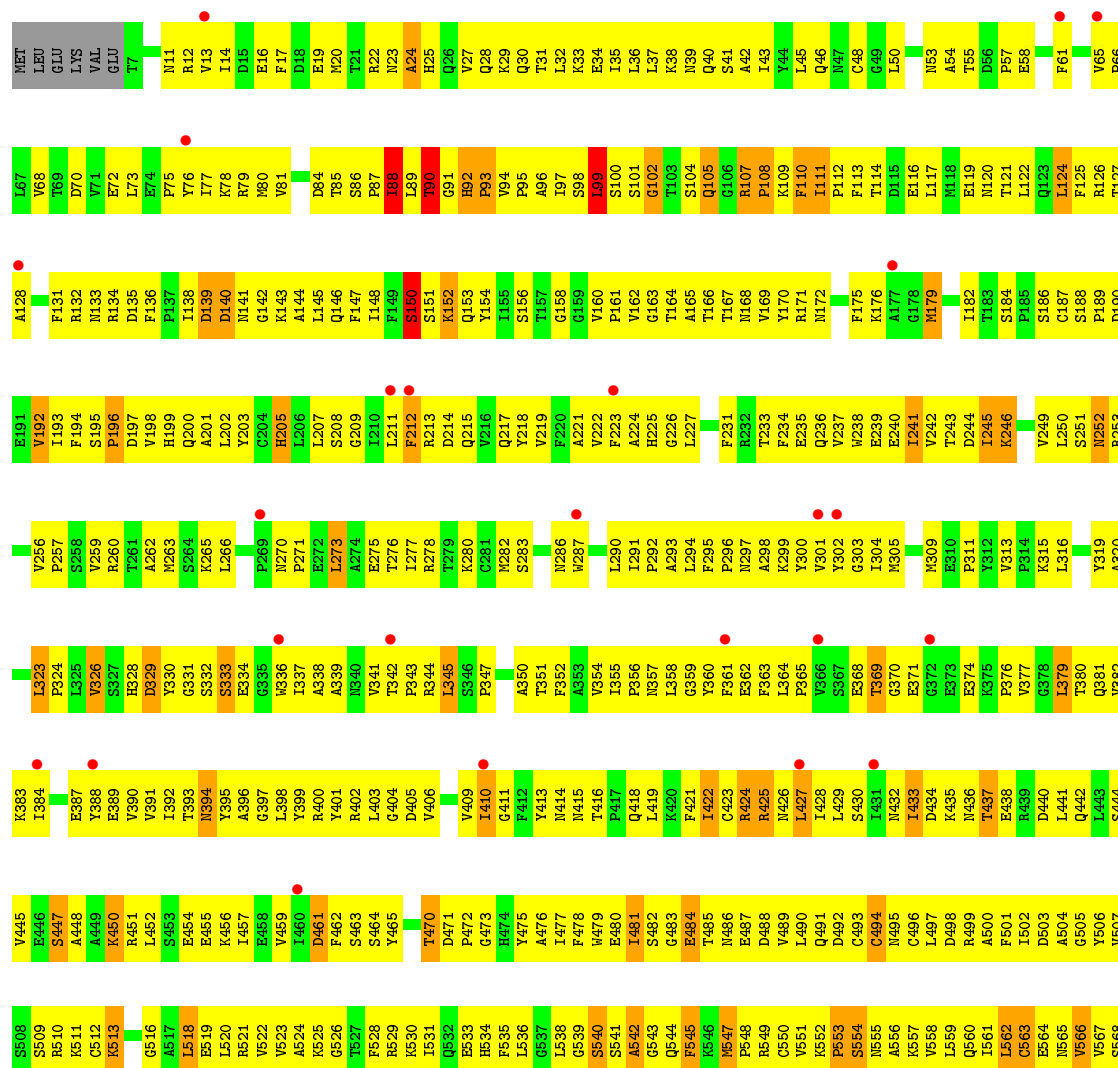
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

- Molecule 1: Jasmonic acid-amido synthetase JAR1

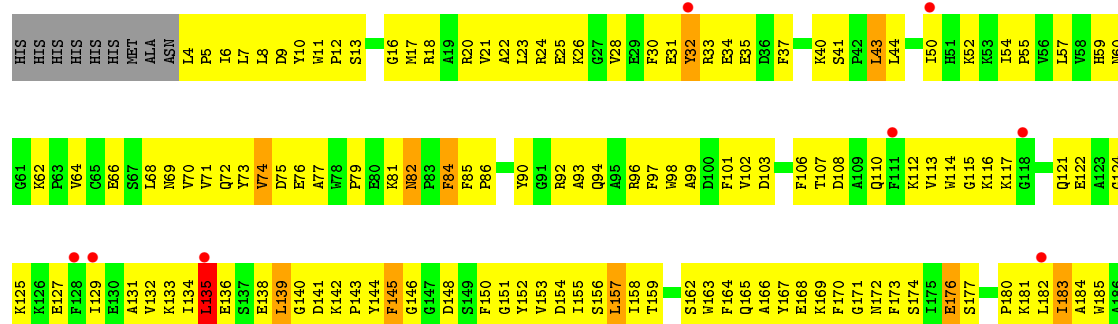


- Molecule 1: Jasmonic acid-amido synthetase JAR1



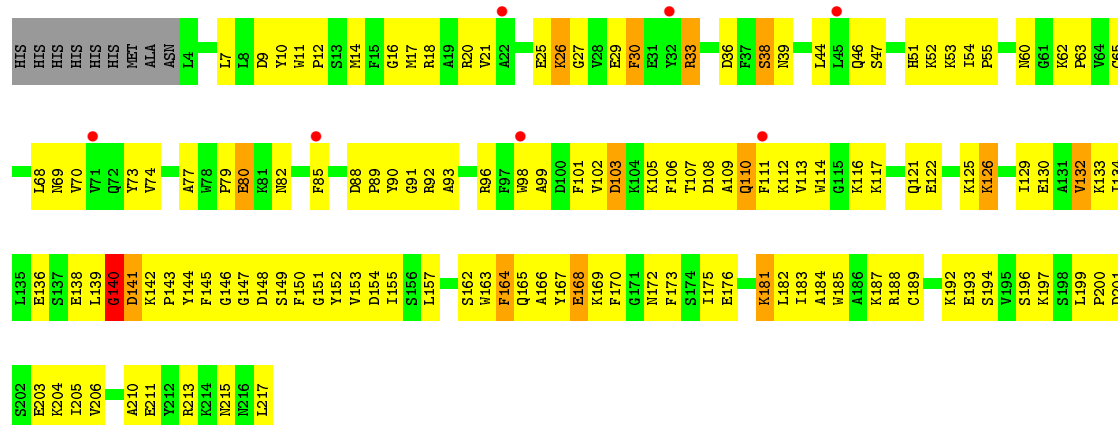


• Molecule 2: Glutathione S-transferase U20

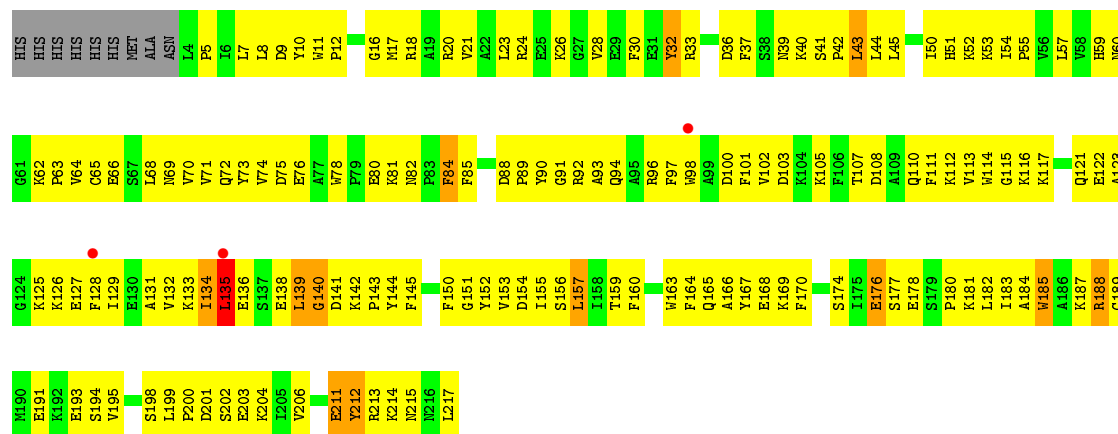




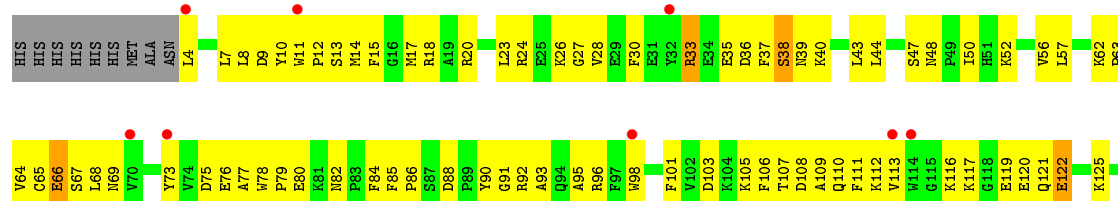
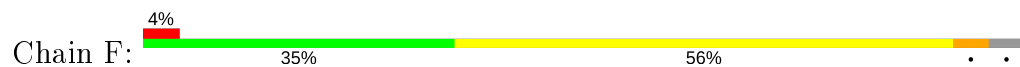
• Molecule 2: Glutathione S-transferase U20

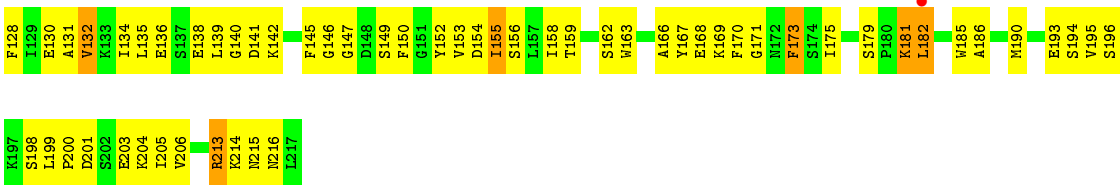


• Molecule 2: Glutathione S-transferase U20



• Molecule 2: Glutathione S-transferase U20





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	53.86 Å 53.85 Å 196.40 Å 92.33° 97.16° 113.48°	Depositor
Resolution (Å)	24.24 – 1.54 24.24 – 1.47	Depositor EDS
% Data completeness (in resolution range)	99.6 (24.24-1.54) 88.7 (24.24-1.47)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.32 (at 1.47 Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.162 , 0.175 0.162 , 0.174	Depositor DCC
R_{free} test set	30425 reflections (10.02%)	wwPDB-VP
Wilson B-factor (Å ²)	-1.6	Xtriage
Anisotropy	-0.387	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.60 , 263.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.053 for k,h,-h-k-l 0.000 for -k,-h,l 0.000 for -h,-k,h+k+l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	18113	wwPDB-VP
Average B, all atoms (Å ²)	6.0	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 71.06 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.8038e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² 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	0.55	0/4581	0.79	4/6219 (0.1%)
1	D	0.56	0/4581	0.80	2/6219 (0.0%)
2	B	0.65	0/1799	0.81	3/2428 (0.1%)
2	C	0.54	0/1799	0.66	1/2428 (0.0%)
2	E	0.65	0/1799	0.77	3/2428 (0.1%)
2	F	0.57	0/1799	0.67	0/2428
All	All	0.58	0/16358	0.77	13/22150 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
2	C	0	2
2	F	0	1
All	All	0	4

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	188	ARG	NE-CZ-NH1	-9.17	115.72	120.30
2	B	135	LEU	CB-CG-CD1	-8.81	96.02	111.00
2	E	188	ARG	NE-CZ-NH1	-8.56	116.02	120.30
1	A	99	LEU	CA-CB-CG	8.09	133.91	115.30
2	E	135	LEU	CB-CG-CD1	-7.24	98.70	111.00
2	B	188	ARG	NE-CZ-NH2	7.02	123.81	120.30
1	A	428	ILE	N-CA-C	-5.88	95.12	111.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	99	LEU	CA-CB-CG	5.63	128.25	115.30
1	A	518	LEU	CA-CB-CG	5.51	127.98	115.30
2	E	188	ARG	NE-CZ-NH2	5.33	122.96	120.30
1	D	102	GLY	N-CA-C	-5.27	99.93	113.10
1	A	102	GLY	N-CA-C	-5.20	100.10	113.10
2	C	69	ASN	CB-CA-C	5.19	120.78	110.40

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	427	LEU	Peptide
2	C	140	GLY	Peptide
2	C	165	GLN	Sidechain
2	F	140	GLY	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	4433	617	2
1	D	4479	0	4433	707	2
2	B	1748	0	1704	247	1
2	C	1748	0	1704	175	0
2	E	1748	0	1704	235	1
2	F	1748	0	1704	161	1
3	A	9	0	10	11	0
3	D	9	0	10	6	0
4	A	31	0	2	21	0
4	D	31	0	2	21	0
5	A	15	0	0	7	0
5	D	15	0	0	5	0
6	B	20	0	15	0	0
6	C	20	0	15	1	0
6	E	20	0	15	4	0
6	F	20	0	15	1	0
7	A	453	0	0	90	5

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	258	0	0	68	3
7	C	230	0	0	45	4
7	D	528	0	0	146	4
7	E	258	0	0	52	1
7	F	246	0	0	39	2
All	All	18113	0	15766	2052	18

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 64.

All (2052) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:176:LYS:NZ	1:A:190:ASP:OD2	1.61	1.34
1:D:176:LYS:NZ	1:D:190:ASP:OD2	1.61	1.31
1:D:456:LYS:NZ	2:E:201:ASP:OD2	1.79	1.15
1:D:107:ARG:HH11	1:D:107:ARG:HG3	1.02	1.13
1:D:499:ARG:O	2:E:188:ARG:NH1	1.85	1.09
1:D:500:ALA:HA	2:E:188:ARG:HH12	1.01	1.09
2:B:98:TRP:O	7:B:401:HOH:O	1.70	1.08
2:F:66:GLU:OE2	7:F:401:HOH:O	1.73	1.07
1:A:454:GLU:OE2	7:A:701:HOH:O	1.72	1.05
1:A:456:LYS:NZ	2:B:201:ASP:OD2	1.89	1.05
2:C:36:ASP:OD2	7:C:401:HOH:O	1.74	1.05
2:E:98:TRP:CH2	2:E:135:LEU:HD11	1.93	1.03
2:B:98:TRP:CH2	2:B:135:LEU:HD11	1.95	1.01
1:D:477:ILE:HG12	1:D:518:LEU:HD11	1.43	1.00
1:A:495:ASN:O	7:A:702:HOH:O	1.78	1.00
1:A:448:ALA:HB2	1:A:496:CYS:HB3	1.42	1.00
1:D:187:CYS:SG	7:D:940:HOH:O	2.21	0.98
2:C:181:LYS:HE3	1:D:95:PRO:HD3	1.45	0.97
2:B:75:ASP:O	7:B:402:HOH:O	1.82	0.96
2:B:20:ARG:NH2	7:B:403:HOH:O	1.98	0.95
2:E:132:VAL:HG23	2:E:182:LEU:HD13	1.49	0.95
2:E:26:LYS:NZ	2:E:82:ASN:O	2.00	0.95
1:A:152:LYS:HE2	1:A:565:ASN:HB2	1.46	0.95
1:D:541:SER:O	1:D:543:GLY:N	1.99	0.95
1:D:363:PHE:HD2	1:D:382:VAL:HG21	1.31	0.94
2:E:176:GLU:OE2	7:E:402:HOH:O	1.82	0.94
1:A:82:ASP:OD2	7:A:703:HOH:O	1.85	0.94
1:A:541:SER:O	1:A:543:GLY:N	2.01	0.93

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:138:ILE:HA	1:D:217:GLN:HE21	1.31	0.93
1:D:98:SER:HB2	1:D:111:ILE:HG23	1.49	0.93
1:D:152:LYS:HE2	1:D:565:ASN:HB2	1.50	0.93
1:D:305:MET:SD	7:D:1042:HOH:O	2.27	0.93
1:D:498:ASP:HB3	1:D:510:ARG:HH22	1.33	0.93
1:D:152:LYS:NZ	1:D:561:ILE:O	2.00	0.93
1:D:500:ALA:CA	2:E:188:ARG:HH12	1.82	0.93
1:A:197:ASP:OD2	7:A:704:HOH:O	1.87	0.92
2:B:18:ARG:NH2	7:B:406:HOH:O	2.02	0.92
1:D:455:GLU:OE2	7:D:702:HOH:O	1.88	0.92
2:C:141:ASP:OD2	2:C:181:LYS:NZ	2.02	0.91
1:D:116:GLU:OE2	7:D:701:HOH:O	1.87	0.90
1:A:500:ALA:CA	2:B:188:ARG:HH12	1.84	0.90
2:C:145:PHE:HB3	2:C:153:VAL:HG13	1.52	0.90
1:D:500:ALA:HA	2:E:188:ARG:NH1	1.86	0.89
2:B:60:ASN:ND2	7:B:408:HOH:O	2.05	0.89
1:A:521:ARG:O	7:A:705:HOH:O	1.88	0.89
4:A:602:ATP:O4'	7:A:706:HOH:O	1.90	0.89
1:D:119:GLU:OE2	7:D:703:HOH:O	1.91	0.89
1:A:498:ASP:HB3	1:A:510:ARG:HH22	1.37	0.88
1:A:166:THR:HG22	3:A:601:ILE:HG23	1.56	0.88
1:D:108:PRO:HG2	1:D:552:LYS:H	1.37	0.88
1:A:500:ALA:CB	2:B:188:ARG:HH12	1.87	0.88
1:A:477:ILE:HG12	1:A:518:LEU:HD11	1.55	0.87
2:E:168:GLU:OE1	7:E:403:HOH:O	1.92	0.87
1:D:496:CYS:SG	7:E:438:HOH:O	2.31	0.87
1:A:400:ARG:NH1	7:A:714:HOH:O	2.07	0.86
1:A:444:SER:O	7:A:707:HOH:O	1.91	0.86
1:D:445:VAL:HG22	1:D:479:TRP:HE1	1.39	0.86
2:B:8:LEU:HD22	2:B:33:ARG:HH21	1.37	0.86
1:D:105:GLN:O	7:D:704:HOH:O	1.91	0.86
1:D:499:ARG:CZ	2:E:184:ALA:HB1	2.06	0.86
2:E:97:PHE:O	7:F:401:HOH:O	1.94	0.86
2:E:134:ILE:HD12	2:F:50:ILE:HG21	1.59	0.85
1:A:107:ARG:HH11	1:A:107:ARG:HG3	1.41	0.85
1:D:242:VAL:HG12	1:D:277:ILE:HD13	1.58	0.85
2:E:144:TYR:O	7:E:404:HOH:O	1.93	0.84
1:A:423:CYS:SG	1:A:541:SER:OG	2.36	0.84
1:A:35:ILE:HD13	1:A:394:ASN:HA	1.59	0.84
1:A:165:ALA:H	1:A:557:LYS:HE3	1.43	0.84
1:A:198:VAL:HA	1:A:201:ALA:HB3	1.59	0.84

