



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 12, 2021 – 02:06 PM EDT

PDB ID : 1XNW  
Title : Acyl-CoA Carboxylase Beta Subunit from *S. coelicolor* (PccB), apo form #2, mutant D422I  
Authors : Diacovich, L.; Mitchell, D.L.; Pham, H.; Gago, G.; Melgar, M.M.; Khosla, C.; Gramajo, H.; Tsai, S.-C.  
Deposited on : 2004-10-05  
Resolution : 2.60 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Xtriage (Phenix) : 1.13  
EDS : 2.23.2  
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) : 2.23.2

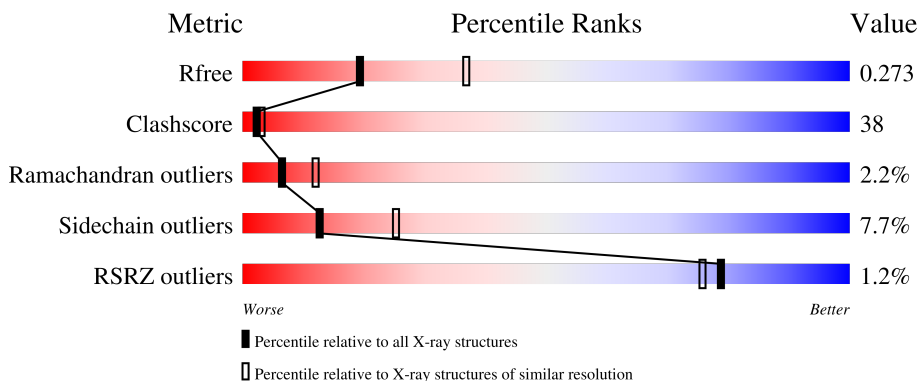
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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.



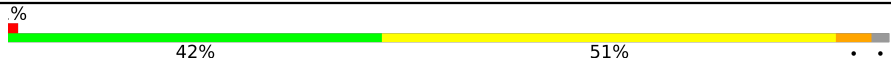
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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

Mol	Chain	Length	Quality of chain
1	A	530	 2% 45% 48% 5%
1	B	530	 % 49% 45%
1	C	530	 % 39% 51% 8%
1	D	530	 % 48% 46%
1	E	530	 2% 45% 48% 5%

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Mol	Chain	Length	Quality of chain
1	F	530	 <p>A horizontal bar chart representing the quality of the chain. The bar is divided into segments: a small red segment at the start, followed by a green segment labeled '42%', a yellow segment labeled '51%', and a small grey segment at the end. A '%' symbol is positioned above the bar on the left side.</p>

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 24754 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 propionyl-CoA carboxylase complex B subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	521	3953	2483	698	759	13	0	0	0
1	B	521	3953	2483	698	759	13	0	0	0
1	C	521	3953	2483	698	759	13	0	0	0
1	D	521	3953	2483	698	759	13	0	0	0
1	E	521	3953	2483	698	759	13	0	0	0
1	F	521	3953	2483	698	759	13	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	422	ILE	ASP	engineered mutation	UNP Q9X4K7
B	422	ILE	ASP	engineered mutation	UNP Q9X4K7
C	422	ILE	ASP	engineered mutation	UNP Q9X4K7
D	422	ILE	ASP	engineered mutation	UNP Q9X4K7
E	422	ILE	ASP	engineered mutation	UNP Q9X4K7
F	422	ILE	ASP	engineered mutation	UNP Q9X4K7

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	173	Total 173	O 173	0	0
2	B	167	Total 167	O 167	0	0
2	C	184	Total 184	O 184	0	0

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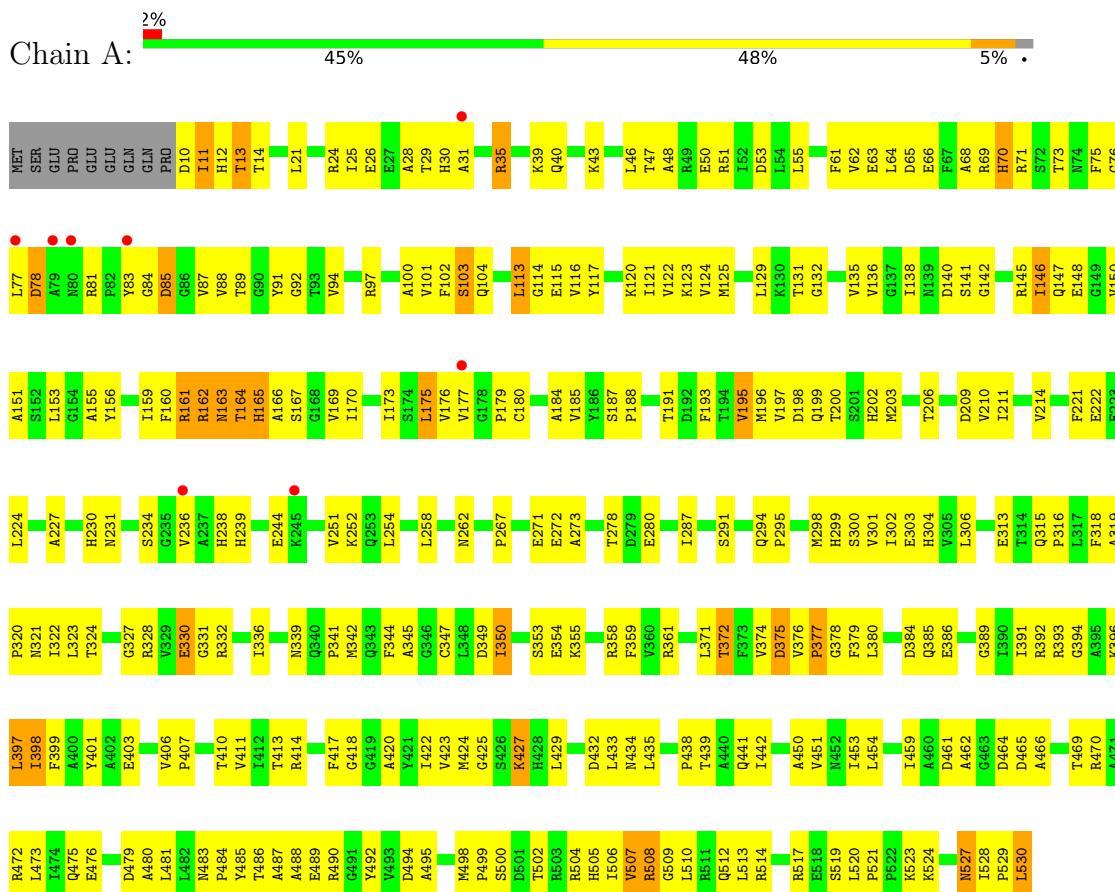
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
2	D	154	Total 154	O 154	0	0
2	E	176	Total 176	O 176	0	0
2	F	182	Total 182	O 182	0	0

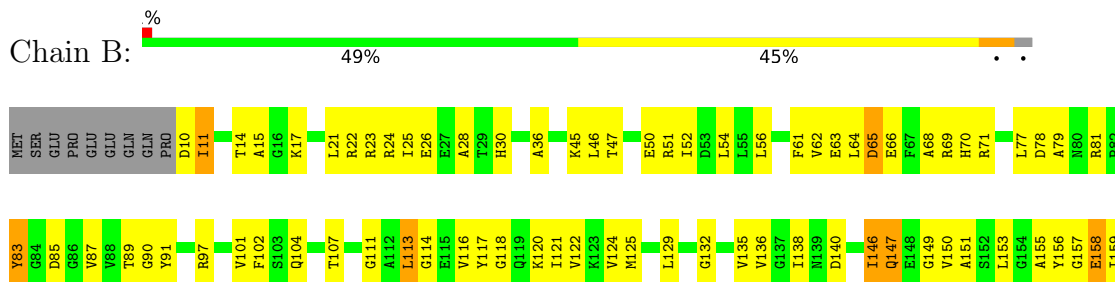
### 3 Residue-property plots

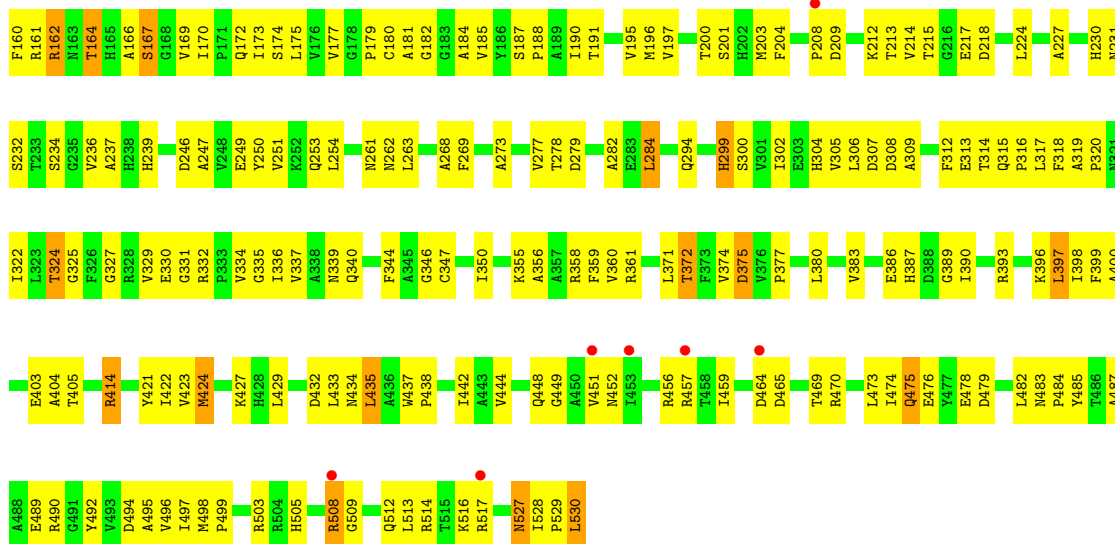
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: propionyl-CoA carboxylase complex B subunit

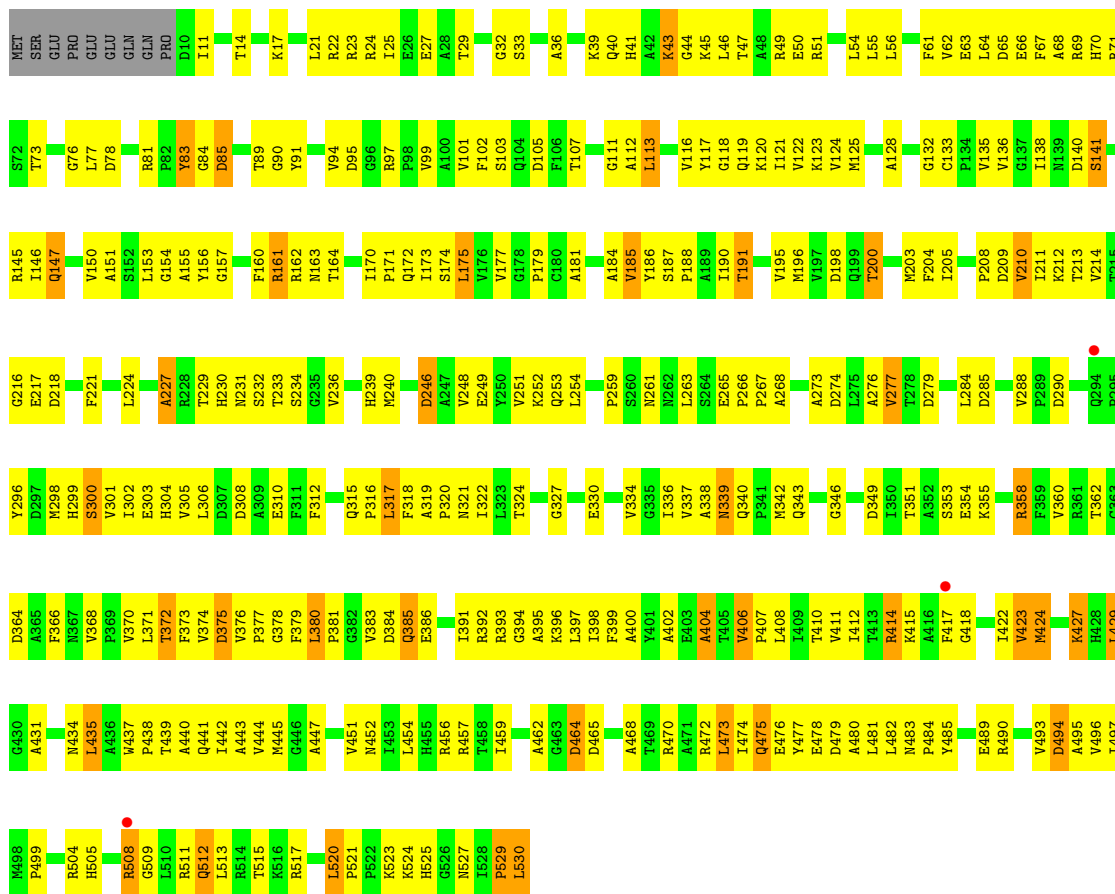
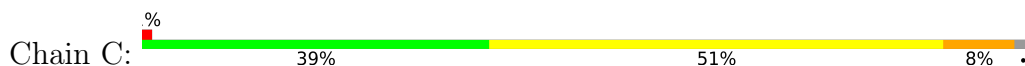


- Molecule 1: propionyl-CoA carboxylase complex B subunit





• Molecule 1: propionyl-CoA carboxylase complex B subunit



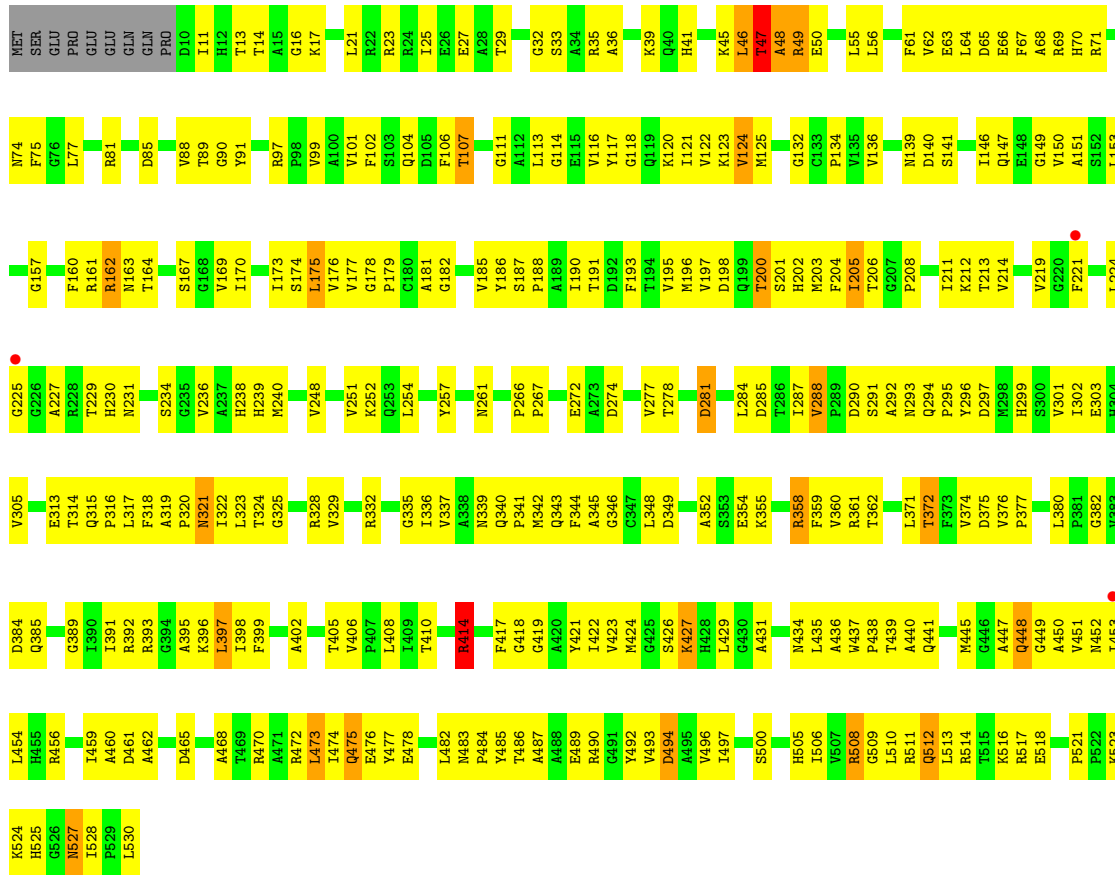
• Molecule 1: propionyl-CoA carboxylase complex B subunit







● Molecule 1: propionyl-CoA carboxylase complex B subunit



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	79.85Å 219.49Å 135.69Å 90.00° 102.99° 90.00°	Depositor
Resolution (Å)	49.05 – 2.60 74.81 – 2.60	Depositor EDS
% Data completeness (in resolution range)	87.7 (49.05-2.60) 87.6 (74.81-2.60)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.13	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.50 (at 2.58Å)	Xtrriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.261 , 0.276 0.267 , 0.273	Depositor DCC
$R_{free}$ test set	2808 reflections (2.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	42.0	Xtrriage
Anisotropy	0.956	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 40.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	24754	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	60.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.23% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

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	0/4033	0.67	0/5478
1	B	0.46	0/4033	0.65	0/5478
1	C	0.47	0/4033	0.66	0/5478
1	D	0.46	0/4033	0.66	0/5478
1	E	0.48	0/4033	0.66	0/5478
1	F	0.46	0/4033	0.65	0/5478
All	All	0.47	0/24198	0.66	0/32868

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	B	0	1
1	C	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	83	TYR	Sidechain
1	C	83	TYR	Sidechain

### 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	3953	0	3887	327	0
1	B	3953	0	3887	301	0
1	C	3953	0	3887	350	0
1	D	3953	0	3887	283	0
1	E	3953	0	3887	334	0
1	F	3953	0	3887	393	0
2	A	173	0	0	64	0
2	B	167	0	0	63	0
2	C	184	0	0	68	0
2	D	154	0	0	48	0
2	E	176	0	0	72	0
2	F	182	0	0	76	0
All	All	24754	0	23322	1802	0

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 38.

