



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 11, 2024 – 05:46 PM EDT

PDB ID : 1BVU  
Title : GLUTAMATE DEHYDROGENASE FROM THERMOCOCCUS LITORALIS  
Authors : Baker, P.J.; Britton, K.L.; Yip, K.S.; Stillman, T.J.; Rice, D.W.  
Deposited on : 1999-07-20  
Resolution : 2.50 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

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

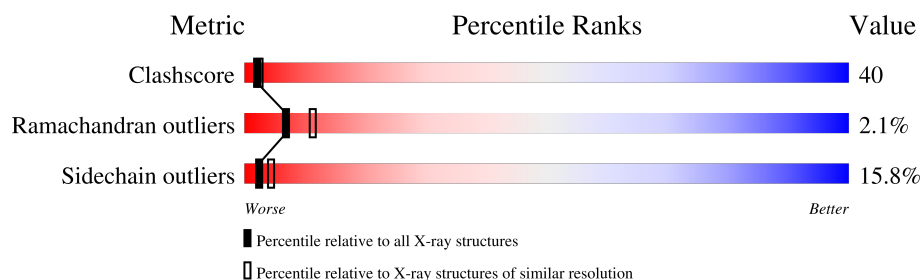
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 Å.

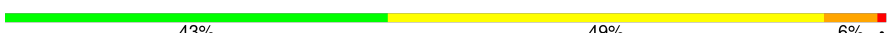
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	418	 37% 50% 12%
1	B	418	 45% 46% 7%
1	C	418	 45% 43% 11%
1	D	418	 39% 49% 11%
1	E	418	 43% 49% 6% •
1	F	418	 44% 47% 9%

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 19566 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 PROTEIN (GLUTAMATE DEHYDROGENASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	416	Total	C	N	O	S	0	0	0
			3261	2076	547	620	18			
1	B	416	Total	C	N	O	S	0	0	0
			3261	2076	547	620	18			
1	C	416	Total	C	N	O	S	0	0	0
			3261	2076	547	620	18			
1	D	416	Total	C	N	O	S	0	0	0
			3261	2076	547	620	18			
1	E	416	Total	C	N	O	S	0	0	0
			3261	2076	547	620	18			
1	F	416	Total	C	N	O	S	0	0	0
			3261	2076	547	620	18			

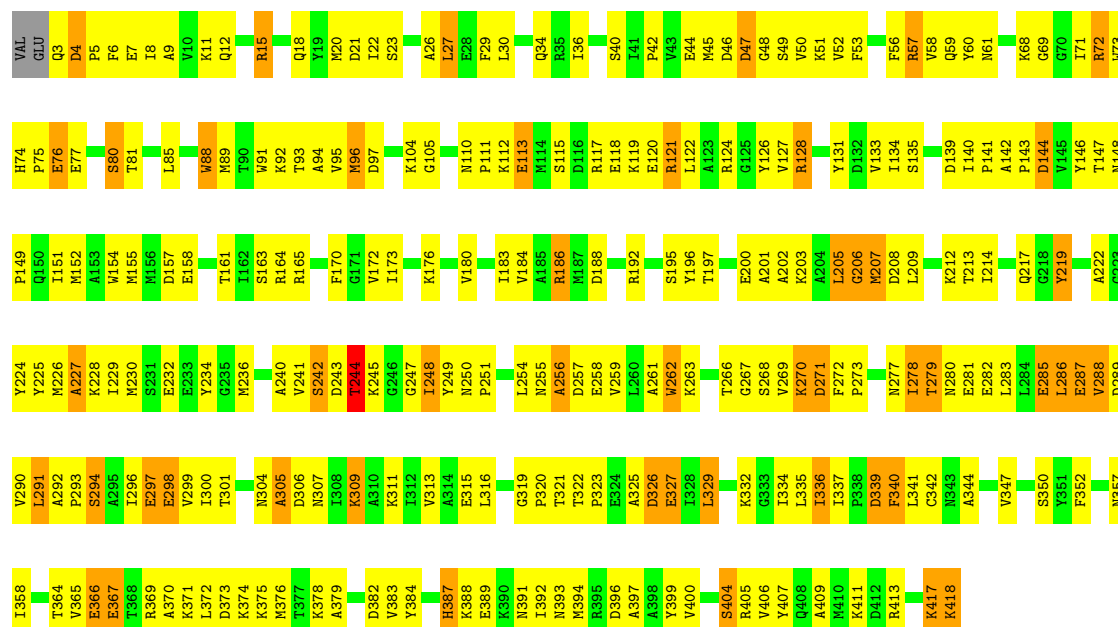
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

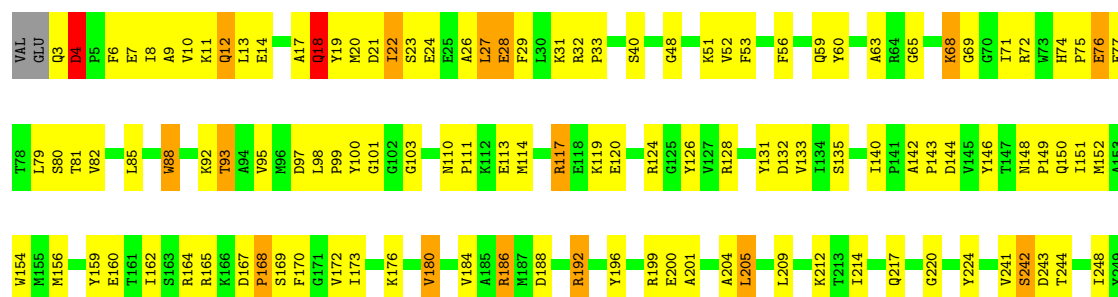
#### • Molecule 1: PROTEIN (GLUTAMATE DEHYDROGENASE)

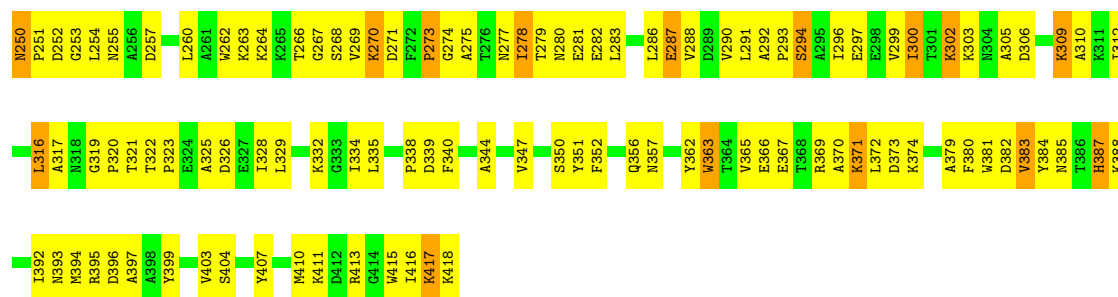
Chain A: 



#### • Molecule 1: PROTEIN (GLUTAMATE DEHYDROGENASE)

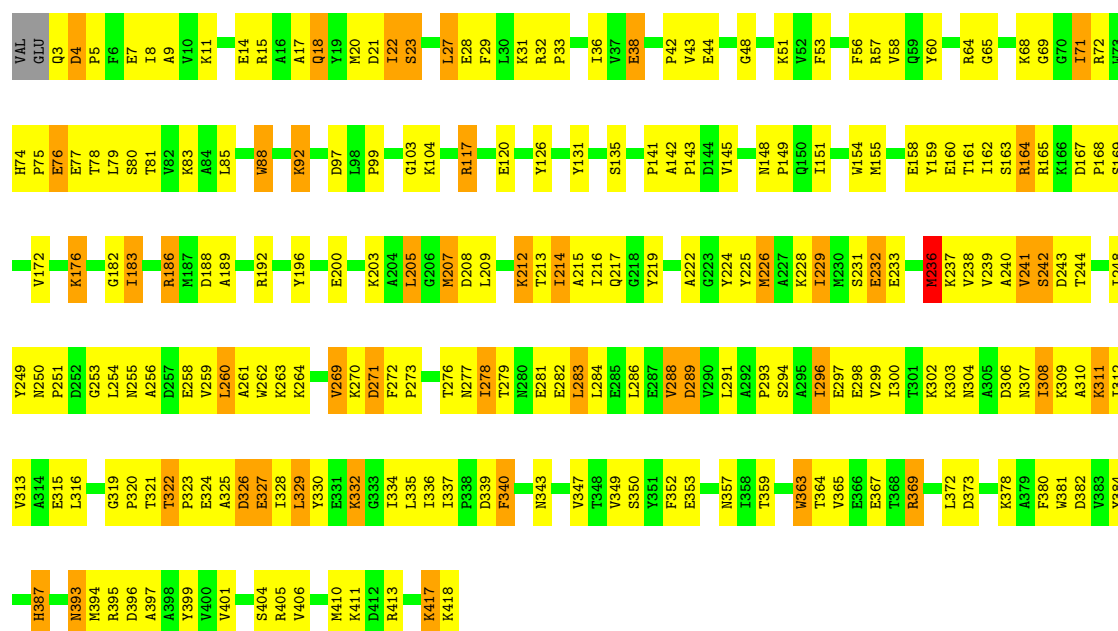
Chain B: 





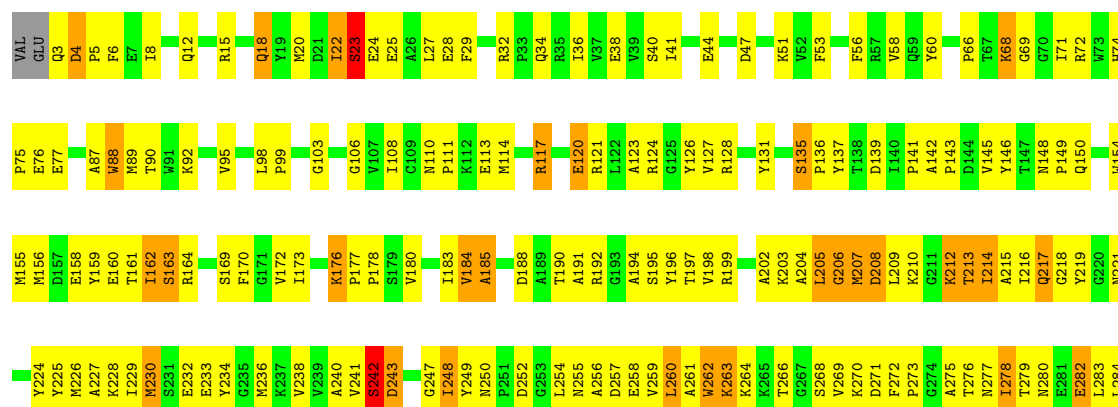
• Molecule 1: PROTEIN (GLUTAMATE DEHYDROGENASE)

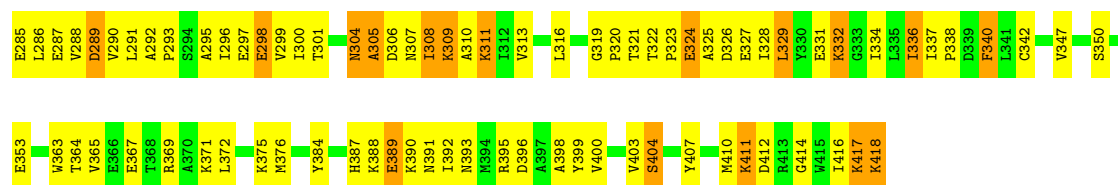
Chain C: 45% 43% 11%



• Molecule 1: PROTEIN (GLUTAMATE DEHYDROGENASE)

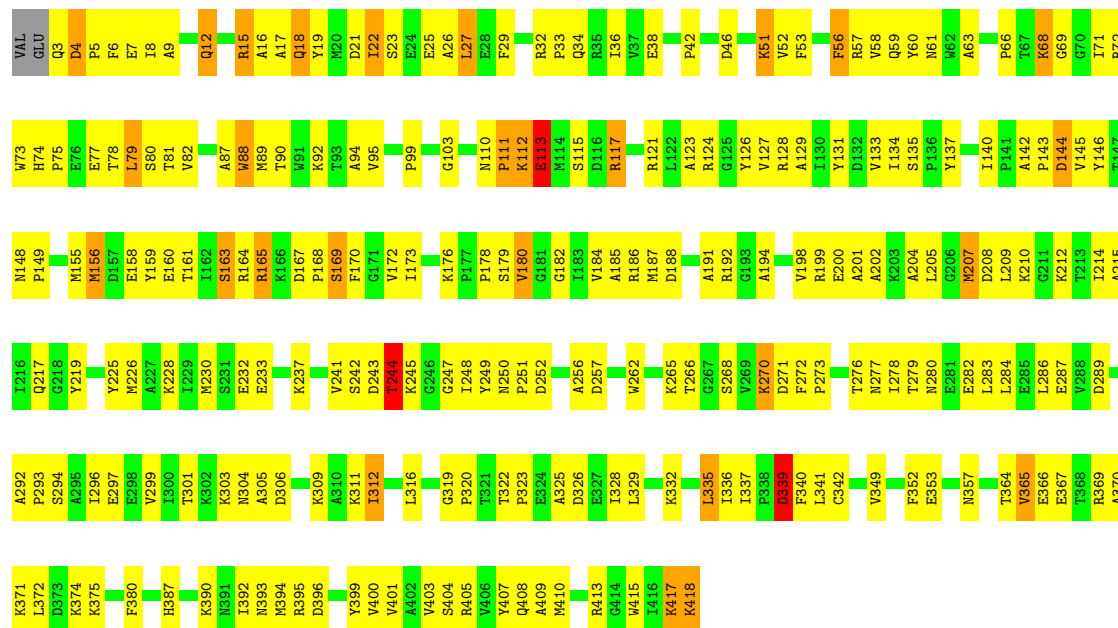
Chain D: 39% 49% 11%





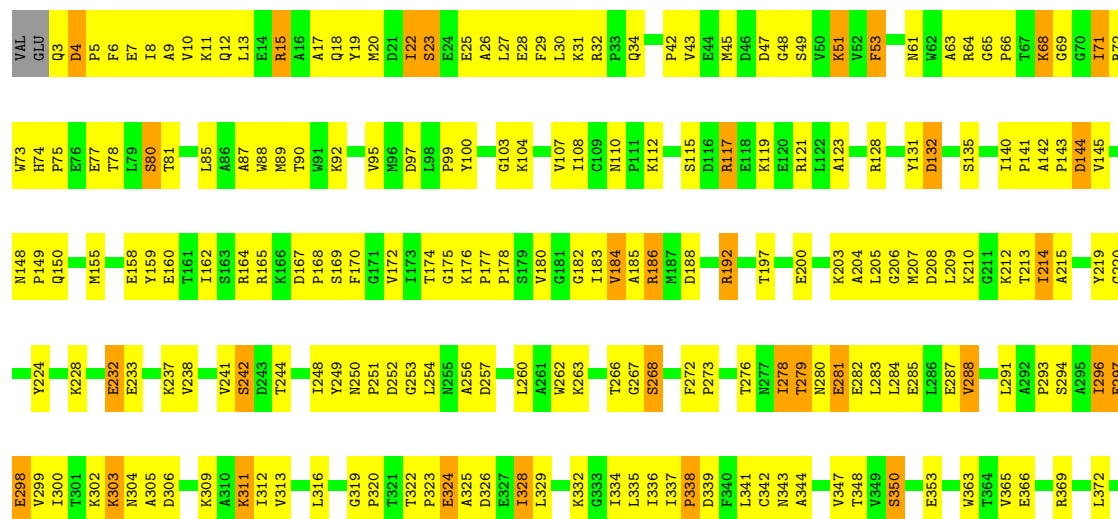
• Molecule 1: PROTEIN (GLUTAMATE DEHYDROGENASE)

Chain E: 43% 49% 6%



• Molecule 1: PROTEIN (GLUTAMATE DEHYDROGENASE)

Chain F: 44% 47% 9%





## 4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	141.90Å 197.50Å 125.70Å 90.00° 113.60° 90.00°	Depositor
Resolution (Å)	10.00 – 2.50	Depositor
% Data completeness (in resolution range)	87.0 (10.00-2.50)	Depositor
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	TNT	Depositor
R, $R_{free}$	(Not available) , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	19566	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	50.0	wwPDB-VP



## 5 Model quality

### 5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.68	0/3331	0.89	4/4511 (0.1%)
1	B	0.70	0/3331	0.91	4/4511 (0.1%)
1	C	0.70	0/3331	0.90	3/4511 (0.1%)
1	D	0.70	0/3331	0.89	1/4511 (0.0%)
1	E	0.72	0/3331	0.94	3/4511 (0.1%)
1	F	0.70	0/3331	0.90	0/4511
All	All	0.70	0/19986	0.90	15/27066 (0.1%)

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	164	ARG	NE-CZ-NH2	7.26	123.93	120.30
1	C	164	ARG	NE-CZ-NH1	-6.32	117.14	120.30
1	A	128	ARG	NE-CZ-NH1	6.13	123.36	120.30
1	B	250	ASN	C-N-CD	-6.09	107.20	120.60
1	B	316	LEU	CB-CG-CD2	-6.05	100.71	111.00
1	D	139	ASP	CB-CG-OD1	5.88	123.60	118.30
1	A	57	ARG	NE-CZ-NH1	-5.85	117.38	120.30
1	A	128	ARG	NE-CZ-NH2	-5.78	117.41	120.30
1	A	121	ARG	NE-CZ-NH2	-5.33	117.64	120.30
1	B	52	VAL	CB-CA-C	-5.12	101.66	111.40
1	E	312	ILE	CB-CA-C	-5.12	101.36	111.60
1	E	165	ARG	NE-CZ-NH2	5.08	122.84	120.30
1	C	413	ARG	NE-CZ-NH1	-5.07	117.76	120.30
1	E	156	MET	CG-SD-CE	-5.05	92.12	100.20
1	B	101	GLY	N-CA-C	-5.03	100.53	113.10

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3261	0	3254	331	0
1	B	3261	0	3254	229	0
1	C	3261	0	3254	260	0
1	D	3261	0	3254	300	0
1	E	3261	0	3254	262	0
1	F	3261	0	3254	241	0
All	All	19566	0	19524	1572	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 40.

