



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 19, 2020 – 08:10 pm BST

PDB ID : 5ECR
Title : Crystal Structure of FIN219-FIP1 complex with JA, VAL and Mg
Authors : Chen, C.Y.; Cheng, Y.S.
Deposited on : 2015-10-20
Resolution : 1.72 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

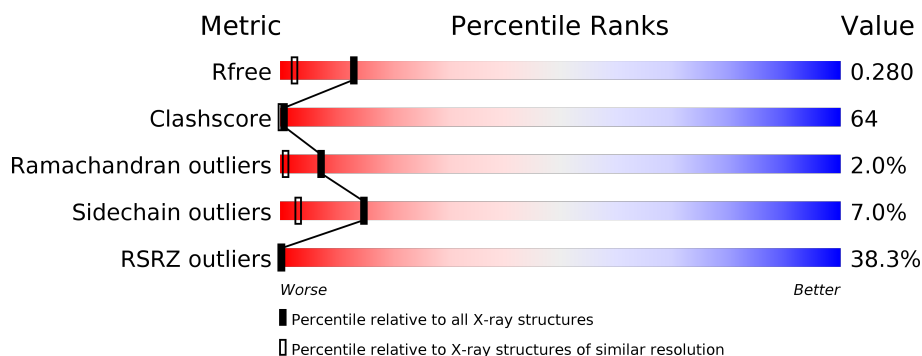
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.72 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	5722 (1.74-1.70)
Clashscore	141614	6152 (1.74-1.70)
Ramachandran outliers	138981	6051 (1.74-1.70)
Sidechain outliers	138945	6051 (1.74-1.70)
RSRZ outliers	127900	5629 (1.74-1.70)

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>52%</div> <div> <div>23%</div> <div>67%</div> <div>8%</div> <div>..</div> </div> </div>
1	D	575	<div> <div>41%</div> <div> <div>23%</div> <div>66%</div> <div>9%</div> <div>..</div> </div> </div>
2	B	223	<div> <div>26%</div> <div> <div>38%</div> <div>55%</div> <div>..</div> </div> </div>
2	C	223	<div> <div>22%</div> <div> <div>29%</div> <div>58%</div> <div>9%</div> <div>.</div> </div> </div>
2	E	223	<div> <div>33%</div> <div> <div>33%</div> <div>61%</div> <div>..</div> </div> </div>
2	F	223	<div> <div>22%</div> <div> <div>30%</div> <div>57%</div> <div>9%</div> <div>..</div> </div> </div>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	VAL	A	602	-	-	X	-

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 17885 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

There are 24 discrepancies between the modelled and reference sequences:

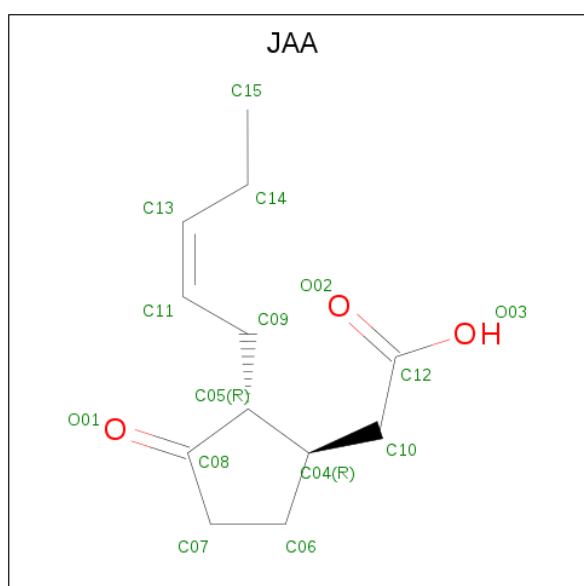
Chain	Residue	Modelled	Actual	Comment	Reference
B	-5	HIS	-	expression tag	UNP Q8L7C9
B	-4	HIS	-	expression tag	UNP Q8L7C9
B	-3	HIS	-	expression tag	UNP Q8L7C9
B	-2	HIS	-	expression tag	UNP Q8L7C9
B	-1	HIS	-	expression tag	UNP Q8L7C9
B	0	HIS	-	expression tag	UNP Q8L7C9
C	-5	HIS	-	expression tag	UNP Q8L7C9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

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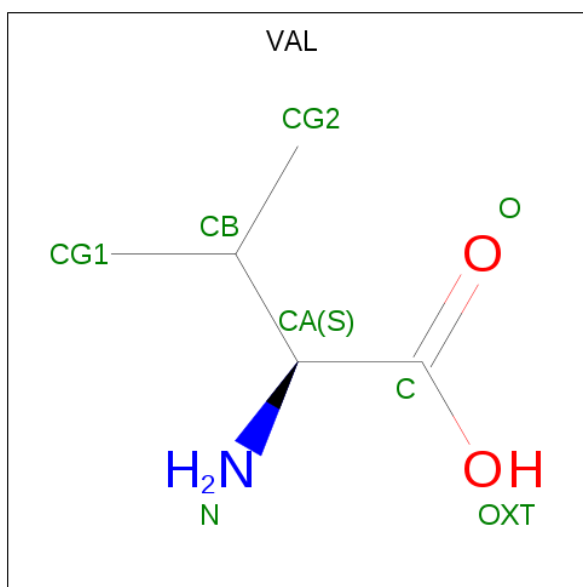
Chain	Residue	Modelled	Actual	Comment	Reference
E	-5	HIS	-	expression tag	UNP Q8L7C9
E	-4	HIS	-	expression tag	UNP Q8L7C9
E	-3	HIS	-	expression tag	UNP Q8L7C9
E	-2	HIS	-	expression tag	UNP Q8L7C9
E	-1	HIS	-	expression tag	UNP Q8L7C9
E	0	HIS	-	expression tag	UNP Q8L7C9
F	-5	HIS	-	expression tag	UNP Q8L7C9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

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



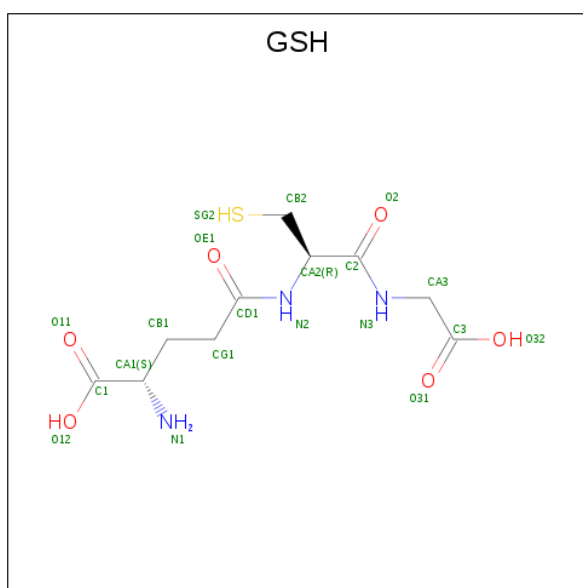
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			15	12	3		
3	D	1	Total	C	O	0	0
			15	12	3		

- Molecule 4 is VALINE (three-letter code: VAL) (formula: C₅H₁₁NO₂).



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

- Molecule 5 is GLUTATHIONE (three-letter code: GSH) (formula: C₁₀H₁₇N₃O₆S).



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

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

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	1	Total	Mg	0	0
			1	1		

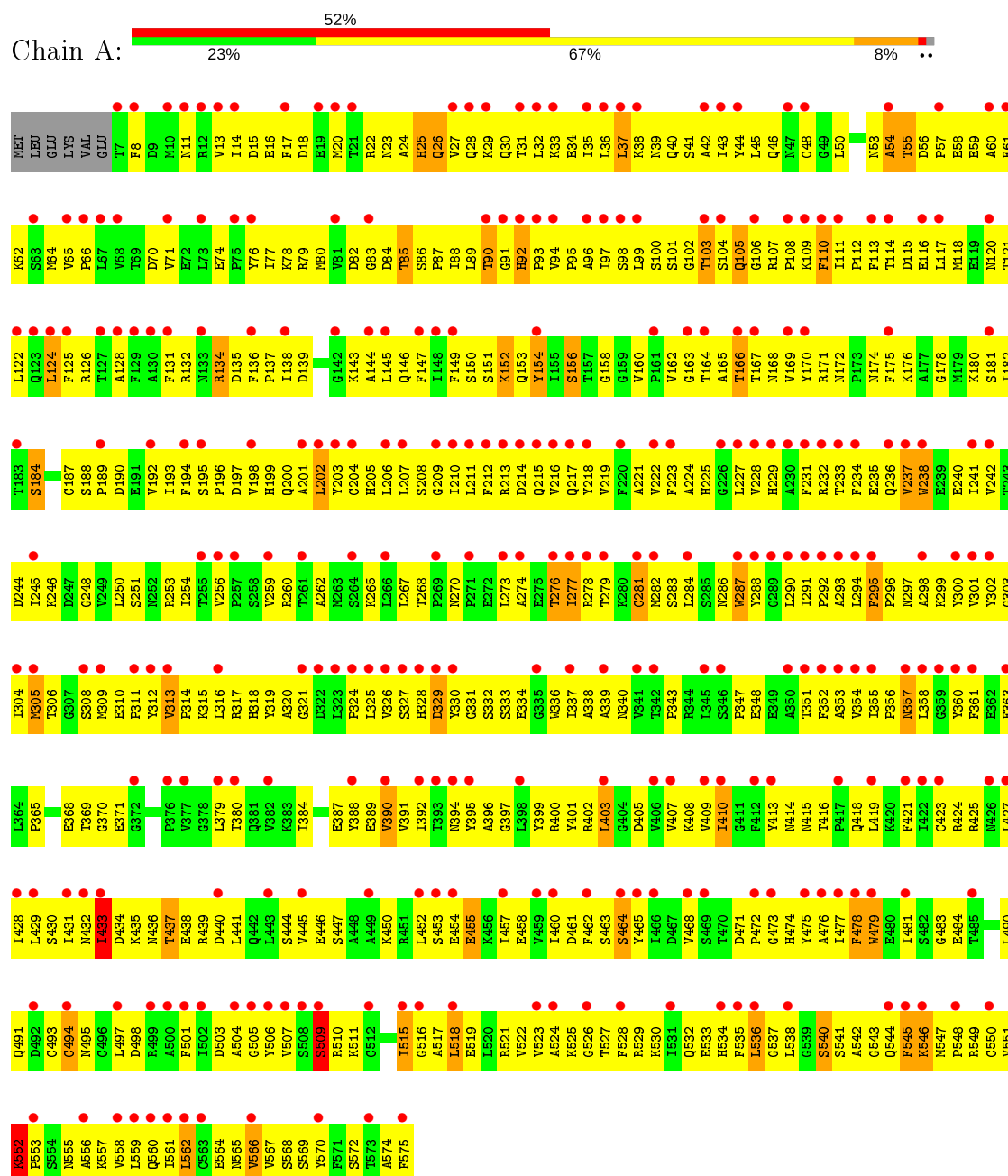
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	512	Total	O	0	0
			512	512		
7	B	203	Total	O	0	0
			203	203		
7	C	198	Total	O	0	0
			198	198		
7	D	510	Total	O	0	0
			510	510		
7	E	186	Total	O	0	0
			186	186		
7	F	199	Total	O	0	0
			199	199		

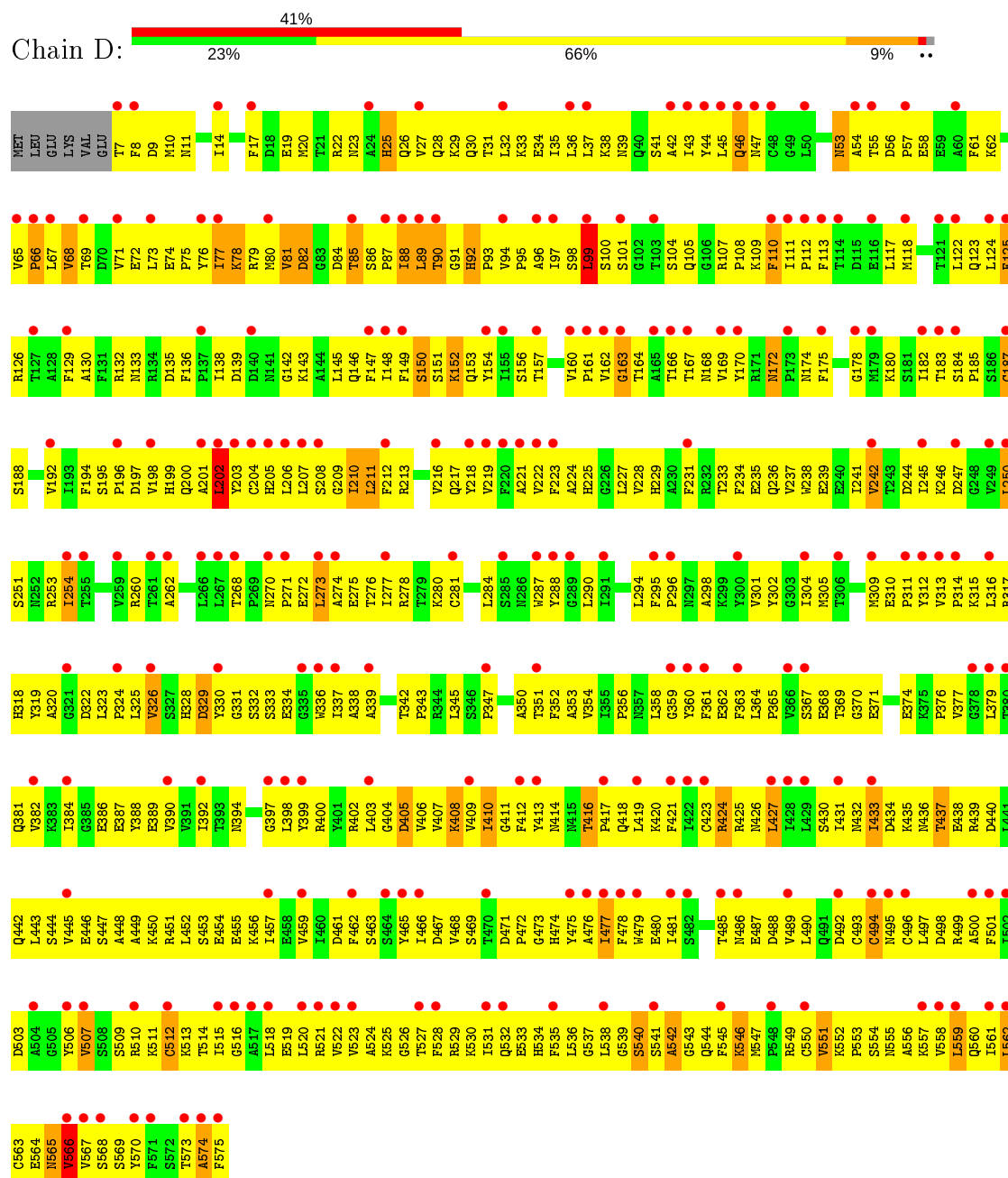
3 Residue-property plots

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.

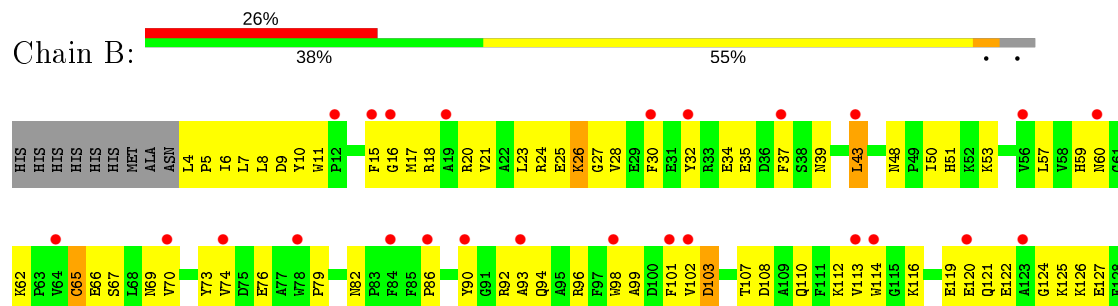
- Molecule 1: Jasmonic acid-amido synthetase JAR1

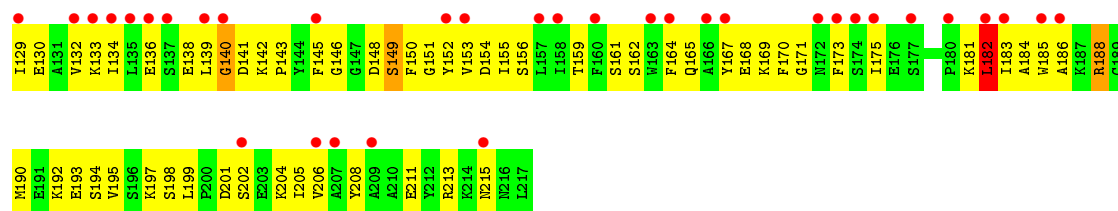


- Molecule 1: Jasmonic acid-amido synthetase JAR1

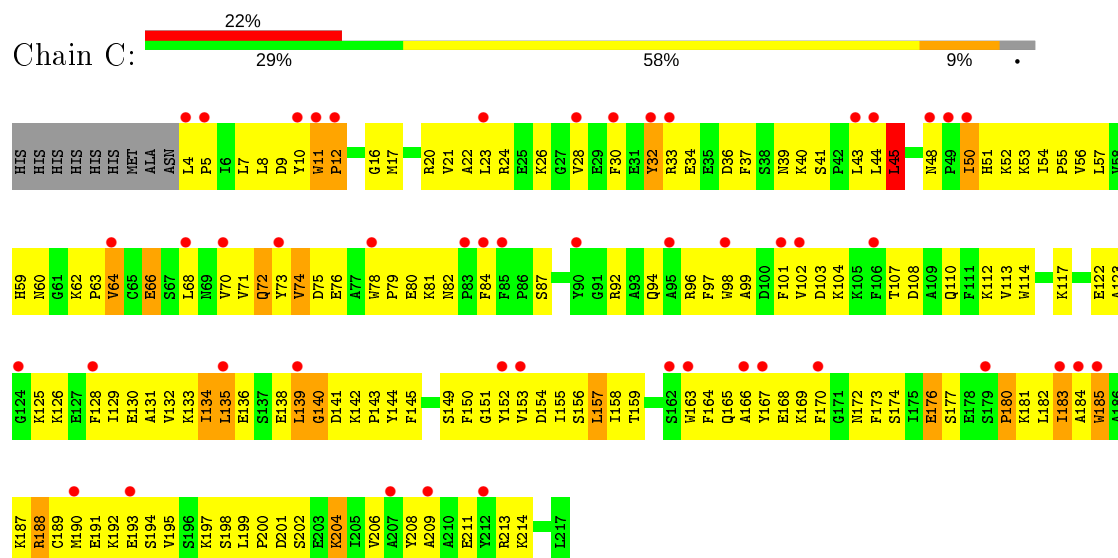


- Molecule 2: Glutathione S-transferase U20

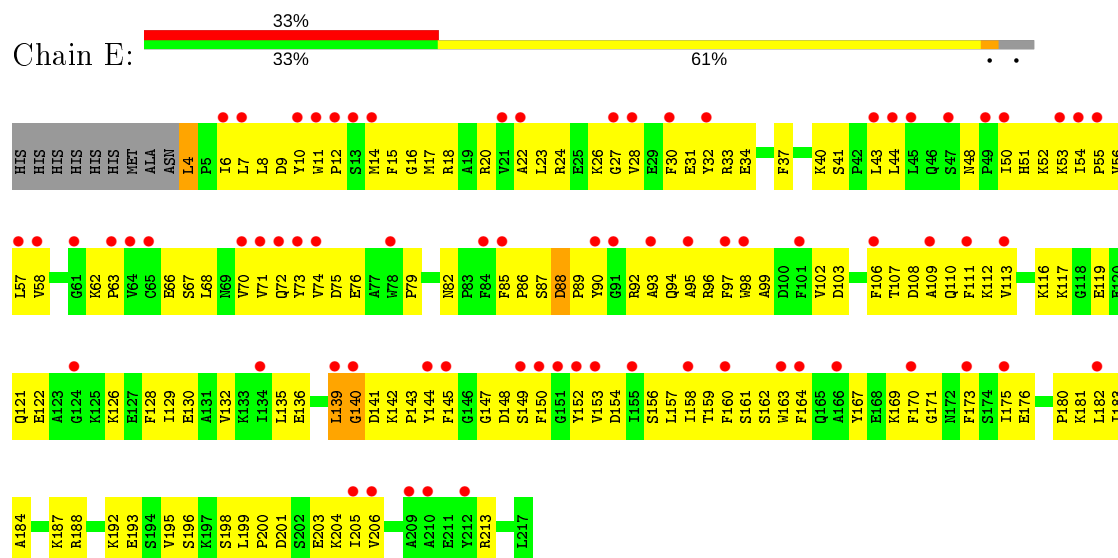




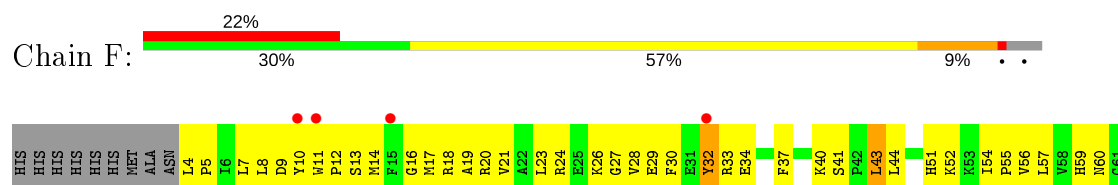
• Molecule 2: Glutathione S-transferase U20

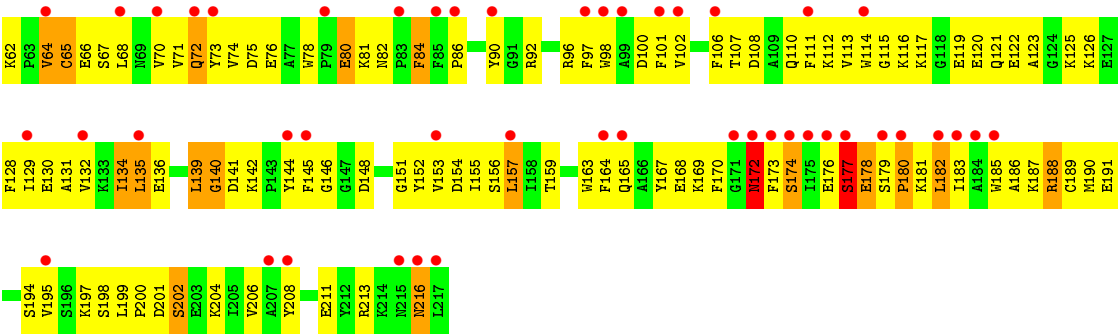


• Molecule 2: Glutathione S-transferase U20



• 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	53.84Å 53.85Å 193.64Å 90.03° 90.04° 113.41°	Depositor
Resolution (Å)	24.20 – 1.72 24.21 – 1.72	Depositor EDS
% Data completeness (in resolution range)	99.6 (24.20-1.72) 99.5 (24.21-1.72)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.05 (at 1.72Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.262 , 0.281 0.262 , 0.280	Depositor DCC
R_{free} test set	21132 reflections (10.01%)	wwPDB-VP
Wilson B-factor (Å ²)	10.3	Xtriage
Anisotropy	0.106	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 218.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.099 for -h,-k,l 0.088 for k,h,-l 0.097 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	17885	wwPDB-VP
Average B, all atoms (Å ²)	12.0	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 52.28 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.9763e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GSH, MG, 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	0.48	0/4581	0.79	6/6219 (0.1%)
1	D	0.48	0/4581	0.79	6/6219 (0.1%)
2	B	0.38	0/1799	0.58	1/2428 (0.0%)
2	C	0.47	0/1799	0.72	4/2428 (0.2%)
2	E	0.41	0/1799	0.63	0/2428
2	F	0.51	0/1799	0.73	1/2428 (0.0%)
All	All	0.46	0/16358	0.74	18/22150 (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	2
1	D	0	2
2	E	0	1
2	F	0	1
All	All	0	6

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	238	TRP	CA-CB-CG	7.72	128.38	113.70
2	C	188	ARG	NE-CZ-NH1	-7.70	116.45	120.30
2	C	188	ARG	NE-CZ-NH2	6.85	123.72	120.30
2	F	188	ARG	NE-CZ-NH1	-6.77	116.92	120.30
1	A	562	LEU	CA-CB-CG	6.47	130.18	115.30
1	D	559	LEU	CA-CB-CG	6.08	129.30	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	211	LEU	CA-CB-CG	6.01	129.12	115.30
1	D	562	LEU	CA-CB-CG	5.80	128.65	115.30
2	B	182	LEU	CA-CB-CG	5.60	128.18	115.30
1	A	552	LYS	C-N-CD	5.29	139.51	128.40
1	A	287	TRP	CA-CB-CG	-5.22	103.79	113.70
1	D	99	LEU	CA-CB-CG	5.19	127.24	115.30
1	D	202	LEU	CB-CG-CD1	5.17	119.79	111.00
2	C	45	LEU	CA-CB-CG	5.14	127.11	115.30
1	A	237	VAL	N-CA-C	5.13	124.85	111.00
1	A	124	LEU	CA-CB-CG	5.10	127.04	115.30
2	C	11	TRP	C-N-CD	5.08	139.06	128.40
1	D	163	GLY	N-CA-C	5.05	125.72	113.10

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	427	LEU	Peptide
1	A	431	ILE	Peptide
1	D	427	LEU	Peptide
1	D	565	ASN	Peptide
2	E	140	GLY	Peptide
2	F	177	SER	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4479	0	4434	704	6
1	D	4479	0	4434	630	5
2	B	1748	0	1704	195	1
2	C	1748	0	1704	243	2
2	E	1748	0	1704	181	0
2	F	1748	0	1704	209	1
3	A	15	0	0	4	0
3	D	15	0	0	2	0
4	A	8	0	8	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	8	0	8	2	0
5	B	20	0	15	4	0
5	C	20	0	15	1	0
5	E	20	0	15	1	0
5	F	20	0	15	3	0
6	D	1	0	0	0	0
7	A	512	0	0	129	4
7	B	203	0	0	28	4
7	C	198	0	0	61	3
7	D	510	0	0	105	4
7	E	186	0	0	26	1
7	F	199	0	0	47	1
All	All	17885	0	15760	2041	22