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:400:ARG:NH1	7:D:720:HOH:O	2.10	0.83
1:D:107:ARG:HG3	1:D:107:ARG:NH1	1.79	0.83
1:D:244:ASP:OD2	7:D:705:HOH:O	1.97	0.83
2:B:26:LYS:HD2	2:B:74:VAL:HG13	1.61	0.83
2:C:52:LYS:NZ	7:C:406:HOH:O	2.06	0.83
1:A:500:ALA:HB2	2:B:188:ARG:HH12	1.44	0.83
1:A:111:ILE:HD13	1:A:334:GLU:HG2	1.59	0.82
2:B:10:TYR:O	7:B:403:HOH:O	1.96	0.82
2:F:216:ASN:N	7:F:405:HOH:O	2.09	0.82
1:A:138:ILE:HA	1:A:217:GLN:HE21	1.44	0.82
1:A:199:HIS:HB3	1:A:525:LYS:H	1.42	0.82
1:A:39:ASN:ND2	1:A:90:THR:O	2.12	0.82
1:D:448:ALA:HB2	1:D:496:CYS:HB3	1.61	0.82
1:D:548:PRO:O	7:D:708:HOH:O	1.98	0.82
1:A:174:ASN:ND2	7:A:721:HOH:O	2.11	0.82
1:A:163:GLY:HA2	1:A:560:GLN:HB2	1.60	0.82
3:D:601:ILE:OXT	7:D:707:HOH:O	1.98	0.82
2:F:117:LYS:HG3	2:F:213:ARG:HH11	1.45	0.82
1:A:153:GLN:HA	1:A:560:GLN:HG2	1.62	0.82
1:A:472:PRO:O	7:A:709:HOH:O	1.97	0.81
2:F:110:GLN:OE1	2:F:167:TYR:OH	1.97	0.81
2:F:101:PHE:HZ	2:F:131:ALA:HB1	1.44	0.81
1:D:164:THR:OG1	1:D:557:LYS:O	1.97	0.81
1:D:329:ASP:HB3	1:D:339:ALA:HA	1.61	0.81
2:B:8:LEU:HD21	2:B:43:LEU:HD11	1.61	0.81
2:E:114:TRP:HA	2:E:170:PHE:HD2	1.46	0.81
1:D:126:ARG:NH1	7:D:719:HOH:O	2.09	0.81
1:D:432:ASN:HA	7:D:704:HOH:O	1.79	0.81
1:A:432:ASN:OD1	1:A:434:ASP:N	2.13	0.81
2:F:169:LYS:NZ	2:F:206:VAL:HG13	1.95	0.81
1:D:198:VAL:HA	1:D:201:ALA:HB3	1.62	0.80
1:A:499:ARG:NE	2:B:184:ALA:HB1	1.95	0.80
1:D:488:ASP:OD1	7:D:706:HOH:O	1.97	0.80
2:F:145:PHE:HB3	2:F:153:VAL:HG13	1.63	0.80
1:A:145:LEU:HD13	1:A:209:GLY:HA3	1.63	0.80
2:B:132:VAL:HG23	2:B:182:LEU:HD13	1.64	0.80
1:D:23:ASN:ND2	7:D:731:HOH:O	2.15	0.80
1:D:132:ARG:O	1:D:136:PHE:N	2.14	0.80
1:A:451:ARG:NH2	7:A:726:HOH:O	2.14	0.80
4:A:602:ATP:N6	5:A:603:JAA:O02	2.15	0.79
1:D:423:CYS:SG	1:D:541:SER:OG	2.40	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:331:GLY:HA3	1:A:336:TRP:HA	1.63	0.79
1:A:363:PHE:HD2	1:A:382:VAL:HG21	1.45	0.79
2:B:25:GLU:OE2	7:B:405:HOH:O	2.01	0.79
1:D:141:ASN:ND2	7:D:728:HOH:O	2.13	0.79
1:D:445:VAL:HA	1:D:479:TRP:CZ2	2.18	0.79
2:E:8:LEU:HD22	2:E:33:ARG:HH21	1.45	0.79
1:D:490:LEU:HD22	1:D:522:VAL:HG21	1.65	0.79
2:E:64:VAL:HG23	2:E:70:VAL:HG22	1.64	0.79
1:A:187:CYS:SG	7:A:752:HOH:O	2.41	0.78
1:D:531:ILE:HG13	1:D:558:VAL:HG22	1.64	0.78
1:A:261:THR:HG22	1:A:265:LYS:HE3	1.64	0.78
2:C:142:LYS:HG2	1:D:41:SER:HB2	1.64	0.78
2:B:122:GLU:HA	2:B:125:LYS:HE2	1.63	0.78
1:D:145:LEU:HD13	1:D:209:GLY:HA3	1.65	0.78
1:D:432:ASN:OD1	1:D:434:ASP:N	2.15	0.78
2:E:80:GLU:O	7:E:405:HOH:O	2.01	0.78
1:A:332:SER:OG	1:A:333:SER:N	2.17	0.78
2:E:98:TRP:CD1	2:E:153:VAL:HG11	2.18	0.78
1:D:488:ASP:OD1	7:D:711:HOH:O	2.01	0.78
1:D:509:SER:O	1:D:513:LYS:N	2.14	0.78
1:A:132:ARG:O	1:A:136:PHE:N	2.11	0.78
1:A:332:SER:HB3	1:A:538:LEU:HD13	1.66	0.78
2:B:211:GLU:OE1	7:B:404:HOH:O	2.00	0.78
2:B:114:TRP:HA	2:B:170:PHE:HD2	1.48	0.78
1:D:99:LEU:HB3	1:D:557:LYS:H	1.49	0.78
2:E:151:GLY:O	7:E:406:HOH:O	2.02	0.78
2:E:114:TRP:CD1	2:E:167:TYR:HE1	2.02	0.78
1:D:197:ASP:OD1	7:D:710:HOH:O	2.01	0.77
2:E:98:TRP:CZ2	2:E:135:LEU:HD11	2.20	0.77
1:D:406:VAL:O	1:D:541:SER:OG	2.02	0.77
1:D:519:GLU:OE2	1:D:569:SER:OG	2.02	0.77
1:A:535:PHE:O	1:A:538:LEU:HB3	1.84	0.77
1:D:448:ALA:HB3	1:D:479:TRP:HH2	1.49	0.77
1:A:150:SER:O	7:A:711:HOH:O	2.02	0.77
1:D:168:ASN:ND2	4:D:603:ATP:O2A	2.14	0.77
1:D:564:GLU:OE2	7:D:709:HOH:O	2.01	0.77
1:D:134:ARG:O	7:D:712:HOH:O	2.01	0.76
2:C:29:GLU:OE2	7:C:403:HOH:O	2.03	0.76
1:A:152:LYS:HG2	1:A:565:ASN:H	1.49	0.76
1:D:111:ILE:HD13	1:D:334:GLU:HG2	1.66	0.76
1:D:361:PHE:O	7:D:713:HOH:O	2.03	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:301:GSH:O32	7:E:407:HOH:O	2.04	0.76
2:E:60:ASN:ND2	7:E:421:HOH:O	2.18	0.76
1:A:10:MET:SD	7:A:987:HOH:O	2.43	0.76
1:A:519:GLU:OE2	1:A:569:SER:OG	2.02	0.76
2:B:35:GLU:OE2	7:B:407:HOH:O	2.04	0.76
1:A:439:ARG:NH2	7:A:729:HOH:O	2.15	0.76
1:A:529:ARG:NH1	1:A:533:GLU:OE2	2.18	0.76
2:C:138:GLU:OE2	7:C:404:HOH:O	2.03	0.76
4:D:603:ATP:C2'	4:D:603:ATP:N3	2.48	0.76
2:F:194:SER:O	2:F:198:SER:OG	2.03	0.76
1:A:98:SER:HB2	1:A:111:ILE:HG23	1.67	0.76
1:D:540:SER:OG	1:D:544:GLN:NE2	2.19	0.76
1:D:58:GLU:OE2	1:D:360:TYR:OH	2.03	0.75
1:D:88:ILE:HD12	1:D:89:LEU:H	1.51	0.75
1:A:500:ALA:HA	2:B:188:ARG:HH12	1.52	0.75
1:D:299:LYS:HB2	1:D:300:TYR:HD1	1.51	0.75
2:C:142:LYS:HA	1:D:39:ASN:ND2	2.00	0.75
1:D:73:LEU:HD22	1:D:89:LEU:HD13	1.69	0.75
1:A:87:PRO:HD3	1:A:93:PRO:HG3	1.67	0.75
1:A:88:ILE:HD12	1:A:89:LEU:H	1.51	0.75
2:C:85:PHE:HB3	2:C:92:ARG:HG2	1.69	0.75
4:A:602:ATP:N3	4:A:602:ATP:C2'	2.50	0.75
1:D:35:ILE:HD13	1:D:394:ASN:HA	1.69	0.75
1:D:199:HIS:HB3	1:D:525:LYS:H	1.49	0.75
1:D:166:THR:HG22	3:D:601:ILE:HG23	1.69	0.75
1:D:144:ALA:O	7:D:715:HOH:O	2.04	0.74
1:D:198:VAL:HG13	1:D:565:ASN:ND2	2.02	0.74
1:D:475:TYR:HB2	1:D:518:LEU:HB2	1.68	0.74
2:F:179:SER:OG	7:F:402:HOH:O	2.05	0.74
1:D:153:GLN:HA	1:D:560:GLN:HG2	1.70	0.74
2:F:117:LYS:HG3	2:F:213:ARG:NH1	2.02	0.74
3:A:601:ILE:HG13	4:A:602:ATP:H2	1.52	0.74
1:A:151:SER:OG	1:A:565:ASN:OD1	2.05	0.74
1:A:77:ILE:HD13	1:A:112:PRO:HD3	1.68	0.74
1:D:535:PHE:O	1:D:538:LEU:HB3	1.88	0.73
1:A:496:CYS:SG	7:B:417:HOH:O	2.27	0.73
1:A:442:GLN:NE2	7:A:742:HOH:O	2.20	0.73
2:C:147:GLY:O	7:C:405:HOH:O	2.06	0.73
2:E:203:GLU:OE2	7:E:401:HOH:O	2.06	0.73
1:A:219:VAL:HB	1:A:295:PHE:CZ	2.24	0.73
2:B:11:TRP:CD1	2:B:12:PRO:HD3	2.24	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:242:VAL:HG21	1:A:278:ARG:HH21	1.52	0.73
1:D:345:LEU:HD13	1:D:350:ALA:HA	1.71	0.73
1:D:463:SER:HB2	1:D:528:PHE:HE1	1.54	0.73
2:E:88:ASP:O	7:E:409:HOH:O	2.07	0.73
1:A:108:PRO:HG2	1:A:552:LYS:H	1.54	0.73
1:A:428:ILE:O	7:A:712:HOH:O	2.06	0.73
1:A:499:ARG:NH2	2:B:184:ALA:O	2.22	0.73
1:D:19:GLU:O	1:D:23:ASN:ND2	2.19	0.73
1:D:400:ARG:NH1	7:D:750:HOH:O	2.20	0.73
1:D:221:ALA:HB1	1:D:529:ARG:HH12	1.54	0.73
2:B:76:GLU:HG3	2:C:89:PRO:HB3	1.71	0.73
1:D:163:GLY:HA2	1:D:560:GLN:HB2	1.69	0.73
3:D:601:ILE:HG13	4:D:603:ATP:H2	1.53	0.73
2:E:26:LYS:HG2	2:E:81:LYS:NZ	2.04	0.73
1:A:492:ASP:HB3	2:B:187:LYS:HD3	1.69	0.72
1:A:84:ASP:OD2	7:A:713:HOH:O	2.07	0.72
2:E:111:PHE:O	7:E:408:HOH:O	2.06	0.72
1:A:28:GLN:NE2	7:A:745:HOH:O	2.21	0.72
1:D:143:LYS:HA	1:D:184:SER:HB2	1.71	0.72
1:A:113:PHE:HB2	4:A:602:ATP:O1B	1.89	0.72
2:C:73:TYR:OH	7:C:407:HOH:O	2.08	0.72
2:F:215:ASN:O	7:F:403:HOH:O	2.06	0.72
2:C:140:GLY:HA3	1:D:38:LYS:HB3	1.72	0.72
2:F:150:PHE:HE1	2:F:155:ILE:HG13	1.55	0.72
1:D:547:MET:SD	7:D:804:HOH:O	2.47	0.72
1:A:200:GLN:NE2	7:A:746:HOH:O	2.22	0.72
1:A:223:PHE:HE2	1:A:545:PHE:HZ	1.36	0.72
2:B:33:ARG:NH2	7:B:427:HOH:O	2.22	0.72
2:E:28:VAL:O	7:E:410:HOH:O	2.08	0.72
1:D:405:ASP:HB2	1:D:541:SER:HB3	1.72	0.72
2:E:195:VAL:HG23	2:E:199:LEU:HD13	1.71	0.72
2:F:193:GLU:HA	2:F:196:SER:HB3	1.72	0.72
1:A:345:LEU:HD13	1:A:350:ALA:HA	1.71	0.72
1:A:199:HIS:N	1:A:524:ALA:HB1	2.04	0.72
1:D:107:ARG:HH22	1:D:552:LYS:HD3	1.55	0.72
1:D:198:VAL:HG22	1:D:524:ALA:HB3	1.71	0.71
1:A:34:GLU:OE2	7:A:715:HOH:O	2.08	0.71
2:E:32:TYR:H	2:E:32:TYR:HD2	1.39	0.71
1:D:286:ASN:ND2	7:D:754:HOH:O	2.21	0.71
2:C:149:SER:O	7:C:405:HOH:O	2.07	0.71
1:D:242:VAL:HG21	1:D:278:ARG:HH21	1.54	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199:HIS:H	1:A:524:ALA:HB1	1.54	0.71
2:E:163:TRP:HB3	2:E:167:TYR:CZ	2.25	0.71
1:A:171:ARG:NH1	7:A:754:HOH:O	2.24	0.71
1:A:195:SER:OG	1:A:197:ASP:OD1	2.09	0.71
1:A:107:ARG:CZ	1:A:433:ILE:HG13	2.21	0.71
1:D:246:LYS:HZ2	1:D:271:PRO:HA	1.54	0.71
2:F:20:ARG:NH1	7:F:420:HOH:O	2.24	0.71
2:E:8:LEU:HD21	2:E:43:LEU:HD11	1.72	0.71
2:F:122:GLU:OE1	7:F:404:HOH:O	2.08	0.71
1:A:73:LEU:HD22	1:A:89:LEU:HD13	1.72	0.71
2:C:90:TYR:O	2:C:93:ALA:HB3	1.91	0.71
1:D:165:ALA:H	1:D:557:LYS:HE3	1.56	0.71
1:D:169:VAL:HG22	4:D:603:ATP:O2'	1.91	0.71
2:F:64:VAL:N	7:F:415:HOH:O	2.20	0.71
1:A:152:LYS:HB2	1:A:561:ILE:HA	1.72	0.70
2:B:174:SER:O	7:B:410:HOH:O	2.08	0.70
1:D:326:VAL:HG12	7:D:776:HOH:O	1.91	0.70
1:D:416:THR:OG1	7:D:714:HOH:O	2.04	0.70
1:A:534:HIS:CG	1:A:557:LYS:HE2	2.26	0.70
1:D:246:LYS:NZ	1:D:271:PRO:HA	2.06	0.70
1:D:529:ARG:NH1	1:D:533:GLU:OE2	2.24	0.70
1:A:317:ARG:NH1	7:A:753:HOH:O	2.24	0.70
1:D:243:THR:O	7:D:716:HOH:O	2.09	0.70
1:D:395:TYR:O	7:D:718:HOH:O	2.09	0.70
2:E:136:GLU:HG3	2:E:181:LYS:HD3	1.74	0.70
2:F:82:ASN:OD1	7:F:406:HOH:O	2.10	0.70
2:B:23:LEU:HD22	2:B:28:VAL:HG11	1.72	0.70
2:F:26:LYS:NZ	2:F:82:ASN:O	2.24	0.70
1:A:99:LEU:HD13	1:A:558:VAL:H	1.57	0.70
1:D:470:THR:O	7:D:717:HOH:O	2.09	0.70
2:E:76:GLU:OE2	2:F:96:ARG:NH1	2.24	0.70
1:D:150:SER:HB2	1:D:167:THR:HA	1.74	0.70
2:F:122:GLU:OE2	7:F:407:HOH:O	2.10	0.70
1:A:152:LYS:HA	1:A:564:GLU:HB2	1.73	0.69
1:D:139:ASP:OD2	1:D:142:GLY:HA3	1.92	0.69
2:E:26:LYS:HG2	2:E:81:LYS:HZ1	1.56	0.69
2:B:75:ASP:HB2	2:B:84:PHE:CE2	2.27	0.69
1:A:164:THR:OG1	1:A:557:LYS:O	2.10	0.69
1:A:331:GLY:O	4:A:602:ATP:N6	2.24	0.69
2:B:214:LYS:O	7:B:411:HOH:O	2.09	0.69
1:A:99:LEU:HB3	1:A:557:LYS:H	1.57	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:219:VAL:HG11	1:D:291:ILE:HG21	1.74	0.69
1:A:143:LYS:NZ	1:A:187:CYS:HA	2.08	0.69
1:A:329:ASP:HB3	1:A:339:ALA:HA	1.74	0.69
1:A:483:GLY:O	7:A:719:HOH:O	2.09	0.69
5:D:602:JAA:O02	4:D:603:ATP:N6	2.26	0.69
2:E:188:ARG:HD2	2:E:191:GLU:OE2	1.92	0.69
1:A:500:ALA:HA	2:B:188:ARG:NH1	2.06	0.69
1:A:513:LYS:HZ2	1:A:575:PHE:HB3	1.56	0.69
1:D:217:GLN:HE22	1:D:299:LYS:HD3	1.57	0.69
1:D:332:SER:HA	4:D:603:ATP:N6	2.07	0.69
2:C:92:ARG:NH1	2:C:96:ARG:HH22	1.91	0.69
2:E:204:LYS:NZ	7:E:401:HOH:O	1.74	0.69
1:A:479:TRP:HZ2	1:A:497:LEU:HD21	1.58	0.69
1:A:226:GLY:HA3	1:A:529:ARG:HH11	1.57	0.69
2:B:84:PHE:CD1	2:B:152:TYR:HB2	2.28	0.69
1:D:117:LEU:O	7:D:721:HOH:O	2.11	0.69
1:D:234:PHE:HD2	1:D:290:LEU:HD21	1.55	0.69
1:D:151:SER:OG	1:D:565:ASN:OD1	2.11	0.69
1:D:87:PRO:HD3	1:D:93:PRO:HG3	1.75	0.68
1:A:504:ALA:O	1:A:507:VAL:HB	1.93	0.68
1:A:516:GLY:O	7:A:717:HOH:O	2.09	0.68
1:D:102:GLY:HA3	1:D:426:ASN:HD21	1.57	0.68
1:D:226:GLY:HA3	1:D:529:ARG:HH11	1.58	0.68
1:A:351:THR:OG1	7:A:710:HOH:O	2.02	0.68
2:B:34:GLU:O	7:B:412:HOH:O	2.11	0.68
2:C:53:LYS:O	7:C:409:HOH:O	2.12	0.68
1:A:402:ARG:O	7:A:722:HOH:O	2.12	0.68
1:A:447:SER:OG	2:B:191:GLU:OE1	2.12	0.68
1:D:202:LEU:HA	1:D:205:HIS:HB2	1.75	0.68
1:D:113:PHE:HB2	4:D:603:ATP:O1B	1.93	0.68
2:E:68:LEU:HA	2:E:71:VAL:HG12	1.74	0.68
2:E:165:GLN:OE1	7:E:412:HOH:O	2.11	0.68
2:B:26:LYS:NZ	2:B:82:ASN:O	2.27	0.68
1:D:110:PHE:CE1	1:D:556:ALA:HB2	2.28	0.68
1:D:20:MET:SD	7:D:937:HOH:O	2.51	0.68
1:D:437:THR:O	1:D:440:ASP:N	2.27	0.68
1:D:99:LEU:HB2	1:D:556:ALA:H	1.59	0.68
1:A:464:SER:O	1:A:551:VAL:N	2.23	0.67
1:A:509:SER:O	1:A:513:LYS:N	2.15	0.67
1:A:153:GLN:H	1:A:564:GLU:HB2	1.59	0.67
2:B:18:ARG:NH2	7:B:425:HOH:O	2.25	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:158:GLY:O	7:D:724:HOH:O	2.12	0.67
1:D:169:VAL:N	4:D:603:ATP:O3'	2.27	0.67
1:A:495:ASN:CB	1:A:499:ARG:HH11	2.07	0.67
1:D:456:LYS:NZ	2:E:204:LYS:HE2	2.07	0.67
2:F:132:VAL:O	7:F:409:HOH:O	2.12	0.67
1:A:34:GLU:OE2	7:A:720:HOH:O	2.11	0.67
1:D:492:ASP:OD1	2:E:176:GLU:HG3	1.95	0.67
1:A:22:ARG:HA	1:A:415:ASN:HB2	1.77	0.67
2:C:146:GLY:O	7:C:408:HOH:O	2.11	0.67
2:E:17:MET:HE2	2:E:200:PRO:HD2	1.76	0.67
2:F:138:GLU:OE2	7:F:408:HOH:O	2.11	0.67
2:B:73:TYR:HE1	2:C:96:ARG:HH11	1.42	0.67
1:D:332:SER:OG	1:D:333:SER:N	2.24	0.67
2:E:62:LYS:NZ	7:E:430:HOH:O	2.26	0.67
1:D:419:LEU:O	7:D:726:HOH:O	2.12	0.67
1:D:39:ASN:ND2	1:D:90:THR:O	2.27	0.67
1:A:150:SER:HB2	1:A:167:THR:HA	1.77	0.67
1:A:332:SER:HA	4:A:602:ATP:N6	2.10	0.67
2:B:144:TYR:HB3	2:B:154:ASP:OD2	1.95	0.67
2:E:144:TYR:HB3	2:E:154:ASP:OD2	1.93	0.67
2:F:35:GLU:HG3	2:F:44:LEU:HD22	1.77	0.67
1:A:304:ILE:HG13	1:A:328:HIS:HB3	1.76	0.67
2:B:77:ALA:O	7:B:413:HOH:O	2.12	0.67
1:D:120:ASN:OD1	7:D:725:HOH:O	2.12	0.67
2:E:91:GLY:N	7:E:409:HOH:O	2.25	0.67
1:A:146:GLN:N	7:A:752:HOH:O	2.23	0.67
1:A:424:ARG:HB2	1:A:425:ARG:HE	1.59	0.67
1:D:22:ARG:NH1	1:D:414:ASN:OD1	2.27	0.67
1:D:352:PHE:HD2	1:D:421:PHE:HE2	1.43	0.67
1:D:534:HIS:CG	1:D:557:LYS:HE2	2.30	0.67
2:C:136:GLU:OE2	7:C:410:HOH:O	2.13	0.67
1:D:406:VAL:N	7:D:766:HOH:O	2.23	0.67
1:A:234:PHE:HD2	1:A:290:LEU:HD21	1.58	0.66
1:A:559:LEU:O	1:A:562:LEU:HB3	1.95	0.66
2:B:64:VAL:HB	2:B:73:TYR:CD2	2.30	0.66
1:D:107:ARG:CZ	1:D:433:ILE:HG13	2.25	0.66
1:A:314:PRO:HB3	1:A:317:ARG:HH12	1.61	0.66
1:A:165:ALA:HA	4:A:602:ATP:O5'	1.94	0.66
1:D:382:VAL:O	7:D:723:HOH:O	2.11	0.66
1:A:219:VAL:HB	1:A:295:PHE:HZ	1.60	0.66
2:E:64:VAL:HB	2:E:73:TYR:CD2	2.29	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:66:GLU:HB2	2:E:69:ASN:HB2	1.77	0.66
1:A:223:PHE:CE2	1:A:545:PHE:HZ	2.14	0.66
1:A:242:VAL:HG12	1:A:277:ILE:HD13	1.76	0.66
1:A:81:VAL:HG22	1:A:97:ILE:HG13	1.77	0.66
1:D:138:ILE:HA	1:D:217:GLN:NE2	2.09	0.66
2:E:93:ALA:O	2:F:69:ASN:ND2	2.27	0.66
1:A:498:ASP:HB3	1:A:510:ARG:NH2	2.10	0.66
1:D:108:PRO:HG2	1:D:552:LYS:N	2.10	0.66
1:D:559:LEU:O	1:D:562:LEU:HB3	1.96	0.66
2:E:211:GLU:OE1	7:E:413:HOH:O	2.14	0.66
2:E:75:ASP:HB2	2:E:84:PHE:CE2	2.31	0.66
1:A:158:GLY:O	7:A:724:HOH:O	2.13	0.66
1:A:500:ALA:CA	2:B:188:ARG:NH1	2.56	0.66
1:D:381:GLN:OE1	7:D:727:HOH:O	2.13	0.66
1:D:164:THR:HG23	1:D:557:LYS:HG3	1.78	0.66
1:A:552:LYS:HD2	1:A:553:PRO:HD2	1.77	0.65
1:A:134:ARG:O	7:A:728:HOH:O	2.15	0.65
1:D:175:PHE:O	1:D:179:MET:HB2	1.96	0.65
1:D:376:PRO:O	7:D:732:HOH:O	2.15	0.65
1:A:152:LYS:NZ	1:A:561:ILE:O	2.29	0.65
2:B:215:ASN:ND2	7:B:434:HOH:O	2.30	0.65
1:D:168:ASN:O	1:D:172:ASN:HB2	1.96	0.65
2:E:178:GLU:O	7:E:415:HOH:O	2.15	0.65
2:F:138:GLU:OE1	7:F:410:HOH:O	2.12	0.65
1:A:419:LEU:O	7:A:727:HOH:O	2.15	0.65
1:A:152:LYS:HD3	1:A:561:ILE:HG23	1.79	0.65
2:C:166:ALA:HA	2:C:169:LYS:HG2	1.78	0.65
2:F:101:PHE:HE2	2:F:135:LEU:HG	1.61	0.65
1:A:197:ASP:N	1:A:197:ASP:OD1	2.30	0.65
1:D:342:THR:O	1:D:345:LEU:HG	1.96	0.65
1:D:454:GLU:OE1	7:E:412:HOH:O	2.13	0.65
2:E:8:LEU:HD13	2:E:44:LEU:HB2	1.79	0.65
2:B:125:LYS:HB3	7:B:516:HOH:O	1.96	0.65
1:D:169:VAL:O	1:D:175:PHE:HB2	1.97	0.65
1:D:401:TYR:O	7:D:730:HOH:O	2.14	0.65
2:E:211:GLU:HA	2:E:214:LYS:HE3	1.78	0.65
2:C:121:GLN:NE2	7:C:422:HOH:O	2.29	0.65
1:D:199:HIS:HB2	1:D:525:LYS:HG3	1.79	0.65
2:E:98:TRP:CE3	2:E:101:PHE:HB2	2.32	0.64
1:A:494:CYS:HA	1:A:497:LEU:HD12	1.79	0.64
2:C:139:LEU:HG	2:C:142:LYS:HB3	1.79	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:280:LYS:O	7:D:733:HOH:O	2.15	0.64
7:D:711:HOH:O	2:E:176:GLU:OE1	2.14	0.64
2:B:187:LYS:O	7:B:417:HOH:O	2.15	0.64
2:B:98:TRP:CZ3	2:B:135:LEU:HD11	2.32	0.64
1:D:135:ASP:OD2	7:D:734:HOH:O	2.15	0.64
2:F:101:PHE:HE1	2:F:105:LYS:HE3	1.62	0.64
1:A:513:LYS:NZ	1:A:575:PHE:HB3	2.12	0.64
1:A:463:SER:HB2	1:A:528:PHE:HE1	1.63	0.64
1:D:343:PRO:HD2	7:D:734:HOH:O	1.98	0.64
7:A:701:HOH:O	2:B:162:SER:HA	1.96	0.64
1:D:445:VAL:HA	1:D:479:TRP:HZ2	1.63	0.64
2:E:69:ASN:OD1	7:E:416:HOH:O	2.15	0.64
1:A:139:ASP:OD2	1:A:142:GLY:HA3	1.96	0.64
1:A:499:ARG:HB3	7:B:416:HOH:O	1.96	0.64
1:A:574:ALA:HB2	2:B:180:PRO:HB2	1.80	0.64
2:B:188:ARG:NE	7:B:416:HOH:O	2.15	0.64
1:D:152:LYS:HD3	1:D:561:ILE:HG23	1.80	0.64
2:F:39:ASN:OD1	7:F:411:HOH:O	2.15	0.64
1:A:219:VAL:HG11	1:A:291:ILE:HG21	1.80	0.64
1:A:107:ARG:NH2	1:A:552:LYS:HB2	2.13	0.64
2:B:103:ASP:OD1	7:B:415:HOH:O	2.15	0.64
2:B:139:LEU:O	2:B:141:ASP:N	2.30	0.64
2:E:11:TRP:CD1	2:E:12:PRO:HD3	2.33	0.64
2:E:166:ALA:HA	2:E:169:LYS:HG2	1.80	0.64
1:A:115:ASP:OD1	7:A:730:HOH:O	2.15	0.64
1:A:479:TRP:CZ2	1:A:497:LEU:HD21	2.32	0.64
1:D:16:GLU:OE2	7:D:735:HOH:O	2.15	0.64
2:E:100:ASP:HB3	7:F:401:HOH:O	1.98	0.64
2:B:164:PHE:HD2	2:B:183:ILE:HD12	1.63	0.64
2:B:64:VAL:HG23	2:B:70:VAL:HG22	1.79	0.64
1:D:219:VAL:HB	1:D:295:PHE:CZ	2.33	0.64
1:D:300:TYR:HB2	7:D:776:HOH:O	1.98	0.64
1:D:153:GLN:H	1:D:564:GLU:HB2	1.62	0.64
2:E:23:LEU:HD22	2:E:28:VAL:HG11	1.79	0.64
2:E:63:PRO:O	7:E:417:HOH:O	2.15	0.64
2:C:38:SER:HB2	7:C:401:HOH:O	1.97	0.63
2:E:7:LEU:HD21	2:E:23:LEU:HD12	1.79	0.63
1:D:90:THR:HA	1:D:399:TYR:HE2	1.63	0.63
1:D:518:LEU:HD12	1:D:519:GLU:N	2.14	0.63
2:F:159:THR:HA	2:F:199:LEU:HD21	1.80	0.63
1:A:168:ASN:O	1:A:172:ASN:HB2	1.99	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:205:ILE:HG22	7:B:488:HOH:O	1.97	0.63
2:B:33:ARG:NH1	2:B:41:SER:OG	2.29	0.63
1:D:134:ARG:NH1	7:D:734:HOH:O	2.30	0.63
1:D:363:PHE:HE1	1:D:390:VAL:HG13	1.60	0.63
1:A:172:ASN:ND2	7:A:772:HOH:O	2.30	0.63
1:D:472:PRO:O	7:D:737:HOH:O	2.15	0.63
1:D:66:PRO:HG2	7:D:722:HOH:O	1.99	0.63
2:E:115:GLY:N	7:E:408:HOH:O	2.32	0.63
2:F:44:LEU:O	7:F:412:HOH:O	2.16	0.63
2:F:101:PHE:CZ	2:F:131:ALA:HB1	2.31	0.63
1:A:70:ASP:HB2	1:A:104:SER:HB2	1.80	0.63
1:A:58:GLU:HG2	1:A:62:LYS:HE2	1.81	0.63
2:C:7:LEU:HD21	2:C:9:ASP:OD2	1.99	0.63
1:D:198:VAL:HG13	1:D:565:ASN:HD21	1.63	0.63
1:D:442:GLN:HG2	1:D:462:PHE:CZ	2.34	0.63
1:A:110:PHE:CE1	1:A:556:ALA:HB2	2.33	0.63
1:A:445:VAL:HG22	1:A:479:TRP:HE1	1.64	0.63
1:D:405:ASP:OD1	1:D:540:SER:HB2	1.99	0.63
1:D:331:GLY:O	4:D:603:ATP:N6	2.32	0.63
1:D:362:GLU:HB2	7:D:1013:HOH:O	1.97	0.63
1:D:495:ASN:HB3	1:D:499:ARG:HH11	1.64	0.63
1:A:143:LYS:HZ1	1:A:187:CYS:HA	1.62	0.62
1:A:143:LYS:HD2	1:A:212:PHE:HB2	1.81	0.62
1:A:499:ARG:HE	2:B:184:ALA:HB1	1.64	0.62
1:D:138:ILE:HB	1:D:217:GLN:HG3	1.80	0.62
2:E:165:GLN:HG3	7:E:433:HOH:O	1.98	0.62
1:A:146:GLN:HB2	1:A:148:ILE:HG23	1.80	0.62
1:A:150:SER:HB3	1:A:170:TYR:CD2	2.34	0.62
1:A:465:TYR:HD1	1:A:551:VAL:HG23	1.64	0.62
1:D:445:VAL:HG22	1:D:479:TRP:NE1	2.11	0.62
1:A:166:THR:OG1	1:A:167:THR:N	2.31	0.62
1:A:437:THR:OG1	1:A:440:ASP:HB2	1.98	0.62
1:A:147:PHE:O	1:A:529:ARG:NH2	2.31	0.62
2:C:63:PRO:O	7:C:411:HOH:O	2.16	0.62
2:F:15:PHE:HA	2:F:18:ARG:HD2	1.81	0.62
1:A:87:PRO:HB3	1:A:93:PRO:HD3	1.81	0.62
1:A:499:ARG:CZ	2:B:184:ALA:HB1	2.28	0.62
1:D:363:PHE:CD2	1:D:382:VAL:HG21	2.23	0.62
1:D:147:PHE:O	1:D:529:ARG:NH2	2.32	0.62
2:E:122:GLU:HA	2:E:125:LYS:HE2	1.80	0.62
1:D:456:LYS:HZ1	2:E:204:LYS:HE2	1.62	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:TYR:HB2	1:A:563:CYS:HB2	1.80	0.62
2:C:146:GLY:HA3	2:C:151:GLY:HA3	1.81	0.62
2:C:201:ASP:HB3	2:C:203:GLU:HG2	1.81	0.62
1:D:304:ILE:HA	7:D:783:HOH:O	1.99	0.62
2:E:54:ILE:HB	2:E:55:PRO:HA	1.82	0.62
1:A:107:ARG:HD3	1:A:433:ILE:H	1.64	0.62
1:D:124:LEU:HB3	5:D:602:JAA:C15	2.28	0.62
2:E:21:VAL:HG12	2:E:155:ILE:HG12	1.80	0.62
1:A:430:SER:O	7:A:732:HOH:O	2.16	0.62
1:A:406:VAL:O	1:A:541:SER:OG	2.16	0.62
1:A:557:LYS:HD2	4:A:602:ATP:O3G	2.00	0.62
1:D:197:ASP:OD1	1:D:197:ASP:N	2.27	0.62
2:C:181:LYS:HA	1:D:93:PRO:HB2	1.81	0.62
2:B:163:TRP:HB3	2:B:167:TYR:CZ	2.35	0.62
2:B:73:TYR:HA	2:B:76:GLU:OE2	2.00	0.62
1:D:99:LEU:CB	1:D:557:LYS:H	2.11	0.62
2:E:102:VAL:O	2:E:107:THR:HG23	2.00	0.62
2:E:40:LYS:HD2	2:E:52:LYS:HB3	1.82	0.62
1:A:440:ASP:OD2	1:A:502:ILE:HG13	2.00	0.62
2:B:79:PRO:HD2	7:B:568:HOH:O	2.00	0.62
2:C:85:PHE:CE1	2:C:152:TYR:HB2	2.35	0.62
1:A:31:THR:OG1	1:A:357:ASN:HA	2.00	0.62
1:D:331:GLY:HA3	1:D:336:TRP:HA	1.81	0.62
2:E:73:TYR:HA	2:E:76:GLU:OE2	1.99	0.62
2:E:84:PHE:CD1	2:E:152:TYR:HB2	2.35	0.62
2:E:5:PRO:HB3	2:E:57:LEU:HD11	1.82	0.61
2:F:75:ASP:OD1	7:F:413:HOH:O	2.16	0.61
2:F:86:PRO:HD3	2:F:146:GLY:O	2.00	0.61
1:D:195:SER:OG	1:D:197:ASP:OD1	2.18	0.61
1:D:465:TYR:HB3	1:D:476:ALA:HB3	1.82	0.61
2:F:8:LEU:HB2	2:F:56:VAL:HB	1.81	0.61
1:A:157:THR:HG22	1:A:469:SER:HB3	1.82	0.61
1:A:481:ILE:O	7:A:731:HOH:O	2.16	0.61
2:B:107:THR:HG21	7:B:415:HOH:O	1.98	0.61
2:B:24:ARG:HB3	2:B:194:SER:HA	1.82	0.61
1:D:142:GLY:HA2	1:D:215:GLN:HB2	1.83	0.61
1:A:74:GLU:OE2	7:A:735:HOH:O	2.16	0.61
2:C:169:LYS:HD3	2:C:206:VAL:HG13	1.82	0.61
2:E:73:TYR:HE1	2:F:96:ARG:HH11	1.46	0.61
2:C:39:ASN:N	7:C:401:HOH:O	2.32	0.61
1:D:360:TYR:HA	7:D:827:HOH:O	2.01	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:125:LYS:HB3	2:F:173:PHE:HE2	1.64	0.61
1:D:461:ASP:HB3	1:D:528:PHE:CD2	2.35	0.61
1:D:162:VAL:HB	1:D:556:ALA:HB1	1.83	0.61
2:E:72:GLN:HE21	2:F:96:ARG:HD2	1.65	0.61
1:A:150:SER:N	7:A:764:HOH:O	2.27	0.61
1:A:363:PHE:HE1	1:A:390:VAL:HG13	1.64	0.61
1:D:152:LYS:HB2	1:D:561:ILE:HA	1.82	0.61
2:F:169:LYS:HZ3	2:F:206:VAL:HG13	1.66	0.61
2:F:98:TRP:CE2	2:F:138:GLU:HG2	2.36	0.61
1:A:444:SER:O	7:A:736:HOH:O	2.17	0.61
2:C:121:GLN:NE2	7:C:429:HOH:O	2.34	0.61
2:C:129:ILE:HG13	7:C:595:HOH:O	2.01	0.61
1:A:141:ASN:OD1	7:A:733:HOH:O	2.16	0.60
1:D:193:ILE:HG12	1:D:205:HIS:CE1	2.35	0.60
1:A:425:ARG:NH1	7:A:718:HOH:O	2.09	0.60
1:D:88:ILE:CD1	1:D:89:LEU:H	2.14	0.60
1:A:494:CYS:SG	1:A:495:ASN:N	2.74	0.60
1:A:175:PHE:O	1:A:179:MET:HB2	2.01	0.60
1:A:238:TRP:O	1:A:242:VAL:HG13	2.01	0.60
2:C:139:LEU:HD23	1:D:92:HIS:CE1	2.37	0.60
1:D:495:ASN:ND2	1:D:574:ALA:H	1.98	0.60
1:A:68:VAL:HG13	1:A:401:TYR:HD1	1.65	0.60
2:C:14:MET:N	7:C:432:HOH:O	2.35	0.60
2:E:20:ARG:HB3	2:E:198:SER:HB3	1.84	0.60
1:A:540:SER:OG	1:A:544:GLN:NE2	2.35	0.60
2:B:151:GLY:N	2:B:154:ASP:OD2	2.28	0.60
2:C:142:LYS:CG	1:D:41:SER:HB2	2.30	0.60
1:A:302:TYR:HH	1:A:328:HIS:HD1	1.50	0.60
2:B:114:TRP:HA	2:B:170:PHE:CD2	2.32	0.60
2:B:117:LYS:HE3	2:B:213:ARG:NH1	2.16	0.60
1:D:464:SER:O	1:D:551:VAL:HG22	2.01	0.60
2:F:106:PHE:CZ	2:F:132:VAL:HG23	2.37	0.60
1:A:462:PHE:O	1:A:549:ARG:NH1	2.34	0.60
2:C:139:LEU:O	2:C:141:ASP:N	2.34	0.60
2:C:153:VAL:HG12	7:C:448:HOH:O	2.01	0.60
1:A:108:PRO:HG2	1:A:552:LYS:HB3	1.84	0.60
1:A:98:SER:OG	4:A:602:ATP:O3B	2.20	0.60
1:D:361:PHE:HE1	1:D:392:ILE:HG23	1.66	0.60
1:D:352:PHE:CD2	1:D:421:PHE:HE2	2.19	0.60
2:E:97:PHE:CE1	2:F:65:CYS:HB2	2.36	0.60
2:B:136:GLU:HG3	2:B:181:LYS:HD3	1.84	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:117:LYS:HG3	2:C:213:ARG:HH11	1.66	0.59
1:D:445:VAL:HG13	1:D:479:TRP:CE2	2.37	0.59
1:D:531:ILE:HA	1:D:534:HIS:ND1	2.17	0.59
2:E:117:LYS:HA	2:E:121:GLN:HB2	1.84	0.59
2:E:24:ARG:HB3	2:E:194:SER:HA	1.84	0.59
1:A:107:ARG:HH22	1:A:552:LYS:HD3	1.67	0.59
2:B:17:MET:HE2	2:B:200:PRO:HD2	1.83	0.59
2:C:144:TYR:HB2	7:C:405:HOH:O	2.03	0.59
1:D:504:ALA:O	1:D:507:VAL:HB	2.02	0.59
2:B:171:GLY:HA3	7:B:513:HOH:O	2.01	0.59
2:C:145:PHE:O	7:C:413:HOH:O	2.17	0.59
1:D:448:ALA:HB3	1:D:479:TRP:CH2	2.34	0.59
1:D:451:ARG:NH1	1:D:454:GLU:OE1	2.36	0.59
1:D:22:ARG:O	7:D:739:HOH:O	2.17	0.59
2:E:114:TRP:HD1	2:E:167:TYR:CE1	2.21	0.59
2:E:114:TRP:HA	2:E:170:PHE:CD2	2.33	0.59
1:D:27:VAL:O	1:D:31:THR:OG1	2.14	0.59
1:D:22:ARG:HA	1:D:415:ASN:HB2	1.83	0.59
2:E:64:VAL:HB	2:E:73:TYR:CE2	2.38	0.59
1:A:97:ILE:HB	1:A:162:VAL:HB	1.84	0.59
1:D:438:GLU:O	1:D:442:GLN:HG3	2.02	0.59
1:A:108:PRO:HG2	1:A:552:LYS:N	2.18	0.59
1:D:311:PRO:O	7:D:738:HOH:O	2.16	0.59
1:A:143:LYS:HA	1:A:184:SER:HB2	1.84	0.59
1:A:496:CYS:HA	1:A:499:ARG:CZ	2.33	0.59
1:D:305:MET:HB2	7:D:729:HOH:O	2.02	0.59
1:D:320:ALA:O	1:D:323:LEU:HB2	2.03	0.59
1:D:328:HIS:CG	1:D:329:ASP:N	2.69	0.59
1:A:333:SER:HA	7:A:706:HOH:O	2.03	0.59
2:B:94:GLN:OE1	7:B:418:HOH:O	2.17	0.59
1:A:150:SER:CB	1:A:167:THR:HA	2.33	0.59
2:C:25:GLU:OE2	7:C:412:HOH:O	2.16	0.59
2:B:9:ASP:HB2	2:B:20:ARG:HH21	1.68	0.58
1:D:207:LEU:O	1:D:211:LEU:HG	2.03	0.58
1:D:426:ASN:HB3	7:D:782:HOH:O	2.03	0.58
1:A:500:ALA:HB2	2:B:188:ARG:NH1	2.16	0.58
1:D:143:LYS:CA	1:D:184:SER:HB2	2.33	0.58
1:A:435:LYS:HA	1:A:436:ASN:HB2	1.85	0.58
1:A:499:ARG:HH12	2:B:187:LYS:HZ1	1.49	0.58
2:C:215:ASN:O	7:C:416:HOH:O	2.17	0.58
1:D:273:LEU:O	1:D:276:THR:OG1	2.20	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:105:GLN:HA	1:D:430:SER:HB3	1.84	0.58
1:D:499:ARG:NE	2:E:184:ALA:HB1	2.17	0.58
1:D:557:LYS:HD2	4:D:603:ATP:O3G	2.03	0.58
1:A:342:THR:O	1:A:345:LEU:HG	2.04	0.58
1:A:444:SER:HA	1:A:500:ALA:CB	2.34	0.58
2:B:86:PRO:HD3	2:B:146:GLY:O	2.03	0.58
1:D:440:ASP:OD1	1:D:501:PHE:HA	2.02	0.58
1:D:109:LYS:HB3	7:D:801:HOH:O	2.04	0.58
1:D:32:LEU:HD21	1:D:61:PHE:HD2	1.69	0.58
1:D:76:TYR:O	1:D:88:ILE:HG12	2.02	0.58
2:E:50:ILE:HG13	2:E:51:HIS:H	1.68	0.58
2:F:111:PHE:HD2	2:F:112:LYS:HD3	1.68	0.58
1:A:374:GLU:N	7:A:784:HOH:O	2.36	0.58
1:A:105:GLN:HA	1:A:430:SER:HB3	1.84	0.58
1:A:99:LEU:CB	1:A:557:LYS:H	2.15	0.58
2:C:142:LYS:HG3	1:D:39:ASN:HA	1.85	0.58
1:D:333:SER:HB2	7:D:844:HOH:O	2.04	0.58
1:A:17:PHE:CE2	1:A:341:VAL:HG11	2.39	0.58
1:A:317:ARG:NH2	7:A:786:HOH:O	2.36	0.58
3:A:601:ILE:HA	4:A:602:ATP:C2	2.39	0.58
2:C:27:GLY:O	7:C:415:HOH:O	2.17	0.58
1:D:484:GLU:N	7:D:803:HOH:O	2.36	0.58
1:D:70:ASP:HB2	1:D:104:SER:HB2	1.85	0.58
2:F:125:LYS:HE2	2:F:171:GLY:HA2	1.86	0.58
2:E:96:ARG:NH1	2:F:69:ASN:OD1	2.31	0.58
1:A:222:VAL:HB	1:A:533:GLU:CD	2.24	0.58
1:A:473:GLY:O	1:A:516:GLY:N	2.33	0.58
2:C:7:LEU:HG	2:C:9:ASP:HB2	1.85	0.58
1:D:140:ASP:N	1:D:140:ASP:OD1	2.24	0.58
1:D:494:CYS:HB2	1:D:520:LEU:HB3	1.86	0.58
1:D:465:TYR:HD1	1:D:551:VAL:HG23	1.67	0.58
2:B:121:GLN:O	2:B:125:LYS:HG3	2.03	0.58
1:D:150:SER:CB	1:D:167:THR:HA	2.34	0.58
1:D:152:LYS:HG2	1:D:565:ASN:H	1.67	0.58
1:D:33:LYS:NZ	1:D:57:PRO:HG2	2.19	0.58
2:E:45:LEU:HD21	7:E:547:HOH:O	2.03	0.58
2:E:80:GLU:N	7:E:429:HOH:O	2.35	0.58
2:B:181:LYS:HA	2:B:184:ALA:HB3	1.86	0.58
1:D:148:ILE:HD12	1:D:170:TYR:CZ	2.38	0.58
1:D:342:THR:OG1	1:D:413:TYR:OH	2.12	0.58
1:D:435:LYS:HZ2	1:D:438:GLU:HA	1.68	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:114:TRP:HD1	2:E:167:TYR:HE1	1.49	0.58
2:E:26:LYS:CG	2:E:81:LYS:NZ	2.67	0.58
1:A:154:TYR:OH	7:A:716:HOH:O	2.09	0.57
1:A:459:VAL:HG22	1:A:481:ILE:HG22	1.85	0.57
1:A:99:LEU:HD23	1:A:535:PHE:HZ	1.68	0.57
2:B:73:TYR:HD1	2:B:76:GLU:OE2	1.86	0.57
1:D:107:ARG:NH2	1:D:552:LYS:HB2	2.18	0.57
2:E:71:VAL:O	2:E:74:VAL:HB	2.04	0.57
2:E:98:TRP:HD1	2:E:153:VAL:HG11	1.65	0.57
1:A:152:LYS:HZ1	1:A:523:VAL:HG11	1.68	0.57
1:A:444:SER:HA	1:A:500:ALA:HB1	1.86	0.57
1:A:345:LEU:O	7:A:734:HOH:O	2.16	0.57
2:C:44:LEU:O	7:C:414:HOH:O	2.17	0.57
1:D:132:ARG:HD2	1:D:326:VAL:HG11	1.86	0.57
1:D:35:ILE:HA	1:D:395:TYR:CE1	2.39	0.57
1:D:437:THR:OG1	1:D:440:ASP:HB2	2.05	0.57
2:E:32:TYR:OH	7:E:411:HOH:O	2.08	0.57
2:E:54:ILE:O	7:E:418:HOH:O	2.16	0.57
2:E:26:LYS:HE3	2:E:78:TRP:O	2.04	0.57
1:A:347:PRO:HA	1:A:350:ALA:HB2	1.87	0.57
1:A:441:LEU:HD23	1:A:549:ARG:HB3	1.86	0.57
2:B:33:ARG:HH22	2:B:41:SER:CB	2.18	0.57
2:C:188:ARG:NH1	1:D:87:PRO:O	2.37	0.57
1:D:124:LEU:HD11	7:D:872:HOH:O	2.02	0.57
1:D:19:GLU:HG3	7:D:731:HOH:O	2.04	0.57
1:D:253:ARG:NH2	7:D:809:HOH:O	2.37	0.57
1:D:503:ASP:OD1	1:D:504:ALA:N	2.37	0.57
2:E:98:TRP:CH2	2:E:135:LEU:CD1	2.79	0.57
2:F:162:SER:HB3	2:F:199:LEU:HD23	1.86	0.57
2:F:215:ASN:OD1	7:F:414:HOH:O	2.17	0.57
1:A:495:ASN:C	1:A:499:ARG:NH1	2.58	0.57
1:D:13:VAL:O	7:D:742:HOH:O	2.17	0.57
6:E:301:GSH:O2	7:E:418:HOH:O	2.17	0.57
1:A:99:LEU:HB3	1:A:557:LYS:CB	2.34	0.57
1:D:283:SER:O	7:D:740:HOH:O	2.17	0.57
1:D:442:GLN:HG2	1:D:462:PHE:HZ	1.68	0.57
2:B:57:LEU:HB3	2:B:64:VAL:HG22	1.87	0.57
2:B:71:VAL:O	2:B:74:VAL:HB	2.04	0.57
1:D:138:ILE:CA	1:D:217:GLN:HE21	2.13	0.57
1:D:531:ILE:HA	1:D:534:HIS:CE1	2.40	0.57
2:F:145:PHE:N	2:F:154:ASP:OD2	2.37	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:E:416:HOH:O	2:F:96:ARG:NE	2.28	0.57
2:B:193:GLU:N	7:B:441:HOH:O	2.38	0.57
2:C:136:GLU:HG3	2:C:181:LYS:HD3	1.86	0.57
1:D:344:ARG:NH1	7:D:811:HOH:O	2.38	0.57
1:D:336:TRP:HB2	1:D:358:LEU:HD13	1.85	0.57
1:D:104:SER:O	1:D:107:ARG:HB2	2.04	0.57
2:E:11:TRP:O	2:E:200:PRO:HG2	2.05	0.57
2:E:53:LYS:HG2	6:E:301:GSH:HA31	1.87	0.57
1:A:153:GLN:HG3	1:A:171:ARG:HD2	1.87	0.57
1:A:531:ILE:HA	1:A:534:HIS:CE1	2.40	0.57
1:D:222:VAL:HB	1:D:533:GLU:CD	2.25	0.57
1:D:219:VAL:HB	1:D:295:PHE:HZ	1.68	0.57
1:D:522:VAL:O	1:D:567:VAL:HG22	2.05	0.57
1:D:68:VAL:HG23	1:D:72:GLU:HB2	1.86	0.57
2:E:8:LEU:HD22	2:E:33:ARG:NH2	2.18	0.57
2:F:108:ASP:O	2:F:112:LYS:HG2	2.04	0.57
2:F:150:PHE:CE1	2:F:155:ILE:HG13	2.37	0.57
2:F:57:LEU:N	7:F:415:HOH:O	2.37	0.57
1:A:202:LEU:HA	1:A:205:HIS:HB2	1.87	0.56
1:A:25:HIS:NE2	1:A:380:THR:OG1	2.38	0.56
1:A:534:HIS:CE1	1:A:557:LYS:HG2	2.40	0.56
1:D:151:SER:OG	1:D:195:SER:O	2.23	0.56
1:D:521:ARG:NH2	7:D:813:HOH:O	2.38	0.56
1:D:99:LEU:HB3	1:D:557:LYS:CB	2.35	0.56
2:F:106:PHE:HZ	2:F:132:VAL:HG23	1.68	0.56
1:A:221:ALA:HB1	1:A:529:ARG:HH12	1.69	0.56
1:A:437:THR:HG21	1:A:439:ARG:HH21	1.70	0.56
2:C:181:LYS:NZ	1:D:114:THR:HG23	2.20	0.56
1:D:280:LYS:HE2	1:D:293:ALA:HB1	1.86	0.56
1:D:477:ILE:HG12	1:D:518:LEU:CD1	2.28	0.56
2:F:130:GLU:O	2:F:134:ILE:HG13	2.05	0.56
1:D:455:GLU:OE1	1:D:485:THR:HB	2.05	0.56
1:D:488:ASP:OD2	2:E:168:GLU:OE2	2.23	0.56
1:D:76:TYR:O	1:D:79:ARG:HB2	2.05	0.56
1:D:96:ALA:HB3	1:D:113:PHE:CD2	2.39	0.56
2:E:63:PRO:HG3	7:E:439:HOH:O	2.05	0.56
2:F:10:TYR:O	2:F:20:ARG:NH2	2.38	0.56
2:F:15:PHE:HB3	2:F:67:SER:HB3	1.87	0.56
2:F:85:PHE:HB3	2:F:92:ARG:HG2	1.86	0.56
1:A:151:SER:OG	1:A:195:SER:O	2.22	0.56
1:A:206:LEU:O	1:A:210:ILE:HG12	2.05	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:60:ASN:ND2	7:C:439:HOH:O	2.38	0.56
1:D:513:LYS:NZ	1:D:575:PHE:HB3	2.20	0.56
1:A:461:ASP:HB3	1:A:528:PHE:CD2	2.40	0.56
1:A:222:VAL:HG21	3:A:601:ILE:N	2.20	0.56
2:C:145:PHE:N	2:C:154:ASP:OD2	2.39	0.56
2:E:184:ALA:HA	2:E:187:LYS:NZ	2.21	0.56
1:A:238:TRP:HZ3	1:A:278:ARG:HA	1.71	0.56
2:B:194:SER:O	2:B:198:SER:OG	2.14	0.56
2:B:195:VAL:HG23	2:B:199:LEU:HD13	1.87	0.56
1:A:241:ILE:O	1:A:245:ILE:HG12	2.05	0.56
1:A:457:ILE:HB	1:A:482:SER:OG	2.06	0.56
2:B:131:ALA:O	2:B:135:LEU:HB2	2.05	0.56
2:C:142:LYS:HE2	1:D:40:GLN:HG2	1.88	0.56
1:D:441:LEU:O	7:D:743:HOH:O	2.18	0.56
1:D:96:ALA:HA	1:D:161:PRO:O	2.05	0.56
2:E:117:LYS:HD3	7:E:553:HOH:O	2.06	0.56
1:A:410:ILE:HG13	1:A:411:GLY:N	2.21	0.56
1:A:498:ASP:HB2	7:A:702:HOH:O	2.05	0.56
1:A:99:LEU:HB3	1:A:557:LYS:HB2	1.88	0.56
2:C:91:GLY:O	7:C:417:HOH:O	2.18	0.56
1:D:459:VAL:HG22	1:D:481:ILE:HG22	1.86	0.56
2:E:44:LEU:O	7:E:419:HOH:O	2.17	0.56
1:A:169:VAL:O	1:A:175:PHE:HB2	2.06	0.56
1:A:221:ALA:HB3	1:A:227:LEU:HG	1.86	0.56
2:B:103:ASP:HA	7:B:415:HOH:O	2.04	0.56
2:B:110:GLN:HA	2:B:113:VAL:HG12	1.88	0.56
1:D:76:TYR:HB2	1:D:89:LEU:HD11	1.88	0.56
2:F:9:ASP:OD1	2:F:10:TYR:N	2.32	0.56
1:A:238:TRP:CZ3	1:A:278:ARG:HA	2.41	0.56
1:D:53:ASN:O	1:D:57:PRO:HB3	2.05	0.56
1:D:99:LEU:HD13	1:D:558:VAL:H	1.71	0.56
1:A:17:PHE:HE1	1:A:355:ILE:HG12	1.69	0.56
2:B:168:GLU:HG3	7:B:463:HOH:O	2.05	0.56
2:B:25:GLU:O	7:B:420:HOH:O	2.18	0.56
1:D:329:ASP:N	1:D:329:ASP:OD1	2.38	0.56
2:E:114:TRP:CD1	2:E:167:TYR:CE1	2.89	0.56
1:A:19:GLU:O	1:A:23:ASN:ND2	2.24	0.55
1:A:352:PHE:HD2	1:A:421:PHE:HE2	1.54	0.55
2:C:26:LYS:HZ3	2:C:82:ASN:C	2.10	0.55
1:D:201:ALA:O	1:D:205:HIS:N	2.39	0.55
1:D:143:LYS:HD2	1:D:212:PHE:HB2	1.88	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:238:TRP:O	1:D:242:VAL:HG13	2.06	0.55
1:D:17:PHE:HE1	1:D:355:ILE:HG12	1.70	0.55
1:D:464:SER:O	1:D:551:VAL:N	2.34	0.55
2:F:111:PHE:CD2	2:F:112:LYS:HD3	2.41	0.55
1:A:250:LEU:HD21	1:A:260:ARG:HG2	1.86	0.55
1:A:361:PHE:HE1	1:A:392:ILE:HG23	1.71	0.55
1:A:530:LYS:HD3	1:A:561:ILE:HD13	1.87	0.55
1:A:563:CYS:O	1:A:566:VAL:HG13	2.07	0.55
2:B:164:PHE:CD2	2:B:183:ILE:HD12	2.41	0.55
2:F:125:LYS:HB3	2:F:173:PHE:CE2	2.42	0.55
1:A:171:ARG:HH21	1:A:194:PHE:HB3	1.71	0.55
1:A:452:LEU:HB3	1:A:457:ILE:HD11	1.87	0.55
1:A:164:THR:HG23	1:A:557:LYS:HG3	1.89	0.55
1:D:445:VAL:HG21	1:D:462:PHE:CG	2.42	0.55
1:D:496:CYS:HB2	2:E:187:LYS:NZ	2.22	0.55
2:E:141:ASP:OD1	2:E:141:ASP:N	2.38	0.55
2:E:177:SER:HB2	7:E:462:HOH:O	2.06	0.55
2:E:26:LYS:CG	2:E:81:LYS:HZ3	2.20	0.55
2:C:102:VAL:HB	7:C:467:HOH:O	2.07	0.55
1:D:81:VAL:HG22	1:D:97:ILE:HG13	1.89	0.55
1:A:203:TYR:CZ	1:A:241:ILE:HG13	2.41	0.55
1:D:237:VAL:O	7:D:741:HOH:O	2.17	0.55
1:D:337:ILE:O	1:D:354:VAL:HA	2.05	0.55
2:F:201:ASP:OD2	2:F:204:LYS:HE2	2.06	0.55
1:A:140:ASP:OD1	1:A:140:ASP:N	2.20	0.55
1:A:503:ASP:OD1	1:A:504:ALA:N	2.39	0.55
2:B:84:PHE:N	7:B:429:HOH:O	2.39	0.55
2:C:117:LYS:HG3	2:C:213:ARG:NH1	2.21	0.55
2:C:213:ARG:NH1	7:C:436:HOH:O	2.38	0.55
1:D:150:SER:HB3	1:D:170:TYR:CD2	2.41	0.55
2:F:214:LYS:HG2	7:F:533:HOH:O	2.06	0.55
2:F:52:LYS:HD2	7:F:493:HOH:O	2.07	0.55
1:A:492:ASP:O	2:B:187:LYS:HE3	2.07	0.55
1:D:301:VAL:N	7:D:776:HOH:O	2.40	0.55
1:D:78:LYS:NZ	7:D:791:HOH:O	2.32	0.55
1:D:50:LEU:HD11	1:D:65:VAL:HG22	1.88	0.55
2:E:125:LYS:HA	2:E:128:PHE:CD2	2.42	0.55
2:E:57:LEU:HB3	2:E:64:VAL:HG22	1.88	0.55
2:F:107:THR:HG23	2:F:110:GLN:HE21	1.72	0.55
1:A:100:SER:HB3	1:A:109:LYS:HD3	1.88	0.55
1:A:246:LYS:NZ	1:A:271:PRO:HA	2.22	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:170:PHE:CE2	2:B:213:ARG:HD2	2.42	0.55
2:C:193:GLU:HA	2:C:196:SER:HB3	1.88	0.55
1:D:143:LYS:NZ	1:D:187:CYS:HA	2.21	0.55
1:D:328:HIS:CG	1:D:329:ASP:H	2.24	0.55
1:D:487:GLU:HG2	1:D:570:TYR:CZ	2.42	0.55
1:A:107:ARG:HD3	1:A:433:ILE:N	2.21	0.55
1:A:199:HIS:HE2	1:A:200:GLN:HE21	1.53	0.55
1:D:363:PHE:HB3	1:D:388:TYR:HB3	1.89	0.55
1:D:451:ARG:NE	2:E:183:ILE:HD11	2.22	0.55
2:E:28:VAL:O	7:E:420:HOH:O	2.18	0.55
1:A:143:LYS:CD	1:A:212:PHE:HB2	2.37	0.54
1:A:287:TRP:HE3	1:A:290:LEU:HD13	1.71	0.54
1:A:84:ASP:C	1:A:86:SER:H	2.10	0.54
2:B:110:GLN:O	2:B:113:VAL:HG12	2.06	0.54
1:D:164:THR:HG22	7:D:764:HOH:O	2.07	0.54
1:D:199:HIS:N	1:D:524:ALA:HB1	2.21	0.54
1:A:138:ILE:HA	1:A:217:GLN:NE2	2.19	0.54
1:A:437:THR:O	1:A:440:ASP:N	2.36	0.54
1:A:523:VAL:HG13	7:A:705:HOH:O	2.06	0.54
1:A:405:ASP:OD1	1:A:540:SER:HB2	2.07	0.54
2:B:102:VAL:HG12	7:B:406:HOH:O	2.07	0.54
1:D:363:PHE:HD1	1:D:390:VAL:HA	1.71	0.54
2:F:65:CYS:O	2:F:66:GLU:HB2	2.07	0.54
1:A:320:ALA:O	1:A:323:LEU:HB2	2.08	0.54
1:A:323:LEU:O	7:A:738:HOH:O	2.18	0.54
1:A:464:SER:O	1:A:551:VAL:HG22	2.07	0.54
2:B:92:ARG:NH2	7:B:443:HOH:O	2.40	0.54
1:D:235:GLU:HG2	1:D:287:TRP:CG	2.42	0.54
1:A:100:SER:HA	1:A:535:PHE:CE1	2.43	0.54
1:A:531:ILE:HA	1:A:534:HIS:ND1	2.22	0.54
1:A:536:LEU:HB2	1:A:545:PHE:CE1	2.43	0.54
2:C:188:ARG:NH1	7:C:442:HOH:O	2.40	0.54
2:B:166:ALA:HB2	7:B:488:HOH:O	2.08	0.54
1:D:107:ARG:HG2	7:D:704:HOH:O	2.08	0.54
1:D:22:ARG:HG2	1:D:414:ASN:HB3	1.87	0.54
1:A:107:ARG:HH11	1:A:107:ARG:CG	2.16	0.54
1:A:411:GLY:O	1:A:418:GLN:N	2.35	0.54
2:E:5:PRO:HG2	2:E:28:VAL:HG21	1.90	0.54
2:F:121:GLN:NE2	2:F:170:PHE:O	2.40	0.54
1:A:193:ILE:HG22	7:A:764:HOH:O	2.07	0.54
1:D:193:ILE:HG12	1:D:205:HIS:HE1	1.72	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:198:VAL:HG12	7:D:797:HOH:O	2.08	0.54
1:D:429:LEU:HG	1:D:430:SER:H	1.71	0.54
7:D:860:HOH:O	2:E:176:GLU:HG2	2.06	0.54
1:A:101:SER:N	7:A:757:HOH:O	2.25	0.54
2:B:10:TYR:CG	2:B:12:PRO:HD2	2.43	0.54
2:B:117:LYS:HE3	2:B:213:ARG:HH11	1.73	0.54
1:D:165:ALA:HB1	4:D:603:ATP:N3	2.22	0.54
1:D:249:VAL:HG11	7:D:1144:HOH:O	2.08	0.54
2:C:143:PRO:HA	1:D:87:PRO:HB2	1.90	0.54
1:A:150:SER:HB3	1:A:170:TYR:HD2	1.72	0.54
1:A:495:ASN:HB3	1:A:499:ARG:HH11	1.70	0.54
1:D:491:GLN:NE2	1:D:570:TYR:HD2	2.05	0.54
2:E:117:LYS:HE3	2:E:213:ARG:HH11	1.73	0.54
2:E:5:PRO:HG3	2:E:59:HIS:CE1	2.43	0.54
2:E:92:ARG:NE	2:F:76:GLU:OE2	2.41	0.54
1:A:53:ASN:O	1:A:57:PRO:HB3	2.08	0.54
2:B:144:TYR:OH	7:B:421:HOH:O	2.18	0.54
2:C:99:ALA:O	2:C:103:ASP:HB2	2.07	0.54
2:C:9:ASP:OD1	2:C:16:GLY:HA3	2.08	0.54
1:D:521:ARG:HB3	1:D:566:VAL:HG12	1.90	0.54
1:A:152:LYS:CE	1:A:565:ASN:HB2	2.29	0.53
2:B:90:TYR:CZ	2:C:62:LYS:HB3	2.43	0.53
1:D:351:THR:HG21	1:D:410:ILE:HG12	1.90	0.53
1:D:352:PHE:N	7:D:726:HOH:O	2.40	0.53
1:D:424:ARG:HB2	1:D:425:ARG:HE	1.72	0.53
1:D:495:ASN:C	1:D:499:ARG:NH1	2.62	0.53
2:E:184:ALA:HA	2:E:187:LYS:HZ2	1.73	0.53
2:F:169:LYS:HZ2	2:F:206:VAL:HG13	1.70	0.53
1:A:102:GLY:HA3	1:A:426:ASN:HD21	1.73	0.53
1:A:328:HIS:CG	1:A:329:ASP:N	2.76	0.53
1:A:199:HIS:HB2	1:A:525:LYS:HG3	1.89	0.53
1:A:99:LEU:HB2	1:A:556:ALA:H	1.73	0.53
1:D:425:ARG:HB3	1:D:427:LEU:HD12	1.91	0.53
2:B:106:PHE:HB2	7:B:465:HOH:O	2.07	0.53
2:B:13:SER:HB3	7:B:403:HOH:O	2.09	0.53
2:B:99:ALA:HA	7:B:501:HOH:O	2.08	0.53
1:D:111:ILE:HD13	1:D:334:GLU:CG	2.37	0.53
2:C:139:LEU:HG	2:C:142:LYS:H	1.74	0.53
2:E:80:GLU:O	7:E:423:HOH:O	2.19	0.53
1:A:29:LYS:O	1:A:33:LYS:HG2	2.09	0.53
1:A:30:GLN:O	1:A:34:GLU:HG3	2.07	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:171:GLY:O	2:B:173:PHE:HD1	1.91	0.53
2:C:14:MET:O	2:C:17:MET:HB2	2.09	0.53
1:D:392:ILE:HD11	1:D:539:GLY:O	2.09	0.53
1:D:498:ASP:CB	1:D:510:ARG:HH22	2.15	0.53
1:A:142:GLY:HA2	1:A:215:GLN:HB2	1.90	0.53
1:A:448:ALA:HB3	1:A:479:TRP:HH2	1.73	0.53
1:D:107:ARG:NH2	1:D:552:LYS:HD3	2.22	0.53
2:E:115:GLY:O	2:E:116:LYS:HD2	2.09	0.53
1:A:351:THR:HG21	1:A:410:ILE:HG12	1.91	0.53
2:B:214:LYS:NZ	7:B:435:HOH:O	2.33	0.53
1:D:97:ILE:HD13	1:D:112:PRO:HA	1.89	0.53
1:D:199:HIS:CD2	1:D:200:GLN:HG3	2.44	0.53
1:D:215:GLN:OE1	1:D:215:GLN:N	2.40	0.53
1:D:423:CYS:SG	7:D:766:HOH:O	2.59	0.53
2:C:188:ARG:HB2	1:D:87:PRO:HD2	1.91	0.53
1:A:432:ASN:OD1	1:A:433:ILE:N	2.41	0.53
1:A:573:THR:OG1	2:B:176:GLU:OE2	2.16	0.53
2:B:54:ILE:HB	2:B:55:PRO:HA	1.91	0.53
1:D:150:SER:HB2	1:D:167:THR:CA	2.39	0.53
1:D:557:LYS:O	7:D:744:HOH:O	2.19	0.53
2:C:188:ARG:NE	1:D:86:SER:HB2	2.22	0.53
2:E:93:ALA:HB1	2:F:64:VAL:HG13	1.90	0.53
1:A:133:ASN:OD1	1:A:138:ILE:N	2.41	0.53
2:B:200:PRO:HA	7:B:527:HOH:O	2.08	0.53
2:C:143:PRO:O	2:C:185:TRP:HD1	1.92	0.53
1:D:304:ILE:HG13	1:D:328:HIS:HB3	1.91	0.53
1:D:507:VAL:O	1:D:511:LYS:HB2	2.08	0.53
1:A:332:SER:HB3	1:A:538:LEU:CD1	2.38	0.53
1:D:94:VAL:HB	1:D:113:PHE:O	2.09	0.53
1:D:28:GLN:HE21	1:D:356:PRO:HA	1.74	0.53
2:F:116:LYS:O	2:F:213:ARG:NH1	2.42	0.53
1:A:22:ARG:NH1	7:A:802:HOH:O	2.42	0.52
1:D:134:ARG:O	7:D:746:HOH:O	2.19	0.52
1:D:166:THR:OG1	1:D:167:THR:N	2.42	0.52
1:D:389:GLU:OE2	1:D:404:GLY:HA2	2.09	0.52
1:D:222:VAL:HG21	3:D:601:ILE:N	2.24	0.52
2:E:153:VAL:O	2:E:157:LEU:HD23	2.08	0.52
1:A:492:ASP:HA	1:A:495:ASN:HD22	1.74	0.52
2:B:98:TRP:CE3	2:B:101:PHE:HB2	2.44	0.52
1:D:393:THR:HA	1:D:398:LEU:O	2.08	0.52
2:E:98:TRP:HE3	2:E:101:PHE:HB2	1.72	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:37:PHE:CZ	6:F:301:GSH:HA32	2.45	0.52
1:A:40:GLN:HA	7:A:898:HOH:O	2.08	0.52
1:A:429:LEU:HD12	7:A:762:HOH:O	2.08	0.52
2:B:81:LYS:O	7:B:423:HOH:O	2.19	0.52
2:C:181:LYS:HZ1	1:D:114:THR:HG23	1.75	0.52
1:D:423:CYS:HG	1:D:541:SER:HG	1.39	0.52
1:D:510:ARG:NH1	1:D:575:PHE:HE2	2.07	0.52
2:F:132:VAL:HG22	2:F:182:LEU:HD23	1.89	0.52
1:A:107:ARG:NH1	1:A:107:ARG:HG3	2.19	0.52
1:A:162:VAL:O	1:A:560:GLN:HB2	2.10	0.52
1:A:196:PRO:HA	1:A:565:ASN:OD1	2.10	0.52
2:B:7:LEU:HD13	2:B:30:PHE:CD2	2.44	0.52
2:B:31:GLU:OE1	7:B:422:HOH:O	2.19	0.52
2:F:121:GLN:O	2:F:125:LYS:HG3	2.09	0.52
2:F:139:LEU:HG	2:F:142:LYS:HB3	1.91	0.52
1:A:23:ASN:O	1:A:27:VAL:HG12	2.10	0.52
1:A:329:ASP:OD1	1:A:329:ASP:N	2.40	0.52
1:A:465:TYR:HB3	1:A:476:ALA:HB3	1.91	0.52
2:C:188:ARG:CB	1:D:87:PRO:HD2	2.40	0.52
1:D:240:GLU:HB3	7:D:741:HOH:O	2.10	0.52
1:D:574:ALA:O	1:D:575:PHE:HB2	2.10	0.52
2:E:169:LYS:HG3	2:E:170:PHE:N	2.25	0.52
1:A:151:SER:OG	1:A:151:SER:O	2.27	0.52
1:A:439:ARG:O	1:A:443:LEU:HB2	2.09	0.52
2:B:37:PHE:HZ	2:B:54:ILE:HG12	1.75	0.52
1:D:479:TRP:CZ2	1:D:497:LEU:HD21	2.44	0.52
1:D:487:GLU:OE1	1:D:568:SER:HB2	2.10	0.52
2:C:188:ARG:HB2	1:D:86:SER:HB2	1.91	0.52
2:E:98:TRP:CZ2	2:E:157:LEU:HD22	2.44	0.52
1:A:148:ILE:HD12	1:A:170:TYR:CZ	2.45	0.52
1:A:150:SER:OG	1:A:150:SER:O	2.15	0.52
1:A:18:ASP:O	1:A:22:ARG:HG3	2.09	0.52
1:A:451:ARG:NH1	1:A:454:GLU:OE2	2.43	0.52
1:D:104:SER:N	1:D:107:ARG:O	2.35	0.52
1:D:429:LEU:HG	1:D:430:SER:N	2.25	0.52
2:E:127:GLU:OE2	7:E:422:HOH:O	2.18	0.52
2:E:57:LEU:HB3	2:E:64:VAL:CG2	2.39	0.52
2:E:72:GLN:HA	2:E:84:PHE:CE2	2.44	0.52
2:F:158:ILE:HG12	7:F:431:HOH:O	2.08	0.52
1:A:163:GLY:HA3	1:A:168:ASN:HD21	1.74	0.52
2:C:162:SER:HB3	2:C:199:LEU:HD23	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:444:SER:HB2	7:D:743:HOH:O	2.09	0.52
1:D:490:LEU:HD11	7:D:808:HOH:O	2.09	0.52
2:E:178:GLU:OE2	7:E:424:HOH:O	2.19	0.52
1:D:499:ARG:C	2:E:188:ARG:NH1	2.59	0.52
1:A:342:THR:OG1	1:A:413:TYR:OH	2.20	0.52
1:A:169:VAL:HG21	3:A:601:ILE:HD11	1.91	0.52
1:D:479:TRP:NE1	7:D:802:HOH:O	2.34	0.52
2:F:136:GLU:HB2	7:F:409:HOH:O	2.08	0.52
2:F:145:PHE:HB2	2:F:154:ASP:OD2	2.09	0.52
2:F:4:LEU:N	7:F:442:HOH:O	2.43	0.52
1:A:441:LEU:CD2	1:A:549:ARG:HB3	2.39	0.52
1:A:75:PRO:O	1:A:79:ARG:HG3	2.10	0.52
2:B:98:TRP:CZ2	2:B:157:LEU:HD22	2.45	0.52
2:C:148:ASP:N	2:C:148:ASP:OD1	2.37	0.52
1:D:256:VAL:HG11	7:D:710:HOH:O	2.10	0.52
1:D:292:PRO:O	1:D:296:PRO:HA	2.09	0.52
1:D:377:VAL:HG13	7:D:818:HOH:O	2.10	0.52
1:D:520:LEU:HD13	7:D:802:HOH:O	2.10	0.52
1:D:98:SER:HG	4:D:603:ATP:PB	2.32	0.52
1:A:405:ASP:HB2	1:A:541:SER:O	2.09	0.51
2:B:98:TRP:HE3	2:B:101:PHE:HB2	1.74	0.51
2:B:117:LYS:HA	2:B:121:GLN:HB2	1.91	0.51
2:B:153:VAL:O	2:B:157:LEU:HD23	2.10	0.51
2:B:64:VAL:HB	2:B:73:TYR:CE2	2.45	0.51
1:D:88:ILE:O	7:D:747:HOH:O	2.19	0.51
2:F:26:LYS:HB3	2:F:28:VAL:HG23	1.91	0.51
1:A:149:PHE:HE2	1:A:202:LEU:HD13	1.75	0.51
1:A:213:ARG:HH21	1:A:296:PRO:HD3	1.75	0.51
1:A:32:LEU:HD21	1:A:61:PHE:HD2	1.74	0.51
2:B:90:TYR:CD2	2:C:62:LYS:HD3	2.44	0.51
2:C:133:LYS:O	2:C:136:GLU:HB3	2.09	0.51
2:B:76:GLU:CG	2:C:89:PRO:HB3	2.40	0.51
1:D:494:CYS:CB	1:D:520:LEU:HB3	2.39	0.51
2:F:95:ALA:HB1	2:F:152:TYR:HD2	1.75	0.51
2:B:40:LYS:HB3	2:B:44:LEU:HD23	1.92	0.51
1:D:151:SER:HB3	1:D:565:ASN:HD21	1.76	0.51
1:D:552:LYS:C	1:D:554:SER:H	2.14	0.51
1:A:18:ASP:OD1	1:A:414:ASN:ND2	2.43	0.51
1:A:361:PHE:CE1	1:A:392:ILE:HG23	2.45	0.51
1:A:477:ILE:O	7:A:739:HOH:O	2.19	0.51
2:B:188:ARG:NH1	7:B:416:HOH:O	2.44	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:184:ALA:HB1	1:D:85:THR:O	2.11	0.51
1:D:445:VAL:HG23	7:D:743:HOH:O	2.09	0.51
1:D:495:ASN:CB	1:D:499:ARG:NH1	2.74	0.51
1:A:45:LEU:O	1:A:49:GLY:N	2.43	0.51
1:A:507:VAL:O	1:A:511:LYS:HB2	2.11	0.51
1:D:28:GLN:HE21	1:D:356:PRO:CA	2.24	0.51
1:D:199:HIS:H	1:D:524:ALA:HB1	1.76	0.51
2:E:117:LYS:HE3	2:E:213:ARG:NH1	2.26	0.51
2:B:145:PHE:HB3	2:B:153:VAL:HG13	1.92	0.51
2:B:206:VAL:HG23	7:B:447:HOH:O	2.10	0.51
1:D:223:PHE:CE2	1:D:545:PHE:HZ	2.27	0.51
2:B:10:TYR:HH	2:B:208:TYR:HH	1.59	0.51
2:B:201:ASP:HB2	2:B:204:LYS:HG3	1.93	0.51
2:B:33:ARG:HH22	2:B:41:SER:HB2	1.75	0.51
2:C:192:LYS:O	2:C:196:SER:N	2.41	0.51
2:E:26:LYS:HG3	2:E:81:LYS:HZ3	1.76	0.51
2:F:17:MET:HG2	2:F:20:ARG:NH1	2.25	0.51
1:A:168:ASN:HA	7:A:864:HOH:O	2.09	0.51
1:A:132:ARG:HA	1:A:343:PRO:HG3	1.93	0.51
1:A:58:GLU:OE2	1:A:360:TYR:OH	2.28	0.51
1:A:363:PHE:CD2	1:A:382:VAL:HG21	2.36	0.51
2:B:16:GLY:HA2	2:B:55:PRO:HB3	1.93	0.51
2:C:201:ASP:HB2	2:C:204:LYS:HG3	1.92	0.51
1:D:42:ALA:HB3	1:D:45:LEU:HD22	1.92	0.51
1:D:199:HIS:HD1	1:D:524:ALA:CB	2.23	0.51
1:D:535:PHE:HB3	1:D:544:GLN:O	2.11	0.51
2:E:8:LEU:HD22	2:E:33:ARG:HE	1.76	0.51
1:A:113:PHE:HB2	4:A:602:ATP:PB	2.50	0.51
2:B:11:TRP:CG	2:B:12:PRO:HD3	2.45	0.51
1:D:112:PRO:HD2	1:D:397:GLY:HA3	1.92	0.51
2:F:132:VAL:HG11	2:F:175:ILE:HG23	1.92	0.51
1:A:121:THR:HG23	5:A:603:JAA:C13	2.40	0.51
1:A:518:LEU:HD12	1:A:519:GLU:N	2.26	0.51
1:A:476:ALA:HA	1:A:519:GLU:O	2.11	0.51
2:B:12:PRO:O	2:B:163:TRP:CZ2	2.63	0.51
2:C:145:PHE:HB2	2:C:154:ASP:OD2	2.11	0.51
2:C:184:ALA:HB1	1:D:85:THR:HB	1.92	0.51
1:D:100:SER:HA	1:D:535:PHE:CE1	2.45	0.51
1:D:503:ASP:O	1:D:507:VAL:HG23	2.11	0.51
1:A:128:ALA:HB2	1:A:329:ASP:OD2	2.10	0.50
1:A:140:ASP:OD1	7:A:740:HOH:O	2.20	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:424:ARG:HB2	1:A:425:ARG:NE	2.25	0.50
1:D:253:ARG:HD2	7:D:869:HOH:O	2.10	0.50
1:D:213:ARG:HH21	1:D:296:PRO:HD3	1.76	0.50
1:D:510:ARG:CZ	1:D:575:PHE:HE2	2.23	0.50
2:F:20:ARG:HB3	2:F:198:SER:HB3	1.94	0.50
1:A:239:GLU:O	1:A:242:VAL:HG22	2.10	0.50
1:D:33:LYS:O	1:D:37:LEU:N	2.43	0.50
2:F:139:LEU:O	2:F:141:ASP:N	2.45	0.50