All (1802) 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:F:47:THR:HG23	1:F:50:GLU:HB2	1.39	1.00
1:B:147:GLN:H	1:B:147:GLN:NE2	1.60	1.00
1:D:147:GLN:HE21	1:D:147:GLN:H	1.06	0.99
1:F:187:SER:HB3	1:F:188:PRO:HD3	1.46	0.96
1:C:173:ILE:HG21	1:C:251:VAL:HG23	1.48	0.95
1:F:99:VAL:HA	2:F:607:HOH:O	1.64	0.94
1:A:35:ARG:HH12	1:A:39:LYS:HD2	1.32	0.94
1:C:40:GLN:HE21	1:C:45:LYS:HD2	1.32	0.94
1:B:147:GLN:HE21	1:B:147:GLN:N	1.66	0.93
1:D:328:ARG:HA	2:D:602:HOH:O	1.70	0.92
1:A:113:LEU:HD22	1:A:117:TYR:CE1	2.05	0.91
1:C:65:ASP:HB2	1:C:120:LYS:HE3	1.50	0.91
1:A:169:VAL:HG23	2:D:594:HOH:O	1.72	0.90
1:A:146:ILE:HD12	1:A:146:ILE:H	1.37	0.89
1:C:440:ALA:O	1:C:484:PRO:HD3	1.73	0.89
1:C:151:ALA:HB2	1:F:490:ARG:NH1	1.88	0.88
1:F:305:VAL:HG21	1:F:506:ILE:HD12	1.56	0.87
1:B:122:VAL:HG22	2:B:586:HOH:O	1.74	0.86
1:F:173:ILE:HG21	1:F:251:VAL:HG23	1.57	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:398:ILE:HG13	1:F:429:LEU:HD21	1.57	0.86
1:F:65:ASP:HB2	1:F:120:LYS:HE3	1.58	0.86
1:F:372:THR:HB	2:F:546:HOH:O	1.76	0.85
1:E:62:VAL:HG11	1:F:508:ARG:HH21	1.41	0.85
1:B:508:ARG:HD3	1:B:509:GLY:N	1.92	0.85
1:B:147:GLN:H	1:B:147:GLN:HE21	0.85	0.84
1:C:113:LEU:HD22	1:C:117:TYR:CE1	2.13	0.83
1:C:408:LEU:HD23	2:C:681:HOH:O	1.76	0.83
1:D:227:ALA:HB1	1:D:240:MET:HG3	1.61	0.83
1:B:325:GLY:O	1:B:359:PHE:HZ	1.60	0.83
1:A:170:ILE:HG21	2:A:570:HOH:O	1.78	0.82
1:D:62:VAL:HG11	1:E:508:ARG:HH21	1.42	0.82
1:E:148:GLU:HG3	2:E:699:HOH:O	1.80	0.82
1:D:422:ILE:HG23	2:D:547:HOH:O	1.80	0.81
1:A:509:GLY:O	1:A:513:LEU:HD23	1.80	0.81
1:A:510:LEU:HA	2:A:537:HOH:O	1.79	0.81
1:B:173:ILE:HG21	1:B:251:VAL:HG23	1.63	0.81
1:B:138:ILE:HG12	1:B:175:LEU:HD23	1.63	0.81
1:B:497:ILE:HG21	1:B:505:HIS:HE2	1.46	0.81
1:B:64:LEU:HG	2:B:562:HOH:O	1.80	0.80
1:C:408:LEU:HA	2:C:681:HOH:O	1.80	0.80
1:D:508:ARG:HH21	1:F:62:VAL:HG11	1.45	0.80
1:E:254:LEU:HB2	2:E:700:HOH:O	1.80	0.80
1:B:433:LEU:HA	1:B:494:ASP:OD1	1.81	0.80
1:A:489:GLU:HA	1:B:68:ALA:HA	1.63	0.80
1:B:113:LEU:HD22	1:B:117:TYR:CE1	2.16	0.80
1:C:334:VAL:HB	2:C:584:HOH:O	1.82	0.80
1:C:231:ASN:HB3	1:C:317:LEU:HD13	1.62	0.79
1:B:306:LEU:HD13	1:B:327:GLY:HA3	1.64	0.79
1:A:393:ARG:HA	1:A:396:LYS:HE3	1.64	0.79
1:C:211:ILE:HG23	2:C:713:HOH:O	1.82	0.79
1:F:104:GLN:HE21	1:F:140:ASP:H	1.30	0.79
1:D:89:THR:HB	1:D:124:VAL:HG21	1.63	0.79
1:F:451:VAL:HG11	1:F:474:ILE:HA	1.62	0.79
1:F:465:ASP:HB3	1:F:468:ALA:HB3	1.65	0.79
1:D:99:VAL:HA	2:D:603:HOH:O	1.82	0.79
1:B:315:GLN:HB3	2:B:625:HOH:O	1.83	0.78
1:A:267:PRO:HG3	2:A:572:HOH:O	1.83	0.78
1:F:348:LEU:HD21	1:F:424:MET:HE3	1.63	0.78
1:D:148:GLU:HG3	2:D:655:HOH:O	1.81	0.78
1:C:151:ALA:HB2	1:F:490:ARG:HH12	1.47	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:170:ILE:HG21	2:C:641:HOH:O	1.83	0.78
1:D:321:ASN:HA	1:D:343:GLN:HB2	1.66	0.78
1:D:62:VAL:HG11	1:E:508:ARG:NH2	1.99	0.78
1:A:295:PRO:HB2	1:A:342:MET:CE	2.13	0.77
1:C:164:THR:HG23	1:F:399:PHE:CD1	2.20	0.77
1:F:299:HIS:O	1:F:303:GLU:HG3	1.85	0.77
1:C:187:SER:HB3	1:C:188:PRO:HD3	1.66	0.77
1:C:371:LEU:HG	2:C:584:HOH:O	1.84	0.77
1:C:484:PRO:HG2	2:C:651:HOH:O	1.83	0.77
1:D:230:HIS:HA	1:D:234:SER:OG	1.84	0.77
1:C:208:PRO:HG3	1:C:224:LEU:HD22	1.65	0.76
1:D:499:PRO:HB3	2:D:581:HOH:O	1.85	0.76
1:D:508:ARG:HD3	1:D:509:GLY:N	2.01	0.76
1:C:45:LYS:HE2	1:C:200:THR:HG22	1.67	0.76
1:F:472:ARG:NH2	1:F:473:LEU:HD22	2.01	0.76
1:E:146:ILE:H	1:E:146:ILE:HD12	1.51	0.76
1:B:89:THR:HB	1:B:124:VAL:HG21	1.66	0.76
1:C:97:ARG:NH1	1:C:267:PRO:HG3	2.01	0.75
1:C:418:GLY:HA2	1:F:153:LEU:HD21	1.68	0.75
1:C:40:GLN:NE2	1:C:45:LYS:HD2	2.01	0.75
1:C:64:LEU:HG	2:C:571:HOH:O	1.87	0.75
1:D:147:GLN:HE21	1:D:147:GLN:N	1.82	0.75
1:E:161:ARG:HG3	1:E:161:ARG:HH11	1.50	0.75
1:D:432:ASP:O	1:D:433:LEU:HD12	1.86	0.75
1:E:111:GLY:HA2	2:E:598:HOH:O	1.87	0.75
1:F:437:TRP:HB2	2:F:648:HOH:O	1.86	0.75
1:A:62:VAL:HG11	1:C:508:ARG:NH2	2.01	0.75
1:A:422:ILE:HG23	2:A:543:HOH:O	1.87	0.75
1:B:414:ARG:HB2	2:B:597:HOH:O	1.87	0.75
1:D:313:GLU:HG2	1:D:316:PRO:HG3	1.69	0.75
1:A:391:ILE:HD12	1:A:391:ILE:H	1.51	0.74
1:A:424:MET:HB3	2:A:594:HOH:O	1.87	0.74
1:C:153:LEU:HD21	1:F:418:GLY:HA2	1.69	0.74
1:C:483:ASN:HD22	1:C:485:TYR:H	1.35	0.74
1:F:101:VAL:HG23	1:F:136:VAL:O	1.87	0.74
1:A:483:ASN:HD22	1:A:485:TYR:HD2	1.36	0.74
1:C:529:PRO:HG3	1:F:190:ILE:HA	1.69	0.74
1:B:497:ILE:HG21	1:B:505:HIS:NE2	2.02	0.74
1:C:399:PHE:CE1	1:F:164:THR:HG23	2.22	0.74
1:B:325:GLY:O	1:B:359:PHE:CZ	2.40	0.74
1:B:398:ILE:HD12	1:E:160:PHE:HB3	1.67	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:159:ILE:HA	2:B:586:HOH:O	1.88	0.74
1:A:230:HIS:HA	1:A:234:SER:OG	1.88	0.74
1:B:69:ARG:HD2	1:B:81:ARG:HB3	1.67	0.74
1:C:273:ALA:HB2	1:C:330:GLU:HG3	1.69	0.74
1:C:319:ALA:HB2	1:C:351:THR:HB	1.69	0.73
1:E:527:ASN:ND2	2:E:584:HOH:O	2.21	0.73
1:F:508:ARG:HD3	1:F:509:GLY:N	2.03	0.73
1:A:398:ILE:HD12	1:D:160:PHE:HB3	1.69	0.73
1:E:412:ILE:HG23	2:E:627:HOH:O	1.88	0.73
1:F:478:GLU:HA	1:F:482:LEU:HB2	1.69	0.73
1:A:162:ARG:HH11	1:A:162:ARG:HG2	1.53	0.73
1:D:69:ARG:HD2	1:D:81:ARG:O	1.89	0.73
1:D:187:SER:HB3	1:D:188:PRO:HD3	1.69	0.73
1:B:153:LEU:HD21	1:E:418:GLY:HA2	1.69	0.73
1:C:89:THR:HB	1:C:124:VAL:HG21	1.71	0.73
1:B:421:TYR:HA	2:B:629:HOH:O	1.88	0.73
1:E:306:LEU:HD21	1:E:336:ILE:HD11	1.70	0.73
1:C:56:LEU:HD12	1:C:61:PHE:HB2	1.71	0.73
1:B:187:SER:HB3	1:B:188:PRO:HD3	1.72	0.72
1:C:40:GLN:HG3	1:C:45:LYS:HB2	1.71	0.72
1:E:319:ALA:HB3	1:E:355:LYS:HD2	1.71	0.72
1:F:451:VAL:HG21	1:F:474:ILE:HG12	1.71	0.72
1:A:62:VAL:HG11	1:C:508:ARG:HH21	1.52	0.72
1:A:508:ARG:NE	1:B:91:TYR:OH	2.22	0.72
1:C:317:LEU:HD12	1:C:317:LEU:H	1.54	0.72
1:A:97:ARG:NH1	2:A:572:HOH:O	2.22	0.72
1:B:305:VAL:HB	2:B:580:HOH:O	1.89	0.72
1:F:49:ARG:HE	1:F:88:VAL:HG21	1.54	0.72
1:D:427:LYS:NZ	1:D:434:ASN:OD1	2.23	0.72
1:F:118:GLY:HA2	2:F:654:HOH:O	1.89	0.72
1:A:28:ALA:HB2	1:A:83:TYR:HD1	1.53	0.72
1:C:372:THR:HG23	1:C:410:THR:HA	1.70	0.72
1:F:337:VAL:HB	2:F:546:HOH:O	1.90	0.72
1:A:427:LYS:HB2	1:A:434:ASN:OD1	1.90	0.72
1:E:395:ALA:O	1:E:398:ILE:HG23	1.90	0.72
1:C:444:VAL:HA	1:F:153:LEU:HD11	1.72	0.72
1:D:197:VAL:O	1:D:227:ALA:HB2	1.89	0.72
1:B:160:PHE:HB3	1:E:398:ILE:HD11	1.71	0.71
1:C:162:ARG:HG2	1:C:162:ARG:HH11	1.55	0.71
1:A:508:ARG:HD3	1:A:509:GLY:N	2.04	0.71
1:D:68:ALA:HA	1:E:489:GLU:HA	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:505:HIS:HA	1:F:508:ARG:HD2	1.72	0.71
1:A:254:LEU:HB2	2:A:660:HOH:O	1.89	0.71
1:A:386:GLU:HG3	1:D:224:LEU:HD11	1.72	0.71
1:A:398:ILE:HG22	1:A:423:VAL:HG22	1.71	0.71
1:D:147:GLN:H	1:D:147:GLN:NE2	1.87	0.71
1:E:374:VAL:HB	1:E:412:ILE:HD13	1.72	0.71
1:F:483:ASN:HD22	1:F:485:TYR:HD2	1.38	0.71
1:D:467:GLU:HA	1:D:470:ARG:HB3	1.71	0.71
1:C:434:ASN:HB2	2:C:690:HOH:O	1.90	0.71
1:F:140:ASP:OD1	1:F:178:GLY:HA3	1.90	0.70
1:F:13:THR:O	1:F:17:LYS:HG2	1.91	0.70
1:A:63:GLU:OE2	1:A:88:VAL:HG13	1.91	0.70
1:C:248:VAL:O	1:C:251:VAL:HG12	1.90	0.70
1:B:69:ARG:HD3	1:B:81:ARG:O	1.91	0.70
1:A:84:GLY:HA2	1:A:120:LYS:HZ2	1.56	0.70
1:E:182:GLY:O	1:E:185:VAL:HG22	1.91	0.70
1:E:465:ASP:HB3	1:E:468:ALA:HB3	1.73	0.70
1:B:495:ALA:HB2	2:B:534:HOH:O	1.91	0.70
1:D:505:HIS:HA	1:D:508:ARG:HD2	1.73	0.70
1:E:185:VAL:O	1:E:188:PRO:HD2	1.91	0.70
1:E:406:VAL:HG22	2:E:677:HOH:O	1.91	0.70
1:F:372:THR:HG23	1:F:410:THR:HA	1.74	0.69
1:C:391:ILE:HG23	2:F:651:HOH:O	1.92	0.69
1:A:508:ARG:NH2	1:B:62:VAL:HG11	2.07	0.69
1:B:160:PHE:HB3	1:E:398:ILE:CD1	2.22	0.69
1:B:422:ILE:HD11	1:E:153:LEU:HB3	1.73	0.69
1:E:158:GLU:HB3	2:E:688:HOH:O	1.92	0.69
1:E:313:GLU:HG2	1:E:316:PRO:HG3	1.73	0.69
1:D:158:GLU:O	1:D:162:ARG:HG2	1.92	0.69
1:A:71:ARG:CZ	1:C:490:ARG:HE	2.05	0.69
1:D:247:ALA:HA	2:D:614:HOH:O	1.92	0.69
1:D:295:PRO:HB2	1:D:342:MET:HE2	1.74	0.69
1:A:187:SER:HB3	1:A:188:PRO:HD3	1.73	0.69
1:E:302:ILE:HD13	1:E:336:ILE:HG21	1.75	0.69
1:E:356:ALA:O	1:E:360:VAL:HG23	1.92	0.69
1:B:478:GLU:HA	1:B:482:LEU:HB2	1.73	0.68
1:F:487:ALA:HB1	1:F:492:TYR:HB2	1.74	0.68
1:B:483:ASN:HD22	1:B:485:TYR:H	1.41	0.68
1:B:302:ILE:HD13	1:B:336:ILE:HG21	1.76	0.68
1:B:432:ASP:O	1:B:433:LEU:HD12	1.93	0.68
1:E:523:LYS:NZ	2:E:599:HOH:O	2.26	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:348:LEU:HD21	1:F:424:MET:CE	2.23	0.68
1:F:434:ASN:HB2	2:F:622:HOH:O	1.93	0.68
1:E:179:PRO:HG3	2:E:625:HOH:O	1.94	0.68
1:F:527:ASN:ND2	2:F:593:HOH:O	2.27	0.68
1:C:427:LYS:NZ	1:C:427:LYS:HB2	2.08	0.68
1:A:513:LEU:N	1:A:513:LEU:HD22	2.08	0.68
1:F:175:LEU:HA	1:F:195:VAL:HG13	1.76	0.68
1:C:524:LYS:HD2	2:F:650:HOH:O	1.93	0.68
1:D:336:ILE:HD12	1:D:336:ILE:N	2.09	0.68
1:E:240:MET:HG2	2:E:624:HOH:O	1.93	0.68
1:E:414:ARG:HA	1:E:440:ALA:HA	1.76	0.68
1:A:70:HIS:HB3	1:A:85:ASP:OD1	1.94	0.68
1:D:528:ILE:O	1:D:530:LEU:HD22	1.94	0.68
1:E:254:LEU:HD13	1:E:312:PHE:HE2	1.58	0.68
1:F:305:VAL:HG21	1:F:506:ILE:CD1	2.23	0.68
1:B:318:PHE:HB3	2:B:625:HOH:O	1.95	0.67
1:C:318:PHE:CZ	1:C:351:THR:HG22	2.29	0.67
1:C:408:LEU:HB2	1:C:431:ALA:HA	1.76	0.67
1:D:74:ASN:HB2	2:D:623:HOH:O	1.94	0.67
1:F:302:ILE:O	1:F:305:VAL:HG12	1.94	0.67
1:F:472:ARG:HH21	1:F:473:LEU:HD22	1.57	0.67
1:B:65:ASP:HB2	1:B:120:LYS:HE3	1.76	0.67
1:D:114:GLY:H	1:D:117:TYR:HB3	1.58	0.67
1:A:113:LEU:HD22	1:A:117:TYR:HE1	1.60	0.67
1:B:324:THR:HG23	1:B:355:LYS:HE2	1.75	0.67
1:E:231:ASN:O	1:E:317:LEU:HB2	1.93	0.67
1:F:162:ARG:HH11	1:F:162:ARG:HG2	1.59	0.67
1:D:508:ARG:NH2	1:F:62:VAL:HG11	2.09	0.67
1:C:470:ARG:HG3	1:C:470:ARG:HH11	1.60	0.67
1:A:35:ARG:HB3	1:A:35:ARG:NH1	2.09	0.67
1:E:113:LEU:HD22	1:E:117:TYR:CE1	2.30	0.67
1:F:70:HIS:HB2	2:F:605:HOH:O	1.95	0.67
1:F:104:GLN:HG2	2:F:708:HOH:O	1.94	0.67
1:F:231:ASN:O	1:F:317:LEU:HB2	1.95	0.67
1:E:120:LYS:HD3	2:E:689:HOH:O	1.93	0.67
1:C:321:ASN:HA	1:C:343:GLN:HB2	1.77	0.66
1:C:156:TYR:HB3	1:C:160:PHE:CE2	2.31	0.66
1:D:197:VAL:HA	2:D:633:HOH:O	1.95	0.66
1:F:150:VAL:O	1:F:153:LEU:HB2	1.96	0.66
1:C:229:THR:HA	2:C:595:HOH:O	1.94	0.66
1:E:230:HIS:HB3	1:E:236:VAL:HG22	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:433:LEU:HA	1:A:494:ASP:OD1	1.96	0.66
1:A:529:PRO:O	1:A:530:LEU:HD13	1.96	0.66
1:C:299:HIS:O	1:C:303:GLU:HG3	1.96	0.66
2:C:698:HOH:O	1:F:358:ARG:HG2	1.95	0.66
1:A:91:TYR:OH	1:C:508:ARG:NE	2.28	0.66
1:C:417:PHE:HA	1:C:443:ALA:O	1.96	0.66
1:B:438:PRO:HG3	1:C:21:LEU:HD22	1.78	0.66
1:C:434:ASN:N	1:C:494:ASP:OD1	2.23	0.66
1:F:514:ARG:HD2	2:F:700:HOH:O	1.94	0.66
1:C:190:ILE:HD12	1:F:399:PHE:HD1	1.60	0.66
1:C:211:ILE:HD11	2:C:579:HOH:O	1.96	0.66
1:E:62:VAL:HG21	1:F:508:ARG:HE	1.61	0.66
1:F:101:VAL:HG23	1:F:136:VAL:HB	1.77	0.66
1:F:523:LYS:HE3	2:F:688:HOH:O	1.96	0.66
1:C:196:MET:HB3	2:C:620:HOH:O	1.94	0.66
1:E:175:LEU:HB3	2:E:593:HOH:O	1.96	0.66
1:F:328:ARG:HB3	2:F:550:HOH:O	1.95	0.66
1:A:14:THR:HB	2:A:574:HOH:O	1.94	0.65
1:B:101:VAL:HG23	1:B:136:VAL:O	1.96	0.65
1:F:377:PRO:HA	1:F:417:PHE:HD2	1.61	0.65
1:A:391:ILE:HD13	2:A:650:HOH:O	1.96	0.65
1:B:459:ILE:HD11	1:B:470:ARG:HB2	1.78	0.65
1:C:45:LYS:CE	1:C:200:THR:HG22	2.25	0.65
1:F:32:GLY:HA3	1:F:107:THR:OG1	1.96	0.65
1:F:198:ASP:HA	1:F:227:ALA:HB3	1.78	0.65
1:A:494:ASP:HB3	1:B:64:LEU:HD22	1.79	0.65
1:D:429:LEU:HD13	2:D:547:HOH:O	1.97	0.65
1:E:334:VAL:HG23	2:E:612:HOH:O	1.96	0.65
1:F:177:VAL:HG12	1:F:197:VAL:CG2	2.26	0.65
1:F:354:GLU:HG3	2:F:628:HOH:O	1.95	0.65
1:F:104:GLN:HE21	1:F:140:ASP:N	1.93	0.65
1:A:84:GLY:HA2	1:A:120:LYS:NZ	2.11	0.65
1:C:437:TRP:HB2	2:C:618:HOH:O	1.95	0.65
1:B:11:ILE:O	1:B:11:ILE:HG13	1.97	0.65
1:B:102:PHE:CD1	1:B:121:ILE:HG23	2.32	0.65
1:C:101:VAL:HG23	1:C:136:VAL:O	1.97	0.65
1:F:162:ARG:HB2	2:F:630:HOH:O	1.95	0.64
1:A:319:ALA:HB3	1:A:355:LYS:HD2	1.78	0.64
1:A:354:GLU:OE1	1:A:393:ARG:HB3	1.97	0.64
2:C:692:HOH:O	1:F:402:ALA:HB1	1.97	0.64
1:E:117:TYR:HA	2:E:689:HOH:O	1.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:61:PHE:HE1	1:C:90:GLY:HA3	1.60	0.64
1:C:508:ARG:HD3	1:C:509:GLY:N	2.12	0.64
1:E:258:LEU:HB2	2:E:571:HOH:O	1.96	0.64
1:A:164:THR:HG23	1:D:399:PHE:CD1	2.32	0.64
1:B:315:GLN:N	1:B:316:PRO:HD3	2.12	0.64
1:B:361:ARG:HD2	1:B:403:GLU:OE2	1.98	0.64
1:C:164:THR:HG23	1:F:399:PHE:CE1	2.33	0.64
1:D:337:VAL:HG11	2:D:601:HOH:O	1.96	0.64
1:E:396:LYS:HG2	2:E:592:HOH:O	1.96	0.64
1:B:162:ARG:HG3	2:B:586:HOH:O	1.96	0.64
1:E:298:MET:SD	1:E:301:VAL:HG21	2.38	0.64
1:F:208:PRO:HA	1:F:211:ILE:HD12	1.79	0.64
1:A:71:ARG:NH2	1:C:490:ARG:HE	1.95	0.64
1:B:508:ARG:NH2	1:C:62:VAL:HG11	2.12	0.64
1:C:336:ILE:N	1:C:336:ILE:HD12	2.13	0.64
1:B:335:GLY:C	1:B:336:ILE:HD12	2.18	0.64
1:B:448:GLN:O	1:B:451:VAL:HG22	1.98	0.64
1:D:433:LEU:HA	1:D:494:ASP:OD1	1.97	0.64
1:A:180:CYS:O	1:A:203:MET:HA	1.98	0.64
1:A:315:GLN:N	1:A:316:PRO:HD3	2.13	0.64
1:B:190:ILE:HD12	1:E:399:PHE:HD1	1.63	0.64
1:E:21:LEU:O	1:E:25:ILE:HG23	1.98	0.64
1:F:175:LEU:HA	1:F:195:VAL:CG1	2.28	0.64
1:B:162:ARG:HG2	1:B:162:ARG:HH11	1.63	0.64
1:C:399:PHE:CD1	1:F:164:THR:HG23	2.33	0.64
1:E:141:SER:O	1:E:179:PRO:HB2	1.98	0.64
1:A:71:ARG:HH21	1:C:490:ARG:HA	1.63	0.63
1:B:527:ASN:ND2	1:E:358:ARG:HE	1.94	0.63
1:C:319:ALA:N	1:C:320:PRO:HD3	2.13	0.63
1:E:529:PRO:O	1:E:530:LEU:HD12	1.97	0.63
1:B:52:ILE:HG13	2:B:590:HOH:O	1.97	0.63
1:E:145:ARG:HB2	2:E:608:HOH:O	1.97	0.63
1:D:173:ILE:HG21	1:D:251:VAL:HG23	1.79	0.63
1:B:279:ASP:O	1:B:282:ALA:HB3	1.98	0.63
1:B:527:ASN:ND2	2:B:585:HOH:O	2.32	0.63
1:C:427:LYS:HB2	1:C:427:LYS:HZ2	1.63	0.63
1:B:499:PRO:HB3	2:B:646:HOH:O	1.97	0.63
1:D:374:VAL:HG13	1:D:424:MET:HG3	1.80	0.63
1:E:398:ILE:HB	2:E:706:HOH:O	1.97	0.63
1:B:231:ASN:HD21	1:B:239:HIS:C	2.01	0.63
1:D:65:ASP:HB2	1:D:120:LYS:HE3	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:505:HIS:HA	1:E:508:ARG:HD2	1.81	0.63
1:C:393:ARG:HA	1:C:396:LYS:HE3	1.81	0.62
1:F:316:PRO:HA	2:F:567:HOH:O	1.98	0.62
1:A:214:VAL:HG11	1:D:381:PRO:HG2	1.80	0.62
1:C:284:LEU:HD13	1:C:304:HIS:CD2	2.33	0.62
1:C:147:GLN:N	1:C:147:GLN:OE1	2.31	0.62
1:C:483:ASN:ND2	1:C:485:TYR:HB2	2.14	0.62
1:E:113:LEU:HD12	2:E:665:HOH:O	1.99	0.62
1:A:392:ARG:HG3	1:A:392:ARG:HH11	1.64	0.62
1:E:18:LEU:HD11	1:F:285:ASP:O	1.98	0.62
1:F:295:PRO:HB2	2:F:536:HOH:O	1.99	0.62
1:F:483:ASN:ND2	1:F:485:TYR:HB2	2.13	0.62
1:F:97:ARG:NH1	1:F:267:PRO:HG3	2.14	0.62
1:C:411:VAL:HG22	1:C:435:LEU:HB2	1.80	0.62
1:D:361:ARG:HD2	1:D:403:GLU:OE2	1.99	0.62
1:E:113:LEU:HD13	1:E:117:TYR:CD1	2.34	0.62
1:E:422:ILE:HG23	2:E:539:HOH:O	1.99	0.62
1:B:121:ILE:HG22	2:B:575:HOH:O	2.00	0.62
1:E:336:ILE:HG13	2:E:612:HOH:O	1.98	0.62
1:D:397:LEU:HD22	1:D:423:VAL:HG13	1.82	0.62
1:F:169:VAL:HG12	1:F:170:ILE:HG23	1.82	0.62
1:F:234:SER:HB2	1:F:236:VAL:HG13	1.81	0.62
1:B:456:ARG:O	1:B:459:ILE:HG22	1.99	0.62
1:D:469:THR:O	1:D:473:LEU:HB2	1.99	0.62
1:A:483:ASN:ND2	1:A:485:TYR:HB2	2.15	0.61
1:B:306:LEU:HB2	2:B:642:HOH:O	2.00	0.61
1:C:71:ARG:NH2	1:C:119:GLN:HE22	1.98	0.61
1:A:231:ASN:O	1:A:318:PHE:HB2	1.99	0.61
1:A:472:ARG:O	1:A:476:GLU:HG3	1.99	0.61
1:A:61:PHE:CZ	1:A:63:GLU:HB2	2.35	0.61
1:E:91:TYR:OH	1:F:508:ARG:NE	2.34	0.61
1:E:505:HIS:O	1:E:508:ARG:HD3	2.00	0.61
1:F:177:VAL:HG12	1:F:197:VAL:HG23	1.80	0.61
1:A:224:LEU:HD12	1:D:383:VAL:HG13	1.80	0.61
1:C:322:ILE:HA	1:C:339:ASN:HA	1.81	0.61
1:F:342:MET:HG2	2:F:657:HOH:O	2.00	0.61
1:A:371:LEU:HD23	2:A:558:HOH:O	1.99	0.61
1:E:208:PRO:HG3	1:E:224:LEU:HD22	1.80	0.61
1:F:185:VAL:HG23	2:F:651:HOH:O	2.00	0.61
1:C:70:HIS:NE2	1:C:81:ARG:HG2	2.14	0.61
1:D:113:LEU:HD22	1:D:117:TYR:CE1	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:70:HIS:HB2	2:C:533:HOH:O	2.00	0.61
1:A:418:GLY:HA2	1:D:153:LEU:HD21	1.83	0.61
1:D:496:VAL:HB	1:F:67:PHE:HE2	1.66	0.61
1:A:453:ILE:HG21	1:D:146:ILE:HD12	1.82	0.61
1:A:47:THR:OG1	1:A:50:GLU:HG3	2.01	0.61
1:A:454:LEU:HD13	1:D:75:PHE:CZ	2.36	0.61
1:A:524:LYS:HD3	1:D:405:THR:OG1	2.01	0.61
1:C:24:ARG:HD3	1:C:83:TYR:OH	2.00	0.61
1:C:173:ILE:HD12	1:C:254:LEU:HD23	1.82	0.61