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

All (2041) 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:152:LYS:HZ1	1:A:530:LYS:NZ	1.21	1.34
1:A:152:LYS:NZ	1:A:530:LYS:HZ1	1.30	1.26
1:D:488:ASP:OD1	7:D:701:HOH:O	1.53	1.24
2:C:188:ARG:NH1	1:D:499:ARG:O	1.70	1.22
2:E:92:ARG:NH1	2:F:76:GLU:OE1	1.79	1.15
1:A:446:GLU:OE2	7:A:701:HOH:O	1.67	1.12
1:D:152:LYS:NZ	1:D:527:THR:OG1	1.81	1.12
2:C:188:ARG:HH12	1:D:500:ALA:HA	1.11	1.11
1:A:176:LYS:NZ	1:A:190:ASP:OD2	1.83	1.10
2:C:9:ASP:OD2	7:C:402:HOH:O	1.71	1.09
1:A:134:ARG:NH1	7:A:702:HOH:O	1.86	1.04
2:C:176:GLU:OE2	1:D:573:THR:OG1	1.76	1.04
2:E:139:LEU:HG	2:E:142:LYS:HB2	1.35	1.01
2:E:26:LYS:HZ3	2:E:74:VAL:HG22	1.24	1.00
1:D:143:LYS:HD2	1:D:212:PHE:HB2	1.44	1.00
1:A:106:GLY:HA3	1:A:432:ASN:HD21	1.27	0.99
1:A:510:ARG:NH1	1:A:516:GLY:O	1.94	0.98
1:A:166:THR:HG22	4:A:602:VAL:HG13	1.44	0.98
2:E:40:LYS:NZ	2:E:52:LYS:O	1.96	0.98
1:A:519:GLU:OE2	1:A:569:SER:OG	1.84	0.96
2:F:60:ASN:ND2	7:F:409:HOH:O	1.99	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:284:LEU:HD13	1:A:287:TRP:H	1.30	0.95
2:F:120:GLU:OE1	7:F:401:HOH:O	1.85	0.94
1:A:152:LYS:HA	1:A:564:GLU:HB2	1.49	0.94
2:B:26:LYS:NZ	2:B:82:ASN:H	1.64	0.94
2:C:184:ALA:HB1	1:D:499:ARG:CZ	1.98	0.93
1:A:491:GLN:OE1	7:A:703:HOH:O	1.87	0.93
1:D:254:ILE:O	1:D:260:ARG:NH1	2.01	0.93
1:A:510:ARG:NH1	1:A:515:ILE:HD12	1.84	0.93
2:C:66:GLU:OE2	7:C:405:HOH:O	1.87	0.92
2:C:92:ARG:NH1	7:C:414:HOH:O	2.03	0.92
2:F:190:MET:SD	7:F:436:HOH:O	2.26	0.92
1:A:39:ASN:ND2	2:B:141:ASP:O	2.01	0.92
1:A:199:HIS:HB3	1:A:525:LYS:H	1.32	0.92
1:D:452:LEU:HB3	1:D:457:ILE:HD11	1.49	0.92
1:A:93:PRO:HG3	2:B:184:ALA:HB3	1.52	0.91
2:C:188:ARG:NH1	1:D:500:ALA:HA	1.84	0.91
2:B:116:LYS:O	2:B:213:ARG:NH1	2.02	0.91
1:D:466:ILE:HB	1:D:552:LYS:HA	1.53	0.91
1:A:498:ASP:O	7:A:704:HOH:O	1.88	0.91
1:D:99:LEU:HB3	1:D:557:LYS:H	1.32	0.91
2:B:145:PHE:HB3	2:B:153:VAL:HG13	1.52	0.91
1:A:208:SER:HA	1:A:211:LEU:HD12	1.52	0.90
1:A:225:HIS:HA	1:A:228:VAL:HG22	1.54	0.90
2:C:136:GLU:HG3	2:C:181:LYS:HD3	1.54	0.90
1:A:475:TYR:H	1:A:510:ARG:HH22	1.15	0.89
1:A:165:ALA:H	1:A:557:LYS:NZ	1.70	0.89
2:F:122:GLU:OE2	7:F:403:HOH:O	1.89	0.89
1:A:165:ALA:H	1:A:557:LYS:HZ3	0.91	0.89
2:F:26:LYS:NZ	2:F:82:ASN:O	2.06	0.89
2:F:20:ARG:NH1	7:F:404:HOH:O	1.90	0.88
1:A:152:LYS:NZ	1:A:530:LYS:NZ	2.03	0.88
2:C:117:LYS:NZ	7:C:403:HOH:O	1.77	0.88
2:F:136:GLU:OE2	2:F:180:PRO:HD3	1.73	0.88
1:D:172:ASN:ND2	1:D:174:ASN:OD1	2.07	0.88
2:C:26:LYS:NZ	2:C:82:ASN:O	2.07	0.87
2:C:98:TRP:O	7:C:406:HOH:O	1.91	0.87
2:C:41:SER:N	7:C:415:HOH:O	2.03	0.87
1:A:402:ARG:NH1	7:A:726:HOH:O	2.08	0.87
1:A:100:SER:OG	1:A:334:GLU:OE2	1.92	0.86
2:C:176:GLU:OE1	7:D:701:HOH:O	1.93	0.86
1:D:123:GLN:NE2	7:D:713:HOH:O	2.06	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:ARG:NH1	7:A:731:HOH:O	2.09	0.86
1:A:164:THR:HG22	1:A:557:LYS:HD3	1.57	0.86
1:A:165:ALA:N	1:A:557:LYS:HZ3	1.73	0.86
1:A:22:ARG:HA	1:A:415:ASN:HB2	1.56	0.86
2:C:184:ALA:O	1:D:499:ARG:NH2	2.09	0.86
1:D:552:LYS:O	1:D:554:SER:N	2.09	0.86
1:D:309:MET:O	7:D:702:HOH:O	1.92	0.85
1:A:143:LYS:NZ	1:A:187:CYS:HB3	1.91	0.85
1:A:277:ILE:HG23	1:A:278:ARG:HG3	1.58	0.85
1:A:38:LYS:NZ	1:A:395:TYR:OH	2.10	0.85
2:C:168:GLU:OE1	7:C:407:HOH:O	1.93	0.85
1:D:152:LYS:HB2	1:D:561:ILE:HA	1.59	0.85
1:D:93:PRO:HG2	2:E:181:LYS:HA	1.58	0.85
2:F:26:LYS:HG2	2:F:81:LYS:NZ	1.92	0.84
2:F:197:LYS:O	7:F:405:HOH:O	1.94	0.84
1:D:337:ILE:HD13	1:D:539:GLY:HA3	1.59	0.84
2:F:132:VAL:HG23	2:F:182:LEU:HD13	1.57	0.84
1:A:143:LYS:HD3	1:A:212:PHE:HB2	1.59	0.84
1:A:551:VAL:HG11	1:A:559:LEU:HD11	1.60	0.84
1:A:143:LYS:HZ2	1:A:187:CYS:HB3	1.40	0.84
1:D:408:LYS:HG2	1:D:420:LYS:HG2	1.60	0.84
2:E:187:LYS:O	7:E:401:HOH:O	1.96	0.84
2:E:93:ALA:HB1	2:F:73:TYR:HE1	1.43	0.83
2:C:172:ASN:OD1	7:C:408:HOH:O	1.96	0.83
1:A:74:GLU:OE2	7:A:706:HOH:O	1.97	0.83
2:C:193:GLU:HG3	7:C:442:HOH:O	1.79	0.83
2:E:143:PRO:HB2	2:E:188:ARG:HH12	1.44	0.83
2:F:18:ARG:NH2	7:F:414:HOH:O	2.10	0.83
1:D:480:GLU:OE1	7:D:703:HOH:O	1.94	0.83
1:D:509:SER:O	1:D:513:LYS:N	2.10	0.83
1:A:103:THR:HB	1:A:106:GLY:HA2	1.61	0.83
2:E:143:PRO:HB2	2:E:188:ARG:NH1	1.93	0.83
2:C:26:LYS:HG2	2:C:81:LYS:NZ	1.93	0.83
2:F:120:GLU:O	7:F:406:HOH:O	1.97	0.82
1:A:20:MET:HG2	1:A:356:PRO:HG2	1.61	0.82
1:A:87:PRO:HB2	2:B:143:PRO:HA	1.60	0.82
1:D:199:HIS:HB3	1:D:525:LYS:H	1.43	0.82
1:D:405:ASP:HB2	1:D:541:SER:HB3	1.58	0.82
1:A:106:GLY:HA3	1:A:432:ASN:ND2	1.94	0.82
2:E:50:ILE:HG13	2:E:51:HIS:H	1.43	0.82
1:A:225:HIS:HB3	1:A:312:TYR:CE2	2.15	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:79:PRO:O	7:C:410:HOH:O	1.97	0.81
2:C:184:ALA:HB1	1:D:499:ARG:NH1	1.95	0.81
2:E:26:LYS:NZ	2:E:74:VAL:HG22	1.93	0.81
1:A:478:PHE:CZ	1:A:562:LEU:HA	2.15	0.81
1:D:305:MET:SD	7:D:1023:HOH:O	2.38	0.81
1:D:213:ARG:NE	1:D:294:LEU:O	2.12	0.81
2:C:28:VAL:O	7:C:409:HOH:O	1.97	0.81
1:A:138:ILE:HD12	1:A:217:GLN:HB2	1.61	0.81
1:A:45:LEU:HD22	1:A:50:LEU:HD12	1.62	0.81
2:F:156:SER:OG	7:F:402:HOH:O	1.85	0.81
1:D:199:HIS:H	1:D:524:ALA:HB1	1.44	0.81
1:D:42:ALA:HA	2:E:143:PRO:HG3	1.62	0.81
1:D:239:GLU:OE2	7:D:704:HOH:O	1.98	0.81
1:D:499:ARG:HB2	1:D:499:ARG:CZ	2.08	0.80
1:D:531:ILE:HA	1:D:534:HIS:CE1	2.15	0.80
2:F:72:GLN:OE1	7:F:407:HOH:O	1.99	0.80
1:A:551:VAL:HG13	1:A:555:ASN:HB3	1.63	0.80
1:A:424:ARG:NH1	7:A:747:HOH:O	2.15	0.80
1:A:18:ASP:OD1	1:A:414:ASN:ND2	2.14	0.80
2:F:178:GLU:O	7:F:410:HOH:O	2.00	0.80
1:D:150:SER:HB2	1:D:167:THR:HA	1.61	0.80
1:D:87:PRO:HG2	2:E:188:ARG:HD2	1.64	0.80
2:B:24:ARG:HH12	2:B:197:LYS:HE3	1.47	0.79
1:A:198:VAL:HA	1:A:201:ALA:HB3	1.63	0.79
1:A:458:GLU:O	7:A:708:HOH:O	2.01	0.79
2:B:136:GLU:OE2	7:B:401:HOH:O	1.99	0.79
1:D:329:ASP:HB3	1:D:339:ALA:HA	1.62	0.79
1:D:432:ASN:ND2	7:D:735:HOH:O	2.15	0.79
2:C:132:VAL:HG23	2:C:182:LEU:HD13	1.63	0.79
2:C:9:ASP:OD1	7:C:412:HOH:O	2.00	0.79
1:D:145:LEU:HD13	1:D:209:GLY:HA3	1.65	0.79
1:D:445:VAL:HG22	1:D:479:TRP:HE1	1.47	0.79
2:B:145:PHE:HB2	2:B:154:ASP:HB3	1.64	0.79
1:A:145:LEU:HD13	1:A:209:GLY:HA3	1.65	0.79
1:A:306:THR:OG1	1:A:330:TYR:OH	2.01	0.78
1:A:62:LYS:HG2	1:A:400:ARG:NH1	1.99	0.78
1:A:117:LEU:HD11	1:A:333:SER:HA	1.65	0.78
1:D:138:ILE:HB	1:D:217:GLN:HG3	1.64	0.78
1:A:304:ILE:HG13	1:A:328:HIS:HB3	1.65	0.78
1:A:236:GLN:OE1	7:A:710:HOH:O	2.02	0.78
2:B:215:ASN:ND2	7:B:405:HOH:O	2.08	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:152:LYS:HD3	1:D:561:ILE:HG23	1.64	0.78
1:D:44:TYR:HB2	1:D:89:LEU:HG	1.66	0.78
2:B:76:GLU:OE1	7:C:404:HOH:O	2.01	0.78
1:D:268:THR:O	7:D:705:HOH:O	2.02	0.78
1:D:322:ASP:O	7:D:706:HOH:O	2.02	0.78
1:D:442:GLN:HG2	1:D:462:PHE:HZ	1.48	0.78
1:A:150:SER:OG	7:A:709:HOH:O	2.02	0.78
1:A:452:LEU:HD23	1:A:481:ILE:HG12	1.64	0.78
1:A:425:ARG:NH2	7:A:734:HOH:O	2.09	0.78
1:A:332:SER:HG	1:A:534:HIS:HE2	1.32	0.78
1:A:465:TYR:HA	1:A:551:VAL:HB	1.66	0.78
1:D:495:ASN:C	1:D:499:ARG:HH12	1.87	0.77
1:A:224:ALA:HA	1:A:227:LEU:HD12	1.64	0.77
1:A:501:PHE:HB2	1:A:506:TYR:CZ	2.19	0.77
1:A:152:LYS:CE	1:A:530:LYS:HZ1	1.97	0.77
1:D:418:GLN:OE1	7:D:707:HOH:O	2.02	0.77
2:E:40:LYS:NZ	2:E:52:LYS:HB2	1.98	0.77
1:A:464:SER:HG	1:A:550:CYS:HG	1.07	0.77
1:D:99:LEU:HD23	1:D:558:VAL:H	1.49	0.77
1:D:495:ASN:C	1:D:499:ARG:NH1	2.37	0.77
2:B:18:ARG:HD3	2:B:156:SER:HA	1.65	0.77
1:A:413:TYR:OH	7:A:707:HOH:O	1.97	0.77
1:A:527:THR:HG23	1:A:561:ILE:HG21	1.65	0.77
2:F:119:GLU:O	7:F:411:HOH:O	2.03	0.77
1:A:152:LYS:HD2	1:A:561:ILE:HG23	1.65	0.76
2:B:201:ASP:O	7:B:402:HOH:O	2.02	0.76
1:D:439:ARG:NH1	7:D:741:HOH:O	2.17	0.76
2:F:164:PHE:HD2	2:F:183:ILE:HD13	1.49	0.76
1:A:143:LYS:HZ2	1:A:209:GLY:HA2	1.50	0.76
1:A:92:HIS:HE1	2:B:185:TRP:HZ2	1.34	0.76
1:D:198:VAL:HG22	1:D:565:ASN:HD22	1.48	0.76
2:E:70:VAL:HA	2:E:73:TYR:CE2	2.21	0.76
1:A:454:GLU:OE1	7:A:711:HOH:O	2.03	0.76
2:F:8:LEU:HD22	2:F:33:ARG:HH21	1.50	0.76
1:A:340:ASN:OD1	7:A:714:HOH:O	2.04	0.76
2:E:93:ALA:HB1	2:F:73:TYR:CE1	2.21	0.75
1:A:555:ASN:N	7:A:718:HOH:O	2.20	0.75
1:D:389:GLU:OE2	1:D:404:GLY:HA2	1.87	0.75
1:A:238:TRP:HA	1:A:241:ILE:HB	1.69	0.75
1:A:340:ASN:ND2	7:A:755:HOH:O	2.18	0.75
2:C:164:PHE:HD2	2:C:183:ILE:HD12	1.52	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:201:ASP:OD2	1:D:456:LYS:NZ	2.18	0.75
1:A:146:GLN:NE2	7:A:758:HOH:O	2.19	0.75
2:F:56:VAL:HG13	7:F:426:HOH:O	1.85	0.75
2:E:122:GLU:OE2	7:E:402:HOH:O	2.05	0.75
2:B:96:ARG:HH11	2:C:73:TYR:HE1	1.32	0.74
2:F:8:LEU:HD21	2:F:43:LEU:HD11	1.68	0.74
1:A:152:LYS:HG3	1:A:561:ILE:HA	1.69	0.74
2:F:62:LYS:NZ	7:F:408:HOH:O	1.99	0.74
1:D:310:GLU:HG2	1:D:311:PRO:HD3	1.69	0.74
1:A:305:MET:HE3	1:A:347:PRO:HG3	1.69	0.74
2:B:96:ARG:NH1	2:C:73:TYR:CE1	2.54	0.74
1:D:211:LEU:O	7:D:712:HOH:O	2.06	0.74
2:C:64:VAL:HG23	2:C:70:VAL:HG22	1.69	0.74
1:D:246:LYS:HE2	1:D:271:PRO:HA	1.69	0.74
1:A:108:PRO:HB3	1:A:555:ASN:HB2	1.69	0.74
1:A:558:VAL:O	7:A:713:HOH:O	2.04	0.74
2:C:80:GLU:OE2	7:C:417:HOH:O	2.06	0.74
1:D:146:GLN:NE2	7:D:743:HOH:O	2.17	0.74
1:A:361:PHE:O	7:A:712:HOH:O	2.04	0.74
1:A:552:LYS:O	7:A:718:HOH:O	2.06	0.74
2:C:33:ARG:NE	7:C:422:HOH:O	2.12	0.74
1:A:331:GLY:HA2	7:A:764:HOH:O	1.87	0.74
1:A:143:LYS:NZ	1:A:209:GLY:HA2	2.02	0.74
1:D:87:PRO:HB2	2:E:143:PRO:HA	1.69	0.73
1:A:301:VAL:HG11	1:A:316:LEU:HD21	1.69	0.73
1:A:401:TYR:HE2	1:A:403:LEU:HD13	1.52	0.73
1:A:79:ARG:HH22	2:B:188:ARG:NH1	1.85	0.73
2:F:180:PRO:HD2	2:F:181:LYS:HG2	1.68	0.73
1:A:397:GLY:O	7:A:721:HOH:O	2.06	0.73
1:A:548:PRO:O	7:A:716:HOH:O	2.05	0.73
2:C:64:VAL:HB	2:C:73:TYR:CD2	2.22	0.73
1:D:143:LYS:HD3	1:D:187:CYS:HB3	1.71	0.73
1:D:9:ASP:O	7:D:710:HOH:O	2.05	0.73
1:A:479:TRP:NE1	7:A:762:HOH:O	2.20	0.73
1:A:132:ARG:NH1	7:A:754:HOH:O	2.22	0.73
1:A:337:ILE:N	7:A:764:HOH:O	2.21	0.73
2:C:142:LYS:NZ	7:C:401:HOH:O	1.60	0.73
1:D:477:ILE:HG13	1:D:520:LEU:HA	1.71	0.73
1:D:164:THR:OG1	1:D:557:LYS:O	2.07	0.73
1:A:304:ILE:O	7:A:715:HOH:O	2.05	0.73
1:A:304:ILE:O	7:A:722:HOH:O	2.06	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:494:CYS:HA	1:A:497:LEU:HD12	1.69	0.73
2:C:26:LYS:HD2	2:C:74:VAL:HG13	1.70	0.73
2:C:33:ARG:HH22	2:C:43:LEU:HD11	1.53	0.73
2:E:92:ARG:HH12	2:F:76:GLU:CD	1.90	0.73
2:C:191:GLU:OE1	1:D:447:SER:OG	2.07	0.73
2:B:24:ARG:NE	2:B:198:SER:OG	2.20	0.73
2:C:211:GLU:OE1	7:C:418:HOH:O	2.06	0.73
1:A:138:ILE:HG13	1:A:217:GLN:OE1	1.88	0.73
1:A:351:THR:HG21	1:A:410:ILE:HG12	1.71	0.73
2:E:89:PRO:HB3	2:F:76:GLU:HG3	1.71	0.73
2:F:136:GLU:HG3	2:F:181:LYS:HD3	1.71	0.73
1:A:284:LEU:HD22	1:A:287:TRP:HA	1.71	0.72
1:A:529:ARG:NH1	7:A:767:HOH:O	2.22	0.72
1:D:236:GLN:NE2	7:D:748:HOH:O	2.18	0.72
1:D:423:CYS:SG	1:D:541:SER:OG	2.46	0.72
2:B:50:ILE:HG13	2:C:134:ILE:HD12	1.72	0.72
2:F:122:GLU:HA	2:F:125:LYS:HE2	1.69	0.72
2:F:98:TRP:HE3	2:F:101:PHE:HB2	1.54	0.72
1:A:329:ASP:OD1	7:A:717:HOH:O	2.06	0.72
1:A:64:MET:O	7:A:723:HOH:O	2.06	0.72
1:D:426:ASN:ND2	7:D:758:HOH:O	2.21	0.72
2:F:168:GLU:OE2	2:F:176:GLU:OE2	2.06	0.72
1:A:223:PHE:CZ	1:A:536:LEU:HB2	2.24	0.72
1:A:150:SER:O	1:A:171:ARG:NH1	2.23	0.72
1:A:337:ILE:HG12	1:A:361:PHE:CZ	2.24	0.72
2:B:92:ARG:NH2	2:C:76:GLU:OE1	2.22	0.72
1:D:524:ALA:HB2	1:D:567:VAL:HG11	1.71	0.72
2:E:20:ARG:HB3	2:E:24:ARG:NH1	2.04	0.72
1:A:446:GLU:OE2	7:A:728:HOH:O	2.08	0.72
1:D:518:LEU:O	7:D:715:HOH:O	2.08	0.71
1:D:534:HIS:O	7:D:714:HOH:O	2.07	0.71
1:A:331:GLY:HA3	1:A:336:TRP:CE3	2.25	0.71
2:C:189:CYS:HB3	7:C:432:HOH:O	1.89	0.71
1:A:295:PHE:O	7:A:725:HOH:O	2.07	0.71
1:D:152:LYS:HE3	1:D:565:ASN:HB2	1.71	0.71
1:D:198:VAL:HA	1:D:201:ALA:HB3	1.72	0.71
2:B:119:GLU:OE2	7:B:404:HOH:O	2.08	0.71
5:B:301:GSH:O31	7:B:407:HOH:O	2.09	0.71
1:A:139:ASP:O	7:A:727:HOH:O	2.08	0.71
1:A:244:ASP:OD2	7:A:724:HOH:O	2.07	0.71
2:F:117:LYS:HE3	2:F:213:ARG:NH1	2.06	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199:HIS:N	1:A:524:ALA:HB1	2.05	0.71
2:C:26:LYS:HG2	2:C:81:LYS:HZ1	1.52	0.71
1:D:208:SER:O	7:D:716:HOH:O	2.08	0.71
1:A:199:HIS:H	1:A:524:ALA:HB1	1.56	0.70
1:D:301:VAL:HG11	1:D:316:LEU:HD21	1.71	0.70
2:F:176:GLU:O	2:F:180:PRO:HB3	1.91	0.70
2:C:187:LYS:NZ	1:D:496:CYS:HB2	2.06	0.70
2:C:4:LEU:N	7:C:427:HOH:O	2.23	0.70
1:D:10:MET:SD	7:D:754:HOH:O	2.48	0.70
1:D:37:LEU:O	7:D:717:HOH:O	2.08	0.70
2:B:103:ASP:O	7:B:406:HOH:O	2.09	0.70
2:C:139:LEU:HD23	7:C:430:HOH:O	1.90	0.70
1:A:331:GLY:N	1:A:537:GLY:O	2.25	0.70
2:B:24:ARG:NH2	2:B:193:GLU:O	2.25	0.70
1:D:496:CYS:HA	1:D:499:ARG:NH2	2.06	0.70
2:F:75:ASP:HB2	2:F:84:PHE:CE2	2.25	0.70
1:A:332:SER:OG	1:A:333:SER:N	2.23	0.70
1:D:108:PRO:HG2	1:D:552:LYS:H	1.57	0.70
1:A:97:ILE:O	7:A:732:HOH:O	2.09	0.70
2:C:7:LEU:HD21	2:C:23:LEU:HD12	1.74	0.70
1:D:199:HIS:O	7:D:718:HOH:O	2.09	0.70
2:E:201:ASP:O	7:E:404:HOH:O	2.09	0.70
1:D:32:LEU:HA	1:D:35:ILE:HD12	1.72	0.70
1:D:406:VAL:O	1:D:541:SER:OG	2.10	0.70
2:F:98:TRP:CE3	2:F:101:PHE:HB2	2.26	0.70
1:A:246:LYS:NZ	1:A:278:ARG:HH22	1.89	0.70
1:A:181:SER:O	7:A:730:HOH:O	2.08	0.70
1:D:53:ASN:N	2:E:90:TYR:OH	2.24	0.70
1:D:549:ARG:NH1	7:D:726:HOH:O	2.24	0.70
1:A:354:VAL:HG21	1:A:379:LEU:HD21	1.73	0.70
1:A:494:CYS:SG	7:A:703:HOH:O	2.50	0.70
1:A:16:GLU:OE2	7:A:733:HOH:O	2.09	0.69
2:C:139:LEU:HG	2:C:145:PHE:CZ	2.27	0.69
2:C:33:ARG:NH2	2:C:43:LEU:HD21	2.07	0.69
1:D:389:GLU:OE2	1:D:402:ARG:NE	2.25	0.69
1:A:166:THR:OG1	1:A:167:THR:N	2.24	0.69
2:B:20:ARG:HD3	2:B:198:SER:HB3	1.73	0.69
1:D:109:LYS:O	7:D:719:HOH:O	2.09	0.69
1:D:451:ARG:NH1	1:D:454:GLU:OE2	2.25	0.69
1:A:118:MET:SD	7:A:810:HOH:O	2.50	0.69
2:B:18:ARG:NH2	2:B:67:SER:OG	2.25	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:116:LYS:O	2:E:213:ARG:NH1	2.25	0.69
1:A:39:ASN:HA	2:B:142:LYS:HG3	1.73	0.69
2:C:188:ARG:HD2	2:C:191:GLU:OE2	1.92	0.69
2:E:176:GLU:OE2	7:E:405:HOH:O	2.10	0.69
2:B:182:LEU:HD13	2:B:185:TRP:CZ3	2.27	0.69
1:A:464:SER:HB2	1:A:477:ILE:HD13	1.74	0.69
1:A:53:ASN:OD1	1:A:54:ALA:N	2.24	0.69
2:B:18:ARG:HD2	2:B:155:ILE:HD12	1.74	0.69
1:D:549:ARG:NH2	7:D:769:HOH:O	2.26	0.69
2:F:11:TRP:CD1	2:F:12:PRO:HD3	2.28	0.69
2:F:139:LEU:HG	2:F:145:PHE:CZ	2.27	0.69
1:A:407:VAL:HG22	1:A:541:SER:HB2	1.75	0.69
1:A:22:ARG:NH1	7:A:779:HOH:O	2.25	0.69
2:C:101:PHE:O	7:C:419:HOH:O	2.09	0.69
1:A:109:LYS:HE2	1:A:111:ILE:HD11	1.73	0.69
1:D:332:SER:OG	1:D:333:SER:N	2.26	0.69
2:E:180:PRO:HD2	2:E:181:LYS:HG3	1.74	0.69
1:A:483:GLY:O	7:A:736:HOH:O	2.11	0.69
2:C:144:TYR:HB3	2:C:154:ASP:OD2	1.93	0.69
1:D:107:ARG:NH2	1:D:552:LYS:HB3	2.08	0.69
1:D:514:THR:O	7:D:724:HOH:O	2.11	0.69
2:E:119:GLU:OE2	7:E:406:HOH:O	2.11	0.69
1:D:38:LYS:HB3	2:E:140:GLY:HA3	1.74	0.69
1:A:224:ALA:HB1	1:A:316:LEU:HD22	1.75	0.68
3:A:601:JAA:O02	7:A:737:HOH:O	2.11	0.68
1:A:99:LEU:HB3	1:A:557:LYS:HB2	1.75	0.68
1:D:54:ALA:O	7:D:721:HOH:O	2.10	0.68
1:D:487:GLU:HG2	1:D:570:TYR:CZ	2.29	0.68
1:D:495:ASN:HB3	1:D:499:ARG:NH1	2.07	0.68
2:E:159:THR:HA	2:E:199:LEU:HD21	1.74	0.68
2:F:30:PHE:O	7:F:413:HOH:O	2.10	0.68
1:A:38:LYS:HZ2	1:A:395:TYR:HE1	1.40	0.68
2:F:64:VAL:N	7:F:426:HOH:O	2.27	0.68
1:A:184:SER:HB2	1:A:217:GLN:NE2	2.09	0.68
1:A:202:LEU:HD21	1:A:529:ARG:HH22	1.57	0.68
2:B:142:LYS:NZ	2:B:145:PHE:O	2.19	0.68
1:D:461:ASP:OD1	7:D:723:HOH:O	2.11	0.68
1:D:77:ILE:CG1	1:D:110:PHE:HB3	2.24	0.68
2:E:40:LYS:HZ1	2:E:52:LYS:HB2	1.55	0.68
2:E:66:GLU:OE2	7:E:408:HOH:O	2.12	0.68
1:A:552:LYS:HG3	1:A:553:PRO:HD2	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:560:GLN:OE1	7:A:735:HOH:O	2.10	0.68
1:D:147:PHE:CE1	1:D:202:LEU:HD13	2.28	0.68
1:D:245:ILE:O	7:D:705:HOH:O	2.10	0.68
2:F:119:GLU:OE2	7:F:416:HOH:O	2.12	0.68
1:A:560:GLN:HB3	7:A:784:HOH:O	1.94	0.68
2:C:59:HIS:O	7:C:421:HOH:O	2.12	0.68
1:D:81:VAL:HG11	1:D:110:PHE:CE2	2.29	0.68
1:D:81:VAL:O	7:D:709:HOH:O	2.11	0.68
1:A:168:ASN:O	1:A:172:ASN:HB2	1.94	0.68
1:A:30:GLN:HA	1:A:33:LYS:HG2	1.75	0.68
1:D:104:SER:HB2	1:D:109:LYS:HB2	1.75	0.68
1:A:171:ARG:O	7:A:738:HOH:O	2.12	0.68
2:B:113:VAL:O	7:B:408:HOH:O	2.11	0.68
1:D:125:PHE:HE2	1:D:328:HIS:CE1	2.12	0.68
1:D:125:PHE:HE2	1:D:328:HIS:HE1	1.41	0.68
1:D:22:ARG:HH11	1:D:414:ASN:CG	1.96	0.68
1:D:199:HIS:N	1:D:524:ALA:HB1	2.08	0.68
2:C:104:LYS:NZ	7:C:413:HOH:O	2.02	0.67
1:D:56:ASP:OD2	7:D:722:HOH:O	2.11	0.67
2:F:106:PHE:O	7:F:417:HOH:O	2.12	0.67
1:A:231:PHE:O	1:A:235:GLU:HB3	1.93	0.67
1:A:399:TYR:O	7:A:740:HOH:O	2.12	0.67
1:A:445:VAL:HG21	1:A:462:PHE:CG	2.29	0.67
1:D:183:THR:O	7:D:729:HOH:O	2.12	0.67
1:D:143:LYS:HG2	1:D:216:VAL:HG22	1.76	0.67
1:A:339:ALA:HB2	1:A:355:ILE:HD11	1.77	0.67
1:D:66:PRO:O	7:D:728:HOH:O	2.12	0.67
1:A:435:LYS:HE3	1:A:438:GLU:HB3	1.76	0.67
1:A:440:ASP:O	7:A:705:HOH:O	2.12	0.67
1:A:445:VAL:HG13	1:A:479:TRP:HE1	1.59	0.67
1:A:96:ALA:HA	1:A:162:VAL:HA	1.77	0.67
1:D:210:ILE:HA	1:D:213:ARG:HG3	1.76	0.67
2:F:26:LYS:O	7:F:415:HOH:O	2.11	0.67
2:F:81:LYS:N	7:F:423:HOH:O	2.22	0.67
1:A:86:SER:HB2	2:B:188:ARG:HE	1.60	0.67
2:B:82:ASN:OD1	7:B:409:HOH:O	2.12	0.67
2:C:11:TRP:CD1	2:C:12:PRO:HD3	2.30	0.67
1:D:336:TRP:HB2	1:D:358:LEU:HD13	1.77	0.67
1:D:519:GLU:OE2	1:D:569:SER:OG	2.06	0.67
1:D:542:ALA:O	7:D:725:HOH:O	2.11	0.67
1:A:300:TYR:HA	7:A:741:HOH:O	1.93	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:340:ASN:HB2	1:A:352:PHE:CD2	2.30	0.67
1:A:423:CYS:HB3	1:A:542:ALA:HB3	1.75	0.67
2:C:68:LEU:HA	2:C:71:VAL:HG12	1.76	0.67
1:D:490:LEU:HD22	1:D:522:VAL:HG21	1.77	0.67
2:B:154:ASP:OD1	2:B:155:ILE:N	2.27	0.67
2:E:31:GLU:OE2	7:E:407:HOH:O	2.12	0.67
2:F:136:GLU:OE2	2:F:180:PRO:CD	2.43	0.67
2:C:22:ALA:HA	2:C:155:ILE:HD13	1.76	0.66
2:C:57:LEU:O	7:C:420:HOH:O	2.11	0.66
1:D:154:TYR:HD2	1:D:559:LEU:HD13	1.60	0.66
1:D:87:PRO:HD2	2:E:188:ARG:HB2	1.77	0.66
2:F:211:GLU:HG3	7:F:456:HOH:O	1.93	0.66
2:B:51:HIS:CD2	2:B:53:LYS:HE2	2.30	0.66
2:F:98:TRP:CD1	2:F:153:VAL:HG11	2.30	0.66
1:A:353:ALA:HB2	1:A:413:TYR:HD2	1.59	0.66
1:A:109:LYS:NZ	1:A:401:TYR:CZ	2.64	0.66
1:A:474:HIS:HA	1:A:510:ARG:HH12	1.59	0.66
2:C:187:LYS:HG2	1:D:451:ARG:HD3	1.76	0.66
2:F:114:TRP:CD1	2:F:167:TYR:HE1	2.13	0.66
2:F:165:GLN:HG2	2:F:206:VAL:HG21	1.77	0.66
1:D:353:ALA:HB2	1:D:413:TYR:CD2	2.30	0.66
1:A:103:THR:HB	1:A:106:GLY:CA	2.24	0.66
1:A:329:ASP:OD1	1:A:330:TYR:N	2.28	0.66
1:A:92:HIS:CE1	2:B:185:TRP:HZ2	2.13	0.66
2:C:23:LEU:HD22	2:C:28:VAL:HG11	1.78	0.66
1:A:128:ALA:HA	1:A:131:PHE:CE2	2.30	0.66
2:C:151:GLY:O	7:C:424:HOH:O	2.13	0.66
2:C:84:PHE:CD1	2:C:152:TYR:HB2	2.30	0.66
1:D:386:GLU:OE1	1:D:387:GLU:N	2.28	0.66
2:E:169:LYS:HZ2	2:E:206:VAL:HG21	1.60	0.66
2:F:163:TRP:HB3	2:F:167:TYR:CZ	2.31	0.66
2:F:24:ARG:HB3	2:F:194:SER:HA	1.78	0.66
2:F:7:LEU:HD21	2:F:23:LEU:HD12	1.78	0.66
1:A:324:PRO:O	7:A:741:HOH:O	2.12	0.66
1:A:424:ARG:HD2	1:A:425:ARG:NH1	2.11	0.66
1:D:105:GLN:HA	1:D:430:SER:HB3	1.76	0.66
2:C:187:LYS:HD3	1:D:492:ASP:HB3	1.78	0.66
1:D:147:PHE:CD2	1:D:529:ARG:NH1	2.63	0.65
1:D:205:HIS:O	7:D:727:HOH:O	2.12	0.65
2:E:57:LEU:HB3	2:E:73:TYR:OH	1.97	0.65
1:A:402:ARG:NH2	7:A:798:HOH:O	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:75:ASP:HB2	2:C:84:PHE:CE2	2.30	0.65
1:D:195:SER:OG	1:D:197:ASP:OD1	2.14	0.65
2:F:26:LYS:HG2	2:F:81:LYS:HZ3	1.61	0.65
1:A:458:GLU:OE2	7:A:744:HOH:O	2.13	0.65
1:D:168:ASN:O	1:D:172:ASN:HB3	1.96	0.65
1:D:313:VAL:HG23	1:D:325:LEU:HD12	1.79	0.65
2:E:92:ARG:NH1	2:F:76:GLU:CD	2.49	0.65
2:F:23:LEU:HD22	2:F:28:VAL:HG11	1.78	0.65
1:D:241:ILE:O	1:D:245:ILE:HG12	1.97	0.65
2:E:159:THR:HG22	2:E:199:LEU:HD11	1.78	0.65
5:F:301:GSH:N1	7:F:430:HOH:O	2.30	0.65
1:A:421:PHE:CD1	1:A:541:SER:HA	2.32	0.65
2:C:166:ALA:HB3	7:C:484:HOH:O	1.95	0.65
2:C:40:LYS:HB3	2:C:44:LEU:HD23	1.78	0.65
1:D:23:ASN:OD1	1:D:26:GLN:HB3	1.96	0.65
2:F:153:VAL:O	2:F:157:LEU:HD23	1.96	0.65
1:A:94:VAL:HG21	1:A:112:PRO:HA	1.79	0.65
1:A:41:SER:HA	2:B:148:ASP:HA	1.78	0.65
2:B:132:VAL:O	2:B:136:GLU:HG2	1.97	0.65
1:D:314:PRO:HB3	1:D:317:ARG:HH12	1.61	0.65
2:F:122:GLU:HG3	7:F:470:HOH:O	1.96	0.65
1:A:432:ASN:O	7:A:746:HOH:O	2.14	0.65
1:A:455:GLU:OE1	7:A:739:HOH:O	2.12	0.65
1:D:533:GLU:O	7:D:731:HOH:O	2.14	0.65
1:D:77:ILE:HG13	1:D:110:PHE:HB3	1.77	0.65
2:E:4:LEU:HD13	2:E:31:GLU:HB2	1.79	0.65
1:A:286:ASN:HA	1:A:287:TRP:CE3	2.32	0.65
2:C:214:LYS:NZ	7:C:411:HOH:O	1.99	0.65
2:C:98:TRP:HE3	2:C:101:PHE:HB2	1.62	0.65
1:A:126:ARG:NH1	7:A:795:HOH:O	2.29	0.64
1:A:445:VAL:HG13	1:A:479:TRP:NE1	2.12	0.64
1:A:484:GLU:O	7:A:742:HOH:O	2.13	0.64
1:D:359:GLY:O	7:D:734:HOH:O	2.15	0.64
1:A:547:MET:O	7:A:743:HOH:O	2.13	0.64
1:D:312:TYR:N	7:D:773:HOH:O	2.27	0.64
1:D:152:LYS:HG2	1:D:565:ASN:H	1.61	0.64
2:E:8:LEU:HD21	7:E:403:HOH:O	1.97	0.64
1:D:445:VAL:HG21	1:D:462:PHE:CG	2.32	0.64
1:D:480:GLU:OE2	1:D:526:GLY:N	2.30	0.64
2:B:96:ARG:NH1	2:C:73:TYR:HE1	1.91	0.64
2:E:107:THR:HA	2:E:110:GLN:HG2	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:VAL:O	1:A:175:PHE:HB2	1.97	0.64
1:A:290:LEU:HD12	1:A:293:ALA:HB3	1.78	0.64
1:D:273:LEU:HA	1:D:276:THR:HG23	1.79	0.64
1:D:382:VAL:O	7:D:736:HOH:O	2.15	0.64
1:D:328:HIS:NE2	3:D:601:JAA:O03	2.29	0.64
2:F:132:VAL:HG22	2:F:179:SER:HB2	1.80	0.64
1:A:464:SER:OG	1:A:550:CYS:SG	2.32	0.64
1:D:151:SER:OG	1:D:565:ASN:ND2	2.29	0.64
1:D:367:SER:HB2	1:D:386:GLU:OE2	1.98	0.64
1:A:97:ILE:HB	1:A:162:VAL:HB	1.80	0.64
1:D:200:GLN:HA	1:D:203:TYR:CE2	2.33	0.64
1:D:463:SER:OG	7:D:726:HOH:O	2.12	0.64
1:D:477:ILE:HD12	1:D:497:LEU:HD13	1.79	0.64
1:D:139:ASP:O	7:D:733:HOH:O	2.15	0.64
1:D:180:LYS:O	7:D:737:HOH:O	2.15	0.64
1:D:98:SER:HB3	1:D:557:LYS:HE3	1.79	0.64
1:A:143:LYS:CD	1:A:212:PHE:HB2	2.26	0.64
1:A:151:SER:HB3	1:A:565:ASN:HD21	1.62	0.64
1:D:162:VAL:O	1:D:560:GLN:HB2	1.98	0.64
1:A:424:ARG:HD2	1:A:425:ARG:HH11	1.61	0.64
1:A:332:SER:HB2	1:A:538:LEU:HA	1.79	0.64
2:C:139:LEU:O	2:C:141:ASP:N	2.30	0.64
1:A:22:ARG:HG2	1:A:414:ASN:HB3	1.81	0.63
2:C:45:LEU:HD12	7:C:444:HOH:O	1.98	0.63
1:A:432:ASN:O	1:A:433:ILE:HG23	1.99	0.63
2:B:90:TYR:O	2:B:93:ALA:HB3	1.99	0.63
1:D:386:GLU:O	7:D:738:HOH:O	2.15	0.63
1:A:313:VAL:HG22	1:A:314:PRO:HD3	1.81	0.63
2:F:176:GLU:N	2:F:176:GLU:OE1	2.29	0.63
1:A:143:LYS:HZ2	1:A:187:CYS:CB	2.11	0.63
1:A:91:GLY:O	7:A:748:HOH:O	2.15	0.63
2:C:98:TRP:CZ2	2:C:157:LEU:HD22	2.34	0.63
1:D:270:ASN:HB3	1:D:273:LEU:HD11	1.79	0.63
1:D:288:TYR:HA	1:D:318:HIS:CD2	2.33	0.63
1:A:105:GLN:HB2	1:A:430:SER:HB2	1.81	0.63
1:A:217:GLN:O	1:A:299:LYS:N	2.29	0.63
1:A:361:PHE:CE1	1:A:392:ILE:HG22	2.34	0.62