All (1572) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:329:LEU:HD23	1:A:334:ILE:CD1	1.54	1.36
1:E:29:PHE:CD1	1:E:410:MET:HE1	1.64	1.32
1:D:255:ASN:O	1:D:259:VAL:HG23	1.25	1.30
1:A:279:THR:HG22	1:A:282:GLU:OE2	1.28	1.27
1:A:329:LEU:CD2	1:A:334:ILE:HD12	1.63	1.27
1:C:384:TYR:HD1	1:C:394:MET:CE	1.49	1.25
1:E:29:PHE:CD1	1:E:410:MET:CE	2.21	1.22
1:C:225:TYR:O	1:C:229:ILE:HG13	1.35	1.20
1:C:214:ILE:HG22	1:C:236:MET:HE2	1.22	1.19
1:D:283:LEU:HA	1:D:286:LEU:CD1	1.74	1.17
1:E:188:ASP:OD2	1:E:192:ARG:NH1	1.80	1.15
1:C:384:TYR:CD1	1:C:394:MET:CE	2.30	1.14
1:A:279:THR:HG23	1:A:282:GLU:HG3	1.18	1.14
1:C:3:GLN:HG2	1:C:4:ASP:H	1.02	1.12
1:D:241:VAL:HG12	1:D:242:SER:H	1.13	1.12
1:C:384:TYR:HD1	1:C:394:MET:HE3	1.06	1.11
1:A:209:LEU:HA	1:A:212:LYS:HG3	1.20	1.11
1:B:3:GLN:HG2	1:B:4:ASP:H	1.10	1.10
1:C:214:ILE:CG2	1:C:236:MET:HE2	1.80	1.10
1:D:283:LEU:CA	1:D:286:LEU:HD12	1.82	1.10
1:A:110:ASN:ND2	1:A:113:GLU:OE2	1.87	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:74:HIS:ND1	1:B:75:PRO:HD2	1.69	1.06
1:C:329:LEU:HD23	1:C:334:ILE:HD12	1.08	1.06
1:C:329:LEU:HD23	1:C:334:ILE:CD1	1.84	1.05
1:A:321:THR:HG22	1:A:322:THR:H	1.20	1.05
1:E:12:GLN:OE1	1:E:88:TRP:HH2	1.37	1.04
1:A:283:LEU:O	1:A:286:LEU:HB2	1.57	1.03
1:E:88:TRP:CZ2	1:E:399:TYR:OH	2.11	1.03
1:A:279:THR:HG23	1:A:282:GLU:CG	1.87	1.03
1:D:241:VAL:CG1	1:D:242:SER:H	1.72	1.03
1:A:279:THR:CG2	1:A:282:GLU:OE2	2.07	1.02
1:B:325:ALA:O	1:B:329:LEU:HD12	1.59	1.02
1:F:29:PHE:CD2	1:F:410:MET:CE	2.43	1.02
1:B:29:PHE:CD2	1:B:410:MET:HE1	1.95	1.02
1:C:214:ILE:HG22	1:C:236:MET:CE	1.90	1.01
1:C:213:THR:OG1	1:C:288:VAL:HG12	1.60	1.01
1:D:241:VAL:HG12	1:D:242:SER:N	1.67	1.01
1:F:184:VAL:HG12	1:F:185:ALA:N	1.67	1.01
1:A:287:GLU:HG3	1:A:309:LYS:HD2	1.43	1.00
1:C:384:TYR:CD1	1:C:394:MET:HE3	1.96	1.00
1:B:29:PHE:HD2	1:B:410:MET:HE1	1.25	0.99
1:C:51:LYS:HG2	1:C:53:PHE:CE1	1.97	0.98
1:B:294:SER:HB3	1:B:316:LEU:CB	1.92	0.98
1:C:297:GLU:HG3	1:C:298:GLU:HG3	1.45	0.97
1:E:262:TRP:O	1:E:266:THR:HB	1.63	0.97
1:F:184:VAL:CG1	1:F:185:ALA:N	2.27	0.97
1:E:29:PHE:HD1	1:E:410:MET:HE1	1.29	0.96
1:C:3:GLN:HG2	1:C:4:ASP:N	1.79	0.96
1:C:3:GLN:CG	1:C:4:ASP:H	1.78	0.96
1:D:279:THR:N	1:D:282:GLU:OE1	1.99	0.95
1:A:170:PHE:O	1:A:176:LYS:NZ	1.99	0.95
1:C:300:ILE:O	1:C:322:THR:HG23	1.67	0.95
1:C:208:ASP:O	1:C:212:LYS:NZ	1.98	0.95
1:C:384:TYR:CD1	1:C:394:MET:HE1	2.01	0.95
1:E:364:THR:OG1	1:E:367:GLU:HG3	1.64	0.95
1:B:29:PHE:CD2	1:B:410:MET:CE	2.50	0.95
1:F:29:PHE:CD2	1:F:410:MET:HE3	2.00	0.95
1:E:323:PRO:O	1:E:326:ASP:HB2	1.68	0.94
1:A:20:MET:CE	1:A:400:VAL:HA	1.98	0.94
1:A:321:THR:HG22	1:A:322:THR:N	1.80	0.94
1:B:7:GLU:O	1:B:11:LYS:HG3	1.68	0.94
1:E:12:GLN:OE1	1:E:88:TRP:CH2	2.20	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:248:ILE:HD12	1:A:254:LEU:HD13	1.50	0.93
1:B:279:THR:OG1	1:B:282:GLU:HG3	1.68	0.93
1:C:183:ILE:HD13	1:C:353:GLU:HB2	1.49	0.93
1:D:184:VAL:O	1:D:185:ALA:CB	2.16	0.93
1:B:321:THR:HG22	1:B:322:THR:N	1.82	0.93
1:A:48:GLY:HA2	1:E:117:ARG:NH2	1.84	0.92
1:D:255:ASN:O	1:D:259:VAL:CG2	2.17	0.92
1:E:176:LYS:NZ	1:E:353:GLU:OE2	2.01	0.92
1:C:270:LYS:HG3	1:C:277:ASN:HD21	1.32	0.92
1:F:184:VAL:CG1	1:F:185:ALA:H	1.81	0.92
1:F:208:ASP:O	1:F:212:LYS:NZ	2.01	0.92
1:C:393:ASN:ND2	1:C:396:ASP:H	1.69	0.91
1:B:148:ASN:HB2	1:B:149:PRO:HD2	1.51	0.91
1:B:242:SER:HB3	1:B:283:LEU:HD13	1.52	0.91
1:F:323:PRO:O	1:F:326:ASP:HB2	1.71	0.91
1:C:384:TYR:HA	1:C:394:MET:HE1	1.51	0.91
1:C:329:LEU:CD2	1:C:334:ILE:HD12	2.00	0.90
1:A:279:THR:CG2	1:A:282:GLU:HG3	1.98	0.90
1:E:4:ASP:O	1:E:8:ILE:HG13	1.72	0.90
1:F:3:GLN:NE2	1:F:80:SER:OG	2.03	0.90
1:A:209:LEU:HA	1:A:212:LYS:CG	2.02	0.90
1:C:5:PRO:HA	1:C:8:ILE:HD12	1.53	0.89
1:C:243:ASP:OD2	1:C:269:VAL:HG22	1.72	0.89
1:C:188:ASP:OD2	1:C:192:ARG:NH1	2.05	0.89
1:D:170:PHE:O	1:D:176:LYS:HE3	1.73	0.89
1:C:148:ASN:HB2	1:C:149:PRO:HD2	1.54	0.89
1:F:188:ASP:OD2	1:F:192:ARG:NH1	2.06	0.89
1:A:48:GLY:HA2	1:E:117:ARG:HH22	1.38	0.88
1:D:3:GLN:HG2	1:D:4:ASP:H	1.38	0.88
1:B:3:GLN:HG2	1:B:4:ASP:N	1.86	0.88
1:B:63:ALA:HB2	1:B:415:TRP:CZ3	2.08	0.88
1:C:120:GLU:HA	1:C:154:TRP:CE3	2.09	0.88
1:C:29:PHE:CD2	1:C:410:MET:CE	2.56	0.88
1:A:315:GLU:OE2	1:A:336:ILE:CD1	2.22	0.87
1:C:241:VAL:HG12	1:C:242:SER:N	1.87	0.87
1:A:51:LYS:HG2	1:A:53:PHE:CE1	2.09	0.87
1:A:188:ASP:O	1:A:192:ARG:HB3	1.73	0.87
1:B:294:SER:HB3	1:B:316:LEU:HB3	1.57	0.87
1:E:219:TYR:CD1	1:E:241:VAL:HG11	2.10	0.87
1:D:322:THR:HB	1:D:323:PRO:HD2	1.55	0.86
1:E:167:ASP:HB2	1:E:168:PRO:HD2	1.55	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:214:ILE:HD12	1:D:290:VAL:CG1	2.06	0.86
1:E:68:LYS:HD3	1:E:140:ILE:HB	1.56	0.86
1:A:400:VAL:O	1:A:404:SER:HB3	1.76	0.86
1:E:322:THR:HB	1:E:323:PRO:HD2	1.58	0.85
1:E:270:LYS:HG2	1:E:277:ASN:HD21	1.41	0.85
1:C:335:LEU:HD23	1:C:336:ILE:N	1.90	0.85
1:D:262:TRP:CH2	1:D:273:PRO:HD3	2.10	0.85
1:C:224:TYR:CD1	1:C:260:LEU:CD2	2.59	0.85
1:C:323:PRO:O	1:C:326:ASP:HB2	1.77	0.85
1:F:392:ILE:HD12	1:F:396:ASP:HB3	1.56	0.85
1:A:20:MET:HE2	1:A:400:VAL:HA	1.56	0.85
1:C:4:ASP:HB3	1:C:5:PRO:HD3	1.58	0.84
1:B:22:ILE:HG12	1:B:23:SER:N	1.92	0.84
1:C:397:ALA:O	1:C:401:VAL:HG23	1.78	0.84
1:D:3:GLN:C	1:D:5:PRO:HD2	1.97	0.84
1:A:322:THR:O	1:A:326:ASP:N	2.10	0.84
1:C:15:ARG:HG3	1:C:18:GLN:NE2	1.92	0.84
1:B:3:GLN:CG	1:B:4:ASP:H	1.90	0.84
1:E:3:GLN:NE2	1:E:80:SER:OG	2.10	0.84
1:F:3:GLN:O	1:F:5:PRO:HD2	1.76	0.83
1:D:214:ILE:HD12	1:D:290:VAL:HG12	1.59	0.83
1:D:279:THR:HG22	1:D:282:GLU:OE1	1.79	0.83
1:A:249:TYR:CE2	1:A:251:PRO:HG3	2.13	0.83
1:A:126:TYR:HD2	1:A:155:MET:HE2	1.44	0.83
1:A:321:THR:CG2	1:A:322:THR:H	1.91	0.82
1:D:283:LEU:HA	1:D:286:LEU:HD12	0.89	0.82
1:B:241:VAL:CG1	1:B:242:SER:N	2.42	0.82
1:F:142:ALA:HB1	1:F:143:PRO:HD2	1.61	0.82
1:C:48:GLY:C	1:F:117:ARG:HH22	1.82	0.82
1:F:29:PHE:CD2	1:F:410:MET:HE1	2.13	0.82
1:C:224:TYR:CD1	1:C:260:LEU:HD22	2.13	0.82
1:F:142:ALA:HB1	1:F:143:PRO:CD	2.09	0.82
1:B:294:SER:HB3	1:B:316:LEU:HB2	1.61	0.82
1:E:296:ILE:HD12	1:E:299:VAL:CG1	2.09	0.81
1:E:167:ASP:HB2	1:E:168:PRO:CD	2.10	0.81
1:B:69:GLY:HA3	1:B:103:GLY:O	1.79	0.81
1:C:186:ARG:HG2	1:C:186:ARG:HH11	1.43	0.81
1:E:184:VAL:HG12	1:E:185:ALA:N	1.96	0.81
1:E:51:LYS:HG2	1:E:53:PHE:CE1	2.15	0.81
1:E:226:MET:HE3	1:E:230:MET:SD	2.21	0.81
1:A:329:LEU:HD22	1:A:334:ILE:HG21	1.63	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:186:ARG:HH11	1:C:186:ARG:CG	1.94	0.80
1:F:379:ALA:O	1:F:383:VAL:HG23	1.81	0.80
1:A:291:LEU:HD22	1:A:293:PRO:HD3	1.63	0.80
1:E:172:VAL:HG22	1:E:172:VAL:O	1.81	0.80
1:A:249:TYR:CZ	1:A:251:PRO:HG3	2.16	0.80
1:C:142:ALA:HB1	1:C:143:PRO:HD2	1.62	0.80
1:E:3:GLN:HG2	1:E:5:PRO:HD3	1.61	0.80
1:C:214:ILE:CG2	1:C:236:MET:CE	2.53	0.80
1:D:184:VAL:O	1:D:185:ALA:HB3	1.81	0.80
1:A:329:LEU:CD2	1:A:334:ILE:CD1	2.37	0.80
1:D:3:GLN:HG2	1:D:4:ASP:N	1.95	0.80
1:D:188:ASP:OD2	1:D:192:ARG:NH1	2.15	0.80
1:D:120:GLU:HB2	1:D:154:TRP:CE3	2.17	0.80
1:E:184:VAL:O	1:E:185:ALA:HB3	1.81	0.80
1:E:242:SER:HB3	1:E:283:LEU:HD13	1.62	0.80
1:B:328:ILE:O	1:B:332:LYS:HB2	1.82	0.79
1:A:30:LEU:HD22	1:A:91:TRP:HH2	1.47	0.79
1:E:74:HIS:ND1	1:E:75:PRO:HD2	1.96	0.79
1:A:407:TYR:OH	1:A:418:LYS:O	1.99	0.79
1:A:228:LYS:O	1:A:232:GLU:HB2	1.82	0.79
1:D:29:PHE:CD1	1:D:410:MET:HE1	2.17	0.78
1:A:3:GLN:O	1:A:4:ASP:C	2.20	0.78
1:C:237:LYS:O	1:C:239:VAL:HG13	1.83	0.78
1:D:4:ASP:O	1:D:8:ILE:HG13	1.84	0.78
1:C:225:TYR:O	1:C:229:ILE:CG1	2.27	0.78
1:C:255:ASN:O	1:C:259:VAL:HG23	1.82	0.78
1:B:74:HIS:ND1	1:B:75:PRO:CD	2.46	0.78
1:E:3:GLN:C	1:E:7:GLU:HG3	2.04	0.78
1:B:148:ASN:HB2	1:B:149:PRO:CD	2.14	0.78
1:A:364:THR:HG23	1:A:367:GLU:OE1	1.83	0.78
1:A:417:LYS:HG2	1:C:117:ARG:NH2	1.98	0.77
1:B:29:PHE:HE1	1:E:42:PRO:HG3	1.49	0.77
1:C:29:PHE:CD2	1:C:410:MET:HE3	2.19	0.77
1:D:194:ALA:O	1:D:197:THR:OG1	2.02	0.77
1:E:22:ILE:HD11	1:E:26:ALA:HB3	1.64	0.77
1:D:262:TRP:CZ3	1:D:273:PRO:CD	2.67	0.77
1:E:3:GLN:NE2	1:E:80:SER:CB	2.46	0.77
1:B:323:PRO:O	1:B:326:ASP:HB2	1.83	0.77
1:B:321:THR:CG2	1:B:322:THR:N	2.47	0.77
1:A:200:GLU:OE2	1:A:203:LYS:NZ	2.18	0.77
1:E:117:ARG:O	1:E:121:ARG:HG3	1.85	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:PRO:HA	1:A:8:ILE:HD12	1.67	0.77
1:F:184:VAL:O	1:F:185:ALA:HB3	1.84	0.76
1:A:120:GLU:HG3	1:A:154:TRP:CD2	2.19	0.76
1:A:117:ARG:NH1	1:B:417:LYS:HG2	2.00	0.76
1:A:417:LYS:HG2	1:C:117:ARG:CZ	2.15	0.76
1:D:322:THR:HB	1:D:323:PRO:CD	2.15	0.76
1:F:393:ASN:ND2	1:F:396:ASP:H	1.83	0.76
1:D:120:GLU:HB2	1:D:154:TRP:CD2	2.20	0.76
1:A:44:GLU:CG	1:E:117:ARG:HH21	1.97	0.76
1:B:172:VAL:O	1:B:172:VAL:HG22	1.86	0.76
1:C:48:GLY:O	1:F:117:ARG:NH2	2.12	0.76
1:C:324:GLU:O	1:C:328:ILE:HG13	1.86	0.76
1:E:3:GLN:HE21	1:E:80:SER:CB	1.98	0.76
1:D:399:TYR:O	1:D:403:VAL:HG23	1.85	0.76
1:E:322:THR:HB	1:E:323:PRO:CD	2.15	0.76
1:A:225:TYR:O	1:A:229:ILE:HG13	1.85	0.75
1:E:170:PHE:O	1:E:176:LYS:HE2	1.86	0.75
1:C:393:ASN:HD22	1:C:396:ASP:H	1.30	0.75
1:D:307:ASN:O	1:D:309:LYS:HG2	1.86	0.75
1:E:22:ILE:HD11	1:E:26:ALA:CB	2.16	0.75
1:F:322:THR:HB	1:F:323:PRO:HD2	1.68	0.75
1:C:241:VAL:HG12	1:C:242:SER:H	1.50	0.75
1:A:209:LEU:CA	1:A:212:LYS:HG3	2.11	0.74
1:E:270:LYS:O	1:E:271:ASP:HB2	1.85	0.74
1:A:30:LEU:HD22	1:A:91:TRP:CH2	2.22	0.74
1:E:29:PHE:CD1	1:E:410:MET:HE3	2.20	0.74
1:C:214:ILE:HG13	1:C:215:ALA:N	2.03	0.74
1:D:29:PHE:CD1	1:D:410:MET:CE	2.71	0.74
1:D:276:THR:HG22	1:D:277:ASN:N	2.02	0.74
1:E:110:ASN:O	1:E:111:PRO:C	2.25	0.74
1:A:262:TRP:O	1:A:266:THR:N	2.16	0.74
1:D:213:THR:HB	1:D:288:VAL:CG1	2.17	0.74
1:F:63:ALA:HB2	1:F:415:TRP:CZ3	2.22	0.74
1:E:22:ILE:HD13	1:E:27:LEU:HD23	1.70	0.74
1:A:48:GLY:CA	1:E:117:ARG:HH22	2.00	0.73
1:B:111:PRO:HG2	1:B:146:TYR:CD2	2.23	0.73
1:E:3:GLN:NE2	1:E:80:SER:HB2	2.02	0.73
1:E:29:PHE:CG	1:E:410:MET:HE1	2.23	0.73
1:B:270:LYS:HG2	1:B:277:ASN:ND2	2.03	0.73
1:B:371:LYS:HB3	1:B:371:LYS:HZ3	1.54	0.73
1:A:94:ALA:O	1:A:405:ARG:NH1	2.21	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:131:TYR:HE1	1:B:159:TYR:CE1	2.07	0.73
1:D:51:LYS:HD3	1:D:53:PHE:CZ	2.23	0.73
1:D:248:ILE:HD13	1:D:269:VAL:HG23	1.71	0.73
1:E:29:PHE:CG	1:E:410:MET:CE	2.72	0.73
1:F:34:GLN:OE1	1:F:61:ASN:HA	1.89	0.73
1:F:228:LYS:O	1:F:232:GLU:HB2	1.89	0.72
1:A:176:LYS:NZ	1:A:357:ASN:OD1	2.18	0.72
1:B:371:LYS:HB3	1:B:371:LYS:NZ	2.02	0.72
1:C:241:VAL:CG1	1:C:242:SER:N	2.51	0.72
1:D:393:ASN:ND2	1:D:396:ASP:OD2	2.22	0.72
1:F:184:VAL:C	1:F:186:ARG:H	1.91	0.72
1:A:74:HIS:ND1	1:A:75:PRO:HD2	2.04	0.72
1:F:184:VAL:HG12	1:F:185:ALA:H	1.44	0.72
1:D:229:ILE:HG23	1:D:233:GLU:CD	2.11	0.72
1:E:3:GLN:HG2	1:E:5:PRO:CD	2.19	0.71
1:B:344:ALA:O	1:B:347:VAL:HG12	1.90	0.71
1:C:167:ASP:HB2	1:C:168:PRO:CD	2.19	0.71
1:D:3:GLN:CG	1:D:4:ASP:H	2.04	0.71
1:E:92:LYS:O	1:E:95:VAL:HG12	1.90	0.71
1:F:186:ARG:O	1:F:186:ARG:HG3	1.88	0.71
1:A:279:THR:OG1	1:A:281:GLU:HG2	1.89	0.71
1:B:117:ARG:NH1	1:C:417:LYS:HG2	2.05	0.71
1:C:291:LEU:HG	1:C:293:PRO:HD3	1.72	0.71
1:C:384:TYR:O	1:C:387:HIS:HD2	1.74	0.71
1:E:179:SER:O	1:E:180:VAL:HG13	1.89	0.71
1:F:250:ASN:OD1	1:F:251:PRO:HD2	1.90	0.71
1:A:226:MET:HG2	1:A:316:LEU:HD11	1.72	0.71
1:D:213:THR:HB	1:D:288:VAL:HG13	1.71	0.71
1:F:51:LYS:HG2	1:F:53:PHE:CE1	2.26	0.71
1:C:241:VAL:CG1	1:C:242:SER:H	2.03	0.71
1:D:313:VAL:HB	1:D:336:ILE:HG12	1.73	0.71
1:C:29:PHE:HD2	1:C:410:MET:HE3	1.56	0.70
1:B:3:GLN:O	1:B:7:GLU:N	2.23	0.70
1:C:15:ARG:HG3	1:C:18:GLN:HE22	1.55	0.70
1:C:183:ILE:HD13	1:C:353:GLU:CB	2.20	0.70
1:A:126:TYR:CD2	1:A:155:MET:CE	2.74	0.70
1:C:176:LYS:O	1:C:182:GLY:HA3	1.92	0.70
1:E:66:PRO:HB3	1:E:137:TYR:O	1.92	0.70
1:E:219:TYR:HD1	1:E:241:VAL:HG11	1.56	0.70
1:B:379:ALA:O	1:B:383:VAL:HG23	1.90	0.70
1:B:142:ALA:HB1	1:B:143:PRO:HD2	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:148:ASN:HB2	1:C:149:PRO:CD	2.18	0.70
1:E:22:ILE:CD1	1:E:26:ALA:HB3	2.21	0.70
1:C:365:VAL:O	1:C:369:ARG:HG3	1.91	0.70
1:A:44:GLU:HG3	1:E:117:ARG:HH21	1.56	0.70
1:A:144:ASP:N	1:A:147:THR:OG1	2.21	0.70
1:A:3:GLN:HB3	1:A:80:SER:HB3	1.74	0.70
1:C:248:ILE:HD13	1:C:269:VAL:O	1.92	0.70
1:F:337:ILE:HG22	1:F:342:CYS:HB2	1.74	0.70
1:B:384:TYR:O	1:B:387:HIS:HD2	1.74	0.70
1:D:213:THR:CG2	1:D:288:VAL:HG13	2.21	0.70
1:F:29:PHE:HD2	1:F:410:MET:HE1	1.52	0.69
1:A:144:ASP:H	1:A:147:THR:HG1	1.38	0.69
1:B:29:PHE:CD2	1:B:410:MET:HE3	2.26	0.69
1:E:270:LYS:HG2	1:E:277:ASN:ND2	2.06	0.69
1:A:96:MET:HE1	1:A:376:MET:SD	2.32	0.69
1:A:315:GLU:OE2	1:A:336:ILE:HD12	1.91	0.69
1:B:288:VAL:O	1:B:310:ALA:HA	1.92	0.69
1:C:335:LEU:HD23	1:C:336:ILE:H	1.54	0.69
1:D:288:VAL:O	1:D:310:ALA:HA	1.93	0.69
1:A:12:GLN:NE2	1:A:88:TRP:HH2	1.90	0.69
1:C:27:LEU:HD13	1:C:31:LYS:HE3	1.72	0.69
1:F:3:GLN:C	1:F:5:PRO:HD2	2.12	0.69
1:A:50:VAL:CG2	1:F:417:LYS:HG2	2.22	0.69
1:A:148:ASN:HB2	1:A:149:PRO:HD2	1.73	0.69
1:A:250:ASN:HB3	1:A:254:LEU:CD2	2.23	0.69
1:A:296:ILE:HD11	1:A:299:VAL:HG12	1.72	0.69
1:A:358:ILE:HD11	1:C:359:THR:O	1.92	0.69
1:B:262:TRP:O	1:B:266:THR:HB	1.92	0.69
1:C:339:ASP:OD1	1:C:339:ASP:N	2.21	0.69
1:D:213:THR:O	1:D:288:VAL:HG12	1.93	0.69
1:D:160:GLU:HG2	1:D:169:SER:HB3	1.75	0.69
1:D:411:LYS:O	1:D:414:GLY:N	2.23	0.69
1:D:230:MET:O	1:D:234:TYR:HB2	1.91	0.69
1:D:242:SER:HA	1:D:247:GLY:HA2	1.75	0.68
1:E:12:GLN:CD	1:E:88:TRP:HH2	1.95	0.68
1:F:399:TYR:O	1:F:403:VAL:HG23	1.93	0.68
1:A:126:TYR:CD2	1:A:155:MET:HE2	2.27	0.68
1:D:304:ASN:O	1:D:307:ASN:N	2.20	0.68
1:B:321:THR:HG22	1:B:322:THR:O	1.93	0.68
1:C:69:GLY:HA3	1:C:103:GLY:O	1.94	0.68
1:D:400:VAL:O	1:D:404:SER:OG	2.10	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:184:VAL:CG1	1:E:185:ALA:N	2.56	0.68
1:C:33:PRO:HB3	1:C:60:TYR:CD1	2.29	0.68
1:E:88:TRP:CH2	1:E:399:TYR:OH	2.47	0.68
1:E:156:MET:SD	1:E:156:MET:C	2.72	0.68
