



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:25 PM GMT

PDB ID : 1FFT  
Title : The structure of ubiquinol oxidase from Escherichia coli  
Authors : Abramson, J.; Riistama, S.; Larsson, G.; Jasaitis, A.; Svensson-Ek, M.; Puustinen, A.; Iwata, S.; Wikstrom, M.  
Deposited on : 2000-07-26  
Resolution : 3.50 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  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

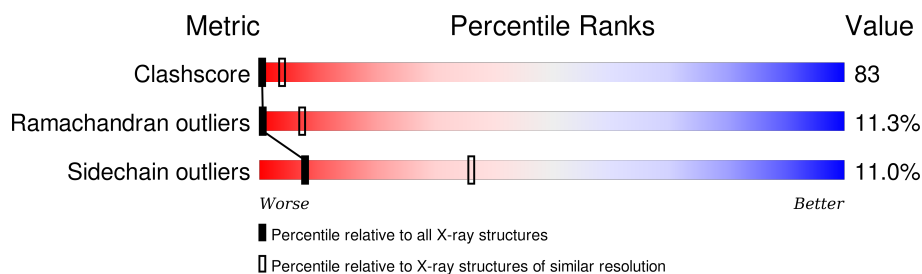
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.50 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))
Clashscore	102246	1157 (3.60-3.40)
Ramachandran outliers	100387	1120 (3.60-3.40)
Sidechain outliers	100360	1121 (3.60-3.40)


The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	663	
1	F	663	
2	B	315	
2	G	315	
3	C	204	
3	H	204	
4	D	109	

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Mol	Chain	Length	Quality of chain
4	I	109	 70% 30%

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 16136 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 UBIQUINOL OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	501	Total	C	N	O	S	312	0	0
			3954	2654	630	639	31			
1	F	501	Total	C	N	O	S	312	0	0
			3954	2654	630	639	31			

- Molecule 2 is a protein called UBIQUINOL OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	257	Total	C	N	O	S	155	0	0
			2015	1320	324	361	10			
2	G	257	Total	C	N	O	S	155	0	0
			2015	1320	324	361	10			

- Molecule 3 is a protein called UBIQUINOL OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	185	Total	C	N	O	S	157	0	0
			1451	970	229	240	12			
3	H	185	Total	C	N	O	S	157	0	0
			1451	970	229	240	12			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	1	MET	-	CLONING ARTIFACT	UNP P0ABJ3
C	2	ALA	-	CLONING ARTIFACT	UNP P0ABJ3
C	3	THR	-	CLONING ARTIFACT	UNP P0ABJ3
C	4	ASP	-	CLONING ARTIFACT	UNP P0ABJ3
C	5	THR	-	CLONING ARTIFACT	UNP P0ABJ3
C	6	LEU	-	CLONING ARTIFACT	UNP P0ABJ3
C	7	THR	-	CLONING ARTIFACT	UNP P0ABJ3
C	8	HIS	-	CLONING ARTIFACT	UNP P0ABJ3

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Chain	Residue	Modelled	Actual	Comment	Reference
C	9	ALA	-	CLONING ARTIFACT	UNP P0ABJ3
C	10	THR	-	CLONING ARTIFACT	UNP P0ABJ3
C	11	ALA	-	CLONING ARTIFACT	UNP P0ABJ3
C	12	HIS	-	CLONING ARTIFACT	UNP P0ABJ3
C	13	ALA	-	CLONING ARTIFACT	UNP P0ABJ3
C	14	HIS	-	CLONING ARTIFACT	UNP P0ABJ3
C	15	GLU	-	CLONING ARTIFACT	UNP P0ABJ3
C	16	HIS	-	CLONING ARTIFACT	UNP P0ABJ3
C	17	GLY	-	CLONING ARTIFACT	UNP P0ABJ3
C	18	HIS	-	CLONING ARTIFACT	UNP P0ABJ3
C	19	HIS	-	CLONING ARTIFACT	UNP P0ABJ3
C	20	ASP	-	CLONING ARTIFACT	UNP P0ABJ3
C	21	ALA	-	CLONING ARTIFACT	UNP P0ABJ3
C	22	GLY	-	CLONING ARTIFACT	UNP P0ABJ3
C	23	GLY	-	CLONING ARTIFACT	UNP P0ABJ3
C	24	THR	-	CLONING ARTIFACT	UNP P0ABJ3
H	1	MET	-	CLONING ARTIFACT	UNP P0ABJ3
H	2	ALA	-	CLONING ARTIFACT	UNP P0ABJ3
H	3	THR	-	CLONING ARTIFACT	UNP P0ABJ3
H	4	ASP	-	CLONING ARTIFACT	UNP P0ABJ3
H	5	THR	-	CLONING ARTIFACT	UNP P0ABJ3
H	6	LEU	-	CLONING ARTIFACT	UNP P0ABJ3
H	7	THR	-	CLONING ARTIFACT	UNP P0ABJ3
H	8	HIS	-	CLONING ARTIFACT	UNP P0ABJ3
H	9	ALA	-	CLONING ARTIFACT	UNP P0ABJ3
H	10	THR	-	CLONING ARTIFACT	UNP P0ABJ3
H	11	ALA	-	CLONING ARTIFACT	UNP P0ABJ3
H	12	HIS	-	CLONING ARTIFACT	UNP P0ABJ3
H	13	ALA	-	CLONING ARTIFACT	UNP P0ABJ3
H	14	HIS	-	CLONING ARTIFACT	UNP P0ABJ3
H	15	GLU	-	CLONING ARTIFACT	UNP P0ABJ3
H	16	HIS	-	CLONING ARTIFACT	UNP P0ABJ3
H	17	GLY	-	CLONING ARTIFACT	UNP P0ABJ3
H	18	HIS	-	CLONING ARTIFACT	UNP P0ABJ3
H	19	HIS	-	CLONING ARTIFACT	UNP P0ABJ3
H	20	ASP	-	CLONING ARTIFACT	UNP P0ABJ3
H	21	ALA	-	CLONING ARTIFACT	UNP P0ABJ3
H	22	GLY	-	CLONING ARTIFACT	UNP P0ABJ3
H	23	GLY	-	CLONING ARTIFACT	UNP P0ABJ3
H	24	THR	-	CLONING ARTIFACT	UNP P0ABJ3

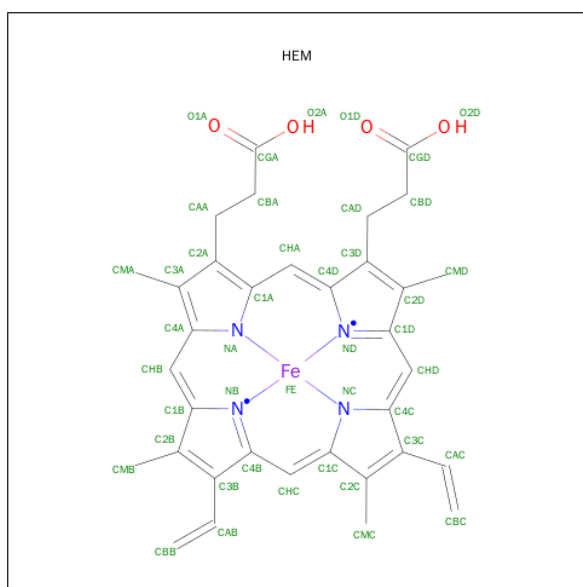
- Molecule 4 is a protein called UBIQUINOL OXIDASE.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	D	109	Total	C	N	O	0	0	0
			545	327	109	109			
4	I	109	Total	C	N	O	0	0	0
			545	327	109	109			

- Molecule 5 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

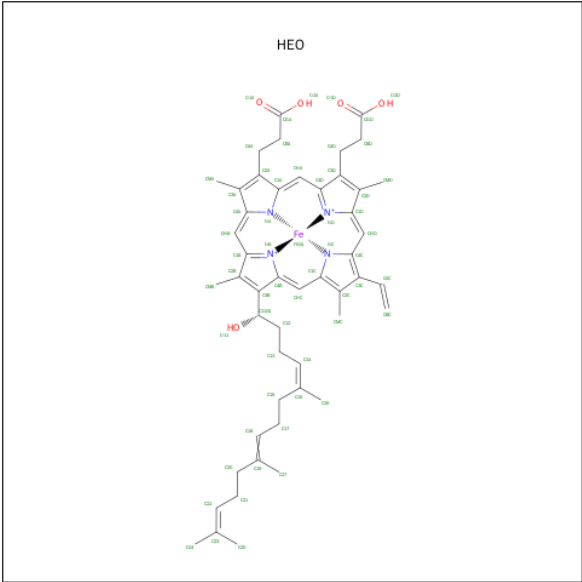
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Cu	0	0
			1	1		
5	F	1	Total	Cu	0	0
			1	1		

- Molecule 6 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	Fe	N	O	0
			43	34	1	4	4	0
6	F	1	Total	C	Fe	N	O	0
			43	34	1	4	4	0

- Molecule 7 is HEME O (three-letter code: HEO) (formula:  $C_{49}H_{58}FeN_4O_5$ ).



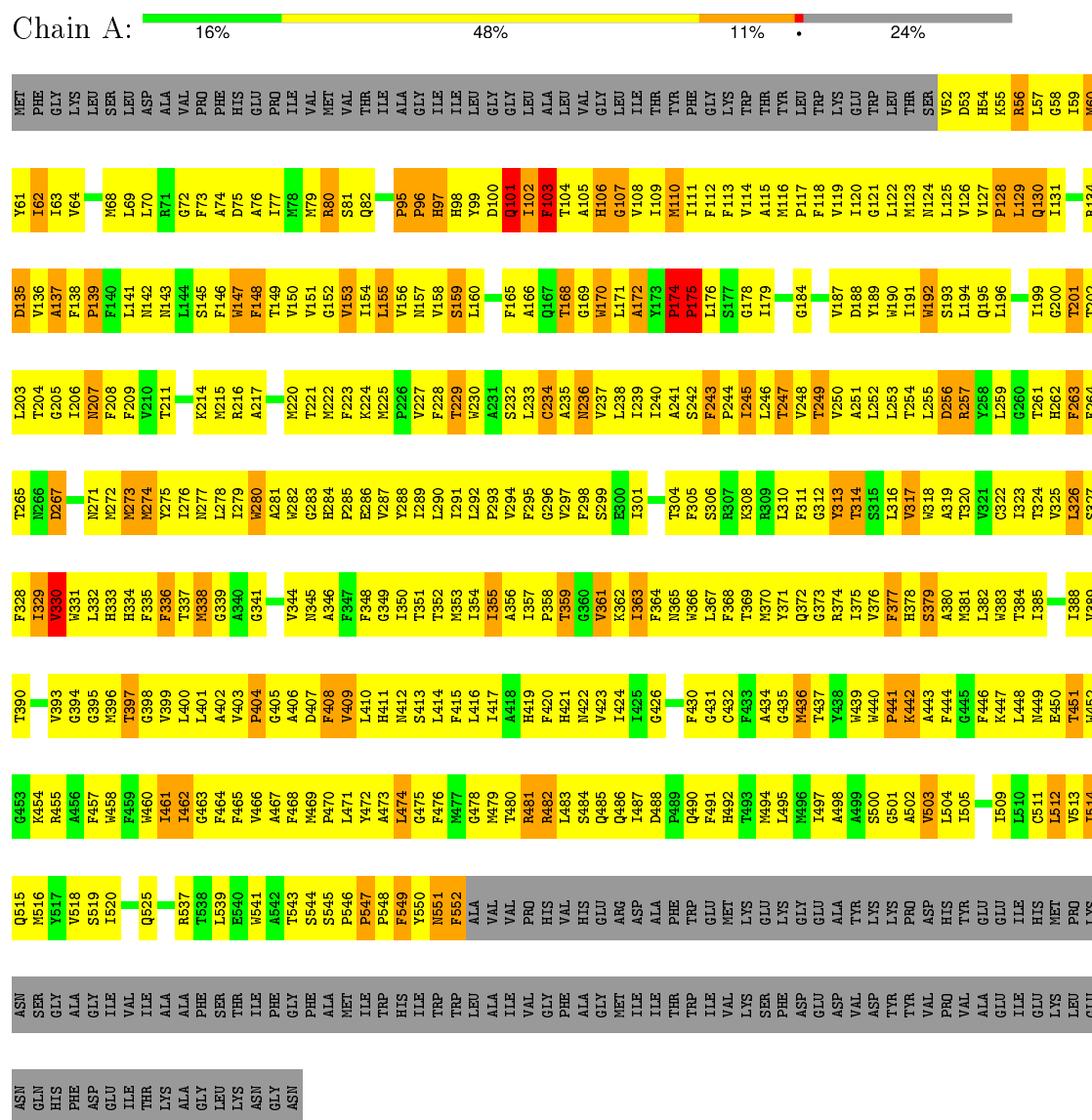
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	Fe	N	O	0	0
			59	49	1	4	5		
7	F	1	Total	C	Fe	N	O	0	0
			59	49	1	4	5		

### 3 Residue-property plots

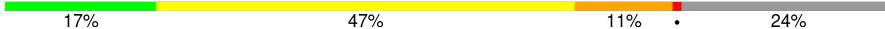
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

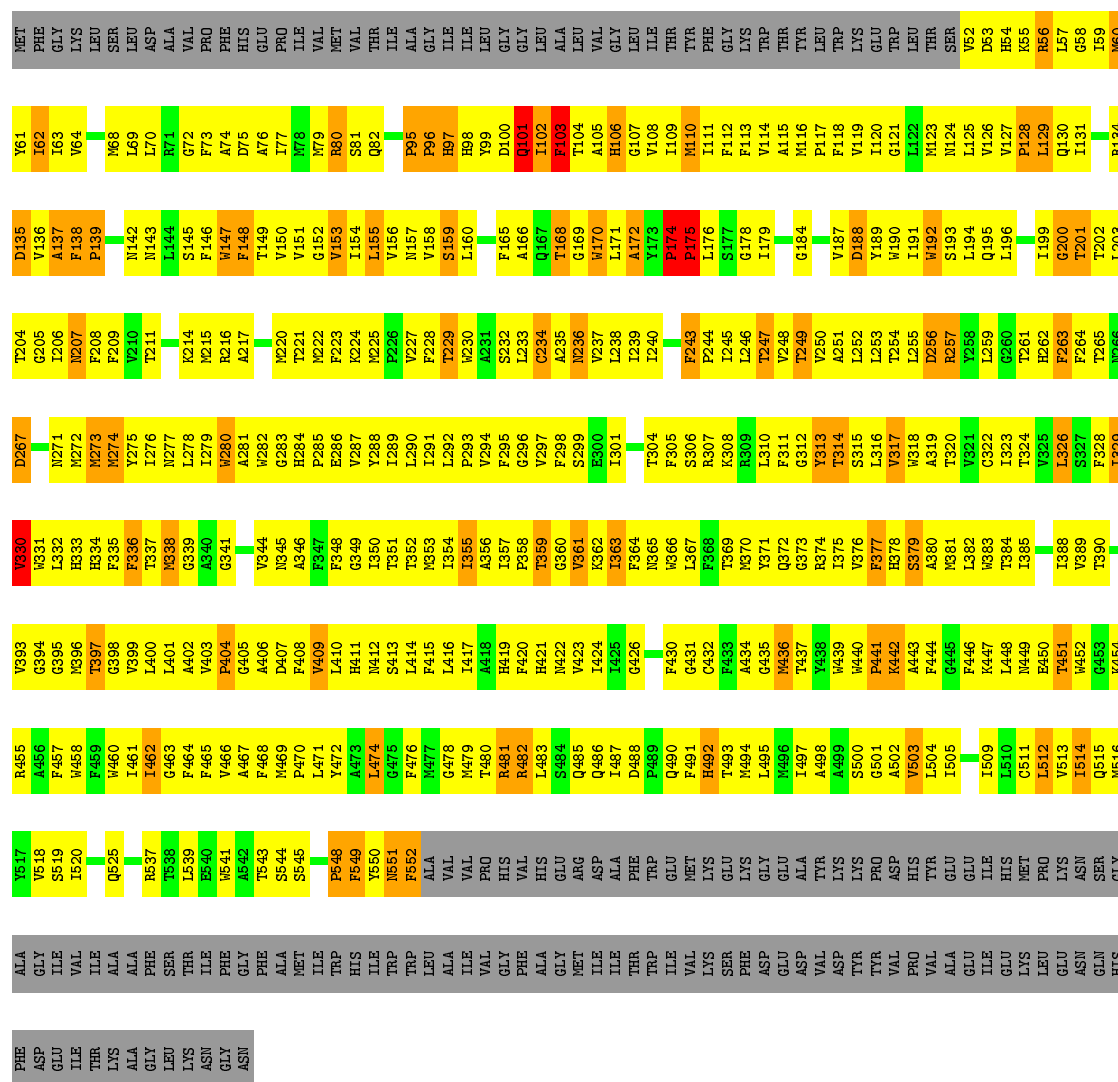
Note EDS was not executed.

#### • Molecule 1: UBIQUINOL OXIDASE




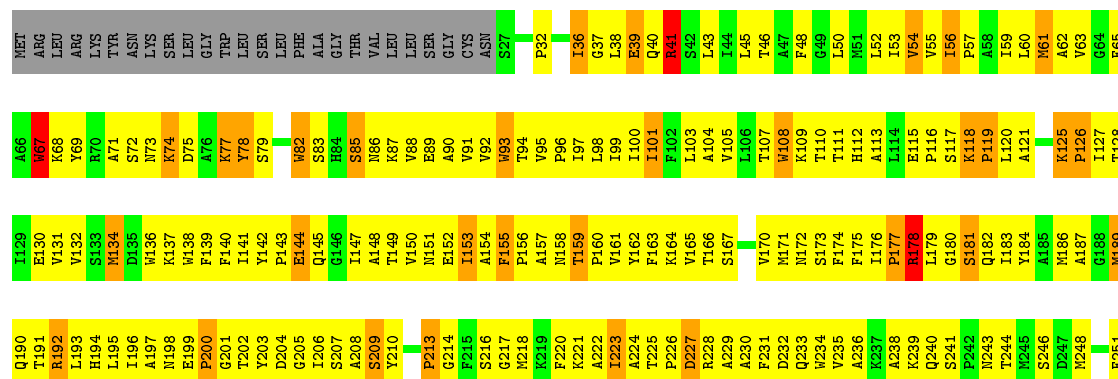


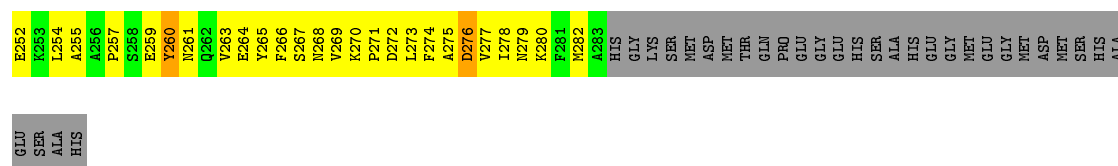
Chain F: 



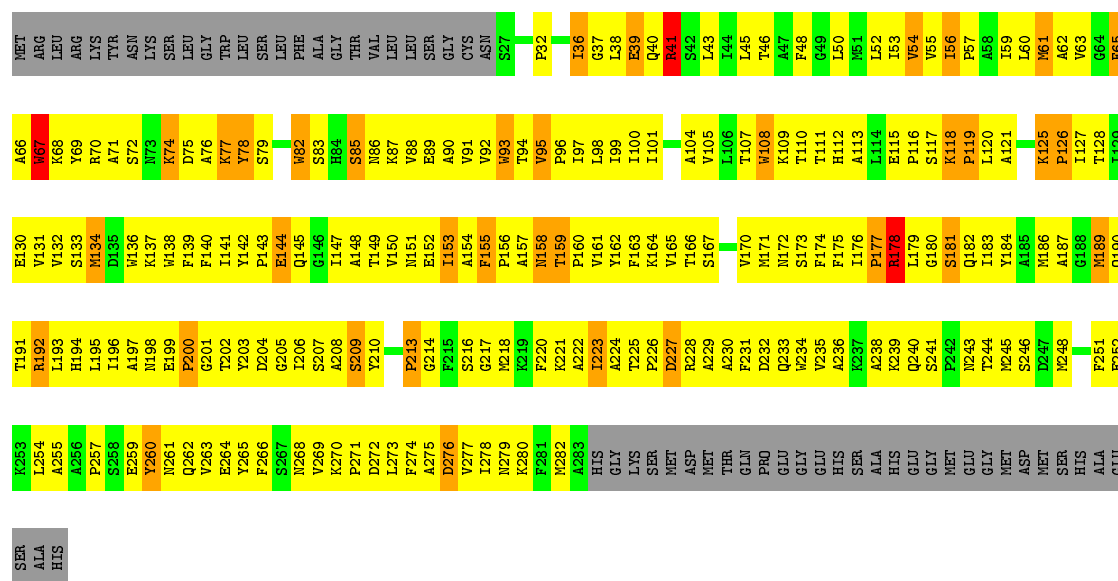
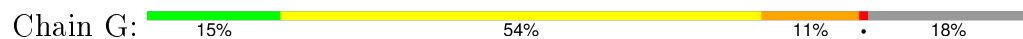
## • Molecule 2: UBIQUINOL OXIDASE

Chain B: 

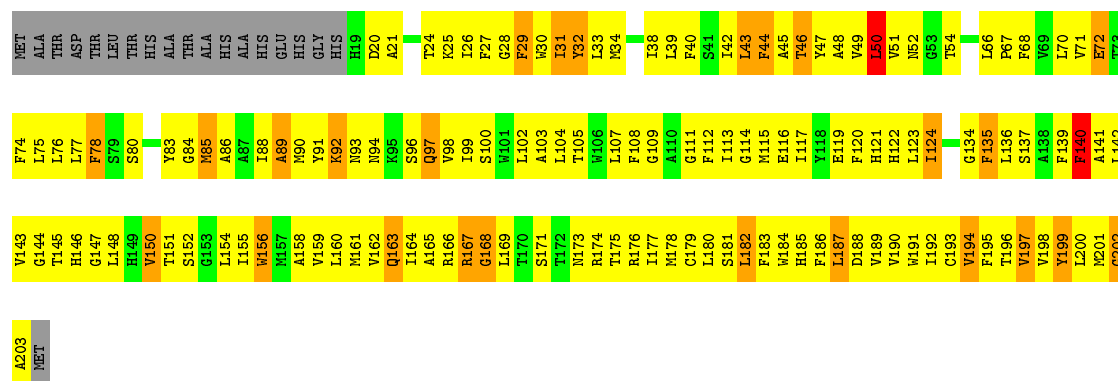




- Molecule 2: UBIQUINOL OXIDASE

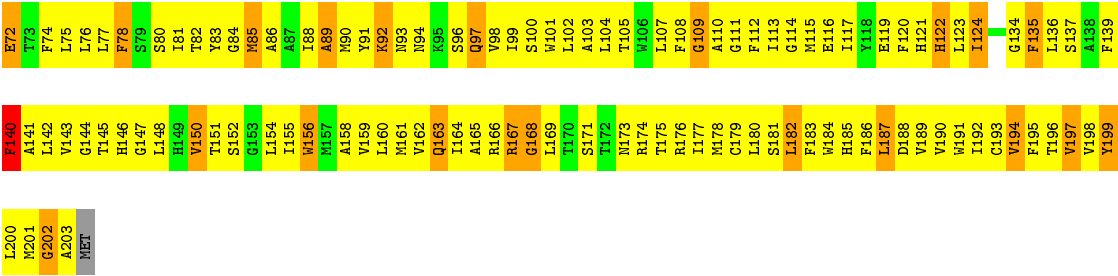


- Molecule 3: UBIQUINOL OXIDASE

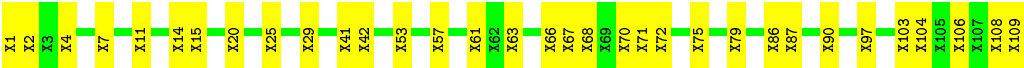


- Molecule 3: UBIQUINOL OXIDASE





● Molecule 4: UBIQUINOL OXIDASE



● Molecule 4: UBIQUINOL OXIDASE



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	92.10 Å   372.50 Å   232.70 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	40.00 – 3.50	Depositor
% Data completeness (in resolution range)	(Not available) (40.00-3.50)	Depositor
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	?	Depositor
R, $R_{free}$	(Not available) , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	16136	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, HEO, CU

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	0.46	1/4086 (0.0%)	0.71	4/5573 (0.1%)
1	F	0.44	0/4086	0.68	2/5573 (0.0%)
2	B	0.43	0/2074	0.65	0/2825
2	G	0.43	0/2074	0.67	0/2825
3	C	0.47	0/1494	0.66	0/2030
3	H	0.43	0/1494	0.65	0/2030
All	All	0.45	1/15308 (0.0%)	0.68	6/20856 (0.0%)

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

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	174	PRO	C-N	-9.24	1.16	1.34

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	174	PRO	C-N-CD	-12.28	93.59	120.60
1	A	175	PRO	CB-CA-C	7.79	131.48	112.00
1	F	175	PRO	CB-CA-C	7.42	130.56	112.00
1	F	174	PRO	C-N-CD	-6.30	106.74	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	547	PRO	CA-N-CD	-6.28	102.72	111.50
1	A	546	PRO	C-N-CD	-6.03	107.33	120.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	174	PRO	Mainchain
1	F	174	PRO	Mainchain

## 5.2 Too-close contacts [i](#)

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	3954	0	3975	658	0
1	F	3954	0	3975	661	0
2	B	2015	0	2016	317	0
2	G	2015	0	2016	348	0
3	C	1451	0	1458	254	0
3	H	1451	0	1458	265	0
4	D	545	0	114	57	0
4	I	545	0	115	55	0
5	A	1	0	0	0	0
5	F	1	0	0	0	0
6	A	43	0	30	18	0
6	F	43	0	30	17	0
7	A	59	0	56	16	0
7	F	59	0	56	14	0
All	All	16136	0	15299	2417	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 83.