1:D:46:GLN:NE2	7:D:749:HOH:O	2.29	0.62
1:D:448:ALA:HB2	1:D:496:CYS:HB3	1.81	0.62
2:E:121:GLN:NE2	2:E:170:PHE:O	2.32	0.62
2:E:24:ARG:NE	7:E:419:HOH:O	2.30	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:10:TYR:HH	2:F:208:TYR:HH	1.47	0.62
1:A:92:HIS:NE2	2:B:136:GLU:O	2.31	0.62
2:E:90:TYR:O	2:E:94:GLN:HG2	1.99	0.62
2:F:33:ARG:NH1	2:F:41:SER:OG	2.31	0.62
1:A:113:PHE:HD1	1:A:117:LEU:HD13	1.64	0.62
1:D:132:ARG:HA	1:D:343:PRO:HG3	1.82	0.62
1:A:236:GLN:NE2	7:A:797:HOH:O	2.29	0.62
2:C:98:TRP:CE3	2:C:101:PHE:HB2	2.34	0.62
1:A:240:GLU:HB3	7:A:757:HOH:O	1.98	0.62
2:C:102:VAL:HG23	7:C:406:HOH:O	2.00	0.62
2:E:23:LEU:HD22	2:E:28:VAL:HB	1.81	0.62
1:A:79:ARG:NH1	2:B:188:ARG:HH22	1.98	0.62
1:A:76:TYR:O	1:A:88:ILE:HD12	1.99	0.62
2:B:110:GLN:HB2	2:B:167:TYR:CE2	2.34	0.62
2:C:114:TRP:CD1	2:C:167:TYR:HE1	2.18	0.62
2:E:48:ASN:ND2	7:E:409:HOH:O	2.32	0.62
2:F:19:ALA:N	7:F:429:HOH:O	2.32	0.62
1:D:208:SER:HA	1:D:211:LEU:HG	1.82	0.62
2:B:195:VAL:HG13	2:B:199:LEU:HD13	1.82	0.62
2:B:114:TRP:O	7:B:412:HOH:O	2.16	0.61
2:B:121:GLN:NE2	2:B:170:PHE:O	2.34	0.61
1:A:93:PRO:HG2	2:B:181:LYS:HA	1.81	0.61
1:D:166:THR:OG1	1:D:561:ILE:HD11	2.00	0.61
2:B:125:LYS:NZ	7:B:403:HOH:O	2.05	0.61
1:D:126:ARG:HD3	1:D:182:ILE:HD13	1.81	0.61
1:D:475:TYR:CZ	1:D:506:TYR:HE1	2.18	0.61
2:E:93:ALA:CB	2:F:73:TYR:HE1	2.12	0.61
2:C:53:LYS:HG2	5:C:301:GSH:HA31	1.81	0.61
2:C:64:VAL:N	7:C:420:HOH:O	2.11	0.61
1:D:22:ARG:NH1	1:D:414:ASN:OD1	2.33	0.61
1:D:25:HIS:O	1:D:29:LYS:HG2	2.00	0.61
1:D:507:VAL:HG12	1:D:510:ARG:NH2	2.16	0.61
2:E:8:LEU:HD13	2:E:44:LEU:HB2	1.81	0.61
1:A:461:ASP:HB3	1:A:528:PHE:CD2	2.34	0.61
2:B:9:ASP:OD1	2:B:10:TYR:N	2.29	0.61
2:E:53:LYS:O	7:E:409:HOH:O	2.16	0.61
2:F:111:PHE:O	7:F:419:HOH:O	2.16	0.61
1:A:244:ASP:HB2	1:A:250:LEU:HA	1.83	0.61
2:B:139:LEU:CD2	2:B:142:LYS:H	2.14	0.61
2:B:24:ARG:HH22	2:B:197:LYS:HB2	1.64	0.61
1:D:364:LEU:HD12	1:D:402:ARG:HH22	1.66	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:114:TRP:HA	2:C:170:PHE:HD2	1.66	0.61
2:E:51:HIS:HB3	2:E:53:LYS:HG3	1.82	0.61
1:A:224:ALA:HB3	1:A:312:TYR:CE1	2.36	0.61
1:A:286:ASN:HA	1:A:287:TRP:HE3	1.64	0.61
1:A:149:PHE:CB	1:A:530:LYS:HZ3	2.14	0.61
1:D:94:VAL:HG11	1:D:112:PRO:HB3	1.83	0.61
1:D:150:SER:HB3	1:D:170:TYR:CD2	2.35	0.61
2:C:32:TYR:HD2	2:C:32:TYR:H	1.49	0.61
1:D:337:ILE:HD13	1:D:539:GLY:CA	2.30	0.61
1:D:420:LYS:NZ	7:D:774:HOH:O	2.27	0.61
1:A:242:VAL:HG21	1:A:278:ARG:HD3	1.82	0.60
1:A:309:MET:HB3	1:A:312:TYR:CE2	2.36	0.60
1:A:109:LYS:NZ	1:A:401:TYR:OH	2.28	0.60
1:A:547:MET:SD	1:A:549:ARG:NH2	2.71	0.60
2:B:139:LEU:HD21	2:B:142:LYS:O	2.00	0.60
1:D:233:THR:HA	1:D:236:GLN:HE21	1.66	0.60
1:D:20:MET:HE2	1:D:356:PRO:HG2	1.83	0.60
1:D:413:TYR:CD2	1:D:418:GLN:HG2	2.35	0.60
2:B:73:TYR:OH	7:B:411:HOH:O	2.16	0.60
1:D:122:LEU:HD23	7:D:828:HOH:O	2.01	0.60
1:D:362:GLU:HG3	1:D:400:ARG:NH2	2.15	0.60
1:D:110:PHE:CE1	1:D:556:ALA:HB2	2.36	0.60
1:D:76:TYR:O	1:D:79:ARG:HB2	2.01	0.60
1:A:232:ARG:O	1:A:235:GLU:HG2	2.01	0.60
1:A:295:PHE:HD1	1:A:298:ALA:HB2	1.65	0.60
2:B:59:HIS:CE1	2:B:60:ASN:HD22	2.19	0.60
2:C:122:GLU:HA	2:C:125:LYS:HE2	1.83	0.60
1:D:150:SER:CB	1:D:167:THR:HA	2.32	0.60
1:D:153:GLN:HA	1:D:560:GLN:HG2	1.83	0.60
1:D:462:PHE:O	1:D:549:ARG:NH1	2.35	0.60
2:F:183:ILE:HD12	2:F:186:ALA:HB3	1.83	0.60
1:A:246:LYS:HZ3	1:A:278:ARG:HH22	1.49	0.60
1:A:92:HIS:ND1	2:B:181:LYS:HB3	2.16	0.60
2:C:201:ASP:HB2	2:C:204:LYS:HG3	1.84	0.60
1:D:339:ALA:O	7:D:740:HOH:O	2.16	0.60
1:D:559:LEU:HA	1:D:562:LEU:HB2	1.83	0.60
1:A:353:ALA:HB2	1:A:413:TYR:CD2	2.37	0.60
2:B:139:LEU:HG	2:B:142:LYS:HB2	1.84	0.60
2:C:202:SER:OG	1:D:454:GLU:OE2	2.17	0.60
1:A:465:TYR:HB3	1:A:476:ALA:HB3	1.83	0.60
1:D:535:PHE:HB3	1:D:544:GLN:O	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:176:GLU:O	2:F:177:SER:HB2	2.00	0.60
2:C:73:TYR:HA	2:C:76:GLU:OE2	2.02	0.60
1:D:495:ASN:O	1:D:499:ARG:NH1	2.35	0.60
2:F:144:TYR:HB3	2:F:154:ASP:OD2	2.01	0.60
2:F:8:LEU:HB2	2:F:56:VAL:HB	1.84	0.60
2:F:64:VAL:HB	2:F:73:TYR:CD2	2.37	0.60
1:A:363:PHE:O	7:A:750:HOH:O	2.17	0.60
1:D:467:ASP:OD1	1:D:474:HIS:N	2.32	0.60
2:E:41:SER:OG	7:E:403:HOH:O	2.06	0.60
1:A:524:ALA:O	7:A:749:HOH:O	2.17	0.60
2:B:120:GLU:O	7:B:414:HOH:O	2.17	0.60
1:D:425:ARG:NH2	7:D:791:HOH:O	2.33	0.60
1:A:223:PHE:HD2	1:A:225:HIS:CD2	2.19	0.60
1:A:41:SER:H	2:B:142:LYS:HG2	1.65	0.60
1:D:122:LEU:O	1:D:126:ARG:HG2	2.02	0.60
1:D:454:GLU:HG2	7:D:798:HOH:O	2.01	0.60
1:D:152:LYS:HA	1:D:564:GLU:HB2	1.84	0.60
2:E:92:ARG:CZ	2:E:96:ARG:HH12	2.13	0.60
1:A:28:GLN:OE1	1:A:379:LEU:HD22	2.02	0.59
1:A:437:THR:O	1:A:440:ASP:N	2.35	0.59
2:C:64:VAL:HB	2:C:73:TYR:CE2	2.37	0.59
1:D:148:ILE:O	1:D:205:HIS:HE1	1.84	0.59
1:D:506:TYR:HB3	1:D:510:ARG:HH21	1.67	0.59
1:D:513:LYS:NZ	1:D:575:PHE:HB3	2.16	0.59
2:E:58:VAL:HG22	2:E:63:PRO:HB3	1.82	0.59
2:F:67:SER:OG	5:F:301:GSH:O12	2.13	0.59
2:F:70:VAL:O	2:F:73:TYR:HB2	2.02	0.59
1:A:42:ALA:HB1	1:A:44:TYR:CE1	2.38	0.59
1:A:149:PHE:HB2	1:A:530:LYS:HZ3	1.66	0.59
2:B:66:GLU:N	7:B:420:HOH:O	2.21	0.59
1:D:223:PHE:CZ	1:D:533:GLU:HA	2.36	0.59
1:A:113:PHE:CD1	1:A:117:LEU:HD13	2.37	0.59
2:B:150:PHE:HB2	2:B:192:LYS:HZ2	1.67	0.59
2:C:163:TRP:HB3	2:C:167:TYR:CZ	2.36	0.59
2:C:183:ILE:HG12	1:D:492:ASP:CG	2.22	0.59
2:E:92:ARG:NH1	2:E:96:ARG:HH12	1.99	0.59
2:F:195:VAL:HG23	2:F:199:LEU:HD13	1.84	0.59
2:F:82:ASN:O	7:F:420:HOH:O	2.17	0.59
1:A:260:ARG:NE	7:A:796:HOH:O	2.29	0.59
1:A:287:TRP:CD1	1:A:290:LEU:HD13	2.37	0.59
1:D:473:GLY:O	1:D:516:GLY:N	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:50:ILE:HD12	2:F:101:PHE:CZ	2.37	0.59
2:F:114:TRP:HA	2:F:170:PHE:HD2	1.66	0.59
1:A:154:TYR:OH	1:A:156:SER:OG	2.19	0.59
1:A:248:GLY:HA2	1:A:267:LEU:HD22	1.83	0.59
1:A:93:PRO:HG3	2:B:184:ALA:CB	2.27	0.59
2:B:96:ARG:NH1	2:C:73:TYR:CD1	2.69	0.59
1:D:61:PHE:O	1:D:65:VAL:HG12	2.02	0.59
1:A:407:VAL:HG11	1:A:419:LEU:HD13	1.84	0.59
1:D:219:VAL:HB	1:D:295:PHE:CZ	2.37	0.59
2:E:8:LEU:O	2:E:55:PRO:HA	2.02	0.59
1:A:473:GLY:O	1:A:516:GLY:N	2.34	0.59
2:C:180:PRO:HG2	1:D:574:ALA:HA	1.85	0.59
2:B:107:THR:HA	2:B:110:GLN:HG2	1.85	0.59
1:D:409:VAL:N	7:D:738:HOH:O	2.31	0.59
2:E:136:GLU:OE2	2:E:181:LYS:HD3	2.02	0.59
1:A:184:SER:HB2	1:A:217:GLN:HE21	1.68	0.59
1:A:24:ALA:O	7:A:752:HOH:O	2.17	0.59
1:A:314:PRO:HB3	1:A:317:ARG:HH12	1.66	0.58
1:A:40:GLN:HG2	2:B:142:LYS:HD2	1.85	0.58
1:A:79:ARG:NH2	2:B:188:ARG:NH1	2.51	0.58
1:D:209:GLY:N	7:D:727:HOH:O	2.36	0.58
1:D:73:LEU:HD22	1:D:89:LEU:HD13	1.84	0.58
2:F:164:PHE:CD2	2:F:183:ILE:HD13	2.34	0.58
2:C:26:LYS:HE2	2:C:75:ASP:HA	1.85	0.58
1:A:291:ILE:HB	1:A:320:ALA:HA	1.84	0.58
1:A:401:TYR:CE2	1:A:403:LEU:HD13	2.37	0.58
1:A:434:ASP:OD2	7:A:751:HOH:O	2.17	0.58
1:A:99:LEU:HB2	1:A:557:LYS:H	1.68	0.58
2:B:165:GLN:HB3	7:B:486:HOH:O	2.02	0.58
2:F:165:GLN:OE1	2:F:202:SER:HB2	2.02	0.58
2:E:62:LYS:HD3	2:F:90:TYR:CD2	2.39	0.58
1:A:48:CYS:HB3	1:A:65:VAL:HG22	1.85	0.58
1:D:521:ARG:NH2	1:D:563:CYS:SG	2.77	0.58
2:F:188:ARG:HD2	2:F:191:GLU:OE2	2.03	0.58
1:D:417:PRO:O	7:D:742:HOH:O	2.17	0.58
2:E:116:LYS:O	7:E:410:HOH:O	2.17	0.58
2:F:142:LYS:HB3	7:F:424:HOH:O	2.03	0.58
1:A:107:ARG:HH21	1:A:433:ILE:HG12	1.68	0.58
1:A:424:ARG:HG3	1:A:425:ARG:H	1.68	0.58
1:A:90:THR:HG23	1:A:397:GLY:CA	2.33	0.58
2:B:152:TYR:O	2:B:155:ILE:HG13	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:98:TRP:CZ2	2:C:135:LEU:HD21	2.38	0.58
1:D:62:LYS:HE2	1:D:376:PRO:HG2	1.85	0.58
1:D:80:MET:SD	1:D:87:PRO:HA	2.44	0.58
2:F:33:ARG:HH12	2:F:41:SER:CB	2.16	0.58
2:F:9:ASP:HB3	7:F:482:HOH:O	2.04	0.58
1:A:152:LYS:CG	1:A:561:ILE:HA	2.33	0.58
1:A:48:CYS:SG	1:A:65:VAL:HG13	2.44	0.58
1:A:79:ARG:HH22	2:B:188:ARG:HH12	1.51	0.58
1:D:480:GLU:OE2	1:D:527:THR:N	2.36	0.58
1:D:153:GLN:H	1:D:564:GLU:HB2	1.68	0.58
1:D:88:ILE:HD12	1:D:89:LEU:HB2	1.85	0.58
1:A:149:PHE:HB2	1:A:530:LYS:NZ	2.19	0.58
1:A:36:LEU:HD22	1:A:61:PHE:HZ	1.68	0.58
2:E:8:LEU:HD12	2:E:56:VAL:HB	1.85	0.58
1:D:143:LYS:N	7:D:765:HOH:O	2.29	0.58
1:D:231:PHE:HB3	1:D:290:LEU:HD13	1.85	0.58
2:F:84:PHE:CD1	2:F:152:TYR:HB2	2.38	0.58
2:B:125:LYS:HB3	2:B:173:PHE:HE2	1.68	0.57
2:C:140:GLY:N	2:C:181:LYS:HZ3	2.02	0.57
2:C:51:HIS:ND1	7:C:423:HOH:O	2.33	0.57
1:D:38:LYS:O	2:E:142:LYS:HG3	2.02	0.57
1:A:445:VAL:HG22	7:A:762:HOH:O	2.04	0.57
1:A:450:LYS:HA	1:A:453:SER:HB3	1.86	0.57
2:B:125:LYS:O	2:B:129:ILE:HG12	2.04	0.57
1:D:363:PHE:HB3	1:D:388:TYR:HB3	1.85	0.57
1:D:44:TYR:CB	1:D:89:LEU:HG	2.34	0.57
2:F:135:LEU:HD13	2:F:182:LEU:HD11	1.86	0.57
1:A:274:ALA:HB1	1:A:278:ARG:CZ	2.34	0.57
1:A:287:TRP:HD1	1:A:290:LEU:HD13	1.68	0.57
1:D:11:ASN:O	1:D:14:ILE:HG13	2.04	0.57
1:D:407:VAL:HG22	1:D:541:SER:HB2	1.85	0.57
1:D:107:ARG:HH22	1:D:552:LYS:HB3	1.69	0.57
1:D:99:LEU:HD12	1:D:100:SER:N	2.19	0.57
2:E:195:VAL:HG13	2:E:199:LEU:HD13	1.85	0.57
2:F:98:TRP:CZ2	2:F:157:LEU:HD22	2.39	0.57
1:A:23:ASN:OD1	1:A:26:GLN:HG2	2.04	0.57
1:A:348:GLU:OE1	7:A:753:HOH:O	2.18	0.57
2:C:26:LYS:HG2	2:C:81:LYS:HZ3	1.69	0.57
1:D:394:ASN:OD1	1:D:398:LEU:HD11	2.04	0.57
1:A:559:LEU:O	1:A:562:LEU:HG	2.04	0.57
1:D:528:PHE:HA	1:D:531:ILE:HG12	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:330:TYR:OH	1:D:541:SER:N	2.36	0.57
1:A:32:LEU:HB2	1:A:360:TYR:CD1	2.39	0.57
1:D:342:THR:OG1	1:D:413:TYR:OH	2.12	0.57
1:D:377:VAL:O	7:D:745:HOH:O	2.18	0.57
1:D:154:TYR:HB3	1:D:560:GLN:HA	1.86	0.57
2:F:64:VAL:HB	2:F:73:TYR:CE2	2.39	0.57
1:A:122:LEU:HD21	1:A:178:GLY:HA3	1.86	0.57
1:A:338:ALA:HA	1:A:354:VAL:HA	1.85	0.57
1:A:441:LEU:HG	1:A:462:PHE:CE2	2.39	0.57
2:C:70:VAL:O	2:C:73:TYR:HB2	2.04	0.57
1:D:168:ASN:ND2	7:D:732:HOH:O	2.15	0.57
1:D:207:LEU:O	1:D:210:ILE:HG22	2.05	0.57
1:A:435:LYS:HA	1:A:436:ASN:HB2	1.87	0.57
2:C:184:ALA:HB1	1:D:499:ARG:NE	2.19	0.57
1:D:108:PRO:HB2	1:D:554:SER:OG	2.05	0.57
1:D:389:GLU:OE1	7:D:744:HOH:O	2.17	0.57
1:A:237:VAL:HG11	7:A:1029:HOH:O	2.05	0.57
1:A:26:GLN:HA	1:A:29:LYS:HG2	1.86	0.57
1:A:32:LEU:HD21	1:A:61:PHE:HD2	1.70	0.57
2:C:17:MET:SD	2:C:199:LEU:HG	2.44	0.57
1:D:8:PHE:CD1	1:D:182:ILE:HG22	2.39	0.57
1:D:382:VAL:HG13	1:D:388:TYR:CE2	2.40	0.57
2:E:113:VAL:O	7:E:410:HOH:O	2.17	0.57
1:A:231:PHE:HA	1:A:234:PHE:HB3	1.86	0.56
2:B:152:TYR:OH	7:B:413:HOH:O	2.16	0.56
2:B:162:SER:HB3	2:B:199:LEU:HD23	1.86	0.56
1:D:284:LEU:HD13	1:D:287:TRP:H	1.69	0.56
1:A:37:LEU:HD11	2:B:90:TYR:HE2	1.69	0.56
1:D:405:ASP:OD1	1:D:405:ASP:N	2.36	0.56
2:F:98:TRP:CZ2	2:F:135:LEU:HD21	2.40	0.56
1:A:206:LEU:HD12	1:A:207:LEU:N	2.20	0.56
1:D:196:PRO:HA	1:D:565:ASN:OD1	2.06	0.56
2:F:29:GLU:N	7:F:433:HOH:O	2.38	0.56
1:A:132:ARG:O	1:A:136:PHE:N	2.38	0.56
2:C:123:ALA:HB2	7:C:476:HOH:O	2.05	0.56
1:A:207:LEU:HD13	1:A:245:ILE:HD11	1.87	0.56
1:A:506:TYR:HA	1:A:509:SER:HB2	1.87	0.56
1:D:451:ARG:NH1	1:D:454:GLU:OE1	2.38	0.56
2:F:68:LEU:HA	2:F:71:VAL:HG12	1.88	0.56
1:A:174:ASN:ND2	7:A:818:HOH:O	2.39	0.56
2:B:150:PHE:HB2	2:B:192:LYS:NZ	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:99:LEU:HD22	1:D:555:ASN:HB3	1.88	0.56
2:E:85:PHE:CE1	2:E:152:TYR:HB2	2.40	0.56
1:A:233:THR:O	1:A:236:GLN:N	2.39	0.56
1:D:330:TYR:HE1	1:D:536:LEU:O	1.89	0.56
1:A:120:ASN:O	1:A:124:LEU:HG	2.06	0.56
1:A:228:VAL:O	1:A:232:ARG:N	2.38	0.56
2:C:10:TYR:HH	2:C:208:TYR:HH	1.53	0.56
1:D:221:ALA:HB3	1:D:227:LEU:HG	1.87	0.56
1:D:360:TYR:C	1:D:361:PHE:HD1	2.10	0.56
1:A:523:VAL:HG22	1:A:524:ALA:H	1.71	0.56
1:A:101:SER:HB3	1:A:535:PHE:CD2	2.41	0.56
1:A:165:ALA:HB3	4:A:602:VAL:HA	1.87	0.56
1:D:242:VAL:O	1:D:246:LYS:HB2	2.05	0.56
1:D:451:ARG:NH1	1:D:454:GLU:CD	2.59	0.56
2:E:144:TYR:HB3	2:E:154:ASP:OD2	2.06	0.56
2:F:183:ILE:O	2:F:186:ALA:N	2.37	0.56
1:A:86:SER:HB2	2:B:188:ARG:NE	2.21	0.56
1:D:110:PHE:CD2	1:D:554:SER:HA	2.41	0.56
1:D:146:GLN:NE2	7:D:760:HOH:O	2.22	0.56
1:D:166:THR:HG22	4:D:602:VAL:HB	1.87	0.56
1:D:233:THR:O	1:D:237:VAL:HG22	2.06	0.56
2:E:50:ILE:HG13	2:E:51:HIS:N	2.18	0.56
1:A:171:ARG:HB2	7:A:709:HOH:O	2.05	0.56
1:A:363:PHE:HB3	1:A:388:TYR:HB3	1.87	0.56
2:B:37:PHE:CE1	5:B:301:GSH:HA32	2.41	0.56
1:A:523:VAL:HG11	1:A:527:THR:HG21	1.88	0.55
1:D:363:PHE:HD2	1:D:382:VAL:HG21	1.70	0.55
1:D:96:ALA:HA	1:D:161:PRO:O	2.05	0.55
2:F:185:TRP:NE1	2:F:189:CYS:SG	2.79	0.55
2:F:64:VAL:HG23	2:F:70:VAL:HG22	1.88	0.55
1:D:113:PHE:CD1	1:D:117:LEU:HD12	2.40	0.55
1:D:169:VAL:HG23	7:D:770:HOH:O	2.06	0.55
1:D:188:SER:OG	1:D:205:HIS:CD2	2.59	0.55
1:D:434:ASP:HB2	1:D:550:CYS:HB3	1.88	0.55
1:D:47:ASN:OD1	7:D:749:HOH:O	2.18	0.55
1:D:495:ASN:CB	1:D:499:ARG:NH1	2.68	0.55
2:F:17:MET:SD	2:F:199:LEU:HG	2.46	0.55
1:A:97:ILE:HD13	1:A:112:PRO:HA	1.87	0.55
1:A:493:CYS:HB3	7:A:940:HOH:O	2.06	0.55
1:A:92:HIS:CE1	2:B:139:LEU:HD22	2.42	0.55
1:A:79:ARG:HH12	2:B:188:ARG:HH12	1.53	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:135:LEU:HD13	2:C:182:LEU:HD11	1.87	0.55
1:D:101:SER:HB3	1:D:535:PHE:CD2	2.41	0.55
1:D:110:PHE:O	7:D:746:HOH:O	2.18	0.55
1:D:332:SER:HB2	1:D:538:LEU:HA	1.88	0.55
1:D:541:SER:O	1:D:543:GLY:N	2.39	0.55
2:E:173:PHE:HE1	2:E:175:ILE:HG13	1.72	0.55
2:E:193:GLU:OE1	2:E:196:SER:OG	2.23	0.55
1:A:143:LYS:NZ	1:A:208:SER:O	2.39	0.55
1:A:152:LYS:HZ1	1:A:530:LYS:HZ3	1.39	0.55
1:D:149:PHE:HB2	1:D:530:LYS:HE2	1.89	0.55
1:D:223:PHE:HD2	1:D:225:HIS:CE1	2.25	0.55
2:E:20:ARG:HB3	2:E:24:ARG:HH12	1.69	0.55
2:F:123:ALA:HB2	7:F:411:HOH:O	2.05	0.55
1:A:150:SER:OG	1:A:150:SER:O	2.22	0.55
1:A:437:THR:OG1	1:A:440:ASP:HB2	2.07	0.55
1:D:328:HIS:CG	1:D:329:ASP:N	2.74	0.55
1:D:39:ASN:ND2	1:D:399:TYR:OH	2.39	0.55
1:D:68:VAL:HG12	1:D:72:GLU:HB2	1.88	0.55
2:F:170:PHE:C	2:F:172:ASN:H	2.08	0.55
1:A:121:THR:HG22	1:A:336:TRP:CZ2	2.41	0.55
2:C:54:ILE:HB	2:C:55:PRO:HA	1.88	0.55
1:D:164:THR:HA	1:D:557:LYS:HG3	1.87	0.55
1:D:228:VAL:HG13	1:D:319:TYR:HE2	1.72	0.55
1:D:551:VAL:HB	1:D:555:ASN:HB2	1.87	0.55
2:F:73:TYR:HA	2:F:76:GLU:OE2	2.07	0.55
1:A:238:TRP:CA	1:A:241:ILE:HB	2.36	0.55
1:A:340:ASN:ND2	1:A:343:PRO:HA	2.20	0.55
2:C:165:GLN:HA	2:C:168:GLU:OE1	2.07	0.55
1:D:150:SER:O	1:D:150:SER:OG	2.20	0.55
2:E:11:TRP:CG	2:E:12:PRO:HD3	2.41	0.55
2:F:125:LYS:HA	2:F:128:PHE:CE2	2.42	0.55
1:A:169:VAL:HG13	1:A:170:TYR:CD1	2.42	0.55
1:A:28:GLN:HG3	1:A:356:PRO:O	2.07	0.55
1:A:503:ASP:OD2	1:A:505:GLY:N	2.38	0.55
2:B:139:LEU:O	2:B:141:ASP:N	2.40	0.55
2:C:96:ARG:N	7:C:440:HOH:O	2.40	0.55
1:D:437:THR:O	1:D:440:ASP:N	2.40	0.55
1:D:495:ASN:O	1:D:498:ASP:HB2	2.06	0.55
1:D:524:ALA:HB2	1:D:567:VAL:CG1	2.36	0.55
1:D:75:PRO:O	1:D:79:ARG:HG3	2.07	0.55
2:F:200:PRO:HG3	7:F:494:HOH:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:93:ALA:CB	2:F:73:TYR:CE1	2.90	0.55
2:C:87:SER:HB3	7:C:502:HOH:O	2.06	0.55
1:D:43:ILE:O	1:D:46:GLN:HG2	2.07	0.55
1:A:201:ALA:O	1:A:205:HIS:N	2.40	0.55
1:A:228:VAL:O	1:A:232:ARG:HG3	2.06	0.55
2:B:76:GLU:OE2	2:C:92:ARG:NH2	2.40	0.55
2:E:205:ILE:HG12	7:E:404:HOH:O	2.06	0.55
1:A:315:LYS:O	1:A:318:HIS:HB3	2.07	0.54
1:A:78:LYS:NZ	7:A:720:HOH:O	2.06	0.54
2:B:93:ALA:HB1	2:C:73:TYR:CZ	2.43	0.54
2:C:185:TRP:NE1	2:C:189:CYS:SG	2.80	0.54
2:E:201:ASP:OD2	2:E:204:LYS:HE3	2.07	0.54
1:A:15:ASP:OD1	1:A:16:GLU:N	2.40	0.54
1:A:151:SER:HB2	1:A:194:PHE:HA	1.88	0.54
1:A:212:PHE:HB3	1:A:215:GLN:NE2	2.23	0.54
1:A:92:HIS:HD2	2:B:140:GLY:O	1.89	0.54
2:C:209:ALA:HB2	7:C:434:HOH:O	2.06	0.54
2:C:8:LEU:HD22	2:C:33:ARG:NH2	2.22	0.54
1:D:107:ARG:CZ	1:D:433:ILE:HG13	2.38	0.54
1:D:363:PHE:HE1	1:D:390:VAL:HG23	1.71	0.54
1:D:513:LYS:HZ2	1:D:575:PHE:HB3	1.71	0.54
2:E:70:VAL:HA	2:E:73:TYR:HE2	1.71	0.54
2:F:86:PRO:HD3	2:F:146:GLY:O	2.08	0.54
1:A:314:PRO:HA	1:A:317:ARG:NH1	2.22	0.54
1:A:77:ILE:CG2	1:A:110:PHE:HB3	2.37	0.54
2:C:102:VAL:O	2:C:107:THR:HG23	2.07	0.54
2:C:168:GLU:OE2	1:D:488:ASP:OD2	2.26	0.54
2:C:44:LEU:HB3	7:C:415:HOH:O	2.07	0.54
1:D:337:ILE:CD1	1:D:361:PHE:HE2	2.20	0.54
2:E:14:MET:HA	2:E:17:MET:HE3	1.88	0.54
1:A:84:ASP:C	1:A:86:SER:H	2.11	0.54
1:D:202:LEU:HD23	1:D:525:LYS:HD2	1.89	0.54
2:F:121:GLN:O	2:F:125:LYS:HG3	2.08	0.54
1:A:340:ASN:HB2	1:A:352:PHE:CE2	2.42	0.54
2:C:164:PHE:O	2:C:168:GLU:HG3	2.08	0.54
2:C:50:ILE:HD12	7:C:489:HOH:O	2.07	0.54
1:A:118:MET:O	1:A:121:THR:OG1	2.24	0.54
1:A:424:ARG:C	1:A:543:GLY:HA2	2.27	0.54
1:D:42:ALA:HB3	1:D:45:LEU:HD13	1.89	0.54
1:D:425:ARG:NH1	1:D:546:LYS:HE3	2.23	0.54
1:A:193:ILE:HA	1:A:205:HIS:CE1	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:HIS:CE1	2:B:185:TRP:CZ2	2.96	0.54
1:A:32:LEU:HD22	1:A:360:TYR:CE2	2.43	0.54
1:A:369:THR:OG1	1:A:370:GLY:N	2.40	0.54
1:A:334:GLU:OE1	1:A:403:LEU:HD21	2.07	0.54
1:D:10:MET:HA	7:D:710:HOH:O	2.08	0.54
1:D:77:ILE:HG12	1:D:110:PHE:C	2.29	0.54
1:D:22:ARG:NH1	1:D:414:ASN:CG	2.62	0.54
1:D:353:ALA:HB2	1:D:413:TYR:HD2	1.72	0.54
1:D:382:VAL:HG13	1:D:388:TYR:CD2	2.43	0.54
1:D:99:LEU:H	1:D:557:LYS:HB2	1.73	0.54
2:E:107:THR:HG22	2:E:160:PHE:CZ	2.43	0.54
2:E:92:ARG:NH2	7:E:424:HOH:O	2.40	0.54
1:A:203:TYR:HD2	1:A:254:ILE:HD11	1.73	0.54
2:B:108:ASP:O	2:B:112:LYS:HG2	2.08	0.54
2:C:24:ARG:HB3	2:C:194:SER:HA	1.90	0.54
1:D:452:LEU:HD23	1:D:481:ILE:HG21	1.89	0.54
2:C:187:LYS:HZ3	1:D:496:CYS:HB2	1.73	0.54
1:D:551:VAL:HG21	1:D:559:LEU:HD23	1.90	0.54
2:E:17:MET:SD	2:E:200:PRO:HD2	2.48	0.54
1:A:128:ALA:HA	1:A:131:PHE:CD2	2.43	0.53
1:A:83:GLY:H	1:A:158:GLY:HA3	1.72	0.53
1:A:339:ALA:N	1:A:353:ALA:O	2.29	0.53
1:A:526:GLY:HA2	1:A:529:ARG:HB3	1.88	0.53
1:A:152:LYS:CE	1:A:530:LYS:NZ	2.65	0.53
1:A:562:LEU:HB3	7:A:713:HOH:O	2.08	0.53
1:D:195:SER:HB3	1:D:201:ALA:HB2	1.90	0.53
1:D:246:LYS:CE	1:D:271:PRO:HA	2.37	0.53
1:D:76:TYR:HB3	1:D:88:ILE:HD13	1.90	0.53
2:E:193:GLU:HA	2:E:196:SER:OG	2.09	0.53
1:A:94:VAL:HB	1:A:113:PHE:O	2.07	0.53
1:A:154:TYR:CE2	1:A:559:LEU:HB3	2.42	0.53
1:A:216:VAL:HG21	7:A:778:HOH:O	2.07	0.53
1:A:223:PHE:CZ	1:A:533:GLU:HA	2.44	0.53
2:C:98:TRP:CD1	2:C:153:VAL:HG11	2.44	0.53
1:A:233:THR:HG23	1:A:525:LYS:NZ	2.22	0.53
1:A:310:GLU:HG3	1:A:311:PRO:HD3	1.90	0.53
1:A:435:LYS:HE3	1:A:438:GLU:CB	2.38	0.53
2:C:40:LYS:HD2	2:C:52:LYS:HB3	1.91	0.53
1:D:445:VAL:HG21	1:D:462:PHE:CD1	2.43	0.53
1:D:79:ARG:NH1	7:D:800:HOH:O	2.40	0.53
2:F:57:LEU:O	2:F:64:VAL:HG22	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:ALA:HA	7:A:745:HOH:O	2.08	0.53
1:A:287:TRP:HB3	7:A:1021:HOH:O	2.08	0.53
1:A:291:ILE:HG21	1:A:301:VAL:HG22	1.91	0.53
1:A:36:LEU:HD22	1:A:61:PHE:CZ	2.44	0.53
1:D:302:TYR:HD1	1:D:326:VAL:HG13	1.72	0.53
1:D:475:TYR:HB2	1:D:518:LEU:HG	1.90	0.53
1:D:85:THR:HB	2:E:184:ALA:HB1	1.90	0.53
2:F:51:HIS:O	7:F:421:HOH:O	2.17	0.53
2:E:66:GLU:CD	2:F:97:PHE:HD1	2.11	0.53
1:A:11:ASN:O	1:A:14:ILE:HG13	2.08	0.53
1:A:334:GLU:O	1:A:394:ASN:ND2	2.40	0.53
2:B:134:ILE:HG22	2:B:138:GLU:OE2	2.08	0.53
2:C:108:ASP:O	2:C:112:LYS:HG2	2.08	0.53
2:C:125:LYS:HA	2:C:128:PHE:CE2	2.44	0.53
1:D:126:ARG:HD2	1:D:182:ILE:HG21	1.91	0.53
1:D:199:HIS:HA	1:D:525:LYS:HB2	1.91	0.53
2:C:102:VAL:HG21	2:C:157:LEU:HB3	1.91	0.53
1:D:295:PHE:HD1	1:D:298:ALA:HB2	1.74	0.53
2:F:108:ASP:O	2:F:112:LYS:HG2	2.07	0.53
1:A:510:ARG:CZ	1:A:515:ILE:HD12	2.38	0.53
2:B:24:ARG:HG3	2:B:30:PHE:HE1	1.74	0.53
2:C:187:LYS:NZ	2:C:187:LYS:HB2	2.23	0.53
1:D:244:ASP:OD1	1:D:251:SER:HB2	2.09	0.53
1:D:381:GLN:O	7:D:750:HOH:O	2.19	0.53
1:D:495:ASN:CB	1:D:499:ARG:HH12	2.20	0.53
1:D:559:LEU:O	1:D:562:LEU:HB3	2.09	0.53
2:E:53:LYS:HG2	5:E:301:GSH:HA31	1.90	0.53
2:F:26:LYS:HG2	2:F:81:LYS:HZ1	1.71	0.53
1:A:218:TYR:HA	1:A:298:ALA:HB1	1.91	0.53
2:B:168:GLU:OE1	7:B:415:HOH:O	2.18	0.53
2:C:188:ARG:HH12	1:D:500:ALA:CA	2.02	0.53
1:D:139:ASP:OD2	1:D:142:GLY:N	2.42	0.53
1:D:400:ARG:HB2	7:D:728:HOH:O	2.09	0.53
1:D:522:VAL:O	1:D:567:VAL:HG22	2.09	0.53
2:E:26:LYS:HG3	2:E:82:ASN:HD21	1.72	0.53
2:B:201:ASP:HB2	2:B:204:LYS:HG3	1.91	0.53
1:D:534:HIS:CD2	1:D:557:LYS:HD3	2.44	0.53
1:A:538:LEU:HD22	1:A:544:GLN:HE21	1.74	0.53
1:D:206:LEU:O	1:D:210:ILE:HB	2.09	0.53
1:D:251:SER:O	1:D:254:ILE:HG12	2.07	0.53
1:D:465:TYR:HB3	1:D:476:ALA:HB3	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:507:VAL:O	1:D:511:LYS:HB2	2.09	0.53
2:B:165:GLN:O	2:B:168:GLU:HG2	2.09	0.52
2:C:158:ILE:HG12	7:C:432:HOH:O	2.08	0.52
1:D:10:MET:HB2	7:D:881:HOH:O	2.08	0.52
1:D:112:PRO:HD2	1:D:397:GLY:HA3	1.90	0.52
1:D:152:LYS:CE	1:D:565:ASN:HB2	2.37	0.52
1:D:330:TYR:HB2	1:D:352:PHE:CD2	2.43	0.52
2:E:162:SER:HB3	2:E:199:LEU:HD23	1.91	0.52
1:A:137:PRO:O	7:A:756:HOH:O	2.18	0.52
1:A:202:LEU:HD21	1:A:529:ARG:NH2	2.23	0.52
1:A:305:MET:CE	1:A:325:LEU:HG	2.38	0.52
1:A:461:ASP:HB3	1:A:528:PHE:HD2	1.74	0.52
2:B:18:ARG:CD	2:B:156:SER:HA	2.38	0.52
2:B:24:ARG:NH2	2:B:197:LYS:HB2	2.23	0.52
1:D:154:TYR:CD2	1:D:559:LEU:HD13	2.44	0.52
1:D:387:GLU:O	7:D:747:HOH:O	2.18	0.52
1:D:412:PHE:N	7:D:707:HOH:O	2.41	0.52
1:D:432:ASN:O	7:D:751:HOH:O	2.19	0.52
2:E:135:LEU:HD23	2:E:157:LEU:HD21	1.91	0.52
2:F:70:VAL:HA	2:F:73:TYR:CD2	2.44	0.52
1:A:236:GLN:NE2	7:A:729:HOH:O	2.08	0.52
1:D:425:ARG:HG2	1:D:545:PHE:CE1	2.45	0.52
1:A:164:THR:OG1	1:A:166:THR:OG1	2.16	0.52
1:A:26:GLN:HG3	1:A:27:VAL:N	2.25	0.52
1:A:290:LEU:N	1:A:319:TYR:O	2.42	0.52
2:C:5:PRO:HG3	2:C:59:HIS:CE1	2.43	0.52
1:D:235:GLU:HG2	1:D:287:TRP:CG	2.44	0.52
1:A:90:THR:HG23	1:A:397:GLY:HA2	1.91	0.52
1:A:551:VAL:CG1	1:A:555:ASN:HB3	2.36	0.52
2:E:62:LYS:NZ	7:E:426:HOH:O	2.41	0.52
2:E:97:PHE:CE1	2:F:65:CYS:HB2	2.45	0.52
1:D:412:PHE:HB3	1:D:414:ASN:O	2.10	0.52
1:D:437:THR:OG1	1:D:440:ASP:HB2	2.09	0.52
7:C:407:HOH:O	1:D:451:ARG:NH2	2.42	0.52
1:A:151:SER:HA	1:A:194:PHE:HA	1.91	0.52
1:A:292:PRO:HA	7:A:725:HOH:O	2.10	0.52
1:A:478:PHE:CZ	1:A:523:VAL:HB	2.44	0.52
1:D:151:SER:HA	1:D:194:PHE:HA	1.92	0.52
2:F:121:GLN:HB3	7:F:457:HOH:O	2.10	0.52
2:C:142:LYS:HB3	7:C:430:HOH:O	2.09	0.52
2:C:20:ARG:HB3	2:C:198:SER:HB3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:40:LYS:HD3	2:E:52:LYS:HE3	1.91	0.52
2:F:139:LEU:O	2:F:141:ASP:N	2.38	0.52
2:F:170:PHE:C	2:F:172:ASN:N	2.63	0.52
1:A:96:ALA:HB1	1:A:163:GLY:H	1.75	0.52
2:F:131:ALA:O	2:F:135:LEU:HB2	2.09	0.52
1:A:204:CYS:HA	1:A:207:LEU:HD23	1.91	0.52
1:D:337:ILE:HD11	1:D:361:PHE:HE2	1.75	0.52
1:D:364:LEU:HD12	1:D:402:ARG:NH2	2.25	0.52
2:E:150:PHE:CZ	2:E:158:ILE:HD12	2.45	0.52
1:A:365:PRO:HA	1:A:388:TYR:CD1	2.44	0.51
1:A:391:VAL:HG12	1:A:402:ARG:HA	1.93	0.51
2:B:161:SER:HB2	2:B:186:ALA:HB1	1.92	0.51
1:D:33:LYS:O	1:D:37:LEU:HB2	2.10	0.51
1:D:403:LEU:HD22	7:D:803:HOH:O	2.09	0.51
