



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:43 PM GMT

PDB ID : 1GRL  
Title : THE CRYSTAL STRUCTURE OF THE BACTERIAL CHAPERONIN  
GROEL AT 2.8 ANGSTROMS  
Authors : Braig, K.; Otwinowski, Z.; Hegde, R.; Boisvert, D.C.; Joachimiak, A.; Horwich,  
A.L.; Sigler, P.B.  
Deposited on : 1995-03-07  
Resolution : 2.80 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

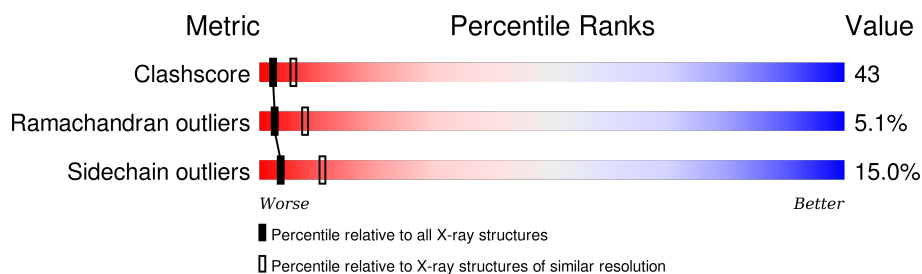
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)

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	548	
1	B	548	
1	C	548	
1	D	548	
1	E	548	
1	F	548	
1	G	548	

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 29274 atoms, of which 5278 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 GROEL (HSP60 CLASS).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	518	Total	C	H	N	O	S	0	0	59
			4182	2149	754	581	681	17			
1	B	518	Total	C	H	N	O	S	0	0	59
			4182	2149	754	581	681	17			
1	C	518	Total	C	H	N	O	S	0	0	59
			4182	2149	754	581	681	17			
1	D	518	Total	C	H	N	O	S	0	0	59
			4182	2149	754	581	681	17			
1	E	518	Total	C	H	N	O	S	0	0	59
			4182	2149	754	581	681	17			
1	F	518	Total	C	H	N	O	S	0	0	59
			4182	2149	754	581	681	17			
1	G	518	Total	C	H	N	O	S	0	0	59
			4182	2149	754	581	681	17			

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	13	GLY	ARG	CONFLICT	UNP P06139
A	126	VAL	ALA	CONFLICT	UNP P06139
A	267	MET	ILE	CONFLICT	UNP P06139
B	13	GLY	ARG	CONFLICT	UNP P06139
B	126	VAL	ALA	CONFLICT	UNP P06139
B	267	MET	ILE	CONFLICT	UNP P06139
C	13	GLY	ARG	CONFLICT	UNP P06139
C	126	VAL	ALA	CONFLICT	UNP P06139
C	267	MET	ILE	CONFLICT	UNP P06139
D	13	GLY	ARG	CONFLICT	UNP P06139
D	126	VAL	ALA	CONFLICT	UNP P06139
D	267	MET	ILE	CONFLICT	UNP P06139
E	13	GLY	ARG	CONFLICT	UNP P06139
E	126	VAL	ALA	CONFLICT	UNP P06139
E	267	MET	ILE	CONFLICT	UNP P06139

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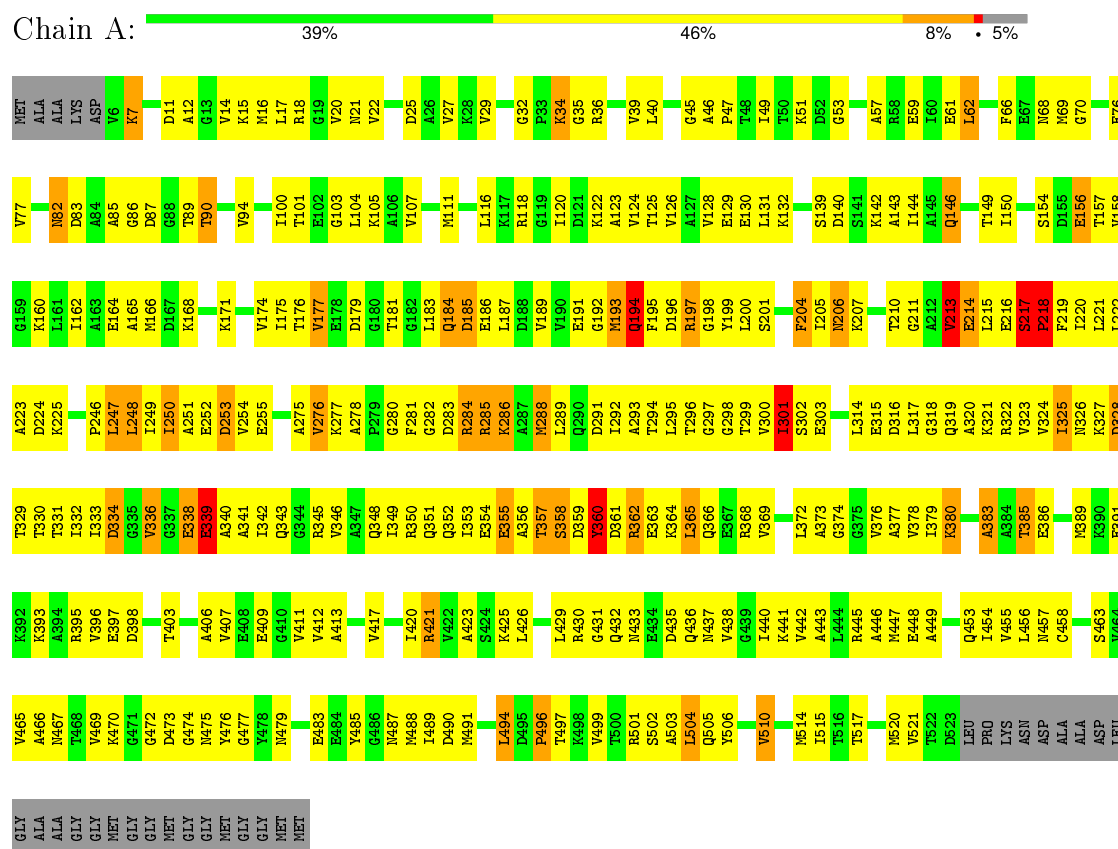
Chain	Residue	Modelled	Actual	Comment	Reference
F	13	GLY	ARG	CONFLICT	UNP P06139
F	126	VAL	ALA	CONFLICT	UNP P06139
F	267	MET	ILE	CONFLICT	UNP P06139
G	13	GLY	ARG	CONFLICT	UNP P06139
G	126	VAL	ALA	CONFLICT	UNP P06139
G	267	MET	ILE	CONFLICT	UNP P06139

### 3 Residue-property plots

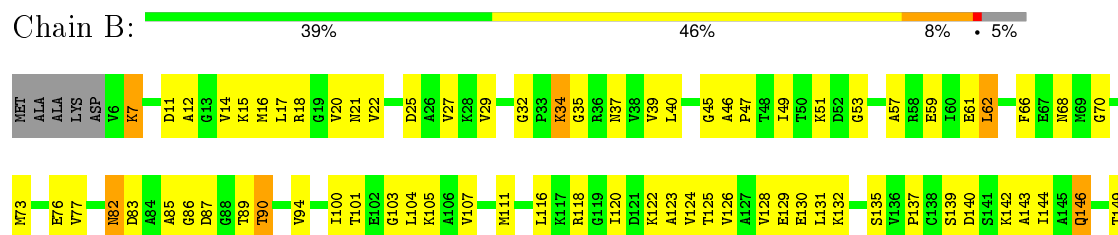
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