1:D:508:ARG:HE	1:F:62:VAL:HG21	1.65	0.61
1:E:101:VAL:HG23	1:E:136:VAL:O	2.00	0.61
1:A:396:LYS:HG2	2:A:677:HOH:O	2.00	0.60
1:A:425:GLY:HA3	2:A:670:HOH:O	2.01	0.60
1:C:456:ARG:O	1:C:459:ILE:HG22	2.01	0.60
1:E:56:LEU:HD13	1:E:92:GLY:HA3	1.83	0.60
1:F:55:LEU:CD2	1:F:136:VAL:HG11	2.31	0.60
1:F:291:SER:HB3	1:F:294:GLN:HB2	1.84	0.60
1:C:435:LEU:HD12	2:C:683:HOH:O	2.01	0.60
1:A:169:VAL:HG21	1:D:521:PRO:HB2	1.84	0.60
1:A:291:SER:HB3	1:A:294:GLN:HB2	1.84	0.60
1:A:302:ILE:HD13	1:A:336:ILE:HG21	1.84	0.60
1:A:459:ILE:HD11	1:A:470:ARG:HB2	1.82	0.60
1:C:231:ASN:O	1:C:317:LEU:HB2	2.01	0.60
1:E:161:ARG:HG3	1:E:161:ARG:NH1	2.16	0.60
1:E:339:ASN:HB2	2:E:569:HOH:O	2.01	0.60
1:F:440:ALA:O	1:F:484:PRO:HD3	2.01	0.60
1:C:208:PRO:HB3	2:C:591:HOH:O	2.00	0.60
1:C:395:ALA:HB2	1:F:186:TYR:HD1	1.66	0.60
1:D:62:VAL:CG1	1:E:508:ARG:HH21	2.13	0.60
1:F:65:ASP:CB	1:F:120:LYS:HE3	2.31	0.60
1:A:73:THR:HG22	1:A:78:ASP:OD2	2.02	0.60
1:E:138:ILE:HG23	2:E:593:HOH:O	2.01	0.60
1:F:340:GLN:CD	1:F:342:MET:HB2	2.22	0.60
1:B:70:HIS:HB2	2:B:621:HOH:O	2.02	0.60
1:B:87:VAL:HG23	1:B:104:GLN:HA	1.83	0.60
1:C:392:ARG:HG3	1:C:392:ARG:HH11	1.67	0.60
1:E:483:ASN:HD22	1:E:485:TYR:H	1.48	0.60
1:A:273:ALA:HB2	1:A:330:GLU:HG3	1.84	0.60
1:D:391:ILE:HA	2:D:640:HOH:O	2.02	0.60
1:E:472:ARG:O	1:E:476:GLU:HG3	2.02	0.60
1:B:22:ARG:O	1:B:25:ILE:HG12	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:397:LEU:HD13	1:B:423:VAL:CG1	2.32	0.59
1:C:386:GLU:OE1	1:F:204:PHE:HA	2.01	0.59
1:A:159:ILE:HG22	2:A:562:HOH:O	2.02	0.59
1:A:487:ALA:HB1	1:A:492:TYR:HB2	1.84	0.59
1:D:39:LYS:O	1:D:43:LYS:HG3	2.03	0.59
1:E:322:ILE:HG13	1:E:338:ALA:O	2.02	0.59
1:F:238:HIS:HA	1:F:315:GLN:HG2	1.84	0.59
1:A:24:ARG:HB3	1:A:83:TYR:HE1	1.67	0.59
1:A:175:LEU:HD22	1:A:177:VAL:HG13	1.84	0.59
1:E:259:PRO:HB2	2:E:600:HOH:O	2.02	0.59
1:E:464:ASP:O	1:E:465:ASP:HB2	2.02	0.59
1:C:186:TYR:HD1	1:F:395:ALA:HB2	1.68	0.59
1:D:284:LEU:O	1:D:287:ILE:HG22	2.02	0.59
1:E:416:ALA:HB3	1:E:442:ILE:HA	1.85	0.59
1:F:198:ASP:HB2	1:F:240:MET:SD	2.43	0.59
1:F:288:VAL:HG23	2:F:677:HOH:O	2.02	0.59
1:A:377:PRO:O	1:A:417:PHE:HB2	2.02	0.59
1:B:151:ALA:HB2	1:E:490:ARG:NH2	2.18	0.59
1:B:527:ASN:HD21	1:E:358:ARG:HE	1.50	0.59
1:C:398:ILE:HD12	1:F:160:PHE:HD2	1.66	0.59
1:F:414:ARG:HA	1:F:439:THR:O	2.02	0.59
1:A:71:ARG:NH2	1:C:490:ARG:HA	2.16	0.59
1:A:151:ALA:HB2	1:D:490:ARG:NH1	2.18	0.59
2:A:694:HOH:O	1:D:358:ARG:HA	2.03	0.59
1:B:169:VAL:HG23	2:E:599:HOH:O	2.01	0.59
1:B:529:PRO:HA	2:B:649:HOH:O	2.02	0.59
1:C:172:GLN:O	1:C:191:THR:HB	2.02	0.59
1:F:97:ARG:CZ	1:F:267:PRO:HG3	2.32	0.59
1:F:121:ILE:O	1:F:125:MET:HG3	2.03	0.59
1:F:472:ARG:HG2	1:F:472:ARG:HH11	1.67	0.59
1:F:377:PRO:O	1:F:417:PHE:HB2	2.02	0.59
1:D:525:HIS:HB2	2:D:573:HOH:O	2.02	0.59
1:F:187:SER:CB	1:F:188:PRO:HD3	2.25	0.59
1:B:508:ARG:NE	1:C:91:TYR:OH	2.36	0.58
1:C:89:THR:HG22	1:C:102:PHE:HB2	1.84	0.58
1:C:370:VAL:HB	2:C:681:HOH:O	2.01	0.58
1:D:496:VAL:HB	1:F:67:PHE:CE2	2.38	0.58
1:A:69:ARG:HD2	1:A:81:ARG:O	2.03	0.58
1:E:199:GLN:HB3	2:E:687:HOH:O	2.02	0.58
1:F:231:ASN:HD21	1:F:239:HIS:CA	2.16	0.58
1:D:175:LEU:HD22	1:D:177:VAL:HG13	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:427:LYS:NZ	1:D:427:LYS:HB2	2.17	0.58
1:D:472:ARG:HG2	2:D:624:HOH:O	2.03	0.58
1:D:478:GLU:HA	1:D:482:LEU:HB2	1.84	0.58
1:F:336:ILE:HD12	1:F:336:ILE:N	2.17	0.58
1:B:427:LYS:NZ	1:B:434:ASN:OD1	2.36	0.58
1:C:230:HIS:HB3	1:C:236:VAL:HG22	1.85	0.58
1:F:55:LEU:HD21	1:F:136:VAL:HG11	1.86	0.58
1:A:302:ILE:HD12	2:A:678:HOH:O	2.04	0.58
1:A:451:VAL:HG13	2:A:681:HOH:O	2.03	0.58
1:E:17:LYS:HE2	2:F:625:HOH:O	2.03	0.58
1:F:104:GLN:HG3	1:F:139:ASN:HA	1.85	0.58
1:F:266:PRO:HG2	2:F:604:HOH:O	2.04	0.58
1:C:525:HIS:HE1	1:F:361:ARG:HE	1.52	0.58
1:E:176:VAL:HG12	1:E:201:SER:HB2	1.84	0.58
1:D:70:HIS:HA	1:D:116:VAL:HG21	1.84	0.58
1:D:490:ARG:HH21	1:F:71:ARG:CZ	2.17	0.58
1:E:24:ARG:NH1	1:E:83:TYR:OH	2.37	0.58
1:F:175:LEU:HD23	1:F:195:VAL:HG13	1.85	0.58
1:A:21:LEU:HD22	1:C:438:PRO:HG3	1.84	0.58
1:C:496:VAL:HG21	2:C:651:HOH:O	2.04	0.58
1:D:414:ARG:HD2	2:D:564:HOH:O	2.03	0.58
1:D:25:ILE:O	1:D:29:THR:HG23	2.04	0.58
1:D:181:ALA:HB2	1:D:204:PHE:CE1	2.39	0.58
1:D:197:VAL:HG12	1:D:198:ASP:H	1.69	0.58
1:E:208:PRO:HG3	1:E:224:LEU:CD2	2.33	0.58
1:F:64:LEU:HG	2:F:551:HOH:O	2.03	0.58
1:B:164:THR:HG23	1:E:399:PHE:CD1	2.39	0.57
1:D:181:ALA:HA	1:D:204:PHE:O	2.03	0.57
1:F:193:PHE:HA	1:F:238:HIS:CE1	2.39	0.57
1:F:196:MET:O	1:F:240:MET:HA	2.04	0.57
1:F:392:ARG:HG3	1:F:392:ARG:HH11	1.69	0.57
1:F:427:LYS:HB2	1:F:427:LYS:NZ	2.19	0.57
1:B:508:ARG:CZ	1:C:62:VAL:HG11	2.35	0.57
1:D:176:VAL:HB	1:D:196:MET:HB3	1.86	0.57
1:D:428:HIS:HB2	2:D:547:HOH:O	2.04	0.57
1:A:295:PRO:HB2	1:A:342:MET:HE2	1.86	0.57
1:C:94:VAL:HG23	1:C:99:VAL:HG11	1.85	0.57
1:D:302:ILE:HD13	1:D:336:ILE:HG21	1.87	0.57
1:E:512:GLN:N	2:E:611:HOH:O	2.30	0.57
1:F:195:VAL:HG23	2:F:600:HOH:O	2.03	0.57
1:F:314:THR:HG23	1:F:325:GLY:HA2	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:324:THR:HA	1:B:336:ILE:O	2.04	0.57
1:A:321:ASN:OD1	1:A:321:ASN:N	2.32	0.57
1:B:70:HIS:NE2	1:B:77:LEU:HD22	2.20	0.57
1:C:63:GLU:HG2	1:C:66:GLU:HB2	1.87	0.57
1:D:505:HIS:O	1:D:508:ARG:HD3	2.05	0.57
1:F:111:GLY:O	1:F:141:SER:HB2	2.03	0.57
1:A:442:ILE:HG22	1:D:150:VAL:HG11	1.84	0.57
1:B:302:ILE:O	1:B:305:VAL:HG22	2.04	0.57
1:C:338:ALA:CB	1:C:373:PHE:HB2	2.33	0.57
1:C:368:VAL:HG23	2:C:550:HOH:O	2.03	0.57
1:D:197:VAL:HG12	1:D:198:ASP:N	2.19	0.57
1:F:319:ALA:N	1:F:320:PRO:HD3	2.19	0.57
1:F:329:VAL:N	2:F:550:HOH:O	2.37	0.57
1:A:177:VAL:HG12	1:A:197:VAL:HG23	1.86	0.57
1:B:36:ALA:HB1	1:B:107:THR:HB	1.87	0.57
1:C:520:LEU:HD12	1:C:520:LEU:H	1.69	0.57
1:D:147:GLN:HB2	2:D:655:HOH:O	2.02	0.57
1:A:124:VAL:HG11	2:A:546:HOH:O	2.03	0.57
1:D:503:ARG:O	1:D:504:ARG:C	2.43	0.57
1:E:386:GLU:HA	1:E:390:ILE:HG22	1.85	0.57
1:B:393:ARG:HA	1:B:396:LYS:HE3	1.87	0.57
1:B:470:ARG:HG2	2:B:682:HOH:O	2.05	0.57
2:B:649:HOH:O	1:E:358:ARG:CZ	2.53	0.57
1:D:180:CYS:HB3	1:D:203:MET:HG2	1.87	0.57
1:F:77:LEU:HD12	2:F:655:HOH:O	2.05	0.57
1:F:278:THR:OG1	1:F:281:ASP:HB2	2.04	0.57
1:A:197:VAL:HG12	1:A:198:ASP:N	2.20	0.57
1:B:47:THR:HG23	1:B:50:GLU:CD	2.25	0.57
1:B:262:ASN:OD1	1:B:263:LEU:N	2.37	0.57
1:A:87:VAL:HG13	1:A:87:VAL:O	2.05	0.56
1:B:120:LYS:NZ	2:B:531:HOH:O	2.38	0.56
1:B:435:LEU:HD22	2:B:596:HOH:O	2.05	0.56
1:B:464:ASP:O	1:B:465:ASP:HB2	2.04	0.56
1:C:124:VAL:HG12	2:C:574:HOH:O	2.05	0.56
1:C:342:MET:HG2	2:C:646:HOH:O	2.04	0.56
1:F:49:ARG:HG3	1:F:49:ARG:HH11	1.69	0.56
1:F:205:ILE:HG23	1:F:206:THR:HG23	1.85	0.56
1:A:173:ILE:HG21	1:A:251:VAL:HG23	1.87	0.56
1:B:505:HIS:C	1:B:508:ARG:HH11	2.08	0.56
1:E:431:ALA:HB1	1:E:434:ASN:HD21	1.70	0.56
1:A:505:HIS:O	1:A:508:ARG:NH1	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:338:ALA:HB2	1:C:373:PHE:HB2	1.87	0.56
1:C:402:ALA:HA	1:C:429:LEU:O	2.05	0.56
1:D:315:GLN:N	1:D:316:PRO:HD3	2.20	0.56
1:D:412:ILE:HG23	2:D:620:HOH:O	2.04	0.56
1:D:422:ILE:O	1:D:429:LEU:HD22	2.05	0.56
1:E:145:ARG:NE	2:E:608:HOH:O	2.38	0.56
1:F:375:ASP:CG	1:F:414:ARG:HB3	2.26	0.56
1:B:250:TYR:OH	1:B:314:THR:HG22	2.05	0.56
1:B:307:ASP:OD2	1:B:330:GLU:N	2.38	0.56
1:C:51:ARG:HH12	1:C:140:ASP:HB2	1.71	0.56
1:E:483:ASN:HB2	1:E:484:PRO:HD2	1.88	0.56
1:D:177:VAL:HG12	1:D:197:VAL:CG2	2.35	0.56
1:E:177:VAL:HG22	2:E:593:HOH:O	2.05	0.56
1:F:521:PRO:HB2	2:F:688:HOH:O	2.05	0.56
1:C:177:VAL:HG11	2:C:605:HOH:O	2.05	0.56
1:C:315:GLN:N	1:C:316:PRO:HD3	2.20	0.56
1:D:467:GLU:HA	1:D:470:ARG:CB	2.36	0.56
1:A:206:THR:CG2	1:A:210:VAL:HB	2.36	0.56
1:B:278:THR:HG23	2:B:693:HOH:O	2.06	0.56
1:C:447:ALA:O	1:C:451:VAL:HG22	2.06	0.56
1:D:238:HIS:HA	1:D:315:GLN:HG2	1.88	0.56
1:D:241:ALA:N	2:D:633:HOH:O	2.38	0.56
1:E:431:ALA:CB	1:E:434:ASN:HD21	2.19	0.56
1:C:472:ARG:HD2	1:C:476:GLU:OE2	2.05	0.56
1:F:517:ARG:O	1:F:518:GLU:HG2	2.05	0.56
1:B:494:ASP:HB3	1:C:64:LEU:HD22	1.88	0.56
1:D:177:VAL:HG12	1:D:197:VAL:HG23	1.88	0.56
1:F:497:ILE:HG13	2:F:687:HOH:O	2.06	0.56
1:C:156:TYR:HB3	1:C:160:PHE:CZ	2.40	0.55
1:D:122:VAL:O	1:D:125:MET:N	2.39	0.55
1:D:398:ILE:CG2	1:D:423:VAL:HG22	2.35	0.55
1:E:113:LEU:HD22	1:E:117:TYR:HE1	1.70	0.55
1:A:399:PHE:CD1	1:D:164:THR:HG23	2.42	0.55
1:A:480:ALA:O	1:A:481:LEU:HD12	2.06	0.55
1:B:508:ARG:HD3	1:B:508:ARG:C	2.26	0.55
1:D:24:ARG:HD3	1:D:83:TYR:OH	2.06	0.55
1:D:505:HIS:C	1:D:508:ARG:HH11	2.08	0.55
1:D:523:LYS:NZ	2:D:594:HOH:O	2.39	0.55
1:E:504:ARG:O	1:E:508:ARG:HD2	2.05	0.55
1:A:153:LEU:HD11	1:D:418:GLY:HA2	1.88	0.55
1:E:10:ASP:HB3	1:E:13:THR:OG1	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:87:VAL:HG13	1:E:120:LYS:HE2	1.88	0.55
1:F:71:ARG:HB2	1:F:71:ARG:NH1	2.21	0.55
1:B:10:ASP:OD1	1:B:11:ILE:N	2.39	0.55
1:B:135:VAL:HG12	1:B:135:VAL:O	2.07	0.55
1:C:121:ILE:O	1:C:125:MET:HG3	2.07	0.55
1:C:398:ILE:HD12	1:F:160:PHE:CD2	2.42	0.55
1:C:306:LEU:HD13	1:C:327:GLY:HA3	1.87	0.55
1:E:180:CYS:SG	1:E:185:VAL:HA	2.47	0.55
1:F:505:HIS:C	1:F:508:ARG:HH11	2.10	0.55
1:B:508:ARG:HE	1:C:62:VAL:HG21	1.70	0.55
1:D:69:ARG:HA	2:D:539:HOH:O	2.07	0.55
1:E:24:ARG:HG2	1:E:24:ARG:HH11	1.70	0.55
1:E:419:GLY:O	1:E:423:VAL:HG23	2.07	0.55
1:A:101:VAL:HG23	1:A:136:VAL:O	2.05	0.55
1:C:24:ARG:HG3	2:C:562:HOH:O	2.06	0.55
1:D:231:ASN:HB3	1:D:317:LEU:HD12	1.89	0.55
1:B:490:ARG:NH1	1:E:151:ALA:HB2	2.21	0.55
1:F:441:GLN:HB3	1:F:482:LEU:HG	1.87	0.55
1:A:299:HIS:O	1:A:303:GLU:HG3	2.07	0.55
2:C:698:HOH:O	1:F:358:ARG:HA	2.06	0.55
1:A:146:ILE:HG12	1:D:453:ILE:HG21	1.87	0.55
1:A:206:THR:HG23	1:A:210:VAL:HB	1.88	0.55
1:A:434:ASN:HB3	2:A:568:HOH:O	2.06	0.55
1:C:337:VAL:O	1:C:372:THR:HA	2.07	0.55
1:D:101:VAL:HG23	1:D:136:VAL:O	2.06	0.55
1:E:121:ILE:HG13	2:E:670:HOH:O	2.07	0.55
1:E:197:VAL:HA	2:E:624:HOH:O	2.07	0.55
1:F:315:GLN:N	1:F:316:PRO:HD3	2.21	0.55
1:F:472:ARG:HG2	1:F:472:ARG:NH1	2.22	0.55
1:D:397:LEU:HD22	1:D:423:VAL:CG1	2.36	0.54
1:A:508:ARG:HD3	1:A:508:ARG:C	2.27	0.54
1:C:150:VAL:O	1:C:153:LEU:N	2.38	0.54
1:C:153:LEU:HD21	1:F:418:GLY:CA	2.37	0.54
1:C:315:GLN:HB2	1:C:355:LYS:HE3	1.89	0.54
1:B:427:LYS:HZ2	1:B:427:LYS:HB2	1.73	0.54
1:D:262:ASN:OD1	1:D:263:LEU:HD13	2.06	0.54
1:F:447:ALA:HA	1:F:477:TYR:CD1	2.42	0.54
1:F:486:THR:O	1:F:489:GLU:HB2	2.08	0.54
2:B:624:HOH:O	1:E:490:ARG:HG3	2.08	0.54
1:E:358:ARG:O	1:E:358:ARG:HD3	2.08	0.54
1:A:374:VAL:HG22	1:A:424:MET:HB3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:231:ASN:HD21	1:C:239:HIS:CA	2.20	0.54
1:D:51:ARG:HB3	1:D:138:ILE:HD13	1.90	0.54
1:D:65:ASP:OD1	1:D:123:LYS:HD2	2.07	0.54
1:D:450:ALA:HB1	1:D:477:TYR:CE2	2.42	0.54
1:F:456:ARG:O	1:F:459:ILE:HG22	2.07	0.54
1:C:268:ALA:HB2	2:C:610:HOH:O	2.08	0.54
1:E:478:GLU:HA	1:E:482:LEU:HB2	1.89	0.54
1:F:49:ARG:H	1:F:49:ARG:HD2	1.73	0.54
1:F:359:PHE:O	1:F:362:THR:N	2.41	0.54
1:A:339:ASN:O	1:A:341:PRO:HD3	2.07	0.54
1:D:288:VAL:HG11	1:D:439:THR:HB	1.89	0.54
1:D:513:LEU:HD22	1:D:513:LEU:N	2.22	0.54
1:A:414:ARG:HA	1:A:439:THR:O	2.08	0.54
1:B:87:VAL:HG11	2:B:657:HOH:O	2.08	0.54
1:E:80:ASN:N	1:E:80:ASN:HD22	2.06	0.54
1:E:432:ASP:O	1:E:433:LEU:HD12	2.08	0.54
1:F:344:PHE:O	1:F:345:ALA:HB3	2.07	0.54
1:A:528:ILE:HG12	2:A:677:HOH:O	2.08	0.54
1:B:173:ILE:HG21	1:B:251:VAL:CG2	2.35	0.54
1:B:346:GLY:HA2	2:B:623:HOH:O	2.07	0.54
1:C:265:GLU:HG2	1:C:266:PRO:HD2	1.90	0.54
1:E:157:GLY:O	1:E:160:PHE:N	2.41	0.54
1:E:185:VAL:C	1:E:188:PRO:HD2	2.28	0.54
1:A:146:ILE:H	1:A:146:ILE:CD1	2.11	0.54
1:A:527:ASN:HD21	1:D:358:ARG:CD	2.21	0.54
1:C:353:SER:CB	1:C:394:GLY:HA2	2.38	0.54
1:D:241:ALA:HB2	2:D:614:HOH:O	2.07	0.54
1:D:414:ARG:HA	1:D:440:ALA:HA	1.90	0.54
1:F:139:ASN:OD1	1:F:176:VAL:HG22	2.08	0.54
1:F:176:VAL:HG12	1:F:201:SER:HB2	1.90	0.54
1:F:203:MET:HB2	1:F:230:HIS:CD2	2.42	0.54
1:A:159:ILE:HA	2:A:583:HOH:O	2.09	0.53
1:A:177:VAL:HG12	1:A:197:VAL:CG2	2.38	0.53
1:B:230:HIS:HA	1:B:234:SER:OG	2.07	0.53
1:C:196:MET:HE2	2:C:620:HOH:O	2.07	0.53
1:C:234:SER:HB2	1:C:236:VAL:HG13	1.89	0.53
1:D:111:GLY:O	1:D:141:SER:HA	2.08	0.53
1:E:46:LEU:HD12	1:E:244:GLU:OE2	2.07	0.53
1:E:175:LEU:HD22	1:E:177:VAL:HG13	1.89	0.53
1:E:428:HIS:HB2	2:E:539:HOH:O	2.08	0.53
1:F:63:GLU:CD	1:F:66:GLU:HB2	2.29	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:177:VAL:HG22	2:F:644:HOH:O	2.07	0.53
1:A:11:ILE:HG23	1:A:12:HIS:ND1	2.23	0.53
1:B:313:GLU:HG2	1:B:316:PRO:HG3	1.90	0.53
1:B:398:ILE:HD11	1:E:190:ILE:HD11	1.89	0.53
1:C:346:GLY:O	1:C:376:VAL:HG23	2.08	0.53
1:C:442:ILE:HB	2:C:547:HOH:O	2.07	0.53
1:B:132:GLY:O	1:B:261:ASN:ND2	2.41	0.53
1:C:185:VAL:O	1:F:391:ILE:HG23	2.08	0.53
1:E:47:THR:OG1	1:E:50:GLU:HG3	2.08	0.53
1:E:147:GLN:HB2	2:E:699:HOH:O	2.06	0.53
1:F:341:PRO:HB2	2:F:657:HOH:O	2.08	0.53
1:F:346:GLY:O	1:F:376:VAL:HG23	2.08	0.53
1:C:364:ASP:O	1:F:524:LYS:HD2	2.08	0.53
1:D:376:VAL:HG21	1:D:420:ALA:HB1	1.90	0.53
1:E:123:LYS:HD2	2:E:609:HOH:O	2.07	0.53
1:E:398:ILE:HG12	1:E:399:PHE:N	2.23	0.53
1:F:497:ILE:HG21	1:F:505:HIS:NE2	2.24	0.53
1:A:55:LEU:HD11	2:A:671:HOH:O	2.08	0.53
1:A:163:ASN:ND2	2:A:562:HOH:O	2.41	0.53
1:A:486:THR:HG23	2:A:598:HOH:O	2.08	0.53
1:B:469:THR:O	1:B:473:LEU:HB2	2.08	0.53
1:C:70:HIS:CE1	1:C:81:ARG:HG2	2.43	0.53
1:C:505:HIS:CA	1:C:508:ARG:HH11	2.22	0.53
1:D:176:VAL:O	1:D:196:MET:HA	2.09	0.53
1:E:67:PHE:CE2	1:F:496:VAL:HB	2.43	0.53
1:D:10:ASP:CG	1:D:11:ILE:H	2.12	0.53
1:D:376:VAL:CG2	1:D:420:ALA:HB1	2.39	0.53
1:F:375:ASP:OD1	1:F:414:ARG:HB3	2.08	0.53
1:C:45:LYS:HE2	1:C:200:THR:O	2.08	0.53
1:C:288:VAL:HG23	2:C:558:HOH:O	2.08	0.53
1:E:483:ASN:ND2	1:E:485:TYR:HB2	2.23	0.53
1:A:28:ALA:HB2	1:A:83:TYR:CD1	2.41	0.53
1:A:141:SER:O	1:A:179:PRO:HB2	2.08	0.53
1:A:450:ALA:HB3	2:A:681:HOH:O	2.09	0.53
1:C:324:THR:HA	1:C:336:ILE:O	2.09	0.53
1:C:530:LEU:HD21	1:F:528:ILE:HD13	1.90	0.53
2:C:650:HOH:O	1:F:149:GLY:HA2	2.08	0.53
1:E:91:TYR:CD1	1:E:91:TYR:C	2.82	0.53
1:E:374:VAL:HG13	1:E:424:MET:HG3	1.91	0.53
1:A:227:ALA:HB1	2:A:597:HOH:O	2.09	0.53
2:A:698:HOH:O	1:B:91:TYR:HB2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:147:GLN:CD	1:C:147:GLN:H	2.11	0.53
1:C:373:PHE:HA	1:C:411:VAL:O	2.08	0.53
1:C:456:ARG:HB3	1:C:456:ARG:NH1	2.23	0.53
1:D:45:LYS:HA	1:D:244:GLU:OE1	2.09	0.53
1:F:101:VAL:CG2	1:F:136:VAL:HB	2.39	0.53
1:C:475:GLN:HE22	1:C:476:GLU:HG3	1.74	0.53
1:D:459:ILE:HD11	1:D:466:ALA:O	2.08	0.53
1:E:321:ASN:OD1	1:E:321:ASN:N	2.38	0.53
1:A:510:LEU:HD23	2:A:537:HOH:O	2.09	0.52
1:B:36:ALA:CB	1:B:107:THR:HB	2.39	0.52
1:B:125:MET:SD	2:B:560:HOH:O	2.58	0.52
1:D:85:ASP:OD2	1:D:116:VAL:HB	2.09	0.52
1:E:315:GLN:N	1:E:316:PRO:HD3	2.24	0.52
1:E:319:ALA:N	1:E:320:PRO:HD3	2.25	0.52
1:A:76:GLY:HA3	2:A:673:HOH:O	2.10	0.52
1:A:164:THR:O	1:A:166:ALA:N	2.42	0.52
1:A:354:GLU:HG2	1:A:396:LYS:HD2	1.91	0.52
1:A:392:ARG:HD3	1:D:236:VAL:HG12	1.91	0.52
1:B:113:LEU:HD22	1:B:117:TYR:HE1	1.72	0.52
1:B:114:GLY:H	1:B:117:TYR:HB3	1.74	0.52
1:C:212:LYS:HG3	1:C:216:GLY:HA2	1.91	0.52
1:C:362:THR:O	1:C:366:PHE:HD2	1.92	0.52
1:E:67:PHE:HE2	1:F:496:VAL:HB	1.73	0.52
1:E:466:ALA:HB2	2:E:602:HOH:O	2.09	0.52
1:F:25:ILE:O	1:F:29:THR:HG23	2.08	0.52
1:F:45:LYS:HB3	2:F:665:HOH:O	2.09	0.52
1:A:62:VAL:HG21	1:C:508:ARG:HE	1.73	0.52
1:C:122:VAL:O	1:C:125:MET:N	2.42	0.52
1:D:205:ILE:HG22	1:D:206:THR:HG23	1.91	0.52
1:D:432:ASP:C	1:D:433:LEU:HD12	2.30	0.52
1:E:528:ILE:O	1:E:530:LEU:HD13	2.10	0.52
1:F:227:ALA:HB2	2:F:554:HOH:O	2.08	0.52
1:C:236:VAL:HG12	1:F:392:ARG:HD3	1.92	0.52
1:C:525:HIS:CE1	1:F:361:ARG:HE	2.28	0.52
1:A:319:ALA:N	1:A:320:PRO:HD3	2.24	0.52
1:B:309:ALA:HA	2:B:642:HOH:O	2.10	0.52
1:C:41:HIS:O	1:C:44:GLY:N	2.35	0.52
1:D:169:VAL:HA	2:D:570:HOH:O	2.10	0.52
1:A:508:ARG:HH21	1:B:62:VAL:HG11	1.75	0.52
1:B:505:HIS:O	1:B:508:ARG:NH1	2.38	0.52
1:D:271:GLU:O	1:D:271:GLU:HG3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:513:LEU:HD22	1:D:513:LEU:H	1.74	0.52