1:D:3:GLN:O	1:D:4:ASP:C	2.32	0.68
1:F:160:GLU:HG2	1:F:169:SER:CB	2.24	0.68
1:F:250:ASN:OD1	1:F:252:ASP:N	2.26	0.68
1:D:279:THR:O	1:D:282:GLU:HB2	1.94	0.68
1:F:3:GLN:O	1:F:5:PRO:CD	2.42	0.68
1:A:3:GLN:HG2	1:A:4:ASP:N	2.09	0.67
1:A:172:VAL:HG22	1:A:172:VAL:O	1.94	0.67
1:C:192:ARG:NH2	1:C:233:GLU:OE2	2.28	0.67
1:D:41:ILE:O	1:D:41:ILE:HG22	1.94	0.67
1:B:241:VAL:HG12	1:B:242:SER:N	2.07	0.67
1:F:160:GLU:HG2	1:F:169:SER:HB3	1.76	0.67
1:A:323:PRO:O	1:A:326:ASP:HB2	1.94	0.67
1:E:401:VAL:O	1:E:405:ARG:HG3	1.94	0.67
1:B:242:SER:OG	1:B:280:ASN:ND2	2.27	0.67
1:B:367:GLU:O	1:B:370:ALA:HB3	1.95	0.67
1:E:212:LYS:HB3	1:E:289:ASP:OD2	1.95	0.67
1:A:240:ALA:HA	1:A:248:ILE:O	1.95	0.67
1:B:117:ARG:CZ	1:C:417:LYS:HG2	2.25	0.67
1:C:5:PRO:CA	1:C:8:ILE:HD12	2.24	0.67
1:C:158:GLU:O	1:C:162:ILE:HG13	1.94	0.67
1:D:163:SER:O	1:D:164:ARG:HB2	1.94	0.67
1:A:249:TYR:CE2	1:A:251:PRO:HD3	2.31	0.66
1:F:228:LYS:HE3	1:F:232:GLU:OE1	1.95	0.66
1:C:142:ALA:HB1	1:C:143:PRO:CD	2.24	0.66
1:D:203:LYS:O	1:D:206:GLY:N	2.24	0.66
1:E:59:GLN:HE22	1:E:133:VAL:HG23	1.61	0.66
1:A:131:TYR:CD2	1:E:164:ARG:HD3	2.30	0.66
1:A:270:LYS:HG2	1:A:277:ASN:HD21	1.61	0.66
1:A:279:THR:CG2	1:A:282:GLU:CG	2.66	0.66
1:F:5:PRO:HG2	1:F:80:SER:HB2	1.76	0.66
1:B:287:GLU:HG3	1:B:309:LYS:HD2	1.77	0.66
1:D:74:HIS:ND1	1:D:75:PRO:HD2	2.10	0.66
1:E:242:SER:HB3	1:E:283:LEU:CD1	2.25	0.66
1:C:315:GLU:HB3	1:C:320:PRO:HG3	1.78	0.66
1:E:192:ARG:NH2	1:E:233:GLU:OE2	2.28	0.66
1:B:339:ASP:OD1	1:B:340:PHE:N	2.24	0.66
1:C:186:ARG:CG	1:C:186:ARG:NH1	2.54	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:248:ILE:HG13	1:D:254:LEU:HD21	1.78	0.66
1:E:46:ASP:OD2	1:E:115:SER:OG	2.07	0.66
1:E:184:VAL:HG12	1:E:185:ALA:H	1.60	0.66
1:F:242:SER:OG	1:F:280:ASN:ND2	2.29	0.66
1:A:250:ASN:HB3	1:A:254:LEU:HD23	1.78	0.66
1:D:224:TYR:OH	1:D:257:ASP:OD1	2.13	0.66
1:E:323:PRO:C	1:E:326:ASP:HB2	2.16	0.66
1:A:96:MET:CE	1:A:376:MET:SD	2.84	0.66
1:A:315:GLU:O	1:A:342:CYS:HB3	1.95	0.66
1:C:297:GLU:O	1:C:299:VAL:HG13	1.96	0.66
1:D:257:ASP:O	1:D:260:LEU:HB3	1.95	0.66
1:D:278:ILE:HB	1:D:282:GLU:CD	2.15	0.66
1:A:34:GLN:HG3	1:A:60:TYR:O	1.96	0.66
1:A:270:LYS:O	1:A:271:ASP:HB2	1.96	0.66
1:C:176:LYS:NZ	1:C:357:ASN:OD1	2.19	0.66
1:B:176:LYS:NZ	1:B:357:ASN:HD21	1.94	0.65
1:D:323:PRO:O	1:D:326:ASP:HB2	1.96	0.65
1:C:228:LYS:NZ	1:C:232:GLU:OE2	2.29	0.65
1:C:393:ASN:ND2	1:C:395:ARG:HB3	2.12	0.65
1:D:249:TYR:HB2	1:D:278:ILE:CD1	2.26	0.65
1:D:297:GLU:HG3	1:D:298:GLU:HG3	1.78	0.65
1:A:44:GLU:CD	1:E:117:ARG:HE	1.99	0.65
1:D:384:TYR:CE2	1:D:388:LYS:NZ	2.65	0.65
1:E:323:PRO:O	1:E:326:ASP:CB	2.44	0.65
1:B:270:LYS:HG2	1:B:277:ASN:HD21	1.61	0.65
1:F:176:LYS:HB2	1:F:176:LYS:NZ	2.11	0.65
1:B:88:TRP:CZ2	1:B:399:TYR:OH	2.49	0.65
1:A:4:ASP:HB3	1:A:5:PRO:HD3	1.79	0.65
1:B:242:SER:HB3	1:B:283:LEU:CD1	2.26	0.65
1:C:186:ARG:O	1:C:186:ARG:HG3	1.97	0.65
1:E:17:ALA:O	1:E:19:TYR:N	2.30	0.65
1:C:214:ILE:HB	1:C:236:MET:HE1	1.78	0.65
1:D:156:MET:SD	1:D:156:MET:C	2.75	0.65
1:E:124:ARG:O	1:E:128:ARG:HG3	1.96	0.65
1:C:258:GLU:O	1:C:261:ALA:HB3	1.96	0.65
1:D:213:THR:CB	1:D:288:VAL:HG13	2.26	0.65
1:E:29:PHE:CE1	1:E:410:MET:HE3	2.31	0.65
1:E:184:VAL:CG1	1:E:185:ALA:H	2.08	0.65
1:E:228:LYS:O	1:E:232:GLU:HB2	1.97	0.65
1:A:249:TYR:OH	1:A:251:PRO:HG3	1.96	0.65
1:A:301:THR:O	1:A:305:ALA:HB2	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:208:ASP:O	1:C:212:LYS:CE	2.44	0.64
1:E:176:LYS:NZ	1:E:357:ASN:HD21	1.94	0.64
1:E:228:LYS:HE2	1:E:257:ASP:OD1	1.97	0.64
1:E:283:LEU:O	1:E:286:LEU:HB2	1.97	0.64
1:D:158:GLU:O	1:D:162:ILE:HG13	1.97	0.64
1:B:6:PHE:O	1:B:9:ALA:HB3	1.97	0.64
1:E:9:ALA:O	1:E:12:GLN:HB2	1.97	0.64
1:F:29:PHE:CG	1:F:410:MET:CE	2.79	0.64
1:D:208:ASP:O	1:D:212:LYS:HE3	1.97	0.64
1:B:371:LYS:NZ	1:B:371:LYS:CB	2.58	0.64
1:E:71:ILE:HD13	1:E:126:TYR:CE2	2.33	0.64
1:D:249:TYR:HB2	1:D:278:ILE:HD13	1.78	0.64
1:F:4:ASP:O	1:F:8:ILE:HG13	1.97	0.64
1:A:322:THR:OG1	1:A:325:ALA:CB	2.46	0.64
1:B:217:GLN:HE22	1:B:299:VAL:HG11	1.62	0.64
1:D:296:ILE:CD1	1:D:299:VAL:CG1	2.76	0.64
1:D:98:LEU:HD23	1:D:375:LYS:NZ	2.12	0.64
1:F:29:PHE:O	1:F:31:LYS:N	2.31	0.64
1:A:322:THR:HB	1:A:323:PRO:HD2	1.80	0.64
1:B:72:ARG:NE	1:B:77:GLU:OE2	2.19	0.64
1:C:278:ILE:HB	1:C:282:GLU:OE1	1.98	0.64
1:C:378:LYS:NZ	1:C:382:ASP:OD2	2.21	0.64
1:F:184:VAL:HG13	1:F:185:ALA:H	1.59	0.64
1:F:339:ASP:N	1:F:339:ASP:OD1	2.29	0.63
1:B:131:TYR:CE1	1:B:159:TYR:CE1	2.86	0.63
1:A:89:MET:HE3	1:A:89:MET:HA	1.79	0.63
1:F:192:ARG:NH2	1:F:233:GLU:OE2	2.31	0.63
1:A:3:GLN:C	1:A:5:PRO:HD2	2.19	0.63
1:A:214:ILE:HA	1:A:288:VAL:HG21	1.81	0.63
1:A:228:LYS:NZ	1:A:257:ASP:OD2	2.31	0.63
1:B:180:VAL:HG23	1:B:180:VAL:O	1.98	0.63
1:C:259:VAL:HG12	1:C:269:VAL:HG12	1.81	0.63
1:C:329:LEU:CD2	1:C:334:ILE:CD1	2.69	0.63
1:A:3:GLN:HG2	1:A:4:ASP:H	1.64	0.63
1:A:207:MET:HG3	1:A:208:ASP:N	2.13	0.63
1:C:219:TYR:CD1	1:C:241:VAL:HG11	2.34	0.63
1:D:18:GLN:O	1:D:18:GLN:HG3	1.99	0.63
1:E:79:LEU:HD12	1:E:79:LEU:O	1.98	0.63
1:F:348:THR:HG21	1:F:372:LEU:HD12	1.80	0.63
1:A:72:ARG:HG2	1:A:144:ASP:HB3	1.80	0.62
1:A:92:LYS:O	1:A:95:VAL:HG12	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:214:ILE:CA	1:A:288:VAL:HG21	2.29	0.62
1:B:367:GLU:O	1:B:371:LYS:HG2	1.98	0.62
1:D:279:THR:HG23	1:D:282:GLU:H	1.64	0.62
1:F:328:ILE:O	1:F:332:LYS:HG3	1.99	0.62
1:A:126:TYR:HD2	1:A:155:MET:CE	2.09	0.62
1:D:3:GLN:CG	1:D:4:ASP:N	2.62	0.62
1:E:3:GLN:O	1:E:6:PHE:N	2.31	0.62
1:A:81:THR:HG22	1:A:85:LEU:HD11	1.80	0.62
1:A:288:VAL:HG22	1:A:290:VAL:H	1.64	0.62
1:E:173:ILE:O	1:E:176:LYS:HE3	1.98	0.62
1:E:296:ILE:HD12	1:E:299:VAL:HG11	1.79	0.62
1:F:176:LYS:HB2	1:F:176:LYS:HZ3	1.64	0.62
1:A:4:ASP:HB3	1:A:5:PRO:CD	2.29	0.62
1:A:296:ILE:CD1	1:A:299:VAL:HG12	2.29	0.62
1:E:3:GLN:C	1:E:5:PRO:HD2	2.20	0.62
1:E:127:VAL:HG23	1:E:155:MET:HG2	1.80	0.62
1:E:159:TYR:O	1:E:163:SER:HB3	1.99	0.62
1:A:205:LEU:O	1:A:206:GLY:C	2.37	0.62
1:A:230:MET:O	1:A:234:TYR:HB2	2.00	0.62
1:D:176:LYS:HB2	1:D:176:LYS:HZ3	1.64	0.62
1:E:72:ARG:HG3	1:E:144:ASP:HB3	1.81	0.62
1:A:329:LEU:HD23	1:A:334:ILE:HD12	0.71	0.62
1:A:248:ILE:HD12	1:A:254:LEU:CD1	2.27	0.62
1:D:184:VAL:O	1:D:185:ALA:HB2	1.99	0.62
1:B:273:PRO:C	1:B:275:ALA:H	2.03	0.62
1:E:226:MET:CE	1:E:230:MET:CG	2.78	0.62
1:A:249:TYR:CE2	1:A:251:PRO:CG	2.82	0.61
1:D:262:TRP:CE3	1:D:273:PRO:HD2	2.35	0.61
1:A:157:ASP:OD2	1:B:413:ARG:HD3	2.00	0.61
1:A:208:ASP:O	1:A:212:LYS:NZ	2.32	0.61
1:A:278:ILE:HG13	1:A:279:THR:N	2.15	0.61
1:D:209:LEU:HA	1:D:212:LYS:HG2	1.82	0.61
1:A:329:LEU:CD2	1:A:334:ILE:HG21	2.30	0.61
1:A:255:ASN:HB3	1:A:258:GLU:HG3	1.82	0.61
1:D:262:TRP:CZ3	1:D:273:PRO:CG	2.84	0.61
1:B:4:ASP:O	1:B:8:ILE:HG13	2.00	0.61
1:C:297:GLU:O	1:C:299:VAL:CG1	2.48	0.61
1:D:304:ASN:O	1:D:306:ASP:N	2.33	0.61
1:A:110:ASN:HD22	1:A:113:GLU:CD	1.96	0.61
1:B:255:ASN:C	1:B:255:ASN:OD1	2.38	0.61
1:C:213:THR:CB	1:C:288:VAL:HG12	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:219:TYR:CD1	1:C:241:VAL:CG1	2.84	0.61
1:F:416:ILE:HD12	1:F:416:ILE:O	2.00	0.61
1:D:296:ILE:HD12	1:D:299:VAL:CG1	2.30	0.61
1:A:127:VAL:CG2	1:A:155:MET:HG2	2.31	0.61
1:A:392:ILE:HD11	1:A:397:ALA:CA	2.31	0.61
1:A:392:ILE:HD11	1:A:397:ALA:HA	1.83	0.61
1:B:291:LEU:O	1:B:293:PRO:HD2	2.01	0.61
1:B:410:MET:HG2	1:B:415:TRP:CE3	2.35	0.61
1:E:16:ALA:O	1:E:17:ALA:C	2.39	0.61
1:E:179:SER:O	1:E:180:VAL:CG1	2.49	0.61
1:D:98:LEU:HB3	1:D:99:PRO:HD2	1.83	0.60
1:E:29:PHE:CE1	1:E:410:MET:CE	2.82	0.60
1:C:224:TYR:CE1	1:C:260:LEU:HD23	2.36	0.60
1:D:301:THR:O	1:D:305:ALA:HB2	2.02	0.60
1:E:127:VAL:CG2	1:E:155:MET:HG2	2.31	0.60
1:A:127:VAL:HG23	1:A:155:MET:HG2	1.83	0.60
1:C:288:VAL:O	1:C:310:ALA:HA	2.01	0.60
1:C:328:ILE:O	1:C:332:LYS:HB2	2.02	0.60
1:A:46:ASP:OD1	1:A:118:GLU:HG3	2.01	0.60
1:C:29:PHE:CD2	1:C:410:MET:HE1	2.37	0.60
1:C:406:VAL:O	1:C:410:MET:HG3	2.01	0.60
1:D:34:GLN:HG3	1:D:60:TYR:O	2.02	0.60
1:D:250:ASN:OD1	1:D:252:ASP:HB2	2.01	0.60
1:D:271:ASP:O	1:D:272:PHE:C	2.39	0.60
1:E:305:ALA:HB3	1:E:328:ILE:HD13	1.83	0.60
1:F:3:GLN:HB3	1:F:80:SER:HB3	1.83	0.60
1:F:250:ASN:OD1	1:F:250:ASN:C	2.38	0.60
1:A:322:THR:OG1	1:A:325:ALA:HB2	2.02	0.60
1:B:74:HIS:CG	1:B:75:PRO:CD	2.85	0.60
1:B:291:LEU:HG	1:B:293:PRO:HD3	1.83	0.60
1:C:213:THR:OG1	1:C:288:VAL:CG1	2.44	0.60
1:D:242:SER:HA	1:D:247:GLY:CA	2.31	0.60
1:B:9:ALA:O	1:B:12:GLN:HB2	2.01	0.59
1:B:321:THR:CG2	1:B:322:THR:H	2.14	0.59
1:E:78:THR:OG1	1:E:81:THR:OG1	2.17	0.59
1:B:241:VAL:HG13	1:B:242:SER:N	2.16	0.59
1:D:3:GLN:O	1:D:5:PRO:HD2	2.02	0.59
1:A:26:ALA:HB2	1:A:407:TYR:CE1	2.37	0.59
1:A:142:ALA:HB1	1:A:143:PRO:HD2	1.84	0.59
1:A:164:ARG:NH2	1:E:131:TYR:HB3	2.16	0.59
1:C:79:LEU:HG	1:C:83:LYS:HD2	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:137:TYR:CE1	1:F:168:PRO:HG3	2.38	0.59
1:F:400:VAL:O	1:F:404:SER:OG	2.19	0.59
1:C:262:TRP:NE1	1:C:270:LYS:O	2.34	0.59
1:E:72:ARG:NE	1:E:77:GLU:OE2	2.32	0.59
1:F:3:GLN:HB3	1:F:80:SER:CB	2.32	0.59
1:F:209:LEU:O	1:F:210:LYS:C	2.40	0.59
1:D:313:VAL:HG23	1:D:334:ILE:CG2	2.33	0.59
1:F:6:PHE:O	1:F:9:ALA:N	2.35	0.59
1:B:120:GLU:HA	1:B:154:TRP:CE3	2.38	0.59
1:C:214:ILE:HG21	1:C:236:MET:HE2	1.81	0.59
1:C:224:TYR:CD1	1:C:260:LEU:HD23	2.36	0.59
1:E:3:GLN:C	1:E:5:PRO:CD	2.71	0.59
1:A:117:ARG:O	1:A:121:ARG:HG3	2.03	0.59
1:A:242:SER:OG	1:A:280:ASN:ND2	2.36	0.59
1:A:297:GLU:O	1:A:299:VAL:HG13	2.01	0.59
1:B:65:GLY:HA3	1:B:99:PRO:O	2.03	0.59
1:D:23:SER:OG	1:D:418:LYS:OXT	2.19	0.59
1:E:77:GLU:OE1	1:E:77:GLU:HA	2.03	0.59
1:E:279:THR:OG1	1:E:282:GLU:HG3	2.03	0.59
1:D:4:ASP:C	1:D:8:ILE:HG13	2.23	0.58
1:C:167:ASP:HB2	1:C:168:PRO:HD2	1.85	0.58
1:B:201:ALA:O	1:B:205:LEU:HD22	2.03	0.58
1:C:74:HIS:ND1	1:C:75:PRO:HD2	2.17	0.58
1:F:281:GLU:O	1:F:285:GLU:HG3	2.03	0.58
1:B:74:HIS:CE1	1:B:75:PRO:HD2	2.37	0.58
1:A:36:ILE:HG12	1:A:58:VAL:HG22	1.85	0.58
1:B:117:ARG:HH21	1:D:44:GLU:CG	2.15	0.58
1:D:213:THR:HG22	1:D:288:VAL:HG13	1.84	0.58
1:E:3:GLN:O	1:E:4:ASP:C	2.41	0.58
1:C:48:GLY:C	1:F:117:ARG:NH2	2.55	0.58
1:F:283:LEU:HD23	1:F:284:LEU:HD23	1.85	0.58
1:A:71:ILE:HD13	1:A:126:TYR:CE2	2.38	0.58
1:C:260:LEU:O	1:C:263:LYS:N	2.36	0.58
1:F:311:LYS:O	1:F:334:ILE:HG23	2.03	0.58
1:C:48:GLY:HA2	1:F:117:ARG:NH2	2.19	0.58
1:F:391:ASN:O	1:F:392:ILE:HG22	2.03	0.58
1:A:242:SER:HA	1:A:247:GLY:HA2	1.86	0.58
1:A:261:ALA:O	1:A:262:TRP:C	2.42	0.58
1:E:71:ILE:O	1:E:144:ASP:CB	2.52	0.58
1:E:194:ALA:O	1:E:198:VAL:HG23	2.03	0.58
1:F:64:ARG:NH2	1:F:97:ASP:HA	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:ASP:O	1:A:7:GLU:HB2	2.03	0.58
1:E:176:LYS:HZ1	1:E:357:ASN:HD21	1.50	0.58
1:F:278:ILE:HB	1:F:282:GLU:HG2	1.86	0.58
1:A:20:MET:HE1	1:A:400:VAL:HA	1.82	0.57
1:A:148:ASN:HB2	1:A:149:PRO:CD	2.33	0.57
1:A:279:THR:CG2	1:A:282:GLU:CD	2.72	0.57
1:B:164:ARG:O	1:B:165:ARG:HB2	2.04	0.57
1:D:208:ASP:O	1:D:212:LYS:HG2	2.04	0.57
1:F:176:LYS:NZ	1:F:353:GLU:OE2	2.36	0.57
1:B:22:ILE:HD13	1:B:27:LEU:HD23	1.85	0.57
1:C:23:SER:OG	1:C:418:LYS:OXT	2.16	0.57
1:F:263:LYS:HA	1:F:268:SER:O	2.04	0.57
1:A:42:PRO:HG3	1:F:29:PHE:HE1	1.68	0.57
1:A:68:LYS:HD2	1:A:140:ILE:O	2.04	0.57
1:C:270:LYS:C	1:C:272:PHE:H	2.07	0.57
1:C:325:ALA:HA	1:C:328:ILE:HD12	1.86	0.57
1:B:176:LYS:HZ1	1:B:357:ASN:HD21	1.51	0.57
1:B:399:TYR:O	1:B:403:VAL:HG23	2.03	0.57
1:C:207:MET:CE	1:C:311:LYS:CD	2.82	0.57
1:D:160:GLU:HG2	1:D:169:SER:CB	2.33	0.57
1:E:184:VAL:O	1:E:185:ALA:CB	2.47	0.57
1:F:262:TRP:O	1:F:266:THR:HB	2.04	0.57
1:B:100:TYR:HE2	1:B:351:TYR:HB2	1.69	0.57
1:C:81:THR:O	1:C:85:LEU:HD12	2.05	0.57
1:C:183:ILE:CD1	1:C:353:GLU:HB2	2.30	0.57
1:C:214:ILE:CB	1:C:236:MET:HE1	2.35	0.57
1:D:276:THR:CG2	1:D:277:ASN:N	2.68	0.57
1:F:87:ALA:O	1:F:90:THR:HB	2.04	0.57
1:B:250:ASN:C	1:B:250:ASN:OD1	2.42	0.57
1:D:319:GLY:N	1:D:320:PRO:CD	2.67	0.57
1:F:291:LEU:HG	1:F:293:PRO:HD3	1.87	0.57
1:B:248:ILE:HG21	1:B:269:VAL:O	2.04	0.57
1:E:3:GLN:O	1:E:5:PRO:HD2	2.04	0.57
1:E:226:MET:HE2	1:E:230:MET:CG	2.35	0.57
1:A:3:GLN:O	1:A:6:PHE:N	2.38	0.57
1:B:10:VAL:O	1:B:13:LEU:HB3	2.05	0.57
1:C:364:THR:HG23	1:C:367:GLU:OE2	2.05	0.57
1:F:393:ASN:HD22	1:F:396:ASP:H	1.53	0.57
1:B:110:ASN:ND2	1:B:113:GLU:OE2	2.38	0.56
1:B:283:LEU:HA	1:B:286:LEU:HG	1.87	0.56
1:D:305:ALA:CB	1:D:328:ILE:HD13	2.34	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:250:ASN:HB3	1:F:254:LEU:HD21	1.87	0.56
1:A:188:ASP:O	1:A:192:ARG:CB	2.49	0.56
1:B:14:GLU:O	1:B:17:ALA:HB3	2.04	0.56
1:D:142:ALA:HB1	1:D:143:PRO:CD	2.35	0.56
1:B:188:ASP:OD2	1:B:192:ARG:NH1	2.37	0.56
1:D:284:LEU:O	1:D:308:ILE:HD12	2.05	0.56
1:F:68:LYS:HD3	1:F:140:ILE:HB	1.87	0.56
1:A:4:ASP:N	1:A:5:PRO:HD2	2.21	0.56
1:C:3:GLN:CG	1:C:4:ASP:N	2.49	0.56
1:F:51:LYS:HD3	1:F:53:PHE:CZ	2.40	0.56
1:B:384:TYR:CE2	1:B:388:LYS:HD3	2.41	0.56
1:D:262:TRP:O	1:D:266:THR:N	2.27	0.56
1:F:3:GLN:O	1:F:4:ASP:C	2.44	0.56
1:F:9:ALA:O	1:F:12:GLN:HB2	2.06	0.56
1:B:384:TYR:O	1:B:387:HIS:CD2	2.58	0.56
1:C:276:THR:HG22	1:C:277:ASN:N	2.20	0.56
1:F:184:VAL:C	1:F:186:ARG:N	2.59	0.56
1:A:68:LYS:HD2	1:A:140:ILE:HB	1.88	0.56
1:B:273:PRO:O	1:B:275:ALA:N	2.39	0.56
1:C:214:ILE:HG13	1:C:215:ALA:O	2.04	0.56
1:A:47:ASP:OD1	1:A:47:ASP:C	2.43	0.56
1:B:117:ARG:HH21	1:D:44:GLU:HG3	1.70	0.56
1:C:92:LYS:HD3	1:C:347:VAL:HG21	1.88	0.56
1:F:220:GLY:O	1:F:224:TYR:HB3	2.05	0.56
1:B:170:PHE:O	1:B:357:ASN:ND2	2.39	0.56
1:D:126:TYR:HD2	1:D:155:MET:HE2	1.70	0.56
1:D:279:THR:O	1:D:282:GLU:N	2.38	0.56
1:A:296:ILE:HG13	1:A:299:VAL:CG1	2.36	0.56
1:C:176:LYS:HE2	1:C:353:GLU:OE2	2.06	0.56
1:E:57:ARG:NH1	1:E:69:GLY:O	2.36	0.56
1:F:322:THR:O	1:F:326:ASP:N	2.38	0.56
1:A:6:PHE:O	1:A:9:ALA:N	2.39	0.55
1:B:305:ALA:HB3	1:B:328:ILE:HD12	1.89	0.55
1:D:126:TYR:CD2	1:D:155:MET:CE	2.89	0.55
1:D:322:THR:CB	1:D:323:PRO:CD	2.79	0.55