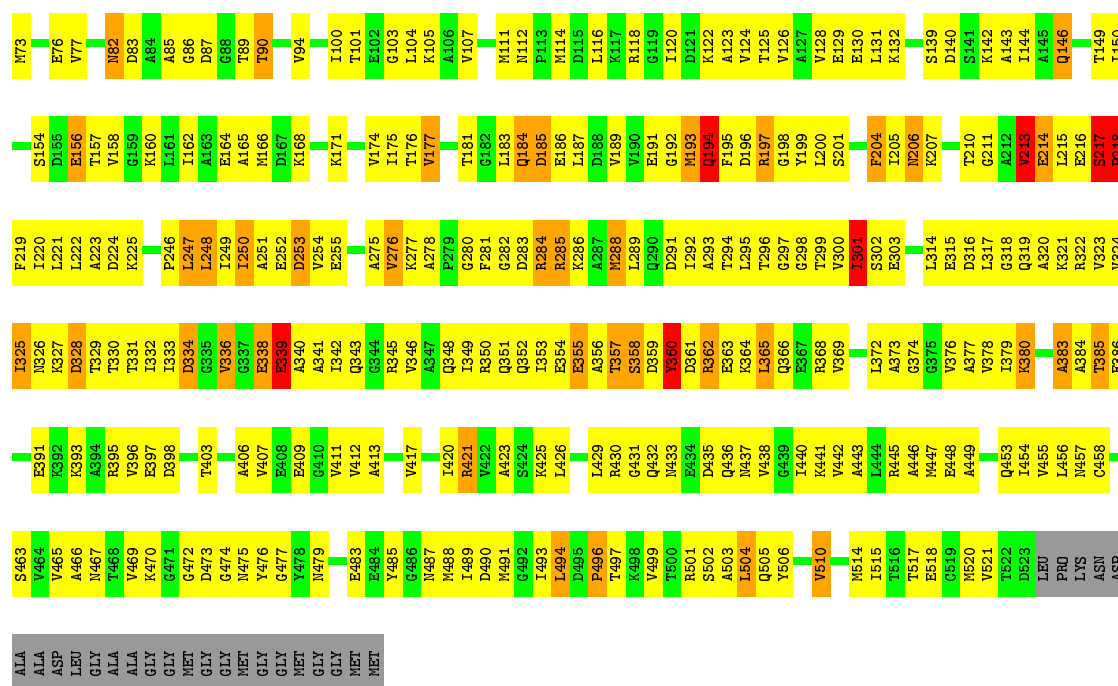
#### • Molecule 1: GROEL (HSP60 CLASS)



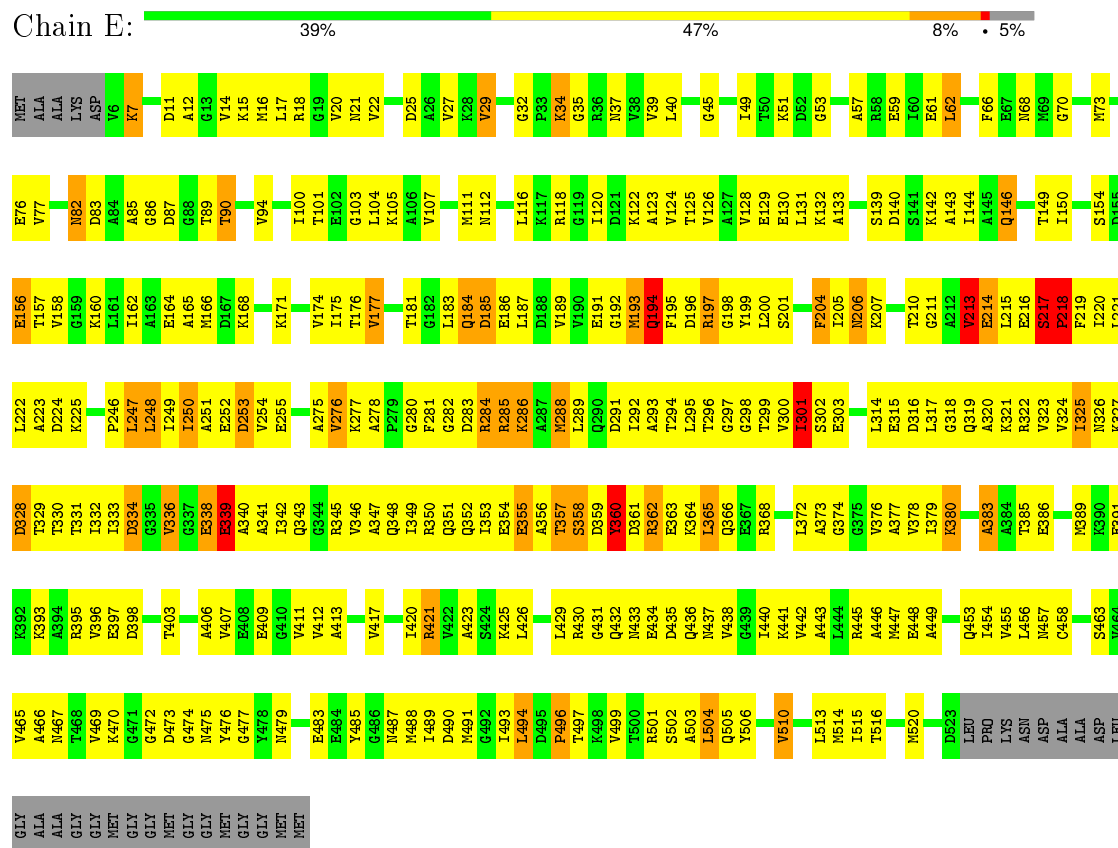
#### • Molecule 1: GROEL (HSP60 CLASS)