All (2417) 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)
3:H:86:ALA:HB1	3:H:91:TYR:CD1	1.43	1.53
3:H:83:TYR:HE1	4:I:14:UNK:CB	1.44	1.30
3:C:78:PHE:HZ	4:D:57:UNK:CB	1.44	1.30
1:A:55:LYS:NZ	1:A:551:ASN:HA	1.44	1.29
3:C:78:PHE:CZ	4:D:57:UNK:CB	2.20	1.24
3:H:78:PHE:CZ	4:I:57:UNK:CB	2.21	1.24
3:H:83:TYR:CE1	4:I:14:UNK:CB	2.21	1.23
3:H:78:PHE:HZ	4:I:57:UNK:CB	1.54	1.20
3:C:30:TRP:CH2	4:D:79:UNK:HA	1.79	1.17
2:G:95:VAL:HG23	2:G:96:PRO:CD	1.73	1.16
3:H:86:ALA:CB	3:H:91:TYR:CD1	2.28	1.14
2:G:148:ALA:HB3	2:G:266:PHE:HB2	1.14	1.14
2:G:95:VAL:HG23	2:G:96:PRO:HD2	1.31	1.13
2:G:244:THR:HB	2:G:268:ASN:HB3	1.26	1.12
2:B:95:VAL:HG23	2:B:96:PRO:HD3	1.27	1.12
2:B:244:THR:HB	2:B:268:ASN:HB3	1.26	1.12
2:B:147:ILE:HG23	2:B:239:LYS:HE3	1.28	1.12
2:G:147:ILE:HG23	2:G:239:LYS:HE3	1.32	1.12
3:H:86:ALA:HB1	3:H:91:TYR:CG	1.86	1.11
2:B:148:ALA:HB3	2:B:266:PHE:HB2	1.13	1.10
1:A:551:ASN:O	1:A:552:PHE:O	1.69	1.08
3:C:30:TRP:CH2	4:D:79:UNK:CA	2.37	1.07
1:F:373:GLY:HA2	2:G:71:ALA:HB1	1.39	1.03
1:F:357:ILE:HG13	2:G:100:ILE:CD1	1.89	1.03
1:A:174:PRO:CB	1:A:175:PRO:HD3	1.87	1.01
1:F:308:LYS:HZ2	1:F:372:GLN:H	1.08	1.01
1:F:195:GLN:HE22	1:F:247:THR:HG22	1.26	1.00
1:F:474:LEU:HD21	1:F:494:MET:HB2	1.45	0.99
1:F:57:LEU:O	1:F:60:MET:HB2	1.63	0.99
1:A:57:LEU:O	1:A:60:MET:HB2	1.63	0.98
3:C:89:ALA:HB2	3:C:174:ARG:HD2	1.41	0.98
3:C:70:LEU:HD21	3:C:115:MET:HB2	1.44	0.98
3:H:86:ALA:HB1	3:H:91:TYR:CE1	1.98	0.98
1:F:357:ILE:HG13	2:G:100:ILE:HD11	1.46	0.97
3:H:89:ALA:HB2	3:H:174:ARG:HD2	1.45	0.97
1:A:195:GLN:HE22	1:A:247:THR:HG22	1.28	0.97
1:F:284:HIS:O	1:F:287:VAL:HG22	1.63	0.97
3:C:88:ILE:HG12	3:C:98:VAL:HG13	1.44	0.97
1:A:308:LYS:NZ	1:A:372:GLN:H	1.63	0.96
2:G:176:ILE:HG21	2:G:179:LEU:HD12	1.46	0.96
1:F:331:TRP:CZ2	4:I:97:UNK:CB	2.49	0.95
2:B:176:ILE:HG21	2:B:179:LEU:HD12	1.46	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:373:GLY:HA2	2:B:71:ALA:HB1	1.47	0.95
1:A:284:HIS:O	1:A:287:VAL:HG22	1.64	0.95
2:B:203:TYR:HB2	2:B:222:ALA:HB3	1.46	0.95
1:A:474:LEU:HD21	1:A:494:MET:HB2	1.49	0.95
3:H:86:ALA:CB	3:H:91:TYR:CE1	2.48	0.95
2:G:203:TYR:HB2	2:G:222:ALA:HB3	1.46	0.94
3:H:70:LEU:HD21	3:H:115:MET:HB2	1.47	0.94
3:H:104:LEU:HA	3:H:107:LEU:HD12	1.49	0.93
4:I:1:UNK:H	4:I:4:UNK:CB	1.80	0.93
4:D:1:UNK:H	4:D:4:UNK:CB	1.80	0.93
1:A:159:SER:HA	1:A:189:TYR:HD1	1.32	0.93
4:I:1:UNK:N	4:I:4:UNK:CB	2.32	0.92
2:G:95:VAL:HG23	2:G:96:PRO:HD3	1.51	0.92
4:D:1:UNK:N	4:D:4:UNK:CB	2.32	0.92
1:F:55:LYS:NZ	1:F:551:ASN:HA	1.85	0.91
3:C:169:LEU:HD23	3:C:174:ARG:HA	1.52	0.91
1:A:308:LYS:HZ2	1:A:372:GLN:H	1.08	0.91
1:F:308:LYS:NZ	1:F:372:GLN:H	1.67	0.91
3:C:30:TRP:HH2	4:D:79:UNK:HA	1.32	0.91
2:G:162:TYR:HA	2:G:194:HIS:CD2	2.06	0.91
1:F:234:CYS:SG	1:F:320:THR:HG22	2.11	0.90
2:G:97:ILE:O	2:G:101:ILE:HG13	1.71	0.90
1:A:424:ILE:HG21	6:A:1001:HEM:HAC	1.54	0.90
1:F:424:ILE:HG21	6:F:1001:HEM:HAC	1.54	0.90
1:F:399:VAL:HG11	7:F:1002:HEO:H252	1.54	0.90
2:B:162:TYR:HA	2:B:194:HIS:CD2	2.07	0.89
3:C:109:GLY:O	3:C:113:ILE:HD13	1.73	0.89
1:A:55:LYS:HZ1	1:A:551:ASN:HA	1.32	0.89
7:F:1002:HEO:H201	2:G:56:ILE:HG21	1.53	0.89
3:H:40:PHE:CD1	3:H:190:VAL:HG11	2.08	0.89
1:A:374:ARG:HB3	2:B:79:SER:HB3	1.53	0.89
3:C:40:PHE:CD1	3:C:190:VAL:HG11	2.08	0.88
1:A:214:LYS:NZ	3:C:24:THR:HA	1.88	0.88
2:G:244:THR:CB	2:G:268:ASN:HB3	2.03	0.88
2:B:244:THR:CB	2:B:268:ASN:HB3	2.03	0.88
3:H:169:LEU:HD23	3:H:174:ARG:HA	1.55	0.88
3:C:160:LEU:HD13	3:C:176:ARG:HD3	1.53	0.88
1:A:237:VAL:HA	1:A:240:ILE:HD12	1.54	0.87
3:C:104:LEU:HA	3:C:107:LEU:HD12	1.54	0.87
1:F:159:SER:HA	1:F:189:TYR:HD1	1.37	0.87
3:H:88:ILE:HA	3:H:98:VAL:HG22	1.56	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:PRO:HB2	1:A:175:PRO:HD3	1.56	0.87
1:A:515:GLN:HG3	1:A:516:MET:N	1.89	0.87
2:B:147:ILE:CG2	2:B:239:LYS:HE3	2.04	0.87
3:H:160:LEU:HD13	3:H:176:ARG:HD3	1.53	0.87
2:B:100:ILE:O	2:B:101:ILE:HG13	1.73	0.87
3:C:88:ILE:HA	3:C:98:VAL:HG22	1.56	0.87
1:A:178:GLY:HA2	1:A:257:ARG:HG2	1.57	0.87
3:H:88:ILE:HG12	3:H:98:VAL:HG13	1.57	0.86
1:F:225:MET:HE1	1:F:233:LEU:HD11	1.56	0.86
1:A:205:GLY:HA2	1:A:236:ASN:OD1	1.76	0.86
1:A:108:VAL:HG22	1:A:170:TRP:HA	1.57	0.86
1:F:395:GLY:HA3	7:F:1002:H2O:H162	1.57	0.86
1:F:205:GLY:HA2	1:F:236:ASN:OD1	1.76	0.86
1:F:515:GLN:HG3	1:F:516:MET:N	1.90	0.86
1:A:331:TRP:CZ2	4:D:97:UNK:CB	2.59	0.85
1:F:237:VAL:HA	1:F:240:ILE:HD12	1.57	0.85
1:F:108:VAL:HG22	1:F:170:TRP:HA	1.58	0.85
1:A:225:MET:HE1	1:A:233:LEU:HD11	1.56	0.85
1:F:178:GLY:HA2	1:F:257:ARG:HG2	1.58	0.85
2:G:264:GLU:HG2	2:G:265:TYR:H	1.41	0.85
1:A:159:SER:HA	1:A:189:TYR:CD1	2.12	0.85
1:A:248:VAL:HG22	3:C:39:LEU:HD12	1.59	0.85
1:A:301:ILE:HD11	1:A:435:GLY:HA2	1.58	0.85
1:A:55:LYS:HZ3	1:A:551:ASN:HA	1.05	0.84
1:A:55:LYS:NZ	1:A:551:ASN:CA	2.36	0.84
3:C:45:ALA:O	3:C:49:VAL:HG23	1.76	0.84
1:A:216:ARG:NH1	1:A:222:MET:HA	1.92	0.84
1:F:174:PRO:CB	1:F:175:PRO:HD3	2.07	0.84
2:G:147:ILE:CG2	2:G:239:LYS:HE3	2.06	0.84
1:A:98:HIS:O	1:A:102:ILE:HG13	1.78	0.83
1:F:168:THR:HB	1:F:172:ALA:HA	1.60	0.83
2:B:126:PRO:HB3	2:B:160:PRO:HB2	1.60	0.83
2:B:195:LEU:HD23	2:B:196:ILE:N	1.93	0.83
1:F:195:GLN:HE22	1:F:247:THR:CG2	1.91	0.83
2:B:264:GLU:HG2	2:B:265:TYR:H	1.43	0.83
1:A:306:SER:HA	1:A:375:ILE:HA	1.59	0.83
1:F:157:ASN:HA	1:F:160:LEU:HD12	1.58	0.83
1:F:301:ILE:HD11	1:F:435:GLY:HA2	1.58	0.83
2:B:93:TRP:O	2:B:96:PRO:HD2	1.79	0.83
2:G:142:TYR:HB3	2:G:145:GLN:HB2	1.60	0.83
1:F:306:SER:HA	1:F:375:ILE:HA	1.59	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:376:VAL:O	1:A:381:MET:HG2	1.79	0.83
1:F:357:ILE:HD11	2:G:100:ILE:HD12	1.59	0.82
1:F:137:ALA:O	1:F:139:PRO:HD3	1.78	0.82
1:A:195:GLN:HE22	1:A:247:THR:CG2	1.91	0.82
1:A:69:LEU:HG	1:A:114:VAL:HG11	1.61	0.82
2:G:195:LEU:HD23	2:G:196:ILE:N	1.94	0.82
1:A:228:PHE:HA	1:A:296:GLY:HA3	1.61	0.82
3:H:72:GLU:OE1	3:H:75:LEU:HD23	1.80	0.82
3:H:156:TRP:NE1	3:H:180:LEU:HD22	1.94	0.82
1:A:157:ASN:HA	1:A:160:LEU:HD12	1.58	0.82
2:B:41:ARG:H	2:B:41:ARG:HD2	1.42	0.82
3:H:45:ALA:O	3:H:49:VAL:HG23	1.79	0.82
1:F:232:SER:O	1:F:236:ASN:HB2	1.80	0.82
2:B:142:TYR:HB3	2:B:145:GLN:HB2	1.60	0.82
3:H:159:VAL:O	3:H:162:VAL:HG12	1.79	0.82
1:F:55:LYS:HZ3	1:F:551:ASN:HA	1.43	0.82
2:B:90:ALA:HA	2:B:93:TRP:HB2	1.62	0.81
1:F:159:SER:HA	1:F:189:TYR:CD1	2.15	0.81
1:F:216:ARG:NH1	1:F:222:MET:HA	1.95	0.81
3:H:90:MET:CE	4:I:67:UNK:CB	2.58	0.81
1:F:228:PHE:HA	1:F:296:GLY:HA3	1.62	0.81
1:F:170:TRP:CZ2	1:F:171:LEU:HD21	2.15	0.81
1:F:373:GLY:HA2	2:G:71:ALA:CB	2.10	0.81
3:C:96:SER:HA	3:C:99:ILE:HD13	1.60	0.81
1:A:234:CYS:SG	1:A:320:THR:HG22	2.21	0.81
1:F:353:MET:HG2	1:F:402:ALA:HB1	1.62	0.81
1:A:395:GLY:HA3	7:A:1002:HEO:H162	1.63	0.81
1:A:480:THR:O	1:A:483:LEU:HG	1.81	0.81
2:G:90:ALA:HA	2:G:93:TRP:HB2	1.64	0.80
1:F:69:LEU:HG	1:F:114:VAL:HG11	1.63	0.80
2:B:192:ARG:HB2	2:B:192:ARG:NH1	1.96	0.80
1:F:357:ILE:CD1	2:G:100:ILE:HD12	2.11	0.80
1:A:175:PRO:O	1:A:179:ILE:HD12	1.81	0.80
1:A:232:SER:O	1:A:236:ASN:HB2	1.81	0.80
1:F:276:ILE:HD13	1:F:338:MET:SD	2.21	0.80
2:G:41:ARG:H	2:G:41:ARG:HD2	1.44	0.80
1:F:357:ILE:CG1	2:G:100:ILE:HD12	2.11	0.80
2:G:192:ARG:NH1	2:G:192:ARG:HB2	1.96	0.80
3:H:189:VAL:O	3:H:192:ILE:HG22	1.81	0.80
3:H:78:PHE:CE1	4:I:57:UNK:CB	2.65	0.80
1:F:249:THR:HG23	1:F:278:LEU:HD12	1.62	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:96:SER:HA	3:H:99:ILE:HD13	1.62	0.80
1:F:331:TRP:HZ2	4:I:97:UNK:CB	1.95	0.80
2:G:126:PRO:HB3	2:G:160:PRO:HB2	1.64	0.80
3:C:185:HIS:CE1	4:D:61:UNK:CB	2.64	0.79
1:F:98:HIS:O	1:F:102:ILE:HG13	1.82	0.79
3:C:159:VAL:O	3:C:162:VAL:HG12	1.82	0.79
2:G:254:LEU:O	2:G:254:LEU:HD13	1.82	0.79
1:A:399:VAL:HG11	7:A:1002:HEO:H252	1.65	0.79
1:F:104:THR:O	1:F:108:VAL:HG23	1.82	0.79
3:H:75:LEU:HD21	4:I:21:UNK:CB	2.13	0.79
2:B:95:VAL:CG2	2:B:96:PRO:HD3	2.09	0.79
2:G:36:ILE:HD11	2:G:38:LEU:HB2	1.64	0.79
1:A:126:VAL:HG11	1:A:439:TRP:CZ2	2.16	0.78
2:G:217:GLY:HA3	2:G:260:TYR:CZ	2.18	0.78
1:A:452:TRP:HA	1:A:455:ARG:HD2	1.64	0.78
1:A:104:THR:O	1:A:108:VAL:HG23	1.82	0.78
2:B:36:ILE:HD11	2:B:38:LEU:HB2	1.64	0.78
3:C:89:ALA:CB	3:C:174:ARG:HD2	2.13	0.78
1:A:249:THR:HG23	1:A:278:LEU:HD12	1.63	0.78
3:H:89:ALA:CB	3:H:174:ARG:HD2	2.14	0.78
3:H:174:ARG:HB3	3:H:177:ILE:HD11	1.66	0.78
1:A:353:MET:HG2	1:A:402:ALA:HB1	1.64	0.78
1:A:159:SER:HB2	1:A:165:PHE:HD1	1.47	0.78
1:F:214:LYS:HE3	3:H:24:THR:HG23	1.66	0.78
2:B:217:GLY:HA3	2:B:260:TYR:CZ	2.18	0.78
3:H:91:TYR:OH	4:I:7:UNK:HA	1.83	0.78
3:C:72:GLU:OE1	3:C:75:LEU:HD23	1.84	0.78
2:G:270:LYS:HE3	2:G:276:ASP:OD1	1.83	0.78
3:C:30:TRP:CH2	4:D:79:UNK:O	2.36	0.78
1:F:214:LYS:NZ	3:H:24:THR:HA	1.99	0.78
1:A:441:PRO:HG3	1:A:447:LYS:HA	1.64	0.77
1:A:137:ALA:O	1:A:139:PRO:HD3	1.82	0.77
2:G:87:LYS:O	2:G:91:VAL:HG23	1.83	0.77
1:A:409:VAL:HG13	2:B:180:GLY:HA2	1.66	0.77
1:A:206:ILE:HG23	3:C:31:ILE:CG2	2.14	0.77
3:H:156:TRP:HE1	3:H:180:LEU:HD22	1.50	0.77
1:A:55:LYS:HZ3	1:A:551:ASN:CA	1.94	0.77
1:F:58:GLY:HA2	1:F:124:ASN:HD22	1.49	0.77
1:F:446:PHE:HZ	1:F:520:ILE:HG12	1.48	0.77
1:A:168:THR:HB	1:A:172:ALA:HA	1.65	0.77
1:A:316:LEU:HD23	1:A:361:VAL:HG12	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:165:VAL:HB	2:B:191:THR:OG1	1.84	0.77
1:F:357:ILE:CG1	2:G:100:ILE:CD1	2.63	0.77
1:F:126:VAL:HG11	1:F:439:TRP:CZ2	2.18	0.77
1:F:409:VAL:HG13	2:G:180:GLY:HA2	1.65	0.77
1:A:214:LYS:HE3	3:C:24:THR:HG23	1.65	0.77
3:C:189:VAL:O	3:C:192:ILE:HG22	1.84	0.77
2:B:175:PHE:CD1	2:B:182:GLN:HB2	2.20	0.77
1:A:339:GLY:O	4:D:104:UNK:CB	2.33	0.77
1:F:389:VAL:HG13	2:G:61:MET:HE1	1.65	0.77
1:F:159:SER:CA	1:F:189:TYR:HD1	1.97	0.77
1:A:446:PHE:HZ	1:A:520:ILE:HG12	1.48	0.77
2:B:87:LYS:O	2:B:91:VAL:HG23	1.84	0.76
1:F:480:THR:O	1:F:483:LEU:HG	1.85	0.76
1:F:110:MET:HB3	6:F:1001:HEM:HBC2	1.67	0.76
1:F:316:LEU:HD23	1:F:361:VAL:HG12	1.65	0.76
3:C:85:MET:HE1	3:C:178:MET:HG3	1.65	0.76
1:A:544:SER:O	1:A:547:PRO:HD3	1.85	0.76
1:A:389:VAL:HG13	2:B:61:MET:HE1	1.66	0.76
1:F:308:LYS:NZ	1:F:372:GLN:HB2	2.00	0.76
1:A:58:GLY:HA2	1:A:124:ASN:HD22	1.49	0.76
2:G:36:ILE:HG12	2:G:39:GLU:H	1.50	0.76
3:C:156:TRP:NE1	3:C:180:LEU:HD22	2.00	0.76
1:A:308:LYS:NZ	1:A:372:GLN:HB2	2.00	0.76
1:F:400:LEU:HD22	2:G:50:LEU:HD21	1.68	0.76
1:F:376:VAL:O	1:F:381:MET:HG2	1.85	0.76
3:C:77:LEU:HD21	3:C:108:PHE:HB2	1.66	0.76
3:H:77:LEU:HA	3:H:80:SER:HB3	1.67	0.76
2:B:270:LYS:HE3	2:B:276:ASP:OD1	1.84	0.76
3:H:90:MET:HE1	4:I:67:UNK:C	2.15	0.75
1:F:57:LEU:HD23	1:F:60:MET:HG3	1.67	0.75
1:F:110:MET:CB	6:F:1001:HEM:HBC2	2.16	0.75
2:B:67:TRP:C	2:B:69:TYR:H	1.89	0.75
1:F:452:TRP:HA	1:F:455:ARG:HD2	1.67	0.75
3:C:30:TRP:CH2	4:D:79:UNK:C	2.69	0.75
1:A:57:LEU:HD23	1:A:60:MET:HG3	1.67	0.75
2:G:67:TRP:C	2:G:69:TYR:H	1.89	0.75
2:G:175:PHE:CD1	2:G:182:GLN:HB2	2.22	0.75
1:A:214:LYS:CE	3:C:24:THR:HG23	2.16	0.75
3:H:90:MET:CE	4:I:67:UNK:C	2.65	0.75
3:H:50:LEU:HD11	3:H:134:GLY:HA3	1.68	0.75
1:F:246:LEU:HD22	1:F:282:TRP:CH2	2.22	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:138:TRP:HZ3	2:G:174:PHE:HD1	1.33	0.74
1:A:159:SER:CA	1:A:189:TYR:HD1	1.98	0.74
1:A:112:PHE:HD2	1:A:194:LEU:HD22	1.51	0.74
2:B:254:LEU:O	2:B:254:LEU:HD13	1.87	0.74
3:C:30:TRP:CH2	4:D:79:UNK:CB	2.69	0.74
2:B:193:LEU:HD23	2:B:194:HIS:N	2.02	0.74
1:F:168:THR:HG23	1:F:176:LEU:HB3	1.68	0.74
3:C:197:VAL:O	3:C:201:MET:HB3	1.87	0.74
2:G:173:SER:N	2:G:208:ALA:HB2	2.02	0.74
1:F:211:THR:HG23	1:F:215:MET:HE3	1.69	0.74
1:F:70:LEU:HD23	1:F:70:LEU:O	1.87	0.74
3:H:99:ILE:N	3:H:99:ILE:HD12	2.03	0.74
1:A:405:GLY:HA2	1:A:408:PHE:CD1	2.23	0.74
1:F:441:PRO:HG3	1:F:447:LYS:HA	1.67	0.74
3:C:50:LEU:HD11	3:C:134:GLY:HA3	1.69	0.74
1:A:110:MET:CB	6:A:1001:HEM:HBC2	2.17	0.74
2:B:175:PHE:HA	2:B:181:SER:O	1.87	0.74
2:G:161:VAL:HG23	2:G:195:LEU:O	1.87	0.74
2:B:184:TYR:CE2	2:B:186:MET:HB2	2.23	0.74
2:G:162:TYR:HA	2:G:194:HIS:HD2	1.50	0.74
2:B:36:ILE:HG12	2:B:39:GLU:H	1.52	0.73
3:H:30:TRP:CH2	4:I:79:UNK:HA	2.23	0.73
1:A:331:TRP:HZ2	4:D:97:UNK:CB	2.00	0.73
1:F:73:PHE:HB3	1:F:77:ILE:HD11	1.69	0.73
2:G:184:TYR:CE2	2:G:186:MET:HB2	2.23	0.73
2:G:193:LEU:HD23	2:G:194:HIS:N	2.02	0.73
2:G:95:VAL:CG2	2:G:96:PRO:HD2	2.15	0.73
3:C:77:LEU:HA	3:C:80:SER:HB3	1.70	0.73
1:A:246:LEU:HD22	1:A:282:TRP:CH2	2.24	0.73
2:B:138:TRP:HZ3	2:B:174:PHE:HD1	1.34	0.73
1:A:110:MET:HB3	6:A:1001:HEM:HBC2	1.70	0.73
3:H:40:PHE:HD1	3:H:190:VAL:HG11	1.50	0.73
1:F:112:PHE:HD2	1:F:194:LEU:HD22	1.52	0.73
1:A:397:THR:HB	1:A:419:HIS:HD1	1.54	0.73
3:H:78:PHE:HZ	4:I:57:UNK:CA	2.01	0.73
1:F:405:GLY:HA2	1:F:408:PHE:CD1	2.23	0.73
2:G:175:PHE:HA	2:G:181:SER:O	1.88	0.73
3:C:174:ARG:HB3	3:C:177:ILE:HD11	1.71	0.73
1:A:276:ILE:HD13	1:A:338:MET:SD	2.28	0.73
3:H:75:LEU:CD2	4:I:21:UNK:CB	2.66	0.73
1:A:349:GLY:O	1:A:353:MET:HG3	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:54:VAL:HA	2:B:57:PRO:CG	2.19	0.73
3:H:197:VAL:O	3:H:201:MET:HB3	1.88	0.73
1:A:221:THR:HG23	1:A:224:LYS:HE3	1.71	0.73
3:C:78:PHE:CE1	4:D:57:UNK:CB	2.72	0.73
1:A:308:LYS:NZ	1:A:372:GLN:N	2.37	0.73
3:C:196:THR:HA	3:C:200:LEU:HD21	1.69	0.73
3:C:40:PHE:HD1	3:C:190:VAL:HG11	1.53	0.73
1:A:111:ILE:HD12	1:A:170:TRP:CE3	2.24	0.72
1:A:482:ARG:NE	6:A:1001:HEM:O1D	2.22	0.72
3:C:197:VAL:HG13	3:C:198:VAL:N	2.04	0.72
2:G:54:VAL:HA	2:G:57:PRO:CG	2.19	0.72
2:G:132:VAL:HG12	2:G:134:MET:SD	2.29	0.72
3:C:30:TRP:HH2	4:D:79:UNK:CA	1.92	0.72
2:G:165:VAL:HB	2:G:191:THR:OG1	1.89	0.72
7:A:1002:HEO:C26	7:A:1002:HEO:H273	2.19	0.72
1:A:201:THR:O	1:A:239:ILE:HG21	1.89	0.72
2:G:95:VAL:CG2	2:G:96:PRO:CD	2.63	0.72
1:F:308:LYS:NZ	1:F:372:GLN:N	2.38	0.72
3:C:144:GLY:O	3:C:148:LEU:HG	1.90	0.72
1:A:174:PRO:CB	1:A:175:PRO:CD	2.65	0.72
1:F:367:LEU:HD13	2:G:63:VAL:HG11	1.70	0.72
2:B:173:SER:N	2:B:208:ALA:HB2	2.05	0.72
1:F:227:VAL:HG11	1:F:299:SER:OG	1.89	0.72
3:H:197:VAL:HG13	3:H:198:VAL:N	2.05	0.72
2:B:101:ILE:O	2:B:105:VAL:HG23	1.90	0.72
1:F:367:LEU:HA	1:F:370:MET:HE3	1.72	0.72
1:F:482:ARG:NE	6:F:1001:HEM:O1D	2.22	0.72
3:C:99:ILE:HD12	3:C:99:ILE:N	2.05	0.72
1:F:406:ALA:HB2	2:G:45:LEU:HD22	1.72	0.72
2:G:36:ILE:HG23	2:G:39:GLU:CD	2.10	0.72
1:F:446:PHE:CZ	1:F:520:ILE:HG12	2.24	0.72
1:A:70:LEU:HD23	1:A:70:LEU:O	1.90	0.72
1:A:308:LYS:CE	1:A:372:GLN:HB2	2.20	0.71
1:A:214:LYS:HZ2	3:C:24:THR:HA	1.53	0.71
1:F:58:GLY:CA	1:F:124:ASN:HD22	2.02	0.71
1:F:138:PHE:HZ	3:H:28:GLY:HA3	1.55	0.71
3:H:77:LEU:HD21	3:H:108:PHE:HB2	1.72	0.71
7:F:1002:HEO:C26	7:F:1002:HEO:H273	2.20	0.71
1:F:308:LYS:HZ2	1:F:372:GLN:N	1.87	0.71
1:F:308:LYS:CE	1:F:372:GLN:HB2	2.21	0.71
3:C:90:MET:HE2	4:D:68:UNK:N	2.04	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:164:ILE:O	3:C:168:GLY:HA2	1.90	0.71
3:C:156:TRP:HE1	3:C:180:LEU:HD13	1.55	0.71
3:H:78:PHE:CE2	3:H:185:HIS:HE1	2.08	0.71
2:G:246:SER:OG	2:G:268:ASN:ND2	2.24	0.71
2:B:161:VAL:HG23	2:B:195:LEU:O	1.90	0.71
3:H:30:TRP:CZ2	4:I:79:UNK:O	2.43	0.71
1:F:201:THR:O	1:F:239:ILE:HG21	1.90	0.71
3:H:196:THR:HA	3:H:200:LEU:HD21	1.73	0.71
1:A:58:GLY:CA	1:A:124:ASN:HD22	2.03	0.71
1:F:292:LEU:HB2	1:F:293:PRO:HD3	1.73	0.71
2:B:235:VAL:O	2:B:239:LYS:HG2	1.90	0.71
2:G:97:ILE:O	2:G:101:ILE:CG1	2.39	0.71
1:F:159:SER:HB2	1:F:165:PHE:HD1	1.56	0.71
2:G:235:VAL:O	2:G:239:LYS:HG2	1.90	0.71
2:B:139:PHE:CE1	2:B:148:ALA:HB1	2.26	0.71
2:G:203:TYR:O	2:G:221:LYS:HA	1.91	0.71
1:A:447:LYS:HG3	1:A:448:LEU:H	1.55	0.71
1:F:397:THR:HB	1:F:419:HIS:HD1	1.56	0.71
1:A:168:THR:HG23	1:A:176:LEU:HB3	1.72	0.70
1:A:292:LEU:HB2	1:A:293:PRO:HD3	1.73	0.70
1:A:227:VAL:HG12	1:A:296:GLY:HA2	1.73	0.70
1:F:481:ARG:HG2	1:F:482:ARG:HG3	1.72	0.70
2:B:147:ILE:HD13	2:B:235:VAL:HA	1.73	0.70
3:H:156:TRP:HE1	3:H:180:LEU:HD13	1.56	0.70
1:F:221:THR:HG23	1:F:224:LYS:HE3	1.73	0.70
1:A:73:PHE:HB3	1:A:77:ILE:HD11	1.73	0.70
2:B:203:TYR:O	2:B:221:LYS:HA	1.91	0.70
1:A:446:PHE:CZ	1:A:520:ILE:HG12	2.25	0.70
1:F:276:ILE:HG22	1:F:335:PHE:CZ	2.27	0.70
2:G:147:ILE:HD13	2:G:235:VAL:HA	1.74	0.70
3:H:158:ALA:O	3:H:161:MET:HB3	1.91	0.70
2:B:45:LEU:HD12	2:B:110:THR:HG21	1.74	0.70
3:C:78:PHE:HZ	4:D:57:UNK:CA	2.05	0.70
1:A:276:ILE:HG22	1:A:335:PHE:CZ	2.27	0.70
2:B:148:ALA:HB3	2:B:266:PHE:CB	2.07	0.70
2:G:125:LYS:H	2:G:126:PRO:CD	2.03	0.70
1:A:227:VAL:HG11	1:A:299:SER:OG	1.91	0.70
2:B:36:ILE:HG23	2:B:39:GLU:CD	2.12	0.70
1:F:225:MET:HE1	1:F:233:LEU:CD1	2.22	0.70
3:C:158:ALA:O	3:C:161:MET:HB3	1.91	0.70
1:F:257:ARG:HH11	1:F:257:ARG:CB	2.04	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:414:LEU:HD12	1:A:471:LEU:HB3	1.74	0.70
3:C:30:TRP:CZ2	4:D:79:UNK:O	2.45	0.69
2:G:45:LEU:HD12	2:G:110:THR:HG21	1.74	0.69
1:F:414:LEU:HD12	1:F:471:LEU:HB3	1.74	0.69
1:A:227:VAL:HG21	1:A:310:LEU:HD22	1.74	0.69
2:B:162:TYR:HA	2:B:194:HIS:HD2	1.53	0.69
3:C:156:TRP:HE1	3:C:180:LEU:HD22	1.56	0.69
1:F:239:ILE:CG1	1:F:289:ILE:HD13	2.22	0.69
1:A:551:ASN:O	1:A:552:PHE:C	2.30	0.69
2:B:125:LYS:H	2:B:126:PRO:CD	2.03	0.69
1:F:313:TYR:O	1:F:317:VAL:HG23	1.93	0.69
1:F:329:ILE:O	1:F:330:VAL:HG13	1.91	0.69
1:A:62:ILE:HD12	1:A:62:ILE:H	1.57	0.69
1:F:227:VAL:HG12	1:F:296:GLY:HA2	1.75	0.69
1:F:227:VAL:HG21	1:F:310:LEU:HD22	1.74	0.69
1:A:382:LEU:HD23	1:A:385:ILE:HD12	1.74	0.69
1:A:220:MET:HG3	1:A:224:LYS:HB2	1.75	0.69
1:F:239:ILE:HG13	1:F:289:ILE:HD13	1.74	0.69
2:G:148:ALA:HB3	2:G:266:PHE:CB	2.08	0.69
3:H:144:GLY:O	3:H:148:LEU:HG	1.93	0.69
3:H:90:MET:HE2	4:I:68:UNK:N	2.08	0.69
2:B:90:ALA:CA	2:B:93:TRP:HB2	2.22	0.69
2:B:205:GLY:HA3	2:B:220:PHE:CE1	2.28	0.69
3:C:77:LEU:HD13	3:C:184:TRP:HZ2	1.56	0.69
1:F:62:ILE:H	1:F:62:ILE:HD12	1.57	0.69
1:A:209:PHE:HE2	3:C:31:ILE:CD1	2.06	0.69
1:A:332:LEU:HB2	1:A:348:PHE:CB	2.23	0.69
3:C:86:ALA:HB1	3:C:91:TYR:CG	2.28	0.69
3:H:98:VAL:C	3:H:99:ILE:HD12	2.13	0.69
4:I:66:UNK:O	4:I:67:UNK:C	2.41	0.69
2:G:139:PHE:CE1	2:G:148:ALA:HB1	2.28	0.69
3:H:164:ILE:O	3:H:168:GLY:HA2	1.93	0.69
1:A:257:ARG:HH11	1:A:257:ARG:CB	2.05	0.69
1:F:440:TRP:HE1	1:F:446:PHE:HE1	1.41	0.69
2:B:199:GLU:OE2	2:B:200:PRO:HD2	1.92	0.68
1:A:211:THR:HG23	1:A:215:MET:HE3	1.74	0.68
1:F:227:VAL:HG11	1:F:299:SER:CB	2.23	0.68
4:D:66:UNK:O	4:D:67:UNK:C	2.41	0.68
1:F:220:MET:HG3	1:F:224:LYS:HB2	1.75	0.68
2:G:90:ALA:CA	2:G:93:TRP:HB2	2.22	0.68
1:A:239:ILE:CG1	1:A:289:ILE:HD13	2.23	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:175:PRO:O	1:F:179:ILE:HD12	1.94	0.68
1:F:349:GLY:O	1:F:353:MET:HG3	1.94	0.68
1:F:551:ASN:O	1:F:552:PHE:HB2	1.93	0.68
3:H:104:LEU:O	3:H:107:LEU:HB2	1.93	0.68
1:F:447:LYS:HG3	1:F:448:LEU:H	1.57	0.68
1:A:152:GLY:O	1:A:156:VAL:HG23	1.94	0.68
1:F:543:THR:HG22	1:F:544:SER:N	2.08	0.68
1:A:481:ARG:HG2	1:A:482:ARG:HG3	1.75	0.68
1:A:403:VAL:HG13	2:B:107:THR:HG23	1.74	0.68
2:G:140:PHE:HB2	2:G:149:THR:OG1	1.94	0.68
1:A:400:LEU:HD22	2:B:50:LEU:HD21	1.75	0.68
1:F:111:ILE:HD11	6:F:1001:HEM:CMD	2.24	0.68
2:G:205:GLY:HA3	2:G:220:PHE:CE1	2.29	0.68
2:G:199:GLU:OE2	2:G:200:PRO:HD2	1.92	0.68
1:F:152:GLY:O	1:F:156:VAL:HG23	1.94	0.68
1:A:252:LEU:HD22	1:A:263:PHE:CZ	2.28	0.68
1:F:174:PRO:CB	1:F:175:PRO:CD	2.72	0.68
1:A:154:ILE:O	1:A:158:VAL:HG23	1.93	0.67
7:A:1002:HEO:H262	7:A:1002:HEO:H273	1.76	0.67
1:A:332:LEU:HB2	1:A:348:PHE:HB3	1.76	0.67
2:G:204:ASP:HA	2:G:220:PHE:O	1.94	0.67
1:F:382:LEU:HD23	1:F:385:ILE:HD12	1.75	0.67
1:F:175:PRO:O	2:G:170:VAL:HG12	1.95	0.67
2:G:50:LEU:O	2:G:54:VAL:HG13	1.94	0.67
2:B:246:SER:OG	2:B:268:ASN:ND2	2.28	0.67
3:H:77:LEU:HD13	3:H:184:TRP:HZ2	1.58	0.67
1:A:225:MET:HE1	1:A:233:LEU:CD1	2.25	0.67
2:B:175:PHE:HB2	2:B:182:GLN:HG3	1.77	0.67
2:B:204:ASP:HA	2:B:220:PHE:O	1.94	0.67
1:A:227:VAL:HG11	1:A:299:SER:CB	2.24	0.67
1:A:329:ILE:O	1:A:330:VAL:HG13	1.93	0.67
7:A:1002:HEO:H241	2:B:100:ILE:HG12	1.77	0.67
1:F:174:PRO:HB3	1:F:175:PRO:HD3	1.77	0.67
1:F:373:GLY:CA	2:G:71:ALA:HB1	2.21	0.67
1:F:257:ARG:HB3	1:F:257:ARG:HH11	1.57	0.67
1:A:220:MET:HA	1:A:224:LYS:HD2	1.75	0.67
1:A:58:GLY:HA3	1:A:125:LEU:HB2	1.77	0.67
1:A:284:HIS:HB3	1:A:285:PRO:HD3	1.76	0.67
1:F:252:LEU:HD22	1:F:263:PHE:CZ	2.29	0.67
1:A:112:PHE:HE1	1:A:286:GLU:OE2	1.78	0.67
3:C:94:ASN:HB2	3:C:97:GLN:NE2	2.10	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:255:LEU:HD23	1:F:259:LEU:HD12	1.77	0.67
1:A:355:ILE:C	1:A:358:PRO:HD2	2.15	0.67
2:G:203:TYR:O	2:G:221:LYS:HG3	1.95	0.67
2:B:140:PHE:HB2	2:B:149:THR:OG1	1.95	0.67
2:G:141:ILE:HD13	2:G:273:LEU:HB3	1.76	0.67
4:I:70:UNK:O	4:I:71:UNK:CB	2.42	0.67
1:F:390:THR:O	1:F:393:VAL:HB	1.94	0.66
3:H:160:LEU:HD22	3:H:176:ARG:NH1	2.10	0.66
1:A:117:PRO:O	1:A:121:GLY:N	2.28	0.66
3:H:84:GLY:O	3:H:88:ILE:HG13	1.94	0.66
1:A:214:LYS:HZ1	3:C:24:THR:HA	1.61	0.66
1:F:58:GLY:HA3	1:F:125:LEU:HB2	1.77	0.66
1:F:316:LEU:HG	1:F:365:ASN:HD22	1.60	0.66
7:F:1002:H2O:H262	7:F:1002:H2O:H273	1.77	0.66
2:G:175:PHE:HB2	2:G:182:GLN:HG3	1.78	0.66
4:I:1:UNK:O	4:I:2:UNK:C	2.41	0.66
3:H:85:MET:O	3:H:88:ILE:HB	1.96	0.66
1:A:390:THR:O	1:A:393:VAL:HB	1.94	0.66
1:F:220:MET:HA	1:F:224:LYS:HD2	1.76	0.66
1:A:313:TYR:O	1:A:317:VAL:HG23	1.96	0.66
1:A:170:TRP:CZ2	1:A:171:LEU:HD21	2.29	0.66
1:F:332:LEU:HB2	1:F:348:PHE:CB	2.25	0.66
1:F:125:LEU:HD23	1:F:125:LEU:O	1.96	0.66
3:C:134:GLY:HA2	3:C:137:SER:HB3	1.78	0.66
1:F:112:PHE:HE1	1:F:286:GLU:OE2	1.79	0.66
4:D:70:UNK:O	4:D:71:UNK:CB	2.42	0.66
1:A:410:LEU:O	1:A:413:SER:HB3	1.95	0.66
2:G:171:MET:HG3	2:G:210:TYR:CE2	2.31	0.66
2:G:98:LEU:HA	2:G:101:ILE:HD12	1.77	0.66
3:H:30:TRP:HZ2	4:I:79:UNK:O	1.77	0.66
1:F:339:GLY:O	4:I:104:UNK:CB	2.43	0.66
2:B:150:VAL:HG12	2:B:151:ASN:HD22	1.60	0.66
1:F:80:ARG:O	1:F:80:ARG:HG3	1.95	0.66
2:B:50:LEU:O	2:B:54:VAL:HG13	1.96	0.66
1:F:367:LEU:HA	1:F:370:MET:CE	2.26	0.66
1:F:117:PRO:O	1:F:121:GLY:N	2.29	0.66
2:G:131:VAL:HB	2:G:165:VAL:HG13	1.78	0.66
2:B:128:THR:HA	2:B:162:TYR:HB2	1.78	0.65
3:C:90:MET:CE	4:D:68:UNK:N	2.58	0.65
4:D:1:UNK:O	4:D:2:UNK:C	2.41	0.65
1:F:346:ALA:HB1	1:F:350:ILE:CD1	2.27	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:69:LEU:HD22	1:F:73:PHE:CD1	2.31	0.65
1:F:187:VAL:O	1:F:191:ILE:HG13	1.96	0.65
2:G:36:ILE:CG1	2:G:39:GLU:H	2.09	0.65
1:F:54:HIS:CD2	1:F:128:PRO:HG2	2.31	0.65
3:H:193:CYS:O	3:H:196:THR:N	2.29	0.65
1:A:257:ARG:HH11	1:A:257:ARG:HB3	1.59	0.65
1:F:257:ARG:HB3	1:F:257:ARG:NH1	2.10	0.65
2:B:131:VAL:HB	2:B:165:VAL:HG13	1.79	0.65
1:F:69:LEU:HD13	1:F:73:PHE:HE1	1.62	0.65
1:A:314:THR:O	1:A:317:VAL:HB	1.96	0.65
1:F:332:LEU:HB2	1:F:348:PHE:HB3	1.79	0.65
2:B:132:VAL:HG12	2:B:134:MET:SD	2.36	0.65
1:F:284:HIS:HB3	1:F:285:PRO:HD3	1.78	0.65
2:G:41:ARG:N	2:G:41:ARG:HH11	1.94	0.65
3:H:25:LYS:O	3:H:29:PHE:HB3	1.97	0.65
1:A:277:ASN:HA	1:A:335:PHE:HZ	1.62	0.65
2:G:128:THR:HA	2:G:162:TYR:HB2	1.79	0.65
3:C:160:LEU:HD22	3:C:176:ARG:NH1	2.12	0.65
1:A:69:LEU:HG	1:A:114:VAL:CG1	2.27	0.65
1:A:203:LEU:HA	1:A:206:ILE:HD12	1.77	0.65
3:H:94:ASN:HB2	3:H:97:GLN:NE2	2.12	0.65
1:F:316:LEU:HG	1:F:365:ASN:ND2	2.12	0.65
1:F:367:LEU:HD23	1:F:370:MET:CE	2.27	0.65
3:H:91:TYR:OH	4:I:6:UNK:C	2.45	0.64
1:A:239:ILE:HG13	1:A:289:ILE:HD13	1.78	0.64
1:A:257:ARG:NH1	1:A:257:ARG:HB3	2.11	0.64
1:A:121:GLY:O	1:A:124:ASN:HB3	1.97	0.64
1:A:332:LEU:H	1:A:348:PHE:HD2	1.44	0.64
1:F:355:ILE:C	1:F:358:PRO:HD2	2.17	0.64
1:A:513:VAL:HA	1:A:516:MET:CE	2.27	0.64
1:F:174:PRO:C	1:F:176:LEU:H	1.99	0.64
3:H:86:ALA:HA	3:H:90:MET:HB2	1.78	0.64
3:C:98:VAL:C	3:C:99:ILE:HD12	2.18	0.64
1:A:159:SER:OG	1:A:189:TYR:CB	2.46	0.64
1:A:159:SER:OG	1:A:189:TYR:HB3	1.97	0.64
1:A:513:VAL:HA	1:A:516:MET:HE2	1.80	0.64
1:F:264:PHE:CE1	1:F:275:TYR:HB2	2.33	0.64
1:A:481:ARG:HG2	1:A:482:ARG:N	2.12	0.64
3:C:74:PHE:HB2	3:C:112:PHE:CD1	2.31	0.64
1:F:216:ARG:HH12	1:F:221:THR:C	2.01	0.64
3:H:26:ILE:HD11	3:H:175:THR:HG23	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:94:ASN:HB2	3:C:97:GLN:HE21	1.62	0.64
1:F:154:ILE:O	1:F:158:VAL:HG23	1.96	0.64
1:A:111:ILE:HD11	6:A:1001:HEM:CMD	2.28	0.64
2:G:67:TRP:C	2:G:69:TYR:N	2.50	0.64
3:C:70:LEU:CD2	3:C:115:MET:HB2	2.22	0.64
1:A:255:LEU:HD23	1:A:259:LEU:HD12	1.80	0.64
1:A:138:PHE:HB2	1:A:207:ASN:ND2	2.12	0.64
3:H:88:ILE:HA	3:H:98:VAL:CG2	2.27	0.64
3:C:192:ILE:HG23	3:C:192:ILE:O	1.97	0.64
1:A:367:LEU:HA	1:A:370:MET:CE	2.27	0.64
2:B:41:ARG:N	2:B:41:ARG:HH11	1.95	0.64
3:H:134:GLY:HA2	3:H:137:SER:HB3	1.80	0.64
3:C:185:HIS:O	3:C:189:VAL:HG23	1.98	0.64
1:F:541:TRP:CE3	1:F:541:TRP:HA	2.33	0.64
3:H:90:MET:HE2	4:I:67:UNK:CB	2.26	0.64
1:A:54:HIS:CD2	1:A:128:PRO:HG2	2.32	0.64
1:F:69:LEU:HD22	1:F:73:PHE:CE1	2.33	0.64
1:A:543:THR:HG22	1:A:544:SER:N	2.12	0.64
1:F:374:ARG:HB3	2:G:79:SER:HB3	1.78	0.64
3:C:88:ILE:HA	3:C:98:VAL:CG2	2.27	0.64
2:B:159:THR:HG21	2:B:228:ARG:HH21	1.63	0.64
1:A:216:ARG:HH12	1:A:221:THR:C	2.01	0.64
1:F:111:ILE:HD12	1:F:170:TRP:CE3	2.33	0.63
1:F:316:LEU:HD21	1:F:365:ASN:HB2	1.80	0.63
3:C:143:VAL:O	3:C:147:GLY:N	2.31	0.63
1:F:513:VAL:HA	1:F:516:MET:HE2	1.81	0.63
1:F:406:ALA:HB2	2:G:45:LEU:CD2	2.28	0.63
1:A:460:TRP:CH2	1:A:509:ILE:HD11	2.33	0.63
1:F:214:LYS:HZ1	3:H:24:THR:HA	1.63	0.63
2:B:95:VAL:HG23	2:B:96:PRO:CD	2.18	0.63
3:H:185:HIS:O	3:H:189:VAL:HG23	1.99	0.63
3:C:193:CYS:O	3:C:196:THR:N	2.31	0.63
1:A:437:THR:HA	1:A:448:LEU:HD12	1.78	0.63
1:A:96:PRO:O	1:A:97:HIS:C	2.35	0.63
1:F:255:LEU:CD2	1:F:259:LEU:HD12	2.29	0.63
2:B:54:VAL:HA	2:B:57:PRO:HG2	1.81	0.63
1:F:512:LEU:HD23	1:F:513:VAL:N	2.13	0.63
1:F:437:THR:HA	1:F:448:LEU:HD12	1.78	0.63
1:A:262:HIS:HB3	1:A:265:THR:HB	1.80	0.63
3:C:70:LEU:HA	3:C:115:MET:HE1	1.80	0.63
2:B:67:TRP:C	2:B:69:TYR:N	2.52	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:359:THR:HB	7:A:1002:HEO:H272	1.80	0.63
1:A:481:ARG:NH2	1:A:482:ARG:HH21	1.97	0.63
3:C:30:TRP:HH2	4:D:79:UNK:C	2.07	0.63
2:G:264:GLU:HG2	2:G:265:TYR:N	2.12	0.63
3:C:85:MET:CE	3:C:178:MET:HG3	2.28	0.63
1:F:314:THR:O	1:F:317:VAL:HB	1.99	0.63
1:F:262:HIS:HB3	1:F:265:THR:HB	1.80	0.63
1:A:277:ASN:HA	1:A:335:PHE:CZ	2.33	0.63
1:F:277:ASN:HA	1:F:335:PHE:HZ	1.64	0.63
3:C:197:VAL:HG13	3:C:198:VAL:HG23	1.80	0.63
1:F:513:VAL:HA	1:F:516:MET:CE	2.28	0.63
1:F:121:GLY:O	1:F:124:ASN:HB3	1.99	0.63
3:C:83:TYR:HE1	4:D:14:UNK:CB	2.11	0.63
1:A:336:PHE:HE2	1:A:404:PRO:HG3	1.63	0.62
7:A:1002:HEO:H201	2:B:56:ILE:HG21	1.80	0.62
2:B:36:ILE:CG1	2:B:39:GLU:H	2.12	0.62
1:F:280:TRP:CE3	1:F:280:TRP:HA	2.34	0.62
2:G:56:ILE:H	2:G:57:PRO:HD2	1.65	0.62
2:G:57:PRO:O	2:G:61:MET:N	2.26	0.62
2:G:59:ILE:O	2:G:63:VAL:HG23	1.98	0.62
1:F:57:LEU:HA	1:F:60:MET:CG	2.29	0.62
2:B:203:TYR:O	2:B:221:LYS:HG3	1.99	0.62
3:H:160:LEU:O	3:H:164:ILE:HG13	1.99	0.62
1:A:541:TRP:CE3	1:A:541:TRP:HA	2.34	0.62
3:H:96:SER:C	3:H:98:VAL:H	2.01	0.62