1:F:46:LEU:HB3	1:F:50:GLU:OE1	2.09	0.52
1:A:328:ARG:HD3	1:A:331:GLY:O	2.10	0.52
1:A:504:ARG:HG3	2:A:531:HOH:O	2.09	0.52
1:D:295:PRO:HB2	1:D:342:MET:CE	2.40	0.52
1:F:321:ASN:OD1	1:F:321:ASN:N	2.38	0.52
1:F:323:LEU:HA	2:F:537:HOH:O	2.10	0.52
1:F:335:GLY:O	1:F:371:LEU:N	2.41	0.52
1:F:397:LEU:HD22	2:F:592:HOH:O	2.10	0.52
1:E:45:LYS:HG2	1:E:200:THR:HG23	1.92	0.52
1:F:483:ASN:HD21	1:F:485:TYR:HB2	1.74	0.52
1:A:495:ALA:HB1	2:A:541:HOH:O	2.10	0.52
1:B:496:VAL:HB	1:C:67:PHE:HE2	1.74	0.52
1:F:483:ASN:HB2	1:F:484:PRO:HD2	1.91	0.52
1:A:432:ASP:O	1:A:433:LEU:HD23	2.09	0.52
1:B:21:LEU:O	1:B:25:ILE:HG23	2.09	0.52
1:B:405:THR:O	1:B:516:LYS:HE2	2.10	0.52
1:C:29:THR:HA	1:C:49:ARG:NE	2.25	0.52
1:F:45:LYS:HE3	1:F:200:THR:HG22	1.92	0.52
1:F:90:GLY:HA2	2:F:551:HOH:O	2.10	0.52
1:F:427:LYS:NZ	1:F:434:ASN:OD1	2.42	0.52
1:A:156:TYR:CE1	1:A:184:ALA:HB2	2.45	0.51
2:A:622:HOH:O	1:B:65:ASP:HA	2.10	0.51
1:C:116:VAL:HG23	2:C:656:HOH:O	2.10	0.51
1:C:340:GLN:HG2	2:C:599:HOH:O	2.11	0.51
1:D:187:SER:CB	1:D:188:PRO:HD3	2.40	0.51
1:F:447:ALA:O	1:F:451:VAL:HG13	2.09	0.51
1:A:507:VAL:HG12	1:A:508:ARG:N	2.24	0.51
1:B:17:LYS:HB2	2:B:593:HOH:O	2.11	0.51
1:B:356:ALA:O	1:B:360:VAL:HG23	2.09	0.51
1:B:442:ILE:HG13	2:B:665:HOH:O	2.09	0.51
1:E:298:MET:HA	1:E:301:VAL:HG23	1.93	0.51
1:E:403:GLU:HG2	2:E:540:HOH:O	2.08	0.51
1:F:238:HIS:HD2	1:F:315:GLN:NE2	2.08	0.51
1:D:121:ILE:O	1:D:125:MET:HG3	2.10	0.51
1:D:395:ALA:O	1:D:398:ILE:HG12	2.10	0.51
1:A:188:PRO:O	1:A:191:THR:OG1	2.28	0.51
1:A:398:ILE:CG2	1:A:423:VAL:HG22	2.40	0.51
1:A:509:GLY:O	1:A:513:LEU:CD2	2.56	0.51
1:B:65:ASP:CB	1:B:120:LYS:HE3	2.40	0.51
1:B:427:LYS:NZ	1:B:427:LYS:HB2	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:284:LEU:HD23	1:D:499:PRO:O	2.10	0.51
1:D:334:VAL:HG13	2:D:602:HOH:O	2.10	0.51
1:E:122:VAL:HG22	2:E:688:HOH:O	2.10	0.51
1:F:523:LYS:CE	2:F:688:HOH:O	2.58	0.51
1:A:483:ASN:ND2	1:A:485:TYR:HD2	2.05	0.51
1:C:71:ARG:HH22	1:C:119:GLN:HE22	1.57	0.51
1:C:470:ARG:HG3	1:C:470:ARG:NH1	2.26	0.51
1:C:497:ILE:HG23	2:C:683:HOH:O	2.10	0.51
1:E:302:ILE:CG2	1:E:336:ILE:HD13	2.41	0.51
1:E:459:ILE:HG12	1:E:470:ARG:HH21	1.76	0.51
1:F:297:ASP:HA	1:F:342:MET:HG3	1.92	0.51
1:F:427:LYS:NZ	2:F:622:HOH:O	2.43	0.51
1:A:69:ARG:CD	1:A:81:ARG:O	2.58	0.51
1:A:391:ILE:HD12	1:A:391:ILE:N	2.23	0.51
2:A:694:HOH:O	1:D:358:ARG:HD3	2.09	0.51
1:D:444:VAL:HG23	2:D:540:HOH:O	2.10	0.51
1:A:483:ASN:HD21	1:A:485:TYR:HB2	1.74	0.51
1:B:322:ILE:CG2	1:B:355:LYS:HD3	2.41	0.51
1:C:208:PRO:C	1:C:210:VAL:H	2.13	0.51
1:D:102:PHE:CD1	1:D:121:ILE:HG23	2.46	0.51
1:D:275:LEU:HD11	1:D:511:ARG:HH12	1.75	0.51
1:F:324:THR:HA	1:F:336:ILE:O	2.10	0.51
1:F:427:LYS:HB2	1:F:427:LYS:HZ3	1.74	0.51
1:A:295:PRO:HB2	1:A:342:MET:HE1	1.91	0.51
1:D:65:ASP:CB	1:D:120:LYS:HE3	2.41	0.51
1:B:396:LYS:HE2	1:B:529:PRO:O	2.10	0.51
1:C:170:ILE:HD13	2:C:641:HOH:O	2.11	0.51
1:C:392:ARG:HG3	1:C:392:ARG:NH1	2.23	0.51
1:C:530:LEU:HD21	1:F:528:ILE:CD1	2.40	0.51
1:F:113:LEU:HD22	1:F:117:TYR:CD1	2.45	0.51
1:A:427:LYS:NZ	1:A:434:ASN:OD1	2.42	0.51
1:C:364:ASP:OD2	1:C:404:ALA:HA	2.11	0.51
1:E:101:VAL:HG22	1:E:102:PHE:N	2.25	0.51
1:A:469:THR:O	1:A:473:LEU:HD13	2.10	0.50
1:C:103:SER:HB2	1:C:138:ILE:HD12	1.92	0.50
1:C:285:ASP:N	2:C:670:HOH:O	2.41	0.50
1:E:156:TYR:CZ	1:E:184:ALA:HB2	2.47	0.50
1:E:264:SER:HB3	2:E:600:HOH:O	2.12	0.50
1:F:55:LEU:HD12	1:F:252:LYS:HG3	1.91	0.50
1:F:56:LEU:HD12	1:F:61:PHE:HB2	1.93	0.50
1:F:224:LEU:O	1:F:229:THR:HG21	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:LEU:HD22	1:C:494:ASP:HB3	1.93	0.50
1:A:375:ASP:CG	1:A:414:ARG:HB3	2.32	0.50
1:B:147:GLN:NE2	1:B:147:GLN:N	2.42	0.50
1:B:399:PHE:CE2	1:B:528:ILE:HB	2.46	0.50
1:C:407:PRO:HB3	1:C:513:LEU:HB3	1.92	0.50
1:D:319:ALA:N	1:D:320:PRO:HD3	2.27	0.50
1:E:324:THR:HA	1:E:336:ILE:O	2.10	0.50
1:E:404:ALA:HB1	2:E:677:HOH:O	2.10	0.50
1:E:440:ALA:O	1:E:484:PRO:HD3	2.11	0.50
1:F:305:VAL:CG2	1:F:506:ILE:HD12	2.37	0.50
1:A:102:PHE:HB3	2:A:546:HOH:O	2.11	0.50
1:C:162:ARG:HG2	1:C:162:ARG:NH1	2.24	0.50
1:E:230:HIS:HA	1:E:234:SER:OG	2.11	0.50
1:F:75:PHE:N	1:F:75:PHE:CD2	2.80	0.50
1:F:301:VAL:HG21	2:F:663:HOH:O	2.12	0.50
1:F:509:GLY:O	1:F:513:LEU:HD23	2.11	0.50
1:A:392:ARG:HG3	1:A:392:ARG:NH1	2.26	0.50
1:B:435:LEU:CD2	2:B:596:HOH:O	2.58	0.50
1:C:175:LEU:HD22	1:C:177:VAL:HG13	1.93	0.50
1:F:238:HIS:HA	1:F:315:GLN:CG	2.41	0.50
1:A:68:ALA:HA	1:C:489:GLU:HA	1.93	0.50
1:A:258:LEU:HD12	2:A:612:HOH:O	2.12	0.50
1:A:298:MET:O	1:A:301:VAL:N	2.44	0.50
1:B:102:PHE:CD2	1:B:102:PHE:O	2.64	0.50
1:B:179:PRO:HD2	2:B:679:HOH:O	2.11	0.50
1:C:91:TYR:CD1	1:C:91:TYR:C	2.84	0.50
1:C:161:ARG:HD3	2:F:578:HOH:O	2.12	0.50
1:C:229:THR:HG23	2:C:595:HOH:O	2.11	0.50
2:C:658:HOH:O	1:F:527:ASN:HB3	2.12	0.50
1:D:392:ARG:HG3	1:D:392:ARG:HH11	1.76	0.50
1:D:390:ILE:HG13	2:D:640:HOH:O	2.11	0.50
1:E:490:ARG:HG2	1:E:490:ARG:HH11	1.76	0.50
1:A:374:VAL:HG12	1:A:375:ASP:N	2.26	0.50
1:C:63:GLU:HG3	1:C:64:LEU:N	2.26	0.50
1:E:152:SER:HA	2:E:665:HOH:O	2.10	0.50
1:E:250:TYR:O	1:E:253:GLN:N	2.44	0.50
1:B:52:ILE:N	2:B:590:HOH:O	2.43	0.50
1:C:475:GLN:NE2	1:C:476:GLU:HG3	2.27	0.50
1:D:438:PRO:HG3	1:F:21:LEU:HD22	1.94	0.50
1:A:121:ILE:O	1:A:124:VAL:HG22	2.12	0.50
1:A:202:HIS:HD2	1:A:222:GLU:HA	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:111:GLY:HA3	2:B:675:HOH:O	2.10	0.50
1:B:247:ALA:O	1:B:250:TYR:N	2.45	0.50
1:C:211:ILE:CG2	1:C:217:GLU:HB2	2.41	0.50
1:C:454:LEU:HD13	1:F:75:PHE:CE1	2.47	0.50
1:D:197:VAL:HB	1:D:200:THR:OG1	2.12	0.50
1:D:357:ALA:HB3	2:D:672:HOH:O	2.10	0.50
1:E:364:ASP:CG	2:E:677:HOH:O	2.50	0.50
1:F:408:LEU:HB2	1:F:431:ALA:HA	1.94	0.50
1:A:29:THR:HG23	2:A:641:HOH:O	2.12	0.49
1:A:122:VAL:HG22	2:A:583:HOH:O	2.11	0.49
1:A:391:ILE:H	1:A:391:ILE:CD1	2.24	0.49
1:A:453:ILE:N	1:A:453:ILE:HD12	2.26	0.49
1:C:89:THR:HA	2:C:707:HOH:O	2.12	0.49
1:D:231:ASN:HD21	1:D:239:HIS:CA	2.24	0.49
1:E:173:ILE:HD11	2:E:632:HOH:O	2.12	0.49
1:E:520:LEU:N	1:E:520:LEU:HD12	2.27	0.49
1:B:150:VAL:HG23	2:B:624:HOH:O	2.12	0.49
1:B:173:ILE:HD13	1:B:251:VAL:HG23	1.94	0.49
1:B:350:ILE:HG21	1:B:393:ARG:NH2	2.27	0.49
1:B:355:LYS:HD2	2:B:625:HOH:O	2.12	0.49
1:B:494:ASP:HA	2:C:696:HOH:O	2.11	0.49
2:B:611:HOH:O	1:E:530:LEU:HG	2.10	0.49
1:C:493:VAL:HA	2:C:690:HOH:O	2.13	0.49
1:E:61:PHE:CE2	1:E:63:GLU:HB2	2.47	0.49
1:F:35:ARG:HH21	1:F:39:LYS:NZ	2.10	0.49
1:A:14:THR:HG23	1:C:439:THR:HG21	1.93	0.49
1:B:483:ASN:HD22	1:B:485:TYR:N	2.09	0.49
1:C:374:VAL:HG22	1:C:424:MET:HB3	1.94	0.49
1:D:508:ARG:NE	1:F:91:TYR:OH	2.45	0.49
1:E:175:LEU:HD21	1:E:247:ALA:HB1	1.94	0.49
1:E:337:VAL:O	1:E:372:THR:HA	2.12	0.49
1:E:376:VAL:HG13	1:E:376:VAL:O	2.12	0.49
1:A:91:TYR:HD1	1:A:92:GLY:N	2.10	0.49
1:A:513:LEU:N	1:A:513:LEU:CD2	2.74	0.49
1:B:89:THR:HB	1:B:124:VAL:CG2	2.38	0.49
1:B:360:VAL:HB	1:B:400:ALA:HB1	1.94	0.49
1:C:373:PHE:HD2	1:C:411:VAL:HB	1.77	0.49
1:D:55:LEU:HD21	1:D:136:VAL:HG11	1.93	0.49
1:D:262:ASN:ND2	2:D:570:HOH:O	2.45	0.49
1:D:302:ILE:HA	2:D:639:HOH:O	2.11	0.49
1:D:503:ARG:HH11	1:D:503:ARG:HG2	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:161:ARG:HD2	2:B:598:HOH:O	2.11	0.49
1:B:246:ASP:HB3	2:B:587:HOH:O	2.13	0.49
1:B:268:ALA:CB	1:B:332:ARG:HG2	2.42	0.49
1:B:336:ILE:HD12	1:B:336:ILE:N	2.28	0.49
1:C:113:LEU:HD22	1:C:117:TYR:CD1	2.47	0.49
1:C:495:ALA:HB3	2:C:683:HOH:O	2.12	0.49
1:D:221:PHE:O	1:D:224:LEU:HB3	2.12	0.49
1:D:335:GLY:O	1:D:371:LEU:N	2.45	0.49
1:E:62:VAL:HG11	1:F:508:ARG:NH2	2.18	0.49
1:E:65:ASP:HB2	1:E:120:LYS:HE3	1.94	0.49
1:E:177:VAL:CA	1:E:201:SER:HB3	2.42	0.49
1:F:497:ILE:HG21	1:F:505:HIS:CE1	2.48	0.49
1:A:48:ALA:O	1:A:51:ARG:HB2	2.12	0.49
1:A:438:PRO:HG3	1:B:21:LEU:HD22	1.93	0.49
1:A:280:GLU:OE2	1:A:280:GLU:N	2.43	0.49
1:A:377:PRO:HG2	1:A:378:GLY:H	1.78	0.49
1:B:47:THR:OG1	1:B:50:GLU:HG3	2.13	0.49
1:B:90:GLY:N	2:B:606:HOH:O	2.46	0.49
1:B:300:SER:O	1:B:304:HIS:ND1	2.46	0.49
1:B:339:ASN:HB2	2:B:696:HOH:O	2.12	0.49
1:C:73:THR:HG22	1:C:78:ASP:HB3	1.95	0.49
1:C:399:PHE:CZ	1:F:164:THR:HG23	2.47	0.49
1:C:418:GLY:HA2	1:F:153:LEU:HD11	1.94	0.49
1:D:185:VAL:HG21	1:D:205:ILE:HG12	1.95	0.49
1:E:273:ALA:O	1:E:275:LEU:HD22	2.13	0.49
1:E:460:ALA:HA	2:E:680:HOH:O	2.11	0.49
1:F:11:ILE:HG13	1:F:11:ILE:O	2.13	0.49
1:A:347:CYS:SG	1:A:377:PRO:HG2	2.53	0.49
1:C:70:HIS:HB3	1:C:85:ASP:OD1	2.13	0.49
1:C:505:HIS:ND1	1:C:508:ARG:NH1	2.60	0.49
1:D:13:THR:HB	1:E:290:ASP:OD1	2.13	0.49
1:D:407:PRO:HB3	1:D:513:LEU:HB3	1.95	0.49
1:D:489:GLU:HA	1:F:68:ALA:HA	1.93	0.49
1:E:121:ILE:O	1:E:124:VAL:HG22	2.12	0.49
1:E:376:VAL:N	1:E:415:LYS:HB2	2.28	0.49
1:E:407:PRO:HB3	1:E:513:LEU:HB3	1.94	0.49
1:F:124:VAL:HB	2:F:565:HOH:O	2.12	0.49
1:F:287:ILE:HG23	1:F:288:VAL:N	2.27	0.49
1:A:10:ASP:CG	1:A:11:ILE:H	2.16	0.49
1:B:399:PHE:CE1	1:E:164:THR:HG23	2.48	0.49
1:C:525:HIS:ND1	1:F:361:ARG:NH2	2.61	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:56:LEU:HD12	1:D:61:PHE:HB2	1.94	0.49
1:E:55:LEU:HD21	1:E:136:VAL:HG21	1.94	0.49
1:E:145:ARG:HD2	1:E:148:GLU:OE2	2.13	0.49
1:E:181:ALA:HA	1:E:204:PHE:O	2.13	0.49
1:E:485:TYR:HA	1:E:488:ALA:HB3	1.93	0.49
1:A:124:VAL:HG21	2:A:546:HOH:O	2.11	0.49
1:A:389:GLY:HA2	2:A:650:HOH:O	2.13	0.49
1:B:484:PRO:HB2	2:B:662:HOH:O	2.12	0.49
1:C:524:LYS:HD3	1:F:405:THR:OG1	2.13	0.49
1:D:475:GLN:HA	1:D:478:GLU:OE1	2.12	0.49
1:E:150:VAL:HG23	2:E:596:HOH:O	2.13	0.49
1:F:208:PRO:HG2	1:F:221:PHE:CE1	2.47	0.49
2:A:589:HOH:O	1:C:495:ALA:HA	2.13	0.48
1:B:403:GLU:HG2	2:B:537:HOH:O	2.12	0.48
1:C:415:LYS:HD3	1:C:417:PHE:HE2	1.77	0.48
1:C:480:ALA:C	1:C:481:LEU:HD22	2.34	0.48
1:D:397:LEU:HD23	1:D:401:TYR:HD2	1.78	0.48
1:D:449:GLY:O	1:D:453:ILE:HD13	2.12	0.48
1:E:302:ILE:HG23	1:E:336:ILE:HD13	1.95	0.48
1:E:312:PHE:HZ	2:E:700:HOH:O	1.95	0.48
1:E:372:THR:CG2	2:E:544:HOH:O	2.60	0.48
1:E:411:VAL:HG22	1:E:435:LEU:HD23	1.94	0.48
1:A:129:LEU:HD13	1:A:166:ALA:HB2	1.95	0.48
1:B:383:VAL:HG21	1:E:219:VAL:HG11	1.95	0.48
1:C:339:ASN:HB3	2:C:543:HOH:O	2.13	0.48
1:D:46:LEU:HB2	1:D:51:ARG:HD2	1.95	0.48
1:D:115:GLU:HB2	1:D:148:GLU:OE1	2.12	0.48
1:D:299:HIS:O	1:D:303:GLU:HG3	2.13	0.48
1:E:63:GLU:HG2	1:E:66:GLU:HB2	1.94	0.48
1:E:507:VAL:HG12	1:E:508:ARG:N	2.26	0.48
1:F:187:SER:HB3	1:F:188:PRO:CD	2.31	0.48
1:F:391:ILE:HA	2:F:709:HOH:O	2.12	0.48
1:A:398:ILE:HD12	1:D:160:PHE:CB	2.42	0.48
1:B:375:ASP:CG	1:B:414:ARG:HB3	2.33	0.48
1:B:473:LEU:HA	1:B:476:GLU:OE1	2.13	0.48
1:B:505:HIS:HA	1:B:508:ARG:HD2	1.95	0.48
1:C:101:VAL:HG22	1:C:102:PHE:N	2.28	0.48
1:C:349:ASP:OD2	1:C:351:THR:OG1	2.30	0.48
1:D:254:LEU:HD13	1:D:312:PHE:HE2	1.78	0.48
1:E:51:ARG:NH2	1:E:244:GLU:OE1	2.41	0.48
1:E:326:PHE:HA	2:E:612:HOH:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:451:VAL:C	1:E:453:ILE:H	2.15	0.48
1:A:35:ARG:HB3	1:A:35:ARG:HH11	1.77	0.48
1:B:56:LEU:HD12	1:B:61:PHE:HB2	1.96	0.48
1:C:174:SER:OG	1:C:191:THR:HG21	2.13	0.48
1:A:195:VAL:HG23	2:A:683:HOH:O	2.14	0.48
1:B:10:ASP:CG	1:B:11:ILE:H	2.17	0.48
1:B:208:PRO:HG3	1:B:224:LEU:HD22	1.95	0.48
1:E:146:ILE:H	1:E:146:ILE:CD1	2.16	0.48
1:B:374:VAL:HG11	2:B:629:HOH:O	2.13	0.48
1:D:224:LEU:O	1:D:229:THR:HG21	2.13	0.48
1:E:24:ARG:HD3	1:F:485:TYR:CE1	2.49	0.48
1:F:212:LYS:C	1:F:214:VAL:H	2.17	0.48
1:F:392:ARG:HG3	1:F:392:ARG:NH1	2.26	0.48
1:B:308:ASP:O	1:B:309:ALA:HB3	2.14	0.48
1:B:509:GLY:O	1:B:513:LEU:CD2	2.61	0.48
1:B:509:GLY:O	1:B:513:LEU:HD22	2.13	0.48
1:C:489:GLU:HB3	2:C:532:HOH:O	2.12	0.48
1:D:509:GLY:O	1:D:513:LEU:CD2	2.60	0.48
1:E:64:LEU:HD22	1:F:494:ASP:HB3	1.95	0.48
1:E:69:ARG:HB2	1:F:489:GLU:HG2	1.95	0.48
1:E:324:THR:HB	1:E:359:PHE:CD2	2.49	0.48
1:E:367:ASN:N	1:E:367:ASN:ND2	2.61	0.48
1:E:427:LYS:HB2	1:E:434:ASN:OD1	2.14	0.48
1:F:173:ILE:HG21	1:F:251:VAL:CG2	2.37	0.48
1:B:234:SER:HB2	1:B:236:VAL:HG13	1.95	0.48
1:B:346:GLY:HA3	2:B:628:HOH:O	2.12	0.48
1:D:73:THR:HA	1:D:78:ASP:OD1	2.12	0.48
1:E:62:VAL:HG12	1:E:62:VAL:O	2.12	0.48
1:F:33:SER:HB2	1:F:36:ALA:HB2	1.96	0.48
1:F:414:ARG:NH1	1:F:414:ARG:HG2	2.29	0.48
1:F:460:ALA:HA	2:F:697:HOH:O	2.12	0.48
1:F:468:ALA:O	1:F:472:ARG:HB2	2.14	0.48
1:F:528:ILE:O	1:F:530:LEU:HD13	2.14	0.48
1:C:320:PRO:O	1:C:343:GLN:HG3	2.14	0.48
1:D:425:GLY:O	1:D:431:ALA:HB2	2.13	0.48
1:F:198:ASP:HB2	1:F:240:MET:CE	2.44	0.48
1:A:160:PHE:HA	2:A:562:HOH:O	2.13	0.48
1:B:299:HIS:HD2	2:B:677:HOH:O	1.96	0.48
1:E:155:ALA:HB3	2:E:665:HOH:O	2.14	0.48
1:A:70:HIS:ND1	1:A:70:HIS:C	2.67	0.47
1:A:406:VAL:HG12	2:A:643:HOH:O	2.12	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:387:HIS:O	1:E:233:THR:HG22	2.14	0.47
2:B:561:HOH:O	1:C:65:ASP:HA	2.14	0.47
1:C:132:GLY:C	1:C:261:ASN:HD22	2.17	0.47
1:C:318:PHE:CE1	1:C:351:THR:HG22	2.49	0.47
1:D:158:GLU:OE2	1:D:161:ARG:NH2	2.47	0.47
1:F:75:PHE:N	1:F:75:PHE:HD2	2.12	0.47
1:F:182:GLY:O	1:F:185:VAL:HG22	2.14	0.47
1:A:135:VAL:HG13	2:A:701:HOH:O	2.14	0.47
1:D:145:ARG:HG2	2:D:655:HOH:O	2.13	0.47
1:E:21:LEU:HD22	1:F:438:PRO:HG3	1.96	0.47
1:E:35:ARG:O	1:E:39:LYS:HG3	2.14	0.47
1:E:118:GLY:O	1:E:121:ILE:N	2.47	0.47
1:F:23:ARG:O	1:F:27:GLU:HG3	2.14	0.47
1:A:131:THR:O	1:C:515:THR:OG1	2.26	0.47
1:A:160:PHE:CE2	1:D:422:ILE:HG21	2.50	0.47
1:B:77:LEU:C	1:B:79:ALA:H	2.17	0.47
1:B:118:GLY:HA3	1:B:155:ALA:HB1	1.96	0.47
1:C:259:PRO:HD3	2:C:550:HOH:O	2.13	0.47
1:C:374:VAL:HB	1:C:412:ILE:HG12	1.96	0.47
1:D:71:ARG:HD3	2:E:668:HOH:O	2.14	0.47
1:D:302:ILE:O	1:D:305:VAL:HG22	2.14	0.47
1:E:322:ILE:HD12	2:E:658:HOH:O	2.13	0.47
1:E:436:ALA:O	1:E:496:VAL:HA	2.14	0.47
1:A:75:PHE:CE2	1:D:454:LEU:HD13	2.49	0.47
1:A:512:GLN:NE2	2:A:698:HOH:O	2.46	0.47
1:A:527:ASN:ND2	1:A:527:ASN:O	2.47	0.47
1:D:334:VAL:HG22	2:D:602:HOH:O	2.14	0.47
1:E:364:ASP:OD2	1:E:404:ALA:HA	2.14	0.47
1:E:528:ILE:HG21	2:E:579:HOH:O	2.13	0.47
1:F:451:VAL:HG21	1:F:474:ILE:CG1	2.42	0.47
1:A:377:PRO:HD3	2:A:534:HOH:O	2.15	0.47
1:A:508:ARG:CZ	1:B:91:TYR:OH	2.63	0.47
1:B:427:LYS:HB2	1:B:434:ASN:OD1	2.13	0.47
1:E:299:HIS:O	1:E:303:GLU:HG3	2.14	0.47
1:E:505:HIS:HA	1:E:508:ARG:CD	2.43	0.47
1:A:89:THR:HB	1:A:124:VAL:HG11	1.97	0.47
1:A:176:VAL:HB	1:A:196:MET:HB3	1.97	0.47
1:A:527:ASN:HD21	1:D:358:ARG:HD3	1.78	0.47
1:B:70:HIS:HE1	1:B:81:ARG:HG2	1.80	0.47
1:B:444:VAL:HA	1:E:153:LEU:HD11	1.95	0.47
1:C:55:LEU:HA	2:C:666:HOH:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:427:LYS:HB2	1:D:427:LYS:HZ2	1.78	0.47
1:E:24:ARG:NH1	1:E:24:ARG:HG2	2.30	0.47
1:F:91:TYR:CD1	1:F:91:TYR:C	2.86	0.47
1:F:345:ALA:HB1	2:F:626:HOH:O	2.15	0.47
1:F:508:ARG:HD3	1:F:508:ARG:C	2.34	0.47
1:A:170:ILE:HG13	1:A:170:ILE:O	2.15	0.47
1:A:380:LEU:HD23	1:A:385:GLN:CD	2.35	0.47
1:A:397:LEU:HD22	1:A:401:TYR:CE2	2.50	0.47
1:C:51:ARG:HH12	1:C:140:ASP:CB	2.27	0.47
1:C:111:GLY:O	1:C:141:SER:HB2	2.15	0.47
1:C:175:LEU:CD2	1:C:177:VAL:HG13	2.45	0.47
1:C:203:MET:CE	1:F:391:ILE:HG21	2.44	0.47
1:C:239:HIS:HA	2:C:601:HOH:O	2.15	0.47
1:C:284:LEU:CD1	1:C:304:HIS:CD2	2.97	0.47
1:D:45:LYS:HD2	2:D:567:HOH:O	2.13	0.47
1:D:115:GLU:O	1:D:119:GLN:HG3	2.15	0.47
1:D:272:GLU:HG2	2:D:600:HOH:O	2.14	0.47
1:D:291:SER:C	1:D:293:ASN:H	2.18	0.47
1:D:291:SER:O	1:D:293:ASN:N	2.47	0.47
1:E:162:ARG:HG2	1:E:162:ARG:HH11	1.79	0.47
1:F:177:VAL:HG12	1:F:197:VAL:HG21	1.95	0.47
1:A:185:VAL:O	1:A:188:PRO:HD2	2.15	0.47
1:A:231:ASN:HD21	1:A:239:HIS:C	2.18	0.47
1:B:322:ILE:HG23	1:B:355:LYS:HD3	1.97	0.47
1:C:47:THR:O	1:C:51:ARG:HG3	2.15	0.47
1:C:173:ILE:HG21	1:C:251:VAL:CG2	2.34	0.47
1:C:302:ILE:O	1:C:305:VAL:HG22	2.15	0.47
1:C:490:ARG:HH12	1:F:151:ALA:HB2	1.80	0.47
1:D:91:TYR:OH	1:E:508:ARG:CZ	2.63	0.47
1:D:399:PHE:HB2	2:D:607:HOH:O	2.15	0.47
1:E:68:ALA:HA	1:F:489:GLU:HA	1.97	0.47
1:F:274:ASP:C	1:F:274:ASP:OD1	2.53	0.47
1:B:231:ASN:ND2	1:B:239:HIS:C	2.68	0.47
1:B:448:GLN:HA	1:B:474:ILE:HD13	1.95	0.47
1:C:422:ILE:HD11	1:F:153:LEU:O	2.15	0.47
1:C:452:ASN:N	1:C:452:ASN:HD22	2.12	0.47