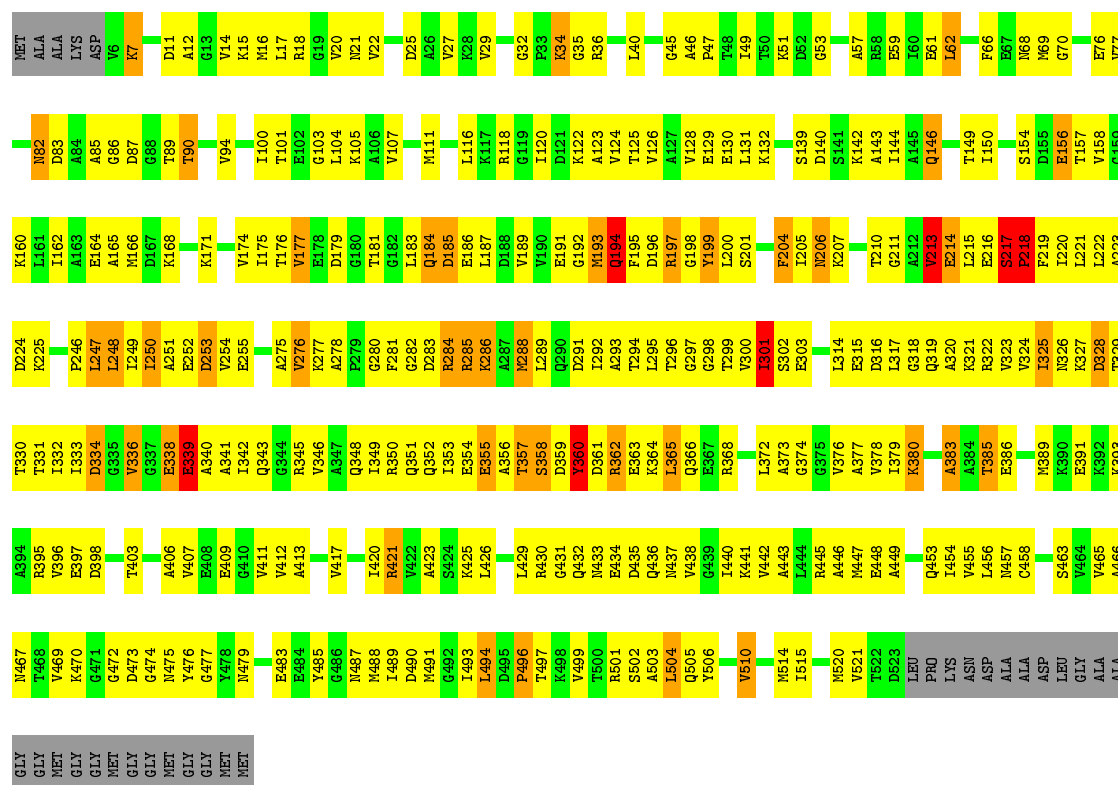


### • Molecule 1: GROEL (HSP60 CLASS)



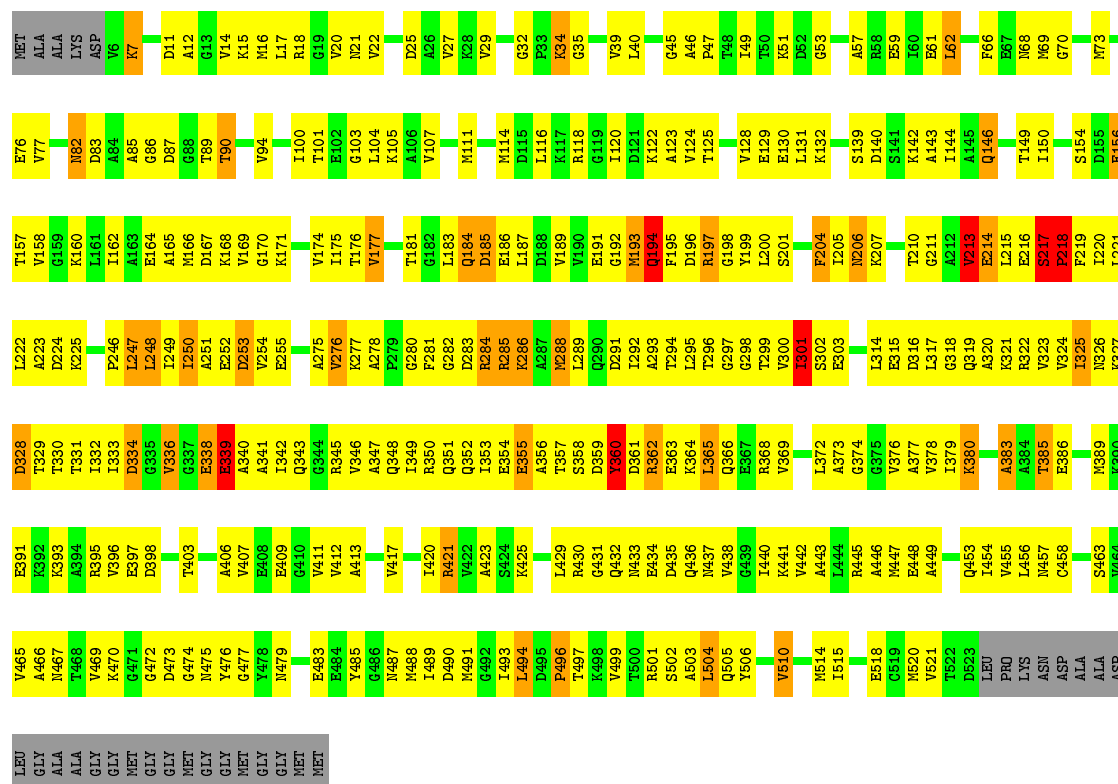
### • Molecule 1: GROEL (HSP60 CLASS)

Chain F: 39% 46% 8% 5%



• Molecule 1: GROEL (HSP60 CLASS)

Chain G: 39% 47% 7% 5%



## 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, $\alpha$ , $\beta$ , $\gamma$	178.00 Å   203.00 Å   278.00 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	8.00 – 2.80	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-2.80)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.326 , 0.368	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	29274	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	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	0.62	0/3389	0.84	2/4571 (0.0%)
1	B	0.62	0/3389	0.84	2/4571 (0.0%)
1	C	0.62	0/3389	0.84	2/4571 (0.0%)
1	D	0.62	0/3389	0.84	2/4571 (0.0%)
1	E	0.62	0/3389	0.84	2/4571 (0.0%)
1	F	0.62	0/3389	0.84	2/4571 (0.0%)
1	G	0.62	0/3389	0.84	2/4571 (0.0%)
All	All	0.62	0/23723	0.84	14/31997 (0.0%)

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	F	360	TYR	N-CA-C	6.51	128.57	111.00
1	B	360	TYR	N-CA-C	6.50	128.55	111.00
1	G	360	TYR	N-CA-C	6.50	128.55	111.00
1	D	360	TYR	N-CA-C	6.49	128.53	111.00
1	E	360	TYR	N-CA-C	6.49	128.52	111.00
1	A	360	TYR	N-CA-C	6.49	128.52	111.00
1	C	360	TYR	N-CA-C	6.49	128.51	111.00
1	E	131	LEU	CA-CB-CG	5.17	127.18	115.30
1	B	131	LEU	CA-CB-CG	5.16	127.18	115.30
1	C	131	LEU	CA-CB-CG	5.15	127.14	115.30
1	A	131	LEU	CA-CB-CG	5.15	127.14	115.30
1	D	131	LEU	CA-CB-CG	5.14	127.13	115.30
1	G	131	LEU	CA-CB-CG	5.14	127.12	115.30
1	F	131	LEU	CA-CB-CG	5.13	127.10	115.30

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	3428	754	3441	314	1
1	B	3428	754	3441	324	9
1	C	3428	754	3440	334	54
1	D	3428	754	3441	323	0
1	E	3428	754	3441	323	18
1	F	3428	754	3440	324	1
1	G	3428	754	3441	315	55
All	All	23996	5278	24085	2090	75

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 43.