1:A:174:PRO:C	1:A:176:LEU:H	2.00	0.62
2:B:56:ILE:H	2:B:57:PRO:HD2	1.65	0.62
3:H:185:HIS:NE2	4:I:57:UNK:O	2.32	0.62
2:G:184:TYR:HE2	2:G:186:MET:HB2	1.63	0.62
3:C:197:VAL:CG1	3:C:198:VAL:N	2.62	0.62
3:C:160:LEU:O	3:C:164:ILE:HG13	1.99	0.62
1:A:248:VAL:CG2	3:C:39:LEU:HD12	2.27	0.62
1:A:407:ASP:OD2	1:A:411:HIS:HB2	1.99	0.62
1:F:359:THR:HB	7:F:1002:HEO:H272	1.80	0.62
2:G:104:ALA:HA	2:G:107:THR:OG1	2.00	0.62
1:F:367:LEU:HD13	2:G:63:VAL:CG1	2.29	0.62
1:F:203:LEU:HA	1:F:206:ILE:HD12	1.80	0.62
1:A:367:LEU:HD23	1:A:370:MET:CE	2.29	0.62
2:B:184:TYR:HE2	2:B:186:MET:HB2	1.64	0.62
1:F:481:ARG:HG2	1:F:482:ARG:N	2.14	0.62
1:F:469:MET:N	1:F:470:PRO:CD	2.62	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:466:VAL:C	1:F:501:GLY:HA3	2.20	0.62
2:G:108:TRP:HZ3	2:G:109:LYS:HE2	1.65	0.62
1:A:174:PRO:HB2	1:A:175:PRO:CD	2.28	0.62
1:A:346:ALA:HB1	1:A:350:ILE:CD1	2.30	0.62
1:A:487:ILE:HA	1:A:492:HIS:CE1	2.34	0.62
1:A:512:LEU:HD23	1:A:513:VAL:N	2.14	0.62
1:F:96:PRO:O	1:F:97:HIS:C	2.35	0.62
1:F:54:HIS:CE1	1:F:55:LYS:HG3	2.35	0.62
2:G:147:ILE:CD1	2:G:235:VAL:HG13	2.29	0.62
1:F:487:ILE:HA	1:F:492:HIS:CE1	2.35	0.62
1:A:551:ASN:C	1:A:552:PHE:O	2.38	0.62
2:B:59:ILE:O	2:B:63:VAL:HG23	1.99	0.62
1:F:330:VAL:O	1:F:333:HIS:ND1	2.32	0.62
1:F:79:MET:SD	1:F:102:ILE:HG22	2.39	0.62
2:G:149:THR:HG22	2:G:265:TYR:HE1	1.64	0.62
3:C:148:LEU:HA	3:C:151:THR:OG1	1.98	0.62
3:C:74:PHE:CZ	3:C:187:LEU:HD22	2.34	0.62
3:H:74:PHE:HA	3:H:77:LEU:HD12	1.82	0.62
1:F:138:PHE:HB2	1:F:207:ASN:ND2	2.14	0.62
3:H:85:MET:N	3:H:88:ILE:HD12	2.14	0.62
1:F:123:MET:HA	1:F:127:VAL:HG23	1.80	0.62
1:F:277:ASN:HA	1:F:335:PHE:CZ	2.34	0.62
1:F:331:TRP:CH2	4:I:97:UNK:CB	2.82	0.62
3:H:197:VAL:CG1	3:H:198:VAL:N	2.62	0.62
1:F:159:SER:OG	1:F:189:TYR:HB3	2.00	0.62
2:B:136:TRP:CE3	2:B:259:GLU:HG2	2.35	0.62
1:A:255:LEU:CD2	1:A:259:LEU:HD12	2.30	0.62
1:A:106:HIS:O	1:A:109:ILE:N	2.32	0.62
1:A:54:HIS:HD2	1:A:128:PRO:HG2	1.64	0.62
1:A:330:VAL:O	1:A:333:HIS:ND1	2.33	0.62
1:A:481:ARG:NH2	1:A:482:ARG:NH2	2.47	0.62
1:F:481:ARG:NH2	1:F:482:ARG:HH21	1.98	0.62
2:B:148:ALA:CB	2:B:266:PHE:HB2	2.08	0.62
1:A:469:MET:N	1:A:470:PRO:CD	2.63	0.62
3:C:66:LEU:N	3:C:67:PRO:HD2	2.14	0.61
1:F:457:PHE:CE2	1:F:461:ILE:HD11	2.35	0.61
1:A:367:LEU:HD13	2:B:63:VAL:HG11	1.82	0.61
1:A:55:LYS:HZ1	1:A:551:ASN:CA	2.03	0.61
1:A:57:LEU:HA	1:A:60:MET:CG	2.30	0.61
3:C:86:ALA:HA	3:C:90:MET:HB2	1.80	0.61
2:B:141:ILE:HD13	2:B:273:LEU:HB3	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:183:PHE:O	3:C:186:PHE:HB3	1.99	0.61
1:A:316:LEU:HG	1:A:365:ASN:ND2	2.16	0.61
1:A:390:THR:HG21	1:A:426:GLY:HA3	1.81	0.61
2:B:171:MET:HG3	2:B:210:TYR:CE2	2.35	0.61
1:F:106:HIS:O	1:F:109:ILE:N	2.33	0.61
3:H:66:LEU:N	3:H:67:PRO:HD2	2.14	0.61
1:F:457:PHE:CD2	1:F:461:ILE:HD11	2.35	0.61
1:A:80:ARG:HG3	1:A:80:ARG:O	2.00	0.61
1:F:54:HIS:NE2	1:F:55:LYS:HG3	2.15	0.61
1:F:57:LEU:HA	1:F:60:MET:HG3	1.82	0.61
3:C:96:SER:C	3:C:98:VAL:H	2.02	0.61
1:F:159:SER:OG	1:F:189:TYR:CB	2.48	0.61
1:F:69:LEU:HG	1:F:114:VAL:CG1	2.30	0.61
1:F:119:VAL:HG22	1:F:123:MET:HE2	1.82	0.61
2:B:264:GLU:HG2	2:B:265:TYR:N	2.15	0.61
3:H:70:LEU:CD2	3:H:115:MET:HB2	2.24	0.61
1:A:252:LEU:HD13	1:A:263:PHE:CE2	2.36	0.61
3:H:91:TYR:OH	4:I:7:UNK:CA	2.49	0.61
2:G:97:ILE:O	2:G:101:ILE:CD1	2.49	0.61
3:H:143:VAL:O	3:H:147:GLY:N	2.33	0.61
3:H:94:ASN:HB2	3:H:97:GLN:HE21	1.65	0.61
1:A:316:LEU:HD21	1:A:365:ASN:HB2	1.83	0.61
3:C:102:LEU:O	3:C:105:THR:HB	2.00	0.61
3:C:25:LYS:O	3:C:29:PHE:HB3	2.01	0.61
3:H:120:PHE:O	3:H:123:LEU:N	2.32	0.61
1:F:333:HIS:HA	1:F:336:PHE:CE1	2.35	0.61
1:F:373:GLY:HA2	2:G:71:ALA:CA	2.30	0.61
1:A:159:SER:HB2	1:A:165:PHE:CD1	2.34	0.61
2:G:136:TRP:CE3	2:G:259:GLU:HG2	2.36	0.61
1:F:466:VAL:HB	1:F:501:GLY:HA2	1.83	0.61
3:H:192:ILE:O	3:H:192:ILE:HG23	2.00	0.61
3:C:30:TRP:HH2	4:D:79:UNK:O	1.79	0.61
1:F:316:LEU:HD21	1:F:365:ASN:CB	2.31	0.61
1:F:354:ILE:HA	2:G:100:ILE:HD13	1.82	0.61
1:A:305:PHE:HE2	1:A:378:HIS:HB2	1.65	0.61
1:A:441:PRO:O	1:A:443:ALA:N	2.34	0.61
3:H:183:PHE:O	3:H:186:PHE:HB3	2.01	0.61
3:C:185:HIS:NE2	4:D:61:UNK:CB	2.64	0.61
1:A:333:HIS:HA	1:A:336:PHE:CE1	2.36	0.61
1:A:316:LEU:HG	1:A:365:ASN:HD22	1.66	0.61
1:A:54:HIS:CE1	1:A:55:LYS:HG3	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:282:TRP:C	1:F:285:PRO:HD2	2.21	0.61
1:F:364:PHE:HA	1:F:367:LEU:HD12	1.83	0.61
2:B:147:ILE:CD1	2:B:235:VAL:HG13	2.31	0.61
1:F:131:ILE:HD12	1:F:216:ARG:HA	1.82	0.61
1:A:125:LEU:O	1:A:125:LEU:HD23	2.01	0.61
1:A:54:HIS:NE2	1:A:55:LYS:HG3	2.16	0.60
1:F:109:ILE:HG22	1:F:114:VAL:HG23	1.83	0.60
1:F:55:LYS:HZ1	1:F:551:ASN:HA	1.62	0.60
2:B:139:PHE:HE1	2:B:148:ALA:HB1	1.66	0.60
1:F:305:PHE:HE2	1:F:378:HIS:HB2	1.65	0.60
1:A:131:ILE:HD12	1:A:216:ARG:HA	1.83	0.60
1:F:441:PRO:O	1:F:443:ALA:N	2.34	0.60
1:A:58:GLY:N	1:A:124:ASN:ND2	2.49	0.60
3:H:178:MET:SD	4:I:68:UNK:CB	2.89	0.60
1:A:280:TRP:HA	1:A:280:TRP:CE3	2.36	0.60
2:B:127:ILE:HD12	2:B:127:ILE:H	1.67	0.60
3:C:85:MET:N	3:C:88:ILE:HD12	2.16	0.60
1:A:450:GLU:OE2	1:A:454:LYS:HE3	2.01	0.60
1:A:264:PHE:CE1	1:A:275:TYR:HB2	2.37	0.60
2:B:137:LYS:NZ	2:B:261:ASN:HD21	1.99	0.60
1:A:187:VAL:O	1:A:191:ILE:HG13	2.01	0.60
2:G:36:ILE:N	2:G:39:GLU:OE2	2.29	0.60
2:B:228:ARG:HG3	2:B:231:PHE:HD2	1.67	0.60
2:B:57:PRO:O	2:B:61:MET:N	2.27	0.60
1:F:235:ALA:O	1:F:238:LEU:HB2	2.01	0.60
2:G:39:GLU:O	2:G:43:LEU:N	2.33	0.60
3:H:197:VAL:HG13	3:H:198:VAL:HG23	1.82	0.60
3:H:74:PHE:CZ	3:H:187:LEU:HD22	2.36	0.60
1:A:440:TRP:HE1	1:A:446:PHE:HE1	1.50	0.60
1:F:442:LYS:HD3	1:F:541:TRP:CZ3	2.37	0.60
3:C:26:ILE:HG22	3:C:27:PHE:N	2.16	0.60
2:B:53:ILE:O	2:B:57:PRO:HD2	2.01	0.60
1:F:54:HIS:HD2	1:F:128:PRO:HG2	1.64	0.60
2:G:54:VAL:HA	2:G:57:PRO:HG2	1.83	0.60
1:F:252:LEU:HD13	1:F:263:PHE:CE2	2.37	0.60
3:C:134:GLY:HA2	3:C:137:SER:CB	2.32	0.60
1:F:336:PHE:HE2	1:F:404:PRO:HG3	1.66	0.60
1:A:442:LYS:HD3	1:A:541:TRP:CZ3	2.37	0.60
1:A:466:VAL:C	1:A:501:GLY:HA3	2.22	0.60
3:H:96:SER:O	3:H:98:VAL:N	2.35	0.60
1:A:205:GLY:O	1:A:240:ILE:HD11	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:481:ARG:NH2	1:F:482:ARG:NH2	2.49	0.60
1:F:69:LEU:HD13	1:F:73:PHE:CE1	2.37	0.60
2:G:148:ALA:CB	2:G:266:PHE:HB2	2.09	0.60
2:G:159:THR:HG21	2:G:228:ARG:HH21	1.66	0.60
3:C:38:ILE:HD13	4:D:90:UNK:CB	2.32	0.60
1:A:457:PHE:CD2	1:A:461:ILE:HD11	2.37	0.60
2:G:56:ILE:HD12	2:G:56:ILE:N	2.16	0.60
1:A:57:LEU:HA	1:A:60:MET:HG3	1.83	0.60
2:G:228:ARG:HG3	2:G:231:PHE:HD2	1.67	0.60
1:F:514:ILE:O	1:F:518:VAL:HG23	2.00	0.60
2:G:251:PHE:CD2	2:G:273:LEU:HD11	2.37	0.60
1:F:457:PHE:O	1:F:461:ILE:HG13	2.00	0.60
2:G:150:VAL:HG12	2:G:151:ASN:HD22	1.65	0.60
1:A:109:ILE:HG22	1:A:114:VAL:HG23	1.84	0.60
1:A:206:ILE:HG23	3:C:31:ILE:HG23	1.83	0.60
2:G:243:ASN:ND2	2:G:265:TYR:O	2.34	0.60
3:C:85:MET:O	3:C:88:ILE:HB	2.02	0.60
1:A:61:TYR:CE1	1:A:146:PHE:HB2	2.37	0.60
1:A:123:MET:HA	1:A:127:VAL:HG23	1.83	0.60
1:A:209:PHE:CE2	3:C:31:ILE:CD1	2.85	0.60
2:G:149:THR:HG22	2:G:265:TYR:CE1	2.36	0.60
2:B:147:ILE:HD13	2:B:235:VAL:HG13	1.84	0.60
3:H:156:TRP:HE1	3:H:180:LEU:CD2	2.15	0.60
2:B:190:GLN:NE2	2:B:192:ARG:HH21	1.99	0.60
3:C:124:ILE:O	3:C:124:ILE:HG22	2.02	0.60
1:F:541:TRP:HE3	1:F:541:TRP:HA	1.67	0.60
1:A:235:ALA:O	1:A:238:LEU:HB2	2.02	0.59
2:G:39:GLU:HB2	2:G:43:LEU:HD12	1.84	0.59
2:B:244:THR:HB	2:B:268:ASN:CB	2.17	0.59
1:F:214:LYS:CE	3:H:24:THR:HG23	2.32	0.59
2:B:227:ASP:CG	2:B:229:ALA:H	2.06	0.59
1:A:364:PHE:HA	1:A:367:LEU:HD12	1.83	0.59
2:B:39:GLU:HB2	2:B:43:LEU:HD12	1.84	0.59
1:F:73:PHE:HB3	1:F:77:ILE:CD1	2.32	0.59
3:C:88:ILE:CG1	3:C:98:VAL:HG13	2.27	0.59
1:A:457:PHE:CE2	1:A:461:ILE:HD11	2.37	0.59
1:F:460:TRP:CH2	1:F:509:ILE:HD11	2.37	0.59
2:G:137:LYS:NZ	2:G:261:ASN:HD21	2.00	0.59
2:G:227:ASP:CG	2:G:229:ALA:H	2.06	0.59
1:A:312:GLY:HA3	1:A:365:ASN:ND2	2.17	0.59
1:A:69:LEU:HD22	1:A:73:PHE:CD1	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:30:TRP:CZ3	4:D:79:UNK:HA	2.35	0.59
2:B:243:ASN:ND2	2:B:265:TYR:O	2.35	0.59
2:G:196:ILE:HG22	2:G:198:ASN:HD21	1.67	0.59
2:B:156:PRO:HG2	2:B:228:ARG:HE	1.68	0.59
1:A:449:ASN:OD1	1:A:451:THR:HB	2.03	0.59
3:C:44:PHE:HE1	3:C:142:LEU:HD21	1.67	0.59
3:H:111:GLY:O	3:H:114:GLY:N	2.34	0.59
1:F:58:GLY:N	1:F:124:ASN:ND2	2.51	0.59
3:H:134:GLY:HA2	3:H:137:SER:CB	2.33	0.59
1:A:79:MET:SD	1:A:102:ILE:HG22	2.42	0.59
1:A:105:ALA:O	1:A:109:ILE:HG13	2.02	0.59
1:A:118:PHE:CZ	1:A:294:VAL:HG22	2.37	0.59
1:F:228:PHE:CE1	1:F:297:VAL:HG23	2.37	0.59
2:G:244:THR:HB	2:G:268:ASN:CB	2.18	0.59
3:C:74:PHE:HZ	3:C:187:LEU:HD22	1.68	0.59
1:A:178:GLY:HA2	1:A:257:ARG:CG	2.31	0.59
1:F:178:GLY:HA2	1:F:257:ARG:CG	2.30	0.59
1:A:464:PHE:HD2	1:A:465:PHE:CE1	2.21	0.59
1:A:282:TRP:C	1:A:285:PRO:HD2	2.22	0.59
1:F:332:LEU:H	1:F:348:PHE:HD2	1.50	0.59
3:C:77:LEU:HD13	3:C:184:TRP:CZ2	2.37	0.59
1:A:192:TRP:CE3	1:A:192:TRP:HA	2.38	0.59
1:A:168:THR:HB	1:A:172:ALA:CA	2.32	0.59
2:G:127:ILE:H	2:G:127:ILE:HD12	1.68	0.59
2:G:147:ILE:HD13	2:G:235:VAL:HG13	1.85	0.59
1:F:375:ILE:HG12	2:G:67:TRP:HE1	1.67	0.59
3:H:124:ILE:O	3:H:124:ILE:HG22	2.03	0.59
3:H:90:MET:HE2	4:I:67:UNK:C	2.32	0.59
3:H:78:PHE:CE2	3:H:185:HIS:CE1	2.90	0.59
1:F:225:MET:SD	1:F:230:TRP:HA	2.43	0.59
2:G:60:LEU:C	2:G:62:ALA:H	2.04	0.59
3:H:74:PHE:HB2	3:H:112:PHE:CD1	2.37	0.59
3:H:74:PHE:HZ	3:H:187:LEU:HD22	1.68	0.59
1:F:206:ILE:HG23	3:H:31:ILE:HG23	1.83	0.59
1:A:436:MET:O	1:A:440:TRP:HB2	2.03	0.59
1:A:126:VAL:HG11	1:A:439:TRP:CE2	2.38	0.59
2:G:87:LYS:HD2	2:G:87:LYS:N	2.18	0.59
3:C:74:PHE:HA	3:C:77:LEU:HD12	1.85	0.59
1:F:156:VAL:HG12	1:F:160:LEU:HD11	1.85	0.59
1:A:512:LEU:O	1:A:515:GLN:HG2	2.02	0.59
1:A:541:TRP:HE3	1:A:541:TRP:HA	1.68	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:280:TRP:O	1:A:331:TRP:HB2	2.03	0.58
2:B:50:LEU:O	2:B:53:ILE:HG22	2.03	0.58
2:B:56:ILE:HD12	2:B:56:ILE:N	2.18	0.58
1:F:168:THR:HB	1:F:172:ALA:CA	2.29	0.58
1:F:390:THR:HG21	1:F:426:GLY:HA3	1.84	0.58
1:F:55:LYS:HD3	1:F:129:LEU:HD21	1.85	0.58
2:G:139:PHE:HE1	2:G:148:ALA:HB1	1.68	0.58
2:B:196:ILE:HG22	2:B:198:ASN:HD21	1.67	0.58
2:B:159:THR:HG21	2:B:228:ARG:NH2	2.18	0.58
1:F:274:MET:HG2	3:H:49:VAL:HG11	1.85	0.58
3:C:68:PHE:O	3:C:72:GLU:HB2	2.02	0.58
1:A:58:GLY:N	1:A:124:ASN:HD22	2.01	0.58
3:C:86:ALA:HB1	3:C:91:TYR:CD1	2.37	0.58
1:A:216:ARG:HH12	1:A:222:MET:HA	1.67	0.58
3:C:26:ILE:HD11	3:C:175:THR:HG23	1.83	0.58
1:A:69:LEU:HD22	1:A:73:PHE:CE1	2.38	0.58
1:F:79:MET:CE	1:F:102:ILE:HG22	2.32	0.58
1:F:366:TRP:O	1:F:369:THR:HB	2.04	0.58
3:C:96:SER:O	3:C:98:VAL:N	2.37	0.58
2:B:108:TRP:HZ3	2:B:109:LYS:HE2	1.69	0.58
2:B:278:ILE:O	2:B:282:MET:HG2	2.03	0.58
1:F:110:MET:HB3	6:F:1001:HEM:CBC	2.33	0.58
1:F:369:THR:O	1:F:369:THR:HG22	2.02	0.58
3:C:96:SER:CA	3:C:99:ILE:HD13	2.30	0.58
2:G:196:ILE:HG22	2:G:198:ASN:ND2	2.17	0.58
1:A:373:GLY:HA2	2:B:71:ALA:CB	2.27	0.58
1:A:381:MET:O	1:A:385:ILE:HG13	2.03	0.58
1:F:58:GLY:N	1:F:124:ASN:HD22	2.01	0.58
1:A:308:LYS:HZ2	1:A:372:GLN:N	1.88	0.58
3:H:113:ILE:HD11	3:H:150:VAL:HG12	1.85	0.58
1:A:466:VAL:HB	1:A:501:GLY:HA2	1.84	0.58
3:H:44:PHE:HE1	3:H:142:LEU:HD21	1.68	0.58
1:F:245:ILE:HD12	1:F:282:TRP:HB2	1.86	0.58
1:F:280:TRP:O	1:F:331:TRP:HB2	2.04	0.58
1:F:373:GLY:HA2	2:G:71:ALA:O	2.03	0.58
1:F:192:TRP:HA	1:F:192:TRP:CE3	2.39	0.58
1:F:105:ALA:O	1:F:109:ILE:HG13	2.03	0.58
2:G:278:ILE:O	2:G:282:MET:HG2	2.04	0.58
1:A:337:THR:HG22	2:B:184:TYR:HB3	1.85	0.58
2:B:87:LYS:HD2	2:B:87:LYS:N	2.19	0.58
1:F:239:ILE:N	1:F:289:ILE:HD11	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:449:ASN:OD1	1:F:451:THR:HB	2.04	0.58
2:G:244:THR:CG2	2:G:268:ASN:HB3	2.33	0.58
3:C:90:MET:CE	4:D:68:UNK:CA	2.82	0.58
3:C:47:TYR:O	3:C:51:VAL:HG13	2.03	0.58
2:B:251:PHE:CD2	2:B:273:LEU:HD11	2.39	0.58
1:F:111:ILE:HD11	6:F:1001:HEM:HMD2	1.86	0.57
1:F:54:HIS:CE1	1:F:135:ASP:HA	2.39	0.57
2:B:177:PRO:C	2:B:179:LEU:H	2.08	0.57
3:H:96:SER:CA	3:H:99:ILE:HD13	2.30	0.57
1:A:209:PHE:HE2	3:C:31:ILE:HD11	1.68	0.57
2:B:95:VAL:O	2:B:99:ILE:HG12	2.03	0.57
1:F:103:PHE:CZ	6:F:1001:HEM:HMA1	2.39	0.57
2:G:53:ILE:O	2:G:57:PRO:HD2	2.03	0.57
3:C:85:MET:SD	3:C:178:MET:HG3	2.44	0.57
3:H:38:ILE:HD13	4:I:90:UNK:CB	2.33	0.57
1:F:155:LEU:HD13	1:F:193:SER:HA	1.85	0.57
1:A:54:HIS:CE1	1:A:135:ASP:HA	2.39	0.57
1:A:55:LYS:HD3	1:A:129:LEU:HD21	1.87	0.57
2:B:39:GLU:O	2:B:43:LEU:HB2	2.04	0.57
2:G:104:ALA:O	2:G:105:VAL:C	2.38	0.57
2:G:162:TYR:CG	2:G:194:HIS:NE2	2.72	0.57
2:B:196:ILE:HG22	2:B:198:ASN:ND2	2.18	0.57
2:G:192:ARG:HH11	2:G:192:ARG:HB2	1.68	0.57
1:A:397:THR:HG21	1:A:472:TYR:OH	2.04	0.57
1:F:464:PHE:HD2	1:F:465:PHE:CE1	2.23	0.57
1:F:549:PHE:H	1:F:549:PHE:HD1	1.52	0.57
1:A:79:MET:CE	1:A:102:ILE:HG22	2.33	0.57
1:A:228:PHE:CE1	1:A:297:VAL:HG23	2.39	0.57
3:C:89:ALA:HB2	3:C:174:ARG:CD	2.25	0.57
3:C:196:THR:HA	3:C:200:LEU:CD2	2.33	0.57
1:A:514:ILE:O	1:A:518:VAL:HG23	2.02	0.57
1:A:248:VAL:HG22	3:C:39:LEU:CD1	2.31	0.57
1:A:156:VAL:HG12	1:A:160:LEU:HD11	1.86	0.57
3:C:29:PHE:HA	3:C:32:TYR:HB2	1.84	0.57
1:F:61:TYR:CE1	1:F:146:PHE:HB2	2.39	0.57
1:F:450:GLU:OE2	1:F:454:LYS:HE3	2.05	0.57
3:H:88:ILE:HG23	3:H:98:VAL:CG1	2.34	0.57
2:B:50:LEU:C	2:B:53:ILE:HG22	2.25	0.57
1:F:407:ASP:OD2	1:F:411:HIS:HB2	2.05	0.57
2:G:179:LEU:HB3	2:G:195:LEU:HD11	1.86	0.57
1:A:492:HIS:HA	1:A:495:LEU:HD12	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:200:LEU:HD12	3:C:201:MET:N	2.18	0.57
1:F:248:VAL:HG22	3:H:39:LEU:HD12	1.87	0.57
2:B:192:ARG:HB2	2:B:192:ARG:HH11	1.68	0.57
1:A:283:GLY:O	1:A:286:GLU:HB3	2.05	0.57
3:C:136:LEU:O	3:C:140:PHE:HB2	2.04	0.57
2:B:136:TRP:HA	2:B:218:MET:HG2	1.87	0.57
1:A:79:MET:HG3	1:A:103:PHE:CZ	2.40	0.57
2:G:173:SER:HB3	2:G:207:SER:O	2.05	0.57
3:C:38:ILE:CD1	4:D:90:UNK:CB	2.82	0.57
3:H:38:ILE:CD1	4:I:90:UNK:CB	2.83	0.57
1:A:239:ILE:N	1:A:289:ILE:HD11	2.20	0.57
1:A:316:LEU:HD21	1:A:365:ASN:CB	2.35	0.57
3:H:134:GLY:O	3:H:137:SER:HB3	2.05	0.57
1:A:549:PHE:HD1	1:A:549:PHE:H	1.53	0.57
1:A:155:LEU:HD13	1:A:193:SER:HA	1.86	0.57
1:A:481:ARG:O	1:A:483:LEU:N	2.38	0.57
1:F:79:MET:HG3	1:F:103:PHE:CZ	2.40	0.57
2:B:162:TYR:CG	2:B:194:HIS:NE2	2.73	0.57
2:G:156:PRO:HG2	2:G:228:ARG:HE	1.70	0.57
3:H:77:LEU:HD13	3:H:184:TRP:CZ2	2.40	0.57
2:B:179:LEU:HB3	2:B:195:LEU:HD11	1.87	0.57
1:A:437:THR:HA	1:A:448:LEU:CD1	2.34	0.57
1:A:457:PHE:O	1:A:461:ILE:HG13	2.04	0.57
1:A:353:MET:O	2:B:100:ILE:HD12	2.05	0.57
2:G:140:PHE:CD2	2:G:153:ILE:HG23	2.40	0.57
1:F:492:HIS:HA	1:F:495:LEU:HD12	1.87	0.57
3:H:70:LEU:HA	3:H:115:MET:HE1	1.87	0.56
3:H:100:SER:O	3:H:103:ALA:HB3	2.05	0.56
3:C:44:PHE:CE1	3:C:142:LEU:HD21	2.40	0.56
3:H:98:VAL:O	3:H:98:VAL:HG12	2.05	0.56
1:F:548:PRO:N	1:F:552:PHE:O	2.38	0.56
2:G:39:GLU:O	2:G:43:LEU:HB2	2.05	0.56
2:B:244:THR:CG2	2:B:268:ASN:HB3	2.35	0.56
2:G:136:TRP:HA	2:G:218:MET:HG2	1.87	0.56
3:H:86:ALA:C	3:H:88:ILE:H	2.08	0.56
3:H:90:MET:CE	4:I:68:UNK:N	2.68	0.56
1:A:367:LEU:HA	1:A:370:MET:HE3	1.87	0.56
1:A:245:ILE:HD12	1:A:282:TRP:HB2	1.87	0.56
2:B:36:ILE:N	2:B:39:GLU:OE2	2.32	0.56
1:F:481:ARG:O	1:F:483:LEU:N	2.39	0.56
2:G:50:LEU:O	2:G:53:ILE:HG22	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:426:GLY:HA2	1:F:430:PHE:CD1	2.41	0.56
2:B:149:THR:HG22	2:B:265:TYR:HE1	1.69	0.56
1:F:381:MET:O	1:F:385:ILE:HG13	2.05	0.56
1:F:474:LEU:HD22	1:F:491:PHE:HA	1.86	0.56
1:F:57:LEU:HD11	1:F:143:ASN:HA	1.87	0.56
3:C:113:ILE:HD11	3:C:150:VAL:HG12	1.87	0.56
3:C:49:VAL:O	3:C:51:VAL:N	2.31	0.56
1:F:436:MET:O	1:F:440:TRP:HB2	2.06	0.56
1:A:442:LYS:HD3	1:A:541:TRP:CE3	2.41	0.56
1:A:251:ALA:O	1:A:254:THR:HB	2.05	0.56
3:C:120:PHE:O	3:C:123:LEU:N	2.36	0.56
1:A:110:MET:HB3	6:A:1001:HEM:CBC	2.35	0.56
1:F:237:VAL:O	1:F:240:ILE:HB	2.05	0.56
1:F:375:ILE:CG1	2:G:67:TRP:HE1	2.19	0.56
3:H:29:PHE:HA	3:H:32:TYR:HB2	1.86	0.56
1:F:442:LYS:HD3	1:F:541:TRP:CE3	2.41	0.56
1:A:271:ASN:HD21	1:A:273:MET:HB2	1.71	0.56
1:F:126:VAL:HG11	1:F:439:TRP:CE2	2.41	0.56
2:G:53:ILE:HG23	2:G:54:VAL:N	2.20	0.56
1:F:159:SER:CA	1:F:189:TYR:CD1	2.81	0.56
3:C:155:ILE:O	3:C:159:VAL:HG23	2.05	0.56
1:A:420:PHE:HA	1:A:423:VAL:HG22	1.87	0.56
1:F:311:PHE:HZ	2:G:88:VAL:HG11	1.70	0.56
1:A:138:PHE:HB2	1:A:207:ASN:HD21	1.69	0.56
3:C:83:TYR:CE1	4:D:14:UNK:CB	2.89	0.56
1:A:366:TRP:O	1:A:369:THR:HB	2.06	0.56
1:A:73:PHE:HB3	1:A:77:ILE:CD1	2.36	0.56
2:B:53:ILE:HG23	2:B:54:VAL:N	2.20	0.56
1:F:312:GLY:HA3	1:F:365:ASN:ND2	2.21	0.56
3:H:77:LEU:HA	3:H:80:SER:CB	2.35	0.56
2:G:248:MET:O	2:G:252:GLU:HG2	2.05	0.56
2:G:50:LEU:C	2:G:53:ILE:HG22	2.26	0.56
3:H:155:ILE:O	3:H:159:VAL:HG23	2.05	0.56
1:A:69:LEU:HD13	1:A:73:PHE:HE1	1.71	0.56
1:F:277:ASN:OD1	1:F:331:TRP:NE1	2.39	0.56
2:G:95:VAL:O	2:G:98:LEU:HB2	2.06	0.56
1:F:437:THR:HA	1:F:448:LEU:CD1	2.35	0.56
2:G:164:LYS:HE3	2:G:274:PHE:CE2	2.40	0.56
2:G:41:ARG:H	2:G:41:ARG:HH11	1.54	0.55
1:F:113:PHE:HE2	1:F:153:VAL:N	2.04	0.55
1:A:333:HIS:CD2	1:A:334:HIS:CD2	2.94	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:60:LEU:C	2:B:62:ALA:H	2.08	0.55
3:C:98:VAL:O	3:C:98:VAL:HG12	2.06	0.55
3:H:113:ILE:O	3:H:117:ILE:HG13	2.05	0.55
2:B:248:MET:O	2:B:252:GLU:HG2	2.06	0.55
3:C:134:GLY:O	3:C:137:SER:HB3	2.06	0.55
1:F:419:HIS:HA	1:F:472:TYR:OH	2.06	0.55
1:F:271:ASN:HD21	1:F:273:MET:HB2	1.72	0.55
1:A:73:PHE:O	1:A:74:ALA:C	2.43	0.55
1:A:474:LEU:HD22	1:A:491:PHE:HA	1.87	0.55
3:H:146:HIS:HE1	3:H:190:VAL:HB	1.71	0.55
1:A:103:PHE:CZ	6:A:1001:HEM:HMA1	2.41	0.55
1:F:330:VAL:HB	1:F:352:THR:OG1	2.06	0.55
3:C:90:MET:HE1	4:D:67:UNK:C	2.36	0.55
1:F:199:ILE:O	1:F:202:THR:HB	2.06	0.55
2:B:165:VAL:HG12	2:B:166:THR:N	2.22	0.55
1:F:283:GLY:O	1:F:286:GLU:HB3	2.06	0.55
2:B:136:TRP:HA	2:B:218:MET:SD	2.47	0.55
3:H:44:PHE:CE1	3:H:142:LEU:HD21	2.41	0.55
1:F:410:LEU:O	1:F:413:SER:HB3	2.06	0.55
1:A:237:VAL:O	1:A:240:ILE:HB	2.06	0.55
1:A:480:THR:HB	1:A:483:LEU:HD11	1.87	0.55
1:F:102:ILE:O	1:F:104:THR:N	2.39	0.55
1:F:288:TYR:OH	1:F:355:ILE:HG21	2.06	0.55
1:F:333:HIS:CD2	1:F:334:HIS:CD2	2.94	0.55
1:F:338:MET:HA	2:G:184:TYR:CG	2.42	0.55
2:B:149:THR:HG22	2:B:265:TYR:CE1	2.41	0.55
1:F:159:SER:HB2	1:F:165:PHE:CD1	2.40	0.55
3:C:42:ILE:O	3:C:45:ALA:HB3	2.06	0.55
2:B:164:LYS:HE3	2:B:274:PHE:CE2	2.41	0.55
1:A:419:HIS:HA	1:A:472:TYR:OH	2.07	0.55
2:G:165:VAL:O	2:G:191:THR:HG23	2.06	0.55
1:A:239:ILE:HG12	1:A:289:ILE:HD13	1.89	0.55
3:C:152:SER:C	3:C:154:LEU:H	2.10	0.55
1:A:384:THR:HG22	1:A:388:ILE:HD11	1.89	0.55
2:G:167:SER:HB3	2:G:187:ALA:HA	1.89	0.55
1:A:238:LEU:CB	1:A:289:ILE:HD11	2.35	0.55
1:A:548:PRO:N	1:A:552:PHE:O	2.40	0.55
1:A:76:ALA:HA	1:A:79:MET:HE3	1.87	0.55
1:F:357:ILE:HB	1:F:358:PRO:HD3	1.87	0.55
3:C:113:ILE:O	3:C:117:ILE:HG13	2.06	0.55
1:A:96:PRO:HB3	1:A:100:ASP:OD1	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:TYR:O	1:A:62:ILE:C	2.45	0.55
1:F:106:HIS:CD2	1:F:107:GLY:N	2.75	0.55
1:F:412:ASN:OD1	2:G:209:SER:HB3	2.07	0.55
2:G:177:PRO:C	2:G:179:LEU:H	2.11	0.55
3:H:148:LEU:HA	3:H:151:THR:OG1	2.06	0.55
1:F:512:LEU:O	1:F:515:GLN:HG2	2.06	0.55
2:B:143:PRO:HG2	2:B:144:GLU:OE2	2.06	0.55
2:G:163:PHE:CD2	2:G:193:LEU:HD22	2.41	0.55
2:G:148:ALA:O	2:G:265:TYR:HD1	1.90	0.55
2:G:40:GLN:HB2	2:G:41:ARG:NH1	2.22	0.55
2:B:148:ALA:O	2:B:265:TYR:HD1	1.90	0.55
1:F:384:THR:HG22	1:F:388:ILE:HD11	1.89	0.55
1:A:57:LEU:HD11	1:A:143:ASN:HA	1.89	0.55
2:G:156:PRO:HD3	2:G:231:PHE:CE2	2.42	0.55
2:G:228:ARG:O	2:G:232:ASP:OD1	2.25	0.55
3:C:77:LEU:HA	3:C:80:SER:CB	2.36	0.55
3:C:195:PHE:CD1	3:C:199:TYR:HB2	2.41	0.55
1:A:415:PHE:CD1	1:A:472:TYR:HD2	2.25	0.55
2:B:173:SER:HB3	2:B:207:SER:O	2.07	0.55
1:F:61:TYR:O	1:F:62:ILE:C	2.45	0.55
2:B:132:VAL:O	2:B:132:VAL:HG12	2.07	0.55
2:B:227:ASP:OD1	2:B:229:ALA:HB3	2.07	0.55
2:G:82:TRP:HE3	2:G:83:SER:H	1.55	0.55
1:A:102:ILE:O	1:A:104:THR:N	2.40	0.55
1:A:106:HIS:CD2	1:A:107:GLY:N	2.75	0.55
1:A:225:MET:SD	1:A:230:TRP:HA	2.47	0.55
2:B:175:PHE:HD2	2:B:206:ILE:HD11	1.72	0.55
1:F:515:GLN:CG	1:F:516:MET:N	2.68	0.55
1:F:515:GLN:O	1:F:518:VAL:HB	2.07	0.55
1:F:104:THR:HG23	6:F:1001:HEM:O2D	2.06	0.54
1:A:515:GLN:CG	1:A:516:MET:N	2.68	0.54
3:H:136:LEU:O	3:H:140:PHE:HB2	2.06	0.54
2:G:165:VAL:HG12	2:G:166:THR:N	2.22	0.54
1:F:394:GLY:HA3	1:F:422:ASN:OD1	2.07	0.54
1:F:96:PRO:HB3	1:F:100:ASP:OD1	2.07	0.54
1:A:110:MET:O	1:A:115:ALA:HB3	2.07	0.54
1:A:359:THR:HB	7:A:1002:HEO:C27	2.37	0.54
1:A:426:GLY:HA2	1:A:430:PHE:CD1	2.42	0.54
1:F:73:PHE:O	1:F:74:ALA:C	2.45	0.54
2:G:36:ILE:CD1	2:G:39:GLU:H	2.20	0.54
2:G:37:GLY:O	2:G:40:GLN:HG2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:159:THR:HG21	2:G:228:ARG:NH2	2.22	0.54
2:B:155:PHE:HA	2:B:231:PHE:CE1	2.42	0.54
1:A:159:SER:CA	1:A:189:TYR:CD1	2.81	0.54
3:H:195:PHE:CD1	3:H:199:TYR:HB2	2.41	0.54
1:A:446:PHE:CZ	1:A:520:ILE:HA	2.42	0.54
1:F:466:VAL:O	1:F:501:GLY:HA3	2.07	0.54
1:F:497:ILE:O	1:F:500:SER:HB2	2.07	0.54
3:H:145:THR:C	3:H:147:GLY:H	2.11	0.54
3:C:156:TRP:HE1	3:C:180:LEU:CD1	2.20	0.54
1:A:497:ILE:O	1:A:500:SER:HB2	2.07	0.54
3:C:111:GLY:O	3:C:114:GLY:N	2.39	0.54
1:F:280:TRP:HE3	1:F:280:TRP:HA	1.73	0.54
3:C:146:HIS:HE1	3:C:190:VAL:HB	1.73	0.54
1:A:310:LEU:HD11	1:A:366:TRP:CD1	2.42	0.54
2:B:50:LEU:HA	2:B:53:ILE:CG2	2.38	0.54
1:F:174:PRO:HB2	1:F:175:PRO:HD3	1.87	0.54
1:F:238:LEU:CB	1:F:289:ILE:HD11	2.36	0.54
1:F:346:ALA:HB1	1:F:350:ILE:HD12	1.89	0.54
2:B:140:PHE:HD2	2:B:149:THR:HG1	1.56	0.54
1:F:306:SER:O	1:F:374:ARG:O	2.26	0.54
3:H:68:PHE:O	3:H:72:GLU:HB2	2.07	0.54
3:H:72:GLU:OE1	3:H:72:GLU:HA	2.07	0.54
3:C:156:TRP:HE1	3:C:180:LEU:CD2	2.20	0.54
1:A:174:PRO:HB3	1:A:175:PRO:HD3	1.82	0.54
1:A:205:GLY:O	1:A:209:PHE:HB2	2.08	0.54
2:B:200:PRO:HA	2:B:224:ALA:O	2.07	0.54
2:B:65:PHE:O	2:B:68:LYS:HE2	2.08	0.54
1:A:209:PHE:HE2	3:C:31:ILE:HD13	1.72	0.54
1:A:332:LEU:HD22	1:A:335:PHE:CB	2.37	0.54
1:A:69:LEU:HD13	1:A:73:PHE:CE1	2.43	0.54
2:B:40:GLN:HB2	2:B:41:ARG:NH1	2.23	0.54
1:F:118:PHE:CZ	1:F:294:VAL:HG22	2.42	0.54
1:F:480:THR:HB	1:F:483:LEU:HD11	1.88	0.54
1:A:515:GLN:O	1:A:518:VAL:HB	2.07	0.54
1:F:446:PHE:CZ	1:F:520:ILE:HA	2.43	0.54
1:A:116:MET:N	1:A:117:PRO:CD	2.70	0.54
2:B:273:LEU:O	2:B:276:ASP:HB2	2.08	0.54
2:G:132:VAL:O	2:G:132:VAL:HG12	2.08	0.54
1:F:251:ALA:O	1:F:254:THR:HB	2.08	0.54
3:H:90:MET:HE3	4:I:67:UNK:CB	2.37	0.54
2:B:88:VAL:O	2:B:91:VAL:HB	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:39:GLU:HG2	2:G:40:GLN:OE1	2.08	0.54
3:C:86:ALA:C	3:C:88:ILE:H	2.11	0.54
2:G:155:PHE:HA	2:G:231:PHE:CE1	2.42	0.54
1:A:216:ARG:HH12	1:A:222:MET:CA	2.21	0.54
2:G:273:LEU:O	2:G:276:ASP:HB2	2.08	0.54
1:A:112:PHE:CE1	1:A:286:GLU:OE2	2.58	0.54
4:D:20:UNK:CB	4:D:53:UNK:CB	2.86	0.54
1:A:187:VAL:O	1:A:190:TRP:HB3	2.08	0.54
3:C:30:TRP:CZ2	4:D:79:UNK:CB	2.91	0.54
2:G:243:ASN:O	2:G:266:PHE:HA	2.07	0.54
2:B:230:ALA:HA	2:B:233:GLN:NE2	2.22	0.54
3:H:156:TRP:HE1	3:H:180:LEU:CD1	2.20	0.54
1:F:216:ARG:HH12	1:F:222:MET:HA	1.72	0.54
2:B:165:VAL:O	2:B:191:THR:HG23	2.08	0.54
1:A:119:VAL:HG22	1:A:123:MET:HE2	1.90	0.54
1:A:277:ASN:OD1	1:A:331:TRP:NE1	2.41	0.54
3:C:88:ILE:HG23	3:C:98:VAL:CG1	2.37	0.54
2:G:197:ALA:C	2:G:198:ASN:HD22	2.11	0.54
3:H:49:VAL:O	3:H:51:VAL:N	2.33	0.54
1:F:397:THR:HG21	1:F:472:TYR:OH	2.07	0.54
1:A:288:TYR:OH	1:A:355:ILE:HG21	2.08	0.53
1:A:369:THR:O	1:A:369:THR:HG22	2.07	0.53
1:F:310:LEU:HD11	1:F:366:TRP:CD1	2.43	0.53
2:G:192:ARG:CZ	2:G:192:ARG:HB2	2.38	0.53
2:G:207:SER:OG	2:G:218:MET:HB2	2.08	0.53
1:A:192:TRP:HA	1:A:192:TRP:HE3	1.73	0.53
1:F:253:LEU:O	1:F:256:ASP:N	2.41	0.53
3:H:152:SER:C	3:H:154:LEU:H	2.11	0.53
1:F:110:MET:O	1:F:115:ALA:HB3	2.08	0.53
1:F:308:LYS:NZ	1:F:372:GLN:CB	2.71	0.53
3:C:196:THR:O	3:C:196:THR:HG22	2.08	0.53
1:A:111:ILE:HD11	6:A:1001:HEM:HMD2	1.91	0.53
1:A:118:PHE:CE2	1:A:294:VAL:HG22	2.43	0.53
1:A:357:ILE:HB	1:A:358:PRO:HD3	1.90	0.53
2:B:50:LEU:HA	2:B:53:ILE:HG22	1.90	0.53
2:G:88:VAL:O	2:G:91:VAL:HB	2.09	0.53
1:A:308:LYS:NZ	1:A:372:GLN:CB	2.71	0.53
2:B:197:ALA:C	2:B:198:ASN:HD22	2.12	0.53
3:C:160:LEU:HD13	3:C:176:ARG:CD	2.33	0.53
1:A:216:ARG:NH1	1:A:222:MET:CA	2.70	0.53
1:F:138:PHE:HB2	1:F:207:ASN:HD21	1.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:227:ASP:OD1	2:G:229:ALA:HB3	2.09	0.53
7:A:1002:HEO:C24	2:B:100:ILE:HG12	2.38	0.53
2:B:41:ARG:H	2:B:41:ARG:HH11	1.56	0.53
2:G:190:GLN:NE2	2:G:192:ARG:HH21	2.06	0.53
1:A:150:VAL:O	1:A:153:VAL:HB	2.08	0.53
1:F:112:PHE:CE1	1:F:286:GLU:OE2	2.59	0.53
2:G:74:LYS:HE2	2:G:75:ASP:OD2	2.08	0.53
1:A:119:VAL:HG22	1:A:123:MET:CE	2.39	0.53
1:F:239:ILE:HG12	1:F:289:ILE:HD13	1.91	0.53
7:F:1002:HEO:H241	2:G:99:ILE:HB	1.90	0.53
2:B:140:PHE:CD2	2:B:153:ILE:HG23	2.44	0.53
2:B:150:VAL:O	2:B:151:ASN:HB2	2.09	0.53
1:A:383:TRP:HB3	1:A:434:ALA:HB2	1.91	0.53
2:B:167:SER:HB3	2:B:187:ALA:HA	1.91	0.53
3:H:89:ALA:HB2	3:H:174:ARG:CD	2.27	0.53
1:A:235:ALA:HB2	1:A:292:LEU:HB2	1.90	0.53
1:A:171:LEU:HD11	1:A:280:TRP:CH2	2.44	0.53
2:G:143:PRO:HG2	2:G:144:GLU:OE2	2.08	0.53
3:C:174:ARG:HD3	3:C:177:ILE:HD11	1.91	0.53
3:C:113:ILE:HD11	3:C:150:VAL:CG1	2.38	0.53
3:H:197:VAL:CG1	3:H:198:VAL:H	2.20	0.53
2:B:192:ARG:HB2	2:B:192:ARG:CZ	2.39	0.53
3:C:72:GLU:OE1	3:C:72:GLU:HA	2.08	0.53
1:F:116:MET:N	1:F:117:PRO:CD	2.71	0.53
1:A:113:PHE:HE2	1:A:153:VAL:N	2.07	0.53
1:A:398:GLY:C	7:A:1002:HEO:HMB3	2.29	0.53
2:B:36:ILE:CD1	2:B:39:GLU:H	2.22	0.53
2:B:90:ALA:HA	2:B:93:TRP:CB	2.35	0.53
1:F:441:PRO:C	1:F:443:ALA:H	2.12	0.53
2:B:136:TRP:CE2	2:B:213:PRO:O	2.61	0.53
1:A:502:ALA:O	1:A:504:LEU:N	2.42	0.53
1:F:316:LEU:HD11	1:F:365:ASN:HB3	1.91	0.53
3:H:113:ILE:HD11	3:H:150:VAL:CG1	2.38	0.53
1:F:301:ILE:HG23	1:F:380:ALA:HB1	1.90	0.53
1:F:415:PHE:CD1	1:F:472:TYR:HD2	2.27	0.53
1:A:466:VAL:O	1:A:501:GLY:HA3	2.09	0.53
3:C:33:LEU:HB2	3:C:34:MET:CE	2.39	0.53
1:F:383:TRP:HB3	1:F:434:ALA:HB2	1.91	0.53
1:A:199:ILE:O	1:A:202:THR:HB	2.09	0.53
1:A:367:LEU:HA	1:A:370:MET:HE2	1.90	0.53
1:A:311:PHE:CZ	2:B:88:VAL:HG21	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:190:TRP:HE3	1:F:191:ILE:HG12	1.74	0.53
1:F:279:ILE:HG22	1:F:280:TRP:N	2.24	0.53
2:G:90:ALA:HA	2:G:93:TRP:CB	2.36	0.53
1:F:57:LEU:HD12	1:F:142:ASN:HD22	1.74	0.53
3:C:197:VAL:CG1	3:C:198:VAL:H	2.20	0.53
1:A:441:PRO:C	1:A:443:ALA:H	2.12	0.53
1:F:192:TRP:HA	1:F:192:TRP:HE3	1.74	0.53
3:H:99:ILE:N	3:H:99:ILE:CD1	2.72	0.53
1:A:104:THR:HG23	6:A:1001:HEM:O2D	2.08	0.53
2:B:39:GLU:HG2	2:B:40:GLN:OE1	2.09	0.53
1:F:174:PRO:HB2	1:F:175:PRO:CD	2.39	0.53
1:F:288:TYR:HE2	1:F:323:ILE:HG23	1.74	0.53
2:G:264:GLU:CG	2:G:265:TYR:H	2.16	0.53
2:G:39:GLU:HG2	2:G:40:GLN:N	2.24	0.53
2:B:228:ARG:O	2:B:232:ASP:OD1	2.27	0.53