1:D:535:PHE:O	1:D:538:LEU:HB3	2.09	0.51
1:A:187:CYS:HB2	1:A:208:SER:HB3	1.92	0.51
1:A:215:GLN:NE2	7:A:824:HOH:O	2.43	0.51
1:A:224:ALA:HB3	1:A:312:TYR:HE1	1.74	0.51
1:A:32:LEU:HB2	1:A:360:TYR:CG	2.45	0.51
2:B:129:ILE:HD12	2:B:175:ILE:HD11	1.92	0.51
2:C:112:LYS:HG3	7:C:450:HOH:O	2.11	0.51
1:D:202:LEU:O	1:D:205:HIS:N	2.43	0.51
2:E:7:LEU:HD11	2:E:32:TYR:CD1	2.45	0.51
2:B:125:LYS:HE2	2:B:171:GLY:HA2	1.93	0.51
2:B:62:LYS:HZ1	2:C:94:GLN:HG3	1.74	0.51
1:D:87:PRO:HD2	2:E:188:ARG:CB	2.40	0.51
1:A:300:TYR:CE1	1:A:302:TYR:HB2	2.46	0.51
1:A:574:ALA:O	1:A:575:PHE:HB2	2.10	0.51
2:B:132:VAL:HG13	2:B:182:LEU:HD23	1.92	0.51
2:C:104:LYS:N	7:C:419:HOH:O	2.43	0.51
2:C:169:LYS:HD3	2:C:206:VAL:HG13	1.93	0.51
1:D:126:ARG:CD	1:D:182:ILE:HG21	2.40	0.51
1:D:351:THR:HG22	1:D:420:LYS:HB3	1.92	0.51
2:E:193:GLU:HB2	7:E:516:HOH:O	2.11	0.51
1:A:405:ASP:HB3	1:A:541:SER:HB3	1.93	0.51
1:A:534:HIS:HA	4:A:602:VAL:N	2.26	0.51
1:A:87:PRO:HB2	2:B:143:PRO:CA	2.37	0.51
2:B:17:MET:HA	2:B:20:ARG:HD2	1.93	0.51
1:D:97:ILE:HG12	1:D:162:VAL:HG22	1.93	0.51
1:D:310:GLU:O	1:D:313:VAL:HG12	2.10	0.51
1:D:566:VAL:HG23	1:D:568:SER:C	2.31	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:73:TYR:HD1	2:F:76:GLU:OE2	1.94	0.51
1:A:151:SER:OG	1:A:195:SER:O	2.29	0.51
1:D:143:LYS:HZ3	1:D:187:CYS:HA	1.74	0.51
1:D:223:PHE:CZ	1:D:536:LEU:HB2	2.46	0.51
1:D:281:CYS:O	1:D:284:LEU:HG	2.10	0.51
1:D:361:PHE:CZ	1:D:392:ILE:HG23	2.46	0.51
1:D:480:GLU:HB3	7:D:703:HOH:O	2.10	0.51
2:E:76:GLU:OE2	2:F:92:ARG:NH2	2.44	0.51
2:F:165:GLN:HG2	2:F:206:VAL:CG2	2.41	0.51
1:A:219:VAL:HB	1:A:295:PHE:CE1	2.45	0.51
1:A:410:ILE:HD11	1:A:418:GLN:OE1	2.10	0.51
2:C:12:PRO:O	2:C:163:TRP:CZ2	2.64	0.51
2:C:194:SER:N	7:C:442:HOH:O	2.43	0.51
1:D:198:VAL:HG13	1:D:565:ASN:HD21	1.74	0.51
1:D:475:TYR:CE1	1:D:506:TYR:HE1	2.28	0.51
1:D:552:LYS:HE3	1:D:554:SER:OG	2.10	0.51
1:A:113:PHE:HE1	1:A:117:LEU:HD22	1.75	0.51
1:A:337:ILE:HG22	1:A:338:ALA:HB2	1.92	0.51
1:A:423:CYS:SG	1:A:543:GLY:N	2.84	0.51
1:A:46:GLN:HB2	2:B:148:ASP:HB2	1.93	0.51
2:C:164:PHE:CD2	2:C:183:ILE:HD12	2.40	0.51
1:D:437:THR:HG21	1:D:439:ARG:HH21	1.75	0.51
2:E:68:LEU:HA	2:E:71:VAL:HG22	1.92	0.51
1:A:131:PHE:HD1	1:A:343:PRO:HG3	1.75	0.51
1:A:503:ASP:CG	1:A:505:GLY:H	2.13	0.51
1:A:37:LEU:HD11	2:B:90:TYR:CE2	2.45	0.51
2:C:141:ASP:N	2:C:141:ASP:OD1	2.44	0.51
2:C:153:VAL:O	2:C:157:LEU:HD23	2.11	0.51
2:E:141:ASP:OD2	2:E:181:LYS:NZ	2.36	0.51
2:E:144:TYR:CZ	2:E:188:ARG:NH1	2.79	0.51
2:F:115:GLY:HA3	7:F:419:HOH:O	2.10	0.51
2:F:117:LYS:HE3	2:F:213:ARG:HH11	1.74	0.51
1:A:156:SER:HB2	1:A:160:VAL:O	2.11	0.51
1:A:45:LEU:HA	1:A:48:CYS:HB2	1.92	0.51
1:A:495:ASN:ND2	7:A:703:HOH:O	2.44	0.51
2:C:125:LYS:HD2	2:C:173:PHE:CE1	2.46	0.51
1:A:154:TYR:HD2	1:A:560:GLN:HA	1.76	0.50
1:A:167:THR:HG21	1:A:560:GLN:HG3	1.92	0.50
2:B:161:SER:HA	2:B:164:PHE:CD2	2.46	0.50
2:C:195:VAL:HG23	2:C:199:LEU:HD13	1.93	0.50
1:D:118:MET:HG3	7:D:828:HOH:O	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:332:SER:CB	1:D:538:LEU:HA	2.41	0.50
1:D:99:LEU:HB2	1:D:556:ALA:H	1.76	0.50
2:F:32:TYR:HD2	2:F:32:TYR:H	1.57	0.50
1:A:56:ASP:O	1:A:60:ALA:N	2.35	0.50
2:B:205:ILE:HG12	7:B:402:HOH:O	2.10	0.50
1:D:20:MET:SD	7:D:713:HOH:O	2.60	0.50
1:A:213:ARG:HA	1:A:216:VAL:CG2	2.41	0.50
1:A:535:PHE:HB3	1:A:544:GLN:O	2.11	0.50
1:D:46:GLN:HG3	1:D:47:ASN:N	2.25	0.50
2:E:171:GLY:HA3	2:E:173:PHE:CE2	2.47	0.50
2:C:125:LYS:HA	2:C:128:PHE:CD2	2.46	0.50
1:D:197:ASP:HA	1:D:567:VAL:HG12	1.94	0.50
1:D:223:PHE:HE2	1:D:532:GLN:HB2	1.77	0.50
2:B:183:ILE:O	2:B:186:ALA:HB3	2.12	0.50
1:D:329:ASP:HB3	1:D:338:ALA:O	2.11	0.50
1:D:337:ILE:O	1:D:354:VAL:HA	2.11	0.50
1:D:337:ILE:HG22	1:D:338:ALA:HB2	1.94	0.50
1:D:529:ARG:NH2	1:D:533:GLU:OE1	2.45	0.50
1:D:76:TYR:O	1:D:88:ILE:HG21	2.12	0.50
1:A:195:SER:HB3	1:A:201:ALA:HB2	1.92	0.50
2:B:37:PHE:O	7:B:416:HOH:O	2.19	0.50
1:D:32:LEU:O	1:D:36:LEU:HD12	2.11	0.50
1:D:529:ARG:HH21	1:D:530:LYS:HD3	1.76	0.50
1:D:33:LYS:NZ	1:D:58:GLU:HB2	2.27	0.50
1:A:279:THR:HA	1:A:282:MET:SD	2.52	0.50
1:A:91:GLY:HA3	2:B:142:LYS:N	2.26	0.50
1:A:237:VAL:O	7:A:757:HOH:O	2.19	0.50
1:A:305:MET:HA	7:A:715:HOH:O	2.12	0.50
1:A:521:ARG:HB3	1:A:566:VAL:HG22	1.94	0.50
1:A:153:GLN:H	1:A:564:GLU:HB2	1.77	0.50
1:A:43:ILE:HD11	1:A:88:ILE:HG23	1.93	0.50
2:C:60:ASN:HB3	7:C:421:HOH:O	2.12	0.50
1:D:17:PHE:HA	1:D:20:MET:HB3	1.93	0.50
1:D:476:ALA:HA	1:D:519:GLU:O	2.12	0.50
2:F:114:TRP:HA	2:F:170:PHE:CD2	2.47	0.50
1:A:291:ILE:HD12	1:A:320:ALA:HB2	1.93	0.50
1:D:270:ASN:HB3	1:D:273:LEU:CD1	2.42	0.50
1:D:467:ASP:CG	1:D:474:HIS:H	2.15	0.50
2:E:110:GLN:HG3	2:E:111:PHE:N	2.25	0.50
2:F:40:LYS:HD2	2:F:52:LYS:HB3	1.93	0.50
1:A:440:ASP:OD1	1:A:501:PHE:HA	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:PRO:HD2	2:B:188:ARG:HB2	1.93	0.49
2:B:153:VAL:O	2:B:156:SER:OG	2.21	0.49
2:C:5:PRO:HB3	2:C:57:LEU:HD11	1.93	0.49
1:D:330:TYR:HE2	1:D:540:SER:H	1.56	0.49
2:F:170:PHE:CD2	2:F:213:ARG:HD2	2.46	0.49
1:A:197:ASP:HA	1:A:567:VAL:HG12	1.94	0.49
1:A:33:LYS:HA	1:A:36:LEU:CD2	2.42	0.49
1:A:421:PHE:CE1	1:A:541:SER:HA	2.47	0.49
1:A:428:ILE:O	7:A:759:HOH:O	2.20	0.49
1:A:103:THR:OG1	1:A:429:LEU:HD11	2.12	0.49
2:B:110:GLN:NE2	7:B:444:HOH:O	2.45	0.49
2:B:94:GLN:O	2:B:98:TRP:HD1	1.95	0.49
1:D:410:ILE:HG13	1:D:418:GLN:HB2	1.94	0.49
2:F:145:PHE:HA	7:F:424:HOH:O	2.11	0.49
2:F:33:ARG:HG3	7:F:518:HOH:O	2.12	0.49
1:A:295:PHE:CD1	1:A:298:ALA:HB2	2.45	0.49
1:A:224:ALA:CB	1:A:316:LEU:HD22	2.43	0.49
2:B:15:PHE:HA	2:B:18:ARG:HG3	1.94	0.49
2:B:9:ASP:OD1	2:B:16:GLY:HA3	2.12	0.49
2:C:98:TRP:CD1	2:C:153:VAL:HG21	2.47	0.49
2:F:172:ASN:O	2:F:173:PHE:HD1	1.94	0.49
2:F:71:VAL:O	2:F:74:VAL:HB	2.13	0.49
1:A:104:SER:C	1:A:106:GLY:N	2.65	0.49
1:A:302:TYR:OH	7:A:719:HOH:O	2.06	0.49
1:A:311:PRO:O	1:A:314:PRO:HD2	2.13	0.49
2:C:57:LEU:O	2:C:64:VAL:HG22	2.13	0.49
1:D:151:SER:HB2	1:D:195:SER:O	2.13	0.49
2:E:132:VAL:HG13	2:E:182:LEU:HD23	1.93	0.49
2:F:110:GLN:HG2	2:F:167:TYR:CE2	2.47	0.49
1:A:104:SER:HB3	1:A:107:ARG:O	2.12	0.49
1:A:149:PHE:CB	1:A:530:LYS:NZ	2.75	0.49
1:A:219:VAL:HB	1:A:295:PHE:CZ	2.47	0.49
1:A:316:LEU:O	1:A:320:ALA:N	2.41	0.49
1:A:387:GLU:HG2	1:A:408:LYS:HB2	1.95	0.49
1:A:163:GLY:HA2	1:A:560:GLN:HB2	1.93	0.49
2:B:124:GLY:HA2	2:B:127:GLU:CD	2.33	0.49
2:E:102:VAL:O	2:E:106:PHE:HB3	2.12	0.49
2:E:129:ILE:HD11	2:E:173:PHE:CD1	2.47	0.49
2:F:140:GLY:N	2:F:181:LYS:NZ	2.60	0.49
1:A:103:THR:CB	1:A:106:GLY:HA2	2.40	0.49
1:A:549:ARG:HG3	7:A:865:HOH:O	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:113:VAL:HG23	7:B:436:HOH:O	2.12	0.49
2:C:129:ILE:HA	2:C:132:VAL:HG12	1.94	0.49
2:C:197:LYS:HE2	7:C:481:HOH:O	2.13	0.49
1:D:145:LEU:HD23	1:D:295:PHE:CZ	2.47	0.49
1:D:342:THR:O	1:D:345:LEU:HG	2.13	0.49
1:D:435:LYS:HD3	1:D:438:GLU:N	2.28	0.49
1:D:110:PHE:CE2	1:D:554:SER:HA	2.48	0.49
2:F:98:TRP:HD1	2:F:153:VAL:HG11	1.77	0.49
2:F:92:ARG:HE	2:F:96:ARG:HH22	1.59	0.49
1:A:200:GLN:HA	7:A:963:HOH:O	2.11	0.49
2:C:130:GLU:OE2	7:C:425:HOH:O	2.20	0.49
2:C:32:TYR:HA	7:C:412:HOH:O	2.12	0.49
1:D:498:ASP:OD1	1:D:518:LEU:HD13	2.12	0.49
2:E:15:PHE:HB3	2:E:67:SER:HB3	1.95	0.49
1:A:8:PHE:CD1	1:A:182:ILE:HG22	2.47	0.49
1:A:308:SER:HB3	1:A:424:ARG:HA	1.94	0.49
1:A:38:LYS:NZ	1:A:395:TYR:CZ	2.78	0.49
1:A:551:VAL:HG11	1:A:559:LEU:CD1	2.38	0.49
2:C:24:ARG:HG3	2:C:30:PHE:CE1	2.47	0.49
1:D:475:TYR:HE1	1:D:515:ILE:HG21	1.76	0.49
1:D:223:PHE:CG	1:D:533:GLU:HG2	2.48	0.49
1:D:543:GLY:O	1:D:544:GLN:HG3	2.13	0.49
2:E:139:LEU:O	2:E:141:ASP:N	2.45	0.49
1:A:524:ALA:HB2	1:A:567:VAL:HG11	1.95	0.49
2:C:44:LEU:HB2	7:C:460:HOH:O	2.13	0.49
2:C:84:PHE:HB2	2:C:152:TYR:N	2.28	0.49
1:D:386:GLU:HB3	7:D:771:HOH:O	2.13	0.49
1:D:452:LEU:HD11	1:D:490:LEU:HD23	1.95	0.49
1:D:94:VAL:HG21	1:D:97:ILE:HG22	1.95	0.49
2:F:125:LYS:O	2:F:129:ILE:HG23	2.13	0.49
2:C:174:SER:OG	7:D:701:HOH:O	2.15	0.49
1:D:398:LEU:O	1:D:398:LEU:HD12	2.13	0.49
2:F:145:PHE:CD2	2:F:157:LEU:HD21	2.47	0.49
2:F:37:PHE:HZ	2:F:54:ILE:HG12	1.77	0.49
1:A:238:TRP:CE3	1:A:277:ILE:HD11	2.48	0.48
1:A:387:GLU:O	1:A:388:TYR:HD1	1.96	0.48
1:A:468:VAL:HG23	7:A:856:HOH:O	2.13	0.48
2:B:125:LYS:HB3	2:B:173:PHE:CE2	2.48	0.48
1:A:41:SER:HB2	2:B:142:LYS:HG2	1.94	0.48
1:D:223:PHE:HZ	1:D:536:LEU:HB2	1.78	0.48
1:D:476:ALA:HB1	1:D:478:PHE:CZ	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:201:ASP:HB2	2:F:204:LYS:HE2	1.94	0.48
2:F:33:ARG:HH12	2:F:41:SER:HB2	1.77	0.48
1:A:104:SER:O	1:A:107:ARG:HG2	2.13	0.48
1:A:225:HIS:HA	1:A:228:VAL:CG2	2.36	0.48
1:A:309:MET:CE	1:A:536:LEU:HD12	2.43	0.48
2:C:32:TYR:CD1	2:C:34:GLU:OE2	2.66	0.48
1:D:509:SER:HA	1:D:512:CYS:SG	2.53	0.48
2:E:98:TRP:HB3	2:E:153:VAL:HG21	1.94	0.48
2:E:24:ARG:CZ	2:E:30:PHE:HZ	2.25	0.48
2:F:14:MET:HG3	2:F:163:TRP:CH2	2.48	0.48
1:A:238:TRP:HA	1:A:241:ILE:CB	2.38	0.48
1:A:284:LEU:HB2	7:A:812:HOH:O	2.12	0.48
1:A:311:PRO:C	1:A:314:PRO:HD2	2.34	0.48
1:A:402:ARG:HD3	7:A:913:HOH:O	2.12	0.48
1:A:452:LEU:HD11	1:A:490:LEU:HD23	1.96	0.48
2:C:44:LEU:HD22	7:C:517:HOH:O	2.14	0.48
2:C:96:ARG:NH1	7:C:404:HOH:O	1.84	0.48
1:D:311:PRO:O	1:D:314:PRO:HD2	2.13	0.48
1:D:496:CYS:HA	1:D:499:ARG:HH22	1.77	0.48
2:E:71:VAL:HG23	2:E:152:TYR:HE1	1.78	0.48
2:F:153:VAL:HA	7:F:402:HOH:O	2.13	0.48
1:A:317:ARG:O	1:A:321:GLY:N	2.45	0.48
2:C:150:PHE:CD1	2:C:192:LYS:HG3	2.48	0.48
1:D:41:SER:HB3	2:E:144:TYR:HB2	1.94	0.48
1:D:407:VAL:HG13	1:D:421:PHE:CE1	2.48	0.48
1:D:73:LEU:HD12	7:D:808:HOH:O	2.13	0.48
2:B:151:GLY:H	2:B:154:ASP:CG	2.17	0.48
2:C:187:LYS:CE	1:D:496:CYS:HB2	2.42	0.48
2:E:129:ILE:HD11	2:E:173:PHE:CE1	2.49	0.48
2:F:151:GLY:N	2:F:154:ASP:OD2	2.47	0.48
1:A:120:ASN:ND2	7:A:828:HOH:O	2.45	0.48
1:A:202:LEU:O	1:A:205:HIS:N	2.46	0.48
1:A:50:LEU:HD13	1:A:61:PHE:CE1	2.49	0.48
1:A:405:ASP:HB2	1:A:540:SER:HB3	1.94	0.48
2:B:15:PHE:HB3	2:B:67:SER:HB3	1.94	0.48
2:C:33:ARG:NH2	2:C:43:LEU:HD11	2.27	0.48
1:D:192:VAL:HG21	1:D:204:CYS:HB3	1.95	0.48
1:D:242:VAL:HA	1:D:245:ILE:HD11	1.95	0.48
2:F:125:LYS:HA	2:F:128:PHE:CD2	2.48	0.48
2:F:139:LEU:HB3	2:F:181:LYS:HE2	1.96	0.48
1:A:70:ASP:HB2	1:A:104:SER:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:295:PHE:C	1:A:297:ASN:H	2.17	0.48
1:A:336:TRP:HB2	1:A:358:LEU:HD13	1.95	0.48
1:A:460:ILE:HG13	7:A:708:HOH:O	2.13	0.48
1:A:464:SER:OG	1:A:465:TYR:N	2.45	0.48
1:A:198:VAL:CG2	1:A:524:ALA:HB3	2.43	0.48
1:A:522:VAL:O	1:A:567:VAL:HG22	2.13	0.48
2:C:68:LEU:HB2	2:C:152:TYR:OH	2.14	0.48
1:D:236:GLN:NE2	7:D:809:HOH:O	2.47	0.48
1:D:219:VAL:HB	1:D:295:PHE:HZ	1.78	0.48
1:D:334:GLU:O	1:D:398:LEU:HD21	2.14	0.48
1:D:410:ILE:HG21	1:D:420:LYS:HB3	1.96	0.48
1:D:492:ASP:O	1:D:495:ASN:HB2	2.13	0.48
1:A:97:ILE:CB	1:A:162:VAL:HB	2.43	0.48
1:A:284:LEU:O	1:A:284:LEU:HD12	2.14	0.48
1:A:302:TYR:OH	7:A:754:HOH:O	2.18	0.48
1:A:85:THR:O	1:A:93:PRO:HB3	2.13	0.48
2:B:182:LEU:HA	2:B:185:TRP:CD2	2.49	0.48
2:B:182:LEU:HD13	2:B:185:TRP:CE3	2.49	0.48
2:C:10:TYR:CD2	2:C:12:PRO:HD2	2.49	0.48
2:C:37:PHE:HD1	2:C:40:LYS:HG2	1.78	0.48
1:D:53:ASN:O	1:D:57:PRO:HB3	2.13	0.48
2:F:199:LEU:HA	2:F:200:PRO:HD2	1.72	0.48
1:A:433:ILE:CD1	1:A:552:LYS:NZ	2.77	0.48
1:A:452:LEU:CD2	1:A:481:ILE:HG12	2.39	0.48
1:A:82:ASP:OD2	7:A:760:HOH:O	2.20	0.48
2:C:131:ALA:O	2:C:135:LEU:HB2	2.14	0.48
2:C:98:TRP:HZ2	2:C:157:LEU:HD22	1.78	0.48
1:D:198:VAL:CG2	1:D:524:ALA:HB3	2.43	0.48
2:E:68:LEU:O	2:E:72:GLN:HG3	2.14	0.48
1:A:231:PHE:CZ	1:A:291:ILE:HG12	2.49	0.48
1:A:356:PRO:HG3	7:A:917:HOH:O	2.14	0.48
1:A:474:HIS:HB2	1:A:517:ALA:O	2.13	0.48
2:C:17:MET:HE3	2:C:163:TRP:CH2	2.49	0.48
2:E:75:ASP:HA	7:E:455:HOH:O	2.14	0.48
1:A:217:GLN:N	7:A:745:HOH:O	2.47	0.47
1:A:27:VAL:CG1	1:A:356:PRO:HB3	2.43	0.47
2:C:98:TRP:HH2	2:C:135:LEU:HD11	1.79	0.47
1:D:459:VAL:HG22	1:D:481:ILE:HG22	1.95	0.47
1:D:405:ASP:OD2	1:D:540:SER:HB3	2.13	0.47
1:A:268:THR:HA	7:A:861:HOH:O	2.14	0.47
1:A:26:GLN:O	1:A:30:GLN:HB2	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:HIS:ND1	1:A:380:THR:HG21	2.29	0.47
1:A:111:ILE:HG23	1:A:396:ALA:O	2.14	0.47
1:A:41:SER:O	2:B:143:PRO:HG2	2.13	0.47
2:B:102:VAL:O	2:B:107:THR:OG1	2.28	0.47
1:D:374:GLU:OE1	7:D:753:HOH:O	2.20	0.47
1:D:495:ASN:HB3	1:D:499:ARG:HH11	1.77	0.47
2:E:181:LYS:HG3	2:E:181:LYS:H	1.43	0.47
2:F:179:SER:HA	2:F:180:PRO:HD3	1.62	0.47
1:A:92:HIS:CE1	2:B:136:GLU:HA	2.50	0.47
2:B:24:ARG:NH1	2:B:197:LYS:HE3	2.23	0.47
2:C:185:TRP:O	2:C:188:ARG:HB3	2.15	0.47
1:D:126:ARG:NH2	1:D:178:GLY:O	2.47	0.47
1:D:313:VAL:HG13	1:D:314:PRO:HD3	1.96	0.47
1:D:450:LYS:HA	1:D:453:SER:HB3	1.96	0.47
1:D:494:CYS:SG	1:D:495:ASN:N	2.88	0.47
1:A:225:HIS:NE2	1:A:532:GLN:OE1	2.46	0.47
2:B:116:LYS:HD3	2:B:120:GLU:HG2	1.97	0.47
2:B:99:ALA:O	2:B:103:ASP:HB2	2.14	0.47
1:D:157:THR:OG1	1:D:469:SER:HB3	2.14	0.47
2:C:187:LYS:HE3	1:D:493:CYS:HA	1.96	0.47
1:D:97:ILE:HG13	1:D:556:ALA:CB	2.44	0.47
2:F:201:ASP:HB2	2:F:204:LYS:HG3	1.95	0.47
1:A:154:TYR:CE1	1:A:156:SER:HA	2.50	0.47
1:A:305:MET:HE1	1:A:325:LEU:HG	1.96	0.47
2:C:12:PRO:O	2:C:163:TRP:HZ2	1.97	0.47
2:C:153:VAL:HG23	2:C:156:SER:HB2	1.95	0.47
2:C:181:LYS:HA	2:C:184:ALA:HB3	1.97	0.47
2:C:57:LEU:HB3	2:C:64:VAL:HG22	1.96	0.47
1:D:363:PHE:CD2	1:D:382:VAL:HG21	2.48	0.47
1:D:450:LYS:HE2	1:D:450:LYS:HB3	1.65	0.47
1:A:309:MET:SD	1:A:545:PHE:CZ	3.08	0.47
1:A:437:THR:HG21	1:A:439:ARG:HH21	1.79	0.47
1:A:91:GLY:O	1:A:92:HIS:C	2.53	0.47
2:C:159:THR:HA	2:C:199:LEU:HD21	1.96	0.47
2:C:17:MET:HE3	2:C:163:TRP:HH2	1.80	0.47
2:C:33:ARG:CZ	2:C:43:LEU:HD21	2.44	0.47
2:F:129:ILE:HA	2:F:132:VAL:HG12	1.97	0.47
2:F:159:THR:HA	2:F:199:LEU:HD21	1.96	0.47
1:A:99:LEU:H	1:A:557:LYS:HG2	1.79	0.47
1:A:95:PRO:HD3	2:B:181:LYS:HZ2	1.79	0.47
1:D:143:LYS:O	1:D:216:VAL:HA	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:207:LEU:O	1:D:211:LEU:HG	2.14	0.47
2:F:141:ASP:HA	7:F:464:HOH:O	2.15	0.47
1:A:90:THR:N	7:A:789:HOH:O	2.28	0.47
1:D:172:ASN:HD21	1:D:174:ASN:CG	2.17	0.47
2:F:114:TRP:HD1	2:F:167:TYR:CE1	2.33	0.47
2:F:80:GLU:N	7:F:423:HOH:O	2.48	0.47
1:A:225:HIS:HB3	1:A:312:TYR:CD2	2.50	0.47
1:A:311:PRO:HB2	7:A:1024:HOH:O	2.14	0.47
5:B:301:GSH:OE1	7:B:418:HOH:O	2.21	0.47
2:C:138:GLU:HG3	2:C:145:PHE:HE1	1.80	0.47
2:C:24:ARG:HG3	2:C:30:PHE:CZ	2.49	0.47
2:C:16:GLY:HA2	2:C:55:PRO:HB3	1.96	0.47
1:D:147:PHE:HD2	1:D:529:ARG:NH1	2.10	0.47
1:D:78:LYS:HE2	1:D:554:SER:HB3	1.97	0.47
2:E:145:PHE:HB2	2:E:154:ASP:CG	2.36	0.47
2:F:130:GLU:O	2:F:134:ILE:HG22	2.15	0.47
2:F:145:PHE:HB3	2:F:153:VAL:CG1	2.44	0.47
2:F:176:GLU:N	2:F:176:GLU:CD	2.68	0.47
2:F:8:LEU:HD13	2:F:44:LEU:HB2	1.97	0.47
1:A:199:HIS:O	7:A:761:HOH:O	2.20	0.47
1:A:92:HIS:HB2	2:B:141:ASP:OD1	2.15	0.47
2:C:23:LEU:CD2	2:C:28:VAL:HG11	2.43	0.47
2:E:17:MET:SD	2:E:199:LEU:HG	2.55	0.47
2:F:57:LEU:HB3	2:F:64:VAL:HG22	1.97	0.47
2:F:90:TYR:OH	7:F:412:HOH:O	2.09	0.47
1:A:294:LEU:HB3	1:A:295:PHE:CD2	2.50	0.47
1:A:481:ILE:HG22	1:A:483:GLY:H	1.80	0.47
2:C:97:PHE:CE2	2:C:101:PHE:CZ	3.03	0.47
2:C:197:LYS:HE3	2:C:197:LYS:HB3	1.77	0.47
1:D:431:ILE:HD13	1:D:431:ILE:HA	1.68	0.47
1:D:448:ALA:CB	1:D:496:CYS:HB3	2.45	0.47
1:D:526:GLY:O	1:D:530:LYS:HG2	2.15	0.47
1:D:547:MET:HG3	7:D:726:HOH:O	2.15	0.47
2:E:163:TRP:HB3	2:E:167:TYR:CZ	2.49	0.47
2:E:20:ARG:NH1	7:E:429:HOH:O	2.44	0.47
2:F:11:TRP:CG	2:F:12:PRO:HD3	2.49	0.47
1:A:221:ALA:HB3	1:A:227:LEU:HG	1.96	0.46
2:B:202:SER:HB3	7:B:517:HOH:O	2.15	0.46
2:B:65:CYS:O	2:B:66:GLU:HB2	2.14	0.46
2:C:5:PRO:HG2	2:C:28:VAL:CG2	2.45	0.46
1:D:108:PRO:HA	7:D:842:HOH:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:75:PRO:HG2	1:D:76:TYR:HD1	1.80	0.46
2:F:26:LYS:HE2	2:F:75:ASP:HA	1.96	0.46
1:A:223:PHE:HE1	1:A:304:ILE:HD12	1.81	0.46
1:A:441:LEU:HG	1:A:462:PHE:HE2	1.80	0.46
1:D:316:LEU:HD23	1:D:320:ALA:HB2	1.98	0.46
1:D:537:GLY:N	7:D:767:HOH:O	2.37	0.46
2:F:174:SER:O	2:F:174:SER:OG	2.25	0.46
2:F:33:ARG:HH22	2:F:41:SER:HB2	1.81	0.46
1:A:246:LYS:HZ1	1:A:278:ARG:HH22	1.63	0.46
2:C:21:VAL:HG12	2:C:155:ILE:HG12	1.97	0.46
2:C:170:PHE:CD2	2:C:213:ARG:HD2	2.50	0.46
1:D:129:PHE:HZ	1:D:218:TYR:HH	1.63	0.46
1:D:274:ALA:O	1:D:277:ILE:HG13	2.15	0.46
1:D:29:LYS:O	1:D:33:LYS:HG2	2.15	0.46
1:D:82:ASP:HA	7:D:709:HOH:O	2.16	0.46
1:A:97:ILE:H	1:A:162:VAL:HA	1.79	0.46
1:D:152:LYS:HD3	1:D:561:ILE:CG2	2.39	0.46
1:D:219:VAL:HG21	1:D:231:PHE:HZ	1.80	0.46
1:D:238:TRP:O	1:D:242:VAL:HG12	2.16	0.46
1:A:242:VAL:HG11	1:A:278:ARG:HH21	1.80	0.46
2:C:177:SER:HB3	7:C:498:HOH:O	2.16	0.46
1:D:8:PHE:CG	1:D:182:ILE:HG22	2.50	0.46
1:D:489:VAL:O	1:D:492:ASP:HB2	2.15	0.46
1:D:521:ARG:HG3	1:D:569:SER:HB2	1.97	0.46
2:F:16:GLY:HA2	2:F:55:PRO:HB3	1.95	0.46
1:A:110:PHE:CE1	1:A:556:ALA:HB2	2.51	0.46
1:A:145:LEU:HB2	7:A:778:HOH:O	2.15	0.46
1:A:262:ALA:O	1:A:265:LYS:HG2	2.16	0.46
1:A:405:ASP:HB3	1:A:541:SER:CB	2.46	0.46
1:A:476:ALA:HA	1:A:519:GLU:O	2.16	0.46
1:A:390:VAL:CG2	1:A:540:SER:HA	2.45	0.46
1:A:70:ASP:HB3	1:A:109:LYS:HD2	1.98	0.46
2:B:164:PHE:HZ	2:B:182:LEU:HD11	1.81	0.46
1:A:79:ARG:NH1	2:B:188:ARG:HH12	2.13	0.46
1:D:284:LEU:HD13	1:D:287:TRP:N	2.30	0.46
1:D:313:VAL:CG1	1:D:314:PRO:HD3	2.45	0.46
1:D:390:VAL:HG11	1:D:540:SER:CB	2.45	0.46
2:E:22:ALA:HB1	2:E:74:VAL:HG11	1.96	0.46
2:E:26:LYS:HG3	2:E:82:ASN:ND2	2.30	0.46
1:A:222:VAL:HG11	1:A:533:GLU:O	2.16	0.46
1:A:497:LEU:HD11	7:A:940:HOH:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:97:ILE:CG1	1:D:162:VAL:HG13	2.45	0.46
1:D:480:GLU:HB2	1:D:528:PHE:CD1	2.50	0.46
1:D:74:GLU:O	1:D:78:LYS:HB2	2.16	0.46
2:E:154:ASP:O	2:E:158:ILE:HG13	2.16	0.46
2:F:135:LEU:HD13	2:F:182:LEU:CD1	2.46	0.46
1:A:208:SER:O	1:A:211:LEU:HB2	2.16	0.46
1:A:240:GLU:OE2	1:A:253:ARG:NE	2.43	0.46
1:A:34:GLU:C	1:A:38:LYS:HE3	2.35	0.46
1:A:87:PRO:CB	2:B:143:PRO:HA	2.40	0.46
2:B:169:LYS:HD3	2:B:206:VAL:HG13	1.96	0.46
2:C:51:HIS:CD2	7:C:489:HOH:O	2.68	0.46
2:C:57:LEU:HB3	2:C:64:VAL:CG2	2.46	0.46
2:C:187:LYS:HE3	1:D:492:ASP:C	2.36	0.46
2:E:149:SER:HB3	2:E:150:PHE:H	1.60	0.46
2:F:100:ASP:HA	7:F:431:HOH:O	2.16	0.46
1:A:143:LYS:HG3	1:A:144:ALA:N	2.28	0.46
1:A:166:THR:HG23	4:A:602:VAL:OXT	2.15	0.46
1:A:143:LYS:O	1:A:216:VAL:HA	2.16	0.46
1:A:210:ILE:HG12	1:A:294:LEU:HD11	1.98	0.46
1:A:326:VAL:HA	7:A:844:HOH:O	2.16	0.46
1:A:305:MET:CE	1:A:347:PRO:HG3	2.43	0.46
1:D:496:CYS:HA	1:D:499:ARG:CZ	2.46	0.46
2:E:18:ARG:NE	2:E:156:SER:O	2.41	0.46
2:F:201:ASP:OD2	2:F:204:LYS:HE2	2.16	0.46
1:A:17:PHE:HA	1:A:20:MET:HB3	1.97	0.46
1:A:210:ILE:HG12	1:A:294:LEU:HD21	1.98	0.46
1:A:309:MET:SD	1:A:312:TYR:HE2	2.39	0.46
1:D:135:ASP:HB2	7:D:827:HOH:O	2.16	0.46
1:D:439:ARG:O	1:D:443:LEU:HB2	2.16	0.46
1:D:68:VAL:HG11	1:D:73:LEU:HD23	1.97	0.46
2:E:10:TYR:HA	2:E:34:GLU:OE2	2.16	0.46
2:F:185:TRP:O	2:F:188:ARG:HB3	2.16	0.46
2:F:195:VAL:HG22	7:F:436:HOH:O	2.15	0.46
1:A:154:TYR:H	1:A:560:GLN:HA	1.81	0.45
1:A:77:ILE:HG23	1:A:80:MET:SD	2.55	0.45
2:C:97:PHE:CE2	2:C:101:PHE:HZ	2.34	0.45
1:D:451:ARG:HH11	1:D:454:GLU:CD	2.18	0.45
1:D:97:ILE:H	1:D:162:VAL:HA	1.80	0.45
2:E:128:PHE:HE2	2:E:175:ILE:HG12	1.81	0.45
2:F:126:LYS:O	2:F:129:ILE:HG13	2.15	0.45
2:F:5:PRO:HB3	2:F:59:HIS:NE2	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:SER:HA	7:A:732:HOH:O	2.16	0.45
2:B:6:ILE:O	2:B:57:LEU:HA	2.17	0.45
2:B:26:LYS:HZ3	2:B:82:ASN:H	1.56	0.45
1:D:410:ILE:HG13	1:D:411:GLY:N	2.30	0.45
2:E:16:GLY:O	2:E:20:ARG:HG3	2.15	0.45
2:E:9:ASP:OD1	2:E:16:GLY:HA3	2.16	0.45
1:A:101:SER:HB3	1:A:535:PHE:CG	2.52	0.45
1:A:203:TYR:HE1	1:A:241:ILE:HG13	1.81	0.45
1:A:281:CYS:HB3	1:A:287:TRP:HE1	1.80	0.45
1:D:231:PHE:CD1	1:D:290:LEU:HD22	2.50	0.45
1:D:315:LYS:HD2	1:D:315:LYS:HA	1.80	0.45
1:D:506:TYR:C	1:D:510:ARG:HE	2.19	0.45
2:E:23:LEU:HD23	2:E:23:LEU:HA	1.80	0.45
2:E:37:PHE:HA	2:E:40:LYS:HG2	1.97	0.45
2:F:11:TRP:O	7:F:404:HOH:O	2.21	0.45
2:F:32:TYR:CD1	2:F:34:GLU:OE2	2.69	0.45
1:A:128:ALA:HB1	7:A:754:HOH:O	2.16	0.45
1:A:151:SER:CB	1:A:194:PHE:HA	2.47	0.45
1:A:330:TYR:HE2	1:A:352:PHE:CD1	2.34	0.45
2:B:26:LYS:HZ1	2:B:82:ASN:H	1.57	0.45
1:D:370:GLY:HA2	1:D:371:GLU:HA	1.77	0.45
1:D:435:LYS:HB3	1:D:436:ASN:C	2.36	0.45
2:F:23:LEU:CD2	2:F:28:VAL:HG11	2.43	0.45
1:A:152:LYS:HG2	1:A:152:LYS:H	1.58	0.45
1:A:121:THR:HG22	1:A:336:TRP:HZ2	1.80	0.45
1:A:505:GLY:C	1:A:507:VAL:H	2.19	0.45
2:C:150:PHE:CE1	2:C:192:LYS:HG3	2.52	0.45
2:C:8:LEU:HD13	2:C:44:LEU:HB2	1.98	0.45
2:E:205:ILE:HG22	7:E:441:HOH:O	2.15	0.45
2:E:24:ARG:HD2	2:E:198:SER:OG	2.16	0.45
2:F:117:LYS:HA	2:F:121:GLN:HB2	1.98	0.45
1:A:97:ILE:HG23	1:A:111:ILE:H	1.82	0.45
1:A:276:THR:CG2	1:A:277:ILE:N	2.79	0.45
1:A:86:SER:HA	1:A:87:PRO:HD2	1.54	0.45
1:A:91:GLY:HA3	2:B:141:ASP:C	2.36	0.45
1:A:87:PRO:HB3	1:A:91:GLY:O	2.17	0.45
1:A:79:ARG:NH2	2:B:188:ARG:HH12	2.12	0.45
2:C:180:PRO:HB2	1:D:574:ALA:HB2	1.98	0.45
1:D:295:PHE:HA	1:D:296:PRO:HD2	1.86	0.45
2:E:107:THR:HG22	2:E:160:PHE:CE2	2.52	0.45
2:F:5:PRO:HB3	2:F:57:LEU:HD11	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:309:MET:CB	1:A:312:TYR:CE2	3.00	0.45
1:A:76:TYR:CD2	1:A:89:LEU:HD21	2.52	0.45
2:B:17:MET:HA	2:B:20:ARG:CG	2.47	0.45
2:C:144:TYR:HB3	2:C:154:ASP:CG	2.37	0.45
2:C:188:ARG:HA	2:C:188:ARG:HD3	1.84	0.45
1:D:331:GLY:HA3	1:D:336:TRP:HA	1.97	0.45
1:D:34:GLU:O	1:D:38:LYS:HG2	2.17	0.45
1:D:451:ARG:CZ	1:D:489:VAL:HG12	2.46	0.45
2:F:102:VAL:O	2:F:107:THR:HG23	2.16	0.45
1:A:222:VAL:HG23	7:A:819:HOH:O	2.16	0.45
1:A:363:PHE:HD1	1:A:390:VAL:HA	1.82	0.45
1:A:39:ASN:OD1	1:A:399:TYR:OH	2.35	0.45
1:A:498:ASP:OD2	7:A:763:HOH:O	2.21	0.45
1:D:273:LEU:HG	1:D:273:LEU:H	1.42	0.45
1:D:332:SER:HB3	1:D:538:LEU:HD12	1.98	0.45
1:D:69:THR:OG1	1:D:71:VAL:HG12	2.16	0.45
2:E:92:ARG:HG3	2:E:96:ARG:HH12	1.82	0.45
2:F:12:PRO:O	2:F:163:TRP:CZ2	2.70	0.45
2:F:26:LYS:HD2	2:F:74:VAL:CG1	2.47	0.45
1:A:143:LYS:CE	1:A:187:CYS:HB3	2.47	0.45
1:A:206:LEU:HD11	1:A:241:ILE:HD11	1.98	0.45
1:A:358:LEU:HA	7:A:828:HOH:O	2.16	0.45
1:A:525:LYS:HD3	7:A:833:HOH:O	2.15	0.45
1:A:108:PRO:CB	1:A:555:ASN:HB2	2.43	0.45
2:B:122:GLU:OE2	2:B:125:LYS:NZ	2.42	0.45
2:B:165:GLN:HA	2:B:168:GLU:OE2	2.17	0.45
2:C:24:ARG:NH1	2:C:30:PHE:HZ	2.15	0.45
1:D:26:GLN:O	1:D:30:GLN:HB2	2.17	0.45
1:D:288:TYR:HA	1:D:318:HIS:HD2	1.79	0.45
1:D:430:SER:OG	1:D:431:ILE:N	2.49	0.45
1:D:534:HIS:NE2	1:D:557:LYS:HD3	2.32	0.45
2:E:48:ASN:OD1	2:E:50:ILE:HD11	2.16	0.45
1:A:188:SER:HB3	1:A:192:VAL:HG13	1.98	0.45