All (2090) 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:181:THR:O	1:G:282:GLY:CA	1.65	1.39
1:D:282:GLY:CA	1:E:181:THR:O	1.69	1.37
1:F:282:GLY:CA	1:G:181:THR:O	1.72	1.36
1:A:282:GLY:HA3	1:B:181:THR:O	1.28	1.30
1:A:386:GLU:OE2	1:G:285:ARG:NH2	1.71	1.23
1:A:181:THR:O	1:G:282:GLY:HA3	1.08	1.23
1:C:281:PHE:HE2	1:D:385:THR:C	1.41	1.22
1:C:281:PHE:CE2	1:D:385:THR:C	2.18	1.16
1:A:282:GLY:CA	1:B:181:THR:O	1.97	1.12
1:F:282:GLY:HA3	1:G:181:THR:O	1.34	1.12
1:F:282:GLY:HA2	1:G:181:THR:O	1.47	1.08
1:A:285:ARG:NH2	1:B:386:GLU:OE2	1.87	1.06
1:F:281:PHE:HE2	1:G:385:THR:C	1.61	1.04
1:B:285:ARG:NH2	1:C:386:GLU:OE2	1.90	1.04
1:D:282:GLY:HA3	1:E:181:THR:O	0.86	1.03
1:C:214:GLU:HG2	1:C:324:VAL:HG13	1.41	1.03
1:B:214:GLU:HG2	1:B:324:VAL:HG13	1.41	1.03
1:G:214:GLU:HG2	1:G:324:VAL:HG13	1.41	1.02
1:D:214:GLU:HG2	1:D:324:VAL:HG13	1.41	1.02
1:A:214:GLU:HG2	1:A:324:VAL:HG13	1.41	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:214:GLU:HG2	1:E:324:VAL:HG13	1.41	1.02
1:F:214:GLU:HG2	1:F:324:VAL:HG13	1.41	1.02
1:C:281:PHE:HE2	1:D:385:THR:CA	1.75	0.99
1:A:181:THR:O	1:G:282:GLY:HA2	1.62	0.99
1:E:285:ARG:NH2	1:F:386:GLU:OE2	1.95	0.99
1:B:281:PHE:CZ	1:C:389:MET:HB2	1.97	0.98
1:C:281:PHE:CE2	1:D:384:ALA:O	2.18	0.97
1:B:281:PHE:CD2	1:C:386:GLU:HA	1.99	0.96
1:C:281:PHE:CE2	1:D:386:GLU:N	2.36	0.94
1:F:302:SER:C	1:F:303:GLU:CA	2.36	0.93
1:E:360:TYR:CE1	1:F:183:LEU:HD22	2.02	0.93
1:G:302:SER:C	1:G:303:GLU:CA	2.36	0.93
1:E:302:SER:C	1:E:303:GLU:CA	2.36	0.93
1:B:360:TYR:CE1	1:C:183:LEU:HD22	2.03	0.93
1:A:302:SER:C	1:A:303:GLU:CA	2.36	0.93
1:D:288:MET:HG3	1:D:368:ARG:HD2	1.50	0.93
1:B:302:SER:C	1:B:303:GLU:CA	2.36	0.93
1:C:302:SER:C	1:C:303:GLU:CA	2.36	0.93
1:D:302:SER:C	1:D:303:GLU:CA	2.36	0.93
1:A:288:MET:HG3	1:A:368:ARG:HD2	1.50	0.92
1:B:360:TYR:OH	1:C:183:LEU:HD13	1.68	0.92
1:B:288:MET:HG3	1:B:368:ARG:HD2	1.50	0.92
1:B:281:PHE:HA	1:B:285:ARG:HG2	1.52	0.92
1:E:360:TYR:OH	1:F:183:LEU:HD13	1.69	0.92
1:E:288:MET:HG3	1:E:368:ARG:HD2	1.50	0.92
1:C:281:PHE:HA	1:C:285:ARG:HG2	1.52	0.92
1:C:82:ASN:HD21	1:C:89:THR:H	1.16	0.92
1:G:288:MET:HG3	1:G:368:ARG:HD2	1.50	0.92
1:C:288:MET:HG3	1:C:368:ARG:HD2	1.50	0.92
1:G:82:ASN:HD21	1:G:89:THR:H	1.16	0.92
1:A:82:ASN:HD21	1:A:89:THR:H	1.16	0.92
1:A:281:PHE:HA	1:A:285:ARG:HG2	1.52	0.91
1:B:281:PHE:CE2	1:C:386:GLU:HA	2.05	0.91
1:D:82:ASN:HD21	1:D:89:THR:H	1.16	0.91
1:F:288:MET:HG3	1:F:368:ARG:HD2	1.50	0.91
1:D:281:PHE:HA	1:D:285:ARG:HG2	1.52	0.91
1:E:300:VAL:HG21	1:E:317:LEU:HD23	1.52	0.90
1:G:281:PHE:HA	1:G:285:ARG:HG2	1.52	0.90
1:F:300:VAL:HG21	1:F:317:LEU:HD23	1.51	0.90
1:E:281:PHE:HA	1:E:285:ARG:HG2	1.52	0.90
1:E:281:PHE:CE2	1:F:386:GLU:HA	2.06	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:300:VAL:HG21	1:A:317:LEU:HD23	1.51	0.90
1:E:281:PHE:CZ	1:F:389:MET:HB2	2.07	0.89
1:G:300:VAL:HG21	1:G:317:LEU:HD23	1.52	0.89
1:B:300:VAL:HG21	1:B:317:LEU:HD23	1.51	0.89
1:D:300:VAL:HG21	1:D:317:LEU:HD23	1.52	0.89
1:E:281:PHE:CD2	1:F:386:GLU:HA	2.07	0.89
1:F:281:PHE:HA	1:F:285:ARG:HG2	1.52	0.89
1:C:281:PHE:CZ	1:D:384:ALA:O	2.26	0.89
1:C:300:VAL:HG21	1:C:317:LEU:HD23	1.51	0.89
1:B:82:ASN:HD21	1:B:89:THR:H	1.16	0.88
1:F:82:ASN:HD21	1:F:89:THR:H	1.16	0.88
1:E:82:ASN:HD21	1:E:89:THR:H	1.16	0.88
1:D:315:GLU:O	1:D:317:LEU:HG	1.75	0.86
1:A:315:GLU:O	1:A:317:LEU:HG	1.76	0.86
1:G:315:GLU:O	1:G:317:LEU:HG	1.76	0.86
1:C:282:GLY:HA2	1:D:181:THR:O	1.75	0.86
1:F:364:LYS:HZ3	1:F:365:LEU:HD13	1.41	0.85
1:D:364:LYS:HZ3	1:D:365:LEU:HD13	1.41	0.85
1:C:315:GLU:O	1:C:317:LEU:HG	1.76	0.85
1:C:364:LYS:HZ3	1:C:365:LEU:HD13	1.42	0.85
1:B:364:LYS:HZ3	1:B:365:LEU:HD13	1.42	0.85
1:E:315:GLU:O	1:E:317:LEU:HG	1.76	0.85
1:F:315:GLU:O	1:F:317:LEU:HG	1.76	0.85
1:B:315:GLU:O	1:B:317:LEU:HG	1.76	0.85
1:C:281:PHE:CZ	1:D:384:ALA:C	2.50	0.85
1:E:364:LYS:HZ3	1:E:365:LEU:HD13	1.41	0.85
1:G:254:VAL:C	1:G:255:GLU:CA	2.46	0.85
1:G:275:ALA:CA	1:G:276:VAL:N	2.40	0.85
1:A:275:ALA:CA	1:A:276:VAL:N	2.40	0.84
1:G:210:THR:CA	1:G:211:GLY:N	2.41	0.84
1:C:275:ALA:CA	1:C:276:VAL:N	2.40	0.84
1:B:254:VAL:C	1:B:255:GLU:CA	2.46	0.84
1:E:254:VAL:C	1:E:255:GLU:CA	2.46	0.84
1:F:275:ALA:CA	1:F:276:VAL:N	2.40	0.84
1:A:210:THR:CA	1:A:211:GLY:N	2.41	0.84
1:E:210:THR:CA	1:E:211:GLY:N	2.41	0.84
1:B:275:ALA:CA	1:B:276:VAL:N	2.40	0.84