1:A:306:SER:O	1:A:374:ARG:O	2.27	0.53
2:G:125:LYS:H	2:G:126:PRO:HD2	1.71	0.53
1:F:486:GLN:C	1:F:487:ILE:HG13	2.29	0.53
1:F:52:VAL:O	1:F:52:VAL:HG12	2.09	0.53
1:F:187:VAL:O	1:F:190:TRP:HB3	2.09	0.52
1:F:205:GLY:O	1:F:209:PHE:HB2	2.09	0.52
1:F:359:THR:HB	7:F:1002:HEO:C27	2.39	0.52
3:C:193:CYS:O	3:C:194:VAL:C	2.46	0.52
3:H:196:THR:HA	3:H:200:LEU:CD2	2.38	0.52
2:G:136:TRP:CE2	2:G:213:PRO:O	2.61	0.52
1:A:502:ALA:O	1:A:503:VAL:C	2.47	0.52
3:H:102:LEU:O	3:H:105:THR:HB	2.09	0.52
3:C:21:ALA:HA	3:C:24:THR:OG1	2.09	0.52
1:A:301:ILE:HG23	1:A:380:ALA:HB1	1.90	0.52
1:F:225:MET:HG3	1:F:229:THR:HB	1.90	0.52
1:F:378:HIS:O	1:F:379:SER:C	2.48	0.52
1:A:382:LEU:HD23	1:A:385:ILE:CD1	2.39	0.52
2:B:82:TRP:HE3	2:B:83:SER:H	1.57	0.52
3:H:174:ARG:HD3	3:H:177:ILE:HD11	1.92	0.52
1:A:280:TRP:HE3	1:A:280:TRP:HA	1.75	0.52
1:A:548:PRO:O	1:A:550:TYR:N	2.42	0.52
1:F:169:GLY:O	1:F:171:LEU:N	2.43	0.52
1:F:171:LEU:HD11	1:F:280:TRP:CH2	2.44	0.52
3:C:74:PHE:CE2	3:C:188:ASP:HA	2.44	0.52
2:B:67:TRP:CG	2:B:68:LYS:N	2.75	0.52
3:H:47:TYR:O	3:H:51:VAL:HG13	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:394:GLY:HA3	1:A:422:ASN:OD1	2.09	0.52
1:F:502:ALA:O	1:F:504:LEU:N	2.43	0.52
1:F:206:ILE:HG23	3:H:31:ILE:CG2	2.40	0.52
2:G:270:LYS:HZ2	2:G:272:ASP:H	1.56	0.52
3:H:33:LEU:HB2	3:H:34:MET:CE	2.39	0.52
1:A:336:PHE:CE2	1:A:404:PRO:HG3	2.44	0.52
1:F:235:ALA:HB2	1:F:292:LEU:HB2	1.90	0.52
2:G:89:GLU:O	2:G:93:TRP:HB2	2.09	0.52
2:G:67:TRP:CG	2:G:68:LYS:N	2.76	0.52
2:B:177:PRO:O	2:B:179:LEU:N	2.43	0.52
3:H:83:TYR:CZ	4:I:14:UNK:CB	2.88	0.52
2:B:101:ILE:CA	2:B:104:ALA:HB3	2.40	0.52
2:G:95:VAL:CG2	2:G:96:PRO:HD3	2.33	0.52
1:A:373:GLY:HA2	2:B:71:ALA:O	2.10	0.52
3:C:46:THR:O	3:C:49:VAL:HB	2.10	0.52
1:F:543:THR:CG2	1:F:544:SER:N	2.72	0.52
2:G:200:PRO:HA	2:G:224:ALA:O	2.09	0.52
3:H:174:ARG:HB3	3:H:177:ILE:CD1	2.39	0.52
3:C:185:HIS:NE2	4:D:57:UNK:O	2.42	0.52
2:B:37:GLY:O	2:B:40:GLN:HG2	2.10	0.52
2:B:228:ARG:HG3	2:B:231:PHE:CD2	2.44	0.52
3:H:193:CYS:O	3:H:194:VAL:C	2.47	0.52
3:H:74:PHE:CE2	3:H:188:ASP:HA	2.44	0.52
2:B:207:SER:OG	2:B:218:MET:HB2	2.10	0.52
2:B:225:THR:HB	2:B:226:PRO:HD2	1.92	0.52
1:A:54:HIS:ND1	1:A:135:ASP:OD2	2.43	0.52
1:A:225:MET:HG3	1:A:229:THR:HB	1.92	0.52
1:A:312:GLY:O	1:A:316:LEU:HG	2.10	0.52
2:B:138:TRP:CZ3	2:B:174:PHE:HD1	2.23	0.52
1:F:362:LYS:HB3	1:F:366:TRP:CH2	2.45	0.52
2:G:230:ALA:HA	2:G:233:GLN:NE2	2.25	0.52
3:C:145:THR:C	3:C:147:GLY:H	2.12	0.52
1:A:253:LEU:O	1:A:256:ASP:N	2.43	0.52
2:B:39:GLU:HG2	2:B:40:GLN:N	2.25	0.52
1:F:205:GLY:O	1:F:240:ILE:HD11	2.10	0.52
2:B:125:LYS:H	2:B:126:PRO:HD2	1.72	0.52
3:H:21:ALA:HA	3:H:24:THR:OG1	2.10	0.52
4:D:86:UNK:O	4:D:87:UNK:C	2.57	0.52
4:D:11:UNK:O	4:D:15:UNK:N	2.42	0.52
1:A:362:LYS:HB3	1:A:366:TRP:CH2	2.45	0.51
1:F:363:ILE:HG22	1:F:364:PHE:N	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:420:PHE:HA	1:F:423:VAL:HG22	1.91	0.51
2:G:95:VAL:HA	2:G:98:LEU:HD12	1.93	0.51
1:F:474:LEU:CD2	1:F:494:MET:HB2	2.31	0.51
1:F:57:LEU:C	1:F:60:MET:HB2	2.29	0.51
1:F:248:VAL:O	1:F:252:LEU:HG	2.11	0.51
3:H:42:ILE:O	3:H:45:ALA:HB3	2.10	0.51
1:A:68:MET:CE	1:A:153:VAL:HG13	2.40	0.51
1:A:318:TRP:O	1:A:322:CYS:SG	2.69	0.51
1:A:311:PHE:CG	1:A:312:GLY:N	2.79	0.51
1:A:405:GLY:HA2	1:A:408:PHE:HD1	1.73	0.51
1:F:277:ASN:CA	1:F:335:PHE:HZ	2.22	0.51
2:G:50:LEU:HA	2:G:53:ILE:CG2	2.40	0.51
1:F:307:ARG:O	2:G:79:SER:HB2	2.10	0.51
1:F:203:LEU:O	1:F:206:ILE:N	2.42	0.51
2:B:93:TRP:C	2:B:96:PRO:HD2	2.30	0.51
1:F:311:PHE:CZ	2:G:88:VAL:HG21	2.45	0.51
3:C:143:VAL:O	3:C:146:HIS:N	2.44	0.51
3:H:145:THR:C	3:H:147:GLY:N	2.62	0.51
2:G:273:LEU:HA	2:G:276:ASP:HB2	1.91	0.51
3:C:97:GLN:HG2	3:C:97:GLN:O	2.10	0.51
2:G:101:ILE:O	2:G:105:VAL:HG23	2.10	0.51
4:I:11:UNK:O	4:I:15:UNK:N	2.42	0.51
1:A:52:VAL:HG12	1:A:52:VAL:O	2.10	0.51
2:B:74:LYS:HE2	2:B:75:ASP:OD2	2.09	0.51
2:G:159:THR:O	2:G:196:ILE:HD13	2.10	0.51
1:A:298:PHE:CE1	1:A:384:THR:HG23	2.45	0.51
1:F:214:LYS:HZ2	3:H:24:THR:HA	1.73	0.51
1:F:125:LEU:C	1:F:125:LEU:HD23	2.31	0.51
3:C:180:LEU:C	3:C:182:LEU:H	2.13	0.51
1:F:150:VAL:O	1:F:153:VAL:HB	2.10	0.51
1:F:68:MET:CE	1:F:153:VAL:HG13	2.40	0.51
1:F:464:PHE:CD1	1:F:468:PHE:HD1	2.27	0.51
1:F:502:ALA:O	1:F:503:VAL:C	2.49	0.51
1:F:54:HIS:ND1	1:F:135:ASP:OD2	2.44	0.51
3:H:200:LEU:HD12	3:H:201:MET:N	2.25	0.51
3:H:46:THR:O	3:H:49:VAL:HB	2.11	0.51
1:A:451:THR:HG22	1:A:452:TRP:N	2.24	0.51
1:A:211:THR:HG23	1:A:215:MET:CE	2.39	0.51
2:B:273:LEU:HA	2:B:276:ASP:HB2	1.92	0.51
1:F:442:LYS:HB2	1:F:541:TRP:HZ3	1.75	0.51
1:A:255:LEU:HB3	1:A:261:THR:HG21	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:431:GLY:O	1:A:432:CYS:C	2.48	0.51
1:A:356:ALA:O	1:A:359:THR:N	2.42	0.51
1:F:312:GLY:O	1:F:316:LEU:HG	2.10	0.51
1:F:332:LEU:HD22	1:F:335:PHE:CB	2.40	0.51
1:F:73:PHE:O	1:F:77:ILE:HG13	2.11	0.51
2:G:99:ILE:HD13	2:G:99:ILE:N	2.26	0.51
2:B:163:PHE:CD2	2:B:193:LEU:HD22	2.45	0.51
1:A:378:HIS:O	1:A:379:SER:C	2.49	0.51
3:H:180:LEU:C	3:H:182:LEU:H	2.14	0.51
1:A:460:TRP:HZ3	1:A:509:ILE:HG12	1.76	0.51
3:H:91:TYR:OH	4:I:7:UNK:N	2.42	0.51
1:A:108:VAL:CG2	1:A:170:TRP:HA	2.36	0.51
1:A:279:ILE:HG22	1:A:280:TRP:N	2.25	0.51
1:A:277:ASN:CA	1:A:335:PHE:HZ	2.22	0.51
1:A:346:ALA:HB1	1:A:350:ILE:HD12	1.92	0.51
1:F:282:TRP:O	1:F:285:PRO:HD2	2.11	0.51
1:F:356:ALA:O	1:F:359:THR:N	2.42	0.51
1:F:54:HIS:CG	1:F:55:LYS:N	2.79	0.51
2:G:50:LEU:HA	2:G:53:ILE:HG22	1.92	0.51
2:G:65:PHE:O	2:G:68:LYS:HE2	2.11	0.51
1:A:57:LEU:C	1:A:60:MET:HB2	2.30	0.51
1:A:375:ILE:HG21	1:A:381:MET:HE2	1.92	0.51
1:A:316:LEU:HD11	1:A:365:ASN:HB3	1.93	0.51
2:B:175:PHE:HD1	2:B:181:SER:C	2.15	0.51
2:B:85:SER:HB3	2:B:88:VAL:HG13	1.93	0.51
1:F:311:PHE:CG	1:F:312:GLY:N	2.79	0.51
3:C:90:MET:HE1	4:D:68:UNK:HA	1.93	0.51
3:H:69:VAL:HG12	3:H:115:MET:SD	2.51	0.51
3:C:71:VAL:HG22	3:C:191:TRP:HE1	1.76	0.51
1:F:216:ARG:NH1	1:F:222:MET:CA	2.73	0.51
1:F:451:THR:HG22	1:F:452:TRP:N	2.24	0.51
3:H:89:ALA:HB1	3:H:171:SER:HA	1.93	0.50
1:F:108:VAL:CG2	1:F:170:TRP:HA	2.37	0.50
1:F:405:GLY:HA2	1:F:408:PHE:HD1	1.73	0.50
1:A:146:PHE:O	1:A:149:THR:N	2.45	0.50
1:A:138:PHE:HZ	3:C:28:GLY:HA3	1.76	0.50
1:F:169:GLY:O	1:F:172:ALA:N	2.44	0.50
2:G:138:TRP:CZ3	2:G:174:PHE:HD1	2.22	0.50
2:G:36:ILE:HG12	2:G:39:GLU:HB3	1.92	0.50
3:C:76:LEU:HB2	3:C:108:PHE:CE2	2.45	0.50
3:H:76:LEU:HB2	3:H:108:PHE:CE2	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:TRP:HE3	1:A:191:ILE:HG12	1.76	0.50
1:A:274:MET:HA	1:A:274:MET:CE	2.42	0.50
2:G:175:PHE:HD1	2:G:181:SER:C	2.15	0.50
1:A:142:ASN:OD1	1:A:208:PHE:HE1	1.95	0.50
3:C:99:ILE:CD1	3:C:99:ILE:N	2.74	0.50
1:F:160:LEU:HD23	1:F:165:PHE:HB2	1.92	0.50
1:F:159:SER:CB	1:F:189:TYR:HD1	2.24	0.50
1:F:216:ARG:HH12	1:F:222:MET:CA	2.24	0.50
1:A:330:VAL:HG12	1:A:351:THR:HB	1.94	0.50
1:A:353:MET:SD	2:B:107:THR:HG21	2.51	0.50
1:F:170:TRP:CE2	1:F:171:LEU:HD21	2.45	0.50
1:A:142:ASN:OD1	1:A:208:PHE:CE1	2.64	0.50
2:G:155:PHE:HZ	2:G:222:ALA:HB1	1.76	0.50
3:C:145:THR:C	3:C:147:GLY:N	2.63	0.50
3:C:160:LEU:O	3:C:163:GLN:HB3	2.10	0.50
1:A:263:PHE:HE2	3:C:46:THR:HG21	1.75	0.50
1:A:209:PHE:CE2	3:C:31:ILE:HD11	2.45	0.50
1:A:239:ILE:HG22	1:A:239:ILE:O	2.11	0.50
1:A:411:HIS:NE2	1:A:412:ASN:OD1	2.44	0.50
1:F:171:LEU:O	1:F:172:ALA:HB3	2.12	0.50
2:G:127:ILE:HG22	2:G:128:THR:N	2.26	0.50
2:G:175:PHE:HD2	2:G:206:ILE:HD11	1.77	0.50
3:H:47:TYR:O	3:H:49:VAL:N	2.45	0.50
3:H:166:ARG:NE	3:H:167:ARG:HH22	2.09	0.50
2:G:225:THR:HB	2:G:226:PRO:HD2	1.94	0.50
1:A:72:GLY:O	1:A:75:ASP:HB2	2.12	0.50
1:A:295:PHE:HE2	1:A:362:LYS:HG3	1.77	0.50
1:A:209:PHE:CE2	3:C:31:ILE:HD13	2.45	0.50
1:F:374:ARG:N	2:G:71:ALA:O	2.45	0.50
3:H:196:THR:O	3:H:196:THR:HG22	2.12	0.50
1:A:156:VAL:HG12	1:A:160:LEU:CD1	2.41	0.50
2:G:270:LYS:HE3	2:G:276:ASP:CG	2.32	0.50
1:A:203:LEU:O	1:A:206:ILE:N	2.44	0.50
2:B:95:VAL:HA	2:B:98:LEU:HD12	1.94	0.50
1:F:277:ASN:N	1:F:335:PHE:HZ	2.10	0.50
1:F:353:MET:SD	2:G:107:THR:HG21	2.51	0.50
1:F:367:LEU:HD23	1:F:370:MET:HE1	1.93	0.50
1:F:69:LEU:O	1:F:73:PHE:HB2	2.12	0.50
2:G:196:ILE:CG2	2:G:198:ASN:HD21	2.24	0.50
3:H:29:PHE:HZ	3:H:182:LEU:HB3	1.76	0.50
1:F:131:ILE:O	1:F:217:ALA:HB2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:406:ALA:HB2	2:B:45:LEU:CD2	2.42	0.50
1:A:331:TRP:CH2	4:D:97:UNK:CB	2.95	0.50
3:C:150:VAL:HG12	3:C:150:VAL:O	2.10	0.50
1:A:137:ALA:H	1:A:215:MET:HE2	1.76	0.50
2:B:270:LYS:HZ2	2:B:272:ASP:H	1.58	0.50
1:F:155:LEU:HD13	1:F:193:SER:CA	2.42	0.50
1:F:431:GLY:O	1:F:432:CYS:C	2.49	0.50
1:A:54:HIS:CE1	1:A:135:ASP:OD2	2.65	0.50
1:A:111:ILE:CD1	1:A:170:TRP:CE3	2.95	0.50
1:A:330:VAL:HB	1:A:352:THR:OG1	2.12	0.50
2:B:39:GLU:O	2:B:43:LEU:N	2.37	0.50
2:B:97:ILE:O	2:B:101:ILE:HD12	2.12	0.50
2:B:176:ILE:CG2	2:B:179:LEU:HD12	2.30	0.50
1:F:202:THR:O	1:F:206:ILE:HG13	2.11	0.50
1:A:442:LYS:NZ	1:A:543:THR:O	2.45	0.50
1:F:543:THR:HG22	1:F:544:SER:H	1.77	0.50
1:A:169:GLY:O	1:A:171:LEU:N	2.45	0.49
2:B:89:GLU:O	2:B:93:TRP:HB2	2.11	0.49
1:F:54:HIS:CE1	1:F:135:ASP:OD2	2.65	0.49
1:F:551:ASN:O	1:F:552:PHE:CB	2.57	0.49
1:F:298:PHE:CE1	1:F:384:THR:HG23	2.47	0.49
3:H:160:LEU:HD13	3:H:176:ARG:CD	2.33	0.49
4:D:71:UNK:O	4:D:72:UNK:C	2.59	0.49
1:A:202:THR:O	1:A:206:ILE:HG13	2.11	0.49
1:A:417:ILE:HD13	6:A:1001:HEM:HBA2	1.94	0.49
3:C:30:TRP:CZ2	4:D:79:UNK:C	2.95	0.49
1:F:118:PHE:CE2	1:F:294:VAL:HG22	2.46	0.49
1:A:442:LYS:HB2	1:A:541:TRP:HZ3	1.76	0.49
1:F:146:PHE:O	1:F:149:THR:N	2.46	0.49
4:D:108:UNK:O	4:D:109:UNK:CB	2.59	0.49
1:A:120:ILE:HG23	1:A:204:THR:HG21	1.94	0.49
1:A:548:PRO:O	1:A:551:ASN:N	2.45	0.49
1:F:295:PHE:HE2	1:F:362:LYS:HG3	1.77	0.49
1:F:411:HIS:NE2	1:F:412:ASN:OD1	2.45	0.49
3:H:199:TYR:CD1	3:H:199:TYR:N	2.79	0.49
1:A:452:TRP:HA	1:A:455:ARG:CD	2.37	0.49
2:G:132:VAL:O	2:G:134:MET:SD	2.70	0.49
1:A:329:ILE:O	1:A:329:ILE:HG22	2.12	0.49
1:F:119:VAL:HG22	1:F:123:MET:CE	2.41	0.49
1:F:191:ILE:CG2	1:F:250:VAL:HG13	2.43	0.49
3:H:143:VAL:O	3:H:144:GLY:C	2.49	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:136:VAL:HG23	1:F:211:THR:OG1	2.12	0.49
1:A:447:LYS:HG3	1:A:448:LEU:N	2.25	0.49
4:I:71:UNK:O	4:I:72:UNK:C	2.59	0.49
3:C:166:ARG:NE	3:C:167:ARG:HH22	2.09	0.49
1:A:367:LEU:HD23	1:A:370:MET:HE3	1.94	0.49
1:A:169:GLY:HA2	1:A:482:ARG:NH1	2.28	0.49
1:A:54:HIS:CG	1:A:55:LYS:N	2.81	0.49
1:F:482:ARG:NH2	6:F:1001:HEM:CGD	2.76	0.49
2:G:36:ILE:HG12	2:G:39:GLU:N	2.22	0.49
2:B:264:GLU:CG	2:B:265:TYR:H	2.19	0.49
3:C:90:MET:CE	4:D:67:UNK:C	2.90	0.49
1:A:465:PHE:O	1:A:470:PRO:HD3	2.13	0.49
1:F:151:VAL:HG11	1:F:196:LEU:HD13	1.93	0.49
1:A:363:ILE:HG22	1:A:364:PHE:N	2.27	0.49
1:F:336:PHE:CE2	1:F:404:PRO:HG3	2.46	0.49
1:F:485:GLN:HA	1:F:485:GLN:OE1	2.12	0.49
1:A:191:ILE:CG2	1:A:250:VAL:HG13	2.43	0.49
1:F:374:ARG:HB2	2:G:78:TYR:O	2.12	0.49
1:A:374:ARG:CB	2:B:79:SER:HB3	2.35	0.49
1:F:274:MET:CE	1:F:274:MET:HA	2.43	0.49
1:F:155:LEU:HD12	1:F:196:LEU:HD12	1.94	0.49
1:A:169:GLY:O	1:A:172:ALA:N	2.46	0.49
1:A:288:TYR:HE2	1:A:323:ILE:HG23	1.78	0.49
2:B:36:ILE:HG12	2:B:39:GLU:HB3	1.94	0.49
1:A:488:ASP:OD1	1:A:490:GLN:HG3	2.13	0.49
1:A:464:PHE:HA	1:A:505:ILE:HD11	1.94	0.49
1:A:155:LEU:HD13	1:A:193:SER:CA	2.43	0.49
1:A:480:THR:OG1	2:B:206:ILE:HB	2.11	0.49
1:F:72:GLY:O	1:F:75:ASP:HB2	2.13	0.49
2:G:85:SER:HB3	2:G:88:VAL:HG13	1.95	0.49
1:A:373:GLY:CA	2:B:71:ALA:HB1	2.32	0.49
1:A:474:LEU:CD2	1:A:491:PHE:HA	2.43	0.49
3:H:102:LEU:HD23	3:H:161:MET:HE2	1.95	0.49
1:A:155:LEU:HD12	1:A:196:LEU:HD12	1.94	0.49
3:H:91:TYR:HE2	4:I:6:UNK:CB	2.26	0.49
2:B:183:ILE:HG13	2:B:184:TYR:N	2.28	0.49
2:G:157:ALA:O	2:G:158:ASN:C	2.51	0.49
1:A:136:VAL:HG23	1:A:211:THR:OG1	2.13	0.49
3:H:97:GLN:HG2	3:H:97:GLN:O	2.13	0.49
2:B:48:PHE:CE1	2:B:52:LEU:HD11	2.48	0.49
1:A:69:LEU:O	1:A:73:PHE:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:411:HIS:ND1	7:F:1002:HEO:O2A	2.45	0.48
4:I:103:UNK:O	4:I:106:UNK:HA	2.13	0.48
3:C:89:ALA:HB1	3:C:171:SER:HA	1.95	0.48
3:C:174:ARG:HB3	3:C:177:ILE:CD1	2.43	0.48
2:G:176:ILE:CG2	2:G:179:LEU:HD12	2.30	0.48
3:H:160:LEU:O	3:H:163:GLN:HB3	2.12	0.48
1:A:131:ILE:O	1:A:217:ALA:HB2	2.13	0.48
2:G:202:THR:HA	2:G:223:ILE:HA	1.95	0.48
1:F:426:GLY:HA2	1:F:430:PHE:CE1	2.48	0.48
2:G:170:VAL:HG23	2:G:171:MET:O	2.13	0.48
3:C:143:VAL:O	3:C:144:GLY:C	2.50	0.48
3:C:66:LEU:N	3:C:67:PRO:CD	2.75	0.48
2:G:130:GLU:OE1	2:G:141:ILE:O	2.30	0.48
2:B:202:THR:HA	2:B:223:ILE:HA	1.95	0.48
4:D:25:UNK:O	4:D:29:UNK:N	2.46	0.48
2:B:50:LEU:CA	2:B:53:ILE:HG22	2.43	0.48
1:F:120:ILE:HG23	1:F:204:THR:HG21	1.95	0.48
1:F:80:ARG:O	1:F:80:ARG:CG	2.60	0.48
1:F:396:MET:HB3	2:G:53:ILE:HD13	1.95	0.48
3:C:174:ARG:HH11	3:C:177:ILE:HG12	1.78	0.48
1:A:73:PHE:HE2	6:A:1001:HEM:HAB	1.78	0.48
1:F:447:LYS:HG3	1:F:448:LEU:N	2.26	0.48
3:C:29:PHE:HZ	3:C:182:LEU:HB3	1.78	0.48
1:A:466:VAL:O	1:A:466:VAL:HG12	2.13	0.48
1:F:147:TRP:O	1:F:151:VAL:HG23	2.13	0.48
2:G:275:ALA:O	2:G:279:ASN:ND2	2.47	0.48
1:A:73:PHE:O	1:A:77:ILE:HG13	2.14	0.48
2:B:243:ASN:O	2:B:266:PHE:HA	2.13	0.48
1:A:57:LEU:HD12	1:A:142:ASN:HD22	1.78	0.48
3:C:100:SER:O	3:C:103:ALA:HB3	2.14	0.48
3:C:112:PHE:HZ	3:C:191:TRP:CZ3	2.31	0.48
3:H:66:LEU:N	3:H:67:PRO:CD	2.75	0.48
3:H:71:VAL:HG22	3:H:191:TRP:HE1	1.79	0.48
3:C:51:VAL:HG12	3:C:135:PHE:CE2	2.48	0.48
2:G:136:TRP:HA	2:G:218:MET:SD	2.54	0.48
1:A:414:LEU:HD23	1:A:479:MET:HB3	1.96	0.48
1:F:465:PHE:O	1:F:470:PRO:HD3	2.14	0.48
1:A:105:ALA:O	1:A:108:VAL:HB	2.13	0.48
1:F:169:GLY:HA2	1:F:482:ARG:NH1	2.29	0.48
1:F:174:PRO:C	1:F:176:LEU:N	2.66	0.48
1:F:235:ALA:O	1:F:289:ILE:HG12	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:336:PHE:CE2	1:F:404:PRO:HA	2.48	0.48
1:A:382:LEU:HA	1:A:385:ILE:CD1	2.43	0.48
1:A:543:THR:CG2	1:A:544:SER:N	2.75	0.48
1:A:125:LEU:C	1:A:125:LEU:HD23	2.34	0.48
3:C:124:ILE:HD11	3:C:140:PHE:HZ	1.79	0.48
1:F:318:TRP:O	1:F:322:CYS:SG	2.68	0.48
4:I:25:UNK:O	4:I:29:UNK:N	2.46	0.48
1:A:485:GLN:HA	1:A:485:GLN:OE1	2.13	0.48
3:H:96:SER:C	3:H:98:VAL:N	2.67	0.48
1:A:235:ALA:O	1:A:289:ILE:HG12	2.13	0.48
1:A:332:LEU:HB2	1:A:348:PHE:CG	2.49	0.48
2:B:95:VAL:O	2:B:98:LEU:HB2	2.13	0.48
1:F:483:LEU:HD22	2:G:216:SER:HA	1.96	0.48
2:B:236:ALA:HA	2:B:239:LYS:HG3	1.96	0.48
3:H:150:VAL:HG12	3:H:150:VAL:O	2.13	0.48
1:F:486:GLN:HG2	1:F:492:HIS:NE2	2.29	0.48
1:A:332:LEU:CD2	1:A:335:PHE:CG	2.96	0.48
2:B:36:ILE:HG12	2:B:39:GLU:N	2.24	0.48
1:A:379:SER:O	1:A:382:LEU:HB2	2.14	0.48
1:A:464:PHE:CD1	1:A:468:PHE:HD1	2.31	0.48
1:F:330:VAL:HG12	1:F:351:THR:HB	1.96	0.48
2:G:184:TYR:CD2	2:G:186:MET:HB2	2.48	0.48
2:G:56:ILE:N	2:G:57:PRO:HD2	2.27	0.48
2:B:196:ILE:CG2	2:B:198:ASN:HD21	2.26	0.48
3:C:47:TYR:O	3:C:49:VAL:N	2.47	0.48
1:F:464:PHE:HA	1:F:505:ILE:HD11	1.95	0.48
1:A:151:VAL:HG11	1:A:196:LEU:HD13	1.94	0.48
3:C:166:ARG:HB2	3:C:167:ARG:NH2	2.27	0.48
3:H:88:ILE:CG1	3:H:98:VAL:HG13	2.37	0.47
1:A:282:TRP:O	1:A:285:PRO:HD2	2.14	0.47
2:B:101:ILE:HA	2:B:104:ALA:HB3	1.96	0.47
2:B:174:PHE:O	2:B:182:GLN:HA	2.14	0.47
2:B:186:MET:HB3	2:B:189:MET:HG3	1.95	0.47
1:F:105:ALA:O	1:F:108:VAL:HB	2.13	0.47
2:G:177:PRO:O	2:G:179:LEU:N	2.47	0.47
2:G:228:ARG:HG3	2:G:231:PHE:CD2	2.46	0.47
1:A:491:PHE:O	1:A:495:LEU:HG	2.14	0.47
3:C:66:LEU:C	3:C:68:PHE:H	2.18	0.47
1:A:96:PRO:HG2	2:B:213:PRO:HA	1.96	0.47
1:F:488:ASP:OD1	1:F:490:GLN:HG3	2.14	0.47
1:A:253:LEU:O	1:A:256:ASP:HB2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:33:LEU:C	3:H:35:SER:H	2.17	0.47
1:A:233:LEU:O	1:A:234:CYS:C	2.52	0.47
1:F:482:ARG:NH2	6:F:1001:HEM:O2D	2.47	0.47
2:G:95:VAL:O	2:G:99:ILE:HG12	2.14	0.47
3:H:143:VAL:O	3:H:146:HIS:N	2.47	0.47
2:G:136:TRP:HB2	2:G:259:GLU:HA	1.95	0.47
2:G:131:VAL:CG2	2:G:165:VAL:HG22	2.44	0.47
1:F:487:ILE:O	1:F:488:ASP:C	2.52	0.47
1:F:253:LEU:O	1:F:256:ASP:HB2	2.14	0.47
1:A:297:VAL:HG22	1:A:439:TRP:HZ3	1.79	0.47
1:A:330:VAL:HG13	1:A:351:THR:CG2	2.44	0.47
4:D:103:UNK:O	4:D:106:UNK:HA	2.14	0.47
2:G:175:PHE:HD1	2:G:181:SER:O	1.98	0.47
2:G:61:MET:HA	2:G:61:MET:CE	2.44	0.47
1:F:385:ILE:HA	1:F:388:ILE:HD12	1.95	0.47
3:C:96:SER:C	3:C:98:VAL:N	2.67	0.47
1:A:486:GLN:C	1:A:487:ILE:HG13	2.34	0.47
3:C:136:LEU:C	3:C:140:PHE:HB2	2.34	0.47
1:A:422:ASN:HA	1:A:464:PHE:CZ	2.49	0.47
3:H:166:ARG:HB2	3:H:167:ARG:NH2	2.27	0.47
3:H:85:MET:HA	3:H:88:ILE:HD12	1.95	0.47
3:H:78:PHE:HZ	4:I:57:UNK:HA	1.78	0.47
1:F:233:LEU:O	1:F:234:CYS:C	2.52	0.47
1:F:311:PHE:CZ	2:G:88:VAL:HG11	2.48	0.47
1:F:142:ASN:OD1	1:F:208:PHE:CE1	2.67	0.47
3:C:74:PHE:HD1	3:C:77:LEU:HD12	1.79	0.47
3:H:66:LEU:C	3:H:68:PHE:H	2.18	0.47
1:F:211:THR:HG23	1:F:215:MET:CE	2.42	0.47
3:H:47:TYR:C	3:H:49:VAL:H	2.17	0.47
3:H:124:ILE:HD11	3:H:140:PHE:HZ	1.80	0.47
1:A:464:PHE:HD2	1:A:465:PHE:CD1	2.33	0.47
1:A:170:TRP:NE1	1:A:171:LEU:HG	2.29	0.47
1:A:389:VAL:HG12	1:A:390:THR:N	2.29	0.47
2:G:184:TYR:CE2	2:G:189:MET:HE2	2.49	0.47
1:A:474:LEU:CD2	1:A:494:MET:HB2	2.34	0.47
1:A:516:MET:O	1:A:519:SER:N	2.40	0.47
3:C:195:PHE:CD1	3:C:199:TYR:CB	2.98	0.47
3:C:72:GLU:O	3:C:75:LEU:HB3	2.14	0.47
2:G:130:GLU:OE1	2:G:141:ILE:HG22	2.15	0.47
1:F:397:THR:HG23	1:F:415:PHE:CZ	2.49	0.47
1:F:460:TRP:HZ3	1:F:509:ILE:HG12	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:170:VAL:HG23	2:B:171:MET:O	2.15	0.47
1:A:384:THR:O	1:A:388:ILE:HG13	2.14	0.47
3:C:47:TYR:C	3:C:49:VAL:H	2.17	0.47
3:C:199:TYR:CD1	3:C:199:TYR:N	2.81	0.47
2:G:48:PHE:CE1	2:G:52:LEU:HD11	2.49	0.47
3:H:88:ILE:HG23	3:H:98:VAL:HG11	1.95	0.47
2:B:56:ILE:N	2:B:57:PRO:HD2	2.28	0.47
1:F:330:VAL:HG13	1:F:351:THR:CG2	2.44	0.47
2:G:174:PHE:O	2:G:182:GLN:HA	2.15	0.47
1:A:512:LEU:O	1:A:516:MET:HG3	2.14	0.47
3:H:51:VAL:HG12	3:H:135:PHE:CE2	2.49	0.47
4:I:73:UNK:O	4:I:75:UNK:N	2.48	0.47
3:H:120:PHE:O	3:H:121:HIS:C	2.52	0.47
1:A:147:TRP:O	1:A:151:VAL:HG23	2.14	0.47
3:H:174:ARG:CB	3:H:177:ILE:HD11	2.42	0.47
1:A:171:LEU:O	1:A:172:ALA:HB3	2.15	0.47
1:A:277:ASN:N	1:A:335:PHE:HZ	2.13	0.47
1:F:345:ASN:O	1:F:349:GLY:N	2.46	0.47
1:F:375:ILE:HG21	1:F:381:MET:HE2	1.96	0.47
3:C:89:ALA:O	3:C:90:MET:C	2.53	0.47
2:B:157:ALA:O	2:B:158:ASN:C	2.53	0.47
3:C:102:LEU:HB3	3:C:161:MET:HE2	1.96	0.47
3:H:29:PHE:C	3:H:31:ILE:H	2.16	0.47
1:A:406:ALA:HB2	2:B:45:LEU:HD22	1.96	0.47
1:A:412:ASN:CG	2:B:209:SER:HB3	2.35	0.47
2:B:61:MET:CE	2:B:61:MET:HA	2.45	0.47
1:F:306:SER:HB3	1:F:375:ILE:HG13	1.96	0.47
2:B:131:VAL:CG2	2:B:165:VAL:HG22	2.45	0.47
2:B:137:LYS:CE	2:B:261:ASN:ND2	2.78	0.47
3:H:85:MET:CA	3:H:88:ILE:HD12	2.45	0.47
1:A:420:PHE:O	1:A:421:HIS:C	2.52	0.47
1:F:357:ILE:CD1	2:G:100:ILE:CD1	2.89	0.47
1:F:389:VAL:HG12	1:F:390:THR:N	2.30	0.47
2:B:139:PHE:HA	2:B:149:THR:O	2.15	0.47
3:C:152:SER:C	3:C:154:LEU:N	2.68	0.47
3:C:191:TRP:O	3:C:191:TRP:CD1	2.68	0.47
1:F:512:LEU:O	1:F:516:MET:HG3	2.15	0.47
1:A:332:LEU:HD22	1:A:335:PHE:HB2	1.96	0.46
1:F:168:THR:CB	1:F:172:ALA:HA	2.40	0.46
1:F:332:LEU:CD2	1:F:335:PHE:CG	2.97	0.46
1:F:373:GLY:C	1:F:375:ILE:HD12	2.35	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:88:ILE:O	3:C:174:ARG:NE	2.48	0.46
2:B:159:THR:O	2:B:196:ILE:HD13	2.15	0.46
1:A:491:PHE:HD1	1:A:491:PHE:H	1.62	0.46
1:A:511:CYS:SG	1:A:512:LEU:N	2.88	0.46
1:A:156:VAL:O	1:A:160:LEU:HD12	2.15	0.46
1:F:272:MET:C	1:F:274:MET:H	2.18	0.46
2:G:125:LYS:N	2:G:126:PRO:CD	2.71	0.46
4:D:86:UNK:O	4:D:90:UNK:N	2.48	0.46
1:A:482:ARG:NH2	6:A:1001:HEM:CGD	2.79	0.46
7:A:1002:HEO:H241	2:B:99:ILE:HB	1.96	0.46
2:B:184:TYR:CD2	2:B:186:MET:HB2	2.49	0.46
2:B:177:PRO:C	2:B:179:LEU:N	2.69	0.46
2:B:156:PRO:HD3	2:B:231:PHE:CE2	2.51	0.46
3:H:30:TRP:CH2	4:I:79:UNK:CA	2.97	0.46
1:F:458:TRP:O	1:F:462:ILE:HG13	2.15	0.46
3:H:89:ALA:O	3:H:90:MET:C	2.53	0.46
1:F:126:VAL:O	1:F:126:VAL:HG12	2.15	0.46
1:F:238:LEU:HD21	1:F:324:THR:HG23	1.95	0.46
1:F:281:ALA:HA	1:F:331:TRP:CG	2.50	0.46
3:C:197:VAL:CG1	3:C:198:VAL:HG23	2.45	0.46
3:H:102:LEU:HD23	3:H:161:MET:CE	2.45	0.46
3:H:199:TYR:H	3:H:199:TYR:HD1	1.60	0.46
1:F:137:ALA:H	1:F:215:MET:CE	2.29	0.46
2:G:130:GLU:OE1	2:G:141:ILE:HB	2.16	0.46
2:B:130:GLU:OE1	2:B:141:ILE:HG22	2.15	0.46
1:A:397:THR:HG23	1:A:415:PHE:CZ	2.50	0.46
2:B:134:MET:CE	2:B:255:ALA:HB2	2.45	0.46
1:A:272:MET:C	1:A:274:MET:H	2.18	0.46
1:A:295:PHE:CE2	1:A:362:LYS:HG3	2.50	0.46
1:F:103:PHE:CZ	6:F:1001:HEM:CMA	2.99	0.46
1:F:306:SER:HA	1:F:375:ILE:HG23	1.96	0.46
1:F:474:LEU:CD2	1:F:491:PHE:HA	2.45	0.46
3:C:177:ILE:C	3:C:177:ILE:HD12	2.35	0.46
3:C:103:ALA:CA	3:C:161:MET:HE1	2.46	0.46
1:A:452:TRP:O	1:A:455:ARG:HB2	2.15	0.46
3:H:174:ARG:HH11	3:H:177:ILE:HG12	1.80	0.46
1:A:127:VAL:N	1:A:128:PRO:CD	2.77	0.46
1:A:336:PHE:CE2	1:A:404:PRO:HA	2.50	0.46
2:G:67:TRP:O	2:G:69:TYR:N	2.48	0.46
3:C:91:TYR:OH	4:D:7:UNK:CB	2.63	0.46
1:A:308:LYS:HZ1	1:A:372:GLN:CB	2.28	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:102:LEU:HD23	3:C:161:MET:CE	2.45	0.46
3:H:102:LEU:HB3	3:H:161:MET:HE2	1.97	0.46
1:A:374:ARG:HB2	2:B:78:TYR:O	2.16	0.46
2:B:217:GLY:CA	2:B:260:TYR:CZ	2.95	0.46
1:A:441:PRO:C	1:A:443:ALA:N	2.69	0.46
1:A:426:GLY:HA2	1:A:430:PHE:CE1	2.51	0.46
2:G:50:LEU:CA	2:G:53:ILE:HG22	2.45	0.46
2:G:60:LEU:C	2:G:62:ALA:N	2.68	0.46
3:C:90:MET:HE1	4:D:68:UNK:CA	2.46	0.46
2:B:136:TRP:HA	2:B:218:MET:CG	2.45	0.46
3:C:120:PHE:O	3:C:121:HIS:C	2.53	0.46
2:G:152:GLU:OE2	2:G:223:ILE:HG13	2.16	0.46
3:H:171:SER:C	3:H:173:ASN:H	2.18	0.46
1:A:281:ALA:HA	1:A:331:TRP:CG	2.50	0.46
1:A:408:PHE:O	2:B:182:GLN:NE2	2.42	0.46
1:A:482:ARG:NH2	6:A:1001:HEM:O2D	2.49	0.46
2:B:88:VAL:HG23	2:B:89:GLU:N	2.31	0.46
1:F:110:MET:HB2	6:F:1001:HEM:HBC2	1.97	0.46
1:F:297:VAL:HG22	1:F:439:TRP:HZ3	1.81	0.46
1:F:403:VAL:HG13	2:G:107:THR:HG23	1.97	0.46
2:G:186:MET:HB3	2:G:189:MET:HG3	1.97	0.46
1:F:384:THR:O	1:F:388:ILE:HG13	2.16	0.46
1:F:491:PHE:HD1	1:F:491:PHE:H	1.62	0.46
3:C:47:TYR:C	3:C:49:VAL:N	2.68	0.46
2:B:270:LYS:HE3	2:B:276:ASP:CG	2.36	0.46
3:C:134:GLY:CA	3:C:137:SER:HB3	2.45	0.46
1:F:422:ASN:HA	1:F:464:PHE:CZ	2.50	0.46
2:B:277:VAL:O	2:B:280:LYS:HG2	2.16	0.46
2:B:238:ALA:O	2:B:241:SER:N	2.48	0.46
3:H:174:ARG:HD3	3:H:177:ILE:CD1	2.46	0.46
1:A:238:LEU:HD21	1:A:324:THR:HG23	1.96	0.46
1:F:395:GLY:CA	7:F:1002:HEO:H162	2.38	0.46
1:F:127:VAL:N	1:F:128:PRO:CD	2.77	0.46
1:F:239:ILE:HG22	1:F:239:ILE:O	2.15	0.46
2:G:111:THR:O	2:G:111:THR:HG22	2.16	0.46
2:G:238:ALA:O	2:G:241:SER:N	2.48	0.46
2:B:195:LEU:HD23	2:B:195:LEU:C	2.37	0.46
2:B:155:PHE:HZ	2:B:222:ALA:HB1	1.80	0.46
3:H:72:GLU:O	3:H:75:LEU:HB3	2.15	0.46
2:B:125:LYS:N	2:B:126:PRO:CD	2.72	0.46
3:H:47:TYR:C	3:H:49:VAL:N	2.68	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:201:GLY:O	2:G:224:ALA:HB3	2.16	0.46
3:H:152:SER:C	3:H:154:LEU:N	2.68	0.46
2:B:152:GLU:OE2	2:B:223:ILE:HG13	2.16	0.46
1:A:345:ASN:O	1:A:349:GLY:N	2.48	0.46
2:B:46:THR:O	2:B:50:LEU:HG	2.15	0.46
1:F:134:ARG:O	1:F:135:ASP:CG	2.54	0.46
1:F:452:TRP:HA	1:F:455:ARG:CD	2.41	0.46
2:B:214:GLY:O	2:B:218:MET:HG3	2.16	0.46
3:C:92:LYS:HE2	3:C:92:LYS:HB3	1.82	0.46
1:A:110:MET:HB2	6:A:1001:HEM:HBC2	1.96	0.46
2:B:175:PHE:HD1	2:B:181:SER:O	1.99	0.46
2:G:56:ILE:HD11	2:G:99:ILE:HG13	1.98	0.46
2:B:149:THR:HG21	2:B:234:TRP:CH2	2.50	0.46
1:F:441:PRO:C	1:F:443:ALA:N	2.70	0.46
2:G:217:GLY:CA	2:G:260:TYR:CZ	2.96	0.46
1:F:255:LEU:HB3	1:F:261:THR:HG21	1.98	0.46
2:G:150:VAL:O	2:G:151:ASN:HB2	2.17	0.46
1:A:318:TRP:O	1:A:322:CYS:N	2.36	0.46
2:G:277:VAL:O	2:G:280:LYS:HG2	2.16	0.46
2:B:53:ILE:O	2:B:55:VAL:N	2.49	0.45
1:F:102:ILE:O	1:F:105:ALA:N	2.49	0.45
1:F:118:PHE:CD2	1:F:119:VAL:N	2.85	0.45
1:F:292:LEU:CB	1:F:293:PRO:HD3	2.44	0.45
1:F:352:THR:HA	1:F:355:ILE:HG12	1.97	0.45
1:F:76:ALA:HA	1:F:79:MET:HE3	1.98	0.45
2:G:154:ALA:HB3	2:G:234:TRP:CD2	2.51	0.45
2:B:142:TYR:HE1	2:B:234:TRP:HZ3	1.64	0.45
4:D:63:UNK:O	4:D:67:UNK:N	2.50	0.45
3:C:102:LEU:HD23	3:C:161:MET:HE2	1.98	0.45
3:H:136:LEU:C	3:H:140:PHE:HB2	2.36	0.45
1:F:414:LEU:HD23	1:F:479:MET:HB3	1.98	0.45
2:B:137:LYS:CE	2:B:261:ASN:HD21	2.29	0.45
1:F:155:LEU:CD1	1:F:193:SER:HA	2.46	0.45
1:A:118:PHE:CD2	1:A:119:VAL:N	2.85	0.45
1:F:79:MET:HG3	1:F:103:PHE:CE2	2.51	0.45
1:F:277:ASN:O	1:F:281:ALA:HB2	2.16	0.45
1:F:295:PHE:CE2	1:F:362:LYS:HG3	2.51	0.45
2:G:193:LEU:HD23	2:G:193:LEU:C	2.37	0.45
2:B:127:ILE:HG22	2:B:128:THR:N	2.31	0.45
3:C:171:SER:C	3:C:173:ASN:H	2.19	0.45
3:H:199:TYR:HD1	3:H:199:TYR:N	2.13	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:375:ILE:CG1	2:B:67:TRP:HE1	2.29	0.45
1:A:146:PHE:O	1:A:148:PHE:N	2.49	0.45
1:A:168:THR:HB	1:A:172:ALA:CB	2.46	0.45
1:A:335:PHE:HA	1:A:338:MET:CE	2.47	0.45
1:F:120:ILE:HD13	1:F:201:THR:OG1	2.16	0.45
1:F:350:ILE:HA	1:F:353:MET:CE	2.47	0.45
2:G:88:VAL:HG23	2:G:89:GLU:N	2.31	0.45
2:B:233:GLN:O	2:B:236:ALA:HB3	2.17	0.45
3:C:103:ALA:HA	3:C:161:MET:HE1	1.99	0.45
1:A:441:PRO:HG2	1:A:447:LYS:HD2	1.98	0.45
1:A:468:PHE:HA	1:A:471:LEU:HG	1.98	0.45
1:F:61:TYR:CE1	1:F:146:PHE:CD1	3.05	0.45
1:A:126:VAL:HG12	1:A:126:VAL:O	2.16	0.45
1:F:195:GLN:HG2	1:F:250:VAL:HG11	1.97	0.45
1:F:284:HIS:NE2	1:F:288:TYR:CE1	2.84	0.45
2:G:97:ILE:HG12	2:G:101:ILE:HD11	1.98	0.45
2:G:162:TYR:CD1	2:G:194:HIS:NE2	2.85	0.45
1:F:142:ASN:OD1	1:F:208:PHE:HE1	2.00	0.45
3:C:88:ILE:HG23	3:C:98:VAL:HG11	1.97	0.45
3:H:191:TRP:O	3:H:191:TRP:CD1	2.69	0.45
3:H:74:PHE:HD1	3:H:77:LEU:HD12	1.81	0.45
2:B:130:GLU:HA	2:B:164:LYS:HB2	1.99	0.45
1:A:377:PHE:CD1	1:A:377:PHE:N	2.84	0.45
3:C:192:ILE:HG12	3:C:192:ILE:O	2.16	0.45
1:A:79:MET:HG3	1:A:103:PHE:CE2	2.52	0.45
1:A:284:HIS:NE2	1:A:288:TYR:CE1	2.84	0.45
1:F:398:GLY:C	7:F:1002:HEO:HMB3	2.36	0.45
1:F:379:SER:O	1:F:382:LEU:HB2	2.17	0.45
1:F:57:LEU:HD23	1:F:57:LEU:HA	1.79	0.45
3:H:145:THR:O	3:H:147:GLY:N	2.49	0.45
1:A:221:THR:H	1:A:224:LYS:HD2	1.81	0.45
3:C:202:GLY:O	3:C:203:ALA:HB3	2.17	0.45
3:H:91:TYR:O	3:H:92:LYS:C	2.54	0.45
2:B:111:THR:HG22	2:B:111:THR:O	2.17	0.45
1:F:291:ILE:HA	1:F:294:VAL:HG23	1.99	0.45
1:F:353:MET:HE3	2:G:104:ALA:CB	2.47	0.45
2:G:38:LEU:HA	2:G:41:ARG:HD3	1.98	0.45
2:G:236:ALA:HA	2:G:239:LYS:HG3	1.99	0.45
1:F:388:ILE:HG13	1:F:388:ILE:H	1.50	0.45
1:F:308:LYS:HZ1	1:F:372:GLN:CB	2.29	0.45
1:F:56:ARG:O	1:F:60:MET:HG2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:84:GLY:C	3:C:88:ILE:HD12	2.37	0.45
1:A:385:ILE:HA	1:A:388:ILE:HD12	1.98	0.45
3:C:50:LEU:HD11	3:C:134:GLY:CA	2.44	0.45
1:F:464:PHE:HD2	1:F:465:PHE:CD1	2.35	0.45
1:F:377:PHE:N	1:F:377:PHE:CD1	2.84	0.45
1:A:424:ILE:CG2	6:A:1001:HEM:HAC	2.38	0.45
1:A:106:HIS:CD2	1:A:107:GLY:H	2.35	0.45
1:A:277:ASN:O	1:A:281:ALA:HB2	2.17	0.45
1:A:480:THR:HB	1:A:483:LEU:CG	2.46	0.45
2:G:43:LEU:O	2:G:46:THR:OG1	2.31	0.45
1:F:491:PHE:O	1:F:493:THR:N	2.50	0.45