1:A:241:ILE:HA	1:A:244:ASP:OD1	2.16	0.45
1:A:310:GLU:HG3	1:A:311:PRO:CD	2.47	0.45
2:B:48:ASN:HD22	2:B:53:LYS:H	1.65	0.45
2:C:163:TRP:HD1	7:C:484:HOH:O	2.00	0.45
2:C:184:ALA:CB	1:D:499:ARG:NH1	2.75	0.45
1:D:55:THR:C	1:D:57:PRO:HD3	2.36	0.45
2:E:108:ASP:O	2:E:112:LYS:HG2	2.17	0.45
1:A:58:GLU:OE2	1:A:360:TYR:OH	2.34	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:384:ILE:HA	1:A:409:VAL:HG12	1.98	0.44
2:C:8:LEU:CD2	2:C:33:ARG:NH2	2.80	0.44
1:D:150:SER:OG	1:D:170:TYR:HB2	2.17	0.44
1:D:288:TYR:CE1	1:D:318:HIS:HA	2.52	0.44
2:F:145:PHE:HB3	2:F:153:VAL:HG13	1.98	0.44
1:A:224:ALA:HA	1:A:227:LEU:CD1	2.43	0.44
1:A:25:HIS:CD2	1:A:25:HIS:H	2.33	0.44
2:C:11:TRP:CG	2:C:12:PRO:HD3	2.52	0.44
2:C:153:VAL:HG21	7:C:406:HOH:O	2.17	0.44
1:D:133:ASN:OD1	1:D:138:ILE:HG12	2.16	0.44
1:D:150:SER:HB2	1:D:167:THR:CA	2.40	0.44
1:D:188:SER:HB3	1:D:192:VAL:CG1	2.47	0.44
1:D:206:LEU:HD13	1:D:234:PHE:HD1	1.82	0.44
2:F:125:LYS:HB2	7:F:470:HOH:O	2.16	0.44
2:F:173:PHE:HB3	2:F:174:SER:H	1.47	0.44
1:A:176:LYS:O	1:A:180:LYS:HB2	2.18	0.44
2:B:17:MET:HG3	2:B:20:ARG:NH1	2.33	0.44
2:C:128:PHE:O	2:C:132:VAL:HG12	2.17	0.44
1:D:219:VAL:HB	1:D:295:PHE:CE1	2.52	0.44
1:D:338:ALA:HA	1:D:354:VAL:HA	1.99	0.44
1:D:485:THR:OG1	1:D:486:ASN:N	2.50	0.44
1:A:147:PHE:HE1	1:A:206:LEU:HB3	1.83	0.44
1:A:217:GLN:CG	1:A:218:TYR:CD2	3.00	0.44
1:A:232:ARG:HA	1:A:235:GLU:CG	2.48	0.44
1:A:351:THR:N	7:A:787:HOH:O	2.50	0.44
1:A:413:TYR:N	1:A:416:THR:O	2.47	0.44
1:A:498:ASP:OD1	1:A:518:LEU:HD12	2.17	0.44
2:B:23:LEU:HD22	2:B:28:VAL:HG11	1.99	0.44
2:C:187:LYS:HE3	1:D:492:ASP:O	2.18	0.44
2:C:204:LYS:HE2	1:D:456:LYS:HZ3	1.81	0.44
2:C:48:ASN:ND2	7:C:423:HOH:O	2.12	0.44
2:C:68:LEU:HD23	2:C:103:ASP:OD2	2.17	0.44
1:D:329:ASP:OD1	1:D:329:ASP:N	2.50	0.44
1:D:31:THR:O	1:D:35:ILE:HG13	2.18	0.44
1:D:449:ALA:HB1	1:D:459:VAL:HG23	1.98	0.44
1:D:549:ARG:HD3	1:D:549:ARG:HA	1.75	0.44
1:D:92:HIS:ND1	2:E:181:LYS:O	2.51	0.44
2:E:121:GLN:HG3	7:E:410:HOH:O	2.17	0.44
2:E:40:LYS:HZ3	2:E:52:LYS:HB2	1.76	0.44
2:E:92:ARG:CZ	2:E:96:ARG:NH1	2.80	0.44
2:F:10:TYR:CD2	2:F:12:PRO:HD2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:141:ASP:N	2:F:141:ASP:OD1	2.50	0.44
1:A:552:LYS:HA	1:A:552:LYS:HD2	1.53	0.44
1:A:97:ILE:O	1:A:556:ALA:HB1	2.18	0.44
1:A:55:THR:C	1:A:57:PRO:HD3	2.37	0.44
1:A:97:ILE:CG2	1:A:111:ILE:H	2.29	0.44
2:B:7:LEU:HD23	2:B:32:TYR:HD1	1.82	0.44
1:D:122:LEU:HD12	1:D:123:GLN:N	2.33	0.44
1:D:143:LYS:NZ	1:D:187:CYS:HA	2.33	0.44
1:D:328:HIS:CG	1:D:329:ASP:H	2.36	0.44
1:D:38:LYS:HD2	1:D:38:LYS:HA	1.84	0.44
1:D:99:LEU:HD13	1:D:555:ASN:OD1	2.18	0.44
1:D:95:PRO:HD3	2:E:181:LYS:HE3	1.99	0.44
2:E:175:ILE:HB	2:E:183:ILE:HD11	1.99	0.44
2:E:98:TRP:CZ2	2:E:135:LEU:HA	2.52	0.44
1:A:479:TRP:O	1:A:523:VAL:HG12	2.17	0.44
1:A:92:HIS:HB3	2:B:181:LYS:HZ1	1.83	0.44
2:B:62:LYS:NZ	2:C:94:GLN:HG3	2.32	0.44
1:D:194:PHE:O	7:D:757:HOH:O	2.21	0.44
1:D:97:ILE:HG12	1:D:162:VAL:HG13	1.99	0.44
2:E:128:PHE:HD1	7:E:411:HOH:O	2.00	0.44
2:E:92:ARG:NH1	2:E:96:ARG:NH1	2.66	0.44
1:A:70:ASP:OD2	1:A:104:SER:HA	2.18	0.44
1:A:233:THR:CG2	1:A:525:LYS:NZ	2.81	0.44
1:A:527:THR:HB	7:A:749:HOH:O	2.16	0.44
2:B:101:PHE:HA	7:B:474:HOH:O	2.17	0.44
2:B:186:ALA:O	2:B:190:MET:HG2	2.17	0.44
2:C:188:ARG:NH1	1:D:499:ARG:C	2.61	0.44
1:D:434:ASP:O	1:D:435:LYS:HG3	2.18	0.44
1:D:84:ASP:C	1:D:86:SER:H	2.21	0.44
2:F:10:TYR:HB3	2:F:13:SER:HB2	1.99	0.44
1:A:112:PRO:HD2	1:A:396:ALA:O	2.17	0.44
1:A:111:ILE:HA	1:A:112:PRO:HD3	1.78	0.44
1:A:13:VAL:HG11	7:A:771:HOH:O	2.17	0.44
1:A:305:MET:SD	1:A:325:LEU:HG	2.58	0.44
1:A:38:LYS:NZ	1:A:395:TYR:CE1	2.78	0.44
1:A:434:ASP:HB2	1:A:550:CYS:HB3	2.00	0.44
2:B:139:LEU:HD23	2:B:142:LYS:H	1.81	0.44
2:B:151:GLY:O	2:B:155:ILE:HG23	2.18	0.44
2:C:9:ASP:HB2	2:C:20:ARG:NH2	2.33	0.44
1:D:125:PHE:CE1	1:D:129:PHE:HE1	2.36	0.44
1:D:130:ALA:O	7:D:754:HOH:O	2.20	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:203:TYR:OH	1:D:254:ILE:HG23	2.17	0.44
1:D:270:ASN:HA	1:D:271:PRO:HD2	1.75	0.44
1:D:23:ASN:O	1:D:27:VAL:HG23	2.18	0.44
1:D:359:GLY:HA3	1:D:361:PHE:HE1	1.83	0.44
1:D:455:GLU:OE1	1:D:485:THR:HB	2.17	0.44
1:D:81:VAL:HA	1:D:160:VAL:HG11	1.98	0.44
2:E:148:ASP:N	2:E:148:ASP:OD1	2.51	0.44
2:E:88:ASP:HB2	2:E:90:TYR:CE1	2.53	0.44
2:E:95:ALA:O	2:E:99:ALA:N	2.47	0.44
1:A:189:PRO:O	1:A:192:VAL:HG12	2.18	0.44
1:A:190:ASP:HA	1:A:193:ILE:HD12	2.00	0.44
1:A:212:PHE:O	1:A:216:VAL:HG23	2.17	0.44
1:A:23:ASN:O	1:A:27:VAL:HG12	2.17	0.44
1:A:281:CYS:O	1:A:287:TRP:CZ2	2.71	0.44
1:A:409:VAL:HG13	7:A:794:HOH:O	2.17	0.44
1:A:92:HIS:CG	2:B:181:LYS:HE3	2.53	0.44
2:B:26:LYS:NZ	2:B:82:ASN:N	2.49	0.44
2:C:142:LYS:HG2	2:C:144:TYR:H	1.83	0.44
1:D:108:PRO:HB3	1:D:555:ASN:N	2.32	0.44
1:D:10:MET:HE3	1:D:133:ASN:HD22	1.83	0.44
1:D:142:GLY:O	1:D:185:PRO:HD2	2.18	0.44
1:D:496:CYS:N	1:D:499:ARG:HH12	2.16	0.44
1:D:80:MET:HE3	1:D:94:VAL:HG22	2.00	0.44
2:F:188:ARG:HD3	2:F:188:ARG:HA	1.56	0.44
2:F:26:LYS:HD2	2:F:74:VAL:HG13	2.00	0.44
2:F:54:ILE:HB	2:F:55:PRO:HA	2.00	0.44
1:A:138:ILE:HD13	1:A:138:ILE:HA	1.76	0.43
1:A:202:LEU:HA	1:A:205:HIS:HB2	2.00	0.43
1:A:309:MET:SD	1:A:312:TYR:CE2	3.11	0.43
1:A:231:PHE:HB2	1:A:319:TYR:CE2	2.53	0.43
1:A:222:VAL:HG22	3:A:601:JAA:C07	2.48	0.43
1:A:99:LEU:HD22	1:A:555:ASN:OD1	2.18	0.43
1:A:114:THR:OG1	2:B:141:ASP:OD2	2.31	0.43
2:B:51:HIS:HD2	2:B:53:LYS:HE2	1.76	0.43
1:D:534:HIS:CE1	1:D:557:LYS:HD3	2.53	0.43
1:D:7:THR:HG21	7:D:990:HOH:O	2.18	0.43
1:A:109:LYS:HE3	1:A:109:LYS:HB2	1.67	0.43
1:A:229:HIS:O	1:A:233:THR:N	2.47	0.43
1:A:572:SER:HA	7:A:703:HOH:O	2.18	0.43
2:C:195:VAL:HG11	7:C:432:HOH:O	2.18	0.43
2:C:71:VAL:O	2:C:74:VAL:HB	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:164:THR:HG22	1:D:166:THR:H	1.83	0.43
1:D:446:GLU:HG2	7:D:1050:HOH:O	2.19	0.43
2:E:106:PHE:O	7:E:411:HOH:O	2.21	0.43
2:E:68:LEU:HD13	2:E:99:ALA:HB1	2.00	0.43
2:E:82:ASN:N	2:E:82:ASN:OD1	2.51	0.43
2:F:12:PRO:O	2:F:163:TRP:HZ2	2.02	0.43
1:A:143:LYS:HE2	1:A:216:VAL:CG2	2.49	0.43
1:A:309:MET:C	1:A:311:PRO:HD2	2.38	0.43
1:A:99:LEU:HB3	1:A:557:LYS:CB	2.47	0.43
2:B:11:TRP:HZ2	2:B:208:TYR:CE1	2.36	0.43
2:C:99:ALA:HA	7:C:406:HOH:O	2.18	0.43
1:D:132:ARG:O	1:D:136:PHE:N	2.38	0.43
1:D:27:VAL:HG11	1:D:356:PRO:HG2	2.00	0.43
1:D:363:PHE:CE1	1:D:390:VAL:HG23	2.52	0.43
1:D:387:GLU:HG3	1:D:408:LYS:HB2	2.01	0.43
1:D:408:LYS:HG3	1:D:409:VAL:N	2.32	0.43
2:E:135:LEU:HD22	2:E:182:LEU:HD21	1.99	0.43
2:E:15:PHE:HB3	2:E:67:SER:CB	2.48	0.43
1:A:219:VAL:HG13	1:A:301:VAL:HG13	2.00	0.43
1:A:288:TYR:CZ	1:A:321:GLY:HA2	2.53	0.43
1:A:475:TYR:HB2	1:A:518:LEU:HD23	2.00	0.43
1:A:494:CYS:SG	1:A:495:ASN:N	2.91	0.43
1:A:102:GLY:N	1:A:546:LYS:O	2.48	0.43
2:B:121:GLN:O	2:B:125:LYS:HG3	2.19	0.43
1:A:41:SER:OG	2:B:142:LYS:HE3	2.18	0.43
1:D:67:LEU:HB3	7:D:856:HOH:O	2.18	0.43
2:E:126:LYS:O	2:E:130:GLU:HG3	2.18	0.43
1:D:91:GLY:HA3	2:E:142:LYS:HA	1.99	0.43
2:E:201:ASP:HB3	2:E:203:GLU:HG2	2.00	0.43
2:E:37:PHE:HE1	2:E:40:LYS:HZ2	1.67	0.43
2:F:98:TRP:CD1	2:F:153:VAL:HG21	2.53	0.43
2:F:181:LYS:O	2:F:185:TRP:N	2.40	0.43
1:A:195:SER:OG	1:A:259:VAL:HG21	2.17	0.43
1:A:370:GLY:HA2	1:A:371:GLU:HA	1.62	0.43
1:A:423:CYS:HA	7:A:747:HOH:O	2.18	0.43
1:A:434:ASP:O	1:A:435:LYS:HG3	2.18	0.43
1:A:537:GLY:HA3	3:A:601:JAA:O02	2.19	0.43
2:B:65:CYS:SG	2:C:97:PHE:CZ	3.06	0.43
1:D:110:PHE:CD1	1:D:556:ALA:HB2	2.53	0.43
1:D:198:VAL:HG22	1:D:565:ASN:ND2	2.24	0.43
1:D:435:LYS:HA	1:D:436:ASN:HB2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:88:ASP:HA	2:E:89:PRO:HD3	1.86	0.43
2:F:10:TYR:CG	2:F:12:PRO:HD2	2.53	0.43
1:A:151:SER:CA	1:A:194:PHE:HA	2.49	0.43
1:A:250:LEU:HD21	1:A:260:ARG:HG2	2.00	0.43
1:A:274:ALA:O	1:A:278:ARG:NE	2.52	0.43
1:A:478:PHE:HZ	1:A:562:LEU:HA	1.79	0.43
2:B:112:LYS:HB2	7:B:414:HOH:O	2.18	0.43
2:B:93:ALA:HB1	2:C:73:TYR:CE1	2.54	0.43
1:D:413:TYR:O	1:D:416:THR:HG22	2.18	0.43
1:D:92:HIS:H	2:E:141:ASP:C	2.22	0.43
2:E:169:LYS:NZ	2:E:206:VAL:HG11	2.33	0.43
2:E:206:VAL:HA	7:E:441:HOH:O	2.18	0.43
1:A:337:ILE:HG13	7:A:764:HOH:O	2.18	0.43
1:A:475:TYR:HB2	1:A:518:LEU:CD2	2.48	0.43
1:A:527:THR:HG22	1:A:528:PHE:CD1	2.53	0.43
2:C:149:SER:HB3	2:C:150:PHE:H	1.71	0.43
1:D:444:SER:HA	1:D:500:ALA:CB	2.48	0.43
1:D:521:ARG:HH11	1:D:521:ARG:HG3	1.83	0.43
1:D:77:ILE:HG12	1:D:110:PHE:O	2.19	0.43
2:E:16:GLY:O	2:E:20:ARG:NE	2.50	0.43
2:E:85:PHE:CD1	2:E:85:PHE:N	2.87	0.43
2:F:194:SER:O	2:F:198:SER:OG	2.20	0.43
1:A:116:GLU:OE2	1:A:395:TYR:CE1	2.72	0.43
1:A:91:GLY:HA3	2:B:142:LYS:C	2.39	0.43
2:C:54:ILE:N	7:C:428:HOH:O	2.50	0.43
2:C:62:LYS:HA	2:C:63:PRO:HD2	1.87	0.43
2:C:190:MET:HB3	1:D:450:LYS:HG3	2.00	0.43
2:E:109:ALA:HB3	7:E:411:HOH:O	2.18	0.43
1:D:39:ASN:HA	2:E:142:LYS:CG	2.49	0.43
1:D:87:PRO:CB	2:E:143:PRO:HA	2.45	0.43
2:E:164:PHE:CD2	2:E:183:ILE:HG12	2.53	0.43
2:F:4:LEU:HA	2:F:5:PRO:HD3	1.69	0.43
2:F:8:LEU:HD22	2:F:33:ARG:NH2	2.26	0.43
2:F:98:TRP:O	2:F:98:TRP:CE3	2.72	0.43
1:A:135:ASP:HB2	7:A:929:HOH:O	2.17	0.43
1:A:25:HIS:HD2	7:A:889:HOH:O	2.02	0.43
1:A:429:LEU:HD12	1:A:429:LEU:HA	1.79	0.43
1:A:555:ASN:O	1:A:559:LEU:HD22	2.19	0.43
1:A:222:VAL:HG13	3:A:601:JAA:C06	2.48	0.43
1:A:96:ALA:HB3	1:A:113:PHE:CD2	2.53	0.43
1:D:316:LEU:O	1:D:320:ALA:N	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:36:LEU:HD13	1:D:61:PHE:CE2	2.54	0.43
1:D:424:ARG:O	1:D:543:GLY:HA2	2.18	0.43
1:D:96:ALA:O	1:D:113:PHE:HB3	2.19	0.43
2:E:24:ARG:NH1	2:E:198:SER:OG	2.51	0.43
2:E:48:ASN:HB3	2:E:52:LYS:HA	2.01	0.43
2:E:62:LYS:HA	2:E:63:PRO:HD2	1.79	0.43
1:A:213:ARG:HG3	1:A:214:ASP:N	2.34	0.43
1:A:56:ASP:HB2	1:A:59:GLU:HB2	2.01	0.43
1:D:124:LEU:HB3	3:D:601:JAA:C15	2.49	0.43
1:D:362:GLU:HG3	1:D:400:ARG:HH22	1.82	0.43
1:D:575:PHE:O	7:D:756:HOH:O	2.21	0.43
2:E:161:SER:HA	2:E:164:PHE:CG	2.54	0.43
2:E:26:LYS:HB2	2:E:26:LYS:HE2	1.91	0.43
2:F:33:ARG:HH22	2:F:41:SER:CB	2.31	0.43
1:A:291:ILE:HD11	1:A:316:LEU:HD11	2.01	0.42
1:A:303:GLY:O	1:A:327:SER:HA	2.19	0.42
1:A:33:LYS:HA	1:A:36:LEU:HD23	2.00	0.42
1:A:66:PRO:HD3	7:A:723:HOH:O	2.19	0.42
1:A:70:ASP:OD1	1:A:71:VAL:N	2.52	0.42
1:A:97:ILE:HA	1:A:111:ILE:O	2.19	0.42
2:C:104:LYS:NZ	7:C:439:HOH:O	2.39	0.42
2:C:114:TRP:HA	2:C:170:PHE:CD2	2.49	0.42
1:D:402:ARG:NH2	7:D:759:HOH:O	2.21	0.42
1:D:407:VAL:HG21	7:D:920:HOH:O	2.19	0.42
1:A:274:ALA:CB	1:A:278:ARG:CZ	2.96	0.42
1:A:238:TRP:CZ2	1:A:281:CYS:HB2	2.54	0.42
1:A:355:ILE:HA	1:A:356:PRO:HD3	1.49	0.42
1:A:389:GLU:OE2	1:A:402:ARG:HG2	2.19	0.42
2:B:18:ARG:HG2	2:B:159:THR:HG21	2.00	0.42
2:B:86:PRO:HD3	2:B:146:GLY:O	2.20	0.42
2:C:4:LEU:HA	2:C:5:PRO:HD3	1.65	0.42
1:D:224:ALA:HA	1:D:316:LEU:HD12	2.00	0.42
1:D:229:HIS:O	1:D:233:THR:HG23	2.20	0.42
1:D:32:LEU:O	1:D:35:ILE:HB	2.20	0.42
1:D:32:LEU:HD13	1:D:360:TYR:CD2	2.54	0.42
1:D:365:PRO:HD2	1:D:374:GLU:HG2	2.01	0.42
1:D:163:GLY:HA2	1:D:560:GLN:HB2	2.02	0.42
2:F:145:PHE:CE2	2:F:157:LEU:HD21	2.53	0.42
2:F:169:LYS:HD3	2:F:206:VAL:HG13	2.01	0.42
1:A:145:LEU:HD13	1:A:209:GLY:CA	2.43	0.42
1:A:154:TYR:CZ	1:A:559:LEU:HD23	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:SER:HB2	2:B:188:ARG:HB2	2.02	0.42
2:B:15:PHE:O	2:B:18:ARG:HB2	2.19	0.42
2:B:194:SER:O	2:B:198:SER:HB2	2.19	0.42
2:C:17:MET:HE2	2:C:200:PRO:HD2	2.01	0.42
1:D:168:ASN:HB2	7:D:770:HOH:O	2.19	0.42
1:D:28:GLN:HA	7:D:734:HOH:O	2.19	0.42
1:D:452:LEU:HD13	1:D:493:CYS:SG	2.59	0.42
2:F:187:LYS:HG2	2:F:187:LYS:O	2.18	0.42
1:A:248:GLY:O	1:A:267:LEU:HB3	2.20	0.42
2:B:27:GLY:HA2	7:B:503:HOH:O	2.19	0.42
1:D:196:PRO:O	1:D:565:ASN:HA	2.19	0.42
1:D:494:CYS:HB2	1:D:520:LEU:HB3	2.01	0.42
2:F:26:LYS:CG	2:F:81:LYS:HZ3	2.30	0.42
1:A:167:THR:HG21	1:A:560:GLN:CG	2.50	0.42
1:A:244:ASP:HB2	1:A:251:SER:H	1.85	0.42
1:A:504:ALA:O	1:A:507:VAL:HB	2.19	0.42
1:A:524:ALA:HB2	1:A:567:VAL:CG1	2.50	0.42
1:A:532:GLN:NE2	7:A:777:HOH:O	2.25	0.42
2:B:51:HIS:HB2	2:B:53:LYS:HG2	2.01	0.42
1:D:111:ILE:HA	1:D:112:PRO:HD3	1.90	0.42
1:D:184:SER:HB3	7:D:733:HOH:O	2.18	0.42
1:D:253:ARG:NH2	7:D:819:HOH:O	2.52	0.42
1:D:44:TYR:OH	1:D:68:VAL:HG22	2.18	0.42
1:D:501:PHE:CE2	1:D:518:LEU:HD21	2.54	0.42
2:E:150:PHE:CD2	2:E:192:LYS:HD2	2.54	0.42
2:E:6:ILE:HG23	2:E:31:GLU:HB3	2.02	0.42
1:A:213:ARG:HA	1:A:216:VAL:HG23	2.01	0.42
1:A:32:LEU:HD22	1:A:360:TYR:CD2	2.54	0.42
1:A:198:VAL:HG22	1:A:524:ALA:HB3	2.00	0.42
2:B:139:LEU:HD21	2:B:142:LYS:H	1.84	0.42
1:A:95:PRO:HD3	2:B:181:LYS:NZ	2.34	0.42
2:B:197:LYS:HE3	2:B:197:LYS:HB2	1.73	0.42
1:D:305:MET:HB3	1:D:347:PRO:HB3	2.02	0.42
2:F:216:ASN:HA	7:F:459:HOH:O	2.19	0.42
2:F:57:LEU:HB3	2:F:64:VAL:CG2	2.50	0.42
1:A:143:LYS:HZ1	1:A:212:PHE:H	1.67	0.42
1:A:27:VAL:HG11	1:A:356:PRO:HB3	2.01	0.42
1:A:351:THR:HG21	1:A:410:ILE:CG1	2.46	0.42
1:A:152:LYS:HD3	1:A:565:ASN:ND2	2.34	0.42
1:A:92:HIS:HE1	2:B:136:GLU:HA	1.84	0.42
2:B:149:SER:HB2	2:B:150:PHE:H	1.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:65:CYS:O	2:B:69:ASN:HB3	2.19	0.42
1:D:41:SER:HA	2:E:147:GLY:O	2.20	0.42
1:D:534:HIS:CD2	1:D:535:PHE:CD1	3.08	0.42
1:D:534:HIS:HD2	1:D:535:PHE:CD1	2.38	0.42
1:D:98:SER:C	1:D:556:ALA:HB3	2.40	0.42
1:D:97:ILE:HG13	1:D:556:ALA:HB1	2.01	0.42
2:F:140:GLY:N	2:F:181:LYS:HZ1	2.18	0.42
2:F:26:LYS:HE3	2:F:78:TRP:O	2.19	0.42
1:A:222:VAL:HG12	1:A:223:PHE:CD1	2.55	0.42
1:A:238:TRP:CZ3	1:A:277:ILE:HG12	2.55	0.42
1:A:509:SER:HB3	1:A:515:ILE:HG12	2.02	0.42
1:D:384:ILE:H	1:D:384:ILE:HG13	1.60	0.42
1:D:551:VAL:HG23	1:D:555:ASN:H	1.84	0.42
2:E:102:VAL:HA	2:E:106:PHE:HB2	2.01	0.42
2:F:102:VAL:O	2:F:106:PHE:HB3	2.20	0.42
1:A:117:LEU:O	1:A:121:THR:HG23	2.19	0.42
1:A:237:VAL:HB	7:A:757:HOH:O	2.20	0.42
1:A:246:LYS:NZ	1:A:278:ARG:NH2	2.63	0.42
1:A:390:VAL:HG21	1:A:540:SER:HA	2.02	0.42
1:A:98:SER:C	1:A:556:ALA:HB3	2.40	0.42
1:A:566:VAL:HG13	1:A:568:SER:C	2.41	0.42
1:A:79:ARG:HH11	1:A:88:ILE:CD1	2.32	0.42
2:B:21:VAL:O	2:B:25:GLU:HB2	2.19	0.42
2:B:50:ILE:HG13	2:C:134:ILE:CD1	2.47	0.42
2:B:8:LEU:HD21	2:B:43:LEU:HD13	2.01	0.42
2:C:126:LYS:O	2:C:129:ILE:HG13	2.20	0.42
1:D:124:LEU:HD21	1:D:329:ASP:HB2	2.02	0.42
1:D:233:THR:HG22	7:D:748:HOH:O	2.19	0.42
1:D:408:LYS:O	1:D:419:LEU:HA	2.20	0.42
1:D:477:ILE:O	1:D:520:LEU:HD12	2.20	0.42
1:D:101:SER:N	1:D:535:PHE:CZ	2.87	0.42
2:E:7:LEU:CD1	2:E:9:ASP:HB2	2.49	0.42
5:F:301:GSH:N1	7:F:425:HOH:O	2.25	0.42
1:A:94:VAL:HG11	1:A:112:PRO:HB3	2.01	0.42
1:A:198:VAL:O	1:A:202:LEU:HD12	2.20	0.42
1:A:217:GLN:HG3	1:A:218:TYR:HD2	1.84	0.42
1:A:242:VAL:HG11	1:A:278:ARG:NH2	2.34	0.42
1:A:305:MET:HG3	7:A:715:HOH:O	2.20	0.42
1:A:310:GLU:N	1:A:311:PRO:HD2	2.34	0.42
1:A:491:GLN:NE2	1:A:570:TYR:CD2	2.88	0.42
1:A:98:SER:OG	1:A:111:ILE:HB	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:108:PRO:HB3	1:D:555:ASN:CB	2.50	0.42
1:D:10:MET:HE1	1:D:133:ASN:HB3	2.00	0.42
1:D:277:ILE:HD12	1:D:278:ARG:N	2.35	0.42
1:D:364:LEU:HB2	1:D:402:ARG:HH22	1.84	0.42
1:D:523:VAL:HG23	7:D:785:HOH:O	2.20	0.42
2:E:33:ARG:NH2	2:E:43:LEU:HD13	2.35	0.42
2:F:21:VAL:HG12	2:F:155:ILE:HG12	2.01	0.42
1:A:284:LEU:C	1:A:284:LEU:HD12	2.41	0.41
1:A:392:ILE:HG13	1:A:401:TYR:HB3	2.02	0.41
1:A:532:GLN:O	1:A:535:PHE:N	2.49	0.41
2:B:110:GLN:O	2:B:113:VAL:HB	2.20	0.41
2:C:26:LYS:HE3	2:C:78:TRP:O	2.19	0.41
2:C:8:LEU:HG	2:C:56:VAL:HB	2.02	0.41
1:D:118:MET:HG2	1:D:172:ASN:ND2	2.35	0.41
1:D:95:PRO:O	1:D:161:PRO:HB2	2.20	0.41
1:D:254:ILE:N	1:D:254:ILE:HD13	2.35	0.41
1:D:403:LEU:HD23	1:D:403:LEU:HA	1.51	0.41
1:D:465:TYR:HD1	1:D:551:VAL:HG13	1.84	0.41
1:D:485:THR:OG1	7:D:755:HOH:O	2.21	0.41
1:A:224:ALA:HB3	1:A:312:TYR:CD1	2.54	0.41
1:A:31:THR:OG1	1:A:357:ASN:HA	2.20	0.41
1:A:510:ARG:HB3	1:A:575:PHE:CE2	2.55	0.41
2:B:193:GLU:HB3	2:B:197:LYS:HE2	2.01	0.41
2:B:34:GLU:HA	7:B:465:HOH:O	2.20	0.41
2:B:4:LEU:HA	2:B:5:PRO:HD3	1.83	0.41
2:C:36:ASP:O	2:C:39:ASN:N	2.47	0.41
2:C:72:GLN:OE1	7:C:426:HOH:O	2.22	0.41
2:C:81:LYS:HG3	2:C:82:ASN:H	1.85	0.41
1:D:156:SER:OG	7:D:709:HOH:O	2.04	0.41
1:D:169:VAL:O	1:D:175:PHE:HB2	2.20	0.41
1:A:105:GLN:N	7:A:829:HOH:O	2.46	0.41
1:A:107:ARG:NH2	7:A:746:HOH:O	2.53	0.41
1:A:188:SER:HB3	1:A:192:VAL:CG1	2.51	0.41
1:A:238:TRP:HA	1:A:241:ILE:CG1	2.50	0.41
1:A:314:PRO:CB	1:A:317:ARG:HH12	2.33	0.41
1:A:471:ASP:HA	1:A:472:PRO:HA	1.80	0.41
2:B:126:LYS:O	2:B:130:GLU:HG2	2.21	0.41
2:C:8:LEU:HD23	2:C:8:LEU:N	2.35	0.41
1:D:250:LEU:HB2	1:D:254:ILE:HG13	2.02	0.41
1:D:446:GLU:HG3	7:D:824:HOH:O	2.20	0.41
1:D:453:SER:HB2	7:D:786:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:184:ALA:CB	1:D:499:ARG:CZ	2.85	0.41
1:D:90:THR:OG1	1:D:397:GLY:HA2	2.20	0.41
2:F:110:GLN:O	2:F:113:VAL:HG12	2.20	0.41
1:A:145:LEU:HD21	1:A:147:PHE:CZ	2.55	0.41
1:A:196:PRO:HG2	1:A:256:VAL:HG11	2.01	0.41
1:A:282:MET:HG3	1:A:283:SER:N	2.36	0.41
1:A:310:GLU:O	1:A:314:PRO:HD3	2.21	0.41
1:A:384:ILE:HA	1:A:409:VAL:CG1	2.49	0.41
1:A:80:MET:HE1	1:A:94:VAL:HG22	2.02	0.41
2:C:110:GLN:O	2:C:113:VAL:HG12	2.20	0.41
1:D:425:ARG:HH12	1:D:546:LYS:HE3	1.84	0.41
2:B:53:LYS:HD3	5:B:301:GSH:HB13	2.02	0.41
2:B:8:LEU:HD22	2:B:35:GLU:OE2	2.19	0.41
2:C:9:ASP:HB2	2:C:20:ARG:HH21	1.85	0.41
1:D:192:VAL:HA	1:D:195:SER:HB2	2.01	0.41
1:D:445:VAL:HG13	1:D:479:TRP:NE1	2.34	0.41
1:D:521:ARG:HG3	1:D:521:ARG:NH1	2.35	0.41
1:D:480:GLU:HB2	1:D:528:PHE:HD1	1.85	0.41
1:D:94:VAL:HG21	1:D:97:ILE:CG2	2.51	0.41
2:E:86:PRO:HD2	2:E:92:ARG:HA	2.02	0.41
1:A:154:TYR:HE2	1:A:162:VAL:HG22	1.85	0.41
1:A:225:HIS:HB3	1:A:312:TYR:CZ	2.53	0.41
1:A:35:ILE:O	1:A:39:ASN:HB2	2.20	0.41
2:B:70:VAL:O	2:B:74:VAL:HG23	2.20	0.41
2:C:57:LEU:O	2:C:64:VAL:HG13	2.21	0.41
1:D:345:LEU:HD13	1:D:350:ALA:HA	2.02	0.41
1:D:471:ASP:HA	1:D:472:PRO:HA	1.88	0.41
1:D:99:LEU:CB	1:D:556:ALA:H	2.34	0.41
1:A:203:TYR:CD2	1:A:254:ILE:HD11	2.53	0.41
1:A:357:ASN:ND2	7:A:843:HOH:O	2.54	0.41
1:A:452:LEU:O	1:A:457:ILE:HB	2.21	0.41
1:A:527:THR:HG23	1:A:561:ILE:CG2	2.44	0.41
2:C:187:LYS:HB2	2:C:187:LYS:HZ3	1.84	0.41
1:D:19:GLU:O	1:D:23:ASN:HB2	2.21	0.41
1:D:247:ASP:HA	7:D:992:HOH:O	2.19	0.41
1:D:323:LEU:HA	1:D:324:PRO:HD3	1.95	0.41
1:D:425:ARG:HB2	1:D:427:LEU:HB2	2.03	0.41
1:D:68:VAL:HG11	1:D:73:LEU:CD2	2.51	0.41
1:A:117:LEU:O	1:A:120:ASN:HB2	2.21	0.41
1:A:87:PRO:HD3	1:A:93:PRO:HD3	2.03	0.41
2:C:64:VAL:HG12	7:C:447:HOH:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:96:ARG:NH1	2:C:76:GLU:OE2	2.54	0.41
1:D:262:ALA:HB3	7:D:783:HOH:O	2.20	0.41
1:D:295:PHE:N	1:D:295:PHE:CD2	2.88	0.41
1:D:440:ASP:OD1	1:D:501:PHE:HA	2.20	0.41
1:D:91:GLY:HA3	2:E:142:LYS:CA	2.51	0.41
2:F:115:GLY:O	2:F:116:LYS:HD2	2.21	0.41
1:A:77:ILE:HG22	1:A:110:PHE:HB3	2.02	0.41
1:A:223:PHE:HB3	1:A:312:TYR:OH	2.21	0.41
1:A:447:SER:O	1:A:450:LYS:HG2	2.21	0.41
1:A:507:VAL:HG13	1:A:511:LYS:HD2	2.03	0.41
1:A:92:HIS:NE2	2:B:139:LEU:HB3	2.35	0.41
1:A:46:GLN:OE1	2:B:149:SER:HB3	2.20	0.41
2:C:142:LYS:HA	2:C:143:PRO:HD3	1.97	0.41
2:C:151:GLY:N	2:C:154:ASP:OD2	2.54	0.41
2:C:26:LYS:HD2	2:C:74:VAL:CG1	2.47	0.41
2:C:64:VAL:HB	2:C:73:TYR:HD2	1.82	0.41
1:D:187:CYS:HB2	1:D:208:SER:C	2.41	0.41
1:D:222:VAL:O	1:D:304:ILE:N	2.35	0.41
1:D:563:CYS:O	1:D:566:VAL:HG12	2.20	0.41
1:D:79:ARG:HD2	7:D:1040:HOH:O	2.21	0.41
1:A:57:PRO:HG3	7:A:809:HOH:O	2.21	0.41
2:B:5:PRO:HB3	2:B:57:LEU:HD21	2.01	0.41
2:C:7:LEU:HD21	2:C:23:LEU:CD1	2.48	0.41
1:D:29:LYS:HB2	1:D:33:LYS:HE2	2.03	0.41
1:D:222:VAL:HG11	4:D:602:VAL:N	2.36	0.41
1:D:82:ASP:O	7:D:761:HOH:O	2.22	0.41
2:E:54:ILE:H	2:E:54:ILE:HG13	1.72	0.41
1:A:117:LEU:HD11	1:A:333:SER:CA	2.42	0.41
1:A:113:PHE:CE1	1:A:117:LEU:HD22	2.56	0.41
1:A:288:TYR:HA	1:A:318:HIS:O	2.21	0.41
1:A:465:TYR:HD1	1:A:551:VAL:CG1	2.34	0.41
1:D:109:LYS:HE3	1:D:111:ILE:HG13	2.02	0.41
1:D:133:ASN:OD1	1:D:138:ILE:N	2.50	0.41
1:D:92:HIS:HB2	2:E:141:ASP:CB	2.51	0.41
2:E:199:LEU:HA	2:E:200:PRO:HD2	1.97	0.41
2:F:182:LEU:O	2:F:185:TRP:HE3	2.04	0.41
2:F:9:ASP:HB2	2:F:20:ARG:NH2	2.36	0.41
1:A:114:THR:HG22	1:A:115:ASP:H	1.86	0.40
1:A:143:LYS:CE	1:A:212:PHE:HB2	2.50	0.40
1:A:309:MET:HE3	1:A:536:LEU:HD12	2.03	0.40
2:B:211:GLU:OE1	7:B:421:HOH:O	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:143:PRO:HB2	2:C:144:TYR:CD2	2.56	0.40
1:D:108:PRO:HG2	1:D:552:LYS:N	2.30	0.40
1:D:152:LYS:HG3	1:D:565:ASN:CG	2.41	0.40
1:D:330:TYR:HB2	1:D:352:PHE:HD2	1.85	0.40
1:D:363:PHE:HB2	1:D:388:TYR:HD2	1.87	0.40
1:D:449:ALA:O	1:D:452:LEU:HB2	2.21	0.40
1:D:77:ILE:O	1:D:81:VAL:HG12	2.21	0.40
2:F:117:LYS:HE3	2:F:213:ARG:HH12	1.84	0.40
2:F:169:LYS:HB2	2:F:169:LYS:HE3	1.68	0.40
1:A:117:LEU:HA	1:A:120:ASN:ND2	2.37	0.40
1:A:337:ILE:O	1:A:354:VAL:HA	2.22	0.40
1:A:444:SER:OG	7:A:705:HOH:O	1.96	0.40
2:C:17:MET:CE	2:C:200:PRO:HD2	2.52	0.40
2:C:20:ARG:CB	2:C:198:SER:HB3	2.51	0.40
2:B:62:LYS:NZ	2:C:94:GLN:CG	2.84	0.40
1:D:302:TYR:CD1	1:D:326:VAL:HG13	2.53	0.40
1:D:125:PHE:CE2	1:D:328:HIS:CE1	3.02	0.40
2:E:99:ALA:O	2:E:103:ASP:HB2	2.21	0.40
1:A:108:PRO:HB3	1:A:555:ASN:CB	2.43	0.40
1:A:256:VAL:O	1:A:260:ARG:HB2	2.21	0.40
1:A:273:LEU:O	1:A:276:THR:HG22	2.20	0.40
1:A:33:LYS:O	1:A:37:LEU:HB2	2.21	0.40
1:A:77:ILE:CG2	1:A:97:ILE:HD12	2.51	0.40
2:C:153:VAL:HG22	2:C:157:LEU:HD23	2.03	0.40
2:C:211:GLU:O	2:C:214:LYS:HG2	2.21	0.40
1:D:101:SER:HB3	1:D:535:PHE:CE2	2.56	0.40
1:D:147:PHE:CE1	1:D:149:PHE:HE2	2.40	0.40
1:D:329:ASP:CB	1:D:339:ALA:HA	2.44	0.40
1:D:36:LEU:HD22	1:D:61:PHE:CE1	2.57	0.40
1:D:65:VAL:HA	1:D:66:PRO:HD3	1.92	0.40
1:D:68:VAL:CG1	1:D:72:GLU:HB2	2.49	0.40
2:F:110:GLN:HG3	7:F:417:HOH:O	2.22	0.40
1:A:201:ALA:O	1:A:205:HIS:ND1	2.50	0.40
1:A:290:LEU:O	1:A:293:ALA:N	2.54	0.40
1:A:428:ILE:HD13	7:A:1133:HOH:O	2.21	0.40
1:A:78:LYS:HE2	1:A:553:PRO:HG2	2.04	0.40
2:B:133:LYS:HA	2:B:136:GLU:OE2	2.22	0.40
1:A:90:THR:O	2:B:143:PRO:HD3	2.21	0.40
2:B:24:ARG:HE	2:B:198:SER:HG	1.62	0.40
1:D:272:GLU:O	1:D:275:GLU:HB3	2.21	0.40
1:D:365:PRO:HG3	1:D:388:TYR:CZ	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:390:VAL:HG11	1:D:540:SER:OG	2.22	0.40
2:E:117:LYS:HE3	2:E:117:LYS:HB2	1.94	0.40
2:F:10:TYR:O	2:F:20:ARG:NH2	2.42	0.40
1:A:566:VAL:HG12	1:A:566:VAL:O	2.20	0.40
1:A:96:ALA:HB3	1:A:113:PHE:HB3	2.04	0.40
2:B:65:CYS:HB2	7:B:420:HOH:O	2.21	0.40
1:D:198:VAL:HG22	1:D:524:ALA:HB3	2.04	0.40
1:D:354:VAL:HG11	1:D:379:LEU:HD21	2.02	0.40
1:D:506:TYR:O	1:D:510:ARG:HB3	2.21	0.40
2:E:93:ALA:HB2	2:E:96:ARG:NH1	2.36	0.40
2:F:23:LEU:HB3	2:F:28:VAL:CG1	2.51	0.40