1:D:254:VAL:C	1:D:255:GLU:CA	2.46	0.84
1:C:210:THR:CA	1:C:211:GLY:N	2.41	0.84
1:F:363:GLU:HA	1:F:366:GLN:HE21	1.43	0.84
1:B:210:THR:CA	1:B:211:GLY:N	2.41	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:206:ASN:HB3	1:D:213:VAL:HA	1.59	0.84
1:C:206:ASN:HB3	1:C:213:VAL:HA	1.59	0.84
1:A:254:VAL:C	1:A:255:GLU:CA	2.46	0.84
1:A:206:ASN:HB3	1:A:213:VAL:HA	1.59	0.84
1:G:364:LYS:HZ3	1:G:365:LEU:HD13	1.41	0.84
1:E:275:ALA:CA	1:E:276:VAL:N	2.40	0.84
1:C:254:VAL:C	1:C:255:GLU:CA	2.46	0.84
1:D:275:ALA:CA	1:D:276:VAL:N	2.40	0.84
1:D:285:ARG:NH2	1:E:386:GLU:OE2	2.10	0.84
1:F:210:THR:CA	1:F:211:GLY:N	2.41	0.84
1:B:206:ASN:HB3	1:B:213:VAL:HA	1.59	0.84
1:B:363:GLU:HA	1:B:366:GLN:HE21	1.43	0.84
1:D:363:GLU:HA	1:D:366:GLN:HE21	1.43	0.84
1:F:254:VAL:C	1:F:255:GLU:CA	2.46	0.84
1:A:364:LYS:HZ3	1:A:365:LEU:HD13	1.43	0.83
1:G:363:GLU:HA	1:G:366:GLN:HE21	1.43	0.83
1:F:281:PHE:CE2	1:G:385:THR:C	2.52	0.83
1:C:421:ARG:HD2	1:C:474:GLY:O	1.79	0.83
1:E:421:ARG:HD2	1:E:474:GLY:O	1.79	0.83
1:A:363:GLU:HA	1:A:366:GLN:HE21	1.43	0.83
1:D:210:THR:CA	1:D:211:GLY:N	2.41	0.83
1:G:206:ASN:HB3	1:G:213:VAL:HA	1.59	0.83
1:E:206:ASN:HB3	1:E:213:VAL:HA	1.59	0.83
1:A:421:ARG:HD2	1:A:474:GLY:O	1.79	0.83
1:E:218:PRO:HD2	1:E:320:ALA:O	1.79	0.83
1:F:206:ASN:HB3	1:F:213:VAL:HA	1.59	0.83
1:D:218:PRO:HD2	1:D:320:ALA:O	1.79	0.83
1:F:246:PRO:CA	1:F:247:LEU:N	2.42	0.82
1:A:246:PRO:CA	1:A:247:LEU:N	2.42	0.82
1:C:246:PRO:CA	1:C:247:LEU:N	2.42	0.82
1:F:218:PRO:HD2	1:F:320:ALA:O	1.79	0.82
1:B:246:PRO:CA	1:B:247:LEU:N	2.42	0.82
1:G:218:PRO:HD2	1:G:320:ALA:O	1.79	0.82
1:G:421:ARG:HD2	1:G:474:GLY:O	1.79	0.82
1:G:246:PRO:CA	1:G:247:LEU:N	2.42	0.82
1:F:421:ARG:HD2	1:F:474:GLY:O	1.79	0.82
1:B:421:ARG:HD2	1:B:474:GLY:O	1.79	0.82
1:C:363:GLU:HA	1:C:366:GLN:HE21	1.43	0.82
1:C:218:PRO:HD2	1:C:320:ALA:O	1.79	0.82
1:E:246:PRO:CA	1:E:247:LEU:N	2.42	0.82
1:A:314:LEU:CA	1:A:315:GLU:N	2.43	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:314:LEU:CA	1:G:315:GLU:N	2.43	0.82
1:D:221:LEU:HD12	1:D:300:VAL:HG11	1.61	0.82
1:C:206:ASN:C	1:C:207:LYS:CA	2.49	0.82
1:G:224:ASP:C	1:G:225:LYS:CA	2.48	0.82
1:F:206:ASN:C	1:F:207:LYS:CA	2.49	0.81
1:A:218:PRO:HD2	1:A:320:ALA:O	1.79	0.81
1:E:224:ASP:C	1:E:225:LYS:CA	2.48	0.81
1:D:246:PRO:CA	1:D:247:LEU:N	2.42	0.81
1:E:363:GLU:HA	1:E:366:GLN:HE21	1.43	0.81
1:G:206:ASN:C	1:G:207:LYS:CA	2.49	0.81
1:C:281:PHE:CD2	1:D:386:GLU:N	2.47	0.81
1:F:314:LEU:CA	1:F:315:GLU:N	2.43	0.81
1:B:221:LEU:HD12	1:B:300:VAL:HG11	1.61	0.81
1:C:221:LEU:HD12	1:C:300:VAL:HG11	1.61	0.81
1:D:206:ASN:C	1:D:207:LYS:CA	2.49	0.81
1:D:421:ARG:HD2	1:D:474:GLY:O	1.79	0.81
1:B:314:LEU:CA	1:B:315:GLU:N	2.43	0.81
1:D:314:LEU:CA	1:D:315:GLU:N	2.43	0.81
1:B:206:ASN:C	1:B:207:LYS:CA	2.49	0.81
1:C:224:ASP:C	1:C:225:LYS:CA	2.48	0.81
1:B:224:ASP:C	1:B:225:LYS:CA	2.48	0.81
1:B:218:PRO:HD2	1:B:320:ALA:O	1.79	0.81
1:E:314:LEU:CA	1:E:315:GLU:N	2.43	0.81
1:E:206:ASN:C	1:E:207:LYS:CA	2.49	0.81
1:C:177:VAL:HG21	1:C:397:GLU:HG3	1.63	0.81
1:D:224:ASP:C	1:D:225:LYS:CA	2.48	0.81
1:B:177:VAL:HG21	1:B:397:GLU:HG3	1.63	0.81
1:E:221:LEU:HD12	1:E:300:VAL:HG11	1.61	0.81
1:F:221:LEU:HD12	1:F:300:VAL:HG11	1.61	0.81
1:A:221:LEU:HD12	1:A:300:VAL:HG11	1.61	0.81
1:G:221:LEU:HD12	1:G:300:VAL:HG11	1.61	0.81
1:C:314:LEU:CA	1:C:315:GLU:N	2.43	0.81
1:A:224:ASP:C	1:A:225:LYS:CA	2.48	0.81
1:A:206:ASN:C	1:A:207:LYS:CA	2.49	0.80
1:F:224:ASP:C	1:F:225:LYS:CA	2.48	0.80
1:E:166:MET:HG3	1:E:171:LYS:HA	1.62	0.80
1:A:177:VAL:HG21	1:A:397:GLU:HG3	1.63	0.80
1:D:177:VAL:HG21	1:D:397:GLU:HG3	1.63	0.80
1:D:166:MET:HG3	1:D:171:LYS:HA	1.62	0.80
1:D:282:GLY:HA3	1:E:181:THR:C	1.98	0.80
1:F:166:MET:HG3	1:F:171:LYS:HA	1.62	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:281:PHE:CG	1:C:389:MET:HE3	2.17	0.80
1:D:111:MET:SD	1:D:438:VAL:HG11	2.22	0.80
1:A:166:MET:HG3	1:A:171:LYS:HA	1.62	0.80
1:G:177:VAL:HG21	1:G:397:GLU:HG3	1.63	0.80
1:B:166:MET:HG3	1:B:171:LYS:HA	1.62	0.80
1:C:166:MET:HG3	1:C:171:LYS:HA	1.62	0.79
1:C:111:MET:SD	1:C:438:VAL:HG11	2.22	0.79
1:E:177:VAL:HG21	1:E:397:GLU:HG3	1.63	0.79
1:G:166:MET:HG3	1:G:171:LYS:HA	1.62	0.79
1:E:111:MET:SD	1:E:438:VAL:HG11	2.22	0.79
1:D:82:ASN:ND2	1:D:89:THR:H	1.80	0.79
1:E:82:ASN:ND2	1:E:89:THR:H	1.80	0.79
1:B:111:MET:SD	1:B:438:VAL:HG11	2.22	0.79