2:F:18:ARG:NH1	2:F:67:SER:OG	2.38	0.50
2:F:75:ASP:HB2	7:F:433:HOH:O	2.11	0.50
1:A:378:GLY:O	1:A:382:VAL:HG23	2.12	0.50
1:A:44:TYR:HB2	1:A:89:LEU:HD23	1.92	0.50
1:A:552:LYS:C	1:A:554:SER:H	2.14	0.50
2:B:24:ARG:HD2	2:B:198:SER:OG	2.11	0.50
2:B:57:LEU:HB3	2:B:64:VAL:CG2	2.41	0.50
1:D:94:VAL:HG11	1:D:112:PRO:HB3	1.91	0.50
1:D:441:LEU:HD23	1:D:549:ARG:HB3	1.93	0.50
3:D:601:ILE:HA	4:D:603:ATP:C2	2.46	0.50
1:A:233:THR:HG21	1:A:525:LYS:NZ	2.25	0.50
1:A:490:LEU:HD22	1:A:522:VAL:HG21	1.93	0.50
1:D:213:ARG:HG3	1:D:214:ASP:N	2.27	0.50
1:D:35:ILE:HD11	1:D:359:GLY:HA2	1.92	0.50
1:D:382:VAL:HG12	1:D:409:VAL:HG21	1.92	0.50
1:D:413:TYR:O	1:D:416:THR:HG22	2.11	0.50
1:D:43:ILE:N	7:D:747:HOH:O	2.45	0.50
2:B:54:ILE:O	7:B:424:HOH:O	2.20	0.50
1:D:336:TRP:NE1	7:D:721:HOH:O	2.23	0.50
1:D:196:PRO:HA	1:D:565:ASN:OD1	2.12	0.50
2:E:169:LYS:HD3	2:E:206:VAL:HG13	1.94	0.50
2:E:73:TYR:CD1	2:F:96:ARG:NH1	2.75	0.50
1:A:151:SER:HB3	1:A:565:ASN:HD21	1.76	0.50
2:B:28:VAL:HG13	2:B:30:PHE:CD1	2.46	0.50
2:E:169:LYS:HD2	7:E:433:HOH:O	2.12	0.50
1:A:198:VAL:HG22	1:A:524:ALA:HB3	1.93	0.50
2:B:150:PHE:CD1	2:B:192:LYS:HG3	2.47	0.50
1:D:100:SER:HB3	1:D:109:LYS:HD3	1.92	0.50
2:F:154:ASP:OD1	2:F:185:TRP:NE1	2.35	0.50
1:A:104:SER:O	1:A:107:ARG:HB2	2.12	0.50
1:A:96:ALA:HA	1:A:161:PRO:O	2.11	0.50
1:A:522:VAL:O	1:A:567:VAL:HG22	2.11	0.50
2:B:172:ASN:ND2	2:B:172:ASN:O	2.45	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:108:ASP:O	2:C:112:LYS:HG2	2.12	0.50
2:C:125:LYS:HB3	2:C:173:PHE:HE2	1.77	0.50
1:D:152:LYS:CB	1:D:561:ILE:HA	2.41	0.50
1:A:151:SER:HB2	1:A:194:PHE:HA	1.94	0.50
1:A:290:LEU:O	1:A:293:ALA:HB3	2.12	0.50
1:A:314:PRO:HB3	1:A:317:ARG:NH1	2.24	0.50
1:A:434:ASP:HB2	1:A:550:CYS:HB3	1.94	0.50
2:B:170:PHE:CD2	2:B:213:ARG:HD2	2.46	0.50
2:C:130:GLU:O	2:C:134:ILE:HG13	2.12	0.50
1:D:413:TYR:CD2	1:D:418:GLN:HG2	2.47	0.50
2:C:148:ASP:HB2	1:D:46:GLN:HB2	1.94	0.50
2:E:97:PHE:HZ	2:F:48:ASN:HD21	1.59	0.50
1:A:108:PRO:HB3	1:A:554:SER:C	2.32	0.49
2:C:150:PHE:HE2	2:C:189:CYS:HB3	1.77	0.49
1:D:150:SER:OG	1:D:194:PHE:HE1	1.95	0.49
1:D:221:ALA:O	7:D:745:HOH:O	2.19	0.49
2:C:148:ASP:HA	1:D:41:SER:HA	1.94	0.49
1:D:275:GLU:HB2	7:D:847:HOH:O	2.12	0.49
1:D:347:PRO:HA	7:D:729:HOH:O	2.12	0.49
2:F:117:LYS:CG	2:F:213:ARG:HH11	2.20	0.49
1:A:201:ALA:O	1:A:205:HIS:N	2.45	0.49
1:A:21:THR:O	1:A:24:ALA:HB2	2.13	0.49
1:A:55:THR:C	1:A:57:PRO:HD3	2.32	0.49
2:B:8:LEU:HB3	7:B:427:HOH:O	2.11	0.49
2:C:125:LYS:HB3	2:C:173:PHE:CE2	2.47	0.49
1:D:462:PHE:O	1:D:549:ARG:NH1	2.44	0.49
2:E:84:PHE:HD1	2:E:85:PHE:N	2.10	0.49
1:A:172:ASN:OD1	7:A:721:HOH:O	2.19	0.49
1:A:42:ALA:HB3	1:A:45:LEU:HD22	1.95	0.49
1:A:496:CYS:HB2	2:B:187:LYS:CE	2.43	0.49
2:C:102:VAL:O	2:C:106:PHE:HB3	2.12	0.49
2:F:8:LEU:HD21	2:F:43:LEU:HD23	1.93	0.49
1:A:316:LEU:O	1:A:320:ALA:N	2.45	0.49
1:A:35:ILE:HA	1:A:395:TYR:CE1	2.47	0.49
2:B:98:TRP:CD1	2:B:153:VAL:HG11	2.47	0.49
1:A:456:LYS:HZ3	2:B:204:LYS:HE2	1.76	0.49
2:E:185:TRP:O	2:E:188:ARG:HB3	2.12	0.49
1:A:189:PRO:O	1:A:193:ILE:HG13	2.12	0.49
1:A:225:HIS:HB3	1:A:309:MET:SD	2.53	0.49
7:A:965:HOH:O	2:B:190:MET:HG3	2.12	0.49
1:D:17:PHE:CD1	1:D:127:THR:HG21	2.47	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:32:LEU:HB2	1:D:360:TYR:CD1	2.48	0.49
1:D:479:TRP:HZ2	1:D:497:LEU:HD21	1.77	0.49
1:A:222:VAL:HG13	5:A:603:JAA:C06	2.42	0.49
2:C:11:TRP:CD1	2:C:12:PRO:HD3	2.47	0.49
2:C:204:LYS:HD2	7:C:552:HOH:O	2.12	0.49
1:D:99:LEU:HA	1:D:109:LYS:O	2.13	0.49
1:D:11:ASN:O	1:D:14:ILE:HG13	2.13	0.49
1:D:17:PHE:CE1	1:D:355:ILE:HG12	2.48	0.49
1:D:301:VAL:C	7:D:776:HOH:O	2.51	0.49
1:D:540:SER:HG	1:D:544:GLN:NE2	2.07	0.49
1:D:572:SER:O	7:D:748:HOH:O	2.20	0.49
1:A:445:VAL:HG22	1:A:479:TRP:NE1	2.27	0.49
2:B:166:ALA:N	7:B:447:HOH:O	2.45	0.49
2:C:70:VAL:HG21	7:C:465:HOH:O	2.11	0.49
2:C:143:PRO:HD3	1:D:39:ASN:HD21	1.77	0.49
1:D:473:GLY:O	1:D:516:GLY:N	2.34	0.49
2:E:10:TYR:CD2	2:E:12:PRO:HD2	2.47	0.49
2:E:181:LYS:O	2:E:184:ALA:HB3	2.13	0.49
1:A:246:LYS:HZ2	1:A:271:PRO:HA	1.77	0.49
2:B:11:TRP:O	2:B:200:PRO:HG2	2.13	0.49
1:D:259:VAL:HG21	7:D:850:HOH:O	2.12	0.49
1:D:262:ALA:O	1:D:265:LYS:HB2	2.13	0.49
1:D:152:LYS:HA	1:D:564:GLU:HB2	1.94	0.49
1:A:490:LEU:HD21	7:A:1021:HOH:O	2.13	0.49
2:B:188:ARG:HD3	2:B:191:GLU:OE2	2.13	0.49
2:B:73:TYR:CZ	2:C:93:ALA:HB1	2.48	0.49
1:D:379:LEU:N	7:D:713:HOH:O	2.45	0.49
1:D:391:VAL:HG13	1:D:401:TYR:O	2.12	0.49
1:D:334:GLU:HB2	1:D:538:LEU:CD1	2.43	0.49
1:A:337:ILE:O	1:A:354:VAL:HA	2.11	0.48
1:A:363:PHE:HD1	1:A:390:VAL:HA	1.77	0.48
1:A:334:GLU:HB3	1:A:398:LEU:HD11	1.94	0.48
1:A:451:ARG:HD3	2:B:187:LYS:HG2	1.94	0.48
2:B:17:MET:CE	2:B:200:PRO:HD2	2.43	0.48
1:D:146:GLN:OE1	1:D:186:SER:OG	2.25	0.48
1:D:512:CYS:O	1:D:513:LYS:HB2	2.13	0.48
2:E:193:GLU:HG2	7:E:498:HOH:O	2.13	0.48
1:A:154:TYR:HB3	1:A:559:LEU:O	2.13	0.48
1:A:27:VAL:O	1:A:31:THR:OG1	2.12	0.48
1:A:353:ALA:HB2	1:A:413:TYR:CD2	2.47	0.48
1:A:339:ALA:N	1:A:353:ALA:O	2.35	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:ALA:HB1	4:A:602:ATP:N3	2.27	0.48
1:A:62:LYS:HD2	7:A:926:HOH:O	2.12	0.48
2:B:17:MET:HE3	2:B:163:TRP:HH2	1.77	0.48
1:D:122:LEU:HB2	7:D:876:HOH:O	2.13	0.48
1:D:192:VAL:HA	1:D:195:SER:HB2	1.94	0.48
1:D:328:HIS:CD2	1:D:329:ASP:N	2.82	0.48
1:D:332:SER:HB3	1:D:538:LEU:HD13	1.94	0.48
1:D:374:GLU:OE2	7:D:749:HOH:O	2.20	0.48
2:E:165:GLN:HG2	7:E:472:HOH:O	2.13	0.48
2:F:169:LYS:HD3	2:F:206:VAL:HG22	1.95	0.48
1:A:97:ILE:H	1:A:162:VAL:HA	1.78	0.48
2:C:211:GLU:HB3	7:C:425:HOH:O	2.14	0.48
1:D:96:ALA:HB3	1:D:113:PHE:HD2	1.79	0.48
1:D:170:TYR:HA	1:D:175:PHE:CD2	2.48	0.48
1:D:302:TYR:HD1	1:D:326:VAL:HG13	1.78	0.48
2:E:110:GLN:O	2:E:113:VAL:HG12	2.13	0.48
1:A:100:SER:HA	1:A:535:PHE:HE1	1.75	0.48
1:A:90:THR:HA	1:A:399:TYR:HE2	1.76	0.48
1:A:454:GLU:OE2	2:B:202:SER:OG	2.30	0.48
1:A:516:GLY:HA3	7:A:709:HOH:O	2.11	0.48
2:B:23:LEU:HD23	2:B:74:VAL:HG22	1.94	0.48
1:D:222:VAL:HB	1:D:533:GLU:HB3	1.96	0.48
1:D:451:ARG:NH1	1:D:454:GLU:OE2	2.46	0.48
2:E:183:ILE:O	2:E:187:LYS:HG3	2.14	0.48
1:A:223:PHE:HE2	1:A:545:PHE:CZ	2.23	0.48
1:A:302:TYR:HD1	1:A:326:VAL:HG13	1.77	0.48
1:A:496:CYS:N	1:A:499:ARG:NH1	2.62	0.48
2:B:114:TRP:CD1	2:B:167:TYR:HE1	2.32	0.48
2:C:181:LYS:HB2	1:D:92:HIS:CD2	2.49	0.48
1:D:156:SER:OG	1:D:160:VAL:O	2.16	0.48
1:D:448:ALA:CB	1:D:496:CYS:HB3	2.37	0.48
1:D:77:ILE:HG13	1:D:89:LEU:HD12	1.95	0.48
2:E:26:LYS:HE2	2:E:75:ASP:HA	1.95	0.48
1:A:213:ARG:HG3	1:A:214:ASP:N	2.28	0.48
1:A:219:VAL:HB	1:A:295:PHE:CE1	2.49	0.48
1:A:330:TYR:CE2	1:A:539:GLY:HA2	2.48	0.48
1:A:383:LYS:HA	7:A:908:HOH:O	2.13	0.48
1:A:448:ALA:HB3	7:A:707:HOH:O	2.12	0.48
1:D:538:LEU:HD12	1:D:539:GLY:N	2.29	0.48
1:D:552:LYS:HD2	1:D:553:PRO:HD2	1.96	0.48
1:A:401:TYR:HE2	1:A:403:LEU:HD13	1.78	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:434:ASP:HB2	1:A:550:CYS:SG	2.54	0.48
2:B:37:PHE:CZ	2:B:54:ILE:HG12	2.49	0.48
1:D:122:LEU:O	1:D:126:ARG:HB2	2.13	0.48
1:D:133:ASN:OD1	1:D:138:ILE:N	2.46	0.48
1:D:445:VAL:HG13	1:D:479:TRP:NE1	2.29	0.48
2:E:123:ALA:HB1	7:E:488:HOH:O	2.13	0.48
1:A:104:SER:O	1:A:105:GLN:HB2	2.14	0.48
1:A:213:ARG:HH21	1:A:296:PRO:CD	2.27	0.48
2:B:142:LYS:HE2	7:B:553:HOH:O	2.12	0.48
2:C:136:GLU:OE2	2:C:181:LYS:HD2	2.13	0.48
1:D:105:GLN:CA	1:D:430:SER:HB3	2.44	0.48
1:D:189:PRO:O	1:D:193:ILE:HG13	2.14	0.48
1:D:207:LEU:HD12	1:D:207:LEU:HA	1.68	0.48
1:A:273:LEU:O	1:A:277:ILE:HG22	2.13	0.48
1:A:498:ASP:OD1	1:A:498:ASP:N	2.46	0.48
2:C:11:TRP:CG	2:C:12:PRO:HD3	2.49	0.48
1:D:113:PHE:HB2	4:D:603:ATP:PB	2.53	0.48
1:D:225:HIS:HB3	1:D:309:MET:SD	2.53	0.48
1:D:477:ILE:HG13	1:D:497:LEU:HD22	1.96	0.48
1:D:225:HIS:NE2	1:D:529:ARG:HG3	2.29	0.48
1:D:403:LEU:HD21	1:D:538:LEU:HD11	1.96	0.48
2:E:168:GLU:HB3	7:E:493:HOH:O	2.13	0.48
2:E:159:THR:HA	2:E:199:LEU:HD21	1.96	0.48
1:A:117:LEU:HB3	7:A:706:HOH:O	2.13	0.48
1:A:208:SER:HA	1:A:211:LEU:HG	1.95	0.48
1:A:218:TYR:HA	1:A:298:ALA:HB1	1.96	0.48
1:A:223:PHE:CZ	1:A:533:GLU:HA	2.49	0.48
1:A:538:LEU:HG	1:A:544:GLN:NE2	2.29	0.48
1:A:108:PRO:HG2	1:A:552:LYS:CB	2.44	0.48
2:B:138:GLU:HA	7:B:461:HOH:O	2.14	0.48
2:B:153:VAL:HA	2:B:156:SER:OG	2.14	0.48
2:C:16:GLY:O	2:C:20:ARG:HG3	2.14	0.48
1:D:451:ARG:HB2	2:E:187:LYS:HD2	1.95	0.48
1:D:456:LYS:NZ	2:E:204:LYS:CE	2.76	0.48
1:D:330:TYR:OH	1:D:541:SER:N	2.47	0.48
1:D:152:LYS:CE	1:D:565:ASN:HB2	2.33	0.48
2:E:135:LEU:HD12	2:E:135:LEU:HA	1.33	0.48
1:A:332:SER:HA	4:A:602:ATP:C6	2.49	0.47
1:A:168:ASN:ND2	4:A:602:ATP:O2A	2.43	0.47
1:A:76:TYR:O	1:A:79:ARG:HB2	2.14	0.47
2:B:7:LEU:HD11	2:B:23:LEU:CD1	2.43	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:145:PHE:HB2	2:C:154:ASP:CG	2.34	0.47
1:D:287:TRP:HE3	1:D:290:LEU:HD13	1.79	0.47
1:D:303:GLY:HA2	7:D:863:HOH:O	2.13	0.47
1:D:98:SER:HB2	1:D:111:ILE:CG2	2.32	0.47
1:A:282:MET:HA	7:A:847:HOH:O	2.14	0.47
1:A:217:GLN:HE22	1:A:299:LYS:HD3	1.79	0.47
1:A:363:PHE:CE1	1:A:390:VAL:HG22	2.49	0.47
1:A:407:VAL:HG21	1:A:419:LEU:HB3	1.96	0.47
1:A:106:GLY:O	1:A:432:ASN:ND2	2.47	0.47
1:A:435:LYS:HB3	1:A:436:ASN:C	2.35	0.47
2:B:12:PRO:O	2:B:163:TRP:HZ2	1.97	0.47
2:E:90:TYR:CD2	2:F:62:LYS:HD3	2.49	0.47
1:A:292:PRO:HD3	1:A:323:LEU:HD12	1.96	0.47
1:A:111:ILE:HD11	1:A:334:GLU:HA	1.96	0.47
1:A:199:HIS:HA	1:A:525:LYS:HB2	1.96	0.47
2:C:150:PHE:HE1	2:C:155:ILE:HG13	1.79	0.47
1:D:170:TYR:HB3	1:D:194:PHE:CZ	2.49	0.47
1:D:280:LYS:HA	7:D:994:HOH:O	2.14	0.47
1:D:45:LEU:HB3	1:D:50:LEU:HB2	1.96	0.47
1:D:55:THR:C	1:D:57:PRO:HD3	2.34	0.47
1:D:169:VAL:HG22	4:D:603:ATP:C2'	2.44	0.47
2:E:10:TYR:O	2:E:20:ARG:NH2	2.41	0.47
2:E:70:VAL:O	2:E:73:TYR:HB2	2.14	0.47
1:A:125:PHE:CE1	1:A:328:HIS:HE1	2.32	0.47
1:A:222:VAL:HB	1:A:533:GLU:HB3	1.97	0.47
1:A:336:TRP:HB2	1:A:358:LEU:HD13	1.96	0.47
2:B:102:VAL:O	2:B:107:THR:HG23	2.14	0.47
2:B:159:THR:HA	2:B:199:LEU:HD21	1.96	0.47
1:D:98:SER:O	1:D:110:PHE:HA	2.15	0.47
1:D:223:PHE:HE2	1:D:545:PHE:HZ	1.62	0.47
1:A:440:ASP:OD1	1:A:501:PHE:HA	2.13	0.47
1:A:101:SER:HB3	1:A:535:PHE:CD2	2.49	0.47
2:B:90:TYR:CE1	2:C:62:LYS:HB3	2.49	0.47
1:D:334:GLU:HB2	1:D:538:LEU:HD13	1.96	0.47
2:E:17:MET:CE	2:E:200:PRO:HD2	2.43	0.47
1:A:10:MET:O	1:A:14:ILE:HG23	2.14	0.47
1:A:171:ARG:NE	7:A:711:HOH:O	2.46	0.47
1:D:239:GLU:O	1:D:242:VAL:HG22	2.14	0.47
1:D:290:LEU:O	1:D:294:LEU:HG	2.14	0.47
1:D:30:GLN:O	1:D:34:GLU:HG3	2.15	0.47
2:E:125:LYS:HA	2:E:128:PHE:CE2	2.49	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:140:GLY:HA2	7:E:516:HOH:O	2.15	0.47
1:A:450:LYS:NZ	7:A:708:HOH:O	1.97	0.47
1:A:405:ASP:HB2	1:A:541:SER:HB3	1.97	0.47
1:D:370:GLY:HA2	1:D:371:GLU:HA	1.72	0.47
1:D:39:ASN:ND2	1:D:90:THR:C	2.68	0.47
1:A:292:PRO:O	1:A:296:PRO:HA	2.14	0.47
1:A:418:GLN:OE1	7:A:741:HOH:O	2.20	0.47
1:A:438:GLU:O	1:A:442:GLN:HG3	2.13	0.47
1:A:474:HIS:HB3	7:A:709:HOH:O	2.15	0.47
1:A:503:ASP:CG	1:A:505:GLY:H	2.18	0.47
3:A:601:ILE:HG13	4:A:602:ATP:C2	2.44	0.47
2:B:195:VAL:N	7:B:409:HOH:O	2.35	0.47
1:D:291:ILE:HG13	1:D:319:TYR:O	2.14	0.47
1:D:363:PHE:HE2	1:D:379:LEU:HD23	1.80	0.47
1:D:382:VAL:HG13	1:D:388:TYR:CD2	2.50	0.47
1:D:48:CYS:HB2	1:D:50:LEU:CD1	2.44	0.47
1:D:490:LEU:HD13	1:D:568:SER:OG	2.14	0.47
1:D:76:TYR:HB3	1:D:88:ILE:HB	1.96	0.47
1:D:87:PRO:HB3	1:D:93:PRO:HD3	1.97	0.47
2:E:129:ILE:HA	2:E:132:VAL:HG12	1.97	0.47
2:F:38:SER:N	7:F:438:HOH:O	2.42	0.47
1:A:94:VAL:HB	1:A:113:PHE:O	2.15	0.47
2:B:98:TRP:HH2	2:B:135:LEU:HD21	1.80	0.47
1:D:405:ASP:OD1	1:D:405:ASP:N	2.48	0.47
2:C:144:TYR:HB2	1:D:41:SER:HB3	1.96	0.47
2:F:13:SER:O	2:F:17:MET:HG3	2.15	0.47
2:F:90:TYR:O	2:F:93:ALA:HB3	2.15	0.47
1:A:110:PHE:CE2	1:A:554:SER:HA	2.50	0.47
2:B:21:VAL:HG12	2:B:155:ILE:HG12	1.97	0.47
2:C:85:PHE:CD1	2:C:85:PHE:N	2.83	0.47
1:D:107:ARG:HH22	1:D:552:LYS:CD	2.26	0.47
1:D:464:SER:HA	1:D:476:ALA:O	2.15	0.47
1:D:77:ILE:HD13	1:D:110:PHE:O	2.15	0.47
2:E:62:LYS:HD3	2:F:90:TYR:CE1	2.50	0.47
2:F:44:LEU:HD12	7:F:412:HOH:O	2.15	0.47
1:A:226:GLY:HA2	1:A:529:ARG:HD2	1.97	0.47
1:A:223:PHE:HE1	1:A:304:ILE:HD13	1.79	0.47
1:A:330:TYR:OH	1:A:541:SER:N	2.48	0.47
1:A:88:ILE:CD1	1:A:89:LEU:H	2.23	0.47
1:A:499:ARG:NH1	2:B:184:ALA:HB1	2.30	0.47
2:B:8:LEU:HD22	2:B:33:ARG:NH2	2.17	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:405:ASP:HB3	7:D:782:HOH:O	2.14	0.47
1:D:456:LYS:HZ1	2:E:204:LYS:CE	2.27	0.47
1:D:538:LEU:HG	1:D:544:GLN:NE2	2.30	0.47
1:D:162:VAL:O	1:D:560:GLN:HB2	2.15	0.47
2:E:182:LEU:HB2	7:E:451:HOH:O	2.15	0.47
2:E:17:MET:SD	2:E:199:LEU:HG	2.55	0.47
2:F:47:SER:HB2	7:F:412:HOH:O	2.14	0.47
1:A:338:ALA:HA	1:A:354:VAL:HA	1.96	0.46
2:B:5:PRO:HB3	2:B:59:HIS:NE2	2.30	0.46
2:B:97:PHE:CE1	2:C:65:CYS:HB2	2.49	0.46
2:C:217:LEU:O	7:C:418:HOH:O	2.20	0.46
1:D:237:VAL:HB	7:D:919:HOH:O	2.15	0.46
1:D:363:PHE:CD1	1:D:390:VAL:HA	2.49	0.46
1:D:391:VAL:HG13	1:D:401:TYR:C	2.36	0.46
1:A:328:HIS:CD2	1:A:329:ASP:N	2.83	0.46
1:A:331:GLY:CA	1:A:336:TRP:HA	2.41	0.46
1:A:360:TYR:O	1:A:393:THR:HB	2.15	0.46
2:B:141:ASP:OD1	2:B:141:ASP:N	2.48	0.46
2:B:85:PHE:HE2	7:B:443:HOH:O	1.98	0.46
2:C:121:GLN:O	2:C:125:LYS:HG3	2.15	0.46
1:D:165:ALA:O	1:D:169:VAL:HG23	2.15	0.46
1:D:257:PRO:HB2	7:D:923:HOH:O	2.15	0.46
7:C:442:HOH:O	1:D:43:ILE:HD13	2.15	0.46
1:D:199:HIS:CB	1:D:525:LYS:HG3	2.44	0.46
1:A:495:ASN:HB2	1:A:499:ARG:HH11	1.78	0.46
2:B:33:ARG:HH12	2:B:41:SER:CB	2.27	0.46
1:D:451:ARG:HH11	1:D:454:GLU:CD	2.18	0.46
1:D:84:ASP:C	1:D:86:SER:H	2.19	0.46
2:F:119:GLU:HG3	7:F:579:HOH:O	2.15	0.46
2:F:14:MET:HG2	2:F:163:TRP:CD1	2.51	0.46
2:F:195:VAL:HG13	2:F:199:LEU:HD13	1.98	0.46
1:A:94:VAL:HG11	1:A:112:PRO:HB3	1.97	0.46
1:A:199:HIS:CD2	1:A:200:GLN:HG3	2.50	0.46
2:C:70:VAL:O	2:C:74:VAL:HG23	2.16	0.46
1:D:102:GLY:HA3	1:D:426:ASN:ND2	2.28	0.46
1:D:433:ILE:HD11	1:D:552:LYS:NZ	2.31	0.46
1:D:480:GLU:OE1	1:D:528:PHE:HD2	1.99	0.46
2:B:115:GLY:O	2:B:116:LYS:HD2	2.16	0.46
2:B:17:MET:SD	2:B:199:LEU:HG	2.56	0.46
1:D:31:THR:OG1	1:D:357:ASN:HA	2.15	0.46
1:D:501:PHE:HD2	1:D:506:TYR:CE2	2.32	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:108:ASP:O	2:E:112:LYS:HG2	2.15	0.46
2:E:33:ARG:HH12	2:E:41:SER:HB2	1.81	0.46
2:E:42:PRO:HD3	7:E:536:HOH:O	2.15	0.46
2:E:71:VAL:HG13	2:E:152:TYR:HE1	1.79	0.46
1:A:25:HIS:CE1	1:A:380:THR:OG1	2.68	0.46
1:A:34:GLU:HB2	7:A:761:HOH:O	2.16	0.46
1:A:464:SER:HA	1:A:476:ALA:O	2.16	0.46
2:C:150:PHE:CE1	2:C:155:ILE:HG13	2.51	0.46
1:D:223:PHE:HE2	1:D:545:PHE:CZ	2.34	0.46
2:E:213:ARG:O	2:E:217:LEU:HG	2.16	0.46
2:F:18:ARG:HH12	2:F:103:ASP:CG	2.18	0.46
2:B:68:LEU:HD12	2:B:69:ASN:N	2.31	0.46
2:B:26:LYS:HE2	2:B:74:VAL:O	2.16	0.46
2:B:90:TYR:CE2	2:C:62:LYS:HD3	2.50	0.46
2:B:98:TRP:CD1	2:B:153:VAL:HG21	2.50	0.46
1:D:94:VAL:HG21	1:D:112:PRO:HA	1.98	0.46
1:D:401:TYR:HE2	1:D:403:LEU:HD13	1.80	0.46
1:D:540:SER:HG	1:D:544:GLN:HE21	1.64	0.46
2:E:144:TYR:CE1	2:E:150:PHE:HD1	2.33	0.46
2:E:89:PRO:O	2:E:92:ARG:HB2	2.16	0.46
1:A:39:ASN:ND2	1:A:90:THR:C	2.69	0.46
1:A:510:ARG:CZ	1:A:575:PHE:HE2	2.28	0.46
2:C:101:PHE:HE1	2:C:105:LYS:HZ1	1.64	0.46
2:C:169:LYS:HZ1	2:C:210:ALA:HB2	1.81	0.46
1:D:150:SER:OG	1:D:150:SER:O	2.24	0.46
1:D:459:VAL:HG13	7:D:768:HOH:O	2.16	0.46
1:D:436:ASN:ND2	1:D:475:TYR:HE2	2.14	0.46
1:D:90:THR:HB	1:D:91:GLY:H	1.58	0.46
2:C:184:ALA:HB3	1:D:93:PRO:HG2	1.98	0.46
1:A:315:LYS:O	1:A:318:HIS:HB3	2.15	0.46
1:A:225:HIS:NE2	1:A:529:ARG:HG3	2.31	0.46
1:A:531:ILE:HG13	1:A:558:VAL:HG22	1.98	0.46
7:C:405:HOH:O	1:D:41:SER:HB3	2.16	0.46
7:D:860:HOH:O	2:E:180:PRO:HB3	2.14	0.46
1:A:304:ILE:HG23	7:A:725:HOH:O	2.15	0.46
2:B:32:TYR:CD1	2:B:34:GLU:OE2	2.69	0.46
2:C:152:TYR:HB3	7:C:448:HOH:O	2.16	0.46
2:C:201:ASP:CB	2:C:203:GLU:HG2	2.44	0.46
1:D:156:SER:N	7:D:810:HOH:O	2.48	0.46
1:D:332:SER:C	4:D:603:ATP:N7	2.70	0.46
1:D:61:PHE:HB2	7:D:761:HOH:O	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:195:VAL:HG23	2:E:199:LEU:CD1	2.44	0.46
2:E:23:LEU:CD2	2:E:28:VAL:HG11	2.46	0.46
2:E:94:GLN:O	2:E:97:PHE:HB3	2.15	0.46
1:A:412:PHE:N	7:A:741:HOH:O	2.33	0.45
1:A:424:ARG:C	1:A:543:GLY:HA2	2.37	0.45
1:A:501:PHE:HD2	1:A:506:TYR:CE2	2.34	0.45
2:B:108:ASP:O	2:B:112:LYS:HG2	2.16	0.45
2:B:98:TRP:CD2	2:B:138:GLU:OE2	2.69	0.45
2:B:188:ARG:HA	7:B:417:HOH:O	2.16	0.45
2:C:148:ASP:OD2	1:D:46:GLN:HA	2.17	0.45
1:D:143:LYS:HD2	7:D:800:HOH:O	2.15	0.45
1:D:259:VAL:HG11	7:D:832:HOH:O	2.17	0.45
2:E:126:LYS:O	2:E:129:ILE:HG13	2.16	0.45
2:E:5:PRO:HG2	2:E:28:VAL:CG2	2.47	0.45
2:F:18:ARG:HG3	2:F:159:THR:HG21	1.98	0.45
2:B:190:MET:HA	2:B:195:VAL:CG1	2.46	0.45
1:D:223:PHE:CZ	1:D:536:LEU:HB3	2.51	0.45
1:D:495:ASN:HD21	1:D:574:ALA:H	1.63	0.45
2:E:131:ALA:O	2:E:135:LEU:HB2	2.16	0.45
2:F:88:ASP:OD2	2:F:91:GLY:N	2.47	0.45
1:A:163:GLY:HA2	1:A:560:GLN:CB	2.38	0.45
1:A:273:LEU:O	1:A:276:THR:OG1	2.17	0.45
2:B:129:ILE:HA	2:B:132:VAL:HG12	1.98	0.45
2:B:133:LYS:HE2	2:B:133:LYS:HB3	1.80	0.45
1:D:483:GLY:N	7:D:824:HOH:O	2.44	0.45
1:D:33:LYS:HZ2	1:D:57:PRO:HG2	1.81	0.45
2:E:10:TYR:CD2	6:E:301:GSH:SG2	3.10	0.45
2:E:7:LEU:HD13	2:E:30:PHE:CD2	2.52	0.45
2:F:107:THR:HG23	2:F:110:GLN:NE2	2.30	0.45
2:F:147:GLY:HA3	7:F:459:HOH:O	2.16	0.45
2:F:17:MET:SD	2:F:199:LEU:HG	2.55	0.45
1:A:105:GLN:CA	1:A:430:SER:HB3	2.46	0.45
1:A:485:THR:OG1	1:A:486:ASN:N	2.49	0.45
2:C:85:PHE:HD1	2:C:85:PHE:N	2.15	0.45
1:A:111:ILE:HA	1:A:112:PRO:HD3	1.79	0.45
1:A:145:LEU:HD11	1:A:147:PHE:CE1	2.52	0.45
1:A:83:GLY:H	1:A:158:GLY:HA3	1.81	0.45
1:A:138:ILE:CA	1:A:217:GLN:HE21	2.23	0.45
2:C:183:ILE:O	2:C:187:LYS:HG3	2.17	0.45
1:D:236:GLN:OE1	7:D:751:HOH:O	2.21	0.45
1:D:547:MET:HG2	7:D:949:HOH:O	2.15	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:139:LEU:HB3	2:E:181:LYS:HE2	1.98	0.45
2:E:24:ARG:NH1	2:E:30:PHE:HZ	2.15	0.45
1:A:242:VAL:HG12	1:A:277:ILE:CD1	2.45	0.45
2:B:84:PHE:HB2	2:B:152:TYR:N	2.31	0.45
2:C:188:ARG:HA	7:D:756:HOH:O	2.17	0.45
2:C:17:MET:O	2:C:21:VAL:HG23	2.17	0.45
1:D:212:PHE:N	1:D:212:PHE:HD1	2.13	0.45
1:D:464:SER:N	1:D:549:ARG:O	2.49	0.45
2:E:166:ALA:HB3	7:E:504:HOH:O	2.16	0.45
2:F:105:LYS:HB2	7:F:474:HOH:O	2.17	0.45
1:A:107:ARG:NH1	1:A:107:ARG:CG	2.78	0.45
1:A:219:VAL:HG22	1:A:227:LEU:HD22	1.97	0.45
1:A:370:GLY:HA2	1:A:371:GLU:HA	1.73	0.45
1:A:495:ASN:CB	1:A:499:ARG:NH1	2.78	0.45
1:A:526:GLY:O	1:A:530:LYS:HG3	2.17	0.45
1:A:538:LEU:HD12	1:A:539:GLY:N	2.32	0.45
1:A:108:PRO:CG	1:A:552:LYS:H	2.28	0.45
1:A:56:ASP:HA	7:A:747:HOH:O	2.16	0.45
4:A:602:ATP:O1A	7:A:706:HOH:O	2.21	0.45
1:A:97:ILE:HB	1:A:162:VAL:CB	2.47	0.45
2:B:122:GLU:HA	2:B:125:LYS:HB2	1.99	0.45
2:B:165:GLN:HB3	7:B:447:HOH:O	2.16	0.45
1:D:165:ALA:HB1	4:D:603:ATP:C4	2.52	0.45
1:D:465:TYR:CD1	1:D:551:VAL:HG23	2.49	0.45
1:D:452:LEU:HD11	1:D:490:LEU:HD23	1.99	0.45
1:A:363:PHE:CD1	1:A:390:VAL:HA	2.52	0.45
1:A:478:PHE:O	1:A:479:TRP:HD1	2.00	0.45
1:A:448:ALA:CB	1:A:496:CYS:HB3	2.31	0.45
2:C:141:ASP:C	1:D:92:HIS:H	2.20	0.45
1:D:171:ARG:NE	7:D:774:HOH:O	2.48	0.45
1:D:233:THR:O	1:D:236:GLN:HB2	2.16	0.45
1:D:23:ASN:O	1:D:27:VAL:HG12	2.17	0.45
1:D:338:ALA:HA	1:D:354:VAL:HA	1.98	0.45
1:D:534:HIS:CE1	1:D:557:LYS:HG2	2.52	0.45
1:D:434:ASP:O	1:D:550:CYS:HB3	2.17	0.45
1:D:99:LEU:HD22	1:D:557:LYS:HB3	1.99	0.45
1:A:18:ASP:O	1:A:21:THR:OG1	2.32	0.45
1:A:198:VAL:HG13	1:A:565:ASN:HD21	1.82	0.45
1:A:512:CYS:O	1:A:513:LYS:HB2	2.17	0.45
1:A:562:LEU:HD23	1:A:563:CYS:N	2.31	0.45
1:A:74:GLU:N	1:A:75:PRO:HD2	2.32	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:195:SER:C	1:D:197:ASP:H	2.19	0.45
1:D:217:GLN:OE1	1:D:217:GLN:HA	2.17	0.45
1:D:278:ARG:O	1:D:282:MET:HE2	2.17	0.45
2:E:42:PRO:HD3	7:E:456:HOH:O	2.16	0.45
1:A:207:LEU:O	1:A:211:LEU:HG	2.17	0.45
1:A:134:ARG:NH2	1:A:341:VAL:O	2.49	0.45
1:A:124:LEU:HB3	5:A:603:JAA:C15	2.46	0.45
2:C:141:ASP:OD2	1:D:114:THR:HG23	2.17	0.45
1:D:17:PHE:CE2	1:D:341:VAL:HG11	2.52	0.45
1:D:203:TYR:CZ	1:D:241:ILE:HG13	2.52	0.45
1:D:323:LEU:HD23	1:D:324:PRO:HD2	1.99	0.45
1:D:405:ASP:HB2	1:D:541:SER:O	2.17	0.45
1:D:476:ALA:HA	1:D:519:GLU:O	2.17	0.45
1:D:199:HIS:HD1	1:D:524:ALA:HB2	1.82	0.45
1:D:75:PRO:O	1:D:79:ARG:HG3	2.17	0.45
2:E:5:PRO:HB3	2:E:59:HIS:NE2	2.32	0.45
2:F:186:ALA:O	2:F:190:MET:HG2	2.17	0.45
1:A:118:MET:HB2	7:A:772:HOH:O	2.17	0.44
1:A:353:ALA:HB2	1:A:413:TYR:HD2	1.81	0.44
1:A:423:CYS:HB2	1:A:543:GLY:N	2.32	0.44
2:B:197:LYS:HE2	7:B:565:HOH:O	2.15	0.44
2:B:23:LEU:HB3	2:B:28:VAL:HG11	1.98	0.44
2:B:98:TRP:CH2	2:B:135:LEU:CD1	2.84	0.44
1:D:199:HIS:HB3	1:D:525:LYS:N	2.26	0.44
1:D:212:PHE:CD1	1:D:212:PHE:N	2.84	0.44
1:D:451:ARG:NH1	1:D:454:GLU:CD	2.71	0.44
1:D:152:LYS:HZ1	1:D:523:VAL:CG1	2.30	0.44
2:E:181:LYS:HA	2:E:184:ALA:HB3	1.99	0.44
2:F:98:TRP:HB3	2:F:153:VAL:HG21	1.99	0.44
1:A:231:PHE:CZ	1:A:291:ILE:HG12	2.52	0.44
1:A:403:LEU:HD23	1:A:540:SER:OG	2.18	0.44
2:B:145:PHE:CD2	2:B:157:LEU:HD21	2.52	0.44
2:C:122:GLU:HG3	7:C:546:HOH:O	2.17	0.44
2:C:147:GLY:HA2	7:C:408:HOH:O	2.15	0.44
1:D:151:SER:HB2	1:D:194:PHE:HA	2.00	0.44
1:D:479:TRP:CE2	7:D:802:HOH:O	2.71	0.44
2:E:214:LYS:HE2	2:E:214:LYS:HB3	1.68	0.44
2:E:16:GLY:HA2	2:E:55:PRO:HB3	1.98	0.44
2:F:195:VAL:HG21	7:F:431:HOH:O	2.16	0.44
1:A:106:GLY:HA3	7:A:732:HOH:O	2.17	0.44
1:A:415:ASN:N	7:A:793:HOH:O	2.38	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:495:ASN:HB2	1:A:499:ARG:NH1	2.32	0.44
1:A:499:ARG:CZ	1:A:499:ARG:HB2	2.48	0.44
1:A:534:HIS:NE2	1:A:557:LYS:HD3	2.33	0.44
2:B:28:VAL:HG13	2:B:30:PHE:HD1	1.82	0.44
2:B:72:GLN:HA	2:B:84:PHE:CE2	2.51	0.44
1:D:11:ASN:HB3	7:D:900:HOH:O	2.17	0.44
1:D:30:GLN:HA	1:D:30:GLN:OE1	2.16	0.44
1:D:454:GLU:HB2	2:E:202:SER:OG	2.17	0.44
2:F:24:ARG:HD2	2:F:198:SER:OG	2.16	0.44
1:A:32:LEU:HB2	1:A:360:TYR:CD1	2.52	0.44
1:A:166:THR:HA	3:A:601:ILE:HG12	1.98	0.44
1:A:83:GLY:N	1:A:158:GLY:HA3	2.32	0.44
1:A:98:SER:HB2	1:A:111:ILE:CG2	2.44	0.44
2:B:156:SER:O	7:B:425:HOH:O	2.21	0.44
1:D:117:LEU:HG	7:D:963:HOH:O	2.16	0.44
1:D:164:THR:N	7:D:744:HOH:O	2.49	0.44
1:D:190:ASP:HA	1:D:193:ILE:HD12	1.99	0.44
1:D:223:PHE:HD2	1:D:225:HIS:CE1	2.35	0.44
1:D:223:PHE:HD2	1:D:225:HIS:ND1	2.16	0.44
1:D:363:PHE:CE1	1:D:390:VAL:HG22	2.52	0.44
1:D:402:ARG:NH1	7:D:845:HOH:O	2.50	0.44
1:D:457:ILE:HD13	7:D:824:HOH:O	2.17	0.44
2:E:11:TRP:CG	2:E:12:PRO:HD3	2.52	0.44
2:F:145:PHE:HB2	2:F:154:ASP:CG	2.38	0.44
1:A:131:PHE:O	1:A:134:ARG:HB3	2.18	0.44
1:A:43:ILE:HG13	1:A:44:TYR:N	2.32	0.44
2:C:168:GLU:OE1	2:C:175:ILE:HD12	2.18	0.44
1:D:302:TYR:CD1	1:D:326:VAL:HG13	2.52	0.44
1:D:406:VAL:HG13	7:D:835:HOH:O	2.17	0.44
1:D:496:CYS:HA	1:D:499:ARG:CZ	2.47	0.44
1:D:547:MET:HA	1:D:548:PRO:HD3	1.82	0.44
1:D:563:CYS:O	1:D:566:VAL:HG13	2.17	0.44
2:E:57:LEU:O	2:E:64:VAL:HG22	2.18	0.44
2:F:122:GLU:OE2	2:F:125:LYS:HD2	2.18	0.44
1:A:207:LEU:HD13	1:A:241:ILE:CD1	2.47	0.44
1:A:198:VAL:HG13	1:A:565:ASN:ND2	2.32	0.44
2:B:82:ASN:C	2:B:82:ASN:HD22	2.21	0.44
2:C:98:TRP:CZ2	2:C:138:GLU:HB2	2.53	0.44
1:D:212:PHE:HB3	1:D:215:GLN:CD	2.38	0.44
1:D:292:PRO:HB3	1:D:323:LEU:HD12	2.00	0.44
1:D:440:ASP:OD2	7:D:753:HOH:O	2.21	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:141:ASP:CB	1:D:92:HIS:HB2	2.47	0.44
2:E:185:TRP:NE1	2:E:189:CYS:SG	2.91	0.44
1:A:496:CYS:HA	1:A:499:ARG:NH2	2.32	0.44
1:A:92:HIS:ND1	1:A:93:PRO:HD2	2.32	0.44
2:B:70:VAL:O	2:B:73:TYR:HB2	2.17	0.44
2:B:92:ARG:HE	2:B:96:ARG:HH22	1.66	0.44
2:C:106:PHE:CE1	2:C:132:VAL:HG23	2.52	0.44
1:D:403:LEU:HD23	1:D:540:SER:OG	2.18	0.44
2:C:142:LYS:HA	1:D:91:GLY:HA3	2.00	0.44
1:A:143:LYS:HD3	1:A:187:CYS:HB3	2.00	0.44
1:A:393:THR:HA	1:A:398:LEU:O	2.18	0.44
1:A:552:LYS:O	1:A:554:SER:N	2.51	0.44
2:B:144:TYR:HB3	2:B:154:ASP:CG	2.38	0.44
2:B:167:TYR:HB2	7:B:463:HOH:O	2.18	0.44
1:A:499:ARG:NH1	2:B:187:LYS:HZ1	2.14	0.44
1:D:396:ALA:HB3	7:D:789:HOH:O	2.18	0.44
1:D:351:THR:HG21	1:D:410:ILE:CD1	2.48	0.44
1:D:416:THR:N	7:D:825:HOH:O	2.50	0.44
2:E:98:TRP:O	2:E:101:PHE:HB2	2.18	0.44
2:E:182:LEU:HD12	7:E:451:HOH:O	2.16	0.44
2:F:162:SER:HB2	2:F:205:ILE:HD12	2.00	0.44
2:F:23:LEU:HD13	2:F:30:PHE:CD2	2.53	0.44
2:C:142:LYS:NZ	7:C:404:HOH:O	2.50	0.44
2:C:169:LYS:HG3	2:C:170:PHE:N	2.33	0.44
1:D:121:THR:HG23	5:D:602:JAA:C13	2.47	0.44
1:D:223:PHE:HZ	1:D:536:LEU:HB3	1.83	0.44
1:D:32:LEU:HD13	1:D:360:TYR:CG	2.53	0.44
1:D:365:PRO:HA	1:D:388:TYR:CD1	2.53	0.44
1:D:423:CYS:HB2	1:D:542:ALA:C	2.38	0.44
2:F:116:LYS:HD3	2:F:116:LYS:HA	1.91	0.44
3:A:601:ILE:HA	4:A:602:ATP:H2	1.82	0.43
2:C:139:LEU:HA	2:C:139:LEU:HD12	1.45	0.43
1:D:377:VAL:N	7:D:818:HOH:O	2.51	0.43
1:D:513:LYS:HZ3	1:D:575:PHE:HB3	1.80	0.43
1:D:562:LEU:HD23	1:D:563:CYS:N	2.33	0.43
1:D:99:LEU:HB3	1:D:557:LYS:N	2.26	0.43
2:E:12:PRO:O	2:E:163:TRP:CZ2	2.71	0.43
2:F:101:PHE:CE2	2:F:135:LEU:HG	2.49	0.43
2:F:136:GLU:HG3	2:F:181:LYS:HD3	2.00	0.43
1:A:17:PHE:CD1	1:A:127:THR:HG21	2.53	0.43
1:A:22:ARG:NH1	1:A:414:ASN:OD1	2.50	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229:HIS:HA	1:A:232:ARG:HE	1.83	0.43
1:A:245:ILE:HG12	1:A:245:ILE:H	1.45	0.43
1:A:284:LEU:HD13	1:A:287:TRP:H	1.82	0.43
2:C:139:LEU:CG	2:C:142:LYS:HB3	2.47	0.43
2:C:164:PHE:CE2	2:C:183:ILE:HG12	2.53	0.43
2:C:77:ALA:O	7:C:420:HOH:O	2.21	0.43
1:D:107:ARG:CG	1:D:107:ARG:NH1	2.59	0.43
1:D:164:THR:HG23	1:D:557:LYS:CG	2.48	0.43
1:D:223:PHE:HZ	1:D:536:LEU:CB	2.31	0.43
1:D:256:VAL:HA	1:D:257:PRO:HD3	1.76	0.43
1:D:25:HIS:CE1	1:D:380:THR:HG21	2.53	0.43
1:D:329:ASP:CB	1:D:339:ALA:HA	2.41	0.43
1:D:495:ASN:CB	1:D:499:ARG:HH11	2.29	0.43
1:D:435:LYS:NZ	1:D:549:ARG:HB2	2.32	0.43
1:D:98:SER:OG	4:D:603:ATP:O3B	2.25	0.43
2:E:154:ASP:HB2	7:E:406:HOH:O	2.17	0.43
2:E:33:ARG:HH12	2:E:41:SER:CB	2.31	0.43
2:F:40:LYS:HG2	2:F:44:LEU:HD23	2.00	0.43
1:A:114:THR:HG22	1:A:115:ASP:N	2.33	0.43
1:A:187:CYS:HB2	1:A:208:SER:O	2.18	0.43
1:A:219:VAL:HG13	1:A:301:VAL:HG13	2.01	0.43
1:A:256:VAL:HA	1:A:257:PRO:HD3	1.77	0.43
1:A:445:VAL:HG21	1:A:462:PHE:CG	2.52	0.43
1:A:491:GLN:HG2	2:B:176:GLU:OE2	2.18	0.43
2:C:25:GLU:OE1	2:C:194:SER:OG	2.32	0.43
1:D:153:GLN:HG3	1:D:171:ARG:HD2	2.00	0.43
1:D:262:ALA:O	1:D:266:LEU:HG	2.18	0.43
1:D:405:ASP:CB	1:D:541:SER:HB3	2.47	0.43
1:D:99:LEU:HB3	1:D:557:LYS:HB3	1.98	0.43
1:A:170:TYR:HB3	1:A:194:PHE:CZ	2.54	0.43
1:A:212:PHE:HB3	1:A:215:GLN:CD	2.38	0.43
1:A:445:VAL:HA	1:A:479:TRP:CZ2	2.53	0.43
1:A:45:LEU:HG	1:A:50:LEU:HD22	2.01	0.43
1:A:328:HIS:CD2	5:A:603:JAA:O03	2.71	0.43
2:B:195:VAL:HG12	7:B:409:HOH:O	2.19	0.43
2:C:109:ALA:O	2:C:113:VAL:HG23	2.18	0.43
1:D:528:PHE:HB3	1:D:547:MET:HE1	1.99	0.43
1:D:86:SER:HB3	7:D:756:HOH:O	2.17	0.43
1:D:90:THR:OG1	1:D:397:GLY:HA2	2.18	0.43
2:E:140:GLY:N	2:E:181:LYS:NZ	2.67	0.43
2:E:54:ILE:N	7:E:418:HOH:O	2.46	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:151:SER:HB3	1:A:198:VAL:CG1	2.48	0.43
1:A:378:GLY:N	1:A:381:GLN:HB2	2.34	0.43
1:A:464:SER:O	1:A:550:CYS:HA	2.19	0.43
1:A:169:VAL:HG22	4:A:602:ATP:C2'	2.48	0.43
3:A:601:ILE:HD12	5:A:603:JAA:C11	2.49	0.43
1:D:330:TYR:HB3	1:D:338:ALA:HB3	1.99	0.43
2:E:36:ASP:O	2:E:39:ASN:N	2.49	0.43
2:F:76:GLU:O	2:F:79:PRO:HG3	2.18	0.43
2:B:124:GLY:HA2	2:B:127:GLU:OE1	2.19	0.43
2:B:40:LYS:HD2	2:B:52:LYS:HB3	2.01	0.43
2:B:5:PRO:HB3	2:B:57:LEU:HD11	2.00	0.43
1:D:124:LEU:HD13	1:D:336:TRP:CD2	2.54	0.43
2:E:9:ASP:OD2	2:E:32:TYR:HB2	2.18	0.43
2:F:132:VAL:HG13	7:F:409:HOH:O	2.17	0.43
2:F:216:ASN:ND2	7:F:450:HOH:O	2.51	0.43
2:F:68:LEU:HA	2:F:68:LEU:HD23	1.68	0.43
1:A:223:PHE:HZ	1:A:536:LEU:HB3	1.84	0.43
1:A:34:GLU:O	1:A:38:LYS:HG2	2.19	0.43
2:B:7:LEU:HD13	2:B:30:PHE:HD2	1.82	0.43
2:B:81:LYS:HG3	2:B:82:ASN:H	1.84	0.43
2:B:98:TRP:O	2:B:98:TRP:CE3	2.71	0.43
2:C:14:MET:HG2	2:C:163:TRP:CD1	2.54	0.43
2:C:116:LYS:O	2:C:213:ARG:NH1	2.52	0.43
1:D:207:LEU:HD13	1:D:241:ILE:HG12	2.00	0.43
1:D:25:HIS:NE2	1:D:380:THR:OG1	2.51	0.43
1:D:22:ARG:HH11	1:D:414:ASN:HB3	1.83	0.43
2:E:166:ALA:HB2	2:E:206:VAL:HA	2.01	0.43
2:E:81:LYS:HG3	2:E:82:ASN:H	1.83	0.43
1:A:143:LYS:CA	1:A:184:SER:HB2	2.47	0.43
1:A:223:PHE:HD2	1:A:225:HIS:ND1	2.16	0.43
1:A:86:SER:HA	1:A:87:PRO:HD2	1.68	0.43
2:C:175:ILE:HG22	2:C:183:ILE:HG13	2.00	0.43
1:D:198:VAL:HG22	7:D:838:HOH:O	2.19	0.43
1:D:203:TYR:OH	7:D:705:HOH:O	2.15	0.43
1:D:448:ALA:HB1	1:D:493:CYS:HA	1.99	0.43
1:D:488:ASP:HA	7:D:711:HOH:O	2.17	0.43
1:D:199:HIS:HA	1:D:525:LYS:HB2	2.01	0.43
2:E:40:LYS:HA	7:E:448:HOH:O	2.18	0.43
2:F:7:LEU:HG	2:F:9:ASP:HB2	1.99	0.43
1:A:97:ILE:HD13	1:A:112:PRO:HA	2.00	0.43
1:A:330:TYR:O	1:A:338:ALA:N	2.44	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:102:VAL:HG21	2:B:157:LEU:HB3	2.01	0.43
2:B:32:TYR:H	2:B:32:TYR:HD2	1.66	0.43
2:C:7:LEU:O	2:C:33:ARG:HB2	2.19	0.43
1:D:478:PHE:O	1:D:479:TRP:HD1	2.02	0.43
2:E:24:ARG:HG3	2:E:30:PHE:CE1	2.54	0.43
2:E:68:LEU:HB2	2:E:152:TYR:OH	2.19	0.43
1:A:150:SER:OG	1:A:167:THR:HA	2.19	0.43
1:A:447:SER:HB3	1:A:496:CYS:SG	2.59	0.43
1:A:465:TYR:CD1	1:A:551:VAL:HG23	2.49	0.43
2:B:158:ILE:HG23	2:B:159:THR:N	2.34	0.43
1:A:573:THR:HG21	2:B:177:SER:OG	2.19	0.43
2:B:7:LEU:HD21	7:B:460:HOH:O	2.19	0.43
2:C:68:LEU:HA	2:C:68:LEU:HD23	1.82	0.43
1:D:107:ARG:CG	1:D:107:ARG:HH11	1.93	0.43
1:D:208:SER:HA	1:D:211:LEU:HG	2.01	0.43
1:D:252:ASN:OD1	1:D:252:ASN:N	2.51	0.43
1:D:145:LEU:HD23	1:D:295:PHE:CE1	2.54	0.43
1:D:503:ASP:CG	1:D:505:GLY:H	2.22	0.43
2:E:84:PHE:CD1	2:E:85:PHE:N	2.87	0.43
2:E:90:TYR:OH	2:F:63:PRO:HD2	2.19	0.43
2:F:139:LEU:O	2:F:142:LYS:HB2	2.18	0.43
2:F:48:ASN:N	7:F:412:HOH:O	2.46	0.43
1:A:352:PHE:CD2	1:A:421:PHE:HE2	2.35	0.42
2:C:68:LEU:HD22	2:C:152:TYR:CE1	2.53	0.42
1:D:260:ARG:NE	7:D:849:HOH:O	2.52	0.42
1:D:358:LEU:HD12	7:D:757:HOH:O	2.18	0.42
1:D:403:LEU:HA	1:D:403:LEU:HD12	1.73	0.42
1:D:552:LYS:O	1:D:554:SER:N	2.52	0.42
2:F:64:VAL:HG21	2:F:73:TYR:CD2	2.54	0.42
1:A:11:ASN:O	1:A:14:ILE:HG13	2.19	0.42
1:A:308:SER:HB3	1:A:424:ARG:HA	2.01	0.42
1:A:442:GLN:O	1:A:446:GLU:HG3	2.19	0.42
1:A:39:ASN:HD21	1:A:91:GLY:HA3	1.84	0.42
2:B:69:ASN:ND2	2:B:73:TYR:OH	2.52	0.42
1:D:98:SER:N	1:D:111:ILE:O	2.52	0.42
1:D:231:PHE:O	1:D:235:GLU:HG3	2.19	0.42
1:D:494:CYS:SG	1:D:495:ASN:N	2.92	0.42
1:D:534:HIS:NE2	1:D:557:LYS:HD3	2.35	0.42
2:E:72:GLN:HA	2:E:84:PHE:HE2	1.84	0.42
1:A:150:SER:HB2	1:A:167:THR:CA	2.46	0.42
1:A:152:LYS:O	1:A:167:THR:HG21	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:TYR:CE1	1:A:241:ILE:HG13	2.54	0.42
1:A:278:ARG:O	1:A:282:MET:HE2	2.18	0.42
1:A:329:ASP:HB3	1:A:338:ALA:O	2.19	0.42
2:B:102:VAL:O	2:B:106:PHE:HB3	2.19	0.42
1:D:235:GLU:HG2	1:D:287:TRP:CD2	2.55	0.42
1:D:331:GLY:HA2	1:D:539:GLY:CA	2.50	0.42
1:D:77:ILE:CG2	1:D:110:PHE:HB3	2.48	0.42
1:D:84:ASP:OD1	7:D:756:HOH:O	2.22	0.42
2:E:50:ILE:HG13	2:E:51:HIS:N	2.32	0.42
2:F:84:PHE:C	2:F:85:PHE:HD1	2.22	0.42
2:B:9:ASP:HB2	2:B:20:ARG:NH2	2.33	0.42
2:C:107:THR:HG23	2:C:110:GLN:HE21	1.83	0.42
1:D:29:LYS:O	1:D:33:LYS:HG2	2.19	0.42
1:D:36:LEU:HD22	1:D:61:PHE:CZ	2.54	0.42
2:E:7:LEU:HD11	2:E:57:LEU:HD13	2.02	0.42
2:F:120:GLU:OE1	7:F:416:HOH:O	2.21	0.42
1:A:492:ASP:CG	2:B:183:ILE:HG12	2.39	0.42
2:B:79:PRO:HA	7:B:402:HOH:O	2.19	0.42
2:C:142:LYS:HB2	1:D:38:LYS:O	2.18	0.42
1:D:241:ILE:O	1:D:245:ILE:HG12	2.19	0.42
1:D:291:ILE:H	1:D:291:ILE:HG13	1.53	0.42
2:F:163:TRP:NE1	2:F:205:ILE:HD13	2.34	0.42
2:F:213:ARG:C	7:F:405:HOH:O	2.56	0.42
1:A:207:LEU:HA	1:A:207:LEU:HD12	1.80	0.42
1:A:223:PHE:CZ	1:A:536:LEU:HB3	2.54	0.42
1:A:234:PHE:CD2	1:A:290:LEU:HD21	2.45	0.42
1:A:503:ASP:O	1:A:507:VAL:HG23	2.20	0.42
1:A:80:MET:HA	1:A:86:SER:O	2.19	0.42
1:A:94:VAL:HG22	1:A:94:VAL:H	1.55	0.42
2:B:25:GLU:HA	2:B:194:SER:HB3	2.01	0.42
2:B:84:PHE:HE1	2:B:85:PHE:CD2	2.37	0.42
2:C:68:LEU:HD22	2:C:152:TYR:HE1	1.83	0.42
1:D:233:THR:O	1:D:237:VAL:HG22	2.19	0.42
1:D:244:ASP:OD1	1:D:251:SER:HB2	2.20	0.42
1:D:295:PHE:HD2	1:D:298:ALA:HB2	1.85	0.42
1:D:410:ILE:HG13	1:D:411:GLY:N	2.34	0.42
1:D:432:ASN:OD1	1:D:433:ILE:N	2.52	0.42
2:F:11:TRP:CG	2:F:12:PRO:HD3	2.54	0.42
1:A:113:PHE:CG	4:A:602:ATP:O2A	2.73	0.42
1:A:189:PRO:O	1:A:192:VAL:HG13	2.19	0.42
1:A:242:VAL:HG21	1:A:278:ARG:NH2	2.27	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:434:ASP:HB2	1:A:550:CYS:CB	2.50	0.42
1:A:534:HIS:CD2	1:A:557:LYS:HE2	2.55	0.42
2:B:96:ARG:HD3	7:B:443:HOH:O	2.20	0.42
1:D:486:ASN:O	1:D:489:VAL:HG22	2.18	0.42
1:D:547:MET:HB2	1:D:547:MET:HE2	1.88	0.42
4:D:603:ATP:O1B	4:D:603:ATP:O1A	2.38	0.42
2:F:107:THR:O	2:F:110:GLN:HG3	2.20	0.42
2:F:201:ASP:HB3	2:F:203:GLU:HG2	2.01	0.42
1:A:104:SER:N	1:A:107:ARG:O	2.38	0.42
1:A:118:MET:O	1:A:121:THR:HB	2.19	0.42
1:A:262:ALA:O	1:A:266:LEU:HG	2.19	0.42
1:A:338:ALA:HB1	1:A:352:PHE:C	2.39	0.42
1:A:431:ILE:HD13	1:A:431:ILE:HA	1.76	0.42
1:A:433:ILE:HD11	1:A:552:LYS:NZ	2.35	0.42
2:B:122:GLU:CA	2:B:125:LYS:HE2	2.43	0.42
2:B:165:GLN:HA	2:B:168:GLU:OE1	2.20	0.42
2:C:169:LYS:NZ	2:C:206:VAL:HG13	2.34	0.42
1:D:471:ASP:HA	1:D:472:PRO:HA	1.76	0.42
1:D:477:ILE:HB	7:D:802:HOH:O	2.20	0.42
1:D:530:LYS:HD2	1:D:561:ILE:HD13	2.02	0.42
2:E:18:ARG:NH2	2:E:103:ASP:OD1	2.51	0.42
1:A:210:ILE:HD12	1:A:210:ILE:HG23	1.85	0.42
1:A:365:PRO:HA	1:A:388:TYR:CD1	2.55	0.42
2:B:10:TYR:CD2	2:B:12:PRO:HD2	2.54	0.42
1:D:101:SER:HB3	1:D:535:PHE:CD2	2.54	0.42
2:E:108:ASP:O	2:E:111:PHE:HB3	2.20	0.42
2:F:163:TRP:CD1	2:F:205:ILE:HD13	2.55	0.42
1:A:112:PRO:HD2	1:A:397:GLY:HA3	2.01	0.42
1:A:363:PHE:HB3	1:A:388:TYR:HB3	2.02	0.42
1:A:475:TYR:HB2	1:A:518:LEU:HB2	2.02	0.42
1:A:223:PHE:CG	1:A:533:GLU:HG2	2.55	0.42
1:A:510:ARG:NH1	1:A:575:PHE:HE2	2.17	0.42
2:B:34:GLU:N	7:B:412:HOH:O	2.52	0.42
2:C:176:GLU:HB2	2:C:183:ILE:HD12	2.01	0.42
2:C:47:SER:HB2	7:C:414:HOH:O	2.20	0.42
1:D:81:VAL:HG21	1:D:110:PHE:CE2	2.55	0.42
1:D:200:GLN:O	1:D:203:TYR:HB3	2.19	0.42
1:D:224:ALA:HA	1:D:316:LEU:HD22	2.01	0.42
1:D:450:LYS:HE2	1:D:450:LYS:HB3	1.70	0.42
2:E:71:VAL:HG13	2:E:152:TYR:CE1	2.55	0.42
2:F:18:ARG:HH22	2:F:103:ASP:CG	2.23	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:ALA:HB1	4:A:602:ATP:C2	2.55	0.41
1:A:290:LEU:O	1:A:294:LEU:HG	2.20	0.41
1:A:496:CYS:HB2	2:B:187:LYS:NZ	2.34	0.41
1:A:223:PHE:HZ	1:A:536:LEU:CB	2.33	0.41
2:B:187:LYS:HB2	2:B:187:LYS:HE2	1.65	0.41
2:B:201:ASP:O	2:B:205:ILE:HG13	2.20	0.41
2:B:5:PRO:O	2:B:6:ILE:HD13	2.20	0.41
2:B:93:ALA:O	2:B:97:PHE:HB2	2.18	0.41
2:C:111:PHE:HA	2:C:114:TRP:NE1	2.35	0.41
1:D:430:SER:O	7:D:755:HOH:O	2.21	0.41
1:D:99:LEU:HD12	1:D:555:ASN:HB3	2.02	0.41
2:E:7:LEU:HD13	2:E:30:PHE:HD2	1.83	0.41
1:A:166:THR:N	3:A:601:ILE:O	2.52	0.41
1:A:478:PHE:CZ	1:A:562:LEU:HG	2.55	0.41
1:A:68:VAL:HG22	1:A:69:THR:N	2.34	0.41
2:B:190:MET:HA	2:B:195:VAL:HG11	2.02	0.41
2:C:14:MET:HE2	7:C:432:HOH:O	2.20	0.41
1:D:163:GLY:HA2	1:D:560:GLN:CB	2.46	0.41
1:D:457:ILE:HB	1:D:482:SER:OG	2.19	0.41
1:D:486:ASN:HB2	7:D:1023:HOH:O	2.18	0.41
1:D:499:ARG:NH2	2:E:184:ALA:O	2.53	0.41
1:D:512:CYS:O	1:D:513:LYS:CB	2.68	0.41
1:D:526:GLY:CA	1:D:529:ARG:HB3	2.50	0.41
1:D:97:ILE:HB	1:D:162:VAL:HB	2.03	0.41
2:E:114:TRP:CZ3	2:E:212:TYR:HD2	2.38	0.41
2:E:211:GLU:O	2:E:214:LYS:HG2	2.20	0.41
1:A:146:GLN:HB2	1:A:148:ILE:CG2	2.50	0.41
1:A:37:LEU:HA	1:A:37:LEU:HD23	1.88	0.41
1:A:553:PRO:HB3	7:A:703:HOH:O	2.20	0.41
1:A:552:LYS:C	1:A:554:SER:N	2.74	0.41
2:B:150:PHE:CE1	2:B:192:LYS:HG3	2.55	0.41
2:B:192:LYS:HB2	7:B:409:HOH:O	2.21	0.41
2:B:23:LEU:HB3	2:B:28:VAL:CG1	2.51	0.41
2:B:57:LEU:O	2:B:64:VAL:HG22	2.21	0.41
1:D:245:ILE:HG12	1:D:245:ILE:H	1.54	0.41
1:D:332:SER:HA	4:D:603:ATP:C6	2.54	0.41
1:D:459:VAL:N	7:D:817:HOH:O	2.39	0.41
1:D:426:ASN:HB3	1:D:543:GLY:O	2.19	0.41
1:D:110:PHE:HE1	1:D:556:ALA:HB2	1.83	0.41
2:E:174:SER:HB3	7:E:462:HOH:O	2.20	0.41
1:A:477:ILE:N	7:A:739:HOH:O	2.53	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:331:GLY:N	1:A:537:GLY:O	2.49	0.41
2:B:22:ALA:HA	2:B:155:ILE:HD13	2.02	0.41
2:B:169:LYS:HG3	2:B:170:PHE:N	2.34	0.41
2:C:9:ASP:OD1	2:C:10:TYR:N	2.43	0.41
1:D:100:SER:HA	1:D:535:PHE:HE1	1.86	0.41
1:D:22:ARG:NH1	1:D:414:ASN:HB3	2.35	0.41
1:D:28:GLN:NE2	1:D:356:PRO:O	2.53	0.41
1:D:479:TRP:CD1	7:D:802:HOH:O	2.71	0.41
1:D:451:ARG:HE	2:E:183:ILE:HD11	1.84	0.41
2:F:201:ASP:HB2	2:F:204:LYS:HG3	2.02	0.41
2:C:200:PRO:HG2	2:C:205:ILE:HD11	2.02	0.41
2:C:30:PHE:N	2:C:30:PHE:CD2	2.88	0.41
2:B:97:PHE:CZ	2:C:65:CYS:HB2	2.56	0.41
1:D:131:PHE:O	1:D:134:ARG:HB3	2.21	0.41
1:D:150:SER:HB3	1:D:170:TYR:HD2	1.83	0.41
1:D:221:ALA:HB3	1:D:227:LEU:HG	2.01	0.41
1:D:111:ILE:HD11	1:D:334:GLU:HA	2.03	0.41
2:E:107:THR:HG22	2:E:160:PHE:CZ	2.55	0.41
2:E:153:VAL:HG23	2:E:156:SER:HB2	2.01	0.41
2:E:164:PHE:CZ	2:E:182:LEU:HD21	2.55	0.41
2:F:135:LEU:HA	2:F:135:LEU:HD23	1.93	0.41
1:A:222:VAL:HG12	1:A:223:PHE:CD1	2.55	0.41
1:A:412:PHE:N	7:A:823:HOH:O	2.53	0.41
1:A:413:TYR:OH	7:A:710:HOH:O	1.99	0.41
1:A:43:ILE:HB	7:A:978:HOH:O	2.20	0.41
1:A:170:TYR:OH	3:A:601:ILE:HD13	2.21	0.41
2:C:201:ASP:OD2	2:C:204:LYS:HE2	2.21	0.41
2:C:88:ASP:HA	2:C:89:PRO:HD2	1.78	0.41
1:D:328:HIS:CD2	5:D:602:JAA:O03	2.73	0.41
1:D:364:LEU:HD23	1:D:364:LEU:HA	1.83	0.41
1:D:223:PHE:CZ	1:D:533:GLU:HA	2.55	0.41
1:D:108:PRO:HG2	1:D:552:LYS:HB3	2.01	0.41
1:D:98:SER:C	1:D:556:ALA:HB3	2.41	0.41
2:E:138:GLU:HG3	2:E:145:PHE:HE1	1.86	0.41
2:F:105:LYS:NZ	2:F:131:ALA:HB2	2.36	0.41
2:F:40:LYS:HB2	2:F:40:LYS:HE3	1.67	0.41
2:F:67:SER:OG	2:F:68:LEU:N	2.52	0.41
1:A:108:PRO:HB2	1:A:554:SER:OG	2.20	0.41
1:A:125:PHE:HD1	1:A:125:PHE:HA	1.68	0.41
1:A:251:SER:HA	7:A:763:HOH:O	2.20	0.41
1:A:222:VAL:HG22	5:A:603:JAA:C07	2.50	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:62:LYS:HG2	7:B:450:HOH:O	2.20	0.41
1:D:113:PHE:CG	4:D:603:ATP:O2A	2.73	0.41
1:D:154:TYR:HB2	1:D:563:CYS:HB2	2.03	0.41
1:D:393:THR:OG1	1:D:400:ARG:N	2.50	0.41
1:D:452:LEU:HG	1:D:485:THR:HG21	2.03	0.41
1:D:99:LEU:HB2	1:D:556:ALA:N	2.30	0.41
2:F:139:LEU:HG	2:F:142:LYS:H	1.85	0.41
2:F:18:ARG:NH2	2:F:156:SER:HB2	2.35	0.41
2:F:26:LYS:NZ	2:F:82:ASN:C	2.73	0.41
2:F:76:GLU:O	7:F:417:HOH:O	2.22	0.41
1:A:81:VAL:HG21	1:A:110:PHE:CE2	2.56	0.41
1:A:432:ASN:ND2	1:A:434:ASP:OD1	2.53	0.41
1:A:445:VAL:HG21	1:A:462:PHE:CD2	2.56	0.41
1:A:547:MET:HA	1:A:548:PRO:HD3	1.83	0.41
2:C:26:LYS:HD2	2:C:26:LYS:HA	1.94	0.41
1:D:250:LEU:HD12	1:D:251:SER:O	2.20	0.41
1:D:313:VAL:HG22	7:D:1042:HOH:O	2.19	0.41
1:D:332:SER:CB	1:D:538:LEU:HA	2.50	0.41
2:E:105:LYS:HB3	2:E:105:LYS:HE2	1.83	0.41
2:E:90:TYR:CD1	2:F:62:LYS:HB3	2.56	0.41
1:A:171:ARG:HB2	7:A:864:HOH:O	2.20	0.41
1:A:282:MET:HB2	1:A:282:MET:HE2	1.78	0.41
1:A:345:LEU:O	7:A:743:HOH:O	2.21	0.41
1:A:535:PHE:HB3	1:A:544:GLN:O	2.20	0.41
1:A:403:LEU:HD21	1:A:538:LEU:HD11	2.02	0.41
2:B:102:VAL:HG23	7:B:401:HOH:O	2.21	0.41
2:B:153:VAL:HG23	7:B:501:HOH:O	2.20	0.41
2:C:126:LYS:HD2	7:C:564:HOH:O	2.20	0.41
2:E:93:ALA:O	2:E:97:PHE:HB2	2.21	0.41
2:F:182:LEU:N	7:F:402:HOH:O	2.46	0.41
1:A:98:SER:O	1:A:110:PHE:HA	2.21	0.41
1:A:124:LEU:HD13	1:A:336:TRP:CD2	2.55	0.41
1:A:450:LYS:H	1:A:450:LYS:HG2	1.66	0.41
1:A:527:THR:HA	1:A:530:LYS:HD2	2.03	0.41
2:C:18:ARG:NH1	2:C:103:ASP:OD1	2.36	0.41
2:C:80:GLU:HG3	7:C:502:HOH:O	2.21	0.41
1:D:295:PHE:HA	1:D:296:PRO:HD3	1.75	0.41
1:D:328:HIS:N	7:D:783:HOH:O	2.53	0.41
2:C:142:LYS:HE3	1:D:39:ASN:HA	2.02	0.41
2:E:143:PRO:HB2	2:E:144:TYR:CD2	2.56	0.41
2:F:139:LEU:HA	2:F:139:LEU:HD12	1.37	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:ILE:N	1:A:162:VAL:HA	2.36	0.41
1:A:313:VAL:HB	1:A:314:PRO:HD3	2.03	0.41
1:A:35:ILE:HD11	1:A:359:GLY:HA2	2.03	0.41
1:A:382:VAL:HG12	1:A:409:VAL:HG21	2.02	0.41
1:A:487:GLU:HG2	1:A:570:TYR:CZ	2.56	0.41
1:A:392:ILE:HD11	1:A:539:GLY:O	2.21	0.41
1:A:567:VAL:HB	7:A:746:HOH:O	2.20	0.41
2:B:114:TRP:CD1	2:B:167:TYR:CE1	3.09	0.41
2:B:40:LYS:HE2	2:B:40:LYS:HB2	1.66	0.41
2:B:60:ASN:O	2:B:60:ASN:ND2	2.54	0.41
1:D:23:ASN:O	1:D:24:ALA:C	2.59	0.41
1:D:128:ALA:HB2	1:D:329:ASP:OD2	2.21	0.41
1:D:452:LEU:HB3	1:D:457:ILE:HD11	2.03	0.41
1:D:499:ARG:CZ	2:E:184:ALA:CB	2.90	0.41
1:D:441:LEU:CD2	1:D:549:ARG:HB3	2.51	0.41
2:C:143:PRO:CB	1:D:87:PRO:HB2	2.51	0.41
2:E:142:LYS:HA	2:E:143:PRO:HD3	1.94	0.41
1:D:447:SER:OG	2:E:191:GLU:OE1	2.38	0.41
2:F:11:TRP:O	2:F:200:PRO:HG3	2.21	0.41
2:F:77:ALA:HB3	2:F:78:TRP:CE3	2.56	0.41
1:A:190:ASP:HA	1:A:193:ILE:HD12	2.04	0.40
1:A:315:LYS:HA	1:A:315:LYS:HD2	1.84	0.40
1:A:512:CYS:O	1:A:513:LYS:CB	2.69	0.40
2:B:103:ASP:HA	7:B:406:HOH:O	2.21	0.40
1:D:12:ARG:HA	7:D:787:HOH:O	2.21	0.40
1:D:305:MET:HB3	1:D:313:VAL:CG2	2.51	0.40
1:D:422:ILE:HG13	1:D:422:ILE:H	1.61	0.40
1:D:536:LEU:HB2	1:D:545:PHE:CE1	2.56	0.40
1:D:405:ASP:CG	1:D:540:SER:HB2	2.41	0.40
2:E:144:TYR:HB3	2:E:154:ASP:CG	2.41	0.40
2:E:9:ASP:N	2:E:9:ASP:OD1	2.55	0.40
2:F:18:ARG:NH2	2:F:103:ASP:OD1	2.54	0.40
2:F:132:VAL:HG22	2:F:182:LEU:CD2	2.51	0.40
1:A:77:ILE:HD13	1:A:111:ILE:HA	2.03	0.40
1:A:152:LYS:HG3	1:A:565:ASN:CG	2.41	0.40
1:A:244:ASP:CG	1:A:251:SER:HB2	2.42	0.40
1:A:429:LEU:HD13	7:A:889:HOH:O	2.20	0.40
1:A:42:ALA:HB3	1:A:45:LEU:HD13	2.03	0.40
1:A:464:SER:N	1:A:549:ARG:O	2.54	0.40
2:C:141:ASP:OD2	2:C:181:LYS:CE	2.70	0.40
2:C:51:HIS:N	2:C:51:HIS:CD2	2.87	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:131:PHE:HD1	1:D:134:ARG:NH2	2.19	0.40
1:D:263:MET:HA	1:D:266:LEU:HD12	2.04	0.40
1:D:291:ILE:HD12	1:D:320:ALA:HA	2.04	0.40
1:D:295:PHE:C	1:D:297:ASN:H	2.25	0.40
1:D:355:ILE:O	7:D:757:HOH:O	2.22	0.40
1:D:383:LYS:NZ	7:D:779:HOH:O	2.27	0.40
1:D:223:PHE:CG	1:D:533:GLU:HG2	2.56	0.40
1:D:53:ASN:HB3	1:D:54:ALA:H	1.54	0.40
2:E:128:PHE:CD1	2:E:128:PHE:C	2.94	0.40
2:E:66:GLU:O	2:E:70:VAL:HG23	2.21	0.40
2:F:109:ALA:O	2:F:113:VAL:HG23	2.21	0.40
2:F:128:PHE:CE2	2:F:175:ILE:HG12	2.56	0.40
1:A:328:HIS:CG	1:A:329:ASP:H	2.38	0.40
1:A:48:CYS:HB2	1:A:50:LEU:CD1	2.51	0.40
1:A:330:TYR:HE2	1:A:540:SER:H	1.62	0.40
2:B:143:PRO:HB2	2:B:144:TYR:CD2	2.57	0.40
2:B:4:LEU:HA	2:B:5:PRO:HD3	1.76	0.40
2:C:157:LEU:HD23	2:C:185:TRP:CZ3	2.56	0.40
6:C:301:GSH:SG2	7:C:449:HOH:O	2.35	0.40
1:D:145:LEU:HD12	7:D:940:HOH:O	2.21	0.40
1:D:152:LYS:HZ1	1:D:523:VAL:HG11	1.87	0.40
1:D:332:SER:HB3	1:D:538:LEU:CD1	2.51	0.40
1:D:336:TRP:CB	1:D:358:LEU:HD13	2.49	0.40
1:D:444:SER:HB3	7:D:841:HOH:O	2.20	0.40
1:D:434:ASP:HB2	1:D:550:CYS:SG	2.61	0.40
2:C:142:LYS:CA	1:D:91:GLY:HA3	2.52	0.40
2:E:170:PHE:CD2	2:E:213:ARG:HD2	2.56	0.40
2:F:14:MET:CE	2:F:110:GLN:HE22	2.33	0.40
1:A:94:VAL:HG21	1:A:112:PRO:HA	2.03	0.40
1:A:152:LYS:HZ1	1:A:523:VAL:CG1	2.33	0.40
1:A:28:GLN:NE2	1:A:356:PRO:O	2.55	0.40
1:A:407:VAL:CG2	1:A:419:LEU:HB3	2.51	0.40
1:A:55:THR:O	7:A:747:HOH:O	2.22	0.40
2:B:138:GLU:HB3	7:B:551:HOH:O	2.21	0.40
2:C:149:SER:HB3	2:C:150:PHE:H	1.66	0.40
2:C:114:TRP:CD1	2:C:167:TYR:HE1	2.40	0.40
2:C:157:LEU:HD21	2:C:182:LEU:HD11	2.03	0.40
2:C:54:ILE:HB	2:C:55:PRO:HA	2.02	0.40
1:D:131:PHE:CD1	1:D:134:ARG:NH2	2.90	0.40
1:D:227:LEU:HB3	1:D:316:LEU:HD13	2.04	0.40
1:D:218:TYR:HA	1:D:298:ALA:HB1	2.02	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:391:VAL:HG22	1:D:402:ARG:HA	2.04	0.40
1:D:411:GLY:O	1:D:418:GLN:N	2.33	0.40
1:D:552:LYS:C	1:D:554:SER:N	2.75	0.40
1:D:39:ASN:HD21	1:D:91:GLY:HA3	1.87	0.40
1:A:106:GLY:C	1:A:107:ARG:HD2	2.42	0.40
1:A:108:PRO:HB3	1:A:555:ASN:HB2	2.04	0.40
1:A:122:LEU:HA	1:A:122:LEU:HD23	1.95	0.40
1:A:273:LEU:HD12	1:A:273:LEU:HA	1.85	0.40
2:C:136:GLU:HG3	2:C:181:LYS:CD	2.52	0.40
1:D:169:VAL:HB	1:D:170:TYR:CD1	2.57	0.40
1:D:203:TYR:HB2	7:D:855:HOH:O	2.22	0.40
1:D:315:LYS:HA	1:D:315:LYS:HD2	1.86	0.40
3:D:601:ILE:HD12	5:D:602:JAA:C11	2.51	0.40
2:F:166:ALA:HA	2:F:169:LYS:HG2	2.04	0.40
2:F:14:MET:HA	2:F:17:MET:SD	2.62	0.40