All (22) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:211:LEU:O	1:A:509:SER:OG[1_655]	1.76	0.44
1:A:270:ASN:O	1:A:511:LYS:NZ[1_655]	1.80	0.40
1:A:238:TRP:N	2:F:177:SER:OG[1_554]	1.91	0.29
7:B:427:HOH:O	7:C:482:HOH:O[1_455]	1.98	0.22
7:D:1210:HOH:O	7:E:581:HOH:O[1_655]	2.00	0.20
7:A:1075:HOH:O	7:B:533:HOH:O[1_545]	2.07	0.13
1:D:270:ASN:ND2	1:D:510:ARG:O[1_655]	2.10	0.10
1:A:270:ASN:ND2	1:A:510:ARG:O[1_655]	2.10	0.10
7:D:1071:HOH:O	7:D:1097:HOH:O[1_665]	2.11	0.09
7:B:476:HOH:O	7:C:503:HOH:O[1_455]	2.12	0.08
1:D:280:LYS:NZ	1:D:503:ASP:OD1[1_655]	2.12	0.08
1:A:22:ARG:NH2	2:B:173:PHE:O[1_545]	2.13	0.07
7:A:1159:HOH:O	7:A:1172:HOH:O[1_565]	2.13	0.07
7:A:1066:HOH:O	7:F:489:HOH:O[1_554]	2.13	0.07
7:B:502:HOH:O	7:C:527:HOH:O[1_455]	2.13	0.07
1:A:276:THR:OG1	1:A:501:PHE:O[1_655]	2.13	0.07
7:D:953:HOH:O	7:D:1024:HOH:O[1_655]	2.15	0.05
7:A:1161:HOH:O	7:A:1200:HOH:O[1_565]	2.15	0.05
2:C:140:GLY:O	1:D:246:LYS:NZ[1_455]	2.17	0.03
7:D:1019:HOH:O	7:D:1095:HOH:O[1_565]	2.17	0.03
1:D:270:ASN:O	1:D:511:LYS:NZ[1_655]	2.18	0.02
2:C:141:ASP:OD2	1:D:278:ARG:NH2[1_455]	2.18	0.02