1:E:432:ASP:HB2	1:E:513:LEU:HD21	1.97	0.47
1:F:163:ASN:N	2:F:630:HOH:O	2.47	0.47
1:F:521:PRO:HD2	2:F:688:HOH:O	2.15	0.47
1:B:45:LYS:CE	1:B:200:THR:HG22	2.45	0.47
1:B:350:ILE:HG21	1:B:393:ARG:CZ	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:483:ASN:HB2	1:B:484:PRO:HD2	1.96	0.47
1:C:195:VAL:HG23	1:C:239:HIS:HB3	1.96	0.47
1:C:230:HIS:HA	1:C:234:SER:OG	2.14	0.47
1:D:89:THR:HB	1:D:124:VAL:CG2	2.40	0.47
1:E:284:LEU:O	1:E:287:ILE:HG22	2.15	0.47
1:E:322:ILE:HG23	1:E:355:LYS:HD3	1.96	0.47
1:E:473:LEU:O	1:E:474:ILE:C	2.54	0.47
1:F:396:LYS:HD3	2:F:594:HOH:O	2.14	0.47
1:F:459:ILE:HD11	1:F:470:ARG:HB2	1.96	0.47
1:A:10:ASP:HB3	1:A:13:THR:OG1	2.15	0.46
1:C:36:ALA:O	1:C:39:LYS:HB2	2.15	0.46
1:C:65:ASP:HB3	1:C:68:ALA:HB2	1.97	0.46
1:C:392:ARG:HD3	1:F:236:VAL:HG12	1.96	0.46
1:E:339:ASN:O	1:E:341:PRO:HD3	2.15	0.46
1:A:499:PRO:N	2:A:690:HOH:O	2.47	0.46
1:A:502:THR:O	1:A:506:ILE:HG13	2.15	0.46
1:A:508:ARG:CZ	1:B:62:VAL:HG11	2.44	0.46
1:B:46:LEU:HB3	1:B:50:GLU:HB2	1.97	0.46
1:C:77:LEU:HD11	1:C:147:GLN:HB2	1.96	0.46
1:C:150:VAL:O	1:C:151:ALA:C	2.53	0.46
1:C:187:SER:CB	1:C:188:PRO:HD3	2.41	0.46
1:C:529:PRO:CG	1:F:190:ILE:HA	2.44	0.46
1:E:135:VAL:HG13	2:E:557:HOH:O	2.13	0.46
1:E:160:PHE:O	1:E:163:ASN:HB2	2.15	0.46
1:F:398:ILE:HG13	1:F:429:LEU:CD2	2.36	0.46
1:A:498:MET:O	1:A:500:SER:N	2.49	0.46
1:B:497:ILE:HD12	2:B:600:HOH:O	2.15	0.46
1:C:373:PHE:CD2	1:C:411:VAL:HB	2.50	0.46
1:C:381:PRO:HA	1:F:206:THR:HG21	1.97	0.46
1:D:122:VAL:O	1:D:124:VAL:N	2.49	0.46
1:D:176:VAL:HG12	1:D:201:SER:HB2	1.97	0.46
1:D:180:CYS:O	1:D:203:MET:HA	2.15	0.46
1:D:342:MET:HE1	2:D:648:HOH:O	2.15	0.46
1:E:231:ASN:HD21	1:E:239:HIS:C	2.18	0.46
1:E:415:LYS:HD3	1:E:417:PHE:HE2	1.80	0.46
1:F:35:ARG:HH21	1:F:39:LYS:HZ1	1.63	0.46
1:A:62:VAL:HG11	1:C:508:ARG:CZ	2.46	0.46
1:A:162:ARG:HH11	1:A:162:ARG:CG	2.24	0.46
1:A:374:VAL:HG23	2:A:636:HOH:O	2.16	0.46
1:E:277:VAL:HG23	1:E:277:VAL:O	2.15	0.46
1:F:325:GLY:O	1:F:359:PHE:HZ	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:SER:HB2	1:A:236:VAL:HG13	1.98	0.46
1:A:494:ASP:HB3	1:B:64:LEU:CD2	2.43	0.46
1:A:504:ARG:NH2	2:A:556:HOH:O	2.48	0.46
1:B:236:VAL:HG23	1:B:237:ALA:N	2.30	0.46
1:C:55:LEU:HD13	1:C:248:VAL:HG13	1.97	0.46
1:D:398:ILE:HG22	1:D:423:VAL:HG22	1.97	0.46
1:E:291:SER:C	1:E:293:ASN:H	2.19	0.46
1:F:205:ILE:O	1:F:205:ILE:HD13	2.14	0.46
1:F:397:LEU:HB3	2:F:592:HOH:O	2.15	0.46
1:A:13:THR:HG22	1:C:290:ASP:CG	2.36	0.46
1:B:273:ALA:N	1:B:330:GLU:OE1	2.48	0.46
1:B:350:ILE:HG13	1:B:390:ILE:HD13	1.97	0.46
1:C:89:THR:HB	1:C:124:VAL:CG2	2.42	0.46
1:D:334:VAL:N	2:D:602:HOH:O	2.48	0.46
1:D:336:ILE:HA	1:D:371:LEU:O	2.15	0.46
1:D:508:ARG:NE	1:F:62:VAL:HG21	2.31	0.46
1:F:339:ASN:OD1	1:F:376:VAL:HB	2.16	0.46
1:F:472:ARG:HH12	1:F:476:GLU:CD	2.17	0.46
1:A:164:THR:O	1:A:165:HIS:C	2.54	0.46
1:A:167:SER:HA	2:A:532:HOH:O	2.16	0.46
1:A:376:VAL:HA	2:A:534:HOH:O	2.15	0.46
1:B:121:ILE:O	1:B:125:MET:HG3	2.16	0.46
1:B:361:ARG:HB2	2:E:584:HOH:O	2.16	0.46
1:C:457:ARG:HG3	1:C:457:ARG:HH11	1.81	0.46
1:D:46:LEU:N	1:D:244:GLU:OE1	2.49	0.46
1:E:55:LEU:CD2	1:E:136:VAL:HG11	2.46	0.46
1:E:180:CYS:HB3	1:E:203:MET:HG2	1.98	0.46
1:F:132:GLY:O	1:F:261:ASN:ND2	2.47	0.46
1:F:202:HIS:HA	1:F:225:GLY:O	2.15	0.46
1:F:302:ILE:HD11	2:F:613:HOH:O	2.15	0.46
1:A:70:HIS:NE2	1:A:77:LEU:HD23	2.31	0.46
1:A:462:ALA:O	1:A:466:ALA:HB2	2.16	0.46
1:A:508:ARG:HG3	1:B:62:VAL:HG21	1.98	0.46
1:B:490:ARG:NH2	1:C:71:ARG:HD3	2.30	0.46
1:E:395:ALA:O	1:E:396:LYS:C	2.54	0.46
1:F:111:GLY:O	1:F:141:SER:CB	2.63	0.46
1:F:483:ASN:ND2	1:F:485:TYR:H	2.14	0.46
1:A:114:GLY:H	1:A:117:TYR:HB3	1.81	0.46
1:B:102:PHE:CD2	1:B:102:PHE:C	2.89	0.46
1:B:322:ILE:HG23	1:B:322:ILE:O	2.15	0.46
1:B:490:ARG:HH21	1:C:71:ARG:HD3	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:298:MET:O	1:C:301:VAL:N	2.49	0.46
1:C:445:MET:HA	2:C:561:HOH:O	2.16	0.46
1:C:483:ASN:HB2	1:C:484:PRO:HD2	1.98	0.46
1:D:440:ALA:O	1:D:484:PRO:HD3	2.15	0.46
1:D:530:LEU:HD22	1:D:530:LEU:N	2.31	0.46
1:E:10:ASP:CG	1:E:11:ILE:H	2.19	0.46
1:F:257:TYR:CE1	1:F:328:ARG:NH1	2.84	0.46
1:F:291:SER:O	1:F:293:ASN:N	2.49	0.46
1:F:419:GLY:O	1:F:423:VAL:HG23	2.16	0.46
1:F:437:TRP:HD1	2:F:687:HOH:O	1.99	0.46
1:F:512:GLN:HE21	1:F:512:GLN:HB3	1.56	0.46
1:B:397:LEU:HB3	1:B:423:VAL:HG13	1.98	0.46
1:C:186:TYR:CD1	1:F:395:ALA:HB2	2.50	0.46
1:C:379:PHE:HZ	1:C:423:VAL:HG21	1.81	0.46
1:E:47:THR:HG23	1:E:50:GLU:OE1	2.16	0.46
1:E:257:TYR:CE1	1:E:328:ARG:NH1	2.84	0.46
1:F:122:VAL:HG11	1:F:162:ARG:HH21	1.80	0.46
1:F:505:HIS:O	1:F:508:ARG:HD3	2.16	0.46
1:F:511:ARG:HG2	2:F:596:HOH:O	2.16	0.46
1:A:55:LEU:HD21	1:A:136:VAL:HG11	1.98	0.45
1:A:161:ARG:HH11	1:A:161:ARG:HG3	1.81	0.45
1:A:349:ASP:O	1:A:350:ILE:C	2.55	0.45
1:A:513:LEU:HB2	2:A:537:HOH:O	2.16	0.45
1:B:448:GLN:HA	1:B:474:ILE:CD1	2.46	0.45
1:B:474:ILE:O	1:B:478:GLU:HG2	2.16	0.45
1:C:456:ARG:HB3	1:C:456:ARG:CZ	2.46	0.45
1:C:505:HIS:C	1:C:508:ARG:HH11	2.20	0.45
1:D:13:THR:O	1:D:17:LYS:HG3	2.16	0.45
1:D:317:LEU:O	1:D:320:PRO:HG3	2.17	0.45
1:E:55:LEU:HD13	1:E:248:VAL:HG13	1.97	0.45
1:E:199:GLN:HG3	1:E:222:GLU:OE1	2.16	0.45
1:F:352:ALA:HB3	2:F:561:HOH:O	2.15	0.45
1:A:199:GLN:HA	1:A:222:GLU:OE1	2.16	0.45
1:C:22:ARG:O	1:C:25:ILE:HG12	2.16	0.45
1:C:208:PRO:HG3	1:C:224:LEU:CD2	2.42	0.45
1:C:229:THR:O	1:C:233:THR:HB	2.16	0.45
1:C:377:PRO:HG2	1:C:378:GLY:H	1.81	0.45
1:D:291:SER:C	1:D:293:ASN:N	2.70	0.45
1:D:321:ASN:OD1	1:D:321:ASN:N	2.41	0.45
1:D:375:ASP:OD1	1:D:414:ARG:HB3	2.15	0.45
1:E:11:ILE:C	1:E:13:THR:H	2.18	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:160:PHE:CZ	1:F:186:TYR:HB2	2.51	0.45
1:F:398:ILE:HD11	1:F:429:LEU:HD11	1.99	0.45
1:F:423:VAL:HG13	2:F:592:HOH:O	2.15	0.45
1:F:493:VAL:HA	2:F:622:HOH:O	2.15	0.45
1:A:146:ILE:HD12	1:A:146:ILE:N	2.18	0.45
1:A:180:CYS:HB3	1:A:203:MET:HG2	1.99	0.45
1:A:185:VAL:HG22	2:A:548:HOH:O	2.16	0.45
1:A:397:LEU:HD13	1:A:423:VAL:CG1	2.45	0.45
1:C:41:HIS:HE1	1:C:50:GLU:OE1	1.99	0.45
1:C:94:VAL:O	1:C:95:ASP:HB2	2.16	0.45
1:C:146:ILE:HG22	1:F:454:LEU:HD21	1.96	0.45
1:D:99:VAL:HG22	2:D:603:HOH:O	2.16	0.45
1:E:20:ASP:O	1:E:23:ARG:HB3	2.17	0.45
1:E:45:LYS:HG2	1:E:200:THR:CG2	2.46	0.45
1:E:306:LEU:HD11	1:E:336:ILE:CD1	2.47	0.45
1:E:374:VAL:HB	2:E:627:HOH:O	2.15	0.45
1:F:21:LEU:O	1:F:25:ILE:HG23	2.17	0.45
1:A:25:ILE:O	1:A:29:THR:HG23	2.17	0.45
1:A:386:GLU:OE1	1:A:391:ILE:HD11	2.17	0.45
1:B:166:ALA:C	2:E:599:HOH:O	2.54	0.45
1:B:215:THR:C	1:B:217:GLU:H	2.17	0.45
1:C:198:ASP:HB2	1:C:240:MET:HG2	1.97	0.45
1:C:354:GLU:HG2	1:C:396:LYS:HD2	1.99	0.45
1:C:375:ASP:CG	1:C:414:ARG:HB3	2.36	0.45
1:C:376:VAL:O	1:C:415:LYS:HB3	2.17	0.45
1:C:520:LEU:HD12	1:C:520:LEU:N	2.30	0.45
1:E:178:GLY:N	1:E:201:SER:HB3	2.31	0.45
1:E:344:PHE:CD1	1:E:344:PHE:N	2.84	0.45
1:F:113:LEU:HD13	1:F:114:GLY:N	2.32	0.45
1:F:176:VAL:O	1:F:196:MET:HA	2.16	0.45
1:B:24:ARG:HD3	1:B:83:TYR:OH	2.16	0.45
1:C:277:VAL:HA	2:C:712:HOH:O	2.17	0.45
1:C:504:ARG:NH2	2:C:669:HOH:O	2.50	0.45
1:C:521:PRO:HB2	1:F:169:VAL:HG21	1.98	0.45
1:D:250:TYR:OH	1:D:314:THR:HG22	2.17	0.45
1:D:306:LEU:HD13	1:D:327:GLY:HA3	1.98	0.45
1:D:389:GLY:O	1:D:390:ILE:C	2.55	0.45
1:D:397:LEU:HD21	1:D:401:TYR:HE2	1.82	0.45
1:E:275:LEU:HD22	1:E:275:LEU:N	2.31	0.45
1:F:234:SER:CB	1:F:236:VAL:HG13	2.45	0.45
1:F:349:ASP:OD1	1:F:349:ASP:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:GLN:OE1	1:A:140:ASP:N	2.47	0.45
1:A:372:THR:HG21	1:A:401:TYR:OH	2.17	0.45
1:A:494:ASP:O	1:A:495:ALA:HB2	2.17	0.45
1:B:212:LYS:C	1:B:214:VAL:H	2.20	0.45
1:C:161:ARG:O	1:C:162:ARG:C	2.55	0.45
1:C:251:VAL:HG13	1:C:252:LYS:N	2.32	0.45
1:C:379:PHE:O	1:C:381:PRO:HD3	2.16	0.45
1:E:70:HIS:CE1	1:E:78:ASP:HA	2.52	0.45
1:E:113:LEU:HD13	1:E:117:TYR:HD1	1.78	0.45
1:F:48:ALA:O	1:F:50:GLU:N	2.49	0.45
1:F:284:LEU:O	1:F:287:ILE:HG22	2.16	0.45
1:A:193:PHE:HA	1:A:238:HIS:CE1	2.52	0.45
1:B:129:LEU:HA	1:B:170:ILE:HD13	1.99	0.45
1:B:508:ARG:NE	1:C:62:VAL:HG11	2.32	0.45
1:C:118:GLY:HA3	1:C:155:ALA:HB1	1.98	0.45
1:D:170:ILE:HG22	2:D:611:HOH:O	2.15	0.45
1:E:177:VAL:HA	1:E:201:SER:HB3	1.99	0.45
1:F:376:VAL:HG13	1:F:376:VAL:O	2.17	0.45
1:A:113:LEU:HD11	2:A:633:HOH:O	2.17	0.45
1:A:224:LEU:HD11	1:D:386:GLU:HG3	1.99	0.45
1:B:23:ARG:O	1:B:26:GLU:HB3	2.17	0.45
1:B:160:PHE:HB3	1:E:398:ILE:HD12	1.98	0.45
1:B:340:GLN:O	1:B:340:GLN:HG3	2.16	0.45
1:D:253:GLN:HB3	1:D:312:PHE:CE1	2.51	0.45
1:E:114:GLY:H	1:E:117:TYR:HB3	1.81	0.45
1:A:62:VAL:HG21	1:C:508:ARG:NE	2.32	0.45
1:B:169:VAL:HG21	1:E:521:PRO:HB2	1.98	0.45
1:B:437:TRP:HD1	2:B:600:HOH:O	1.99	0.45
1:B:512:GLN:HG3	1:C:91:TYR:CE1	2.52	0.45
2:B:585:HOH:O	1:E:361:ARG:HB2	2.16	0.45
1:E:99:VAL:CG1	1:E:100:ALA:N	2.80	0.45
1:E:206:THR:HB	2:E:617:HOH:O	2.17	0.45
1:E:395:ALA:HA	1:E:398:ILE:HG23	1.98	0.45
1:E:483:ASN:HD22	1:E:485:TYR:N	2.14	0.45
1:F:89:THR:HG22	1:F:102:PHE:HB2	1.99	0.45
1:F:196:MET:CE	1:F:203:MET:HG3	2.47	0.45
1:F:251:VAL:HG13	1:F:252:LYS:N	2.31	0.45
1:F:472:ARG:HH21	1:F:473:LEU:CD2	2.28	0.45
1:F:518:GLU:HB3	2:F:543:HOH:O	2.16	0.45
1:A:361:ARG:HD2	1:A:403:GLU:OE2	2.16	0.45
1:A:490:ARG:HH12	1:D:151:ALA:HB2	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:125:MET:HE2	1:B:135:VAL:HG11	1.99	0.45
1:B:212:LYS:O	1:B:214:VAL:N	2.50	0.45
1:B:284:LEU:HD13	1:B:304:HIS:CD2	2.52	0.45
1:B:457:ARG:HE	1:B:457:ARG:HA	1.82	0.45
1:B:475:GLN:HA	1:B:478:GLU:OE1	2.17	0.45
1:D:299:HIS:CD2	1:D:323:LEU:HD13	2.52	0.45
1:D:354:GLU:HA	2:D:672:HOH:O	2.17	0.45
1:D:491:GLY:O	1:D:492:TYR:C	2.56	0.45
1:E:287:ILE:HG23	1:E:288:VAL:N	2.32	0.45
1:E:487:ALA:HB1	1:E:492:TYR:HB2	1.98	0.45
1:F:141:SER:O	1:F:179:PRO:HB2	2.16	0.45
1:F:449:GLY:O	1:F:453:ILE:HG13	2.17	0.45
1:A:124:VAL:HG23	1:A:125:MET:N	2.32	0.44
1:A:411:VAL:C	2:A:636:HOH:O	2.55	0.44
1:A:417:PHE:O	1:A:420:ALA:HB3	2.17	0.44
1:B:246:ASP:O	1:B:249:GLU:HB3	2.17	0.44
1:C:39:LYS:O	1:C:43:LYS:HG2	2.16	0.44
1:C:418:GLY:HA2	1:F:153:LEU:CD2	2.43	0.44
1:D:528:ILE:O	1:D:528:ILE:HG23	2.17	0.44
1:E:70:HIS:NE2	1:E:81:ARG:HG2	2.32	0.44
1:E:377:PRO:HA	1:E:417:PHE:HD2	1.81	0.44
1:F:74:ASN:HB2	2:F:655:HOH:O	2.17	0.44
1:A:153:LEU:O	1:D:422:ILE:HD11	2.17	0.44
1:A:278:THR:HB	1:A:280:GLU:OE2	2.17	0.44
1:B:146:ILE:HD12	1:B:146:ILE:H	1.82	0.44
1:C:76:GLY:HA2	2:C:636:HOH:O	2.15	0.44
1:E:177:VAL:HG12	1:E:197:VAL:HG21	1.99	0.44
1:F:69:ARG:HD3	1:F:81:ARG:O	2.18	0.44
1:F:377:PRO:HA	1:F:417:PHE:CD2	2.47	0.44
1:F:396:LYS:NZ	2:F:594:HOH:O	2.51	0.44
1:C:61:PHE:CE1	1:C:90:GLY:HA3	2.48	0.44
1:C:184:ALA:C	1:C:186:TYR:H	2.19	0.44
1:D:177:VAL:HA	1:D:201:SER:HB3	1.99	0.44
1:F:104:GLN:CG	1:F:139:ASN:HA	2.47	0.44
1:F:389:GLY:O	1:F:393:ARG:HG3	2.16	0.44
1:A:63:GLU:OE1	1:A:66:GLU:HG3	2.18	0.44
1:A:486:THR:HB	2:A:588:HOH:O	2.17	0.44
1:B:253:GLN:HB3	1:B:312:PHE:CE1	2.52	0.44
1:C:69:ARG:O	1:C:116:VAL:HG21	2.17	0.44
1:C:478:GLU:HA	1:C:482:LEU:HB2	2.00	0.44
1:E:375:ASP:OD1	1:E:415:LYS:HG3	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:417:PHE:HE1	1:F:482:LEU:HD11	1.83	0.44
1:A:372:THR:CG2	2:A:594:HOH:O	2.65	0.44
1:A:527:ASN:HD21	1:D:358:ARG:NE	2.15	0.44
1:B:121:ILE:HG13	2:B:657:HOH:O	2.18	0.44
1:B:156:TYR:CE1	1:B:184:ALA:HB2	2.53	0.44
1:C:284:LEU:HD11	1:C:304:HIS:CG	2.52	0.44
1:C:509:GLY:O	1:C:513:LEU:CD2	2.64	0.44
1:D:128:ALA:CB	1:D:135:VAL:HG22	2.48	0.44
1:E:251:VAL:HG23	1:E:252:LYS:N	2.31	0.44
1:F:227:ALA:HB1	1:F:240:MET:HG3	2.00	0.44
1:A:65:ASP:HB2	1:A:120:LYS:HE3	1.98	0.44
1:B:200:THR:HG22	1:B:200:THR:O	2.17	0.44
1:B:204:PHE:HA	1:E:386:GLU:OE2	2.17	0.44
1:C:393:ARG:NH2	1:F:393:ARG:CZ	2.81	0.44
1:C:495:ALA:HB2	2:C:566:HOH:O	2.18	0.44
1:F:91:TYR:HB2	2:F:535:HOH:O	2.16	0.44
1:F:104:GLN:HB2	1:F:140:ASP:H	1.83	0.44
1:A:262:ASN:C	1:A:262:ASN:OD1	2.56	0.44
1:A:324:THR:HA	1:A:336:ILE:O	2.16	0.44
1:A:372:THR:CG2	1:A:401:TYR:OH	2.66	0.44
1:A:498:MET:C	1:A:500:SER:N	2.69	0.44
1:C:274:ASP:OD1	1:C:276:ALA:HB3	2.18	0.44
1:E:374:VAL:HG12	1:E:375:ASP:N	2.33	0.44
1:F:472:ARG:HH12	1:F:476:GLU:CG	2.30	0.44
1:A:91:TYR:OH	1:C:508:ARG:CZ	2.65	0.44
1:B:45:LYS:HE2	1:B:200:THR:HG22	2.00	0.44
1:B:180:CYS:O	1:B:203:MET:HA	2.18	0.44
1:C:451:VAL:HG21	1:C:474:ILE:HG12	1.99	0.44
1:D:134:PRO:HB2	2:D:603:HOH:O	2.18	0.44
1:E:65:ASP:OD2	1:E:120:LYS:HG2	2.17	0.44
1:E:227:ALA:HB3	2:E:675:HOH:O	2.18	0.44
1:E:361:ARG:HD2	1:E:403:GLU:OE2	2.17	0.44
1:A:69:ARG:O	1:A:116:VAL:HG21	2.18	0.44
1:B:63:GLU:HG2	1:B:66:GLU:HB2	1.98	0.44
1:D:353:SER:OG	1:D:394:GLY:HA2	2.18	0.44
1:E:155:ALA:O	1:E:159:ILE:HG13	2.18	0.44
1:E:230:HIS:HB3	1:E:236:VAL:CG2	2.47	0.44
1:F:113:LEU:HD13	1:F:113:LEU:C	2.39	0.44
1:F:187:SER:CB	1:F:188:PRO:CD	2.94	0.44
1:F:510:LEU:O	1:F:511:ARG:C	2.55	0.44
1:A:203:MET:HB2	1:A:230:HIS:CD2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:377:PRO:HA	1:A:417:PHE:HD2	1.83	0.43
1:A:389:GLY:O	1:A:393:ARG:HG3	2.18	0.43
1:D:354:GLU:HG2	1:D:396:LYS:HD2	2.00	0.43
1:E:21:LEU:O	1:E:21:LEU:HD12	2.18	0.43
1:E:71:ARG:NH1	1:F:490:ARG:NH2	2.66	0.43
1:E:177:VAL:HB	1:E:244:GLU:OE1	2.18	0.43
1:E:239:HIS:HA	2:E:673:HOH:O	2.18	0.43
1:F:440:ALA:HB2	2:F:648:HOH:O	2.18	0.43
1:A:464:ASP:O	1:A:465:ASP:HB2	2.18	0.43
1:A:512:GLN:HG3	1:B:91:TYR:CE1	2.52	0.43
1:A:523:LYS:HE2	1:D:169:VAL:CG2	2.48	0.43
1:B:122:VAL:C	1:B:124:VAL:N	2.69	0.43
1:B:167:SER:N	2:E:599:HOH:O	2.50	0.43
1:B:182:GLY:O	1:B:185:VAL:HG22	2.18	0.43
1:D:315:GLN:HA	2:D:542:HOH:O	2.18	0.43
1:D:395:ALA:O	1:D:396:LYS:C	2.54	0.43
1:E:447:ALA:O	1:E:451:VAL:HG22	2.17	0.43
1:F:323:LEU:HD11	2:F:686:HOH:O	2.17	0.43
1:F:448:GLN:O	1:F:451:VAL:HG22	2.17	0.43
1:A:91:TYR:CD1	1:A:92:GLY:N	2.85	0.43
1:A:508:ARG:CG	1:B:62:VAL:HG21	2.48	0.43
1:B:318:PHE:O	1:B:319:ALA:C	2.56	0.43
1:B:528:ILE:O	1:B:530:LEU:HD13	2.18	0.43
1:C:33:SER:O	1:C:36:ALA:N	2.50	0.43
1:C:298:MET:O	1:C:300:SER:N	2.50	0.43
1:D:36:ALA:HB1	1:D:107:THR:HB	2.00	0.43
1:E:25:ILE:O	1:E:29:THR:HG23	2.18	0.43
1:E:294:GLN:HA	1:E:295:PRO:HD3	1.75	0.43
1:E:490:ARG:HH11	1:E:490:ARG:CG	2.30	0.43
1:A:155:ALA:O	1:A:156:TYR:C	2.56	0.43
1:A:300:SER:O	1:A:304:HIS:ND1	2.49	0.43
1:B:172:GLN:HG2	2:B:666:HOH:O	2.17	0.43
1:B:254:LEU:HD22	2:B:607:HOH:O	2.18	0.43
1:C:473:LEU:HD12	1:C:473:LEU:HA	1.82	0.43
1:C:508:ARG:HD3	1:C:508:ARG:C	2.38	0.43
1:D:40:GLN:HE22	1:D:106:PHE:HD2	1.64	0.43
1:D:295:PRO:CB	1:D:342:MET:HE2	2.45	0.43
1:E:62:VAL:CG1	1:F:508:ARG:HH21	2.20	0.43
1:E:414:ARG:HG3	1:E:439:THR:O	2.18	0.43
1:F:161:ARG:O	1:F:164:THR:N	2.47	0.43
1:F:291:SER:C	1:F:293:ASN:N	2.72	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:402:ALA:HA	1:F:429:LEU:O	2.18	0.43
1:A:40:GLN:HE21	1:A:40:GLN:HA	1.83	0.43
1:B:180:CYS:HB3	1:B:203:MET:HG2	2.01	0.43
1:B:386:GLU:HG3	1:E:224:LEU:HD11	2.00	0.43
1:C:84:GLY:HA2	1:C:120:LYS:NZ	2.34	0.43
1:D:47:THR:HG23	1:D:50:GLU:CD	2.39	0.43
1:E:51:ARG:CZ	1:E:177:VAL:CG2	2.97	0.43
1:E:146:ILE:HD12	1:E:146:ILE:N	2.26	0.43
1:A:24:ARG:HD2	1:C:485:TYR:CE1	2.54	0.43
1:A:442:ILE:HD12	1:A:484:PRO:HA	2.00	0.43
1:A:505:HIS:C	1:A:508:ARG:HH11	2.19	0.43
1:B:158:GLU:OE2	1:B:161:ARG:NH2	2.52	0.43
2:B:649:HOH:O	1:E:358:ARG:HG2	2.19	0.43
1:C:285:ASP:HA	1:C:499:PRO:HB2	2.00	0.43
1:D:386:GLU:C	1:D:388:ASP:H	2.20	0.43
1:E:177:VAL:C	1:E:201:SER:HB3	2.39	0.43
1:E:199:GLN:HE21	1:E:199:GLN:HB2	1.53	0.43
1:E:234:SER:HB2	1:E:236:VAL:HG13	2.00	0.43
1:F:313:GLU:HG2	1:F:316:PRO:HG3	2.00	0.43
1:F:528:ILE:O	1:F:530:LEU:CD1	2.67	0.43
1:C:231:ASN:HD21	1:C:239:HIS:C	2.22	0.43
1:C:308:ASP:HB2	1:C:310:GLU:HG3	2.00	0.43
1:E:250:TYR:O	1:E:251:VAL:C	2.56	0.43
1:E:508:ARG:HD3	1:E:508:ARG:C	2.37	0.43
1:F:518:GLU:CB	2:F:543:HOH:O	2.67	0.43
1:A:145:ARG:HD2	1:A:148:GLU:OE2	2.19	0.43
1:A:164:THR:HG23	1:D:399:PHE:CE1	2.53	0.43
1:B:374:VAL:HG12	1:B:375:ASP:N	2.33	0.43
1:C:512:GLN:HE21	1:C:512:GLN:HB3	1.52	0.43
1:D:423:VAL:O	1:D:425:GLY:N	2.51	0.43