1:F:248:VAL:HG13	3:H:43:LEU:CD2	2.47	0.45
3:C:156:TRP:NE1	3:C:180:LEU:HD13	2.28	0.45
1:A:415:PHE:CD1	1:A:472:TYR:CD2	3.04	0.45
2:B:136:TRP:NE1	2:B:213:PRO:O	2.49	0.45
1:F:468:PHE:HA	1:F:471:LEU:HG	1.98	0.45
1:A:102:ILE:O	1:A:105:ALA:N	2.49	0.45
1:A:292:LEU:CB	1:A:293:PRO:HD3	2.44	0.45
1:A:352:THR:HA	1:A:355:ILE:HG12	1.97	0.45
1:A:367:LEU:HD13	2:B:63:VAL:CG1	2.46	0.45
1:F:329:ILE:O	1:F:329:ILE:HG22	2.17	0.45
2:G:149:THR:HG21	2:G:234:TRP:CH2	2.51	0.45
2:G:240:GLN:O	2:G:241:SER:C	2.53	0.45
2:G:156:PRO:HG3	2:G:231:PHE:CD2	2.52	0.45
1:F:101:GLN:CG	1:F:165:PHE:O	2.65	0.45
3:H:29:PHE:C	3:H:31:ILE:N	2.70	0.45
1:A:80:ARG:CG	1:A:80:ARG:O	2.64	0.45
2:G:137:LYS:CE	2:G:261:ASN:ND2	2.79	0.45
2:B:275:ALA:O	2:B:279:ASN:ND2	2.50	0.45
1:A:175:PRO:HG2	1:A:272:MET:HE2	1.99	0.45
1:A:417:ILE:HA	1:A:420:PHE:CE2	2.51	0.45
1:A:481:ARG:HG2	1:A:482:ARG:H	1.80	0.45
1:F:332:LEU:C	1:F:334:HIS:H	2.20	0.45
1:F:332:LEU:HB2	1:F:348:PHE:CG	2.52	0.45
1:F:417:ILE:HA	1:F:420:PHE:CE2	2.51	0.45
2:G:265:TYR:O	2:G:266:PHE:CD2	2.70	0.45
2:G:46:THR:O	2:G:50:LEU:HG	2.16	0.45
2:B:193:LEU:HD23	2:B:194:HIS:O	2.17	0.45
3:C:145:THR:OG1	3:C:146:HIS:N	2.50	0.45
3:C:150:VAL:HG22	3:C:187:LEU:CD1	2.47	0.45
1:A:248:VAL:O	1:A:252:LEU:HG	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:248:VAL:HG21	3:H:42:ILE:CG2	2.47	0.45
2:G:217:GLY:HA3	2:G:260:TYR:CE1	2.52	0.45
3:H:137:SER:O	3:H:140:PHE:HB3	2.17	0.45
2:B:137:LYS:HE2	2:B:261:ASN:ND2	2.32	0.45
1:A:174:PRO:C	1:A:176:LEU:N	2.69	0.45
1:A:291:ILE:HA	1:A:294:VAL:HG23	1.99	0.45
1:A:311:PHE:HZ	2:B:88:VAL:HG21	1.81	0.45
1:A:332:LEU:HD22	1:A:335:PHE:CG	2.52	0.45
1:A:409:VAL:HG12	2:B:175:PHE:HZ	1.80	0.45
1:F:424:ILE:CG2	6:F:1001:HEM:HAC	2.38	0.45
1:F:369:THR:O	1:F:369:THR:CG2	2.65	0.45
1:F:374:ARG:HD3	2:G:76:ALA:O	2.17	0.45
3:H:197:VAL:CG1	3:H:198:VAL:HG23	2.47	0.45
3:H:134:GLY:CA	3:H:137:SER:HB3	2.46	0.45
1:F:138:PHE:CZ	3:H:28:GLY:HA3	2.44	0.45
1:F:318:TRP:O	1:F:322:CYS:N	2.36	0.45
2:B:240:GLN:O	2:B:241:SER:C	2.53	0.45
1:A:244:PRO:O	1:A:245:ILE:C	2.55	0.44
1:F:395:GLY:O	1:F:399:VAL:HG23	2.17	0.44
2:G:142:TYR:HE1	2:G:234:TRP:HZ3	1.64	0.44
2:B:136:TRP:HB2	2:B:259:GLU:HA	1.98	0.44
1:F:466:VAL:O	1:F:466:VAL:HG12	2.16	0.44
1:A:155:LEU:CD1	1:A:193:SER:HA	2.47	0.44
2:B:56:ILE:O	2:B:60:LEU:N	2.48	0.44
1:F:168:THR:CG2	1:F:176:LEU:HB3	2.41	0.44
2:B:154:ALA:HB3	2:B:234:TRP:CD2	2.52	0.44
2:G:155:PHE:CZ	2:G:222:ALA:HB1	2.52	0.44
1:A:487:ILE:O	1:A:488:ASP:C	2.55	0.44
1:A:116:MET:HB3	1:A:117:PRO:HD3	1.98	0.44
1:F:463:GLY:HA3	1:F:505:ILE:HG13	1.99	0.44
1:A:275:TYR:C	1:A:275:TYR:CD2	2.90	0.44
2:B:225:THR:HB	2:B:226:PRO:CD	2.47	0.44
1:A:115:ALA:O	1:A:290:LEU:HD11	2.17	0.44
2:B:138:TRP:HH2	2:B:174:PHE:HA	1.82	0.44
1:F:244:PRO:O	1:F:245:ILE:C	2.56	0.44
1:F:246:LEU:CD1	1:F:250:VAL:HG23	2.47	0.44
1:F:243:PHE:HA	1:F:282:TRP:CD1	2.53	0.44
1:F:389:VAL:O	1:F:393:VAL:HG23	2.16	0.44
3:C:70:LEU:HD23	3:C:115:MET:HE3	1.99	0.44
3:C:190:VAL:O	3:C:194:VAL:HG23	2.17	0.44
1:A:541:TRP:C	1:A:543:THR:N	2.70	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:PRO:CG	2:B:213:PRO:HA	2.47	0.44
1:A:502:ALA:C	1:A:504:LEU:N	2.68	0.44
1:A:169:GLY:C	1:A:171:LEU:N	2.69	0.44
1:A:316:LEU:CD2	1:A:362:LYS:HA	2.47	0.44
2:B:175:PHE:CD2	2:B:206:ILE:HD11	2.51	0.44
2:B:36:ILE:HG23	2:B:39:GLU:HB3	2.00	0.44
3:C:85:MET:HA	3:C:88:ILE:HD12	1.97	0.44
1:F:274:MET:CE	3:H:49:VAL:HG21	2.47	0.44
3:C:137:SER:O	3:C:140:PHE:HB3	2.18	0.44
2:B:132:VAL:O	2:B:134:MET:SD	2.76	0.44
3:C:26:ILE:CD1	3:C:175:THR:HG23	2.47	0.44
1:A:458:TRP:O	1:A:462:ILE:HG13	2.18	0.44
4:D:41:UNK:O	4:D:42:UNK:C	2.66	0.44
4:I:41:UNK:O	4:I:42:UNK:C	2.66	0.44
1:A:338:MET:HA	2:B:184:TYR:CG	2.53	0.44
1:F:106:HIS:CG	1:F:107:GLY:N	2.84	0.44
1:F:245:ILE:HB	1:F:282:TRP:HB2	2.00	0.44
1:F:400:LEU:HD11	2:G:46:THR:HA	2.00	0.44
1:F:79:MET:SD	1:F:102:ILE:CG2	3.05	0.44
1:A:56:ARG:O	1:A:60:MET:HG2	2.18	0.44
3:C:148:LEU:O	3:C:151:THR:N	2.50	0.44
2:G:45:LEU:CD1	2:G:110:THR:HG21	2.45	0.44
1:F:275:TYR:C	1:F:275:TYR:CD2	2.91	0.44
3:C:26:ILE:C	3:C:28:GLY:N	2.69	0.44
1:F:476:PHE:C	1:F:478:GLY:H	2.21	0.44
1:A:398:GLY:O	7:A:1002:HEO:HMB3	2.17	0.44
1:A:484:SER:H	2:B:216:SER:CB	2.30	0.44
2:B:38:LEU:HA	2:B:41:ARG:HD3	1.99	0.44
1:F:111:ILE:HD11	6:F:1001:HEM:HMD3	1.98	0.44
1:F:127:VAL:HG13	1:F:229:THR:HG23	1.99	0.44
1:F:316:LEU:CD2	1:F:362:LYS:HA	2.48	0.44
1:F:332:LEU:HD22	1:F:335:PHE:CG	2.53	0.44
1:F:98:HIS:O	1:F:99:TYR:C	2.56	0.44
2:G:177:PRO:C	2:G:179:LEU:N	2.71	0.44
2:B:67:TRP:O	2:B:69:TYR:N	2.50	0.44
1:F:248:VAL:CG2	3:H:39:LEU:HD12	2.47	0.44
1:F:116:MET:HB3	1:F:117:PRO:HD3	1.98	0.44
1:A:61:TYR:CE1	1:A:146:PHE:CD1	3.06	0.44
1:A:105:ALA:O	1:A:106:HIS:O	2.36	0.44
1:A:368:PHE:CE1	2:B:88:VAL:HB	2.53	0.44
1:F:105:ALA:O	1:F:106:HIS:O	2.36	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:337:THR:HG22	2:G:184:TYR:HB3	2.00	0.44
1:F:382:LEU:HD23	1:F:385:ILE:CD1	2.45	0.44
1:F:160:LEU:HD23	1:F:165:PHE:CB	2.48	0.44
1:A:157:ASN:CA	1:A:160:LEU:HD12	2.37	0.44
1:F:541:TRP:C	1:F:543:THR:N	2.70	0.44
1:A:466:VAL:HB	1:A:501:GLY:CA	2.48	0.44
1:A:238:LEU:HB2	1:A:289:ILE:HD11	1.98	0.44
2:B:186:MET:HB3	2:B:189:MET:CG	2.47	0.44
1:F:335:PHE:HA	1:F:338:MET:CE	2.48	0.44
1:F:357:ILE:O	1:F:361:VAL:HG23	2.18	0.44
2:G:142:TYR:HA	2:G:143:PRO:HD2	1.87	0.44
1:A:57:LEU:CD1	1:A:143:ASN:HA	2.47	0.44
1:A:59:ILE:O	1:A:60:MET:C	2.56	0.44
3:C:90:MET:HE1	4:D:68:UNK:N	2.31	0.44
1:A:486:GLN:HG2	1:A:492:HIS:NE2	2.33	0.44
1:A:101:GLN:CG	1:A:165:PHE:O	2.66	0.44
3:H:145:THR:OG1	3:H:146:HIS:N	2.51	0.44
3:C:67:PRO:HB2	3:C:195:PHE:CD1	2.52	0.44
1:A:437:THR:HG23	1:A:448:LEU:HD12	2.00	0.44
1:A:150:VAL:O	1:A:153:VAL:CB	2.66	0.44
4:I:75:UNK:O	4:I:79:UNK:N	2.51	0.44
1:F:502:ALA:C	1:F:504:LEU:N	2.68	0.44
1:A:267:ASP:N	1:A:267:ASP:OD1	2.51	0.44
1:A:243:PHE:HA	1:A:282:TRP:CD1	2.53	0.44
1:A:79:MET:C	1:A:81:SER:H	2.20	0.44
2:B:41:ARG:H	2:B:41:ARG:CD	2.23	0.44
4:D:75:UNK:O	4:D:79:UNK:N	2.50	0.44
2:B:147:ILE:CD1	2:B:235:VAL:HA	2.44	0.44
2:B:201:GLY:O	2:B:224:ALA:HB3	2.18	0.44
1:A:159:SER:OG	1:A:189:TYR:HB2	2.16	0.44
3:H:197:VAL:HG13	3:H:198:VAL:H	1.81	0.44
3:H:50:LEU:HD11	3:H:134:GLY:CA	2.43	0.44
1:F:406:ALA:CB	2:G:45:LEU:HD22	2.45	0.44
3:H:139:PHE:O	3:H:141:ALA:N	2.51	0.44
1:A:103:PHE:CZ	6:A:1001:HEM:CMA	3.01	0.43
1:A:106:HIS:CG	1:A:107:GLY:N	2.85	0.43
1:F:106:HIS:CD2	1:F:107:GLY:H	2.36	0.43
1:F:238:LEU:HB2	1:F:289:ILE:HD11	1.99	0.43
1:F:319:ALA:HB1	1:F:362:LYS:HE2	2.00	0.43
1:F:417:ILE:HD13	6:F:1001:HEM:HBA2	2.00	0.43
1:F:55:LYS:HD3	1:F:551:ASN:OD1	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:140:PHE:HD2	2:G:149:THR:OG1	2.01	0.43
2:G:36:ILE:HG23	2:G:39:GLU:HB3	2.00	0.43
3:H:116:GLU:OE1	3:H:143:VAL:HG11	2.18	0.43
3:H:67:PRO:HB2	3:H:195:PHE:CD1	2.52	0.43
1:A:388:ILE:H	1:A:388:ILE:HG13	1.52	0.43
2:G:136:TRP:NE1	2:G:213:PRO:O	2.51	0.43
1:F:68:MET:HE3	1:F:153:VAL:HG13	2.00	0.43
2:B:45:LEU:CD1	2:B:110:THR:HG21	2.46	0.43
1:A:61:TYR:O	1:A:64:VAL:N	2.51	0.43
3:C:94:ASN:HB2	3:C:97:GLN:HB3	2.00	0.43
1:A:476:PHE:C	1:A:478:GLY:H	2.21	0.43
1:F:267:ASP:OD1	1:F:267:ASP:N	2.50	0.43
3:H:88:ILE:O	3:H:174:ARG:NE	2.51	0.43
1:F:169:GLY:C	1:F:171:LEU:N	2.70	0.43
1:F:292:LEU:HA	1:F:295:PHE:CD1	2.52	0.43
1:F:316:LEU:HD22	1:F:362:LYS:HA	2.00	0.43
1:F:330:VAL:CG1	1:F:352:THR:OG1	2.66	0.43
1:F:75:ASP:C	1:F:79:MET:HE2	2.39	0.43
3:C:84:GLY:O	3:C:88:ILE:HG13	2.18	0.43
2:G:195:LEU:C	2:G:195:LEU:HD23	2.39	0.43
1:F:441:PRO:HG2	1:F:447:LYS:HD2	2.00	0.43
3:H:156:TRP:NE1	3:H:180:LEU:HD13	2.29	0.43
1:A:134:ARG:O	1:A:135:ASP:CG	2.56	0.43
1:A:120:ILE:HD13	1:A:201:THR:OG1	2.18	0.43
1:A:277:ASN:HD21	4:D:97:UNK:CB	2.31	0.43
1:F:346:ALA:HA	1:F:350:ILE:HG13	1.99	0.43
1:F:355:ILE:HG22	1:F:355:ILE:O	2.18	0.43
1:F:411:HIS:CE1	1:F:412:ASN:ND2	2.87	0.43
1:F:548:PRO:O	1:F:550:TYR:N	2.51	0.43
2:G:233:GLN:O	2:G:236:ALA:HB3	2.19	0.43
2:B:162:TYR:CD1	2:B:194:HIS:NE2	2.87	0.43
3:H:190:VAL:O	3:H:194:VAL:HG23	2.18	0.43
1:A:137:ALA:H	1:A:215:MET:CE	2.31	0.43
2:G:214:GLY:O	2:G:218:MET:HG3	2.19	0.43
3:H:167:ARG:HH11	3:H:167:ARG:HG3	1.83	0.43
1:A:473:ALA:O	1:A:475:GLY:N	2.50	0.43
1:A:79:MET:O	1:A:81:SER:N	2.52	0.43
3:H:185:HIS:CG	3:H:185:HIS:O	2.70	0.43
1:F:168:THR:O	1:F:172:ALA:HA	2.18	0.43
1:F:328:PHE:O	1:F:331:TRP:HZ3	2.02	0.43
2:G:89:GLU:HB3	2:G:93:TRP:CD2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:239:LYS:HA	2:G:239:LYS:HE2	1.99	0.43
1:A:57:LEU:HA	1:A:57:LEU:HD23	1.79	0.43
1:F:157:ASN:CA	1:F:160:LEU:HD12	2.40	0.43
3:C:199:TYR:HD1	3:C:199:TYR:N	2.15	0.43
1:F:440:TRP:O	1:F:444:PHE:HB2	2.18	0.43
1:F:148:PHE:HA	1:F:148:PHE:HD2	1.70	0.43
1:A:498:ALA:C	1:A:500:SER:H	2.22	0.43
4:I:63:UNK:O	4:I:67:UNK:N	2.52	0.43
3:H:83:TYR:C	3:H:101:TRP:CZ3	2.91	0.43
3:C:78:PHE:HD2	3:C:78:PHE:O	2.01	0.43
1:A:127:VAL:HG13	1:A:229:THR:HG23	2.00	0.43
1:A:357:ILE:N	1:A:358:PRO:CD	2.81	0.43
1:A:389:VAL:O	1:A:393:VAL:HG23	2.18	0.43
1:A:412:ASN:OD1	2:B:209:SER:HB3	2.18	0.43
1:F:412:ASN:CG	2:G:209:SER:HB3	2.38	0.43
2:G:99:ILE:O	2:G:100:ILE:C	2.53	0.43
1:F:57:LEU:CD1	1:F:143:ASN:HA	2.48	0.43
3:C:174:ARG:HD3	3:C:177:ILE:CD1	2.48	0.43
2:G:158:ASN:O	2:G:159:THR:HG23	2.19	0.43
1:F:221:THR:H	1:F:224:LYS:HD2	1.83	0.43
2:B:130:GLU:OE1	2:B:141:ILE:HB	2.19	0.43
2:B:271:PRO:O	2:B:272:ASP:OD1	2.36	0.43
2:G:136:TRP:HA	2:G:218:MET:CG	2.47	0.43
1:F:415:PHE:CD1	1:F:472:TYR:CD2	3.06	0.43
2:G:137:LYS:HE2	2:G:261:ASN:ND2	2.34	0.43
1:F:151:VAL:O	1:F:155:LEU:HB2	2.17	0.43
3:C:139:PHE:O	3:C:141:ALA:N	2.51	0.43
3:H:86:ALA:HB2	3:H:91:TYR:CE1	2.46	0.43
1:A:111:ILE:HD11	6:A:1001:HEM:HMD3	1.99	0.43
1:A:246:LEU:CD1	1:A:250:VAL:HG23	2.49	0.43
1:F:367:LEU:HD13	2:G:63:VAL:CB	2.48	0.43
1:F:420:PHE:O	1:F:421:HIS:C	2.55	0.43
1:F:79:MET:C	1:F:81:SER:H	2.20	0.43
2:G:138:TRP:HH2	2:G:174:PHE:HA	1.82	0.43
2:G:59:ILE:O	2:G:62:ALA:HB3	2.17	0.43
2:B:265:TYR:O	2:B:266:PHE:CD2	2.71	0.43
3:C:84:GLY:O	3:C:85:MET:C	2.57	0.43
3:C:85:MET:CA	3:C:88:ILE:HD12	2.49	0.43
1:A:137:ALA:HB2	1:A:215:MET:HE2	2.00	0.43
1:A:543:THR:HG22	1:A:544:SER:H	1.84	0.43
2:B:130:GLU:OE1	2:B:141:ILE:O	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:137:LYS:CE	2:G:261:ASN:HD21	2.32	0.43
1:A:251:ALA:O	1:A:254:THR:CB	2.66	0.43
3:C:139:PHE:C	3:C:141:ALA:H	2.22	0.43
1:A:325:VAL:O	1:A:327:SER:N	2.47	0.43
1:A:241:ALA:O	1:A:328:PHE:HE2	2.01	0.43
1:A:243:PHE:N	1:A:244:PRO:CD	2.81	0.43
2:B:184:TYR:CE2	2:B:189:MET:HE2	2.54	0.43
2:B:39:GLU:CB	2:B:43:LEU:HD12	2.48	0.43
1:F:404:PRO:HG2	2:G:111:THR:CG2	2.49	0.43
1:F:491:PHE:C	1:F:493:THR:H	2.22	0.43
1:F:59:ILE:O	1:F:60:MET:C	2.56	0.43
2:B:195:LEU:HD23	2:B:196:ILE:C	2.39	0.43
3:H:103:ALA:CA	3:H:161:MET:HE1	2.49	0.43
3:H:150:VAL:HG22	3:H:187:LEU:CD1	2.48	0.43
1:A:356:ALA:HA	7:A:1002:HEO:H262	1.99	0.43
1:F:73:PHE:HE2	6:F:1001:HEM:HAB	1.83	0.43
1:F:239:ILE:O	1:F:243:PHE:HB2	2.18	0.43
1:A:486:GLN:H	1:A:486:GLN:NE2	2.17	0.43
2:G:248:MET:HA	2:G:251:PHE:HB3	2.00	0.43
1:A:442:LYS:HB2	1:A:541:TRP:CZ3	2.52	0.43
4:I:73:UNK:O	4:I:76:UNK:N	2.52	0.43
2:G:134:MET:HG2	2:G:255:ALA:CB	2.48	0.43
1:F:146:PHE:O	1:F:148:PHE:N	2.51	0.43
1:A:151:VAL:O	1:A:155:LEU:HB2	2.17	0.43
1:A:190:TRP:CE3	1:A:191:ILE:HG12	2.53	0.43
1:F:79:MET:O	1:F:81:SER:N	2.52	0.43
2:G:56:ILE:O	2:G:60:LEU:N	2.49	0.43
2:B:193:LEU:HD23	2:B:193:LEU:C	2.39	0.43
1:F:306:SER:HA	1:F:375:ILE:CA	2.40	0.43
3:C:112:PHE:HZ	3:C:191:TRP:CE3	2.37	0.43
1:A:61:TYR:O	1:A:63:ILE:N	2.52	0.43
3:H:84:GLY:O	3:H:85:MET:C	2.57	0.43
3:H:92:LYS:HE2	3:H:92:LYS:HB3	1.85	0.43
1:A:119:VAL:CG2	1:A:293:PRO:HG2	2.48	0.43
1:A:332:LEU:C	1:A:334:HIS:H	2.22	0.43
1:A:319:ALA:HB1	1:A:362:LYS:HE2	2.01	0.43
3:H:78:PHE:CZ	4:I:57:UNK:CA	2.88	0.43
1:F:115:ALA:O	1:F:290:LEU:HD11	2.19	0.43
1:F:201:THR:O	1:F:201:THR:HG22	2.18	0.43
1:F:79:MET:C	1:F:81:SER:N	2.72	0.43
2:G:186:MET:HB3	2:G:189:MET:CG	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:153:ILE:HD11	2:B:220:PHE:CE2	2.54	0.43
1:F:375:ILE:HG21	2:G:67:TRP:CZ2	2.54	0.43
3:C:150:VAL:HG22	3:C:187:LEU:HD11	2.01	0.43
1:F:435:GLY:O	1:F:437:THR:N	2.52	0.43
2:G:130:GLU:HA	2:G:164:LYS:HB2	2.01	0.43
1:F:80:ARG:NH2	1:F:467:ALA:O	2.52	0.43
1:A:80:ARG:NH2	1:A:467:ALA:O	2.52	0.43
3:H:166:ARG:NE	3:H:167:ARG:NH2	2.66	0.43
1:A:480:THR:HB	1:A:483:LEU:CD1	2.48	0.42
1:A:396:MET:HB3	2:B:53:ILE:HD13	2.00	0.42
1:F:243:PHE:N	1:F:244:PRO:CD	2.81	0.42
1:F:119:VAL:CG2	1:F:293:PRO:HG2	2.48	0.42
2:G:41:ARG:H	2:G:41:ARG:CD	2.24	0.42
2:G:39:GLU:CB	2:G:43:LEU:HD12	2.49	0.42
2:G:147:ILE:CD1	2:G:235:VAL:HA	2.45	0.42
1:F:491:PHE:C	1:F:493:THR:N	2.71	0.42
2:B:201:GLY:O	2:B:203:TYR:CE1	2.72	0.42
3:H:103:ALA:HA	3:H:161:MET:HE1	2.01	0.42
1:A:452:TRP:HA	1:A:455:ARG:HB2	2.01	0.42
1:F:150:VAL:O	1:F:153:VAL:CB	2.67	0.42
3:H:26:ILE:CD1	3:H:175:THR:HG23	2.46	0.42
1:A:460:TRP:CZ3	1:A:509:ILE:HG12	2.54	0.42
1:F:466:VAL:HB	1:F:501:GLY:CA	2.48	0.42
1:F:99:TYR:CE1	1:F:103:PHE:HD1	2.37	0.42
1:F:338:MET:HA	2:G:184:TYR:CD1	2.52	0.42
1:F:79:MET:SD	1:F:103:PHE:N	2.92	0.42
2:G:140:PHE:CE1	2:G:153:ILE:HD13	2.53	0.42
4:D:66:UNK:C	4:D:68:UNK:N	2.79	0.42
2:G:203:TYR:O	2:G:221:LYS:CA	2.63	0.42
1:F:101:GLN:HG3	1:F:165:PHE:O	2.19	0.42
1:F:61:TYR:O	1:F:63:ILE:N	2.52	0.42
1:F:442:LYS:HB2	1:F:541:TRP:CZ3	2.53	0.42
2:B:134:MET:HG2	2:B:255:ALA:CB	2.48	0.42
3:H:94:ASN:HB2	3:H:97:GLN:HB3	2.01	0.42
1:A:299:SER:HB3	1:A:310:LEU:HD22	2.00	0.42
1:A:361:VAL:HG22	2:B:93:TRP:CH2	2.55	0.42
1:A:316:LEU:HD22	1:A:362:LYS:HA	2.01	0.42
1:A:79:MET:C	1:A:81:SER:N	2.72	0.42
1:F:292:LEU:O	1:F:295:PHE:HB2	2.19	0.42
1:F:350:ILE:HG12	1:F:353:MET:HE1	2.01	0.42
1:A:305:PHE:CD1	1:A:305:PHE:N	2.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:LEU:HD22	1:A:263:PHE:CE2	2.54	0.42
1:A:228:PHE:CG	1:A:228:PHE:O	2.73	0.42
2:B:50:LEU:O	2:B:53:ILE:CG2	2.67	0.42
1:A:364:PHE:HB3	2:B:92:VAL:HG21	2.02	0.42
1:F:357:ILE:N	1:F:358:PRO:CD	2.82	0.42
1:F:480:THR:HB	1:F:483:LEU:CG	2.48	0.42
2:G:262:GLN:O	2:G:264:GLU:N	2.52	0.42
2:B:140:PHE:CE1	2:B:153:ILE:HD13	2.54	0.42
1:F:516:MET:O	1:F:519:SER:N	2.45	0.42
1:F:502:ALA:O	1:F:505:ILE:N	2.52	0.42
1:A:128:PRO:O	1:A:130:GLN:N	2.53	0.42
1:A:331:TRP:CD2	1:A:348:PHE:HE2	2.38	0.42
1:A:346:ALA:HA	1:A:350:ILE:HG13	2.00	0.42
1:A:350:ILE:HA	1:A:353:MET:HE2	2.01	0.42
1:F:233:LEU:O	1:F:236:ASN:N	2.52	0.42
1:F:337:THR:HG23	2:G:183:ILE:HA	2.02	0.42
3:H:72:GLU:O	3:H:76:LEU:HD23	2.19	0.42
2:G:167:SER:HB3	2:G:187:ALA:CA	2.49	0.42
1:A:549:PHE:CD1	1:A:549:PHE:N	2.87	0.42
1:A:119:VAL:HG13	1:A:120:ILE:N	2.34	0.42
1:A:233:LEU:O	1:A:236:ASN:N	2.52	0.42
1:A:354:ILE:O	1:A:356:ALA:N	2.53	0.42
2:B:54:VAL:C	2:B:56:ILE:N	2.73	0.42
1:F:243:PHE:HA	1:F:282:TRP:NE1	2.34	0.42
1:F:299:SER:HB3	1:F:310:LEU:HD22	2.00	0.42
1:F:333:HIS:HB2	7:F:1002:HEO:HA2	2.00	0.42
1:F:354:ILE:O	1:F:356:ALA:N	2.53	0.42
1:F:320:THR:OG1	1:F:362:LYS:NZ	2.52	0.42
1:F:373:GLY:CA	2:G:71:ALA:O	2.67	0.42
2:G:195:LEU:HD23	2:G:196:ILE:C	2.40	0.42
1:F:137:ALA:HB2	1:F:215:MET:HE2	2.01	0.42
1:F:216:ARG:NH2	1:F:220:MET:O	2.51	0.42
1:A:68:MET:SD	1:A:113:PHE:HB3	2.60	0.42
1:F:264:PHE:CD1	1:F:275:TYR:HB2	2.54	0.42
1:A:195:GLN:NE2	1:A:247:THR:CG2	2.71	0.42
1:A:292:LEU:O	1:A:295:PHE:HB2	2.20	0.42
2:B:89:GLU:HB3	2:B:93:TRP:CD2	2.55	0.42
7:F:1002:HEO:O11	7:F:1002:HEO:HHC	2.19	0.42
1:F:329:ILE:O	1:F:351:THR:HG21	2.19	0.42
1:F:354:ILE:C	1:F:356:ALA:H	2.22	0.42
2:B:239:LYS:HA	2:B:239:LYS:HE2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:156:VAL:HG12	1:F:160:LEU:CD1	2.48	0.42
1:F:437:THR:HG23	1:F:448:LEU:HD12	2.01	0.42
2:B:269:VAL:O	2:B:270:LYS:C	2.56	0.42
1:F:112:PHE:C	1:F:113:PHE:CD1	2.93	0.42
1:F:442:LYS:NZ	1:F:543:THR:O	2.53	0.42
1:A:460:TRP:CZ3	1:A:509:ILE:CD1	3.02	0.42
1:A:201:THR:O	1:A:201:THR:HG22	2.19	0.42
1:A:354:ILE:C	1:A:356:ALA:H	2.22	0.42
1:A:404:PRO:HG2	2:B:111:THR:CG2	2.50	0.42
1:A:99:TYR:CE1	1:A:103:PHE:HD1	2.37	0.42
2:B:140:PHE:CZ	2:B:153:ILE:HD13	2.54	0.42
3:C:89:ALA:O	3:C:91:TYR:O	2.38	0.42
2:B:156:PRO:HG3	2:B:231:PHE:CD2	2.55	0.42
1:F:248:VAL:HG22	3:H:39:LEU:CD1	2.49	0.42
2:G:166:THR:HG23	2:G:167:SER:N	2.34	0.42
2:B:45:LEU:HD12	2:B:110:THR:CG2	2.46	0.42
1:A:148:PHE:HD2	1:A:148:PHE:HA	1.70	0.42
3:H:33:LEU:HB2	3:H:34:MET:HE2	2.01	0.42
1:A:476:PHE:N	1:A:476:PHE:CD1	2.88	0.42
1:A:483:LEU:HD22	2:B:216:SER:HA	2.02	0.42
1:F:335:PHE:O	1:F:337:THR:N	2.53	0.42
2:G:140:PHE:CZ	2:G:153:ILE:HD13	2.54	0.42
2:G:97:ILE:O	2:G:101:ILE:HD12	2.19	0.42
3:H:77:LEU:HD22	3:H:105:THR:HG23	2.02	0.42
1:A:306:SER:HA	1:A:375:ILE:CA	2.41	0.42
2:B:217:GLY:HA3	2:B:260:TYR:CE1	2.55	0.42
2:G:130:GLU:OE1	2:G:141:ILE:CG2	2.68	0.42
1:A:138:PHE:HB3	1:A:141:LEU:HD12	2.02	0.42
1:A:195:GLN:HG2	1:A:250:VAL:HG11	2.00	0.42
1:A:243:PHE:HA	1:A:282:TRP:NE1	2.34	0.42
1:A:395:GLY:O	1:A:399:VAL:HG23	2.20	0.42
1:F:227:VAL:HG11	1:F:299:SER:HB2	2.01	0.42
1:F:191:ILE:HG22	1:F:250:VAL:HG13	2.02	0.42
1:F:337:THR:C	1:F:339:GLY:H	2.24	0.42
1:F:400:LEU:HD13	2:G:50:LEU:CD2	2.50	0.42
2:G:127:ILE:HG21	2:G:142:TYR:HE2	1.84	0.42
1:F:511:CYS:SG	1:F:512:LEU:N	2.93	0.42
3:H:119:GLU:O	3:H:120:PHE:C	2.58	0.42
1:F:498:ALA:C	1:F:500:SER:H	2.24	0.42
1:F:253:LEU:O	1:F:254:THR:C	2.58	0.42
2:B:241:SER:O	2:B:267:SER:OG	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:72:SER:OG	2:B:73:ASN:N	2.53	0.42
3:H:177:ILE:C	3:H:177:ILE:HD12	2.39	0.41
1:A:107:GLY:O	1:A:111:ILE:HG13	2.20	0.41
2:B:40:GLN:HB2	2:B:41:ARG:HH11	1.85	0.41
2:B:39:GLU:HG3	2:B:43:LEU:HD12	2.01	0.41
1:F:356:ALA:HA	7:F:1002:HEO:H262	2.01	0.41
1:F:305:PHE:N	1:F:305:PHE:CD1	2.88	0.41
1:F:306:SER:CB	1:F:375:ILE:HG13	2.50	0.41
3:C:90:MET:HE2	4:D:68:UNK:CA	2.49	0.41
1:A:255:LEU:HB3	1:A:261:THR:CG2	2.50	0.41
3:H:85:MET:SD	3:H:178:MET:HG3	2.61	0.41
4:I:66:UNK:C	4:I:68:UNK:N	2.79	0.41
1:A:168:THR:CB	1:A:172:ALA:HA	2.44	0.41
1:F:111:ILE:CD1	1:F:170:TRP:CE3	3.03	0.41
2:G:183:ILE:HG13	2:G:184:TYR:N	2.35	0.41
2:G:40:GLN:HB2	2:G:41:ARG:HH11	1.85	0.41
2:G:91:VAL:HG12	2:G:92:VAL:HG13	2.02	0.41
1:F:375:ILE:HD12	2:G:71:ALA:O	2.21	0.41
1:A:308:LYS:HE3	1:A:372:GLN:HB2	1.99	0.41
2:B:158:ASN:O	2:B:159:THR:HG23	2.20	0.41
3:H:26:ILE:C	3:H:28:GLY:N	2.70	0.41
1:A:463:GLY:O	1:A:464:PHE:C	2.56	0.41
1:A:461:ILE:HG13	1:A:461:ILE:H	1.61	0.41
3:C:166:ARG:NE	3:C:167:ARG:NH2	2.67	0.41
3:C:139:PHE:C	3:C:141:ALA:N	2.74	0.41
2:G:245:MET:O	2:G:269:VAL:HA	2.21	0.41
3:H:88:ILE:HG23	3:H:98:VAL:HG13	2.01	0.41
1:A:238:LEU:HB3	1:A:289:ILE:HD11	2.02	0.41
2:G:183:ILE:HB	2:G:193:LEU:HD12	2.02	0.41
2:G:36:ILE:O	2:G:39:GLU:OE2	2.38	0.41
2:G:53:ILE:O	2:G:55:VAL:N	2.53	0.41
3:C:70:LEU:HD23	3:C:115:MET:CE	2.50	0.41
2:B:203:TYR:O	2:B:221:LYS:CA	2.65	0.41
1:A:156:VAL:O	1:A:160:LEU:CD1	2.68	0.41
1:F:61:TYR:O	1:F:64:VAL:N	2.53	0.41
2:G:178:ARG:HA	2:G:178:ARG:HD2	1.86	0.41
3:H:84:GLY:C	3:H:88:ILE:HD12	2.41	0.41
1:F:190:TRP:CE3	1:F:191:ILE:HG12	2.52	0.41
2:G:156:PRO:HD3	2:G:231:PHE:CZ	2.54	0.41
3:H:148:LEU:O	3:H:151:THR:N	2.53	0.41
3:C:67:PRO:HB2	3:C:195:PHE:CE1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:202:GLY:O	3:H:203:ALA:HB3	2.20	0.41
3:H:84:GLY:O	3:H:88:ILE:CG1	2.67	0.41
1:A:337:THR:C	1:A:339:GLY:H	2.24	0.41
1:A:176:LEU:HD13	2:B:170:VAL:HG11	2.03	0.41
2:B:60:LEU:C	2:B:62:ALA:N	2.72	0.41
1:F:332:LEU:HD22	1:F:335:PHE:HB2	2.02	0.41
2:G:54:VAL:C	2:G:56:ILE:N	2.74	0.41
2:B:140:PHE:HD2	2:B:149:THR:OG1	2.02	0.41
1:F:306:SER:OG	1:F:375:ILE:HG23	2.21	0.41
1:A:101:GLN:HG3	1:A:165:PHE:O	2.20	0.41
3:C:154:LEU:HD13	3:C:184:TRP:HH2	1.84	0.41
1:A:375:ILE:CG2	1:A:381:MET:HE2	2.49	0.41
1:A:509:ILE:HD13	1:A:509:ILE:HA	1.77	0.41
1:A:383:TRP:CD1	1:A:434:ALA:HA	2.56	0.41
2:G:269:VAL:HG23	2:G:269:VAL:O	2.20	0.41
1:A:316:LEU:O	1:A:319:ALA:HB3	2.21	0.41
3:H:78:PHE:CZ	4:I:57:UNK:HA	2.54	0.41
1:F:480:THR:OG1	2:G:206:ILE:HB	2.20	0.41
2:G:153:ILE:HD11	2:G:220:PHE:CE2	2.55	0.41
2:G:264:GLU:CG	2:G:265:TYR:N	2.79	0.41
4:I:104:UNK:C	4:I:106:UNK:N	2.79	0.41
3:H:82:THR:CG2	4:I:10:UNK:O	2.68	0.41
1:A:168:THR:O	1:A:172:ALA:HA	2.20	0.41
1:A:245:ILE:HB	1:A:282:TRP:HB2	2.03	0.41
1:A:396:MET:HB3	2:B:53:ILE:CD1	2.50	0.41
1:A:79:MET:SD	1:A:102:ILE:CG2	3.09	0.41
4:D:104:UNK:C	4:D:106:UNK:N	2.79	0.41
1:F:316:LEU:O	1:F:319:ALA:HB3	2.21	0.41
2:B:127:ILE:HG21	2:B:142:TYR:HE2	1.85	0.41
3:C:77:LEU:HD22	3:C:105:THR:HG23	2.01	0.41
3:H:195:PHE:CD1	3:H:199:TYR:CB	3.04	0.41
1:F:137:ALA:N	1:F:215:MET:HE1	2.36	0.41
3:C:199:TYR:HD1	3:C:199:TYR:H	1.66	0.41
1:A:112:PHE:C	1:A:113:PHE:CD1	2.93	0.41
1:F:543:THR:CG2	1:F:544:SER:H	2.33	0.41
1:F:461:ILE:H	1:F:461:ILE:HG13	1.61	0.41
2:B:178:ARG:HD2	2:B:178:ARG:HA	1.86	0.41
3:H:86:ALA:C	3:H:88:ILE:N	2.73	0.41
1:A:106:HIS:O	1:A:108:VAL:N	2.53	0.41
1:A:310:LEU:HD11	1:A:366:TRP:HD1	1.85	0.41
3:H:78:PHE:CZ	3:H:185:HIS:CE1	3.09	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:228:PHE:CD1	1:F:297:VAL:HG23	2.56	0.41
1:F:57:LEU:HA	1:F:60:MET:HB2	2.02	0.41
3:C:145:THR:O	3:C:147:GLY:N	2.53	0.41
3:H:150:VAL:HG22	3:H:187:LEU:HD11	2.03	0.41
3:H:81:ILE:HD11	3:H:105:THR:HG21	2.02	0.41
1:A:512:LEU:HD23	1:A:513:VAL:HG23	2.03	0.41
1:A:227:VAL:HG11	1:A:299:SER:HB2	2.01	0.41
2:B:86:ASN:C	2:B:87:LYS:HD2	2.40	0.41
1:A:417:ILE:HD13	6:A:1001:HEM:CBA	2.50	0.41
1:A:335:PHE:O	1:A:337:THR:N	2.54	0.41
1:A:98:HIS:HB3	1:A:102:ILE:HD11	2.03	0.41
1:F:408:PHE:O	2:G:182:GLN:NE2	2.45	0.41
1:F:238:LEU:HB3	1:F:289:ILE:HD11	2.03	0.41
1:F:409:VAL:HG21	2:G:43:LEU:CD2	2.51	0.41
2:G:147:ILE:HG21	2:G:238:ALA:HB3	2.01	0.41
1:A:486:GLN:CD	1:A:486:GLN:N	2.74	0.41
3:H:102:LEU:HD23	3:H:161:MET:HG3	2.03	0.41
1:F:159:SER:OG	1:F:189:TYR:HB2	2.18	0.41
3:C:42:ILE:CG2	3:C:43:LEU:N	2.84	0.41
2:G:271:PRO:O	2:G:272:ASP:OD1	2.39	0.41
2:B:130:GLU:OE1	2:B:141:ILE:CG2	2.69	0.41
1:F:452:TRP:O	1:F:455:ARG:HB2	2.20	0.41
1:A:397:THR:O	1:A:401:LEU:HG	2.20	0.41
3:C:94:ASN:HD22	3:C:97:GLN:HE22	1.68	0.41
1:A:253:LEU:O	1:A:254:THR:C	2.59	0.41
2:G:225:THR:HB	2:G:226:PRO:CD	2.51	0.41
1:F:476:PHE:CD1	1:F:476:PHE:N	2.89	0.41
1:F:341:GLY:O	1:F:344:VAL:N	2.54	0.41
1:A:350:ILE:HA	1:A:353:MET:CE	2.51	0.41
1:A:355:ILE:HG22	1:A:355:ILE:O	2.21	0.41
1:A:481:ARG:O	1:A:483:LEU:HD23	2.21	0.41
1:F:170:TRP:NE1	1:F:171:LEU:HG	2.35	0.41
1:F:120:ILE:CD1	1:F:201:THR:OG1	2.69	0.41
1:F:195:GLN:NE2	1:F:247:THR:CG2	2.71	0.41
1:F:480:THR:HB	1:F:483:LEU:CD1	2.50	0.41
3:C:102:LEU:HD23	3:C:161:MET:HG3	2.03	0.41
3:H:112:PHE:HZ	3:H:191:TRP:CZ3	2.39	0.41
3:C:164:ILE:O	3:C:168:GLY:CA	2.64	0.41
1:A:252:LEU:HD13	1:A:263:PHE:CD2	2.55	0.41
2:B:248:MET:HA	2:B:251:PHE:HB3	2.02	0.41
1:A:68:MET:HE1	1:A:153:VAL:HG13	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:397:THR:O	1:F:401:LEU:HG	2.20	0.41
2:B:89:GLU:HB3	2:B:93:TRP:CE3	2.56	0.40
2:B:91:VAL:HG12	2:B:92:VAL:HG13	2.03	0.40
1:F:170:TRP:CE2	1:F:171:LEU:CD2	3.04	0.40
1:A:513:VAL:HA	1:A:516:MET:HE1	2.01	0.40
1:A:137:ALA:N	1:A:215:MET:HE2	2.35	0.40
2:B:251:PHE:CE2	2:B:273:LEU:HD21	2.56	0.40
2:G:134:MET:CE	2:G:255:ALA:HB2	2.50	0.40
1:A:502:ALA:O	1:A:505:ILE:N	2.54	0.40
1:F:463:GLY:O	1:F:464:PHE:C	2.57	0.40
1:F:251:ALA:O	1:F:254:THR:CB	2.68	0.40
3:H:33:LEU:C	3:H:35:SER:N	2.74	0.40
1:A:341:GLY:O	1:A:344:VAL:N	2.54	0.40
1:F:228:PHE:O	1:F:228:PHE:CG	2.75	0.40
1:F:316:LEU:HD21	1:F:365:ASN:CG	2.41	0.40
1:F:409:VAL:HG21	2:G:43:LEU:HD21	2.03	0.40
1:F:481:ARG:HG2	1:F:482:ARG:H	1.85	0.40
2:G:140:PHE:HD2	2:G:149:THR:HG1	1.69	0.40
2:G:50:LEU:O	2:G:53:ILE:CG2	2.69	0.40
2:G:90:ALA:O	2:G:91:VAL:C	2.59	0.40
2:B:126:PRO:HG3	2:B:160:PRO:HG2	2.03	0.40
1:F:252:LEU:HD22	1:F:263:PHE:CE2	2.56	0.40
1:F:509:ILE:HA	1:F:509:ILE:HD13	1.75	0.40
3:H:110:ALA:O	3:H:114:GLY:N	2.54	0.40
1:A:155:LEU:HA	1:A:155:LEU:HD23	1.89	0.40
1:A:251:ALA:HA	1:A:254:THR:OG1	2.21	0.40
2:B:167:SER:HB3	2:B:187:ALA:CA	2.51	0.40
4:I:108:UNK:O	4:I:109:UNK:CB	2.69	0.40
1:A:420:PHE:CD1	7:A:1002:HEO:HMD3	2.56	0.40
7:A:1002:HEO:HHC	7:A:1002:HEO:O11	2.21	0.40
1:A:79:MET:SD	1:A:103:PHE:N	2.94	0.40
1:A:122:LEU:HA	1:A:122:LEU:HD23	1.83	0.40
1:A:328:PHE:O	1:A:331:TRP:HZ3	2.05	0.40
1:F:360:GLY:O	1:F:361:VAL:C	2.59	0.40
1:F:315:SER:HB3	1:F:365:ASN:HD21	1.86	0.40
2:G:53:ILE:CG2	2:G:54:VAL:N	2.84	0.40
2:G:86:ASN:C	2:G:87:LYS:HD2	2.41	0.40
3:C:177:ILE:HD12	3:C:178:MET:N	2.36	0.40
2:B:155:PHE:CZ	2:B:222:ALA:HB1	2.56	0.40
2:G:254:LEU:C	2:G:254:LEU:HD13	2.41	0.40
2:G:45:LEU:HD12	2:G:110:THR:CG2	2.48	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:26:ILE:HG22	3:H:27:PHE:N	2.35	0.40
1:A:463:GLY:HA3	1:A:505:ILE:HG13	2.03	0.40
1:A:255:LEU:HD22	1:A:259:LEU:HD12	2.03	0.40
1:A:473:ALA:C	1:A:475:GLY:N	2.75	0.40
3:H:122:HIS:ND1	3:H:122:HIS:O	2.54	0.40
1:A:481:ARG:CG	1:A:482:ARG:N	2.80	0.40
2:B:99:ILE:O	2:B:103:LEU:HB2	2.21	0.40
1:F:311:PHE:HZ	2:G:88:VAL:HG21	1.85	0.40
2:G:184:TYR:OH	2:G:189:MET:CE	2.70	0.40
3:C:146:HIS:NE2	3:C:187:LEU:HD23	2.36	0.40
1:F:257:ARG:NH1	1:F:257:ARG:CB	2.74	0.40
1:F:200:GLY:O	1:F:202:THR:N	2.54	0.40
1:A:440:TRP:O	1:A:444:PHE:HB2	2.22	0.40
2:G:278:ILE:HG22	2:G:282:MET:HG3	2.03	0.40
2:G:74:LYS:HE2	2:G:75:ASP:CG	2.42	0.40
3:H:33:LEU:O	3:H:37:CYS:N	2.55	0.40
3:H:139:PHE:C	3:H:141:ALA:N	2.75	0.40
1:A:411:HIS:ND1	7:A:1002:HEO:O2A	2.52	0.40
1:A:122:LEU:CD1	1:A:297:VAL:HG21	2.51	0.40
1:A:242:SER:OG	1:A:282:TRP:HD1	2.05	0.40
1:A:228:PHE:CD1	1:A:297:VAL:HG23	2.56	0.40
1:A:369:THR:CG2	1:A:369:THR:O	2.69	0.40
2:B:43:LEU:O	2:B:46:THR:OG1	2.36	0.40
1:F:187:VAL:O	1:F:188:ASP:C	2.60	0.40
2:G:139:PHE:HA	2:G:149:THR:O	2.21	0.40
3:H:107:LEU:C	3:H:109:GLY:N	2.73	0.40
3:C:116:GLU:OE1	3:C:143:VAL:HG11	2.21	0.40
3:H:191:TRP:C	3:H:193:CYS:H	2.24	0.40
1:A:305:PHE:HD1	1:A:305:PHE:N	2.19	0.40
3:C:51:VAL:HG12	3:C:135:PHE:CZ	2.57	0.40
3:H:94:ASN:HD22	3:H:97:GLN:HE22	1.69	0.40
3:C:119:GLU:O	3:C:120:PHE:C	2.60	0.40
2:G:74:LYS:HG3	2:G:74:LYS:H	1.70	0.40
3:C:33:LEU:HB2	3:C:34:MET:HE2	2.02	0.40
1:F:383:TRP:CD1	1:F:434:ALA:HA	2.57	0.40
3:H:167:ARG:NH1	3:H:167:ARG:HG3	2.36	0.40
1:F:318:TRP:C	1:F:322:CYS:HG	2.23	0.40
2:G:70:ARG:C	2:G:72:SER:H	2.25	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	499/663 (75%)	331 (66%)	110 (22%)	58 (12%)	0	7
1	F	499/663 (75%)	333 (67%)	108 (22%)	58 (12%)	0	7
2	B	255/315 (81%)	162 (64%)	66 (26%)	27 (11%)	0	8
2	G	255/315 (81%)	167 (66%)	58 (23%)	30 (12%)	0	7
3	C	183/204 (90%)	112 (61%)	52 (28%)	19 (10%)	1	8
3	H	183/204 (90%)	107 (58%)	56 (31%)	20 (11%)	0	8
All	All	1874/2364 (79%)	1212 (65%)	450 (24%)	212 (11%)	0	7