All (18) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:270:ASN:O	1:D:511:LYS:NZ[1_565]	2.00	0.20
1:A:278:ARG:NH2	2:B:141:ASP:OD2[1_565]	2.05	0.15
1:A:270:ASN:ND2	1:A:510:ARG:O[1_565]	2.07	0.13
7:D:979:HOH:O	7:D:1014:HOH:O[1_445]	2.09	0.11
7:A:924:HOH:O	7:A:929:HOH:O[1_545]	2.10	0.10
7:B:530:HOH:O	7:C:538:HOH:O[1_565]	2.12	0.08
7:C:462:HOH:O	7:C:498:HOH:O[1_665]	2.12	0.08
7:A:1120:HOH:O	7:F:543:HOH:O[1_454]	2.13	0.07
1:D:270:ASN:ND2	1:D:510:ARG:O[1_565]	2.15	0.05
7:B:480:HOH:O	7:C:478:HOH:O[1_565]	2.15	0.05
7:A:1048:HOH:O	7:A:1102:HOH:O[1_565]	2.15	0.05
2:E:215:ASN:O	2:F:33:ARG:NH2[1_565]	2.16	0.04
7:A:908:HOH:O	7:F:566:HOH:O[1_354]	2.16	0.04
7:D:1203:HOH:O	7:E:638:HOH:O[1_565]	2.16	0.04
7:D:1062:HOH:O	7:D:1146:HOH:O[1_565]	2.16	0.04
7:A:1112:HOH:O	7:A:1119:HOH:O[1_545]	2.16	0.04
7:B:419:HOH:O	7:C:415:HOH:O[1_565]	2.18	0.02
7:D:1140:HOH:O	7:D:1168:HOH:O[1_665]	2.19	0.01