1:E:397:LEU:HD13	1:E:423:VAL:CG1	2.49	0.43
1:E:412:ILE:HG22	1:E:440:ALA:HB1	2.01	0.43
1:F:174:SER:O	1:F:195:VAL:HG12	2.19	0.43
1:F:393:ARG:HB3	2:F:628:HOH:O	2.18	0.43
1:A:193:PHE:HA	1:A:238:HIS:ND1	2.33	0.43
1:A:332:ARG:HG3	1:A:332:ARG:HH11	1.84	0.43
1:A:375:ASP:OD1	1:A:414:ARG:HB3	2.19	0.43
1:B:231:ASN:HD21	1:B:239:HIS:CA	2.32	0.43
1:C:214:VAL:HG12	1:C:214:VAL:O	2.18	0.43
1:D:21:LEU:O	1:D:25:ILE:HG23	2.19	0.43
1:D:367:ASN:HA	1:D:406:VAL:CG1	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:405:THR:N	2:E:677:HOH:O	2.41	0.43
1:F:70:HIS:ND1	1:F:70:HIS:C	2.72	0.43
1:F:291:SER:C	1:F:293:ASN:H	2.22	0.43
1:F:318:PHE:HA	2:F:614:HOH:O	2.19	0.43
1:A:21:LEU:O	1:A:25:ILE:HG23	2.18	0.43
1:A:141:SER:OG	1:A:142:GLY:N	2.50	0.43
1:A:306:LEU:HD13	1:A:327:GLY:HA3	2.01	0.43
1:B:389:GLY:O	1:B:390:ILE:C	2.57	0.43
1:C:154:GLY:O	1:C:155:ALA:C	2.58	0.43
1:C:414:ARG:HA	1:C:440:ALA:HA	2.00	0.43
1:D:122:VAL:O	1:D:123:LYS:C	2.56	0.43
1:D:442:ILE:HG13	2:D:644:HOH:O	2.18	0.43
1:E:47:THR:N	1:E:50:GLU:OE1	2.50	0.43
1:E:157:GLY:O	1:E:160:PHE:HB2	2.19	0.43
1:F:121:ILE:HD12	2:F:654:HOH:O	2.19	0.43
1:F:208:PRO:HG2	1:F:221:PHE:CZ	2.54	0.43
1:F:238:HIS:HD2	1:F:315:GLN:HE21	1.67	0.43
1:B:85:ASP:O	1:B:85:ASP:OD2	2.37	0.42
1:B:157:GLY:O	1:B:159:ILE:N	2.51	0.42
1:B:236:VAL:CG2	1:B:237:ALA:N	2.82	0.42
1:B:377:PRO:HG3	2:B:650:HOH:O	2.19	0.42
1:B:449:GLY:HA2	1:B:452:ASN:ND2	2.34	0.42
1:B:512:GLN:NE2	2:B:545:HOH:O	2.52	0.42
1:C:135:VAL:HG22	2:C:574:HOH:O	2.19	0.42
1:E:87:VAL:HG13	1:E:87:VAL:O	2.18	0.42
1:E:161:ARG:NH1	1:E:161:ARG:CG	2.80	0.42
1:E:197:VAL:HB	1:E:200:THR:HB	2.01	0.42
1:E:455:HIS:O	1:E:457:ARG:N	2.52	0.42
1:F:55:LEU:CD1	1:F:252:LYS:HG3	2.49	0.42
1:F:106:PHE:O	1:F:106:PHE:CD2	2.71	0.42
1:F:134:PRO:N	2:F:607:HOH:O	2.52	0.42
1:B:335:GLY:O	1:B:371:LEU:N	2.49	0.42
1:C:246:ASP:O	1:C:249:GLU:HB3	2.20	0.42
1:C:316:PRO:HD2	2:C:601:HOH:O	2.19	0.42
1:C:462:ALA:C	1:C:464:ASP:N	2.73	0.42
1:D:486:THR:HB	2:D:599:HOH:O	2.18	0.42
1:E:302:ILE:O	1:E:305:VAL:HG22	2.19	0.42
1:E:313:GLU:HG3	2:E:561:HOH:O	2.19	0.42
1:B:268:ALA:HB2	1:B:332:ARG:HG2	2.00	0.42
1:C:227:ALA:HB2	2:C:620:HOH:O	2.19	0.42
1:C:232:SER:HB3	1:C:317:LEU:CB	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:253:GLN:HB3	1:C:312:PHE:CE1	2.55	0.42
1:E:199:GLN:HB2	2:E:691:HOH:O	2.19	0.42
1:E:397:LEU:HD13	1:E:423:VAL:HG11	2.02	0.42
1:E:505:HIS:CD2	2:E:640:HOH:O	2.72	0.42
1:F:322:ILE:HG13	2:F:608:HOH:O	2.18	0.42
1:F:445:MET:HG3	1:F:450:ALA:HB2	2.01	0.42
1:A:353:SER:CB	1:A:394:GLY:HA2	2.49	0.42
1:A:485:TYR:HA	1:A:488:ALA:HB3	2.02	0.42
1:A:530:LEU:HB3	2:D:672:HOH:O	2.20	0.42
1:B:11:ILE:O	1:B:11:ILE:CG1	2.67	0.42
1:B:334:VAL:HG23	1:B:336:ILE:HD11	2.01	0.42
1:B:503:ARG:NH2	2:B:693:HOH:O	2.51	0.42
1:B:505:HIS:CA	1:B:508:ARG:HH11	2.32	0.42
1:C:32:GLY:HA3	1:C:107:THR:OG1	2.19	0.42
1:C:128:ALA:HB2	2:C:574:HOH:O	2.19	0.42
1:C:170:ILE:CD1	2:C:641:HOH:O	2.67	0.42
1:C:443:ALA:HB1	2:C:629:HOH:O	2.18	0.42
1:D:180:CYS:HB3	1:D:203:MET:CG	2.50	0.42
1:E:306:LEU:CD2	1:E:336:ILE:HD11	2.45	0.42
1:E:332:ARG:NH1	1:E:332:ARG:HB2	2.34	0.42
1:E:473:LEU:O	1:E:476:GLU:N	2.52	0.42
1:F:55:LEU:HD21	1:F:136:VAL:HG21	2.00	0.42
1:F:414:ARG:HA	1:F:440:ALA:HA	2.00	0.42
1:A:147:GLN:OE1	1:A:147:GLN:N	2.49	0.42
1:A:379:PHE:O	1:A:380:LEU:C	2.57	0.42
1:A:410:THR:HG22	2:A:636:HOH:O	2.19	0.42
1:C:285:ASP:OD1	1:C:499:PRO:HD2	2.19	0.42
1:C:305:VAL:HG23	1:C:306:LEU:N	2.34	0.42
1:C:358:ARG:HB3	2:C:653:HOH:O	2.20	0.42
1:D:509:GLY:O	1:D:513:LEU:HD22	2.20	0.42
1:E:298:MET:SD	1:E:301:VAL:CG2	3.07	0.42
1:F:122:VAL:O	1:F:123:LYS:C	2.57	0.42
1:F:325:GLY:O	1:F:359:PHE:CZ	2.72	0.42
1:F:380:LEU:O	1:F:380:LEU:HD23	2.19	0.42
1:A:136:VAL:HG21	2:A:671:HOH:O	2.19	0.42
1:A:287:ILE:O	1:A:287:ILE:HG13	2.19	0.42
1:A:332:ARG:NH1	1:A:514:ARG:HH21	2.17	0.42
1:A:344:PHE:CD1	1:A:344:PHE:N	2.88	0.42
1:A:397:LEU:HB3	1:A:423:VAL:HG13	2.02	0.42
1:C:50:GLU:O	1:C:54:LEU:HB2	2.20	0.42
1:C:181:ALA:HB2	1:C:204:PHE:CE1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:62:VAL:HG21	1:F:508:ARG:CG	2.50	0.42
1:E:98:PRO:HB2	2:E:662:HOH:O	2.19	0.42
1:E:177:VAL:HG12	1:E:197:VAL:CG2	2.49	0.42
1:E:298:MET:O	1:E:299:HIS:C	2.58	0.42
1:E:398:ILE:CG1	1:E:399:PHE:N	2.81	0.42
1:E:427:LYS:NZ	2:E:694:HOH:O	2.50	0.42
1:E:459:ILE:HD11	1:E:470:ARG:HB2	2.02	0.42
1:A:374:VAL:CG1	1:A:375:ASP:N	2.83	0.42
1:A:527:ASN:ND2	1:D:358:ARG:HE	2.18	0.42
1:B:146:ILE:HD12	1:B:146:ILE:N	2.35	0.42
1:B:175:LEU:HD12	1:B:195:VAL:HG13	2.01	0.42
1:C:154:GLY:O	1:C:157:GLY:N	2.53	0.42
1:E:469:THR:O	1:E:473:LEU:HD13	2.19	0.42
1:F:173:ILE:HD13	1:F:254:LEU:HD23	2.02	0.42
1:F:291:SER:HB3	1:F:294:GLN:CB	2.49	0.42
1:F:332:ARG:N	2:F:550:HOH:O	2.53	0.42
1:F:337:VAL:HG21	1:F:360:VAL:HG22	2.01	0.42
1:F:382:GLY:O	1:F:385:GLN:HB2	2.20	0.42
1:A:39:LYS:O	1:A:43:LYS:HB2	2.19	0.42
1:A:313:GLU:OE1	1:A:323:LEU:HD22	2.20	0.42
1:A:427:LYS:HE2	1:A:494:ASP:OD2	2.20	0.42
1:B:61:PHE:HE1	1:B:90:GLY:HA3	1.84	0.42
1:B:87:VAL:O	1:B:87:VAL:HG13	2.20	0.42
1:B:336:ILE:N	1:B:336:ILE:CD1	2.82	0.42
1:B:396:LYS:HD3	1:E:530:LEU:HG	2.02	0.42
1:C:380:LEU:HD23	1:C:385:GLN:CD	2.40	0.42
1:D:453:ILE:HD12	1:D:453:ILE:N	2.34	0.42
1:F:150:VAL:O	1:F:153:LEU:N	2.44	0.42
1:F:198:ASP:HA	1:F:227:ALA:CB	2.46	0.42
1:A:397:LEU:HD13	1:A:423:VAL:HG12	2.01	0.42
1:A:398:ILE:HD11	1:D:190:ILE:HD11	2.01	0.42
1:B:51:ARG:HB2	2:B:590:HOH:O	2.19	0.42
1:B:69:ARG:O	1:B:116:VAL:HG21	2.20	0.42
1:B:90:GLY:HA2	2:B:562:HOH:O	2.20	0.42
1:B:149:GLY:O	1:E:444:VAL:HB	2.20	0.42
1:C:171:PRO:HG3	1:C:366:PHE:CE1	2.55	0.42
1:C:459:ILE:HD11	1:C:470:ARG:HB2	2.00	0.42
1:C:468:ALA:O	1:C:472:ARG:HB2	2.20	0.42
1:D:99:VAL:HG13	2:D:603:HOH:O	2.19	0.42
1:D:181:ALA:CB	1:D:204:PHE:CE1	3.01	0.42
1:D:182:GLY:O	1:D:205:ILE:HD13	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:361:ARG:CZ	2:E:579:HOH:O	2.68	0.42
1:F:190:ILE:O	1:F:191:THR:C	2.59	0.42
1:F:193:PHE:HA	1:F:238:HIS:ND1	2.34	0.42
1:F:372:THR:HG21	2:F:568:HOH:O	2.19	0.42
1:F:374:VAL:HG13	1:F:424:MET:HG3	2.01	0.42
1:F:461:ASP:HB3	2:F:627:HOH:O	2.19	0.42
1:A:203:MET:HB2	1:A:230:HIS:NE2	2.35	0.42
1:A:315:GLN:N	1:A:316:PRO:CD	2.82	0.42
1:B:85:ASP:OD1	1:B:116:VAL:HB	2.20	0.42
1:B:177:VAL:HG12	1:B:197:VAL:CG2	2.50	0.42
1:B:375:ASP:OD2	1:B:414:ARG:HB3	2.20	0.42
1:C:23:ARG:NH2	1:C:27:GLU:OE2	2.52	0.42
1:C:248:VAL:HG12	2:C:666:HOH:O	2.20	0.42
1:C:383:VAL:HG22	1:F:219:VAL:HG21	2.02	0.42
1:C:505:HIS:HA	1:C:508:ARG:HH11	1.85	0.42
1:D:91:TYR:CD1	1:D:91:TYR:C	2.93	0.42
1:D:419:GLY:O	1:D:420:ALA:C	2.58	0.42
1:E:51:ARG:CZ	1:E:177:VAL:HG21	2.50	0.42
1:E:258:LEU:HG	2:E:560:HOH:O	2.19	0.42
1:E:505:HIS:O	1:E:508:ARG:NH1	2.52	0.42
1:F:116:VAL:O	1:F:120:LYS:HG3	2.20	0.42
1:F:231:ASN:HD21	1:F:239:HIS:C	2.23	0.42
1:F:248:VAL:O	1:F:251:VAL:HG12	2.20	0.42
1:F:315:GLN:HB2	1:F:355:LYS:HE3	2.01	0.42
1:A:11:ILE:O	1:A:11:ILE:HG13	2.20	0.41
1:A:160:PHE:HE2	1:D:422:ILE:HG21	1.84	0.41
1:A:197:VAL:O	1:A:227:ALA:HB2	2.20	0.41
1:A:406:VAL:HB	1:A:407:PRO:CD	2.50	0.41
1:A:461:ASP:O	1:A:462:ALA:HB3	2.20	0.41
1:C:523:LYS:O	1:C:523:LYS:HG2	2.19	0.41
2:C:713:HOH:O	1:F:382:GLY:HA2	2.20	0.41
1:D:234:SER:HB2	1:D:236:VAL:HG13	2.02	0.41
1:E:335:GLY:O	1:E:371:LEU:N	2.53	0.41
1:F:122:VAL:HG13	1:F:162:ARG:NE	2.35	0.41
1:F:281:ASP:O	1:F:500:SER:HA	2.20	0.41
1:F:294:GLN:HA	1:F:295:PRO:HD3	1.84	0.41
1:F:344:PHE:CD1	1:F:344:PHE:N	2.88	0.41
1:A:94:VAL:HG13	1:A:252:LYS:HD2	2.02	0.41
1:A:153:LEU:HD11	1:D:418:GLY:CA	2.50	0.41
1:A:206:THR:HG22	1:A:211:ILE:HG13	2.02	0.41
1:A:398:ILE:CD1	1:D:160:PHE:HB3	2.43	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:528:ILE:O	1:A:530:LEU:HD22	2.21	0.41
1:B:28:ALA:C	1:B:30:HIS:H	2.23	0.41
1:B:122:VAL:O	1:B:125:MET:N	2.53	0.41
1:B:196:MET:HB2	2:B:609:HOH:O	2.20	0.41
1:B:319:ALA:N	1:B:320:PRO:HD3	2.35	0.41
1:B:444:VAL:HB	1:E:149:GLY:C	2.41	0.41
1:B:487:ALA:HB1	1:B:492:TYR:HB2	2.01	0.41
1:C:185:VAL:CG2	1:F:391:ILE:HG12	2.50	0.41
1:C:353:SER:HB3	1:C:394:GLY:HA2	2.01	0.41
1:C:400:ALA:HA	2:C:693:HOH:O	2.20	0.41
2:C:660:HOH:O	1:F:525:HIS:HB2	2.20	0.41
1:D:285:ASP:OD1	1:D:499:PRO:HD2	2.20	0.41
1:D:397:LEU:HD23	1:D:401:TYR:CD2	2.55	0.41
1:D:418:GLY:O	1:D:421:TYR:HB3	2.20	0.41
1:D:439:THR:HG21	1:F:14:THR:HG23	2.02	0.41
1:F:380:LEU:HD23	1:F:380:LEU:C	2.41	0.41
1:A:101:VAL:HG22	1:A:102:PHE:N	2.35	0.41
1:A:413:THR:HA	2:A:544:HOH:O	2.19	0.41
1:A:508:ARG:C	1:A:508:ARG:CD	2.87	0.41
1:B:157:GLY:C	1:B:159:ILE:N	2.73	0.41
1:C:161:ARG:HG3	1:C:161:ARG:HH11	1.85	0.41
1:D:113:LEU:HD22	1:D:117:TYR:HE1	1.84	0.41
1:D:220:GLY:O	1:D:221:PHE:C	2.58	0.41
1:D:281:ASP:O	1:D:284:LEU:HB2	2.19	0.41
1:E:130:LYS:HG3	1:F:516:LYS:HG3	2.02	0.41
1:A:26:GLU:O	1:A:30:HIS:HD2	2.04	0.41
1:A:150:VAL:O	1:A:151:ALA:C	2.59	0.41
1:A:162:ARG:HG2	1:A:162:ARG:H	1.71	0.41
1:A:271:GLU:O	1:A:272:GLU:C	2.59	0.41
1:A:490:ARG:NH1	2:A:579:HOH:O	2.53	0.41
1:B:121:ILE:N	2:B:657:HOH:O	2.52	0.41
1:B:380:LEU:HD23	1:B:380:LEU:O	2.20	0.41
1:B:473:LEU:HD12	1:B:476:GLU:OE1	2.19	0.41
1:B:517:ARG:NH2	2:B:533:HOH:O	2.34	0.41
1:C:14:THR:O	1:C:17:LYS:HB2	2.21	0.41
1:C:364:ASP:OD1	1:C:406:VAL:HG22	2.21	0.41
1:D:21:LEU:HD22	1:E:438:PRO:HG3	2.01	0.41
1:D:47:THR:O	1:D:51:ARG:HD3	2.20	0.41
1:D:449:GLY:HA2	1:D:452:ASN:HD22	1.85	0.41
1:E:55:LEU:HD21	1:E:136:VAL:HG11	2.02	0.41
1:E:455:HIS:C	1:E:457:ARG:N	2.72	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:181:ALA:HB2	1:F:204:PHE:CE1	2.55	0.41
1:F:422:ILE:HA	1:F:426:SER:HB3	2.01	0.41
1:A:24:ARG:C	1:A:26:GLU:N	2.73	0.41
1:B:498:MET:HE3	1:B:499:PRO:HD2	2.01	0.41
1:C:122:VAL:O	1:C:124:VAL:N	2.53	0.41
1:C:360:VAL:HB	1:C:400:ALA:HB1	2.03	0.41
1:D:231:ASN:O	1:D:317:LEU:HB2	2.20	0.41
1:D:380:LEU:HD23	1:D:385:GLN:NE2	2.35	0.41
1:E:427:LYS:HB2	1:E:427:LYS:NZ	2.36	0.41
1:F:16:GLY:HA3	2:F:573:HOH:O	2.20	0.41
1:F:71:ARG:HB2	1:F:71:ARG:HH11	1.86	0.41
1:F:230:HIS:HB3	1:F:236:VAL:HG22	2.03	0.41
1:F:342:MET:O	1:F:343:GLN:HG2	2.21	0.41
1:F:423:VAL:CG1	2:F:592:HOH:O	2.68	0.41
1:A:324:THR:HB	1:A:359:PHE:CD2	2.55	0.41
1:A:508:ARG:NE	1:B:62:VAL:HG21	2.35	0.41
1:B:269:PHE:O	1:B:331:GLY:HA3	2.21	0.41
1:B:456:ARG:HH12	1:B:457:ARG:CZ	2.32	0.41
2:B:649:HOH:O	1:E:358:ARG:CG	2.69	0.41
1:D:46:LEU:N	1:D:46:LEU:HD12	2.36	0.41
1:D:125:MET:HE3	2:D:541:HOH:O	2.21	0.41
1:D:284:LEU:HA	1:D:284:LEU:HD12	1.81	0.41
1:D:296:TYR:N	1:D:342:MET:HE1	2.36	0.41
1:D:336:ILE:N	1:D:336:ILE:CD1	2.79	0.41
1:E:62:VAL:HG21	1:F:508:ARG:NE	2.32	0.41
1:E:156:TYR:OH	1:E:184:ALA:HB2	2.19	0.41
1:E:486:THR:O	1:E:489:GLU:HB2	2.20	0.41
1:F:85:ASP:O	1:F:85:ASP:CG	2.59	0.41
1:F:147:GLN:HB3	2:F:655:HOH:O	2.18	0.41
1:F:203:MET:HB2	1:F:230:HIS:NE2	2.36	0.41
1:A:100:ALA:HB3	2:A:578:HOH:O	2.19	0.41
1:A:156:TYR:O	1:A:159:ILE:HB	2.20	0.41
1:A:322:ILE:O	1:A:322:ILE:HG23	2.19	0.41
1:A:521:PRO:HD2	1:D:165:HIS:O	2.21	0.41
1:B:162:ARG:HH11	1:B:162:ARG:CG	2.30	0.41
1:B:344:PHE:N	1:B:344:PHE:CD1	2.88	0.41
1:D:463:GLY:HA2	2:D:657:HOH:O	2.21	0.41
1:E:10:ASP:N	2:E:629:HOH:O	2.53	0.41
1:E:316:PRO:HD2	2:E:567:HOH:O	2.20	0.41
1:F:122:VAL:HG11	1:F:162:ARG:NH2	2.36	0.41
1:F:157:GLY:O	1:F:160:PHE:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:ARG:HB3	1:A:83:TYR:CE1	2.51	0.41
1:A:28:ALA:HB3	2:A:641:HOH:O	2.20	0.41
1:A:162:ARG:HG2	1:A:162:ARG:NH1	2.29	0.41
1:A:164:THR:O	1:A:167:SER:N	2.45	0.41
1:A:399:PHE:CG	1:D:164:THR:HG23	2.56	0.41
1:B:437:TRP:HA	2:B:600:HOH:O	2.20	0.41
1:B:489:GLU:O	1:C:68:ALA:HA	2.20	0.41
1:C:112:ALA:HB3	1:C:145:ARG:HE	1.86	0.41
1:C:153:LEU:O	1:F:422:ILE:HD11	2.20	0.41
1:C:319:ALA:N	1:C:320:PRO:CD	2.84	0.41
1:C:346:GLY:O	1:C:377:PRO:HD2	2.20	0.41
1:C:440:ALA:O	1:C:483:ASN:HA	2.20	0.41
1:D:67:PHE:CE2	1:E:496:VAL:HB	2.56	0.41
1:D:325:GLY:O	1:D:359:PHE:CZ	2.74	0.41
1:E:254:LEU:CD1	1:E:312:PHE:HE2	2.30	0.41
1:E:322:ILE:CG2	1:E:355:LYS:HD3	2.51	0.41
1:E:462:ALA:C	1:E:464:ASP:N	2.72	0.41
1:F:41:HIS:HA	1:F:45:LYS:O	2.21	0.41
1:F:336:ILE:HA	1:F:371:LEU:O	2.21	0.41
1:A:40:GLN:HA	1:A:40:GLN:NE2	2.36	0.41
1:A:103:SER:HA	1:A:138:ILE:HB	2.03	0.41
1:A:132:GLY:N	2:A:609:HOH:O	2.54	0.41
1:A:150:VAL:HG23	1:A:151:ALA:N	2.36	0.41
1:A:299:HIS:HA	2:A:678:HOH:O	2.21	0.41
1:A:490:ARG:HA	1:B:71:ARG:HH21	1.86	0.41
1:B:14:THR:O	1:B:15:ALA:C	2.58	0.41
1:B:61:PHE:CE1	1:B:90:GLY:HA3	2.55	0.41
1:B:155:ALA:O	1:B:159:ILE:HG13	2.21	0.41
1:B:177:VAL:HA	1:B:201:SER:HB3	2.03	0.41
1:B:197:VAL:O	1:B:227:ALA:HB2	2.21	0.41
1:C:40:GLN:O	1:C:41:HIS:C	2.59	0.41
1:C:105:ASP:HA	2:C:614:HOH:O	2.21	0.41
1:C:156:TYR:CE1	1:C:184:ALA:HB2	2.56	0.41
1:C:393:ARG:NH2	1:F:393:ARG:NH1	2.69	0.41
1:C:407:PRO:HB3	1:C:513:LEU:CB	2.51	0.41
2:C:705:HOH:O	1:F:211:ILE:HD13	2.20	0.41
1:D:16:GLY:HA3	2:D:579:HOH:O	2.20	0.41
1:D:55:LEU:CD2	1:D:136:VAL:HG11	2.50	0.41
1:D:478:GLU:C	1:D:480:ALA:H	2.23	0.41
1:E:101:VAL:CG2	1:E:102:PHE:N	2.84	0.41
1:E:339:ASN:ND2	2:E:658:HOH:O	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:350:ILE:O	1:E:354:GLU:HG3	2.21	0.41
1:F:70:HIS:O	1:F:81:ARG:HD2	2.21	0.41
1:F:322:ILE:HG21	2:F:710:HOH:O	2.20	0.41
1:F:377:PRO:HG3	2:F:632:HOH:O	2.20	0.41
1:F:475:GLN:HE21	1:F:475:GLN:HB3	1.72	0.41
1:A:46:LEU:HD12	1:A:244:GLU:OE2	2.21	0.41
1:B:157:GLY:O	1:B:160:PHE:N	2.54	0.41
1:D:439:THR:CG2	1:F:14:THR:HG23	2.51	0.41
1:E:148:GLU:HB3	2:E:587:HOH:O	2.21	0.41
1:E:156:TYR:CE1	1:E:184:ALA:HB2	2.55	0.41
1:E:194:THR:OG1	1:E:237:ALA:HA	2.21	0.41
1:B:91:TYR:CD1	1:B:91:TYR:C	2.94	0.40
1:B:329:VAL:O	1:B:330:GLU:HB2	2.21	0.40
1:B:508:ARG:C	1:B:508:ARG:CD	2.89	0.40
1:C:141:SER:O	1:C:179:PRO:O	2.39	0.40
1:C:422:ILE:O	1:C:423:VAL:C	2.59	0.40
1:C:434:ASN:O	1:C:494:ASP:OD1	2.37	0.40
1:E:62:VAL:HG21	1:F:508:ARG:HG3	2.03	0.40
1:F:162:ARG:NH1	1:F:162:ARG:CG	2.83	0.40
1:F:212:LYS:O	1:F:214:VAL:N	2.54	0.40
1:F:440:ALA:O	1:F:483:ASN:HA	2.21	0.40
1:A:344:PHE:O	1:A:345:ALA:HB3	2.22	0.40
1:C:212:LYS:HD3	1:C:218:ASP:HB2	2.03	0.40
1:C:339:ASN:HB3	2:C:573:HOH:O	2.20	0.40
1:C:364:ASP:CG	1:C:404:ALA:HA	2.40	0.40
1:E:459:ILE:HG23	1:E:460:ALA:N	2.36	0.40
1:F:359:PHE:O	1:F:360:VAL:C	2.58	0.40
1:B:181:ALA:HB2	1:B:204:PHE:CE1	2.57	0.40
1:B:185:VAL:HB	1:E:391:ILE:HD13	2.04	0.40
1:B:232:SER:HB3	1:B:317:LEU:HB3	2.03	0.40
1:B:307:ASP:CG	1:B:330:GLU:H	2.24	0.40
1:B:337:VAL:O	1:B:372:THR:HA	2.21	0.40
1:C:163:ASN:N	2:C:539:HOH:O	2.54	0.40
1:C:511:ARG:HD2	2:C:556:HOH:O	2.22	0.40
1:D:429:LEU:HA	1:D:429:LEU:HD12	1.80	0.40
1:D:487:ALA:HB1	1:D:492:TYR:HB2	2.03	0.40
1:E:60:SER:HB2	1:E:93:THR:H	1.87	0.40
1:E:101:VAL:HG13	2:E:607:HOH:O	2.21	0.40
1:E:244:GLU:O	1:E:248:VAL:HG23	2.22	0.40
1:E:344:PHE:O	1:E:345:ALA:HB3	2.20	0.40
1:F:48:ALA:C	1:F:50:GLU:N	2.74	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:482:LEU:HD13	2:F:691:HOH:O	2.21	0.40
1:A:508:ARG:HE	1:B:62:VAL:HG21	1.87	0.40
1:E:65:ASP:HA	2:F:590:HOH:O	2.21	0.40
1:E:187:SER:N	1:E:188:PRO:CD	2.84	0.40
1:E:445:MET:HG3	1:E:450:ALA:HB2	2.04	0.40
1:F:101:VAL:HG22	1:F:102:PHE:N	2.36	0.40
1:A:454:LEU:HD13	1:D:75:PHE:CE1	2.57	0.40
1:B:174:SER:OG	1:B:191:THR:HG21	2.22	0.40
1:B:374:VAL:HG13	1:B:424:MET:HG3	2.04	0.40
1:B:451:VAL:HG21	1:B:474:ILE:CG1	2.52	0.40
1:C:208:PRO:O	1:C:210:VAL:N	2.55	0.40
1:C:472:ARG:CD	1:C:476:GLU:OE2	2.70	0.40
1:D:332:ARG:HA	1:D:333:PRO:HD3	1.88	0.40
1:D:397:LEU:HD21	1:D:401:TYR:CE2	2.56	0.40
1:D:455:HIS:O	1:D:459:ILE:HG22	2.22	0.40
1:E:114:GLY:O	1:E:117:TYR:HB3	2.22	0.40
1:E:157:GLY:O	1:E:158:GLU:C	2.60	0.40
1:F:301:VAL:HG13	1:F:437:TRP:HH2	1.85	0.40
1:F:418:GLY:O	1:F:421:TYR:HB3	2.21	0.40
1:F:436:ALA:O	1:F:496:VAL:HA	2.20	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	519/530 (98%)	444 (86%)	65 (12%)	10 (2%)	8	15
1	B	519/530 (98%)	440 (85%)	68 (13%)	11 (2%)	7	13
1	C	519/530 (98%)	430 (83%)	70 (14%)	19 (4%)	3	4
1	D	519/530 (98%)	437 (84%)	71 (14%)	11 (2%)	7	13