1:E:22:ILE:CD1	1:E:27:LEU:CD2	2.85	0.55
1:C:7:GLU:O	1:C:11:LYS:HG3	2.05	0.55
1:D:248:ILE:HD13	1:D:269:VAL:CG2	2.35	0.55
1:F:205:LEU:O	1:F:206:GLY:C	2.44	0.55
1:D:240:ALA:HB1	1:D:283:LEU:HD12	1.89	0.55
1:A:3:GLN:HB3	1:A:80:SER:CB	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:71:ILE:HD13	1:C:126:TYR:CE2	2.42	0.55
1:D:217:GLN:OE1	1:D:284:LEU:HD21	2.06	0.55
1:B:88:TRP:CH2	1:B:399:TYR:OH	2.59	0.55
1:B:241:VAL:HG13	1:B:242:SER:H	1.71	0.55
1:C:297:GLU:HA	1:C:320:PRO:HA	1.88	0.55
1:D:248:ILE:CG1	1:D:254:LEU:HD21	2.36	0.55
1:F:18:GLN:NE2	1:F:19:TYR:CE2	2.68	0.55
1:F:115:SER:O	1:F:119:LYS:HG3	2.07	0.55
1:F:337:ILE:O	1:F:338:PRO:C	2.45	0.55
1:A:409:ALA:O	1:A:413:ARG:HG3	2.07	0.55
1:B:204:ALA:HB1	1:B:384:TYR:CE1	2.42	0.55
1:C:249:TYR:HB2	1:C:278:ILE:HD13	1.89	0.55
1:D:384:TYR:HE2	1:D:388:LYS:NZ	2.03	0.55
1:E:23:SER:CB	1:E:418:LYS:OXT	2.54	0.55
1:A:304:ASN:O	1:A:305:ALA:C	2.45	0.55
1:D:407:TYR:OH	1:D:418:LYS:O	2.24	0.55
1:E:22:ILE:CD1	1:E:27:LEU:HD23	2.35	0.55
1:A:164:ARG:O	1:A:165:ARG:HB2	2.06	0.55
1:B:68:LYS:HD2	1:B:140:ILE:O	2.06	0.55
1:B:302:LYS:HG3	1:B:303:LYS:N	2.22	0.55
1:B:321:THR:HG22	1:B:322:THR:H	1.66	0.55
1:C:349:VAL:O	1:C:352:PHE:HB2	2.07	0.55
1:D:297:GLU:HB2	1:D:319:GLY:O	2.07	0.55
1:F:184:VAL:O	1:F:185:ALA:CB	2.52	0.55
1:A:315:GLU:HG3	1:A:337:ILE:O	2.07	0.55
1:B:410:MET:HG2	1:B:415:TRP:HE3	1.72	0.55
1:C:196:TYR:HE2	1:C:372:LEU:HD23	1.72	0.55
1:D:176:LYS:HB2	1:D:176:LYS:NZ	2.22	0.55
1:F:65:GLY:HA3	1:F:99:PRO:O	2.06	0.55
1:F:66:PRO:HD2	1:F:99:PRO:O	2.07	0.55
1:D:213:THR:C	1:D:288:VAL:CG1	2.75	0.55
1:A:95:VAL:CG1	1:A:96:MET:N	2.70	0.54
1:A:392:ILE:HD12	1:A:396:ASP:CB	2.37	0.54
1:D:289:ASP:OD1	1:D:289:ASP:N	2.39	0.54
1:E:160:GLU:HG2	1:E:169:SER:CB	2.37	0.54
1:E:250:ASN:C	1:E:250:ASN:OD1	2.46	0.54
1:B:323:PRO:HA	1:B:326:ASP:OD2	2.07	0.54
1:D:213:THR:HB	1:D:288:VAL:HG12	1.89	0.54
1:E:23:SER:HB3	1:E:418:LYS:OXT	2.08	0.54
1:F:142:ALA:CB	1:F:143:PRO:CD	2.78	0.54
1:A:319:GLY:N	1:A:320:PRO:CD	2.69	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:202:ALA:HB1	1:D:207:MET:CG	2.37	0.54
1:E:3:GLN:O	1:E:7:GLU:HG3	2.06	0.54
1:F:69:GLY:HA3	1:F:103:GLY:O	2.08	0.54
1:F:158:GLU:O	1:F:162:ILE:HG13	2.07	0.54
1:F:188:ASP:OD2	1:F:192:ARG:HD2	2.08	0.54
1:F:407:TYR:OH	1:F:418:LYS:O	2.12	0.54
1:A:242:SER:HB3	1:A:283:LEU:HD13	1.89	0.54
1:A:315:GLU:OE2	1:A:336:ILE:HD13	2.06	0.54
1:A:335:LEU:HD11	1:A:394:MET:HE2	1.89	0.54
1:D:71:ILE:HD13	1:D:126:TYR:CE2	2.42	0.54
1:C:207:MET:HE2	1:C:311:LYS:HD3	1.90	0.54
1:C:381:TRP:O	1:C:382:ASP:C	2.46	0.54
1:D:47:ASP:OD1	1:D:47:ASP:C	2.46	0.54
1:D:416:ILE:HD12	1:D:418:LYS:OXT	2.07	0.54
1:E:19:TYR:O	1:E:390:LYS:NZ	2.38	0.54
1:E:33:PRO:HB3	1:E:60:TYR:CD1	2.42	0.54
1:E:111:PRO:HG2	1:E:146:TYR:CD2	2.42	0.54
1:E:184:VAL:C	1:E:186:ARG:H	2.08	0.54
1:A:387:HIS:CD2	1:A:388:LYS:N	2.76	0.54
1:B:142:ALA:HB1	1:B:143:PRO:CD	2.37	0.54
1:C:276:THR:CG2	1:C:277:ASN:N	2.70	0.54
1:E:160:GLU:HG2	1:E:169:SER:HB3	1.90	0.54
1:F:250:ASN:OD1	1:F:251:PRO:CD	2.55	0.54
1:B:167:ASP:O	1:B:169:SER:N	2.39	0.54
1:B:291:LEU:O	1:B:293:PRO:CD	2.56	0.54
1:D:75:PRO:HD2	1:D:76:GLU:H	1.73	0.54
1:E:3:GLN:HB3	1:E:80:SER:CB	2.37	0.54
1:E:94:ALA:O	1:E:405:ARG:NH1	2.34	0.54
1:A:281:GLU:O	1:A:285:GLU:HG3	2.08	0.54
1:E:167:ASP:O	1:E:169:SER:N	2.36	0.54
1:F:391:ASN:O	1:F:392:ILE:CG2	2.56	0.54
1:A:222:ALA:O	1:A:226:MET:HB2	2.08	0.54
1:A:285:GLU:O	1:A:309:LYS:HE3	2.07	0.54
1:D:389:GLU:HG3	1:D:390:LYS:N	2.21	0.54
1:F:71:ILE:HD11	1:F:141:PRO:CB	2.38	0.54
1:D:384:TYR:OH	1:D:388:LYS:NZ	2.31	0.53
1:E:73:TRP:O	1:E:145:VAL:HG12	2.08	0.53
1:F:304:ASN:O	1:F:305:ALA:C	2.45	0.53
1:A:120:GLU:HG3	1:A:154:TRP:CE2	2.42	0.53
1:C:289:ASP:N	1:C:289:ASP:OD1	2.39	0.53
1:D:4:ASP:O	1:D:8:ILE:CG1	2.55	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:313:VAL:HG23	1:D:334:ILE:HG21	1.91	0.53
1:E:399:TYR:O	1:E:403:VAL:HG23	2.08	0.53
1:A:12:GLN:NE2	1:A:88:TRP:CH2	2.75	0.53
1:A:184:VAL:C	1:A:186:ARG:H	2.11	0.53
1:A:352:PHE:CZ	1:A:371:LYS:HB3	2.44	0.53
1:B:48:GLY:HA2	1:D:117:ARG:NH2	2.23	0.53
1:C:97:ASP:HB2	1:C:405:ARG:NH1	2.22	0.53
1:D:219:TYR:CD2	1:D:219:TYR:O	2.61	0.53
1:D:228:LYS:NZ	1:D:232:GLU:OE1	2.42	0.53
1:E:226:MET:HE3	1:E:230:MET:CG	2.36	0.53
1:F:250:ASN:HB3	1:F:254:LEU:CD2	2.38	0.53
1:A:213:THR:C	1:A:288:VAL:HG23	2.29	0.53
1:A:339:ASP:O	1:A:342:CYS:N	2.41	0.53
1:B:26:ALA:O	1:B:27:LEU:C	2.46	0.53
1:C:283:LEU:O	1:C:286:LEU:HB2	2.08	0.53
1:C:393:ASN:ND2	1:C:396:ASP:N	2.48	0.53
1:D:98:LEU:HD23	1:D:375:LYS:HZ2	1.71	0.53
1:D:172:VAL:O	1:D:172:VAL:HG22	2.08	0.53
1:D:242:SER:OG	1:D:243:ASP:N	2.42	0.53
1:E:323:PRO:CA	1:E:326:ASP:HB2	2.39	0.53
1:B:184:VAL:CG1	1:B:184:VAL:O	2.56	0.53
1:A:321:THR:CG2	1:A:322:THR:N	2.51	0.53
1:E:170:PHE:O	1:E:357:ASN:ND2	2.42	0.53
1:B:6:PHE:O	1:B:9:ALA:N	2.41	0.53
1:B:68:LYS:HD3	1:B:140:ILE:HB	1.91	0.53
1:C:278:ILE:HD11	1:C:283:LEU:HD12	1.91	0.53
1:D:127:VAL:HG23	1:D:155:MET:HG2	1.89	0.53
1:A:126:TYR:CD2	1:A:155:MET:HE1	2.44	0.53
1:D:4:ASP:O	1:D:8:ILE:N	2.28	0.53
1:D:124:ARG:O	1:D:128:ARG:HG3	2.09	0.53
1:D:276:THR:HG22	1:D:277:ASN:H	1.71	0.53
1:B:373:ASP:OD1	1:B:373:ASP:C	2.46	0.53
1:D:127:VAL:CG2	1:D:155:MET:HG2	2.38	0.53
1:D:250:ASN:C	1:D:252:ASP:H	2.12	0.53
1:D:322:THR:O	1:D:326:ASP:N	2.32	0.53
1:E:271:ASP:O	1:E:272:PHE:C	2.47	0.53
1:F:418:LYS:OXT	1:F:418:LYS:HG3	2.09	0.53
1:A:81:THR:HG22	1:A:85:LEU:CD1	2.39	0.52
1:B:347:VAL:O	1:B:350:SER:OG	2.27	0.52
1:D:209:LEU:HA	1:D:212:LYS:CG	2.38	0.52
1:E:94:ALA:O	1:E:405:ARG:HD2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:416:ILE:HD12	1:F:416:ILE:C	2.28	0.52
1:A:115:SER:O	1:A:119:LYS:HG3	2.10	0.52
1:A:209:LEU:CA	1:A:212:LYS:CG	2.81	0.52
1:F:220:GLY:O	1:F:224:TYR:CB	2.57	0.52
1:A:279:THR:N	1:A:282:GLU:OE2	2.42	0.52
1:B:72:ARG:HG2	1:B:144:ASP:OD2	2.09	0.52
1:E:3:GLN:O	1:E:5:PRO:CD	2.57	0.52
1:E:172:VAL:O	1:E:172:VAL:CG2	2.53	0.52
1:F:78:THR:OG1	1:F:81:THR:OG1	2.04	0.52
1:F:200:GLU:O	1:F:203:LYS:HB2	2.09	0.52
1:A:92:LYS:HE2	1:A:344:ALA:HA	1.91	0.52
1:A:250:ASN:HB3	1:A:254:LEU:HD21	1.91	0.52
1:B:72:ARG:NH2	1:B:77:GLU:OE1	2.24	0.52
1:C:72:ARG:HE	1:C:77:GLU:CD	2.12	0.52
1:C:212:LYS:N	1:C:212:LYS:CD	2.73	0.52
1:B:59:GLN:HE22	1:B:133:VAL:HG23	1.75	0.52
1:D:72:ARG:O	1:D:106:GLY:HA2	2.10	0.52
1:D:229:ILE:HG23	1:D:233:GLU:CG	2.40	0.52
1:D:322:THR:O	1:D:325:ALA:HB3	2.08	0.52
1:E:123:ALA:HA	1:E:155:MET:HE3	1.92	0.52
1:F:71:ILE:HD11	1:F:141:PRO:HB3	1.91	0.52
1:B:3:GLN:N	1:B:6:PHE:HB3	2.25	0.52
1:C:250:ASN:HB3	1:C:254:LEU:HD21	1.90	0.52
1:E:3:GLN:HB3	1:E:80:SER:HB3	1.90	0.52
1:E:319:GLY:N	1:E:320:PRO:CD	2.72	0.52
1:E:370:ALA:O	1:E:374:LYS:HG3	2.08	0.52
1:D:248:ILE:HG23	1:D:269:VAL:HG23	1.92	0.52
1:E:297:GLU:HB2	1:E:319:GLY:O	2.09	0.52
1:A:34:GLN:OE1	1:A:61:ASN:HA	2.10	0.52
1:B:17:ALA:O	1:B:20:MET:N	2.36	0.52
1:B:176:LYS:HE2	1:B:180:VAL:O	2.10	0.52
1:A:48:GLY:C	1:E:117:ARG:HH22	2.13	0.52
1:A:259:VAL:HG12	1:A:269:VAL:HG23	1.90	0.52
1:E:74:HIS:CE1	1:E:75:PRO:HD2	2.45	0.52
1:A:72:ARG:HG2	1:A:144:ASP:OD2	2.10	0.52
1:A:370:ALA:O	1:A:374:LYS:HG3	2.10	0.52
1:A:392:ILE:CD1	1:A:397:ALA:N	2.73	0.52
1:B:209:LEU:HA	1:B:212:LYS:HG2	1.92	0.52
1:D:328:ILE:O	1:D:332:LYS:HB2	2.10	0.52
1:D:336:ILE:O	1:D:338:PRO:HD3	2.09	0.52
1:E:249:TYR:CE2	1:E:251:PRO:HD3	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:74:HIS:ND1	1:F:75:PRO:HD2	2.25	0.52
1:A:110:ASN:ND2	1:A:113:GLU:HG3	2.25	0.51
1:C:321:THR:HG22	1:C:322:THR:N	2.24	0.51
1:C:393:ASN:HD21	1:C:395:ARG:HB3	1.76	0.51
1:D:141:PRO:HB2	1:D:173:ILE:HG13	1.90	0.51
1:F:291:LEU:O	1:F:293:PRO:HD2	2.09	0.51
1:F:337:ILE:O	1:F:338:PRO:O	2.28	0.51
1:D:74:HIS:ND1	1:D:75:PRO:CD	2.73	0.51
1:F:205:LEU:HD11	1:F:335:LEU:HD23	1.92	0.51
1:F:344:ALA:O	1:F:347:VAL:HG12	2.10	0.51
1:B:172:VAL:O	1:B:172:VAL:CG2	2.56	0.51
1:B:294:SER:CB	1:B:316:LEU:HB2	2.36	0.51
1:E:339:ASP:O	1:E:341:LEU:N	2.43	0.51
1:F:29:PHE:HB3	1:F:410:MET:CE	2.41	0.51
1:F:29:PHE:C	1:F:31:LYS:H	2.14	0.51
1:E:148:ASN:HB2	1:E:149:PRO:HD2	1.93	0.51
1:E:294:SER:HB3	1:E:316:LEU:HB2	1.91	0.51
1:A:217:GLN:HB3	1:A:293:PRO:HA	1.92	0.51
1:B:186:ARG:HG3	1:B:186:ARG:O	2.09	0.51
1:C:322:THR:HB	1:C:323:PRO:CD	2.41	0.51
1:D:364:THR:HG23	1:D:367:GLU:OE1	2.11	0.51
1:E:112:LYS:C	1:E:113:GLU:HG3	2.30	0.51
1:E:176:LYS:HB2	1:E:176:LYS:HZ2	1.75	0.51
1:A:131:TYR:O	1:A:134:ILE:HG13	2.10	0.51
1:B:18:GLN:NE2	1:B:19:TYR:CE2	2.78	0.51
1:B:81:THR:HG22	1:B:85:LEU:HD11	1.93	0.51
1:B:214:ILE:HA	1:B:290:VAL:O	2.10	0.51
1:C:48:GLY:CA	1:F:117:ARG:NH2	2.73	0.51
1:D:72:ARG:HE	1:D:77:GLU:CD	2.14	0.51
1:B:3:GLN:O	1:B:6:PHE:N	2.44	0.51
1:B:270:LYS:O	1:B:271:ASP:HB2	2.10	0.51
1:C:270:LYS:C	1:C:272:PHE:N	2.64	0.51
1:D:321:THR:CG2	1:D:322:THR:N	2.74	0.51
1:D:325:ALA:HA	1:D:328:ILE:HD12	1.92	0.51
1:F:411:LYS:O	1:F:414:GLY:N	2.43	0.51
1:A:3:GLN:O	1:A:4:ASP:O	2.29	0.51
1:A:323:PRO:C	1:A:326:ASP:HB2	2.31	0.51
1:A:329:LEU:HD22	1:A:334:ILE:CG2	2.36	0.51
1:B:48:GLY:C	1:D:117:ARG:HH22	2.13	0.51
1:B:111:PRO:HG2	1:B:146:TYR:HD2	1.72	0.51
1:C:164:ARG:O	1:C:165:ARG:HB2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:TYR:CE2	1:A:251:PRO:CD	2.93	0.51
1:B:297:GLU:CB	1:B:319:GLY:O	2.59	0.51
1:B:322:THR:HB	1:B:323:PRO:CD	2.40	0.51
1:C:270:LYS:O	1:C:272:PHE:N	2.44	0.51
1:D:321:THR:HG22	1:D:322:THR:N	2.25	0.51
1:E:69:GLY:HA3	1:E:103:GLY:O	2.11	0.51
1:A:241:VAL:CG1	1:A:242:SER:N	2.73	0.50
1:B:93:THR:HG21	1:B:100:TYR:HB2	1.93	0.50
1:D:110:ASN:ND2	1:D:113:GLU:HG3	2.26	0.50
1:E:228:LYS:NZ	1:E:232:GLU:OE2	2.43	0.50
1:D:262:TRP:CZ3	1:D:273:PRO:HG3	2.46	0.50
1:F:66:PRO:HG2	1:F:100:TYR:HD1	1.76	0.50
1:A:89:MET:HA	1:A:89:MET:CE	2.42	0.50
1:B:124:ARG:O	1:B:128:ARG:HG3	2.11	0.50
1:B:356:GLN:OE1	1:B:362:TYR:HA	2.12	0.50
1:D:22:ILE:HA	1:D:407:TYR:CE2	2.47	0.50
1:D:249:TYR:O	1:D:275:ALA:HB1	2.11	0.50
1:F:170:PHE:O	1:F:176:LYS:CE	2.59	0.50
1:B:24:GLU:O	1:B:28:GLU:HB2	2.11	0.50
1:B:312:ILE:HA	1:B:335:LEU:O	2.12	0.50
1:C:323:PRO:HA	1:C:326:ASP:HB2	1.94	0.50
1:D:29:PHE:CG	1:D:410:MET:HE1	2.46	0.50
1:D:242:SER:OG	1:D:280:ASN:ND2	2.45	0.50
1:D:284:LEU:HB3	1:D:308:ILE:HD11	1.93	0.50
1:A:72:ARG:HG2	1:A:144:ASP:CB	2.40	0.50
1:A:248:ILE:HG12	1:A:269:VAL:HG22	1.92	0.50
1:D:29:PHE:CD1	1:D:410:MET:HE3	2.46	0.50
1:D:126:TYR:CD2	1:D:155:MET:HE1	2.46	0.50
1:F:299:VAL:HG23	1:F:300:ILE:HG13	1.92	0.50
1:D:262:TRP:CH2	1:D:273:PRO:CD	2.83	0.50
1:D:296:ILE:HD11	1:D:299:VAL:HG12	1.94	0.50
1:E:34:GLN:HG3	1:E:60:TYR:O	2.12	0.50
1:F:172:VAL:HG22	1:F:172:VAL:O	2.10	0.50
1:A:245:LYS:CD	1:A:268:SER:HB2	2.42	0.50
1:A:335:LEU:HD11	1:A:394:MET:CE	2.42	0.50
1:C:38:GLU:HG2	1:D:36:ILE:HD12	1.93	0.50
1:C:205:LEU:HD23	1:C:207:MET:CE	2.41	0.50
1:E:208:ASP:C	1:E:208:ASP:OD1	2.50	0.50
1:F:25:GLU:OE1	1:F:418:LYS:HG2	2.12	0.50
1:F:89:MET:O	1:F:92:LYS:HB3	2.12	0.50
1:F:117:ARG:O	1:F:121:ARG:HG3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:160:GLU:HG2	1:F:169:SER:OG	2.11	0.50
1:F:238:VAL:O	1:F:254:LEU:N	2.32	0.50
1:A:120:GLU:HG3	1:A:154:TRP:CG	2.47	0.50
1:B:167:ASP:HB2	1:B:168:PRO:HD2	1.93	0.50
1:C:20:MET:HG3	1:C:22:ILE:HG22	1.94	0.50
1:A:30:LEU:HD21	1:A:406:VAL:HG11	1.93	0.50
1:B:114:MET:HB3	1:B:119:LYS:HG3	1.93	0.50
1:B:263:LYS:O	1:B:267:GLY:N	2.42	0.50
1:C:207:MET:CE	1:C:311:LYS:HD2	2.41	0.50
1:D:117:ARG:O	1:D:121:ARG:HG3	2.12	0.50
1:A:417:LYS:HD2	1:A:417:LYS:N	2.26	0.49
1:D:4:ASP:N	1:D:5:PRO:HD2	2.27	0.49
1:D:229:ILE:HG23	1:D:233:GLU:HG3	1.94	0.49
1:D:304:ASN:O	1:D:305:ALA:C	2.50	0.49
1:F:3:GLN:O	1:F:5:PRO:N	2.45	0.49
1:F:72:ARG:NH2	1:F:77:GLU:OE1	2.39	0.49
1:A:96:MET:O	1:A:97:ASP:CB	2.60	0.49
1:C:200:GLU:HB3	1:C:380:PHE:CD2	2.46	0.49
1:C:260:LEU:O	1:C:263:LYS:HB3	2.12	0.49
1:C:384:TYR:O	1:C:387:HIS:CD2	2.59	0.49
1:E:71:ILE:O	1:E:144:ASP:HB3	2.11	0.49
1:E:312:ILE:HA	1:E:335:LEU:O	2.12	0.49
1:A:373:ASP:O	1:A:374:LYS:C	2.50	0.49
1:D:297:GLU:HA	1:D:320:PRO:HA	1.94	0.49
1:A:263:LYS:HD2	1:A:268:SER:HA	1.94	0.49
1:B:381:TRP:O	1:B:382:ASP:C	2.49	0.49
1:D:142:ALA:HB1	1:D:143:PRO:HD2	1.95	0.49
1:D:214:ILE:HG13	1:D:215:ALA:N	2.27	0.49
1:D:300:ILE:HA	1:D:304:ASN:ND2	2.28	0.49
1:D:305:ALA:HB3	1:D:328:ILE:HD13	1.93	0.49
1:E:68:LYS:CD	1:E:140:ILE:O	2.61	0.49
1:E:325:ALA:O	1:E:329:LEU:HD12	2.13	0.49
1:F:164:ARG:O	1:F:165:ARG:HB2	2.13	0.49
1:F:324:GLU:O	1:F:328:ILE:HG13	2.13	0.49
1:F:329:LEU:HD13	1:F:336:ILE:HD11	1.94	0.49
1:A:3:GLN:CG	1:A:4:ASP:N	2.75	0.49
1:A:339:ASP:O	1:A:341:LEU:N	2.45	0.49
1:B:262:TRP:O	1:B:266:THR:N	2.40	0.49
1:D:258:GLU:O	1:D:261:ALA:HB3	2.11	0.49
1:E:352:PHE:CZ	1:E:371:LYS:HB3	2.47	0.49
1:F:17:ALA:O	1:F:20:MET:N	2.36	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:PRO:HG3	1:A:146:TYR:CD2	2.48	0.49
1:A:117:ARG:HE	1:A:117:ARG:HA	1.78	0.49
1:A:224:TYR:O	1:A:227:ALA:HB3	2.13	0.49
1:B:81:THR:O	1:B:85:LEU:HD12	2.12	0.49
1:C:4:ASP:O	1:C:8:ILE:HD12	2.13	0.49
1:C:43:VAL:HG12	1:C:44:GLU:N	2.26	0.49
1:C:74:HIS:CG	1:C:75:PRO:HD2	2.48	0.49
1:C:77:GLU:HG3	1:C:78:THR:N	2.28	0.49
1:F:10:VAL:O	1:F:13:LEU:HB3	2.13	0.49
1:B:278:ILE:HG13	1:B:279:THR:O	2.13	0.49
1:C:71:ILE:CD1	1:C:126:TYR:CE2	2.96	0.49
1:C:214:ILE:CB	1:C:236:MET:CE	2.90	0.49
1:D:216:ILE:HG12	1:D:292:ALA:HB3	1.93	0.49
1:E:279:THR:HG23	1:E:282:GLU:OE2	2.12	0.49
1:E:323:PRO:HA	1:E:326:ASP:HB2	1.95	0.49
1:C:14:GLU:O	1:C:17:ALA:HB3	2.13	0.49
1:C:131:TYR:CE1	1:C:159:TYR:CE1	3.00	0.49
1:C:161:THR:HG21	1:F:128:ARG:CZ	2.43	0.49
1:D:202:ALA:HB1	1:D:207:MET:HG2	1.95	0.49
1:E:3:GLN:O	1:E:5:PRO:N	2.46	0.49
1:E:200:GLU:HB3	1:E:380:PHE:CD2	2.48	0.49
1:F:238:VAL:O	1:F:253:GLY:HA2	2.13	0.49
1:F:341:LEU:HD22	1:F:383:VAL:HG21	1.95	0.49
1:A:372:LEU:O	1:A:373:ASP:C	2.51	0.49