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	567/575 (99%)	506 (89%)	47 (8%)	14 (2%)	5	0
1	D	567/575 (99%)	505 (89%)	43 (8%)	19 (3%)	3	0
2	B	212/223 (95%)	196 (92%)	14 (7%)	2 (1%)	17	3
2	C	212/223 (95%)	199 (94%)	10 (5%)	3 (1%)	11	1
2	E	212/223 (95%)	192 (91%)	19 (9%)	1 (0%)	29	9
2	F	212/223 (95%)	196 (92%)	14 (7%)	2 (1%)	17	3
All	All	1982/2042 (97%)	1794 (90%)	147 (7%)	41 (2%)	7	0

All (41) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	369	THR
1	A	513	LYS
1	A	540	SER
1	A	542	ALA
1	D	369	THR
1	D	513	LYS
1	D	540	SER
1	D	542	ALA
1	A	368	GLU
1	A	553	PRO
2	B	140	GLY
1	D	150	SER
1	D	553	PRO
2	E	140	GLY
1	A	426	ASN
1	A	437	THR
1	A	541	SER
2	C	140	GLY
1	D	368	GLU
1	D	433	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	437	THR
2	F	27	GLY
1	A	88	ILE
1	A	93	PRO
1	A	150	SER
2	C	141	ASP
1	D	90	THR
2	F	66	GLU
2	C	79	PRO
1	D	88	ILE
1	D	93	PRO
1	D	196	PRO
1	D	394	ASN
2	B	66	GLU
1	D	24	ALA
1	D	105	GLN
1	A	566	VAL
1	D	566	VAL
1	A	433	ILE
1	D	428	ILE
1	D	481	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%)	444 (89%)	55 (11%)	6	0
1	D	499/505 (99%)	444 (89%)	55 (11%)	6	0
2	B	187/195 (96%)	171 (91%)	16 (9%)	10	1
2	C	187/195 (96%)	172 (92%)	15 (8%)	12	1
2	E	187/195 (96%)	173 (92%)	14 (8%)	13	1
2	F	187/195 (96%)	174 (93%)	13 (7%)	15	1
All	All	1746/1790 (98%)	1578 (90%)	168 (10%)	8	0