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	519/530 (98%)	441 (85%)	71 (14%)	7 (1%)	12	24
1	F	519/530 (98%)	435 (84%)	73 (14%)	11 (2%)	7	13
All	All	3114/3180 (98%)	2627 (84%)	418 (13%)	69 (2%)	6	12

All (69) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	375	ASP
1	B	11	ILE
1	D	448	GLN
1	F	448	GLN
1	A	11	ILE
1	A	115	GLU
1	A	165	HIS
1	A	350	ILE
1	B	213	THR
1	B	375	ASP
1	C	11	ILE
1	C	85	ASP
1	C	209	ASP
1	C	227	ALA
1	C	375	ASP
1	C	404	ALA
1	C	464	ASP
1	D	140	ASP
1	D	424	MET
1	E	140	ASP
1	E	232	SER
1	F	213	THR
1	B	78	ASP
1	B	140	ASP
1	C	191	THR
1	C	414	ARG
1	D	375	ASP
1	D	387	HIS
1	E	375	ASP
1	F	48	ALA
1	F	167	SER
1	F	414	ARG
1	F	452	ASN
1	F	462	ALA

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Mol	Chain	Res	Type
1	A	221	PHE
1	B	167	SER
1	B	424	MET
1	D	11	ILE
1	E	250	TYR
1	F	47	THR
1	A	31	ALA
1	A	85	ASP
1	A	507	VAL
1	B	158	GLU
1	B	404	ALA
1	C	123	LYS
1	C	296	TYR
1	C	385	GLN
1	C	423	VAL
1	C	424	MET
1	C	477	TYR
1	C	529	PRO
1	D	123	LYS
1	D	292	ALA
1	D	462	ALA
1	E	107	THR
1	E	267	PRO
1	F	146	ILE
1	F	292	ALA
1	B	414	ARG
1	C	185	VAL
1	C	221	PHE
1	D	404	ALA
1	E	251	VAL
1	F	296	TYR
1	C	210	VAL
1	B	146	ILE
1	A	377	PRO
1	D	390	ILE