1:B:281:PHE:CE2	1:C:389:MET:HB2	2.18	0.79
1:G:111:MET:SD	1:G:438:VAL:HG11	2.22	0.79
1:A:111:MET:SD	1:A:438:VAL:HG11	2.22	0.79
1:F:177:VAL:HG21	1:F:397:GLU:HG3	1.63	0.79
1:A:82:ASN:ND2	1:A:89:THR:H	1.80	0.79
1:D:363:GLU:HA	1:D:366:GLN:NE2	1.97	0.79
1:F:111:MET:SD	1:F:438:VAL:HG11	2.22	0.79
1:G:82:ASN:ND2	1:G:89:THR:H	1.80	0.79
1:F:82:ASN:ND2	1:F:89:THR:H	1.80	0.79
1:B:363:GLU:HA	1:B:366:GLN:NE2	1.97	0.78
1:C:82:ASN:ND2	1:C:89:THR:H	1.80	0.78
1:A:363:GLU:HA	1:A:366:GLN:NE2	1.97	0.78
1:B:82:ASN:ND2	1:B:89:THR:H	1.80	0.78
1:G:363:GLU:HA	1:G:366:GLN:NE2	1.97	0.78
1:C:363:GLU:HA	1:C:366:GLN:NE2	1.97	0.78
1:C:128:VAL:O	1:C:132:LYS:HG2	1.84	0.78
1:E:294:THR:HG21	1:E:345:ARG:HD2	1.66	0.78
1:F:194:GLN:NE2	1:F:331:THR:HG22	1.99	0.78
1:A:294:THR:HG21	1:A:345:ARG:HD2	1.66	0.78
1:B:294:THR:HG21	1:B:345:ARG:HD2	1.66	0.78
1:E:363:GLU:HA	1:E:366:GLN:NE2	1.97	0.78
1:G:128:VAL:O	1:G:132:LYS:HG2	1.84	0.78
1:F:363:GLU:HA	1:F:366:GLN:NE2	1.97	0.78
1:C:194:GLN:NE2	1:C:331:THR:HG22	1.99	0.78
1:F:294:THR:HG21	1:F:345:ARG:HD2	1.66	0.78
1:F:27:VAL:HG12	1:F:90:THR:HG23	1.66	0.78
1:D:294:THR:HG21	1:D:345:ARG:HD2	1.66	0.78
1:A:385:THR:C	1:G:281:PHE:HE2	1.87	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:194:GLN:NE2	1:B:331:THR:HG22	1.99	0.78
1:G:194:GLN:NE2	1:G:331:THR:HG22	1.99	0.78
1:G:294:THR:HG21	1:G:345:ARG:HD2	1.66	0.78
1:G:174:VAL:HG13	1:G:376:VAL:HA	1.65	0.78
1:E:466:ALA:O	1:E:470:LYS:HB2	1.84	0.77
1:D:128:VAL:O	1:D:132:LYS:HG2	1.84	0.77
1:A:174:VAL:HG13	1:A:376:VAL:HA	1.65	0.77
1:A:194:GLN:NE2	1:A:331:THR:HG22	1.99	0.77
1:E:194:GLN:NE2	1:E:331:THR:HG22	1.99	0.77
1:G:27:VAL:HG12	1:G:90:THR:HG23	1.66	0.77
1:C:294:THR:HG21	1:C:345:ARG:HD2	1.66	0.77
1:F:466:ALA:O	1:F:470:LYS:HB2	1.84	0.77
1:F:174:VAL:HG13	1:F:376:VAL:HA	1.65	0.77
1:F:128:VAL:O	1:F:132:LYS:HG2	1.84	0.77
1:D:466:ALA:O	1:D:470:LYS:HB2	1.84	0.77
1:B:128:VAL:O	1:B:132:LYS:HG2	1.84	0.77
1:E:27:VAL:HG12	1:E:90:THR:HG23	1.66	0.77
1:C:27:VAL:HG12	1:C:90:THR:HG23	1.66	0.77
1:D:194:GLN:NE2	1:D:331:THR:HG22	1.99	0.77
1:C:466:ALA:O	1:C:470:LYS:HB2	1.84	0.77
1:A:27:VAL:HG12	1:A:90:THR:HG23	1.66	0.77
1:D:27:VAL:HG12	1:D:90:THR:HG23	1.66	0.77
1:B:174:VAL:HG13	1:B:376:VAL:HA	1.65	0.77
1:C:411:VAL:HG21	1:C:494:LEU:HG	1.68	0.76
1:D:411:VAL:HG21	1:D:494:LEU:HG	1.68	0.76
1:E:128:VAL:O	1:E:132:LYS:HG2	1.84	0.76
1:A:128:VAL:O	1:A:132:LYS:HG2	1.84	0.76
1:G:466:ALA:O	1:G:470:LYS:HB2	1.84	0.76
1:F:411:VAL:HG21	1:F:494:LEU:HG	1.68	0.76
1:B:27:VAL:HG12	1:B:90:THR:HG23	1.66	0.76
1:D:174:VAL:HG13	1:D:376:VAL:HA	1.65	0.76
1:B:411:VAL:HG21	1:B:494:LEU:HG	1.68	0.76
1:E:411:VAL:HG21	1:E:494:LEU:HG	1.68	0.76
1:A:411:VAL:HG21	1:A:494:LEU:HG	1.68	0.76
1:C:438:VAL:O	1:C:442:VAL:HG23	1.86	0.76
1:B:438:VAL:O	1:B:442:VAL:HG23	1.86	0.76
1:D:73:MET:HG2	1:E:49:ILE:HD11	1.66	0.76
1:C:69:MET:CE	1:D:39:VAL:HG12	2.15	0.76
1:G:411:VAL:HG21	1:G:494:LEU:HG	1.68	0.76
1:C:174:VAL:HG13	1:C:376:VAL:HA	1.65	0.76
1:B:466:ALA:O	1:B:470:LYS:HB2	1.84	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:174:VAL:HG13	1:E:376:VAL:HA	1.65	0.76
1:A:438:VAL:O	1:A:442:VAL:HG23	1.86	0.76
1:C:281:PHE:CE2	1:D:384:ALA:C	2.59	0.76
1:D:438:VAL:O	1:D:442:VAL:HG23	1.86	0.76
1:B:281:PHE:CE2	1:C:389:MET:CB	2.69	0.75
1:G:438:VAL:O	1:G:442:VAL:HG23	1.86	0.75
1:B:281:PHE:CZ	1:C:389:MET:CB	2.68	0.75
1:A:466:ALA:O	1:A:470:LYS:HB2	1.84	0.75
1:F:295:LEU:HD23	1:F:372:LEU:HD23	1.69	0.75
1:C:220:ILE:HA	1:C:248:LEU:HB3	1.69	0.75
1:E:295:LEU:HD23	1:E:372:LEU:HD23	1.69	0.75
1:B:285:ARG:CZ	1:C:386:GLU:OE2	2.34	0.75
1:B:220:ILE:HA	1:B:248:LEU:HB3	1.69	0.75
1:F:438:VAL:O	1:F:442:VAL:HG23	1.86	0.75
1:E:438:VAL:O	1:E:442:VAL:HG23	1.86	0.74
1:G:295:LEU:HD23	1:G:372:LEU:HD23	1.69	0.74
1:C:295:LEU:HD23	1:C:372:LEU:HD23	1.69	0.74
1:D:112:ASN:ND2	1:E:458:CYS:O	2.19	0.74
1:B:295:LEU:HD23	1:B:372:LEU:HD23	1.69	0.74
1:D:295:LEU:HD23	1:D:372:LEU:HD23	1.69	0.74
1:B:292:ILE:O	1:B:296:THR:HG22	1.88	0.74
1:E:292:ILE:O	1:E:296:THR:HG22	1.88	0.74
1:C:292:ILE:O	1:C:296:THR:HG22	1.88	0.74
1:F:292:ILE:O	1:F:296:THR:HG22	1.88	0.74
1:F:220:ILE:HA	1:F:248:LEU:HB3	1.69	0.74
1:D:220:ILE:HA	1:D:248:LEU:HB3	1.69	0.74
1:F:340:ALA:HA	1:F:343:GLN:HG3	1.68	0.74
1:G:340:ALA:HA	1:G:343:GLN:HG3	1.69	0.74
1:D:292:ILE:O	1:D:296:THR:HG22	1.88	0.74