All (212) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	96	PRO
1	A	102	ILE
1	A	106	HIS
1	A	135	ASP
1	A	175	PRO
1	A	330	VAL
1	A	336	PHE
1	A	379	SER
1	A	451	THR
1	A	482	ARG
1	A	549	PHE
2	B	85	SER
2	B	101	ILE
2	B	116	PRO
2	B	118	LYS
2	B	119	PRO
3	C	97	GLN
3	C	197	VAL
1	F	96	PRO
1	F	102	ILE

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Mol	Chain	Res	Type
1	F	106	HIS
1	F	135	ASP
1	F	175	PRO
1	F	330	VAL
1	F	336	PHE
1	F	379	SER
1	F	451	THR
1	F	482	ARG
1	F	549	PHE
1	F	551	ASN
2	G	85	SER
2	G	116	PRO
2	G	118	LYS
2	G	119	PRO
3	H	97	GLN
3	H	197	VAL
1	A	62	ILE
1	A	95	PRO
1	A	97	HIS
1	A	103	PHE
1	A	110	MET
1	A	129	LEU
1	A	139	PRO
1	A	147	TRP
1	A	166	ALA
1	A	184	GLY
1	A	304	THR
1	A	355	ILE
1	A	363	ILE
1	A	442	LYS
1	A	481	ARG
1	A	525	GLN
1	A	551	ASN
2	B	67	TRP
2	B	113	ALA
2	B	125	LYS
2	B	178	ARG
2	B	200	PRO
2	B	223	ILE
2	B	263	VAL
3	C	20	ASP
3	C	50	LEU