All (168) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	PHE
1	A	13	VAL
1	A	19	GLU
1	A	80	MET
1	A	88	ILE
1	A	90	THR
1	A	92	HIS
1	A	94	VAL
1	A	99	LEU
1	A	110	PHE
1	A	111	ILE
1	A	125	PHE
1	A	139	ASP
1	A	140	ASP
1	A	150	SER
1	A	169	VAL
1	A	182	ILE
1	A	192	VAL
1	A	197	ASP
1	A	205	HIS
1	A	241	ILE
1	A	242	VAL
1	A	245	ILE
1	A	273	LEU
1	A	299	LYS
1	A	329	ASP
1	A	333	SER
1	A	345	LEU
1	A	379	LEU
1	A	384	ILE
1	A	387	GLU
1	A	410	ILE
1	A	422	ILE
1	A	423	CYS
1	A	425	ARG
1	A	427	LEU
1	A	430	SER
1	A	431	ILE
1	A	433	ILE
1	A	438	GLU
1	A	447	SER
1	A	455	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	457	ILE
1	A	461	ASP
1	A	482	SER
1	A	488	ASP
1	A	494	CYS
1	A	502	ILE
1	A	509	SER
1	A	514	THR
1	A	518	LEU
1	A	545	PHE
1	A	562	LEU
1	A	563	CYS
1	A	573	THR
2	B	32	TYR
2	B	43	LEU
2	B	50	ILE
2	B	74	VAL
2	B	82	ASN
2	B	84	PHE
2	B	134	ILE
2	B	135	LEU
2	B	139	LEU
2	B	145	PHE
2	B	148	ASP
2	B	157	LEU
2	B	176	GLU
2	B	183	ILE
2	B	185	TRP
2	B	202	SER
2	C	26	LYS
2	C	30	PHE
2	C	33	ARG
2	C	38	SER
2	C	46	GLN
2	C	80	GLU
2	C	103	ASP
2	C	110	GLN
2	C	126	LYS
2	C	132	VAL
2	C	164	PHE
2	C	168	GLU
2	C	172	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	181	LYS
2	C	197	LYS
1	D	80	MET
1	D	88	ILE
1	D	90	THR
1	D	92	HIS
1	D	99	LEU
1	D	107	ARG
1	D	108	PRO
1	D	110	PHE
1	D	111	ILE
1	D	124	LEU
1	D	125	PHE
1	D	139	ASP
1	D	140	ASP
1	D	150	SER
1	D	152	LYS
1	D	179	MET
1	D	182	ILE
1	D	188	SER
1	D	192	VAL
1	D	205	HIS
1	D	212	PHE
1	D	241	ILE
1	D	245	ILE
1	D	246	LYS
1	D	252	ASN
1	D	273	LEU
1	D	323	LEU
1	D	326	VAL
1	D	329	ASP
1	D	333	SER
1	D	345	LEU
1	D	369	THR
1	D	379	LEU
1	D	384	ILE
1	D	387	GLU
1	D	410	ILE
1	D	422	ILE
1	D	424	ARG
1	D	425	ARG
1	D	427	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	447	SER
1	D	450	LYS
1	D	461	ASP
1	D	470	THR
1	D	484	GLU
1	D	494	CYS
1	D	502	ILE
1	D	518	LEU
1	D	545	PHE
1	D	547	MET
1	D	554	SER
1	D	562	LEU
1	D	563	CYS
1	D	572	SER
1	D	573	THR
2	E	32	TYR
2	E	37	PHE
2	E	43	LEU
2	E	65	CYS
2	E	84	PHE
2	E	133	LYS
2	E	134	ILE
2	E	135	LEU
2	E	139	LEU
2	E	157	LEU
2	E	176	GLU
2	E	185	TRP
2	E	211	GLU
2	E	212	TYR
2	F	33	ARG
2	F	36	ASP
2	F	38	SER
2	F	80	GLU
2	F	122	GLU
2	F	132	VAL
2	F	149	SER
2	F	155	ILE
2	F	168	GLU
2	F	173	PHE
2	F	181	LYS
2	F	182	LEU
2	F	213	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	GLN
1	A	174	ASN
1	A	217	GLN
2	B	48	ASN
2	B	60	ASN
2	B	110	GLN
2	C	51	HIS
2	C	72	GLN
2	C	121	GLN
1	D	120	ASN
1	D	205	HIS
1	D	217	GLN
1	D	495	ASN
1	D	544	GLN
1	D	565	ASN
2	E	60	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