### 5.3.2 Protein sidechains

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	412/421 (98%)	377 (92%)	35 (8%)	10	21
1	B	412/421 (98%)	386 (94%)	26 (6%)	18	36
1	C	412/421 (98%)	373 (90%)	39 (10%)	8	16
1	D	412/421 (98%)	386 (94%)	26 (6%)	18	36
1	E	412/421 (98%)	376 (91%)	36 (9%)	10	20
1	F	412/421 (98%)	383 (93%)	29 (7%)	15	30
All	All	2472/2526 (98%)	2281 (92%)	191 (8%)	13	25

All (191) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	THR
1	A	35	ARG
1	A	53	ASP
1	A	70	HIS
1	A	78	ASP
1	A	103	SER
1	A	113	LEU
1	A	123	LYS
1	A	146	ILE
1	A	161	ARG
1	A	162	ARG
1	A	163	ASN
1	A	164	THR
1	A	175	LEU
1	A	195	VAL
1	A	200	THR
1	A	209	ASP
1	A	330	GLU
1	A	358	ARG
1	A	372	THR
1	A	384	ASP
1	A	397	LEU
1	A	398	ILE
1	A	427	LYS
1	A	429	LEU
1	A	435	LEU
1	A	441	GLN
1	A	475	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	479	ASP
1	A	508	ARG
1	A	517	ARG
1	A	519	SER
1	A	520	LEU
1	A	527	ASN
1	A	530	LEU
1	B	54	LEU
1	B	65	ASP
1	B	97	ARG
1	B	113	LEU
1	B	147	GLN
1	B	162	ARG
1	B	164	THR
1	B	209	ASP
1	B	218	ASP
1	B	277	VAL
1	B	284	LEU
1	B	294	GLN
1	B	299	HIS
1	B	324	THR
1	B	347	CYS
1	B	358	ARG
1	B	372	THR
1	B	397	LEU
1	B	429	LEU
1	B	435	LEU
1	B	475	GLN
1	B	479	ASP
1	B	508	ARG
1	B	514	ARG
1	B	527	ASN
1	B	530	LEU
1	C	43	LYS
1	C	46	LEU
1	C	113	LEU
1	C	133	CYS
1	C	141	SER
1	C	147	GLN
1	C	161	ARG
1	C	175	LEU
1	C	200	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C	205	ILE
1	C	213	THR
1	C	246	ASP
1	C	263	LEU
1	C	277	VAL
1	C	279	ASP
1	C	300	SER
1	C	317	LEU
1	C	339	ASN
1	C	358	ARG
1	C	372	THR
1	C	380	LEU
1	C	384	ASP
1	C	397	LEU
1	C	406	VAL
1	C	427	LYS
1	C	429	LEU
1	C	435	LEU
1	C	441	GLN
1	C	465	ASP
1	C	473	LEU
1	C	475	GLN
1	C	479	ASP
1	C	494	ASP
1	C	508	ARG
1	C	512	GLN
1	C	517	ARG
1	C	520	LEU
1	C	527	ASN
1	C	530	LEU
1	D	51	ARG
1	D	71	ARG
1	D	78	ASP
1	D	97	ARG
1	D	113	LEU
1	D	130	LYS
1	D	147	GLN
1	D	164	THR
1	D	175	LEU
1	D	199	GLN
1	D	205	ILE
1	D	218	ASP

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	D	246	ASP
1	D	284	LEU
1	D	353	SER
1	D	358	ARG
1	D	372	THR
1	D	429	LEU
1	D	435	LEU
1	D	444	VAL
1	D	470	ARG
1	D	475	GLN
1	D	490	ARG
1	D	508	ARG
1	D	512	GLN
1	D	527	ASN
1	E	13	THR
1	E	27	GLU
1	E	46	LEU
1	E	54	LEU
1	E	80	ASN
1	E	113	LEU
1	E	146	ILE
1	E	156	TYR
1	E	161	ARG
1	E	162	ARG
1	E	175	LEU
1	E	187	SER
1	E	199	GLN
1	E	213	THR
1	E	218	ASP
1	E	246	ASP
1	E	263	LEU
1	E	280	GLU
1	E	330	GLU
1	E	358	ARG
1	E	367	ASN
1	E	372	THR
1	E	398	ILE
1	E	427	LYS
1	E	429	LEU
1	E	435	LEU
1	E	441	GLN
1	E	465	ASP

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Mol	Chain	Res	Type
1	E	475	GLN
1	E	490	ARG
1	E	494	ASP
1	E	505	HIS
1	E	508	ARG
1	E	512	GLN
1	E	513	LEU
1	E	527	ASN
1	F	46	LEU
1	F	47	THR
1	F	49	ARG
1	F	107	THR
1	F	124	VAL
1	F	162	ARG
1	F	175	LEU
1	F	200	THR
1	F	205	ILE
1	F	272	GLU
1	F	277	VAL
1	F	281	ASP
1	F	288	VAL
1	F	290	ASP
1	F	321	ASN
1	F	358	ARG
1	F	372	THR
1	F	384	ASP
1	F	397	LEU
1	F	406	VAL
1	F	414	ARG
1	F	427	LYS
1	F	435	LEU
1	F	473	LEU
1	F	475	GLN
1	F	494	ASP
1	F	508	ARG
1	F	512	GLN
1	F	527	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (79) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	HIS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	40	GLN
1	A	172	GLN
1	A	202	HIS
1	A	231	ASN
1	A	294	GLN
1	A	315	GLN
1	A	452	ASN
1	A	483	ASN
1	A	512	GLN
1	A	527	ASN
1	B	30	HIS
1	B	119	GLN
1	B	147	GLN
1	B	163	ASN
1	B	231	ASN
1	B	387	HIS
1	B	452	ASN
1	B	475	GLN
1	B	483	ASN
1	B	512	GLN
1	B	527	ASN
1	C	30	HIS
1	C	40	GLN
1	C	41	HIS
1	C	119	GLN
1	C	163	ASN
1	C	172	GLN
1	C	231	ASN
1	C	261	ASN
1	C	387	HIS
1	C	441	GLN
1	C	452	ASN
1	C	475	GLN
1	C	483	ASN
1	C	512	GLN
1	C	527	ASN
1	D	30	HIS
1	D	40	GLN
1	D	119	GLN
1	D	147	GLN
1	D	163	ASN
1	D	199	GLN

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Mol	Chain	Res	Type
1	D	231	ASN
1	D	294	GLN
1	D	367	ASN
1	D	452	ASN
1	D	512	GLN
1	D	527	ASN
1	E	40	GLN
1	E	80	ASN
1	E	119	GLN
1	E	163	ASN
1	E	199	GLN
1	E	231	ASN
1	E	299	HIS
1	E	367	ASN
1	E	434	ASN
1	E	441	GLN
1	E	448	GLN
1	E	455	HIS
1	E	483	ASN
1	E	512	GLN
1	E	527	ASN
1	F	30	HIS
1	F	40	GLN
1	F	74	ASN
1	F	104	GLN
1	F	147	GLN
1	F	163	ASN
1	F	172	GLN
1	F	231	ASN
1	F	294	GLN
1	F	315	GLN
1	F	367	ASN
1	F	475	GLN
1	F	483	ASN
1	F	512	GLN
1	F	527	ASN

### 5.3.3 RNA

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	521/530 (98%)	0.02	8 (1%) 73 70	36, 57, 77, 113	0
1	B	521/530 (98%)	-0.05	7 (1%) 77 73	37, 57, 78, 116	0
1	C	521/530 (98%)	-0.01	3 (0%) 89 88	37, 59, 76, 111	0
1	D	521/530 (98%)	-0.05	5 (0%) 82 80	38, 57, 77, 117	0
1	E	521/530 (98%)	0.08	13 (2%) 57 51	35, 57, 77, 115	0
1	F	521/530 (98%)	-0.01	3 (0%) 89 88	40, 60, 76, 113	0
All	All	3126/3180 (98%)	-0.00	39 (1%) 79 76	35, 58, 77, 117	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	453	ILE	3.7
1	D	464	ASP	3.3
1	A	77	LEU	3.1
1	D	517	ARG	3.0
1	D	508	ARG	2.8
1	A	83	TYR	2.8
1	D	462	ALA	2.7
1	E	221	PHE	2.7
1	B	464	ASP	2.6
1	A	31	ALA	2.6
1	A	79	ALA	2.6
1	E	203	MET	2.5
1	B	508	ARG	2.5
1	E	200	THR	2.4
1	B	451	VAL	2.3
1	B	208	PRO	2.3
1	F	453	ILE	2.2
1	C	508	ARG	2.2
1	F	225	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	236	VAL	2.2
1	F	221	PHE	2.2
1	A	177	VAL	2.2
1	E	383	VAL	2.2
1	E	457	ARG	2.2
1	E	236	VAL	2.1
1	B	457	ARG	2.1
1	A	80	ASN	2.1
1	E	43	LYS	2.1
1	C	417	PHE	2.1
1	E	36	ALA	2.1
1	B	517	ARG	2.1
1	E	508	ARG	2.1
1	C	294	GLN	2.1
1	D	453	ILE	2.1
1	A	245	LYS	2.1
1	E	31	ALA	2.1
1	E	242	GLY	2.1
1	E	35	ARG	2.0
1	E	77	LEU	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.