1:G:292:ILE:O	1:G:296:THR:HG22	1.88	0.74
1:A:292:ILE:O	1:A:296:THR:HG22	1.88	0.74
1:C:340:ALA:HA	1:C:343:GLN:HG3	1.69	0.74
1:D:501:ARG:HH11	1:D:505:GLN:HE22	1.35	0.73
1:B:501:ARG:HH11	1:B:505:GLN:HE22	1.35	0.73
1:E:501:ARG:HH11	1:E:505:GLN:HE22	1.36	0.73
1:A:295:LEU:HD23	1:A:372:LEU:HD23	1.69	0.73
1:C:281:PHE:CE2	1:D:385:THR:CA	2.66	0.73
1:G:220:ILE:HA	1:G:248:LEU:HB3	1.69	0.73
1:C:501:ARG:HH11	1:C:505:GLN:HE22	1.36	0.73
1:F:501:ARG:HH11	1:F:505:GLN:HE22	1.35	0.73
1:D:340:ALA:HA	1:D:343:GLN:HG3	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:340:ALA:HA	1:E:343:GLN:HG3	1.69	0.73
1:G:501:ARG:HH11	1:G:505:GLN:HE22	1.35	0.73
1:B:340:ALA:HA	1:B:343:GLN:HG3	1.69	0.73
1:A:220:ILE:HA	1:A:248:LEU:HB3	1.69	0.73
1:A:501:ARG:HH11	1:A:505:GLN:HE22	1.36	0.73
1:D:197:ARG:HH11	1:D:197:ARG:HG2	1.54	0.73
1:A:197:ARG:HG2	1:A:197:ARG:HH11	1.54	0.73
1:A:340:ALA:HA	1:A:343:GLN:HG3	1.69	0.73
1:E:197:ARG:HG2	1:E:197:ARG:HH11	1.54	0.73
1:A:363:GLU:O	1:A:366:GLN:HG2	1.88	0.73
1:B:363:GLU:O	1:B:366:GLN:HG2	1.88	0.73
1:F:281:PHE:CE2	1:G:386:GLU:N	2.57	0.73
1:E:220:ILE:HA	1:E:248:LEU:HB3	1.69	0.73
1:G:363:GLU:O	1:G:366:GLN:HG2	1.88	0.72
1:C:363:GLU:O	1:C:366:GLN:HG2	1.88	0.72
1:G:197:ARG:HG2	1:G:197:ARG:HH11	1.54	0.72
1:B:197:ARG:HG2	1:B:197:ARG:HH11	1.54	0.72
1:D:363:GLU:O	1:D:366:GLN:HG2	1.88	0.72
1:F:363:GLU:O	1:F:366:GLN:HG2	1.88	0.72
1:E:363:GLU:O	1:E:366:GLN:HG2	1.88	0.72
1:A:411:VAL:CG2	1:A:494:LEU:HG	2.20	0.72
1:C:282:GLY:CA	1:D:181:THR:O	2.38	0.72
1:F:192:GLY:HA3	1:F:376:VAL:HG23	1.72	0.72
1:E:192:GLY:HA3	1:E:376:VAL:HG23	1.72	0.72
1:G:192:GLY:HA3	1:G:376:VAL:HG23	1.72	0.72
1:D:411:VAL:CG2	1:D:494:LEU:HG	2.20	0.72
1:D:192:GLY:HA3	1:D:376:VAL:HG23	1.72	0.72
1:F:197:ARG:HG2	1:F:197:ARG:HH11	1.54	0.72
1:B:281:PHE:CD2	1:C:386:GLU:CA	2.73	0.71
1:A:192:GLY:HA3	1:A:376:VAL:HG23	1.72	0.71
1:E:411:VAL:CG2	1:E:494:LEU:HG	2.20	0.71
1:G:411:VAL:CG2	1:G:494:LEU:HG	2.20	0.71
1:C:192:GLY:HA3	1:C:376:VAL:HG23	1.72	0.71
1:C:197:ARG:HH11	1:C:197:ARG:HG2	1.54	0.71
1:B:192:GLY:HA3	1:B:376:VAL:HG23	1.72	0.71
1:E:198:GLY:HA2	1:E:326:ASN:O	1.91	0.71
1:D:198:GLY:HA2	1:D:326:ASN:O	1.91	0.71
1:F:166:MET:CG	1:F:171:LYS:HA	2.21	0.71
1:B:197:ARG:HG2	1:B:197:ARG:NH1	2.06	0.71
1:C:197:ARG:HG2	1:C:197:ARG:NH1	2.06	0.71
1:G:166:MET:CG	1:G:171:LYS:HA	2.21	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:198:GLY:HA2	1:C:326:ASN:O	1.91	0.71
1:B:198:GLY:HA2	1:B:326:ASN:O	1.91	0.71
1:E:166:MET:CG	1:E:171:LYS:HA	2.21	0.71
1:D:166:MET:CG	1:D:171:LYS:HA	2.21	0.71
1:C:411:VAL:CG2	1:C:494:LEU:HG	2.20	0.71
1:F:198:GLY:HA2	1:F:326:ASN:O	1.91	0.71
1:D:197:ARG:NH1	1:D:197:ARG:HG2	2.06	0.71
1:A:198:GLY:HA2	1:A:326:ASN:O	1.91	0.70
1:G:198:GLY:HA2	1:G:326:ASN:O	1.91	0.70
1:B:411:VAL:CG2	1:B:494:LEU:HG	2.20	0.70
1:A:166:MET:CG	1:A:171:LYS:HA	2.21	0.70
1:F:411:VAL:CG2	1:F:494:LEU:HG	2.20	0.70
1:A:197:ARG:NH1	1:A:197:ARG:HG2	2.06	0.70
1:C:166:MET:CG	1:C:171:LYS:HA	2.21	0.70
1:E:197:ARG:HG2	1:E:197:ARG:NH1	2.06	0.70
1:B:166:MET:CG	1:B:171:LYS:HA	2.21	0.70
1:G:197:ARG:HG2	1:G:197:ARG:NH1	2.06	0.69
1:F:197:ARG:HG2	1:F:197:ARG:NH1	2.06	0.69
1:B:281:PHE:CD2	1:C:389:MET:HE3	2.27	0.69
1:D:360:TYR:CE1	1:E:183:LEU:HD22	2.27	0.69
1:E:325:ILE:HG22	1:E:326:ASN:N	2.08	0.69
1:F:325:ILE:HG22	1:F:326:ASN:N	2.08	0.69
1:C:521:VAL:HB	1:D:40:LEU:HD23	1.75	0.69
1:D:325:ILE:HG22	1:D:326:ASN:N	2.08	0.69
1:E:281:PHE:CE2	1:F:389:MET:HB2	2.27	0.69
1:C:325:ILE:HG22	1:C:326:ASN:N	2.08	0.69
1:G:325:ILE:HG22	1:G:326:ASN:N	2.08	0.69
1:A:216:GLU:HA	1:A:322:ARG:HG2	1.75	0.68
1:E:281:PHE:CE2	1:F:389:MET:CB	2.76	0.68
1:D:216:GLU:HA	1:D:322:ARG:HG2	1.75	0.68
1:G:216:GLU:HA	1:G:322:ARG:HG2	1.75	0.68
1:B:216:GLU:HA	1:B:322:ARG:HG2	1.75	0.68
1:D:125:THR:O	1:D:129:GLU:HG3	1.93	0.68
1:B:325:ILE:HG22	1:B:326:ASN:N	2.08	0.68
1:C:216:GLU:HA	1:C:322:ARG:HG2	1.75	0.68
1:A:125:THR:O	1:A:129:GLU:HG3	1.93	0.68
1:E:281:PHE:CZ	1:F:389:MET:CB	2.76	0.68
1:F:125:THR:O	1:F:129:GLU:HG3	1.93	0.68
1:E:216:GLU:HA	1:E:322:ARG:HG2	1.75	0.68
1:B:324:VAL:O	1:B:324:VAL:HG12	1.94	0.68
1:B:125:THR:O	1:B:129:GLU:HG3	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:125:THR:O	1:E:129:GLU:HG3	1.93	0.68
1:F:216:GLU:HA	1:F:322:ARG:HG2	1.75	0.68
1:C:125:THR:O	1:C:129:GLU:HG3	1.93	0.68