1:B:81:THR:O	1:B:85:LEU:CD1	2.61	0.49
1:B:131:TYR:CZ	1:B:162:ILE:HG22	2.47	0.49
1:B:322:THR:HB	1:B:323:PRO:HD2	1.94	0.49
1:C:297:GLU:C	1:C:299:VAL:HG13	2.32	0.49
1:C:324:GLU:O	1:C:328:ILE:CG1	2.59	0.49
1:F:169:SER:O	1:F:172:VAL:HG12	2.13	0.49
1:F:224:TYR:CE1	1:F:260:LEU:HD22	2.47	0.49
1:B:352:PHE:O	1:B:356:GLN:HG3	2.13	0.49
1:C:219:TYR:CG	1:C:241:VAL:HG11	2.48	0.49
1:C:219:TYR:OH	1:C:256:ALA:HA	2.12	0.49
1:D:4:ASP:HB3	1:D:5:PRO:HD3	1.95	0.49
1:D:205:LEU:O	1:D:206:GLY:O	2.30	0.49
1:D:304:ASN:OD1	1:D:304:ASN:N	2.24	0.49
1:E:365:VAL:CG2	1:E:366:GLU:N	2.75	0.49
1:F:365:VAL:CG2	1:F:366:GLU:OE2	2.60	0.49
1:A:384:TYR:O	1:A:387:HIS:HD2	1.95	0.48
1:B:250:ASN:O	1:B:253:GLY:N	2.35	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:315:GLU:HB3	1:C:320:PRO:CG	2.42	0.48
1:D:337:ILE:HG22	1:D:342:CYS:HB2	1.94	0.48
1:E:23:SER:OG	1:E:26:ALA:N	2.35	0.48
1:A:243:ASP:O	1:A:244:THR:C	2.52	0.48
1:C:212:LYS:N	1:C:212:LYS:HD3	2.28	0.48
1:D:4:ASP:N	1:D:5:PRO:CD	2.76	0.48
1:F:296:ILE:HD12	1:F:299:VAL:CG1	2.43	0.48
1:F:323:PRO:O	1:F:326:ASP:CB	2.53	0.48
1:B:319:GLY:N	1:B:320:PRO:CD	2.76	0.48
1:D:209:LEU:O	1:D:212:LYS:HB2	2.13	0.48
1:D:219:TYR:HB2	1:D:241:VAL:HG13	1.94	0.48
1:D:416:ILE:O	1:D:416:ILE:HG13	2.10	0.48
1:F:263:LYS:O	1:F:267:GLY:N	2.44	0.48
1:A:161:THR:HG21	1:E:128:ARG:NH2	2.29	0.48
1:B:71:ILE:HD13	1:B:126:TYR:CE2	2.48	0.48
1:C:164:ARG:NE	1:F:131:TYR:HD2	2.11	0.48
1:C:321:THR:CG2	1:C:322:THR:N	2.76	0.48
1:A:151:ILE:HG22	1:A:152:MET:HE3	1.94	0.48
1:D:241:VAL:CG1	1:D:242:SER:N	2.34	0.48
1:D:296:ILE:HD11	1:D:299:VAL:CG1	2.43	0.48
1:E:117:ARG:O	1:E:121:ARG:CG	2.60	0.48
1:E:304:ASN:O	1:E:305:ALA:C	2.50	0.48
1:F:263:LYS:O	1:F:267:GLY:CA	2.62	0.48
1:A:296:ILE:HG13	1:A:299:VAL:HG11	1.94	0.48
1:A:365:VAL:O	1:A:366:GLU:C	2.49	0.48
1:B:393:ASN:O	1:B:396:ASP:N	2.46	0.48
1:E:142:ALA:HB1	1:E:143:PRO:HD2	1.94	0.48
1:A:208:ASP:O	1:A:212:LYS:CG	2.61	0.48
1:A:213:THR:OG1	1:A:288:VAL:HG23	2.14	0.48
1:B:17:ALA:O	1:B:19:TYR:N	2.47	0.48
1:B:167:ASP:HB2	1:B:168:PRO:CD	2.44	0.48
1:B:200:GLU:HB3	1:B:380:PHE:CD2	2.48	0.48
1:D:224:TYR:O	1:D:227:ALA:HB3	2.13	0.48
1:D:262:TRP:CD1	1:D:268:SER:O	2.67	0.48
1:D:279:THR:O	1:D:280:ASN:C	2.51	0.48
1:E:22:ILE:HD13	1:E:27:LEU:CD2	2.43	0.48
1:E:36:ILE:HG12	1:E:58:VAL:HG22	1.94	0.48
1:E:178:PRO:C	1:E:180:VAL:H	2.16	0.48
1:F:249:TYR:N	1:F:276:THR:O	2.38	0.48
1:F:294:SER:HB3	1:F:316:LEU:HB2	1.95	0.48
1:A:74:HIS:CG	1:A:75:PRO:HD2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:47:ASP:OD1	1:F:49:SER:HB3	2.14	0.48
1:A:269:VAL:O	1:A:269:VAL:HG13	2.14	0.48
1:B:74:HIS:CG	1:B:75:PRO:HD3	2.48	0.48
1:C:217:GLN:HE22	1:C:299:VAL:HG21	1.78	0.48
1:D:262:TRP:CE3	1:D:273:PRO:CD	2.96	0.48
1:E:68:LYS:HD2	1:E:140:ILE:O	2.13	0.48
1:E:72:ARG:HG2	1:E:145:VAL:HB	1.95	0.48
1:A:45:MET:C	1:A:47:ASP:H	2.15	0.48
1:B:51:LYS:HD3	1:B:53:PHE:CZ	2.49	0.48
1:E:22:ILE:HD11	1:E:26:ALA:HB1	1.96	0.48
1:E:209:LEU:O	1:E:210:LYS:C	2.45	0.48
1:E:241:VAL:HG12	1:E:242:SER:H	1.78	0.48
1:A:249:TYR:CD2	1:A:251:PRO:HD3	2.49	0.47
1:B:322:THR:CB	1:B:323:PRO:CD	2.92	0.47
1:C:27:LEU:CD1	1:C:31:LYS:HE3	2.40	0.47
1:C:33:PRO:HB3	1:C:60:TYR:HD1	1.76	0.47
1:D:3:GLN:O	1:D:6:PHE:N	2.47	0.47
1:D:276:THR:CG2	1:D:277:ASN:H	2.27	0.47
1:B:148:ASN:CB	1:B:149:PRO:CD	2.85	0.47
1:C:343:ASN:OD1	1:C:343:ASN:C	2.52	0.47
1:B:262:TRP:CD1	1:B:268:SER:O	2.68	0.47
1:E:160:GLU:CG	1:E:169:SER:HB3	2.44	0.47
1:E:179:SER:C	1:E:180:VAL:HG13	2.34	0.47
1:F:25:GLU:OE1	1:F:418:LYS:CG	2.63	0.47
1:F:160:GLU:CG	1:F:169:SER:HB3	2.42	0.47
1:A:241:VAL:HG12	1:A:242:SER:N	2.29	0.47
1:B:352:PHE:CZ	1:B:371:LYS:HB2	2.49	0.47
1:C:120:GLU:HA	1:C:154:TRP:CZ3	2.49	0.47
1:D:311:LYS:O	1:D:334:ILE:HG23	2.14	0.47
1:E:409:ALA:O	1:E:413:ARG:HG3	2.15	0.47
1:E:184:VAL:C	1:E:186:ARG:N	2.66	0.47
1:E:219:TYR:OH	1:E:256:ALA:HB1	2.15	0.47
1:E:237:LYS:HD3	1:E:252:ASP:O	2.14	0.47
1:F:329:LEU:HD23	1:F:334:ILE:HD12	1.97	0.47
1:F:366:GLU:CD	1:F:366:GLU:H	2.18	0.47
1:B:196:TYR:O	1:B:199:ARG:HB3	2.15	0.47
1:B:300:ILE:O	1:B:322:THR:HG23	2.15	0.47
1:D:25:GLU:OE2	1:D:417:LYS:N	2.47	0.47
1:D:296:ILE:HD12	1:D:299:VAL:HG13	1.95	0.47
1:E:22:ILE:HD12	1:E:27:LEU:CD2	2.44	0.47
1:F:297:GLU:O	1:F:298:GLU:C	2.52	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:GLN:CG	1:A:4:ASP:H	2.27	0.47
1:A:74:HIS:CE1	1:A:75:PRO:HD2	2.49	0.47
1:B:93:THR:HG22	1:B:98:LEU:HD12	1.96	0.47
1:C:72:ARG:NH2	1:C:77:GLU:OE1	2.38	0.47
1:C:238:VAL:O	1:C:253:GLY:HA2	2.14	0.47
1:C:262:TRP:CZ3	1:C:273:PRO:CD	2.97	0.47
1:E:248:ILE:HA	1:E:276:THR:O	2.14	0.47
1:E:280:ASN:O	1:E:283:LEU:HB3	2.15	0.47
1:F:339:ASP:O	1:F:342:CYS:N	2.46	0.47
1:F:391:ASN:C	1:F:392:ILE:CG2	2.82	0.47
1:A:74:HIS:ND1	1:A:75:PRO:CD	2.74	0.47
1:A:323:PRO:O	1:A:326:ASP:CB	2.62	0.47
1:A:417:LYS:CG	1:C:117:ARG:CZ	2.92	0.47
1:C:270:LYS:CG	1:C:271:ASP:N	2.78	0.47
1:D:296:ILE:HD12	1:D:297:GLU:O	2.15	0.47
1:E:226:MET:HE2	1:E:230:MET:HG3	1.97	0.47
1:F:248:ILE:C	1:F:278:ILE:HD13	2.35	0.47
1:A:164:ARG:CZ	1:E:131:TYR:HB3	2.45	0.47
1:A:219:TYR:OH	1:A:256:ALA:CB	2.63	0.47
1:B:29:PHE:HD1	1:E:52:VAL:HG21	1.79	0.47
1:B:72:ARG:HH21	1:B:77:GLU:CD	2.15	0.47
1:D:126:TYR:HD2	1:D:155:MET:CE	2.25	0.47
1:F:279:THR:O	1:F:282:GLU:HB3	2.14	0.47
1:F:343:ASN:OD1	1:F:343:ASN:O	2.33	0.47
1:A:96:MET:HE2	1:A:376:MET:SD	2.55	0.47
1:A:250:ASN:CB	1:A:254:LEU:HD21	2.45	0.47
1:A:268:SER:C	1:A:270:LYS:H	2.17	0.47
1:A:288:VAL:CG2	1:A:289:ASP:N	2.77	0.47
1:A:392:ILE:HD12	1:A:396:ASP:HB2	1.96	0.47
1:D:192:ARG:NH2	1:D:233:GLU:OE2	2.48	0.47
1:D:285:GLU:OE1	1:D:307:ASN:CB	2.63	0.47
1:D:347:VAL:HA	1:D:350:SER:OG	2.15	0.47
1:F:45:MET:HG2	1:F:49:SER:O	2.15	0.47
1:A:214:ILE:HG22	1:A:236:MET:HE2	1.96	0.46
1:A:292:ALA:HB1	1:A:316:LEU:HD12	1.97	0.46
1:C:240:ALA:O	1:C:241:VAL:HG23	2.15	0.46
1:D:238:VAL:O	1:D:254:LEU:HD12	2.15	0.46
1:D:297:GLU:O	1:D:299:VAL:HG13	2.15	0.46
1:E:176:LYS:NZ	1:E:176:LYS:HB2	2.30	0.46
1:A:300:ILE:HA	1:A:304:ASN:HD21	1.80	0.46
1:A:322:THR:OG1	1:A:325:ALA:HB3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:392:ILE:HD12	1:A:397:ALA:N	2.30	0.46
1:B:11:LYS:O	1:B:12:GLN:C	2.53	0.46
1:C:219:TYR:CD1	1:C:241:VAL:HG13	2.50	0.46
1:C:327:GLU:O	1:C:330:TYR:HB3	2.15	0.46
1:D:213:THR:C	1:D:288:VAL:HG12	2.34	0.46
1:D:240:ALA:CB	1:D:283:LEU:HD12	2.45	0.46
1:E:111:PRO:O	1:E:113:GLU:N	2.45	0.46
1:F:248:ILE:HG13	1:F:248:ILE:O	2.14	0.46
1:A:131:TYR:HA	1:A:134:ILE:HD11	1.97	0.46
1:B:220:GLY:O	1:B:224:TYR:HB3	2.15	0.46
1:B:383:VAL:HG12	1:B:397:ALA:HB3	1.97	0.46
1:C:216:ILE:O	1:C:241:VAL:HA	2.14	0.46
1:D:176:LYS:NZ	1:D:353:GLU:OE2	2.49	0.46
1:F:297:GLU:HA	1:F:320:PRO:HA	1.97	0.46
1:D:288:VAL:HG12	1:D:289:ASP:H	1.80	0.46
1:E:226:MET:CE	1:E:230:MET:HG2	2.46	0.46
1:A:45:MET:C	1:A:47:ASP:N	2.68	0.46
1:A:95:VAL:HG13	1:A:96:MET:N	2.30	0.46
1:A:270:LYS:O	1:A:271:ASP:CB	2.62	0.46
1:C:296:ILE:H	1:C:296:ILE:HG13	1.58	0.46
1:C:363:TRP:CD1	1:C:363:TRP:N	2.84	0.46
1:D:270:LYS:O	1:D:271:ASP:HB2	2.16	0.46
1:D:285:GLU:O	1:D:309:LYS:HE2	2.15	0.46
1:E:63:ALA:HB2	1:E:415:TRP:CZ3	2.50	0.46
1:E:249:TYR:OH	1:E:251:PRO:HG3	2.15	0.46
1:F:170:PHE:O	1:F:176:LYS:HE2	2.15	0.46
1:C:9:ALA:CB	1:C:88:TRP:HZ3	2.28	0.46
1:C:322:THR:CB	1:C:323:PRO:CD	2.93	0.46
1:D:148:ASN:HB2	1:D:149:PRO:HD2	1.98	0.46
1:E:337:ILE:HG22	1:E:342:CYS:HB2	1.97	0.46
1:F:176:LYS:HD2	1:F:180:VAL:O	2.16	0.46
1:A:186:ARG:O	1:A:186:ARG:HG3	2.15	0.46
1:A:250:ASN:CB	1:A:254:LEU:CD2	2.92	0.46
1:C:57:ARG:NH2	1:C:69:GLY:O	2.43	0.46
1:D:88:TRP:CH2	1:D:399:TYR:OH	2.69	0.46
1:D:329:LEU:H	1:D:329:LEU:HG	1.59	0.46
1:F:53:PHE:N	1:F:53:PHE:CD1	2.83	0.46
1:B:75:PRO:HD2	1:B:76:GLU:H	1.80	0.46
1:D:263:LYS:HD2	1:D:268:SER:HA	1.98	0.46
1:D:372:LEU:O	1:D:376:MET:HG2	2.16	0.46
1:E:199:ARG:O	1:E:202:ALA:HB3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:167:ASP:HB2	1:F:168:PRO:CD	2.46	0.46
1:A:47:ASP:OD1	1:A:47:ASP:O	2.34	0.46
1:A:89:MET:CE	1:A:89:MET:CA	2.94	0.46
1:C:65:GLY:HA3	1:C:99:PRO:O	2.15	0.46
1:F:22:ILE:O	1:F:23:SER:O	2.34	0.46
1:F:313:VAL:O	1:F:313:VAL:HG12	2.15	0.46
1:A:73:TRP:CH2	1:A:122:LEU:HD23	2.51	0.46
1:A:124:ARG:O	1:A:128:ARG:HG3	2.16	0.46
1:D:87:ALA:O	1:D:90:THR:HB	2.15	0.46
1:D:259:VAL:HA	1:D:272:PHE:CE1	2.51	0.46
1:D:262:TRP:O	1:D:263:LYS:C	2.54	0.46
1:D:300:ILE:HD13	1:D:308:ILE:HG13	1.98	0.46
1:E:217:GLN:HB3	1:E:293:PRO:HA	1.98	0.46
1:E:243:ASP:O	1:E:245:LYS:N	2.49	0.46
1:F:73:TRP:CD1	1:F:107:VAL:HG23	2.51	0.46
1:F:329:LEU:HD23	1:F:334:ILE:CD1	2.45	0.46
1:B:329:LEU:HD23	1:B:334:ILE:HD13	1.97	0.45
1:C:222:ALA:O	1:C:226:MET:HB2	2.15	0.45
1:D:120:GLU:HB2	1:D:154:TRP:CZ3	2.49	0.45
1:D:219:TYR:OH	1:D:256:ALA:HA	2.16	0.45
1:E:56:PHE:O	1:E:126:TYR:OH	2.29	0.45
1:F:110:ASN:OD1	1:F:112:LYS:HB2	2.16	0.45
1:A:72:ARG:NH2	1:A:77:GLU:OE1	2.24	0.45
1:D:225:TYR:O	1:D:226:MET:C	2.53	0.45
1:D:248:ILE:HD11	1:D:254:LEU:CD2	2.46	0.45
1:E:79:LEU:HD12	1:E:79:LEU:C	2.35	0.45
1:F:26:ALA:HB2	1:F:407:TYR:CE1	2.52	0.45
1:F:43:VAL:HB	1:F:53:PHE:HE1	1.81	0.45
1:F:72:ARG:HG2	1:F:144:ASP:HB3	1.98	0.45
1:A:3:GLN:N	1:A:6:PHE:HB3	2.31	0.45
1:A:117:ARG:HA	1:A:117:ARG:NE	2.31	0.45
1:D:301:THR:HA	1:D:325:ALA:HB2	1.98	0.45
1:E:29:PHE:CG	1:E:410:MET:HE2	2.52	0.45
1:E:74:HIS:ND1	1:E:75:PRO:CD	2.72	0.45
1:E:110:ASN:HB3	1:E:113:GLU:OE2	2.16	0.45
1:F:220:GLY:O	1:F:224:TYR:N	2.43	0.45
1:F:365:VAL:HG23	1:F:366:GLU:N	2.32	0.45
1:A:322:THR:O	1:A:325:ALA:HB3	2.16	0.45
1:B:294:SER:HA	1:B:317:ALA:HB2	1.97	0.45
1:C:417:LYS:HD2	1:C:417:LYS:N	2.31	0.45
1:F:176:LYS:O	1:F:182:GLY:HA3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:209:LEU:O	1:F:212:LYS:HG2	2.17	0.45
1:F:391:ASN:C	1:F:392:ILE:HG23	2.35	0.45
1:A:30:LEU:HD21	1:A:406:VAL:CG1	2.46	0.45
1:A:296:ILE:CD1	1:A:299:VAL:CG1	2.94	0.45
1:B:160:GLU:HG2	1:B:169:SER:HB3	1.99	0.45
1:C:224:TYR:CG	1:C:260:LEU:CD2	3.00	0.45
1:E:301:THR:OG1	1:E:303:LYS:HB2	2.15	0.45
1:F:324:GLU:H	1:F:324:GLU:HG2	1.25	0.45
1:A:262:TRP:CH2	1:A:273:PRO:HD3	2.51	0.45
1:A:329:LEU:CD2	1:A:334:ILE:HD13	2.39	0.45
1:C:64:ARG:NH2	1:C:97:ASP:HA	2.31	0.45
1:C:117:ARG:NH2	1:F:48:GLY:O	2.46	0.45
1:E:34:GLN:OE1	1:E:61:ASN:HA	2.17	0.45
1:A:208:ASP:O	1:A:212:LYS:CE	2.65	0.45
1:B:184:VAL:O	1:B:184:VAL:HG12	2.17	0.45
1:C:71:ILE:CD1	1:C:126:TYR:HE2	2.30	0.45
1:D:58:VAL:O	1:D:103:GLY:HA2	2.17	0.45
1:E:87:ALA:O	1:E:90:THR:HB	2.17	0.45
1:F:313:VAL:HB	1:F:336:ILE:HG12	1.99	0.45
1:A:20:MET:HE2	1:A:400:VAL:CA	2.39	0.45
1:B:173:ILE:O	1:B:173:ILE:CG2	2.65	0.45
1:B:184:VAL:C	1:B:186:ARG:H	2.20	0.45
1:C:384:TYR:HA	1:C:394:MET:CE	2.35	0.45
1:E:142:ALA:HB1	1:E:143:PRO:CD	2.47	0.45
1:B:209:LEU:HA	1:B:212:LYS:CG	2.46	0.45
1:C:373:ASP:C	1:C:373:ASP:OD1	2.56	0.45
1:D:217:GLN:O	1:D:217:GLN:CG	2.64	0.45
1:E:111:PRO:HG2	1:E:146:TYR:HD2	1.81	0.45
1:E:170:PHE:O	1:E:176:LYS:CE	2.62	0.45
1:E:266:THR:HG22	1:E:268:SER:H	1.82	0.45
1:E:339:ASP:OD1	1:E:339:ASP:N	2.50	0.45
1:E:393:ASN:O	1:E:396:ASP:N	2.50	0.45
1:F:170:PHE:O	1:F:176:LYS:HE3	2.17	0.45
1:B:186:ARG:O	1:B:186:ARG:CG	2.64	0.45
1:B:329:LEU:HD23	1:B:334:ILE:CD1	2.47	0.45
1:C:205:LEU:HD12	1:C:205:LEU:HA	1.66	0.45
1:C:277:ASN:O	1:C:278:ILE:HG22	2.17	0.45
1:E:26:ALA:HB2	1:E:407:TYR:CE1	2.52	0.45
1:C:43:VAL:CG1	1:C:44:GLU:N	2.80	0.44
1:E:51:LYS:HG2	1:E:53:PHE:HE1	1.78	0.44
1:E:201:ALA:O	1:E:202:ALA:C	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:GLY:O	1:A:141:PRO:HA	2.17	0.44
1:B:79:LEU:O	1:B:82:VAL:HB	2.18	0.44
1:C:4:ASP:O	1:C:8:ILE:CD1	2.65	0.44
1:C:304:ASN:N	1:C:304:ASN:OD1	2.51	0.44
1:D:68:LYS:HD2	1:D:68:LYS:HA	1.69	0.44
1:D:340:PHE:HE1	1:D:398:ALA:HB1	1.81	0.44
1:E:59:GLN:HE22	1:E:133:VAL:CG2	2.26	0.44
1:E:249:TYR:CE2	1:E:251:PRO:HG3	2.52	0.44
1:B:250:ASN:OD1	1:B:251:PRO:HD2	2.16	0.44
1:B:266:THR:O	1:B:266:THR:CG2	2.66	0.44
1:B:393:ASN:O	1:B:394:MET:C	2.55	0.44
1:D:12:GLN:CD	1:D:88:TRP:HH2	2.21	0.44
1:D:38:GLU:HG3	1:D:56:PHE:CD1	2.53	0.44
1:A:128:ARG:HD2	1:A:158:GLU:OE2	2.17	0.44
1:C:131:TYR:HE1	1:C:159:TYR:CE1	2.35	0.44
1:C:319:GLY:N	1:C:320:PRO:CD	2.81	0.44
1:D:272:PHE:HA	1:D:273:PRO:HD2	1.85	0.44
1:E:123:ALA:O	1:E:155:MET:HE2	2.18	0.44
1:E:148:ASN:HB2	1:E:149:PRO:CD	2.47	0.44
1:E:156:MET:HE1	1:E:170:PHE:CE1	2.53	0.44
1:F:3:GLN:C	1:F:5:PRO:CD	2.82	0.44
1:F:72:ARG:HG2	1:F:144:ASP:OD2	2.17	0.44
1:F:89:MET:O	1:F:92:LYS:N	2.51	0.44
1:F:297:GLU:H	1:F:297:GLU:HG3	1.12	0.44
1:A:201:ALA:O	1:A:202:ALA:C	2.56	0.44
1:A:270:LYS:HE2	1:A:277:ASN:ND2	2.33	0.44
1:B:257:ASP:O	1:B:260:LEU:N	2.50	0.44
1:D:248:ILE:HG23	1:D:269:VAL:CG2	2.47	0.44
1:A:219:TYR:OH	1:A:256:ALA:HA	2.18	0.44
1:B:131:TYR:CE1	1:B:159:TYR:HE1	2.33	0.44
1:C:74:HIS:CE1	1:C:76:GLU:HB2	2.52	0.44
1:D:160:GLU:CG	1:D:169:SER:HB3	2.46	0.44
1:D:269:VAL:O	1:D:272:PHE:HB2	2.18	0.44
1:F:3:GLN:NE2	1:F:80:SER:HG	2.10	0.44
1:A:93:THR:O	1:A:97:ASP:N	2.51	0.44
1:B:279:THR:HG1	1:B:282:GLU:HG3	1.80	0.44
1:B:338:PRO:HD3	1:B:394:MET:HB3	1.99	0.44
1:D:150:GLN:OE1	1:D:154:TRP:NE1	2.50	0.44
1:D:319:GLY:N	1:D:320:PRO:HD2	2.32	0.44
1:E:71:ILE:HD13	1:E:126:TYR:HE2	1.81	0.44
1:E:74:HIS:CG	1:E:75:PRO:CD	3.01	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:201:ALA:O	1:E:204:ALA:N	2.50	0.44
1:A:209:LEU:C	1:A:212:LYS:HG2	2.38	0.44
1:A:209:LEU:O	1:A:236:MET:HG2	2.18	0.44
1:C:158:GLU:O	1:C:158:GLU:HG3	2.18	0.44
1:C:270:LYS:HG3	1:C:277:ASN:ND2	2.14	0.44
1:D:249:TYR:CB	1:D:278:ILE:HD13	2.46	0.44
1:E:176:LYS:O	1:E:182:GLY:HA3	2.17	0.44
1:B:3:GLN:CG	1:B:4:ASP:N	2.57	0.44
1:B:3:GLN:O	1:B:4:ASP:C	2.56	0.44
1:D:126:TYR:CD2	1:D:155:MET:HE2	2.50	0.44
1:D:328:ILE:O	1:D:331:GLU:HB2	2.18	0.44
1:E:110:ASN:HD22	1:E:113:GLU:CG	2.31	0.44
1:A:197:THR:O	1:A:201:ALA:N	2.50	0.43
1:A:259:VAL:CG1	1:A:269:VAL:HG23	2.48	0.43