10 ligands are modelled in this entry.

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	GSH	C	301	-	12,19,19	1.68	4 (33%)	15,24,24	3.03	7 (46%)
6	GSH	E	301	-	12,19,19	1.57	3 (25%)	15,24,24	3.24	8 (53%)
6	GSH	F	301	-	12,19,19	1.62	4 (33%)	15,24,24	2.71	6 (40%)
5	JAA	D	602	-	12,15,15	5.85	7 (58%)	12,19,19	2.58	6 (50%)
4	ATP	A	602	-	26,33,33	4.81	18 (69%)	31,52,52	3.38	16 (51%)
5	JAA	A	603	-	12,15,15	5.85	7 (58%)	12,19,19	2.53	5 (41%)
4	ATP	D	603	-	26,33,33	5.03	15 (57%)	31,52,52	3.23	14 (45%)
6	GSH	B	301	-	12,19,19	1.67	4 (33%)	15,24,24	2.93	6 (40%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	GSH	C	301	-	-	4/18/24/24	-
6	GSH	E	301	-	-	2/18/24/24	-
6	GSH	F	301	-	-	2/18/24/24	-
5	JAA	D	602	-	-	3/7/22/22	0/1/1/1
4	ATP	A	602	-	-	6/18/38/38	0/3/3/3
5	JAA	A	603	-	-	6/7/22/22	0/1/1/1
4	ATP	D	603	-	-	6/18/38/38	0/3/3/3
6	GSH	B	301	-	-	3/18/24/24	-

All (62) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	602	JAA	C05-C08	-13.31	1.30	1.52
5	A	603	JAA	C05-C08	-12.52	1.31	1.52
4	D	603	ATP	C4-N3	12.34	1.52	1.35
4	D	603	ATP	C5'-C4'	-11.42	1.16	1.51
4	A	602	ATP	C4-N3	11.34	1.51	1.35
4	A	602	ATP	C5'-C4'	-11.16	1.16	1.51
5	A	603	JAA	C06-C04	-10.92	1.25	1.53
5	D	602	JAA	C06-C04	-10.50	1.26	1.53
4	D	603	ATP	C3'-C4'	-9.95	1.27	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	602	ATP	C3'-C4'	-9.73	1.28	1.53
4	D	603	ATP	C2'-C1'	-8.65	1.40	1.53
4	A	602	ATP	C2'-C3'	-7.81	1.32	1.53
4	D	603	ATP	C2'-C3'	-7.67	1.32	1.53
5	D	602	JAA	C07-C08	7.33	1.63	1.51
5	A	603	JAA	C10-C04	-7.05	1.44	1.53
5	A	603	JAA	C07-C08	6.67	1.61	1.51
4	A	602	ATP	C2'-C1'	-6.59	1.43	1.53
5	D	602	JAA	C10-C04	-5.94	1.46	1.53
4	D	603	ATP	C2-N1	5.07	1.43	1.33
4	A	602	ATP	C2-N1	5.05	1.43	1.33
5	A	603	JAA	C05-C04	5.05	1.67	1.54
5	D	602	JAA	C05-C04	4.69	1.66	1.54
4	D	603	ATP	C6-N6	-4.62	1.17	1.34
4	A	602	ATP	O3'-C3'	-4.47	1.32	1.43
4	A	602	ATP	C6-N6	-4.29	1.18	1.34
4	D	603	ATP	O3'-C3'	-4.18	1.33	1.43
4	D	603	ATP	C5-C4	-3.75	1.31	1.40
4	A	602	ATP	C5-C4	-3.71	1.31	1.40
4	D	603	ATP	C2-N3	-3.47	1.26	1.32
4	D	603	ATP	C5-N7	-3.30	1.27	1.39
4	A	602	ATP	O2'-C2'	-3.29	1.35	1.43
4	A	602	ATP	C2-N3	-3.07	1.27	1.32
4	D	603	ATP	PG-O1G	3.04	1.60	1.50
4	A	602	ATP	C5-N7	-3.04	1.28	1.39
6	F	301	GSH	CD1-N2	2.94	1.40	1.34
6	B	301	GSH	C2-N3	2.91	1.40	1.33
6	E	301	GSH	CD1-N2	2.91	1.40	1.34
6	C	301	GSH	CD1-N2	2.86	1.40	1.34
6	B	301	GSH	CA2-N2	-2.78	1.40	1.45
6	B	301	GSH	CD1-N2	2.68	1.39	1.34
4	A	602	ATP	PA-O5'	2.67	1.70	1.59
4	D	603	ATP	O2'-C2'	-2.61	1.36	1.43
4	A	602	ATP	O4'-C4'	-2.60	1.39	1.45
6	E	301	GSH	C2-N3	2.57	1.39	1.33
5	A	603	JAA	C06-C07	2.53	1.58	1.53
6	B	301	GSH	CA3-N3	-2.53	1.41	1.46
6	F	301	GSH	C2-N3	2.52	1.39	1.33
4	A	602	ATP	O4'-C1'	2.51	1.44	1.41
6	F	301	GSH	CA2-N2	-2.50	1.40	1.45
6	C	301	GSH	C2-N3	2.50	1.39	1.33
5	D	602	JAA	C06-C07	2.43	1.58	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	603	ATP	O4'-C4'	-2.36	1.39	1.45
4	A	602	ATP	PG-O1G	2.34	1.58	1.50
6	C	301	GSH	CB2-CA2	-2.33	1.50	1.53
4	A	602	ATP	PA-O2A	-2.26	1.44	1.55
6	C	301	GSH	CA2-N2	-2.21	1.41	1.45
6	E	301	GSH	CA2-N2	-2.16	1.41	1.45
6	F	301	GSH	CA3-N3	-2.15	1.41	1.46
5	A	603	JAA	C09-C05	-2.12	1.51	1.54
4	A	602	ATP	PG-O3G	-2.11	1.46	1.54
4	D	603	ATP	PG-O2G	-2.10	1.46	1.54
5	D	602	JAA	O01-C08	-2.07	1.18	1.21

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	602	ATP	C4-C5-N7	-10.23	98.74	109.40
4	D	603	ATP	C4-C5-N7	-9.66	99.33	109.40
6	B	301	GSH	CA2-CB2-SG2	-8.37	104.79	114.19
6	E	301	GSH	CA3-N3-C2	-8.09	110.69	122.34
4	A	602	ATP	PA-O3A-PB	-7.57	106.85	132.83
6	F	301	GSH	CA2-CB2-SG2	-7.13	106.17	114.19
6	C	301	GSH	CA2-CB2-SG2	-6.90	106.44	114.19
4	D	603	ATP	PA-O3A-PB	-6.84	109.35	132.83
4	D	603	ATP	O2'-C2'-C3'	6.45	132.68	111.82
5	D	602	JAA	C06-C07-C08	-5.83	99.57	105.42
4	A	602	ATP	O2'-C2'-C3'	5.27	128.86	111.82
6	E	301	GSH	CA2-CB2-SG2	-5.22	108.33	114.19
5	A	603	JAA	C06-C07-C08	-5.14	100.26	105.42
4	A	602	ATP	N3-C2-N1	-4.96	120.93	128.68
6	C	301	GSH	CA3-N3-C2	-4.92	115.26	122.34
4	A	602	ATP	PA-O5'-C5'	-4.69	94.15	121.68
4	D	603	ATP	O2G-PG-O3B	4.57	119.96	104.64
4	D	603	ATP	N3-C2-N1	-4.42	121.76	128.68
6	C	301	GSH	CB2-CA2-C2	-4.30	100.90	109.76
4	D	603	ATP	PA-O5'-C5'	-4.27	96.65	121.68
4	A	602	ATP	C2'-C3'-C4'	4.18	110.77	102.64
4	A	602	ATP	O2G-PG-O3B	4.14	118.52	104.64
6	F	301	GSH	CA3-N3-C2	-3.97	116.62	122.34
4	A	602	ATP	O4'-C4'-C3'	3.93	112.90	105.11
6	B	301	GSH	C3-CA3-N3	-3.84	103.02	110.43
6	B	301	GSH	CA3-N3-C2	-3.84	116.82	122.34
4	D	603	ATP	C2'-C3'-C4'	3.80	110.03	102.64

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	603	JAA	C06-C04-C10	-3.65	107.13	113.67
4	A	602	ATP	O4'-C4'-C5'	3.63	121.32	109.37
6	E	301	GSH	CB2-CA2-N2	-3.59	106.16	111.28
4	A	602	ATP	C5-C6-N6	3.44	125.58	120.35
5	D	602	JAA	C09-C11-C13	-3.40	113.78	126.40
5	A	603	JAA	C09-C11-C13	-3.35	113.95	126.40
5	D	602	JAA	C06-C04-C10	-3.31	107.74	113.67
6	F	301	GSH	CG1-CD1-N2	-3.19	110.30	115.83
6	E	301	GSH	CA2-C2-N3	3.18	122.96	116.54
6	C	301	GSH	CG1-CD1-N2	-3.14	110.38	115.83
6	E	301	GSH	CG1-CD1-N2	-3.12	110.42	115.83
6	C	301	GSH	CB1-CG1-CD1	3.04	119.83	113.04
4	D	603	ATP	C3'-C2'-C1'	2.99	105.48	100.98
6	E	301	GSH	CA2-N2-CD1	2.97	129.29	121.65
6	E	301	GSH	C3-CA3-N3	-2.88	104.89	110.43
6	C	301	GSH	CB2-CA2-N2	-2.83	107.24	111.28
4	D	603	ATP	O4'-C4'-C3'	2.83	110.72	105.11
4	A	602	ATP	PB-O3B-PG	-2.75	123.39	132.83
6	F	301	GSH	CB1-CG1-CD1	2.64	118.94	113.04
5	A	603	JAA	O01-C08-C07	2.63	129.37	125.56
4	D	603	ATP	O4'-C4'-C5'	2.60	117.94	109.37
4	D	603	ATP	C5-C6-N6	2.60	124.30	120.35
6	B	301	GSH	CG1-CD1-N2	-2.55	111.40	115.83
6	C	301	GSH	CA2-N2-CD1	2.55	128.20	121.65
4	D	603	ATP	O5'-C5'-C4'	-2.50	100.38	108.99
4	D	603	ATP	PB-O3B-PG	-2.50	124.24	132.83
4	D	603	ATP	O3'-C3'-C4'	2.47	118.18	111.05
4	A	602	ATP	C3'-C2'-C1'	2.42	104.63	100.98
4	A	602	ATP	C2-N1-C6	2.41	122.87	118.75
4	A	602	ATP	C5-C6-N1	-2.40	114.91	120.35
4	A	602	ATP	O3'-C3'-C2'	2.31	119.31	111.82
5	A	603	JAA	C05-C09-C11	2.27	117.66	112.94
6	F	301	GSH	CB2-CA2-C2	-2.23	105.16	109.76
6	E	301	GSH	O2-C2-N3	-2.21	118.25	122.99
5	D	602	JAA	O01-C08-C07	2.19	128.74	125.56
6	F	301	GSH	CA2-N2-CD1	2.18	127.27	121.65
4	A	602	ATP	C1'-N9-C4	-2.15	122.87	126.64
6	B	301	GSH	CA2-N2-CD1	2.12	127.11	121.65
5	D	602	JAA	C05-C09-C11	2.11	117.33	112.94
5	D	602	JAA	C06-C04-C05	2.08	106.34	103.34
6	B	301	GSH	CB2-CA2-N2	-2.08	108.32	111.28

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	301	GSH	N1-CA1-CB1-CG1
6	C	301	GSH	C1-CA1-CB1-CG1
6	C	301	GSH	N2-CA2-CB2-SG2
6	C	301	GSH	C2-CA2-CB2-SG2
6	E	301	GSH	N2-CA2-CB2-SG2
6	E	301	GSH	C2-CA2-CB2-SG2
4	A	602	ATP	PB-O3B-PG-O2G
4	A	602	ATP	C5'-O5'-PA-O3A
5	A	603	JAA	C05-C04-C10-C12
5	A	603	JAA	C06-C04-C10-C12
5	A	603	JAA	C11-C13-C14-C15
6	B	301	GSH	N2-CA2-CB2-SG2
6	B	301	GSH	C2-CA2-CB2-SG2
6	F	301	GSH	N1-CA1-CB1-CG1
6	F	301	GSH	C1-CA1-CB1-CG1
4	A	602	ATP	C3'-C4'-C5'-O5'
5	A	603	JAA	C05-C09-C11-C13
5	D	602	JAA	C11-C13-C14-C15
5	D	602	JAA	C04-C05-C09-C11
5	A	603	JAA	C04-C05-C09-C11
4	D	603	ATP	PB-O3B-PG-O2G
4	D	603	ATP	PB-O3B-PG-O3G
5	D	602	JAA	C08-C05-C09-C11
5	A	603	JAA	C08-C05-C09-C11
6	B	301	GSH	C3-CA3-N3-C2
4	D	603	ATP	PB-O3B-PG-O1G
4	A	602	ATP	PB-O3B-PG-O3G
4	D	603	ATP	C5'-O5'-PA-O3A
4	A	602	ATP	C5'-O5'-PA-O1A
4	D	603	ATP	C5'-O5'-PA-O1A
4	A	602	ATP	PG-O3B-PB-O3A
4	D	603	ATP	PG-O3B-PB-O3A

There are no ring outliers.