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Mol	Chain	Res	Type
3	C	89	ALA
3	C	165	ALA
3	C	168	GLY
3	C	194	VAL
3	C	199	TYR
3	C	202	GLY
1	F	95	PRO
1	F	97	HIS
1	F	103	PHE
1	F	110	MET
1	F	129	LEU
1	F	139	PRO
1	F	147	TRP
1	F	166	ALA
1	F	184	GLY
1	F	234	CYS
1	F	355	ILE
1	F	363	ILE
1	F	442	LYS
1	F	481	ARG
1	F	525	GLN
2	G	67	TRP
2	G	113	ALA
2	G	125	LYS
2	G	178	ARG
2	G	223	ILE
2	G	263	VAL
3	H	20	ASP
3	H	50	LEU
3	H	52	ASN
3	H	89	ALA
3	H	109	GLY
3	H	165	ALA
3	H	168	GLY
3	H	194	VAL
3	H	199	TYR
3	H	202	GLY
1	A	82	GLN
1	A	101	GLN
1	A	128	PRO
1	A	137	ALA
1	A	200	GLY

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Mol	Chain	Res	Type
1	A	201	THR
1	A	234	CYS
1	A	273	MET
1	A	326	LEU
1	A	338	MET
1	A	474	LEU
2	B	112	HIS
2	B	117	SER
2	B	121	ALA
2	B	209	SER
2	B	213	PRO
2	B	260	TYR
3	C	48	ALA
3	C	52	ASN
3	C	54	THR
3	C	92	LYS
3	C	93	ASN
3	C	140	PHE
1	F	62	ILE
1	F	82	GLN
1	F	101	GLN
1	F	128	PRO
1	F	137	ALA
1	F	200	GLY
1	F	201	THR
1	F	273	MET
1	F	304	THR
1	F	338	MET
1	F	436	MET
2	G	77	LYS
2	G	112	HIS
2	G	117	SER
2	G	121	ALA
2	G	200	PRO
2	G	209	SER
2	G	213	PRO
2	G	260	TYR
3	H	48	ALA
3	H	54	THR
3	H	92	LYS
3	H	140	PHE
1	A	60	MET