1:A:323:PRO:O	1:A:327:GLU:OE2	2.36	0.43
1:B:29:PHE:CD1	1:E:52:VAL:HG21	2.52	0.43
1:C:164:ARG:CZ	1:F:131:TYR:HB3	2.48	0.43
1:C:322:THR:HB	1:C:323:PRO:HD2	2.00	0.43
1:D:135:SER:OG	1:D:136:PRO:N	2.51	0.43
1:D:262:TRP:O	1:D:264:LYS:N	2.51	0.43
1:E:126:TYR:O	1:E:129:ALA:HB3	2.18	0.43
1:F:3:GLN:HB3	1:F:80:SER:OG	2.18	0.43
1:F:383:VAL:HG12	1:F:394:MET:HE3	2.00	0.43
1:A:3:GLN:O	1:A:7:GLU:N	2.49	0.43
1:A:74:HIS:CE1	1:A:76:GLU:HB2	2.53	0.43
1:D:195:SER:HB2	1:D:234:TYR:HE2	1.83	0.43
1:D:202:ALA:HB1	1:D:207:MET:HG3	1.99	0.43
1:D:324:GLU:O	1:D:325:ALA:C	2.56	0.43
1:F:74:HIS:CG	1:F:75:PRO:HD2	2.53	0.43
1:A:30:LEU:CD2	1:A:91:TRP:HH2	2.22	0.43
1:A:245:LYS:HD3	1:A:268:SER:HB2	2.00	0.43
1:B:164:ARG:HA	1:B:164:ARG:HD2	1.74	0.43
1:C:15:ARG:HG3	1:C:15:ARG:O	2.18	0.43
1:C:250:ASN:HA	1:C:251:PRO:HD3	1.80	0.43
1:C:328:ILE:O	1:C:332:LYS:N	2.51	0.43
1:D:212:LYS:HA	1:D:212:LYS:HD3	1.36	0.43
1:A:291:LEU:O	1:A:293:PRO:HD2	2.18	0.43
1:D:296:ILE:CD1	1:D:299:VAL:HG12	2.48	0.43
1:D:384:TYR:HE2	1:D:388:LYS:HZ3	1.65	0.43
1:E:322:THR:O	1:E:326:ASP:N	2.51	0.43
1:F:219:TYR:OH	1:F:256:ALA:HB1	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:279:THR:OG1	1:F:282:GLU:HB2	2.17	0.43
1:A:50:VAL:HG23	1:F:417:LYS:HG2	1.99	0.43
1:A:57:ARG:NE	1:A:139:ASP:OD2	2.44	0.43
1:A:128:ARG:CZ	1:E:161:THR:HG21	2.48	0.43
1:B:392:ILE:HG21	1:B:392:ILE:HD13	1.74	0.43
1:B:404:SER:O	1:B:407:TYR:HB3	2.18	0.43
1:C:279:THR:H	1:C:282:GLU:HG3	1.83	0.43
1:D:214:ILE:HA	1:D:288:VAL:HG11	2.01	0.43
1:E:207:MET:CG	1:E:208:ASP:N	2.80	0.43
1:B:48:GLY:CA	1:D:117:ARG:HH22	2.32	0.43
1:B:51:LYS:HG2	1:B:53:PHE:CE1	2.53	0.43
1:B:250:ASN:HA	1:B:251:PRO:HD3	1.48	0.43
1:C:270:LYS:HG2	1:C:271:ASP:N	2.34	0.43
1:D:74:HIS:O	1:D:108:ILE:HA	2.19	0.43
1:D:192:ARG:HG2	1:D:372:LEU:HD23	2.01	0.43
1:D:411:LYS:O	1:D:412:ASP:C	2.57	0.43
1:A:366:GLU:HG3	1:A:367:GLU:N	2.34	0.43
1:B:48:GLY:HA2	1:D:117:ARG:HH22	1.83	0.43
1:C:92:LYS:HG3	1:C:340:PHE:O	2.19	0.43
1:C:208:ASP:O	1:C:212:LYS:CD	2.66	0.43
1:C:319:GLY:N	1:C:320:PRO:HD3	2.34	0.43
1:D:145:VAL:O	1:D:145:VAL:HG12	2.18	0.43
1:E:208:ASP:O	1:E:212:LYS:HE2	2.18	0.43
1:E:296:ILE:CD1	1:E:299:VAL:CG1	2.91	0.43
1:F:11:LYS:O	1:F:12:GLN:C	2.57	0.43
1:F:213:THR:OG1	1:F:288:VAL:HA	2.19	0.43
1:A:104:LYS:HG3	1:A:105:GLY:H	1.84	0.43
1:A:111:PRO:CG	1:A:146:TYR:CD2	3.02	0.43
1:B:156:MET:C	1:B:156:MET:SD	2.97	0.43
1:F:77:GLU:HB3	1:F:108:ILE:HG12	2.01	0.43
1:A:340:PHE:O	1:A:344:ALA:HB2	2.18	0.43
1:B:33:PRO:HB3	1:B:60:TYR:CD1	2.54	0.43
1:C:164:ARG:HH21	1:F:132:ASP:CG	2.22	0.43
1:C:207:MET:HE2	1:C:311:LYS:CD	2.46	0.43
1:C:284:LEU:HD13	1:C:299:VAL:O	2.19	0.43
1:D:72:ARG:NE	1:D:77:GLU:OE2	2.38	0.43
1:D:148:ASN:C	1:D:148:ASN:OD1	2.57	0.43
1:E:27:LEU:HD22	1:E:27:LEU:HA	1.74	0.43
1:E:192:ARG:HD3	1:E:369:ARG:HG2	2.01	0.43
1:E:214:ILE:HG12	1:E:215:ALA:N	2.33	0.43
1:F:284:LEU:HD23	1:F:284:LEU:N	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:319:GLY:N	1:F:320:PRO:CD	2.81	0.43
1:F:322:THR:O	1:F:325:ALA:N	2.52	0.43
1:A:96:MET:O	1:A:97:ASP:HB3	2.19	0.42
1:D:197:THR:O	1:D:198:VAL:C	2.57	0.42
1:D:205:LEU:HA	1:D:205:LEU:HD12	1.64	0.42
1:E:33:PRO:HB3	1:E:60:TYR:HD1	1.81	0.42
1:F:123:ALA:HB1	1:F:155:MET:HG3	2.01	0.42
1:A:304:ASN:HA	1:A:307:ASN:ND2	2.34	0.42
1:B:150:GLN:OE1	1:B:154:TRP:NE1	2.52	0.42
1:B:385:ASN:HD22	1:B:388:LYS:HE2	1.83	0.42
1:D:284:LEU:HD13	1:D:299:VAL:O	2.18	0.42
1:E:15:ARG:O	1:E:15:ARG:HG3	2.15	0.42
1:E:366:GLU:CD	1:E:366:GLU:H	2.23	0.42
1:F:66:PRO:HG2	1:F:100:TYR:CD1	2.53	0.42
1:F:214:ILE:HG13	1:F:215:ALA:N	2.34	0.42
1:A:68:LYS:NZ	1:A:141:PRO:O	2.52	0.42
1:B:26:ALA:HB2	1:B:416:ILE:HD13	2.00	0.42
1:C:79:LEU:O	1:C:83:LYS:HG3	2.19	0.42
1:E:270:LYS:HE2	1:E:270:LYS:HB3	1.26	0.42
1:F:27:LEU:HD23	1:F:27:LEU:HA	1.80	0.42
1:F:183:ILE:HG12	1:F:353:GLU:HB2	2.02	0.42
1:A:196:TYR:O	1:A:200:GLU:HG2	2.20	0.42
1:B:12:GLN:CD	1:B:88:TRP:HH2	2.23	0.42
1:C:42:PRO:HB3	1:D:29:PHE:HE2	1.85	0.42
1:C:161:THR:HG21	1:F:128:ARG:NH2	2.34	0.42
1:C:172:VAL:HG22	1:C:172:VAL:O	2.19	0.42
1:C:260:LEU:O	1:C:261:ALA:C	2.57	0.42
1:D:288:VAL:HG12	1:D:289:ASP:N	2.34	0.42
1:E:25:GLU:OE1	1:E:418:LYS:HG3	2.20	0.42
1:E:72:ARG:HH21	1:E:77:GLU:CD	2.22	0.42
1:E:417:LYS:HA	1:E:417:LYS:HD2	1.63	0.42
1:A:59:GLN:HE22	1:A:133:VAL:HB	1.83	0.42
1:B:23:SER:OG	1:B:418:LYS:OXT	2.18	0.42
1:C:277:ASN:C	1:C:278:ILE:CG2	2.87	0.42
1:C:308:ILE:H	1:C:308:ILE:HG12	1.53	0.42
1:D:224:TYR:CE1	1:D:256:ALA:HB1	2.54	0.42
1:E:404:SER:O	1:E:407:TYR:HB3	2.19	0.42
1:F:197:THR:O	1:F:200:GLU:HB2	2.20	0.42
1:A:196:TYR:CD2	1:A:373:ASP:HA	2.55	0.42
1:B:63:ALA:HB2	1:B:415:TRP:CH2	2.53	0.42
1:C:237:LYS:O	1:C:238:VAL:C	2.58	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:323:PRO:O	1:C:326:ASP:CB	2.58	0.42
1:D:120:GLU:HA	1:D:154:TRP:CE3	2.54	0.42
1:D:145:VAL:O	1:D:146:TYR:HB2	2.20	0.42
1:D:214:ILE:CA	1:D:288:VAL:HG11	2.50	0.42
1:E:156:MET:HE2	1:E:170:PHE:CD1	2.54	0.42
1:F:403:VAL:O	1:F:403:VAL:HG12	2.19	0.42
1:A:286:LEU:HD23	1:A:286:LEU:HA	1.70	0.42
1:B:292:ALA:HA	1:B:293:PRO:HD2	1.89	0.42
1:B:365:VAL:H	1:B:365:VAL:HG22	1.61	0.42
1:C:36:ILE:HG12	1:C:58:VAL:HG22	2.02	0.42
1:C:176:LYS:HE2	1:C:176:LYS:HB2	1.64	0.42
1:C:214:ILE:HB	1:C:236:MET:CE	2.46	0.42
1:C:243:ASP:C	1:C:243:ASP:OD1	2.58	0.42
1:C:262:TRP:CH2	1:C:273:PRO:HD3	2.55	0.42
1:C:313:VAL:O	1:C:313:VAL:HG12	2.20	0.42
1:C:365:VAL:O	1:C:369:ARG:CG	2.64	0.42
1:D:66:PRO:HD2	1:D:99:PRO:O	2.19	0.42
1:D:69:GLY:HA3	1:D:103:GLY:O	2.20	0.42
1:D:131:TYR:CE1	1:D:159:TYR:CE1	3.08	0.42
1:F:177:PRO:HA	1:F:178:PRO:HD3	1.79	0.42
1:F:365:VAL:HG22	1:F:366:GLU:OE2	2.19	0.42
1:A:29:PHE:CE2	1:F:42:PRO:HG3	2.54	0.42
1:A:364:THR:O	1:A:367:GLU:HB2	2.20	0.42
1:B:192:ARG:HG2	1:B:372:LEU:HD21	2.02	0.42
1:B:204:ALA:HB1	1:B:384:TYR:CZ	2.55	0.42
1:B:363:TRP:CD1	1:B:363:TRP:N	2.87	0.42
1:C:250:ASN:HB3	1:C:254:LEU:CD2	2.50	0.42
1:C:299:VAL:O	1:C:299:VAL:HG23	2.19	0.42
1:D:123:ALA:HB1	1:D:155:MET:HG3	2.01	0.42
1:D:262:TRP:CZ2	1:D:273:PRO:HD3	2.53	0.42
1:D:292:ALA:HA	1:D:293:PRO:HD2	1.68	0.42
1:F:15:ARG:O	1:F:18:GLN:HG2	2.19	0.42
1:F:17:ALA:C	1:F:19:TYR:N	2.71	0.42
1:F:131:TYR:CE1	1:F:159:TYR:CE1	3.08	0.42
1:F:219:TYR:OH	1:F:256:ALA:HA	2.20	0.42
1:A:224:TYR:CZ	1:A:228:LYS:HD2	2.54	0.42
1:A:313:VAL:HB	1:A:336:ILE:HG12	2.02	0.42
1:B:250:ASN:OD1	1:B:252:ASP:N	2.53	0.42
1:D:217:GLN:HB2	1:D:283:LEU:CD2	2.50	0.42
1:D:291:LEU:HG	1:D:293:PRO:HD3	2.02	0.42
1:E:78:THR:O	1:E:82:VAL:HG23	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:176:LYS:NZ	1:F:176:LYS:CB	2.83	0.42
1:F:392:ILE:HG21	1:F:392:ILE:HD13	1.84	0.42
1:A:339:ASP:C	1:A:341:LEU:N	2.73	0.42
1:B:214:ILE:HD12	1:B:290:VAL:CG1	2.50	0.42
1:C:148:ASN:CB	1:C:149:PRO:CD	2.84	0.42
1:D:196:TYR:O	1:D:199:ARG:HB3	2.20	0.42
1:D:205:LEU:HD13	1:D:205:LEU:N	2.35	0.42
1:D:209:LEU:O	1:D:236:MET:HG2	2.20	0.42
1:D:283:LEU:O	1:D:286:LEU:HB2	2.19	0.42
1:A:255:ASN:O	1:A:258:GLU:N	2.52	0.41
1:B:260:LEU:O	1:B:264:LYS:HG2	2.18	0.41
1:D:110:ASN:HA	1:D:111:PRO:HD2	1.92	0.41
1:D:177:PRO:HA	1:D:178:PRO:HD3	1.87	0.41
1:F:242:SER:HB3	1:F:283:LEU:HD13	2.01	0.41
1:A:45:MET:N	1:A:49:SER:O	2.35	0.41
1:A:241:VAL:HG12	1:A:269:VAL:HG21	2.02	0.41
1:D:110:ASN:O	1:D:114:MET:HG3	2.20	0.41
1:D:203:LYS:O	1:D:204:ALA:C	2.57	0.41
1:D:260:LEU:HD12	1:D:260:LEU:O	2.21	0.41
1:D:285:GLU:OE1	1:D:307:ASN:HB2	2.20	0.41
1:E:365:VAL:HG22	1:E:366:GLU:N	2.34	0.41
1:F:73:TRP:NE1	1:F:107:VAL:CG2	2.84	0.41
1:F:149:PRO:O	1:F:150:GLN:C	2.59	0.41
1:F:203:LYS:O	1:F:204:ALA:C	2.58	0.41
1:F:224:TYR:OH	1:F:257:ASP:OD1	2.30	0.41
1:F:365:VAL:HG23	1:F:366:GLU:OE2	2.20	0.41
1:A:40:SER:HB2	1:A:52:VAL:CG1	2.50	0.41
1:B:280:ASN:O	1:B:281:GLU:C	2.58	0.41
1:F:174:THR:HG1	1:F:350:SER:HG	1.57	0.41
1:F:272:PHE:HA	1:F:273:PRO:HD2	1.77	0.41
1:A:15:ARG:O	1:A:18:GLN:HG3	2.21	0.41
1:A:340:PHE:CE1	1:A:399:TYR:CE1	3.09	0.41
1:B:286:LEU:HD23	1:B:286:LEU:HA	1.63	0.41
1:C:209:LEU:HD22	1:C:236:MET:SD	2.61	0.41
1:D:137:TYR:CZ	1:F:168:PRO:HG3	2.55	0.41
1:D:190:THR:HG22	1:D:191:ALA:N	2.35	0.41
1:D:218:GLY:HA3	1:D:295:ALA:HB2	2.03	0.41
1:D:271:ASP:O	1:D:272:PHE:O	2.39	0.41
1:E:59:GLN:NE2	1:E:133:VAL:HG23	2.32	0.41
1:E:186:ARG:HA	1:E:349:VAL:HG11	2.01	0.41
1:F:213:THR:OG1	1:F:288:VAL:HG12	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:ARG:HG2	1:A:144:ASP:CG	2.40	0.41
1:A:184:VAL:C	1:A:186:ARG:N	2.73	0.41
1:A:263:LYS:O	1:A:267:GLY:N	2.41	0.41
1:B:287:GLU:HA	1:B:309:LYS:HB2	2.02	0.41
1:B:371:LYS:HG2	1:B:371:LYS:H	1.30	0.41
1:C:15:ARG:O	1:C:18:GLN:NE2	2.53	0.41
1:E:164:ARG:O	1:E:165:ARG:HB2	2.19	0.41
1:E:243:ASP:O	1:E:244:THR:C	2.58	0.41
1:A:23:SER:OG	1:A:418:LYS:OXT	2.24	0.41
1:A:173:ILE:O	1:A:173:ILE:CG2	2.64	0.41
1:A:323:PRO:HA	1:A:326:ASP:HB2	2.02	0.41
1:A:335:LEU:HD12	1:A:336:ILE:N	2.35	0.41
1:B:12:GLN:HE21	1:B:12:GLN:HB3	1.56	0.41
1:C:343:ASN:OD1	1:C:343:ASN:O	2.39	0.41
1:D:120:GLU:CB	1:D:154:TRP:CE3	2.98	0.41
1:D:292:ALA:O	1:D:293:PRO:C	2.58	0.41
1:E:128:ARG:HD2	1:E:158:GLU:OE2	2.20	0.41
1:F:280:ASN:O	1:F:283:LEU:HB3	2.20	0.41
1:F:387:HIS:HB2	1:F:392:ILE:O	2.20	0.41
1:A:205:LEU:HA	1:A:205:LEU:HD12	1.77	0.41
1:A:397:ALA:O	1:A:400:VAL:HB	2.19	0.41
1:B:27:LEU:HD12	1:B:31:LYS:HE3	2.02	0.41
1:B:128:ARG:CZ	1:D:161:THR:HG21	2.51	0.41
1:B:299:VAL:HG23	1:B:300:ILE:N	2.36	0.41
1:B:371:LYS:HZ3	1:B:371:LYS:CB	2.22	0.41
1:C:4:ASP:HB3	1:C:5:PRO:CD	2.40	0.41
1:D:336:ILE:O	1:D:336:ILE:HG22	2.18	0.41
1:F:85:LEU:HD23	1:F:85:LEU:HA	1.89	0.41
1:A:172:VAL:O	1:A:172:VAL:CG2	2.64	0.41
1:A:372:LEU:O	1:A:375:LYS:N	2.54	0.41
1:C:120:GLU:CA	1:C:154:TRP:CE3	2.93	0.41
1:C:294:SER:HB3	1:C:316:LEU:HB2	2.03	0.41
1:E:178:PRO:C	1:E:180:VAL:N	2.73	0.41
1:A:44:GLU:HG3	1:E:117:ARG:NH2	2.31	0.41
1:A:248:ILE:CD1	1:A:254:LEU:HD13	2.36	0.41
1:A:283:LEU:HA	1:A:286:LEU:HG	2.03	0.41
1:A:294:SER:HB3	1:A:316:LEU:HB2	2.03	0.41
1:A:336:ILE:HD13	1:A:336:ILE:HG23	1.81	0.41
1:A:340:PHE:HE1	1:A:399:TYR:CE1	2.39	0.41
1:B:142:ALA:C	1:B:152:MET:SD	3.00	0.41
1:C:126:TYR:HD2	1:C:155:MET:HE2	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:160:GLU:HG2	1:C:169:SER:HB3	2.03	0.41
1:C:207:MET:HE1	1:C:311:LYS:CD	2.51	0.41
1:C:241:VAL:O	1:C:242:SER:HB3	2.20	0.41
1:C:304:ASN:HA	1:C:307:ASN:HD22	1.85	0.41
1:C:307:ASN:O	1:C:309:LYS:HG3	2.21	0.41
1:D:98:LEU:HD23	1:D:375:LYS:HZ3	1.83	0.41
1:D:141:PRO:HD2	1:D:172:VAL:O	2.21	0.41
1:D:276:THR:HG22	1:D:277:ASN:O	2.21	0.41
1:E:393:ASN:O	1:E:394:MET:C	2.58	0.41
1:F:3:GLN:O	1:F:6:PHE:N	2.53	0.41
1:F:85:LEU:HB3	1:F:104:LYS:HD3	2.02	0.41
1:F:302:LYS:O	1:F:303:LYS:C	2.58	0.41
1:F:416:ILE:HD13	1:F:418:LYS:OXT	2.21	0.41
1:A:8:ILE:O	1:A:12:GLN:HG3	2.21	0.41
1:A:27:LEU:HD23	1:A:27:LEU:HA	1.77	0.41
1:A:224:TYR:OH	1:A:228:LYS:HD2	2.21	0.41
1:B:13:LEU:O	1:B:14:GLU:C	2.57	0.41
1:B:394:MET:H	1:B:394:MET:HG2	1.58	0.41
1:C:401:VAL:HG23	1:C:401:VAL:H	1.66	0.41
1:D:92:LYS:O	1:D:95:VAL:HG12	2.20	0.41
1:D:163:SER:O	1:D:164:ARG:CB	2.62	0.41
1:E:265:LYS:HD2	1:E:265:LYS:HA	1.83	0.41
1:F:141:PRO:O	1:F:142:ALA:HB2	2.20	0.41
1:A:73:TRP:O	1:A:146:TYR:HB2	2.21	0.40
1:B:92:LYS:O	1:B:95:VAL:HG12	2.20	0.40
1:B:299:VAL:HG23	1:B:300:ILE:CG1	2.51	0.40
1:E:272:PHE:HA	1:E:273:PRO:HD2	1.88	0.40
1:F:29:PHE:HB3	1:F:410:MET:HE2	2.03	0.40
1:F:208:ASP:OD1	1:F:209:LEU:N	2.54	0.40
1:A:164:ARG:HD2	1:A:164:ARG:HA	1.76	0.40
1:A:170:PHE:HB3	1:A:176:LYS:HZ2	1.86	0.40
1:A:184:VAL:O	1:A:184:VAL:CG1	2.68	0.40
1:A:202:ALA:HB2	1:A:209:LEU:HD21	2.03	0.40
1:A:272:PHE:HA	1:A:273:PRO:HD2	1.94	0.40
1:A:322:THR:HB	1:A:323:PRO:CD	2.49	0.40
1:A:378:LYS:HE2	1:A:382:ASP:OD1	2.21	0.40
1:A:379:ALA:O	1:A:383:VAL:HG23	2.21	0.40
1:E:192:ARG:HG2	1:E:372:LEU:HD23	2.02	0.40
1:E:292:ALA:HB1	1:E:316:LEU:HD12	2.03	0.40
1:F:73:TRP:NE1	1:F:107:VAL:HG21	2.35	0.40
1:F:224:TYR:CZ	1:F:260:LEU:HD22	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226:MET:HG2	1:A:316:LEU:CD1	2.47	0.40
1:A:240:ALA:CA	1:A:248:ILE:O	2.65	0.40
1:A:279:THR:O	1:A:282:GLU:HB2	2.20	0.40
1:B:93:THR:O	1:B:97:ASP:N	2.54	0.40
1:C:141:PRO:HD2	1:C:172:VAL:O	2.21	0.40
1:E:123:ALA:HA	1:E:155:MET:CE	2.50	0.40
1:E:134:ILE:HD12	1:E:159:TYR:CE1	2.56	0.40
1:F:208:ASP:O	1:F:212:LYS:HG2	2.21	0.40
1:F:249:TYR:HB2	1:F:278:ILE:HD12	2.03	0.40
1:A:4:ASP:O	1:A:8:ILE:N	2.42	0.40
1:A:344:ALA:O	1:A:347:VAL:HG12	2.22	0.40
1:C:261:ALA:O	1:C:264:LYS:HB2	2.21	0.40
1:D:209:LEU:CA	1:D:212:LYS:HG2	2.49	0.40
1:E:178:PRO:O	1:E:180:VAL:N	2.54	0.40
1:E:247:GLY:O	1:E:248:ILE:HG23	2.22	0.40
1:F:337:ILE:CG2	1:F:342:CYS:HB2	2.45	0.40
1:A:89:MET:HB3	1:A:89:MET:HE2	1.76	0.40
1:A:131:TYR:CE2	1:E:164:ARG:HD3	2.56	0.40
1:A:209:LEU:C	1:A:212:LYS:CG	2.89	0.40
1:A:213:THR:C	1:A:288:VAL:CG2	2.90	0.40
1:A:277:ASN:O	1:A:278:ILE:HG22	2.21	0.40
1:B:192:ARG:HG2	1:B:372:LEU:CD2	2.52	0.40
1:B:273:PRO:C	1:B:275:ALA:N	2.71	0.40
1:C:3:GLN:O	1:C:4:ASP:C	2.60	0.40
1:C:17:ALA:HB2	1:C:27:LEU:HD21	2.02	0.40
1:D:131:TYR:HE1	1:D:159:TYR:CE1	2.39	0.40
1:D:240:ALA:HB1	1:D:283:LEU:CD1	2.52	0.40
1:D:367:GLU:O	1:D:371:LYS:HG3	2.22	0.40
1:E:66:PRO:HD2	1:E:99:PRO:O	2.22	0.40
1:E:176:LYS:CE	1:E:357:ASN:HD21	2.34	0.40
1:E:191:ALA:HB3	1:E:225:TYR:HB3	2.03	0.40
1:F:22:ILE:C	1:F:23:SER:O	2.59	0.40
1:F:29:PHE:CB	1:F:410:MET:CE	3.00	0.40
1:F:149:PRO:HA	1:F:175:GLY:O	2.22	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	414/418 (99%)	355 (86%)	48 (12%)	11 (3%)	5	7
1	B	414/418 (99%)	370 (89%)	39 (9%)	5 (1%)	13	24
1	C	414/418 (99%)	355 (86%)	53 (13%)	6 (1%)	11	20
1	D	414/418 (99%)	356 (86%)	49 (12%)	9 (2%)	6	10
1	E	414/418 (99%)	366 (88%)	38 (9%)	10 (2%)	6	9
1	F	414/418 (99%)	359 (87%)	45 (11%)	10 (2%)	6	9
All	All	2484/2508 (99%)	2161 (87%)	272 (11%)	51 (2%)	7	11