7 monomers are involved in 58 short contacts:

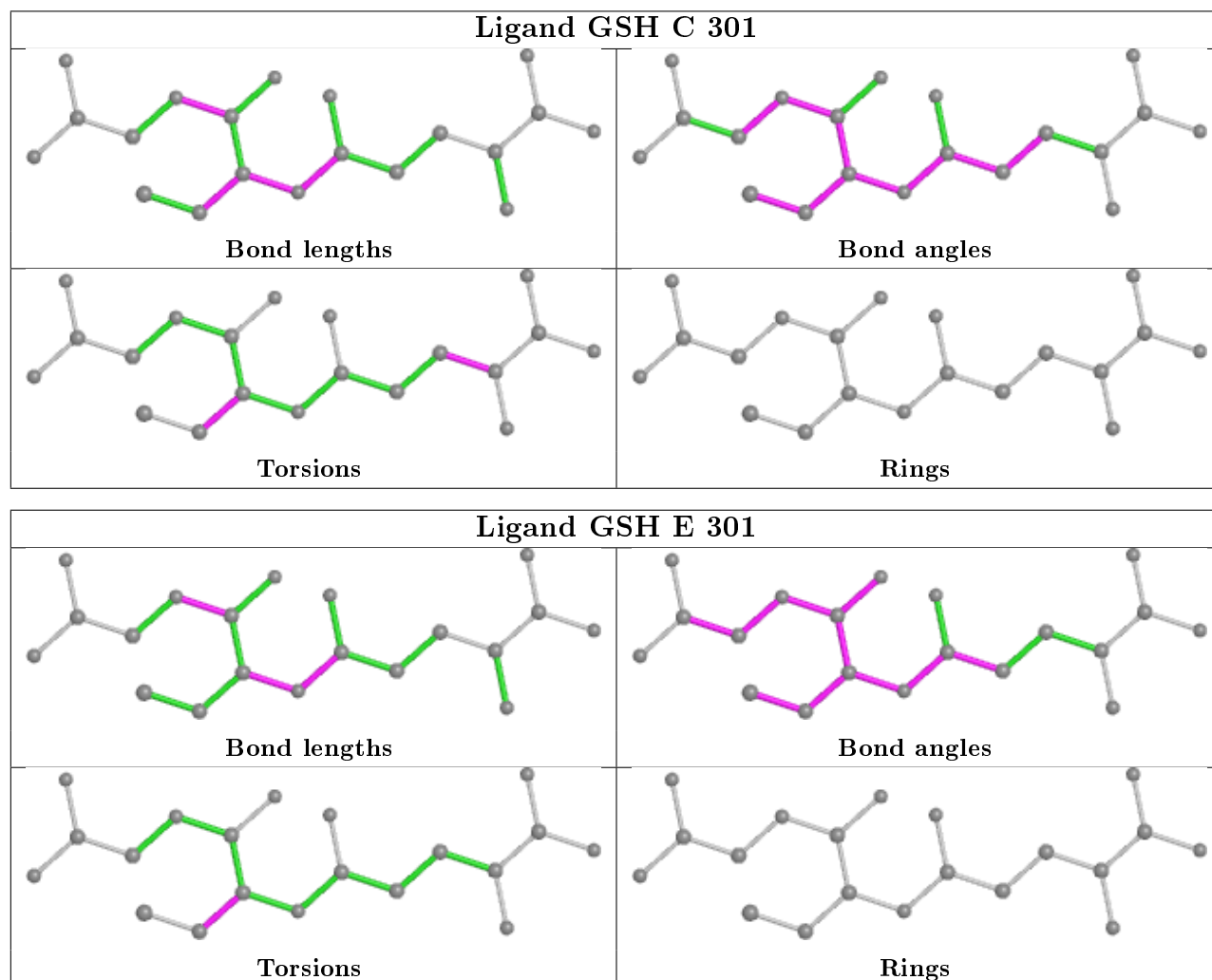
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	301	GSH	1	0
6	E	301	GSH	4	0
6	F	301	GSH	1	0
5	D	602	JAA	5	0

Continued on next page...

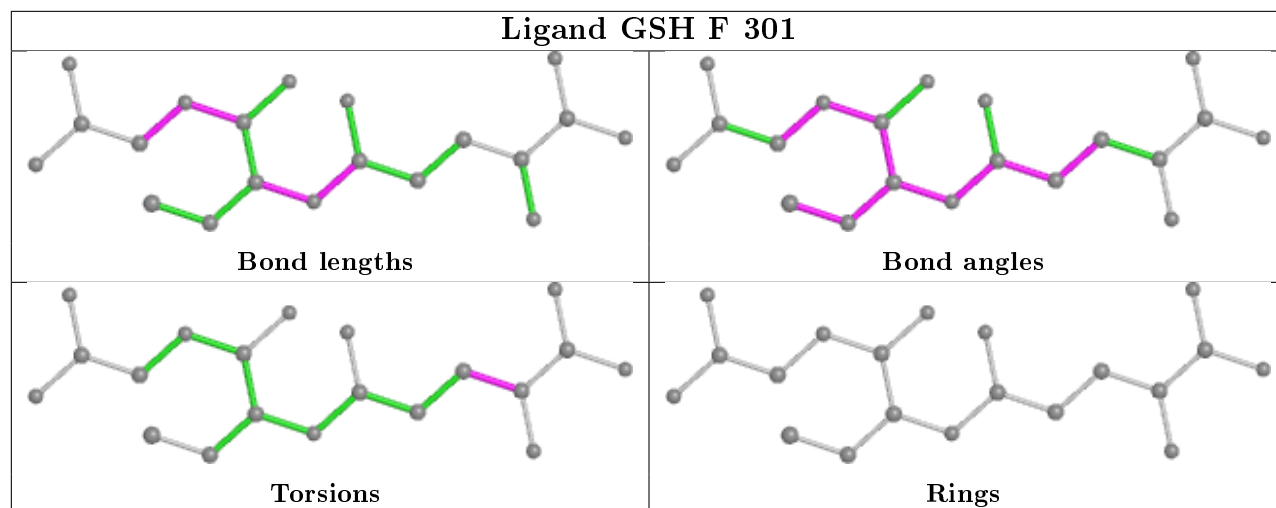
Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	602	ATP	21	0
5	A	603	JAA	7	0
4	D	603	ATP	21	0

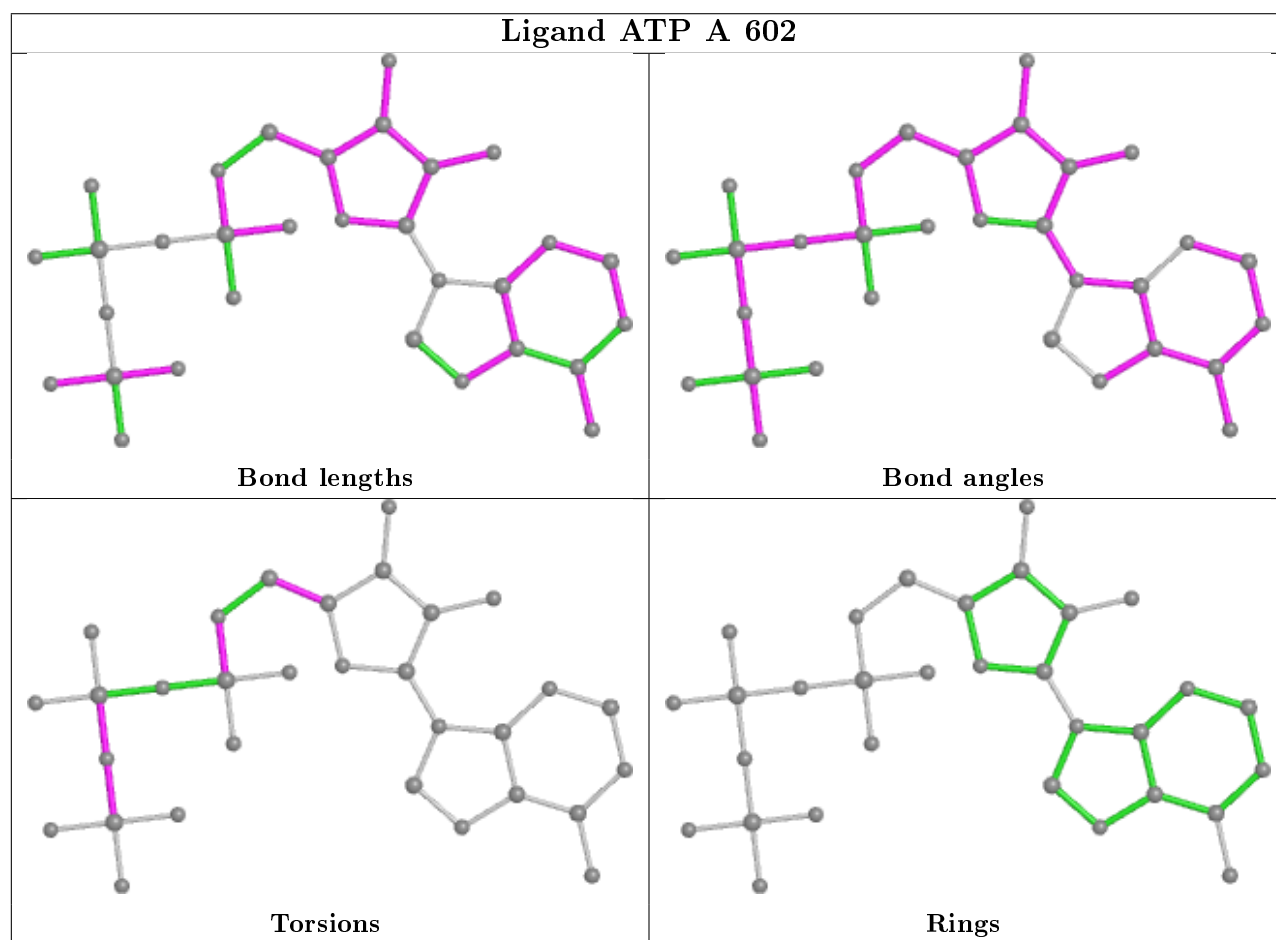
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

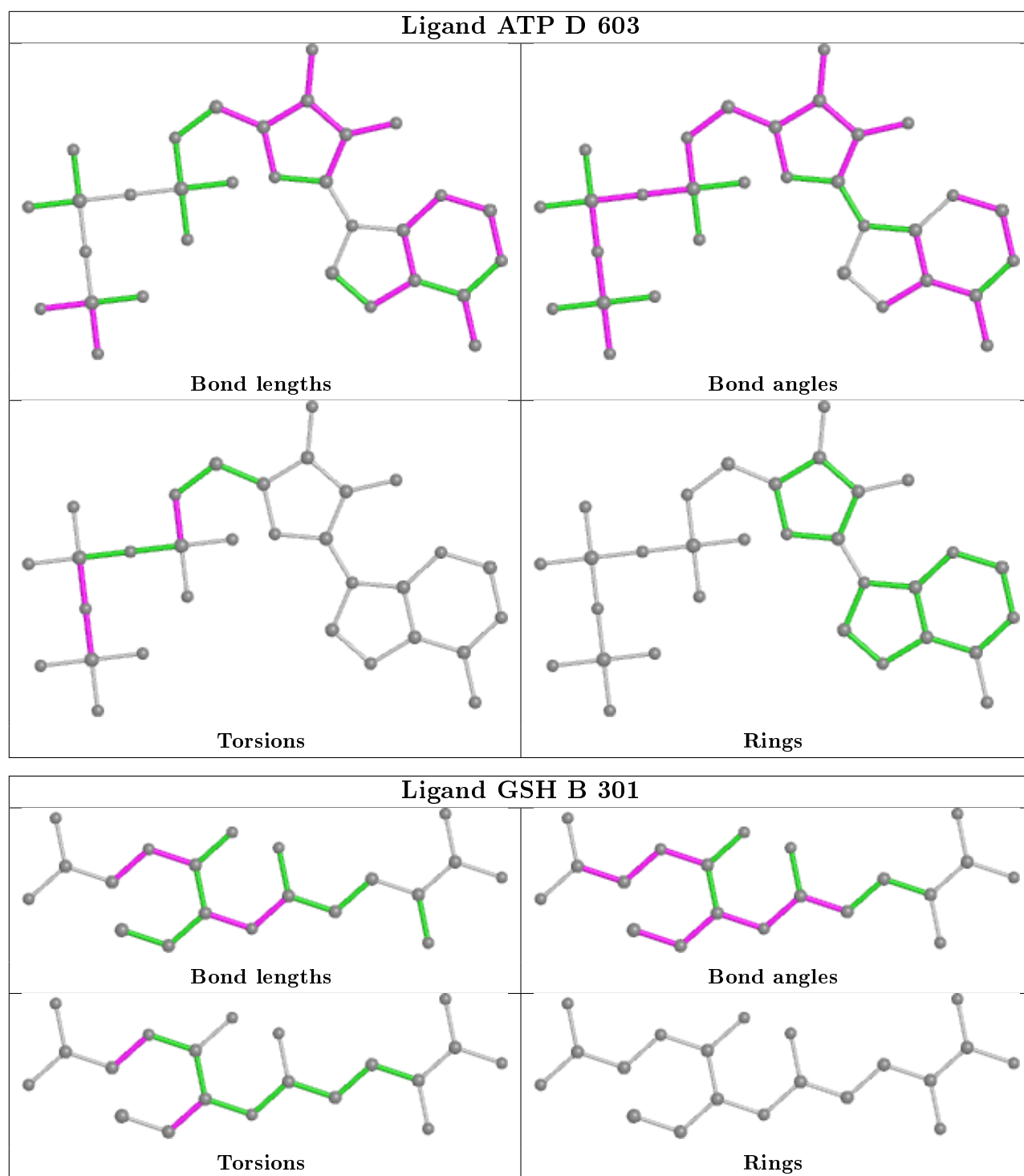


Ligand GSH F 301



Ligand ATP A 602





5.7 Other polymers [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	569/575 (98%)	0.81	25 (4%) 34 39	3, 7, 7, 16	0
1	D	569/575 (98%)	0.83	26 (4%) 32 36	3, 7, 7, 16	0
2	B	214/223 (95%)	0.63	9 (4%) 36 41	2, 3, 7, 11	0
2	C	214/223 (95%)	0.80	7 (3%) 46 53	7, 7, 7, 7	0
2	E	214/223 (95%)	0.62	3 (1%) 75 79	2, 3, 7, 11	0
2	F	214/223 (95%)	0.80	9 (4%) 36 41	7, 7, 7, 7	0
All	All	1994/2042 (97%)	0.77	79 (3%) 38 44	2, 7, 7, 16	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	427	LEU	4.2
1	D	212	PHE	3.4
1	D	427	LEU	3.2
1	D	372	GLY	3.2
1	A	8	PHE	3.0
2	B	32	TYR	2.8
2	E	98	TRP	2.8
1	D	388	TYR	2.8
1	D	366	VAL	2.8
1	A	372	GLY	2.7
1	A	342	THR	2.7
2	B	129	ILE	2.7
1	A	388	TYR	2.7
2	C	32	TYR	2.6
1	D	431	ILE	2.6
1	A	65	VAL	2.6
2	F	73	TYR	2.6
2	C	111	PHE	2.6
1	A	431	ILE	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	570	TYR	2.6
2	F	114	TRP	2.5
1	A	575	PHE	2.5
1	D	361	PHE	2.5
1	D	269	PRO	2.4
1	A	366	VAL	2.4
1	D	384	ILE	2.4
2	B	50	ILE	2.4
1	A	336	TRP	2.4
2	F	98	TRP	2.4
1	A	175	PHE	2.3
2	B	118	GLY	2.3
1	D	177	ALA	2.3
1	A	223	PHE	2.3
1	A	494	CYS	2.3
2	F	4	LEU	2.3
1	D	65	VAL	2.3
2	C	71	VAL	2.3
1	D	575	PHE	2.3
2	C	85	PHE	2.3
1	A	449	ALA	2.3
1	A	124	LEU	2.3
1	D	128	ALA	2.2
2	E	135	LEU	2.2
2	F	182	LEU	2.2
1	D	336	TRP	2.2
2	B	111	PHE	2.2
2	E	128	PHE	2.2
1	A	428	ILE	2.2
1	D	410	ILE	2.2
1	D	302	TYR	2.2
1	D	13	VAL	2.2
1	A	177	ALA	2.1
1	A	493	CYS	2.1
1	D	76	TYR	2.1
2	F	70	VAL	2.1
1	D	287	TRP	2.1
1	A	325	LEU	2.1
2	B	135	LEU	2.1
1	D	460	ILE	2.1
2	C	98	TRP	2.1
2	F	11	TRP	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	211	LEU	2.1
2	C	45	LEU	2.1
2	C	22	ALA	2.1
1	D	301	VAL	2.1
1	A	528	PHE	2.1
1	D	61	PHE	2.1
1	D	223	PHE	2.1
2	B	182	LEU	2.1
2	F	32	TYR	2.0
2	F	113	VAL	2.0
1	A	48	CYS	2.0
1	A	61	PHE	2.0
1	A	501	PHE	2.0
2	B	128	PHE	2.0
1	A	211	LEU	2.0
1	A	68	VAL	2.0
2	B	208	TYR	2.0
1	D	342	THR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	JAA	D	602	15/15	0.95	0.13	6,7,7,7	0
4	ATP	A	602	31/31	0.96	0.12	6,7,7,7	0
6	GSH	E	301	20/20	0.96	0.13	6,6,7,7	0
5	JAA	A	603	15/15	0.96	0.12	6,7,7,7	0
4	ATP	D	603	31/31	0.96	0.12	6,7,7,7	0

Continued on next page...

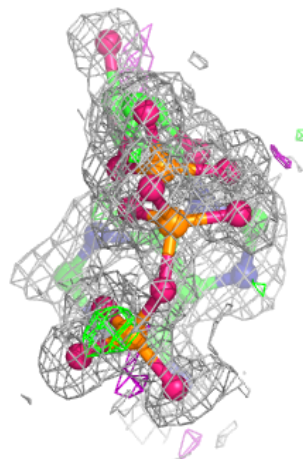
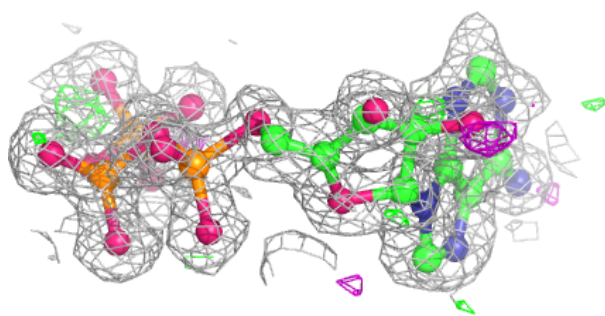
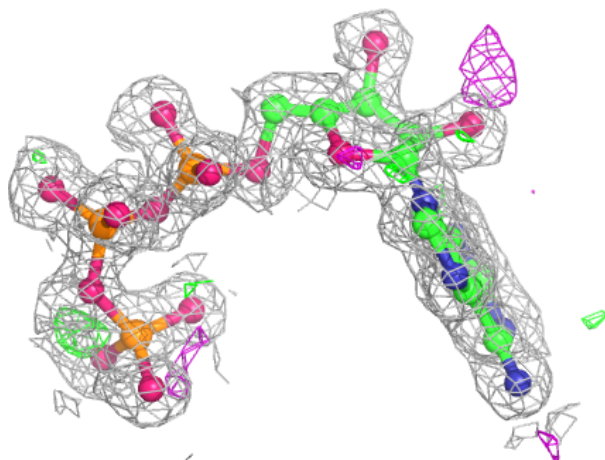
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	GSH	B	301	20/20	0.96	0.13	6,7,7,7	0
3	ILE	D	601	9/9	0.97	0.11	6,6,7,7	0
6	GSH	C	301	20/20	0.97	0.13	6,7,7,7	0
3	ILE	A	601	9/9	0.97	0.11	6,6,7,7	0
6	GSH	F	301	20/20	0.97	0.12	6,7,7,7	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.

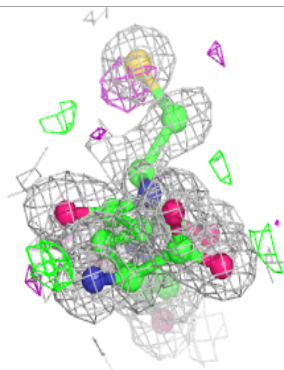
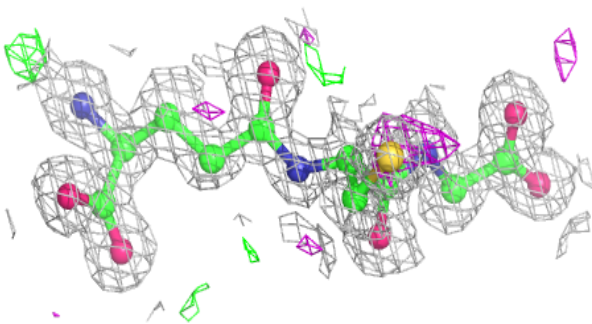
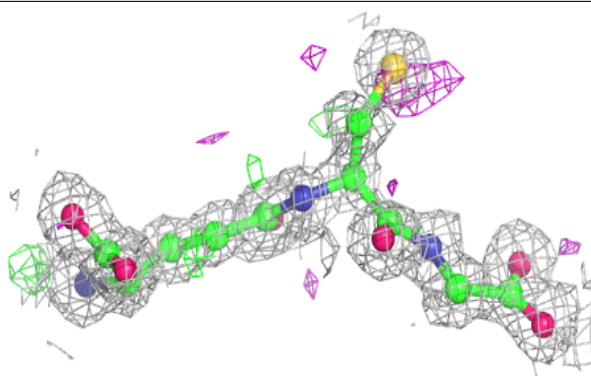
Electron density around ATP A 602:

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

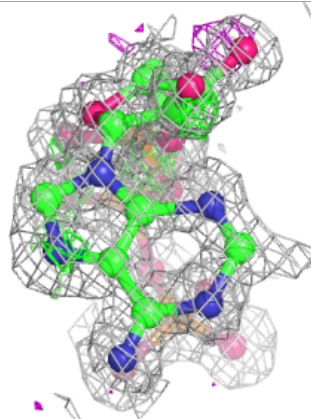
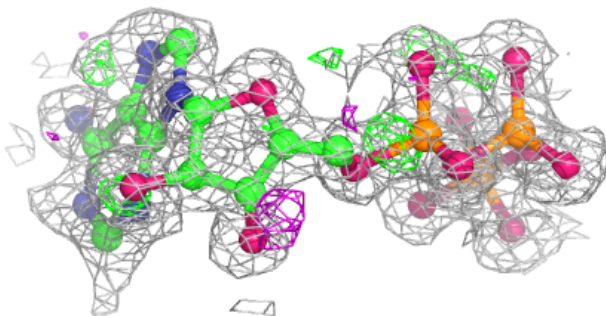
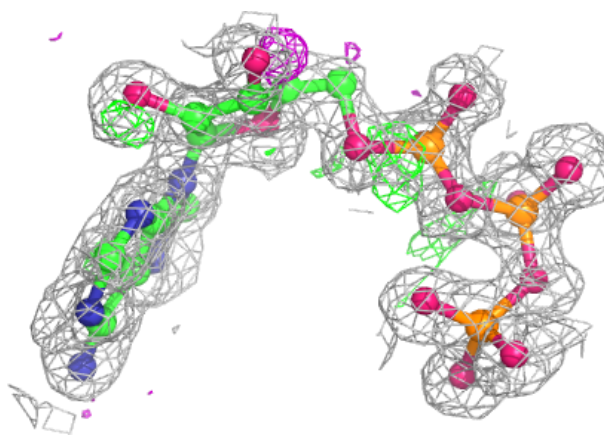


Electron density around GSH E 301:

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

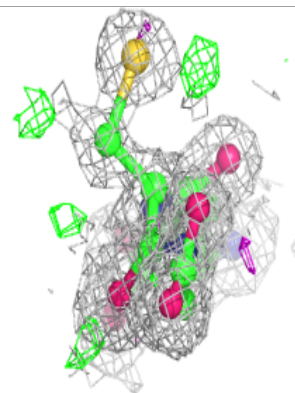
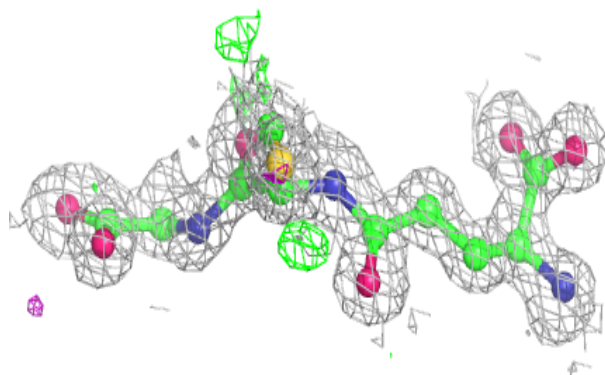
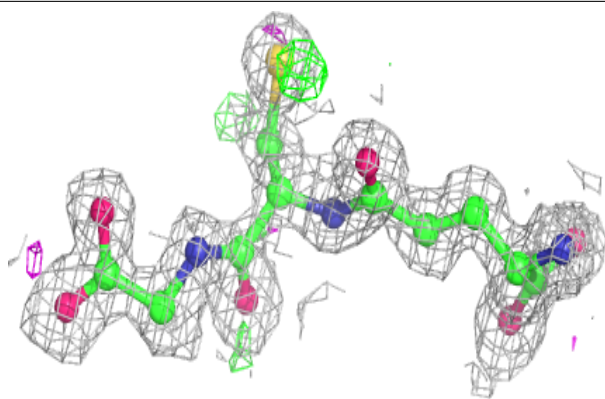
**Electron density around ATP D 603:**

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

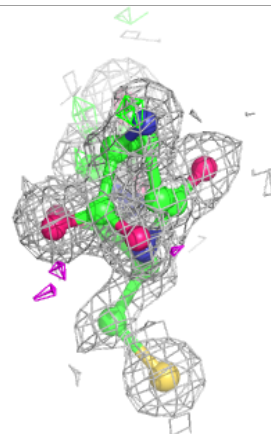
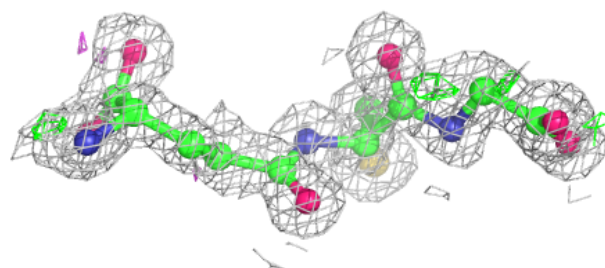
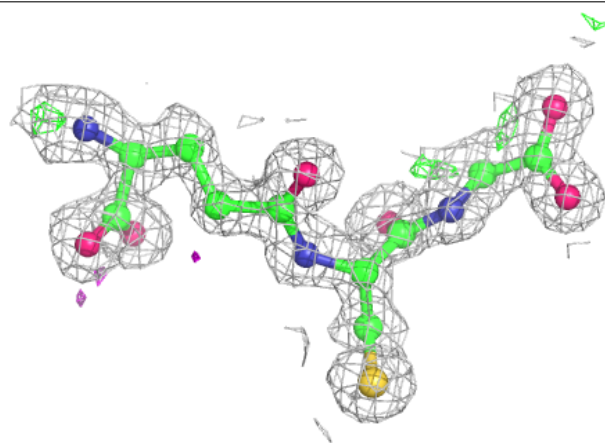


Electron density around GSH B 301:

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

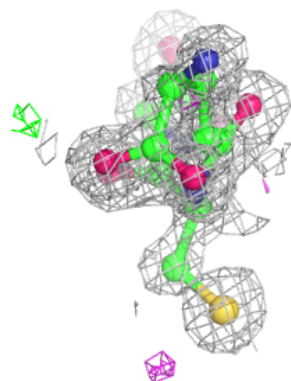
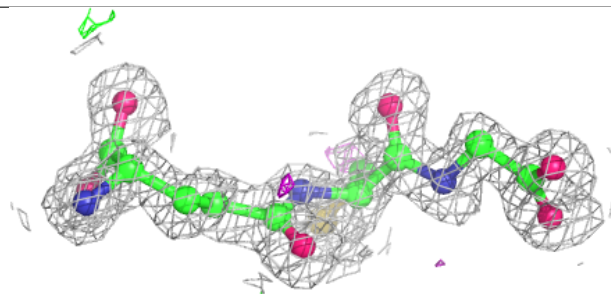
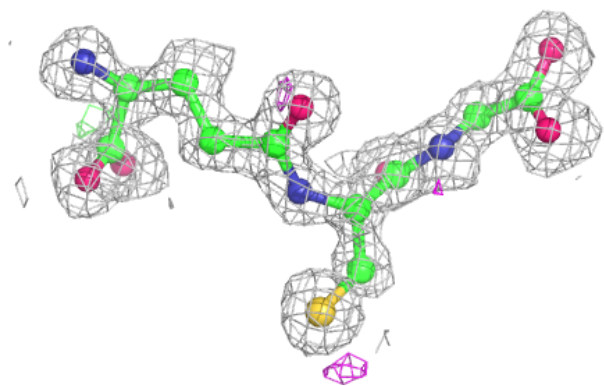
**Electron density around GSH C 301:**

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



Electron density around GSH 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.