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%)	513 (90%)	41 (7%)	13 (2%)	6	1
1	D	567/575 (99%)	504 (89%)	53 (9%)	10 (2%)	8	1
2	B	212/223 (95%)	197 (93%)	12 (6%)	3 (1%)	11	2
2	C	212/223 (95%)	193 (91%)	15 (7%)	4 (2%)	8	1
2	E	212/223 (95%)	192 (91%)	18 (8%)	2 (1%)	17	4
2	F	212/223 (95%)	191 (90%)	14 (7%)	7 (3%)	4	0
All	All	1982/2042 (97%)	1790 (90%)	153 (8%)	39 (2%)	7	1

All (39) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	433	ILE
1	A	540	SER
1	D	433	ILE
1	D	540	SER
1	D	542	ALA
2	F	177	SER
2	F	180	PRO
1	A	166	THR
1	A	437	THR
1	A	566	VAL
2	C	140	GLY
1	D	53	ASN
1	D	437	THR
1	D	566	VAL
2	F	140	GLY
2	F	174	SER
1	A	54	ALA
1	A	92	HIS
1	A	368	GLU
2	B	26	LYS

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Mol	Chain	Res	Type
2	B	140	GLY
1	D	368	GLU
1	D	574	ALA
2	F	66	GLU
1	A	105	GLN
1	A	329	ASP
2	B	79	PRO
1	D	369	THR
2	F	172	ASN
1	A	85	THR
2	C	66	GLU
2	C	180	PRO
1	D	553	PRO
1	A	509	SER
2	F	27	GLY
1	A	296	PRO
2	E	27	GLY
2	E	79	PRO
2	C	12	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	499/505 (99%)	461 (92%)	38 (8%)	13	2
1	D	499/505 (99%)	458 (92%)	41 (8%)	11	2
2	B	187/195 (96%)	180 (96%)	7 (4%)	34	14
2	C	187/195 (96%)	172 (92%)	15 (8%)	12	2
2	E	187/195 (96%)	183 (98%)	4 (2%)	53	35
2	F	187/195 (96%)	170 (91%)	17 (9%)	9	1
All	All	1746/1790 (98%)	1624 (93%)	122 (7%)	15	3

All (122) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	HIS
1	A	26	GLN
1	A	37	LEU
1	A	55	THR
1	A	90	THR
1	A	103	THR
1	A	110	PHE
1	A	125	PHE
1	A	134	ARG
1	A	152	LYS
1	A	154	TYR
1	A	156	SER
1	A	184	SER
1	A	202	LEU
1	A	276	THR
1	A	277	ILE
1	A	281	CYS
1	A	295	PHE
1	A	305	MET
1	A	313	VAL
1	A	357	ASN
1	A	390	VAL
1	A	403	LEU
1	A	410	ILE
1	A	433	ILE
1	A	455	GLU
1	A	463	SER
1	A	464	SER
1	A	478	PHE
1	A	479	TRP
1	A	494	CYS
1	A	509	SER
1	A	515	ILE
1	A	518	LEU
1	A	536	LEU
1	A	545	PHE
1	A	546	LYS
1	A	552	LYS
2	B	39	ASN
2	B	43	LEU
2	B	65	CYS
2	B	103	ASP
2	B	149	SER

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Mol	Chain	Res	Type
2	B	182	LEU
2	B	188	ARG
2	C	32	TYR
2	C	45	LEU
2	C	50	ILE
2	C	64	VAL
2	C	72	GLN
2	C	74	VAL
2	C	133	LYS
2	C	134	ILE
2	C	135	LEU
2	C	139	LEU
2	C	157	LEU
2	C	176	GLU
2	C	183	ILE
2	C	185	TRP
2	C	204	LYS
1	D	25	HIS
1	D	46	GLN
1	D	66	PRO
1	D	68	VAL
1	D	77	ILE
1	D	78	LYS
1	D	81	VAL
1	D	82	ASP
1	D	85	THR
1	D	88	ILE
1	D	89	LEU
1	D	90	THR
1	D	92	HIS
1	D	99	LEU
1	D	110	PHE
1	D	125	PHE
1	D	150	SER
1	D	152	LYS
1	D	172	ASN
1	D	187	CYS
1	D	202	LEU
1	D	210	ILE
1	D	242	VAL
1	D	250	LEU
1	D	254	ILE

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Mol	Chain	Res	Type
1	D	273	LEU
1	D	326	VAL
1	D	329	ASP
1	D	405	ASP
1	D	408	LYS
1	D	410	ILE
1	D	416	THR
1	D	424	ARG
1	D	468	VAL
1	D	477	ILE
1	D	494	CYS
1	D	507	VAL
1	D	512	CYS
1	D	546	LYS
1	D	551	VAL
1	D	566	VAL
2	E	4	LEU
2	E	87	SER
2	E	88	ASP
2	E	139	LEU
2	F	32	TYR
2	F	43	LEU
2	F	64	VAL
2	F	65	CYS
2	F	72	GLN
2	F	80	GLU
2	F	84	PHE
2	F	134	ILE
2	F	135	LEU
2	F	139	LEU
2	F	148	ASP
2	F	157	LEU
2	F	172	ASN
2	F	178	GLU
2	F	182	LEU
2	F	202	SER
2	F	216	ASN

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	26	GLN

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Mol	Chain	Res	Type
1	A	146	GLN
1	A	217	GLN
1	A	394	ASN
1	A	491	GLN
1	A	565	ASN
2	B	60	ASN
2	C	72	GLN
1	D	39	ASN
1	D	123	GLN
1	D	172	ASN
1	D	205	HIS
1	D	236	GLN
1	D	318	HIS
1	D	565	ASN
2	F	110	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 9 ligands modelled in this entry, 1 is monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	GSH	F	301	-	12,19,19	1.71	3 (25%)	15,24,24	3.03	5 (33%)
3	JAA	A	601	-	12,15,15	5.81	6 (50%)	12,19,19	2.80	5 (41%)
5	GSH	B	301	-	12,19,19	1.75	3 (25%)	15,24,24	2.27	6 (40%)
5	GSH	C	301	-	12,19,19	1.73	3 (25%)	15,24,24	3.71	8 (53%)
3	JAA	D	601	6	12,15,15	5.83	6 (50%)	12,19,19	3.19	7 (58%)
5	GSH	E	301	-	12,19,19	1.74	3 (25%)	15,24,24	2.87	5 (33%)

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
5	GSH	F	301	-	-	3/18/24/24	-
3	JAA	A	601	-	-	2/7/22/22	0/1/1/1
5	GSH	B	301	-	-	4/18/24/24	-
5	GSH	C	301	-	-	4/18/24/24	-
3	JAA	D	601	6	-	4/7/22/22	0/1/1/1
5	GSH	E	301	-	-	9/18/24/24	-

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	JAA	C05-C08	-12.68	1.31	1.52
3	D	601	JAA	C05-C08	-12.43	1.31	1.52
3	A	601	JAA	C06-C04	-11.43	1.23	1.53
3	D	601	JAA	C06-C04	-11.29	1.24	1.53
3	D	601	JAA	C10-C04	-6.39	1.45	1.53
3	D	601	JAA	C07-C08	6.15	1.61	1.51
3	A	601	JAA	C10-C04	-6.11	1.45	1.53
3	A	601	JAA	C07-C08	5.76	1.60	1.51
3	D	601	JAA	C05-C04	4.76	1.66	1.54
3	A	601	JAA	C05-C04	4.65	1.66	1.54
3	D	601	JAA	C09-C05	-4.34	1.48	1.54
3	A	601	JAA	C09-C05	-3.89	1.48	1.54
5	B	301	GSH	C2-N3	3.36	1.41	1.33
5	F	301	GSH	CA2-N2	-3.34	1.38	1.45
5	E	301	GSH	C2-N3	3.27	1.40	1.33
5	C	301	GSH	CA2-N2	-3.17	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	301	GSH	CA2-N2	-3.03	1.39	1.45
5	B	301	GSH	CD1-N2	2.84	1.40	1.34
5	F	301	GSH	C2-N3	2.81	1.39	1.33
5	C	301	GSH	C2-N3	2.72	1.39	1.33
5	B	301	GSH	CA2-N2	-2.60	1.40	1.45
5	C	301	GSH	CD1-N2	2.35	1.39	1.34
5	E	301	GSH	CD1-N2	2.30	1.38	1.34
5	F	301	GSH	CD1-N2	2.09	1.38	1.34

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	301	GSH	CA2-CB2-SG2	-9.99	102.97	114.19
5	F	301	GSH	CA2-CB2-SG2	-9.27	103.78	114.19
5	E	301	GSH	CA2-CB2-SG2	-6.67	106.70	114.19
3	D	601	JAA	C07-C06-C04	-6.28	97.85	104.41
5	B	301	GSH	CA2-CB2-SG2	-6.15	107.28	114.19
5	E	301	GSH	CB2-CA2-N2	-6.02	102.70	111.28
3	D	601	JAA	C09-C11-C13	-5.69	105.26	126.40
3	A	601	JAA	O01-C08-C05	5.02	132.05	125.58
3	A	601	JAA	C09-C11-C13	-4.67	109.04	126.40
5	F	301	GSH	CB2-CA2-N2	-4.65	104.65	111.28
5	C	301	GSH	CB2-CA2-N2	-4.59	104.74	111.28
5	C	301	GSH	CA3-N3-C2	-4.44	115.95	122.34
3	A	601	JAA	C07-C08-C05	-4.16	102.01	109.05
3	A	601	JAA	C06-C04-C10	-4.15	106.24	113.67
5	C	301	GSH	CG1-CD1-N2	-4.06	108.79	115.83
5	C	301	GSH	CB1-CG1-CD1	3.62	121.12	113.04
5	E	301	GSH	CB1-CG1-CD1	3.55	120.97	113.04
3	D	601	JAA	O01-C08-C05	3.55	130.15	125.58
5	E	301	GSH	CG1-CD1-N2	-3.48	109.79	115.83
5	C	301	GSH	CG1-CB1-CA1	-3.39	105.94	113.84
3	D	601	JAA	C06-C04-C10	-3.34	107.69	113.67
5	C	301	GSH	C2-CA2-N2	-3.16	102.57	111.16
5	F	301	GSH	C3-CA3-N3	-3.12	104.42	110.43
3	D	601	JAA	C06-C07-C08	-3.09	102.32	105.42
3	D	601	JAA	C07-C08-C05	-3.08	103.84	109.05
5	C	301	GSH	OE1-CD1-CG1	2.75	127.05	122.02
5	B	301	GSH	C2-CA2-N2	-2.69	103.83	111.16
5	F	301	GSH	CG1-CD1-N2	-2.59	111.34	115.83
5	E	301	GSH	OE1-CD1-CG1	2.50	126.58	122.02
5	B	301	GSH	CB2-CA2-N2	-2.41	107.84	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	301	GSH	CA3-N3-C2	-2.36	118.94	122.34
3	D	601	JAA	C10-C04-C05	2.32	120.11	114.74
5	B	301	GSH	CB1-CG1-CD1	2.25	118.06	113.04
5	B	301	GSH	CG1-CD1-N2	-2.07	112.25	115.83
3	A	601	JAA	C07-C06-C04	-2.06	102.26	104.41
5	F	301	GSH	C2-CA2-N2	-2.03	105.62	111.16

There are no chirality outliers.

All (26) torsion outliers are listed below:

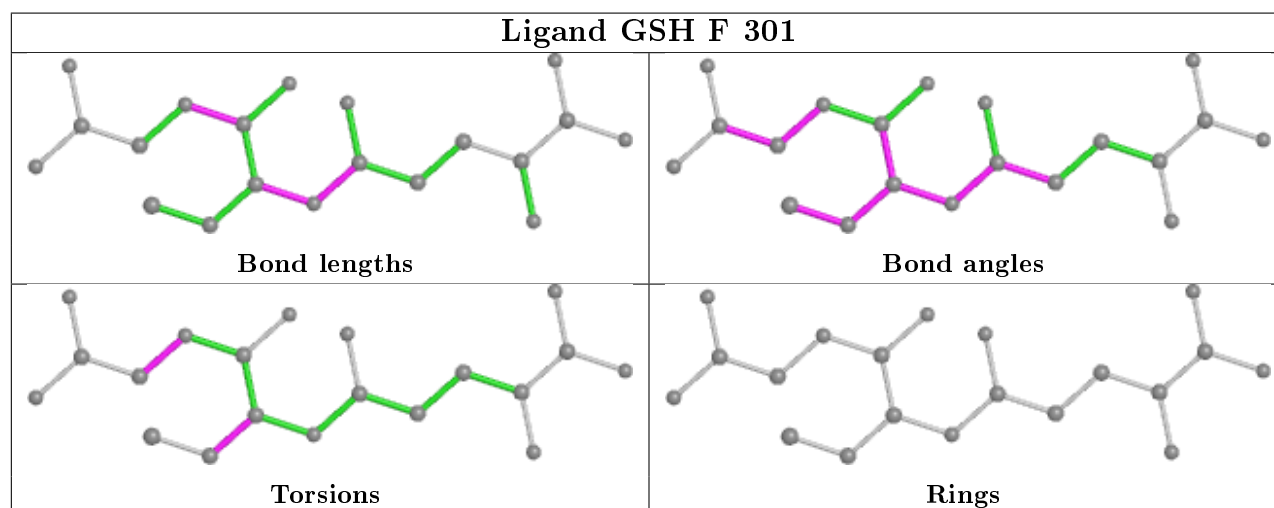
Mol	Chain	Res	Type	Atoms
5	F	301	GSH	N2-CA2-CB2-SG2
5	F	301	GSH	C2-CA2-CB2-SG2
5	B	301	GSH	N1-CA1-CB1-CG1
5	B	301	GSH	C1-CA1-CB1-CG1
5	B	301	GSH	C2-CA2-CB2-SG2
5	C	301	GSH	N2-CA2-CB2-SG2
5	C	301	GSH	C2-CA2-CB2-SG2
3	D	601	JAA	C04-C05-C09-C11
3	D	601	JAA	C09-C11-C13-C14
3	D	601	JAA	C11-C13-C14-C15
5	E	301	GSH	N2-CA2-CB2-SG2
5	E	301	GSH	C2-CA2-CB2-SG2
3	A	601	JAA	C09-C11-C13-C14
5	C	301	GSH	CA1-CB1-CG1-CD1
5	E	301	GSH	CA1-CB1-CG1-CD1
3	A	601	JAA	C05-C09-C11-C13
3	D	601	JAA	C08-C05-C09-C11
5	E	301	GSH	C1-CA1-CB1-CG1
5	B	301	GSH	N2-CA2-CB2-SG2
5	E	301	GSH	C3-CA3-N3-C2
5	E	301	GSH	OE1-CD1-CG1-CB1
5	F	301	GSH	C3-CA3-N3-C2
5	C	301	GSH	C3-CA3-N3-C2
5	E	301	GSH	O2-C2-CA2-N2
5	E	301	GSH	N2-CD1-CG1-CB1
5	E	301	GSH	N3-C2-CA2-N2

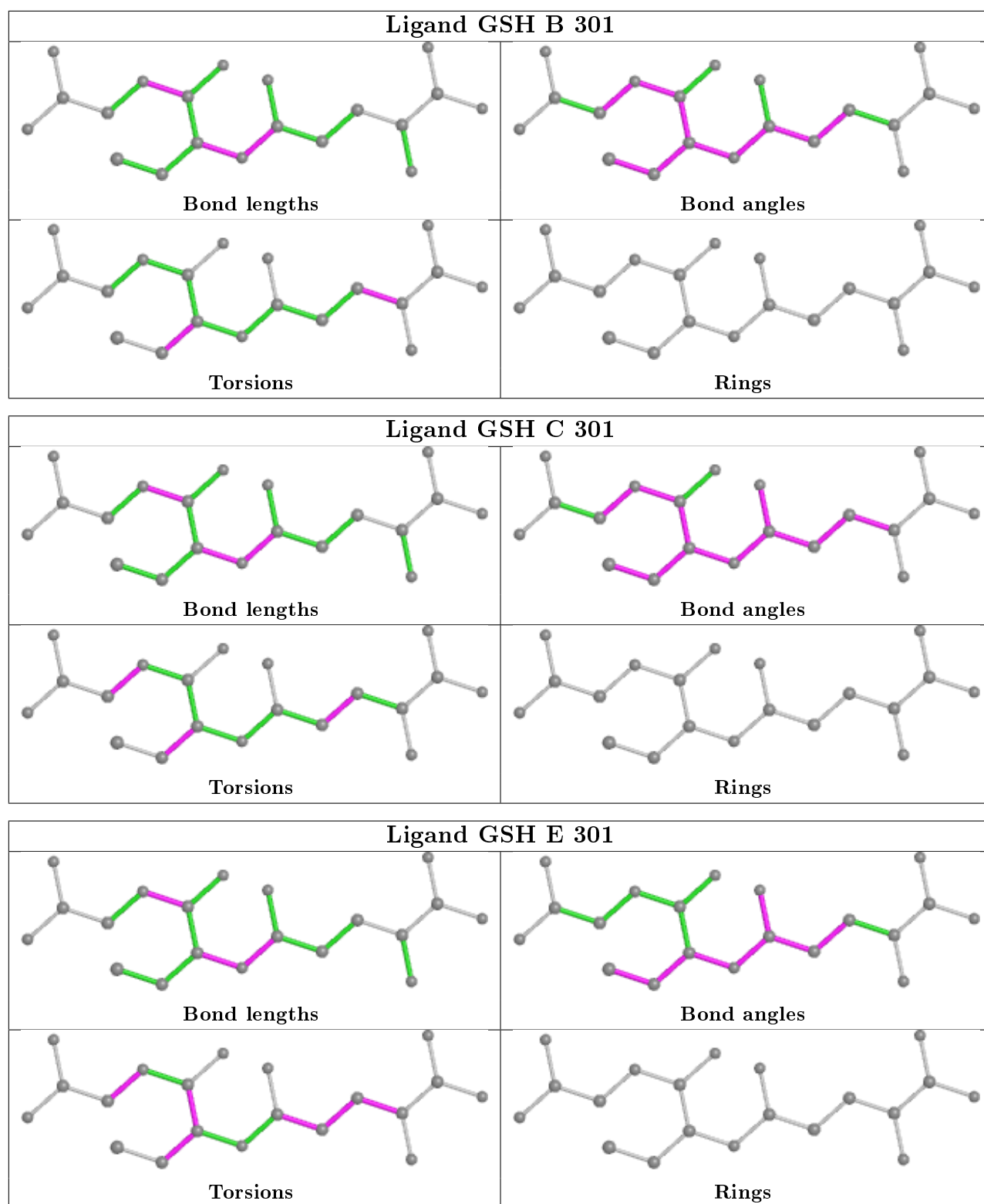
There are no ring outliers.

6 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	F	301	GSH	3	0
3	A	601	JAA	4	0
5	B	301	GSH	4	0
5	C	301	GSH	1	0
3	D	601	JAA	2	0
5	E	301	GSH	1	0

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





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	2.35	298 (52%) 0 0	5, 17, 25, 32	0
1	D	569/575 (98%)	1.84	235 (41%) 0 0	4, 12, 19, 26	0
2	B	214/223 (95%)	1.51	59 (27%) 0 0	6, 13, 21, 28	0
2	C	214/223 (95%)	1.24	49 (22%) 0 0	3, 7, 11, 18	0
2	E	214/223 (95%)	1.65	73 (34%) 0 0	7, 12, 20, 26	0
2	F	214/223 (95%)	1.46	50 (23%) 0 0	4, 9, 14, 22	0
All	All	1994/2042 (97%)	1.82	764 (38%) 0 0	3, 12, 22, 32	0

All (764) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	27	VAL	9.8
2	E	97	PHE	9.0
1	A	515	ILE	9.0
2	F	174	SER	8.7
1	A	429	LEU	8.5
1	A	36	LEU	8.2
1	D	161	PRO	8.0
1	A	294	LEU	7.9
1	A	17	PHE	7.4
1	A	432	ASN	7.4
2	C	90	TYR	7.3
1	A	210	ILE	7.2
1	A	346	SER	7.2
2	E	95	ALA	7.1
2	B	123	ALA	6.6
1	A	13	VAL	6.6
1	A	287	TRP	6.6
2	F	176	GLU	6.6
1	A	202	LEU	6.4

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Mol	Chain	Res	Type	RSRZ
1	A	523	VAL	6.3
1	A	284	LEU	6.3
2	F	172	ASN	6.2
1	A	305	MET	6.2
1	A	506	TYR	6.1
1	D	361	PHE	6.1
1	A	309	MET	6.0
1	D	173	PRO	5.8
1	A	423	CYS	5.8
1	A	125	PHE	5.7
1	A	459	VAL	5.7
1	D	566	VAL	5.7
1	A	354	VAL	5.7
1	A	457	ILE	5.7
1	A	233	THR	5.5
1	A	377	VAL	5.5
1	A	531	ILE	5.5
1	A	274	ALA	5.4
1	A	500	ALA	5.4
2	B	132	VAL	5.3
1	A	237	VAL	5.2
1	D	517	ALA	5.2
1	A	295	PHE	5.2
1	A	35	ILE	5.2
1	A	468	VAL	5.2
1	A	556	ALA	5.1
2	B	140	GLY	5.1
1	D	203	TYR	5.1
1	A	60	ALA	5.1
1	D	114	THR	5.0
1	A	301	VAL	5.0
1	A	48	CYS	5.0
1	A	145	LEU	5.0
2	E	70	VAL	5.0
1	A	279	THR	4.9
1	A	65	VAL	4.9
1	D	507	VAL	4.9
1	A	66	PRO	4.9
1	D	506	TYR	4.9
2	B	139	LEU	4.9
1	A	238	TRP	4.9
1	A	169	VAL	4.9

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Mol	Chain	Res	Type	RSRZ
1	A	257	PRO	4.8
1	A	37	LEU	4.8
1	D	155	ILE	4.8
1	D	398	LEU	4.8
1	A	406	VAL	4.8
1	A	104	SER	4.8
1	A	475	TYR	4.8
1	A	234	PHE	4.8
1	D	475	TYR	4.8
1	A	538	LEU	4.7
2	F	180	PRO	4.7
1	D	466	ILE	4.6
1	A	220	PHE	4.6
1	A	392	ILE	4.6
1	D	271	PRO	4.6
1	A	8	PHE	4.6
1	A	497	LEU	4.5
1	D	523	VAL	4.5
1	A	507	VAL	4.5
1	D	77	ILE	4.5
1	A	563	CYS	4.5
1	D	262	ALA	4.5
1	D	162	VAL	4.5
1	D	202	LEU	4.5
1	D	111	ILE	4.5
1	A	154	TYR	4.5
2	C	10	TYR	4.5
2	B	153	VAL	4.4
1	A	170	TYR	4.4
2	B	135	LEU	4.4
1	A	110	PHE	4.4
1	D	46	GLN	4.4
1	A	113	PHE	4.3
1	D	160	VAL	4.3
1	A	433	ILE	4.3
1	A	460	ILE	4.3
1	D	515	ILE	4.3
1	D	89	LEU	4.3
1	D	409	VAL	4.3
1	A	469	SER	4.2
1	A	546	LYS	4.2
1	D	288	TYR	4.2