All (51) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	ASP
1	B	4	ASP
1	C	4	ASP
1	D	4	ASP
1	D	305	ALA
1	E	18	GLN
1	E	112	LYS
1	E	340	PHE
1	F	4	ASP
1	F	23	SER
1	F	30	LEU
1	A	244	THR
1	A	298	GLU
1	A	340	PHE
1	B	18	GLN
1	C	236	MET
1	D	23	SER
1	D	185	ALA
1	D	206	GLY
1	D	262	TRP

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Mol	Chain	Res	Type
1	E	180	VAL
1	E	244	THR
1	E	339	ASP
1	F	388	LYS
1	A	256	ALA
1	A	339	ASP
1	C	271	ASP
1	E	113	GLU
1	F	7	GLU
1	F	389	GLU
1	B	274	GLY
1	C	241	VAL
1	D	242	SER
1	D	263	LYS
1	E	4	ASP
1	F	402	ALA
1	A	262	TRP
1	A	271	ASP
1	B	168	PRO
1	D	180	VAL
1	E	169	SER
1	F	338	PRO
1	A	206	GLY
1	A	227	ALA
1	A	305	ALA
1	C	189	ALA
1	E	111	PRO
1	F	184	VAL
1	F	303	LYS
1	B	180	VAL
1	C	145	VAL