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Mol	Chain	Res	Type
1	A	153	VAL
1	A	170	TRP
1	A	361	VAL
1	A	436	MET
1	A	539	LEU
2	B	32	PRO
2	B	54	VAL
2	B	77	LYS
1	F	153	VAL
1	F	170	TRP
1	F	326	LEU
1	F	474	LEU
1	F	539	LEU
2	G	32	PRO
3	H	93	ASN
1	A	172	ALA
1	A	207	ASN
1	A	313	TYR
1	A	317	VAL
1	A	371	TYR
1	A	462	ILE
2	B	56	ILE
2	B	177	PRO
1	F	60	MET
1	F	172	ALA
1	F	207	ASN
1	F	317	VAL
1	F	361	VAL
1	F	371	TYR
1	F	492	HIS
2	G	54	VAL
2	G	65	PHE
2	G	66	ALA
2	G	108	TRP
2	G	133	SER
2	G	177	PRO
3	H	181	SER
1	A	404	PRO
1	A	408	PHE
2	B	41	ARG
2	B	108	TRP
3	C	124	ILE

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Mol	Chain	Res	Type
3	C	181	SER
1	F	174	PRO
1	F	313	TYR
1	F	462	ILE
1	F	503	VAL
2	G	41	ARG
2	G	56	ILE
2	G	158	ASN
3	H	124	ILE
1	A	503	VAL
2	B	257	PRO
1	F	404	PRO
1	F	441	PRO
2	G	126	PRO
2	G	257	PRO
3	C	150	VAL
3	H	150	VAL
1	A	107	GLY
1	A	441	PRO
2	B	126	PRO
1	A	245	ILE
1	A	329	ILE
1	F	329	ILE
1	F	138	PHE

### 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	413/547 (76%)	373 (90%)	40 (10%)	10	42
1	F	413/547 (76%)	373 (90%)	40 (10%)	10	42
2	B	215/262 (82%)	188 (87%)	27 (13%)	5	28
2	G	215/262 (82%)	187 (87%)	28 (13%)	5	27
3	C	152/166 (92%)	133 (88%)	19 (12%)	6	29

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	H	152/166 (92%)	134 (88%)	18 (12%)	6	31
All	All	1560/1950 (80%)	1388 (89%)	172 (11%)	8	36

All (172) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	ASP
1	A	56	ARG
1	A	80	ARG
1	A	95	PRO
1	A	101	GLN
1	A	103	PHE
1	A	130	GLN
1	A	145	SER
1	A	148	PHE
1	A	155	LEU
1	A	159	SER
1	A	168	THR
1	A	188	ASP
1	A	192	TRP
1	A	223	PHE
1	A	229	THR
1	A	236	ASN
1	A	243	PHE
1	A	247	THR
1	A	249	THR
1	A	256	ASP
1	A	257	ARG
1	A	263	PHE
1	A	267	ASP
1	A	274	MET
1	A	280	TRP
1	A	314	THR
1	A	326	LEU
1	A	330	VAL
1	A	359	THR
1	A	377	PHE
1	A	397	THR
1	A	409	VAL
1	A	416	LEU
1	A	461	ILE
1	A	512	LEU

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Mol	Chain	Res	Type
1	A	514	ILE
1	A	537	ARG
1	A	545	SER
1	A	552	PHE
2	B	36	ILE
2	B	39	GLU
2	B	41	ARG
2	B	61	MET
2	B	67	TRP
2	B	74	LYS
2	B	77	LYS
2	B	78	TYR
2	B	82	TRP
2	B	93	TRP
2	B	94	THR
2	B	115	GLU
2	B	118	LYS
2	B	119	PRO
2	B	120	LEU
2	B	134	MET
2	B	144	GLU
2	B	153	ILE
2	B	155	PHE
2	B	159	THR
2	B	172	ASN
2	B	178	ARG
2	B	181	SER
2	B	189	MET
2	B	192	ARG
2	B	227	ASP
2	B	276	ASP
3	C	29	PHE
3	C	31	ILE
3	C	32	TYR
3	C	43	LEU
3	C	44	PHE
3	C	46	THR
3	C	50	LEU
3	C	72	GLU
3	C	78	PHE
3	C	85	MET
3	C	122	HIS

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Mol	Chain	Res	Type
3	C	135	PHE
3	C	140	PHE
3	C	156	TRP
3	C	163	GLN
3	C	167	ARG
3	C	179	CYS
3	C	182	LEU
3	C	187	LEU
1	F	53	ASP
1	F	56	ARG
1	F	80	ARG
1	F	95	PRO
1	F	101	GLN
1	F	103	PHE
1	F	130	GLN
1	F	145	SER
1	F	148	PHE
1	F	155	LEU
1	F	159	SER
1	F	168	THR
1	F	188	ASP
1	F	192	TRP
1	F	223	PHE
1	F	229	THR
1	F	236	ASN
1	F	243	PHE
1	F	247	THR
1	F	249	THR
1	F	256	ASP
1	F	257	ARG
1	F	263	PHE
1	F	267	ASP
1	F	274	MET
1	F	280	TRP
1	F	314	THR
1	F	326	LEU
1	F	330	VAL
1	F	359	THR
1	F	377	PHE
1	F	397	THR
1	F	409	VAL
1	F	416	LEU

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Mol	Chain	Res	Type
1	F	512	LEU
1	F	514	ILE
1	F	537	ARG
1	F	545	SER
1	F	548	PRO
1	F	552	PHE
2	G	36	ILE
2	G	39	GLU
2	G	41	ARG
2	G	61	MET
2	G	67	TRP
2	G	74	LYS
2	G	77	LYS
2	G	78	TYR
2	G	82	TRP
2	G	93	TRP
2	G	94	THR
2	G	95	VAL
2	G	115	GLU
2	G	118	LYS
2	G	119	PRO
2	G	120	LEU
2	G	134	MET
2	G	144	GLU
2	G	153	ILE
2	G	155	PHE
2	G	159	THR
2	G	172	ASN
2	G	178	ARG
2	G	181	SER
2	G	189	MET
2	G	192	ARG
2	G	227	ASP
2	G	276	ASP
3	H	29	PHE
3	H	32	TYR
3	H	43	LEU
3	H	44	PHE
3	H	46	THR
3	H	50	LEU
3	H	72	GLU
3	H	78	PHE

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Mol	Chain	Res	Type
3	H	85	MET
3	H	122	HIS
3	H	135	PHE
3	H	140	PHE
3	H	156	TRP
3	H	163	GLN
3	H	167	ARG
3	H	179	CYS
3	H	182	LEU
3	H	187	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	124	ASN
1	A	142	ASN
1	A	143	ASN
1	A	195	GLN
1	A	266	ASN
1	A	345	ASN
1	A	365	ASN
1	A	372	GLN
1	A	486	GLN
1	A	492	HIS
2	B	151	ASN
2	B	168	ASN
2	B	190	GLN
2	B	198	ASN
2	B	233	GLN
2	B	261	ASN
2	B	268	ASN
3	C	94	ASN
3	C	97	GLN
1	F	124	ASN
1	F	142	ASN
1	F	143	ASN
1	F	195	GLN
1	F	266	ASN
1	F	345	ASN
1	F	365	ASN
2	G	151	ASN
2	G	168	ASN

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Mol	Chain	Res	Type
2	G	190	GLN
2	G	198	ASN
2	G	233	GLN
2	G	261	ASN
2	G	268	ASN
3	H	94	ASN
3	H	97	GLN
3	H	185	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
6	HEM	A	1001	1	30,50,50	2.74	8 (26%)	24,82,82	2.80	7 (29%)
7	HEO	A	1002	1	49,66,66	1.14	5 (10%)	59,102,102	1.33	8 (13%)
6	HEM	F	1001	1	30,50,50	2.76	9 (30%)	24,82,82	2.79	7 (29%)
7	HEO	F	1002	1	49,66,66	1.16	5 (10%)	59,102,102	1.32	9 (15%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	HEM	A	1001	1	-	0/10/54/54	0/0/8/8
7	HEO	A	1002	1	-	0/28/114/114	0/0/8/8
6	HEM	F	1001	1	-	0/10/54/54	0/0/8/8
7	HEO	F	1002	1	-	0/28/114/114	0/0/8/8

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	1001	HEM	C3B-C4B	-8.20	1.44	1.51
6	A	1001	HEM	C3B-C4B	-7.57	1.45	1.51
6	F	1001	HEM	C2D-C3D	-6.41	1.35	1.54
6	A	1001	HEM	C2D-C3D	-6.28	1.35	1.54
6	F	1001	HEM	C3C-CAC	-6.13	1.39	1.51
6	A	1001	HEM	C3C-CAC	-6.08	1.39	1.51
6	F	1001	HEM	C3D-C4D	-5.31	1.44	1.51
6	A	1001	HEM	C3D-C4D	-5.14	1.45	1.51
6	A	1001	HEM	C2C-C1C	-4.20	1.44	1.52
7	A	1002	HEO	C3C-CAC	-3.89	1.39	1.47
7	F	1002	HEO	C3C-CAC	-3.84	1.39	1.47
6	F	1001	HEM	C2C-C1C	-3.62	1.45	1.52
7	A	1002	HEO	C3C-C2C	-3.61	1.35	1.40
7	F	1002	HEO	C3C-C2C	-3.41	1.35	1.40
7	F	1002	HEO	CHA-C4D	-2.35	1.35	1.41
7	A	1002	HEO	CHA-C4D	-2.14	1.36	1.41
6	F	1001	HEM	C2D-C1D	-2.06	1.45	1.51
6	F	1001	HEM	C4C-NC	2.20	1.38	1.36
7	F	1002	HEO	C14-C15	2.23	1.37	1.33
6	A	1001	HEM	C4C-NC	2.24	1.38	1.36
7	A	1002	HEO	C18-C19	2.24	1.37	1.33
7	A	1002	HEO	C14-C15	2.29	1.37	1.33
6	F	1001	HEM	C1C-NC	2.34	1.38	1.36
7	F	1002	HEO	C18-C19	2.68	1.38	1.33
6	A	1001	HEM	C1C-NC	3.03	1.39	1.36
6	F	1001	HEM	CBB-CAB	4.11	1.53	1.29
6	A	1001	HEM	CBB-CAB	4.19	1.53	1.29

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1001	HEM	C3B-CAB-CBB	-9.58	109.76	124.46
6	F	1001	HEM	C3B-CAB-CBB	-9.46	109.95	124.46
7	A	1002	HEO	C1D-ND-C4D	-3.25	102.03	105.00
7	F	1002	HEO	C1D-ND-C4D	-3.16	102.12	105.00
7	A	1002	HEO	C4C-CHD-C1D	-2.61	123.66	129.26
7	F	1002	HEO	C4C-CHD-C1D	-2.59	123.70	129.26
7	A	1002	HEO	C13-C14-C15	-2.50	122.33	127.76
7	F	1002	HEO	C13-C14-C15	-2.42	122.50	127.76
7	F	1002	HEO	C17-C18-C19	-2.41	122.53	127.76
7	A	1002	HEO	C17-C18-C19	-2.40	122.54	127.76
7	A	1002	HEO	C13-C12-C11	-2.40	111.33	114.51
7	F	1002	HEO	C1C-CHC-C4B	-2.31	124.30	129.26
7	F	1002	HEO	C13-C12-C11	-2.30	111.45	114.51
7	A	1002	HEO	C1C-CHC-C4B	-2.14	124.66	129.26
7	F	1002	HEO	C4B-NB-C1B	-2.12	103.07	105.00
7	F	1002	HEO	C3D-C4D-ND	2.11	112.55	110.35
7	A	1002	HEO	C3D-C4D-ND	2.18	112.62	110.35
7	F	1002	HEO	C3C-C4C-NC	2.45	112.37	109.21
7	A	1002	HEO	C3C-C4C-NC	2.52	112.47	109.21
6	F	1001	HEM	CMD-C2D-C3D	2.69	126.25	114.35
6	A	1001	HEM	CMD-C2D-C3D	2.71	126.31	114.35
6	A	1001	HEM	C2D-C3D-C4D	2.74	106.15	101.50
6	F	1001	HEM	C2D-C3D-C4D	2.76	106.18	101.50
6	F	1001	HEM	CAD-C3D-C4D	3.89	126.17	112.47
6	A	1001	HEM	CAD-C3D-C4D	4.01	126.61	112.47
6	A	1001	HEM	CMC-C2C-C3C	4.09	126.74	116.53
6	A	1001	HEM	CMB-C2B-C3B	4.15	126.89	116.53
6	F	1001	HEM	CMC-C2C-C3C	4.19	126.99	116.53
6	F	1001	HEM	CMB-C2B-C3B	4.22	127.07	116.53
6	A	1001	HEM	CAD-C3D-C2D	4.77	126.92	113.22
6	F	1001	HEM	CAD-C3D-C2D	4.93	127.40	113.22

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 65 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1001	HEM	18	0
7	A	1002	HEO	16	0
6	F	1001	HEM	17	0
7	F	1002	HEO	14	0

## 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 ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.