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Mol	Chain	Res	Type	RSRZ
2	F	165	GLN	4.2
1	A	67	LEU	4.2
1	A	241	ILE	4.2
2	F	173	PHE	4.2
1	A	129	PHE	4.2
1	A	545	PHE	4.2
2	B	183	ILE	4.2
1	D	457	ILE	4.1
2	E	61	GLY	4.1
2	E	173	PHE	4.1
2	B	64	VAL	4.1
2	B	70	VAL	4.1
1	A	326	VAL	4.0
1	A	131	PHE	4.0
1	D	76	TYR	4.0
1	D	313	VAL	4.0
1	A	477	ILE	4.0
1	D	428	ILE	4.0
1	D	397	GLY	4.0
1	A	136	PHE	4.0
1	A	149	PHE	4.0
1	A	211	LEU	3.9
2	F	73	TYR	3.9
2	E	49	PRO	3.9
1	A	428	ILE	3.9
1	D	481	ILE	3.9
2	B	175	ILE	3.9
2	F	114	TRP	3.9
1	A	535	PHE	3.9
1	D	42	ALA	3.9
1	A	345	LEU	3.9
2	E	71	VAL	3.9
1	A	312	TYR	3.9
1	D	65	VAL	3.9
1	D	113	PHE	3.9
1	A	324	PRO	3.9
1	A	38	LYS	3.8
2	F	179	SER	3.8
1	D	266	LEU	3.8
2	B	185	TRP	3.8
1	A	230	ALA	3.8
1	A	431	ILE	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	466	ILE	3.8
1	D	71	VAL	3.8
2	C	153	VAL	3.8
2	E	57	LEU	3.8
1	A	558	VAL	3.8
1	D	204	CYS	3.8
1	A	311	PRO	3.8
2	C	193	GLU	3.8
1	A	14	ILE	3.8
2	E	158	ILE	3.8
2	F	175	ILE	3.8
2	E	74	VAL	3.8
1	A	175	PHE	3.7
1	A	19	GLU	3.7
1	D	219	VAL	3.7
1	A	353	ALA	3.7
1	A	166	THR	3.7
1	A	526	GLY	3.7
1	D	304	ILE	3.7
1	D	32	LEU	3.7
1	A	42	ALA	3.7
2	E	206	VAL	3.7
1	D	380	THR	3.7
1	D	462	PHE	3.7
1	D	274	ALA	3.7
1	A	443	LEU	3.7
2	F	68	LEU	3.7
1	A	407	VAL	3.7
1	D	85	THR	3.7
1	A	327	SER	3.7
2	F	90	TYR	3.7
1	A	352	PHE	3.7
1	D	149	PHE	3.7
2	F	177	SER	3.6
1	A	116	GLU	3.6
2	F	144	TYR	3.6
1	D	531	ILE	3.6
2	B	78	TRP	3.6
1	A	388	TYR	3.6
1	A	43	ILE	3.6
1	A	325	LEU	3.6
1	A	379	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
1	D	528	PHE	3.6
1	A	313	VAL	3.6
1	A	330	TYR	3.6
1	A	33	LYS	3.6
1	A	122	LEU	3.6
1	A	198	VAL	3.6
1	D	167	THR	3.6
1	D	287	TRP	3.6
1	D	154	TYR	3.6
1	A	290	LEU	3.6
1	A	403	LEU	3.6
2	F	99	ALA	3.5
1	A	282	MET	3.5
1	A	454	GLU	3.5
1	A	524	ALA	3.5
2	F	64	VAL	3.5
2	F	183	ILE	3.5
1	A	281	CYS	3.5
2	B	202	SER	3.5
1	A	393	THR	3.5
1	D	179	MET	3.5
1	D	250	LEU	3.5
2	E	139	LEU	3.5
1	A	147	PHE	3.5
1	D	476	ALA	3.5
1	D	285	SER	3.5
2	F	98	TRP	3.5
1	D	571	PHE	3.5
1	D	7	THR	3.5
2	E	109	ALA	3.5
1	A	323	LEU	3.4
1	A	473	GLY	3.4
1	A	57	PRO	3.4
1	D	550	CYS	3.4
1	A	28	GLN	3.4
1	A	217	GLN	3.4
1	D	429	LEU	3.4
1	D	242	VAL	3.4
1	D	522	VAL	3.4
2	E	175	ILE	3.4
2	B	60	ASN	3.4
2	E	98	TRP	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	536	LEU	3.4
1	D	206	LEU	3.4
2	C	28	VAL	3.4
1	D	182	ILE	3.4
1	D	384	ILE	3.4
1	D	561	ILE	3.4
1	A	339	ALA	3.3
1	D	316	LEU	3.3
1	D	419	LEU	3.3
1	A	203	TYR	3.3
2	E	21	VAL	3.3
1	D	147	PHE	3.3
1	A	419	LEU	3.3
2	E	134	ILE	3.3
1	D	192	VAL	3.3
1	D	479	TRP	3.3
2	F	132	VAL	3.3
1	A	161	PRO	3.3
1	A	71	VAL	3.3
1	D	520	LEU	3.3
1	A	548	PRO	3.3
2	E	63	PRO	3.3
1	A	218	TYR	3.3
1	A	54	ALA	3.3
1	A	355	ILE	3.3
1	A	103	THR	3.2
1	D	43	ILE	3.2
1	D	208	SER	3.2
2	F	216	ASN	3.2
1	A	214	ASP	3.2
1	A	231	PHE	3.2
1	D	110	PHE	3.2
1	D	516	GLY	3.2
2	F	157	LEU	3.2
2	B	32	TYR	3.2
2	E	90	TYR	3.2
2	F	208	TYR	3.2
1	A	271	PRO	3.2
1	D	314	PRO	3.2
1	D	187	CYS	3.2
1	A	316	LEU	3.2
1	A	341	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	412	PHE	3.2
1	D	412	PHE	3.2
1	D	421	PHE	3.2
1	A	109	LYS	3.2
1	D	512	CYS	3.2
1	D	222	VAL	3.2
2	E	44	LEU	3.2
2	C	170	PHE	3.2
2	E	91	GLY	3.2
1	D	399	TYR	3.2
2	E	10	TYR	3.2
1	A	464	SER	3.2
1	A	81	VAL	3.1
1	D	558	VAL	3.1
2	E	30	PHE	3.1
2	B	134	ILE	3.1
1	A	93	PRO	3.1
1	D	289	GLY	3.1
2	E	124	GLY	3.1
1	A	445	VAL	3.1
1	D	122	LEU	3.1
2	F	153	VAL	3.1
2	E	22	ALA	3.1
2	E	210	ALA	3.1
1	A	465	TYR	3.1
2	E	73	TYR	3.1
1	A	337	ILE	3.1
2	B	158	ILE	3.1
1	A	127	THR	3.1
2	B	206	VAL	3.1
2	F	135	LEU	3.1
1	D	335	GLY	3.1
1	A	561	ILE	3.1
1	A	321	GLY	3.1
1	A	518	LEU	3.1
2	F	102	VAL	3.1
2	E	54	ILE	3.0
1	A	508	SER	3.0
1	A	390	VAL	3.0
2	F	217	LEU	3.0
1	A	269	PRO	3.0
1	A	273	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	311	PRO	3.0
1	D	277	ILE	3.0
1	D	431	ILE	3.0
1	D	573	THR	3.0
2	B	180	PRO	3.0
2	F	171	GLY	3.0
1	A	358	LEU	3.0
1	A	560	GLN	3.0
1	D	337	ILE	3.0
1	D	360	TYR	3.0
1	D	494	CYS	3.0
1	D	570	TYR	3.0
2	C	32	TYR	3.0
1	A	501	PHE	3.0
1	A	181	SER	3.0
1	A	472	PRO	3.0
1	D	124	LEU	3.0
1	D	495	ASN	2.9
2	B	207	ALA	2.9
1	A	289	GLY	2.9
1	D	121	THR	2.9
1	A	148	ILE	2.9
1	A	277	ILE	2.9
1	D	433	ILE	2.9
1	A	83	GLY	2.9
1	A	98	SER	2.9
2	E	50	ILE	2.9
1	A	302	TYR	2.9
1	D	220	PHE	2.9
1	D	363	PHE	2.9
1	D	45	LEU	2.9
1	D	403	LEU	2.9
2	C	49	PRO	2.9
2	E	6	ILE	2.9
1	A	505	GLY	2.9
1	D	413	TYR	2.9
1	D	465	TYR	2.9
2	F	10	TYR	2.9
2	E	28	VAL	2.9
1	A	106	GLY	2.9
1	A	422	ILE	2.9
2	C	83	PRO	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	128	ALA	2.9
1	A	361	PHE	2.8
1	D	125	PHE	2.8
1	A	512	CYS	2.8
1	D	259	VAL	2.8
1	D	489	VAL	2.8
1	D	496	CYS	2.8
1	D	538	LEU	2.8
1	A	322	ASP	2.8
2	E	12	PRO	2.8
2	E	14	MET	2.8
2	C	183	ILE	2.8
1	D	47	ASN	2.8
1	A	223	PHE	2.8
1	A	421	PHE	2.8
1	D	390	VAL	2.8
1	D	535	PHE	2.8
1	D	575	PHE	2.8
1	A	124	LEU	2.8
2	B	102	VAL	2.8
1	D	112	PRO	2.8
1	A	96	ALA	2.8
1	D	165	ALA	2.8
1	A	91	GLY	2.8
1	A	410	ILE	2.8
1	D	148	ILE	2.8
1	D	510	ARG	2.8
2	E	32	TYR	2.8
1	A	259	VAL	2.8
1	D	366	VAL	2.8
2	B	164	PHE	2.8
2	E	43	LEU	2.8
2	F	97	PHE	2.8
1	D	178	GLY	2.8
1	D	477	ILE	2.8
2	B	129	ILE	2.8
1	A	553	PRO	2.8
1	D	169	VAL	2.8
1	D	567	VAL	2.8
1	A	276	THR	2.8
2	E	160	PHE	2.8
1	A	476	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
2	B	93	ALA	2.8
2	B	186	ALA	2.8
2	E	205	ILE	2.7
1	D	541	SER	2.7
2	B	167	TYR	2.7
1	D	69	THR	2.7
1	D	268	THR	2.7
1	D	207	LEU	2.7
1	D	562	LEU	2.7
2	B	56	VAL	2.7
2	E	7	LEU	2.7
1	D	60	ALA	2.7
1	D	568	SER	2.7
2	B	174	SER	2.7
1	A	68	VAL	2.7
1	D	198	VAL	2.7
1	D	216	VAL	2.7
2	C	44	LEU	2.7
2	E	64	VAL	2.7
2	E	93	ALA	2.7
1	D	427	LEU	2.7
1	D	417	PRO	2.7
1	A	61	PHE	2.7
1	A	21	THR	2.7
1	A	90	THR	2.7
1	A	502	ILE	2.7
2	E	166	ALA	2.7
1	D	336	TRP	2.7
1	A	222	VAL	2.7
2	B	182	LEU	2.7
2	E	47	SER	2.7
1	A	328	HIS	2.7
2	E	150	PHE	2.7
1	A	31	THR	2.7
1	A	550	CYS	2.7
2	F	72	GLN	2.7
1	A	99	LEU	2.7
1	D	445	VAL	2.7
2	C	68	LEU	2.7
2	C	185	TRP	2.7
1	D	8	PHE	2.7
1	D	545	PHE	2.7

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Mol	Chain	Res	Type	RSRZ
2	B	173	PHE	2.7
1	D	205	HIS	2.6
1	D	504	ALA	2.6
1	D	392	ILE	2.6
1	A	562	LEU	2.6
1	D	103	THR	2.6
1	A	194	PHE	2.6
1	A	212	PHE	2.6
1	A	478	PHE	2.6
1	A	97	ILE	2.6
1	A	261	THR	2.6
1	D	249	VAL	2.6
2	C	70	VAL	2.6
1	A	300	TYR	2.6
1	D	37	LEU	2.6
1	A	516	GLY	2.6
2	B	98	TRP	2.6
2	C	98	TRP	2.6
1	A	528	PHE	2.6
1	D	55	THR	2.6
1	D	255	THR	2.6
1	D	470	THR	2.6
1	D	492	ASP	2.6
1	A	372	GLY	2.6
1	D	359	GLY	2.6
2	E	155	ILE	2.6
1	A	398	LEU	2.6
1	D	218	TYR	2.6
1	D	464	SER	2.6
1	D	17	PHE	2.6
1	D	501	PHE	2.6
2	B	101	PHE	2.6
1	A	144	ALA	2.6
1	A	350	ALA	2.6
1	D	67	LEU	2.6
1	D	518	LEU	2.6
1	A	44	TYR	2.6
1	A	413	TYR	2.6
1	D	170	TYR	2.6
1	A	453	SER	2.6
1	A	462	PHE	2.5
2	F	164	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	96	ALA	2.5
1	D	221	ALA	2.5
1	A	195	SER	2.5
1	A	481	ILE	2.5
1	D	88	ILE	2.5
2	B	137	SER	2.5
1	A	206	LEU	2.5
1	D	137	PRO	2.5
2	E	45	LEU	2.5
1	D	44	TYR	2.5
1	D	163	GLY	2.5
1	D	300	TYR	2.5
2	C	73	TYR	2.5
1	A	342	THR	2.5
1	A	573	THR	2.5
1	D	48	CYS	2.5
1	A	92	HIS	2.5
1	A	534	HIS	2.5
2	F	15	PHE	2.5
2	F	145	PHE	2.5
1	A	108	PRO	2.5
2	E	55	PRO	2.5
1	A	32	LEU	2.5
1	A	236	GLN	2.5
1	A	395	TYR	2.5
1	A	570	TYR	2.5
1	A	204	CYS	2.5
1	A	10	MET	2.5
1	A	142	GLY	2.5
1	D	500	ALA	2.5
2	F	106	PHE	2.5
2	F	111	PHE	2.5
1	A	499	ARG	2.5
1	A	111	ILE	2.5
2	C	11	TRP	2.5
2	B	113	VAL	2.5
2	E	113	VAL	2.5
2	C	139	LEU	2.5
2	B	177	SER	2.5
2	E	151	GLY	2.5
1	A	376	PRO	2.5
1	D	175	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
2	C	30	PHE	2.5
1	A	94	VAL	2.5
2	C	207	ALA	2.4
1	D	482	SER	2.4
1	D	321	GLY	2.4
1	A	120	ASN	2.4
1	A	304	ILE	2.4
2	B	160	PHE	2.4
1	D	73	LEU	2.4
1	D	559	LEU	2.4
1	A	504	ALA	2.4
2	E	209	ALA	2.4
2	B	163	TRP	2.4
1	A	63	SER	2.4
1	A	288	TYR	2.4
1	D	127	THR	2.4
1	A	359	GLY	2.4
2	E	65	CYS	2.4
2	C	102	VAL	2.4
1	A	73	LEU	2.4
1	A	245	ILE	2.4
1	A	427	LEU	2.4
1	A	449	ALA	2.4
1	D	502	ILE	2.4
2	C	128	PHE	2.4
2	E	149	SER	2.4
1	D	485	THR	2.4
1	A	209	GLY	2.4
2	C	212	TYR	2.4
2	E	27	GLY	2.4
1	A	232	ARG	2.4
1	A	452	LEU	2.4
1	D	36	LEU	2.4
1	D	351	THR	2.4
2	F	129	ILE	2.4
1	A	189	PRO	2.4
1	A	292	PRO	2.4
2	F	86	PRO	2.4
1	A	76	TYR	2.4
1	A	544	GLN	2.4
1	D	312	TYR	2.4
1	D	80	MET	2.4

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Mol	Chain	Res	Type	RSRZ
2	E	78	TRP	2.4
1	A	440	ASP	2.4
2	B	209	ALA	2.4
1	D	90	THR	2.4
1	D	527	THR	2.4
1	A	229	HIS	2.4
1	D	521	ARG	2.3
1	A	207	LEU	2.3
1	D	99	LEU	2.3
2	C	5	PRO	2.3
1	D	129	PHE	2.3
1	A	308	SER	2.3
1	A	357	ASN	2.3
1	A	360	TYR	2.3
2	B	90	TYR	2.3
2	E	144	TYR	2.3
2	C	163	TRP	2.3
1	A	380	THR	2.3
1	A	426	ASN	2.3
1	D	27	VAL	2.3
1	A	227	LEU	2.3
1	D	254	ILE	2.3
2	B	37	PHE	2.3
1	A	298	ALA	2.3
1	D	330	TYR	2.3
2	B	166	ALA	2.3
2	B	172	ASN	2.3
2	B	215	ASN	2.3
1	D	459	VAL	2.3
1	A	266	LEU	2.3
1	A	335	GLY	2.3
1	D	50	LEU	2.3
2	B	120	GLU	2.3
1	A	329	ASP	2.3
1	D	223	PHE	2.3
1	D	295	PHE	2.3
2	B	84	PHE	2.3
1	A	7	THR	2.3
1	A	167	THR	2.3
1	A	485	THR	2.3
1	A	264	SER	2.3
1	D	184	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	215	GLN	2.3
1	D	309	MET	2.3
2	F	70	VAL	2.3
1	D	486	ASN	2.3
1	D	97	ILE	2.3
1	A	75	PRO	2.3
1	D	347	PRO	2.3
2	E	170	PHE	2.3
1	A	11	ASN	2.3
1	A	278	ARG	2.2
1	D	94	VAL	2.2
1	D	296	PRO	2.2
1	D	548	PRO	2.2
2	C	64	VAL	2.2
2	C	162	SER	2.2
1	A	293	ALA	2.2
1	A	559	LEU	2.2
1	D	183	THR	2.2
1	D	379	LEU	2.2
2	C	166	ALA	2.2
2	E	85	PHE	2.2
1	D	324	PRO	2.2
1	A	351	THR	2.2
1	A	409	VAL	2.2
1	D	116	GLU	2.2
2	B	136	GLU	2.2
2	F	195	VAL	2.2
1	A	133	ASN	2.2
1	A	163	GLY	2.2
1	D	532	GLN	2.2
1	A	479	TRP	2.2
2	E	13	SER	2.2
1	A	363	PHE	2.2
1	D	57	PRO	2.2
1	D	87	PRO	2.2
1	D	231	PHE	2.2
2	C	12	PRO	2.2
2	E	101	PHE	2.2
2	E	164	PHE	2.2
1	A	114	THR	2.2
1	D	306	THR	2.2
1	D	201	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	574	ALA	2.2
2	C	95	ALA	2.2
2	E	58	VAL	2.2
1	A	117	LEU	2.2
2	C	179	SER	2.2
1	A	138	ILE	2.2
1	D	245	ILE	2.2
1	D	291	ILE	2.2
2	B	86	PRO	2.2
2	E	72	GLN	2.2
2	E	163	TRP	2.2
1	A	394	ASN	2.2
2	F	215	ASN	2.2
1	D	24	ALA	2.2
2	C	84	PHE	2.2
2	C	152	TYR	2.2
2	E	84	PHE	2.2
2	E	106	PHE	2.2
1	D	557	LYS	2.2
1	A	20	MET	2.2
1	D	101	SER	2.2
1	A	213	ARG	2.2
2	B	74	VAL	2.2
1	D	196	PRO	2.2
2	C	135	LEU	2.2
2	E	182	LEU	2.2
1	D	378	GLY	2.2
1	A	492	ASP	2.2
2	E	11	TRP	2.2
2	F	185	TRP	2.2
2	C	33	ARG	2.1
1	D	212	PHE	2.1
2	C	85	PHE	2.1
1	D	66	PRO	2.1
1	D	423	CYS	2.1
1	A	256	VAL	2.1
2	E	153	VAL	2.1
1	A	12	ARG	2.1
2	C	50	ILE	2.1
1	A	201	ALA	2.1
2	B	19	ALA	2.1
2	C	209	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
2	F	207	ALA	2.1
1	D	270	ASN	2.1
1	A	417	PRO	2.1
1	D	140	ASP	2.1
2	C	78	TRP	2.1
1	A	575	PHE	2.1
1	A	192	VAL	2.1
1	D	267	LEU	2.1
2	B	43	LEU	2.1
2	C	43	LEU	2.1
2	F	184	ALA	2.1
2	B	16	GLY	2.1
1	A	29	LYS	2.1
2	B	133	LYS	2.1
2	B	152	TYR	2.1
2	C	167	TYR	2.1
2	E	53	LYS	2.1
2	B	30	PHE	2.1
2	B	114	TRP	2.1
2	C	101	PHE	2.1
2	C	106	PHE	2.1
1	A	47	ASN	2.1
1	A	255	THR	2.1
1	A	228	VAL	2.1
1	D	339	ALA	2.1
2	C	23	LEU	2.1
1	D	166	THR	2.1
2	E	152	TYR	2.1
2	F	32	TYR	2.1
2	B	145	PHE	2.1
2	F	85	PHE	2.1
2	F	101	PHE	2.1
1	D	54	ALA	2.1
1	D	326	VAL	2.1
2	F	11	TRP	2.1
1	A	509	SER	2.1
1	D	14	ILE	2.1
1	D	157	THR	2.0
1	D	261	THR	2.0
1	A	130	ALA	2.0
1	D	118	MET	2.0
1	A	216	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	382	VAL	2.0
1	D	478	PHE	2.0
2	E	145	PHE	2.0
1	A	291	ILE	2.0
1	A	494	CYS	2.0
1	D	281	CYS	2.0
1	D	422	ILE	2.0
1	D	247	ASP	2.0
2	E	140	GLY	2.0
2	F	79	PRO	2.0
2	F	83	PRO	2.0
2	C	48	ASN	2.0
2	C	190	MET	2.0
2	C	184	ALA	2.0
1	A	123	GLN	2.0
1	D	367	SER	2.0
2	E	212	TYR	2.0
1	A	242	VAL	2.0
1	A	566	VAL	2.0
1	D	382	VAL	2.0
1	D	273	LEU	2.0
2	B	15	PHE	2.0
2	B	157	LEU	2.0
2	C	4	LEU	2.0
2	E	111	PHE	2.0
2	F	182	LEU	2.0
1	A	164	THR	2.0
1	A	183	THR	2.0
1	A	226	GLY	2.0
2	B	12	PRO	2.0
2	C	124	GLY	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](#)

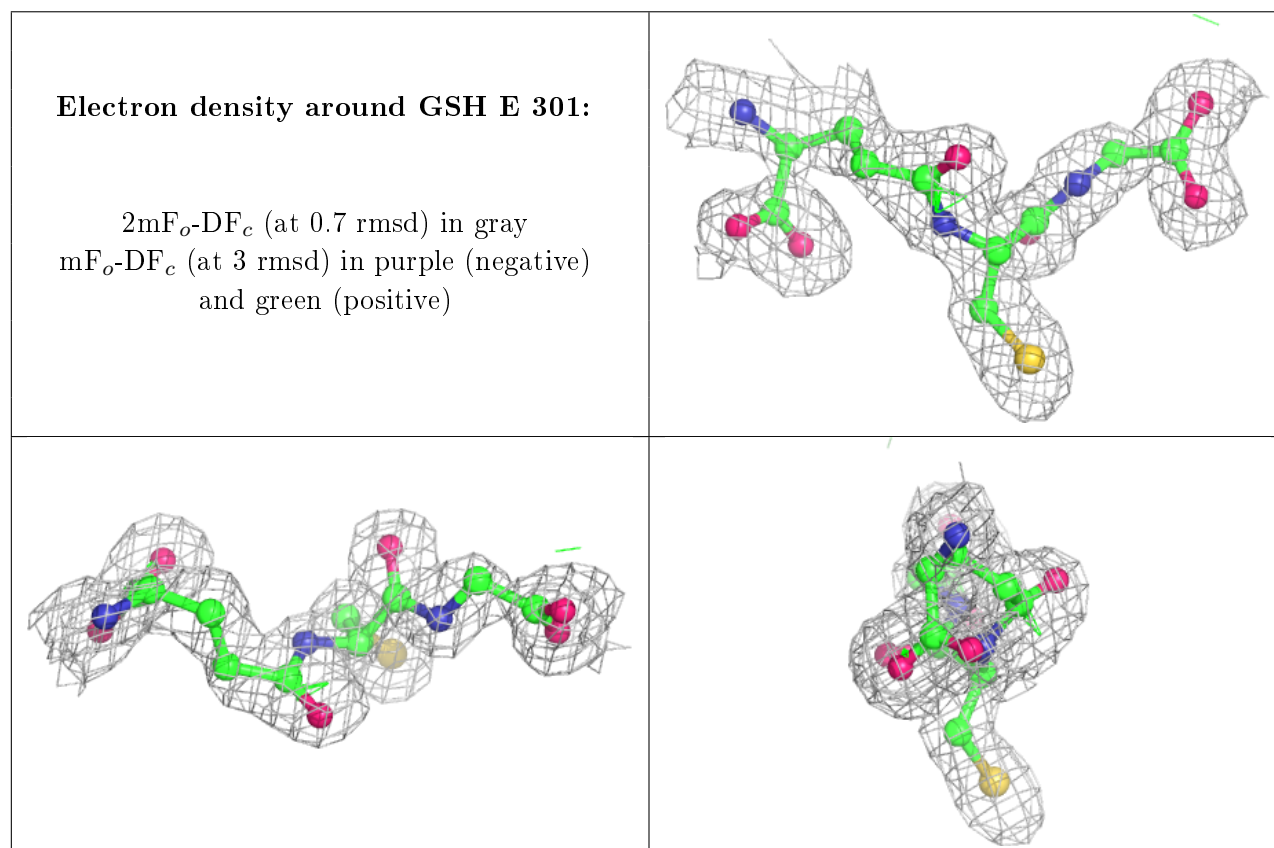
There are no carbohydrates in this entry.

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.

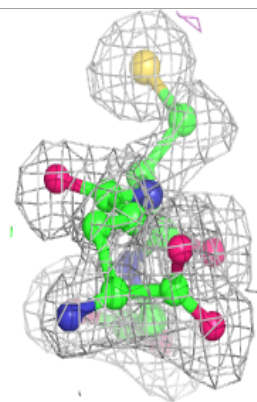
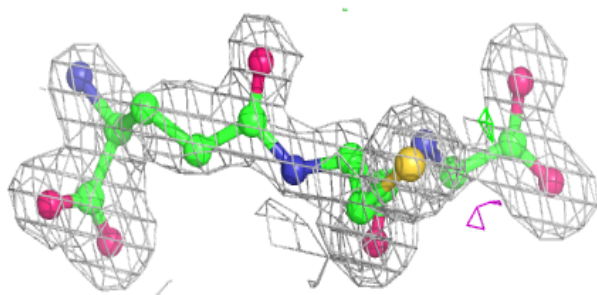
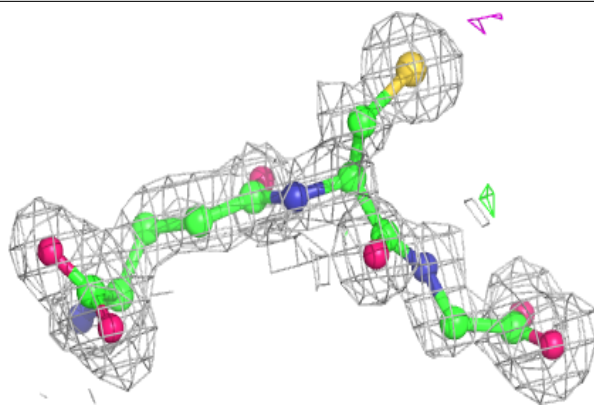
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	VAL	A	602	8/8	0.71	0.22	15,20,22,28	0
4	VAL	D	602	8/8	0.75	0.21	12,17,23,28	0
3	JAA	D	601	15/15	0.81	0.18	7,13,19,20	0
3	JAA	A	601	15/15	0.84	0.20	12,15,20,24	0
5	GSH	E	301	20/20	0.88	0.14	5,13,20,35	0
5	GSH	C	301	20/20	0.89	0.16	4,11,20,27	0
5	GSH	F	301	20/20	0.89	0.14	6,10,14,19	0
5	GSH	B	301	20/20	0.93	0.18	5,21,23,28	0
6	MG	D	603	1/1	0.94	0.21	19,19,19,19	0

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

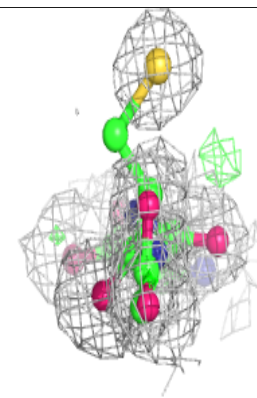
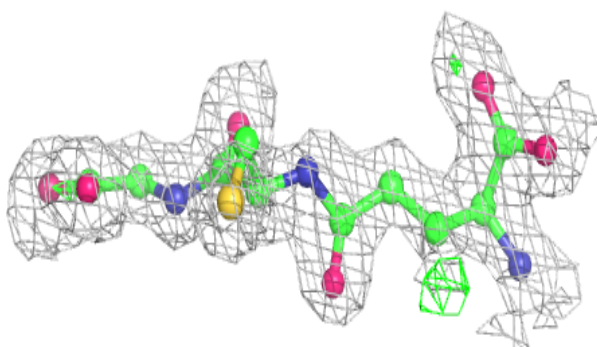
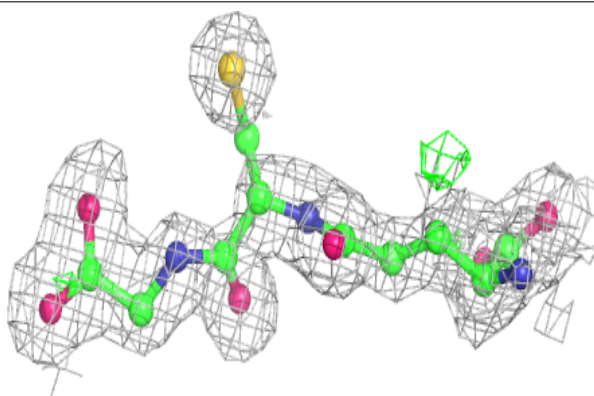


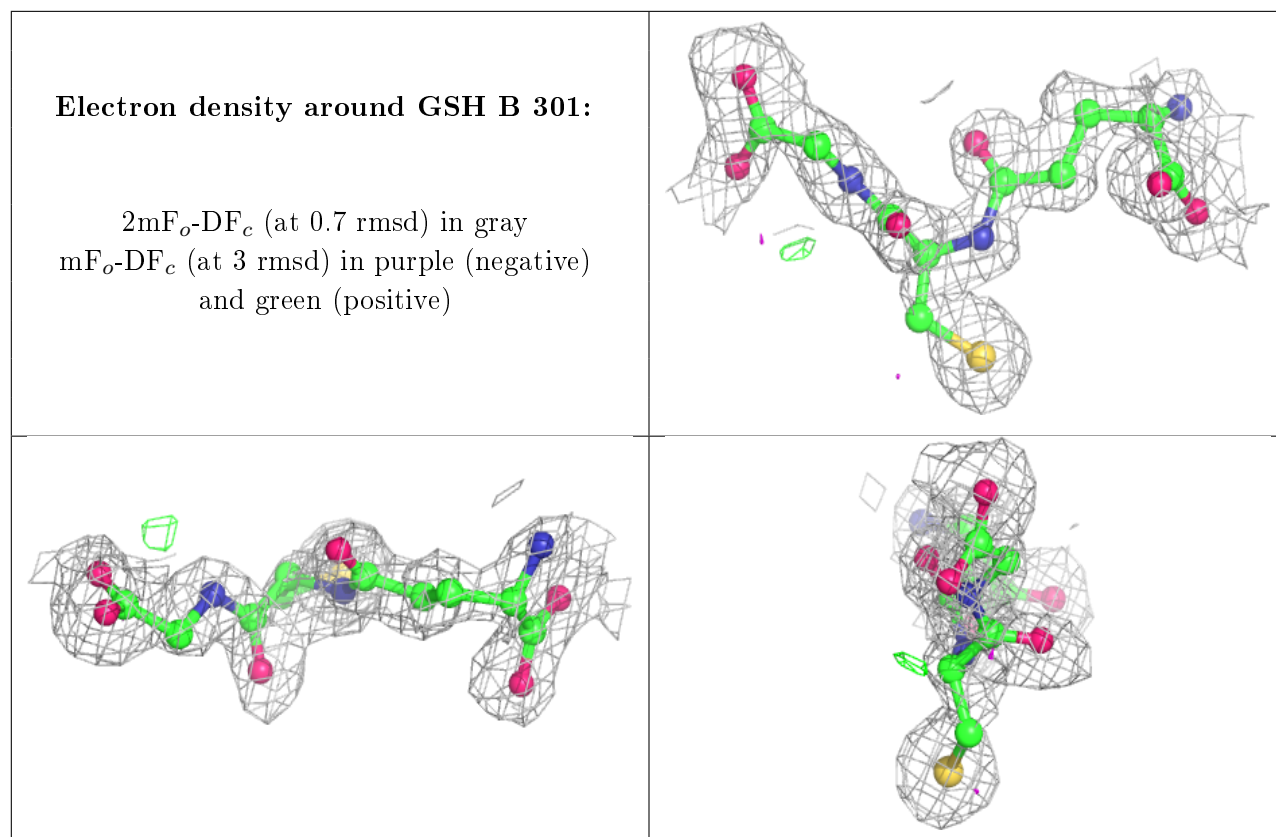
Electron density around GSH C 301:

$2mF_o-DF_c$ (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.