### 5.3.2 Protein sidechains [i](#)

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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	342/344 (99%)	284 (83%)	58 (17%)	2	3
1	B	342/344 (99%)	296 (86%)	46 (14%)	4	7
1	C	342/344 (99%)	277 (81%)	65 (19%)	1	2
1	D	342/344 (99%)	279 (82%)	63 (18%)	1	2
1	E	342/344 (99%)	299 (87%)	43 (13%)	4	8
1	F	342/344 (99%)	292 (85%)	50 (15%)	3	5
All	All	2052/2064 (99%)	1727 (84%)	325 (16%)	2	4

All (325) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	LYS
1	A	15	ARG
1	A	21	ASP
1	A	22	ILE
1	A	27	LEU
1	A	47	ASP
1	A	56	PHE
1	A	72	ARG
1	A	76	GLU
1	A	80	SER
1	A	88	TRP
1	A	96	MET
1	A	112	LYS
1	A	113	GLU
1	A	135	SER
1	A	144	ASP
1	A	163	SER
1	A	180	VAL
1	A	183	ILE
1	A	186	ARG
1	A	195	SER
1	A	205	LEU
1	A	207	MET
1	A	219	TYR
1	A	242	SER
1	A	244	THR
1	A	248	ILE

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Mol	Chain	Res	Type
1	A	270	LYS
1	A	278	ILE
1	A	279	THR
1	A	285	GLU
1	A	286	LEU
1	A	287	GLU
1	A	288	VAL
1	A	291	LEU
1	A	294	SER
1	A	297	GLU
1	A	298	GLU
1	A	306	ASP
1	A	309	LYS
1	A	311	LYS
1	A	326	ASP
1	A	327	GLU
1	A	329	LEU
1	A	332	LYS
1	A	336	ILE
1	A	350	SER
1	A	366	GLU
1	A	367	GLU
1	A	369	ARG
1	A	387	HIS
1	A	389	GLU
1	A	391	ASN
1	A	393	ASN
1	A	404	SER
1	A	411	LYS
1	A	417	LYS
1	A	418	LYS
1	B	4	ASP
1	B	12	GLN
1	B	18	GLN
1	B	21	ASP
1	B	22	ILE
1	B	27	LEU
1	B	28	GLU
1	B	32	ARG
1	B	40	SER
1	B	56	PHE
1	B	68	LYS

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Mol	Chain	Res	Type
1	B	76	GLU
1	B	80	SER
1	B	88	TRP
1	B	93	THR
1	B	117	ARG
1	B	132	ASP
1	B	135	SER
1	B	151	ILE
1	B	186	ARG
1	B	192	ARG
1	B	205	LEU
1	B	242	SER
1	B	243	ASP
1	B	244	THR
1	B	254	LEU
1	B	270	LYS
1	B	273	PRO
1	B	278	ILE
1	B	287	GLU
1	B	294	SER
1	B	296	ILE
1	B	300	ILE
1	B	302	LYS
1	B	306	ASP
1	B	309	LYS
1	B	363	TRP
1	B	366	GLU
1	B	369	ARG
1	B	371	LYS
1	B	374	LYS
1	B	383	VAL
1	B	387	HIS
1	B	395	ARG
1	B	411	LYS
1	B	417	LYS
1	C	18	GLN
1	C	21	ASP
1	C	22	ILE
1	C	23	SER
1	C	27	LEU
1	C	28	GLU
1	C	32	ARG

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Mol	Chain	Res	Type
1	C	38	GLU
1	C	56	PHE
1	C	68	LYS
1	C	71	ILE
1	C	76	GLU
1	C	80	SER
1	C	88	TRP
1	C	92	LYS
1	C	104	LYS
1	C	117	ARG
1	C	135	SER
1	C	151	ILE
1	C	163	SER
1	C	176	LYS
1	C	183	ILE
1	C	186	ARG
1	C	203	LYS
1	C	205	LEU
1	C	207	MET
1	C	212	LYS
1	C	214	ILE
1	C	226	MET
1	C	229	ILE
1	C	231	SER
1	C	232	GLU
1	C	236	MET
1	C	242	SER
1	C	244	THR
1	C	260	LEU
1	C	269	VAL
1	C	278	ILE
1	C	281	GLU
1	C	283	LEU
1	C	288	VAL
1	C	289	ASP
1	C	296	ILE
1	C	302	LYS
1	C	303	LYS
1	C	306	ASP
1	C	308	ILE
1	C	311	LYS
1	C	312	ILE

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Mol	Chain	Res	Type
1	C	322	THR
1	C	326	ASP
1	C	327	GLU
1	C	329	LEU
1	C	332	LYS
1	C	337	ILE
1	C	340	PHE
1	C	350	SER
1	C	363	TRP
1	C	369	ARG
1	C	387	HIS
1	C	393	ASN
1	C	399	TYR
1	C	404	SER
1	C	411	LYS
1	C	417	LYS
1	D	15	ARG
1	D	18	GLN
1	D	20	MET
1	D	22	ILE
1	D	23	SER
1	D	24	GLU
1	D	27	LEU
1	D	28	GLU
1	D	32	ARG
1	D	40	SER
1	D	68	LYS
1	D	88	TRP
1	D	89	MET
1	D	117	ARG
1	D	120	GLU
1	D	135	SER
1	D	162	ILE
1	D	163	SER
1	D	176	LYS
1	D	183	ILE
1	D	184	VAL
1	D	205	LEU
1	D	207	MET
1	D	208	ASP
1	D	210	LYS
1	D	212	LYS

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Mol	Chain	Res	Type
1	D	213	THR
1	D	214	ILE
1	D	217	GLN
1	D	221	ASN
1	D	230	MET
1	D	242	SER
1	D	243	ASP
1	D	248	ILE
1	D	260	LEU
1	D	278	ILE
1	D	282	GLU
1	D	287	GLU
1	D	289	ASP
1	D	298	GLU
1	D	304	ASN
1	D	308	ILE
1	D	309	LYS
1	D	311	LYS
1	D	316	LEU
1	D	324	GLU
1	D	327	GLU
1	D	329	LEU
1	D	332	LYS
1	D	336	ILE
1	D	340	PHE
1	D	363	TRP
1	D	365	VAL
1	D	369	ARG
1	D	387	HIS
1	D	389	GLU
1	D	391	ASN
1	D	392	ILE
1	D	395	ARG
1	D	404	SER
1	D	411	LYS
1	D	417	LYS
1	D	418	LYS
1	E	12	GLN
1	E	15	ARG
1	E	18	GLN
1	E	21	ASP
1	E	22	ILE

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Mol	Chain	Res	Type
1	E	27	LEU
1	E	32	ARG
1	E	38	GLU
1	E	51	LYS
1	E	56	PHE
1	E	68	LYS
1	E	79	LEU
1	E	88	TRP
1	E	89	MET
1	E	113	GLU
1	E	117	ARG
1	E	135	SER
1	E	144	ASP
1	E	163	SER
1	E	187	MET
1	E	205	LEU
1	E	207	MET
1	E	244	THR
1	E	270	LYS
1	E	278	ILE
1	E	284	LEU
1	E	287	GLU
1	E	306	ASP
1	E	309	LYS
1	E	311	LYS
1	E	332	LYS
1	E	335	LEU
1	E	336	ILE
1	E	339	ASP
1	E	365	VAL
1	E	375	LYS
1	E	387	HIS
1	E	392	ILE
1	E	395	ARG
1	E	400	VAL
1	E	408	GLN
1	E	417	LYS
1	E	418	LYS
1	F	15	ARG
1	F	22	ILE
1	F	28	GLU
1	F	32	ARG

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Mol	Chain	Res	Type
1	F	51	LYS
1	F	53	PHE
1	F	68	LYS
1	F	71	ILE
1	F	80	SER
1	F	88	TRP
1	F	95	VAL
1	F	117	ARG
1	F	132	ASP
1	F	135	SER
1	F	144	ASP
1	F	145	VAL
1	F	148	ASN
1	F	186	ARG
1	F	192	ARG
1	F	207	MET
1	F	214	ILE
1	F	232	GLU
1	F	237	LYS
1	F	241	VAL
1	F	242	SER
1	F	244	THR
1	F	268	SER
1	F	278	ILE
1	F	279	THR
1	F	281	GLU
1	F	287	GLU
1	F	288	VAL
1	F	296	ILE
1	F	297	GLU
1	F	298	GLU
1	F	306	ASP
1	F	309	LYS
1	F	311	LYS
1	F	312	ILE
1	F	324	GLU
1	F	328	ILE
1	F	350	SER
1	F	363	TRP
1	F	369	ARG
1	F	375	LYS
1	F	387	HIS

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Mol	Chain	Res	Type
1	F	393	ASN
1	F	404	SER
1	F	410	MET
1	F	411	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	12	GLN
1	A	18	GLN
1	A	150	GLN
1	A	277	ASN
1	A	280	ASN
1	A	307	ASN
1	A	385	ASN
1	A	387	HIS
1	A	391	ASN
1	B	3	GLN
1	B	12	GLN
1	B	150	GLN
1	B	217	GLN
1	B	280	ASN
1	B	357	ASN
1	B	385	ASN
1	B	387	HIS
1	B	408	GLN
1	C	3	GLN
1	C	217	GLN
1	C	277	ASN
1	C	280	ASN
1	C	307	ASN
1	C	387	HIS
1	C	393	ASN
1	D	3	GLN
1	D	280	ASN
1	D	385	ASN
1	E	3	GLN
1	E	150	GLN
1	E	277	ASN
1	E	357	ASN
1	E	385	ASN

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Mol	Chain	Res	Type
1	E	387	HIS
1	E	408	GLN
1	F	3	GLN
1	F	217	GLN
1	F	280	ASN
1	F	393	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

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

There are no ligands in this entry.

### 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.