1:A:324:VAL:O	1:A:324:VAL:HG12	1.94	0.67
1:A:325:ILE:HG22	1:A:326:ASN:N	2.08	0.67
1:A:351:GLN:O	1:A:354:GLU:HB3	1.95	0.67
1:C:324:VAL:HG12	1:C:324:VAL:O	1.94	0.67
1:G:351:GLN:O	1:G:354:GLU:HB3	1.95	0.67
1:G:324:VAL:O	1:G:324:VAL:HG12	1.94	0.67
1:G:125:THR:O	1:G:129:GLU:HG3	1.93	0.67
1:B:351:GLN:O	1:B:354:GLU:HB3	1.95	0.67
1:B:281:PHE:CZ	1:C:389:MET:HG3	2.30	0.67
1:G:501:ARG:HH11	1:G:505:GLN:NE2	1.93	0.67
1:F:351:GLN:O	1:F:354:GLU:HB3	1.95	0.67
1:E:324:VAL:HG12	1:E:324:VAL:O	1.94	0.67
1:D:247:LEU:HG	1:D:248:LEU:N	2.10	0.67
1:E:351:GLN:O	1:E:354:GLU:HB3	1.95	0.67
1:B:501:ARG:HH11	1:B:505:GLN:NE2	1.93	0.67
1:D:324:VAL:HG12	1:D:324:VAL:O	1.94	0.67
1:A:247:LEU:HG	1:A:248:LEU:N	2.10	0.67
1:E:247:LEU:HG	1:E:248:LEU:N	2.10	0.67
1:E:501:ARG:HH11	1:E:505:GLN:NE2	1.93	0.67
1:F:324:VAL:HG12	1:F:324:VAL:O	1.94	0.66
1:F:220:ILE:HD12	1:F:248:LEU:HG	1.77	0.66
1:C:501:ARG:HH11	1:C:505:GLN:NE2	1.93	0.66
1:G:201:SER:O	1:G:204:PHE:HB2	1.95	0.66
1:F:281:PHE:CD2	1:G:386:GLU:CA	2.78	0.66
1:B:247:LEU:HG	1:B:248:LEU:N	2.10	0.66
1:D:351:GLN:O	1:D:354:GLU:HB3	1.95	0.66
1:D:501:ARG:HH11	1:D:505:GLN:NE2	1.93	0.66
1:C:201:SER:O	1:C:204:PHE:HB2	1.96	0.66
1:E:201:SER:O	1:E:204:PHE:HB2	1.96	0.66
1:E:285:ARG:CZ	1:F:386:GLU:OE2	2.44	0.66
1:C:351:GLN:O	1:C:354:GLU:HB3	1.95	0.66
1:A:220:ILE:HD12	1:A:248:LEU:HG	1.77	0.66
1:G:220:ILE:HD12	1:G:248:LEU:HG	1.77	0.66
1:B:476:TYR:HE1	1:B:485:TYR:HB3	1.61	0.66
1:D:476:TYR:HE1	1:D:485:TYR:HB3	1.61	0.66
1:B:201:SER:O	1:B:204:PHE:HB2	1.95	0.66
1:F:501:ARG:HH11	1:F:505:GLN:NE2	1.93	0.66
1:A:501:ARG:HH11	1:A:505:GLN:NE2	1.93	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:220:ILE:HD12	1:E:248:LEU:HG	1.77	0.66
1:E:281:PHE:CG	1:F:389:MET:HE3	2.31	0.66
1:C:220:ILE:HD12	1:C:248:LEU:HG	1.77	0.66
1:B:220:ILE:HD12	1:B:248:LEU:HG	1.77	0.66
1:A:201:SER:O	1:A:204:PHE:HB2	1.96	0.66
1:G:247:LEU:HG	1:G:248:LEU:N	2.10	0.66
1:F:476:TYR:HE1	1:F:485:TYR:HB3	1.61	0.66
1:B:432:GLN:HB2	1:B:436:GLN:NE2	2.11	0.66
1:C:432:GLN:HB2	1:C:436:GLN:NE2	2.11	0.66
1:F:247:LEU:HG	1:F:248:LEU:N	2.10	0.65
1:D:517:THR:HG21	1:E:39:VAL:HG23	1.77	0.65
1:A:432:GLN:HB2	1:A:436:GLN:NE2	2.11	0.65
1:D:201:SER:O	1:D:204:PHE:HB2	1.96	0.65
1:B:123:ALA:HB2	1:B:440:ILE:HG23	1.78	0.65
1:G:432:GLN:HB2	1:G:436:GLN:NE2	2.11	0.65
1:A:476:TYR:HE1	1:A:485:TYR:HB3	1.61	0.65
1:F:281:PHE:CD2	1:G:386:GLU:HA	2.31	0.65
1:G:476:TYR:HE1	1:G:485:TYR:HB3	1.61	0.65
1:A:281:PHE:CE2	1:B:386:GLU:HA	2.31	0.65
1:C:247:LEU:HG	1:C:248:LEU:N	2.10	0.65
1:D:220:ILE:HD12	1:D:248:LEU:HG	1.77	0.65
1:F:201:SER:O	1:F:204:PHE:HB2	1.96	0.65
1:E:281:PHE:CZ	1:F:389:MET:HG3	2.32	0.65
1:A:123:ALA:HB2	1:A:440:ILE:HG23	1.78	0.65
1:F:432:GLN:HB2	1:F:436:GLN:NE2	2.11	0.65
1:F:123:ALA:HB2	1:F:440:ILE:HG23	1.78	0.65
1:D:432:GLN:HB2	1:D:436:GLN:NE2	2.11	0.65
1:E:432:GLN:HB2	1:E:436:GLN:NE2	2.11	0.65
1:A:22:VAL:HG11	1:A:62:LEU:HD21	1.78	0.65
1:E:281:PHE:CD2	1:F:389:MET:HE3	2.32	0.65
1:C:123:ALA:HB2	1:C:440:ILE:HG23	1.78	0.65
1:F:22:VAL:HG11	1:F:62:LEU:HD21	1.78	0.65
1:E:476:TYR:HE1	1:E:485:TYR:HB3	1.61	0.64
1:E:123:ALA:HB2	1:E:440:ILE:HG23	1.78	0.64
1:G:22:VAL:HG11	1:G:62:LEU:HD21	1.78	0.64
1:A:281:PHE:HE2	1:B:385:THR:C	2.00	0.64
1:D:73:MET:HE1	1:D:514:MET:HG2	1.79	0.64
1:G:123:ALA:HB2	1:G:440:ILE:HG23	1.78	0.64
1:D:123:ALA:HB2	1:D:440:ILE:HG23	1.78	0.64
1:C:22:VAL:HG11	1:C:62:LEU:HD21	1.78	0.64
1:B:22:VAL:HG11	1:B:62:LEU:HD21	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:476:TYR:HE1	1:C:485:TYR:HB3	1.61	0.64
1:A:386:GLU:HA	1:G:281:PHE:CD2	2.33	0.64
1:A:517:THR:HG21	1:B:39:VAL:HG23	1.79	0.64
1:D:281:PHE:CE2	1:E:386:GLU:HA	2.33	0.64
1:E:22:VAL:HG11	1:E:62:LEU:HD21	1.78	0.64
1:E:281:PHE:CD2	1:F:386:GLU:CA	2.80	0.64
1:C:69:MET:HE1	1:D:39:VAL:HG12	1.80	0.64
1:D:22:VAL:HG11	1:D:62:LEU:HD21	1.78	0.64
1:A:69:MET:HE2	1:B:39:VAL:HG12	1.79	0.63
1:A:77:VAL:HG11	1:A:510:VAL:HG22	1.81	0.63
1:B:281:PHE:CE1	1:C:389:MET:HG3	2.33	0.63
1:B:77:VAL:HG11	1:B:510:VAL:HG22	1.81	0.63
1:E:77:VAL:HG11	1:E:510:VAL:HG22	1.81	0.63
1:D:144:ILE:HG23	1:D:403:THR:HG21	1.80	0.63
1:F:171:LYS:HB3	1:F:407:VAL:HG11	1.80	0.63
1:D:171:LYS:HB3	1:D:407:VAL:HG11	1.80	0.62
1:G:171:LYS:HB3	1:G:407:VAL:HG11	1.80	0.62
1:F:281:PHE:HE2	1:G:386:GLU:N	1.95	0.62
1:E:247:LEU:HD21	1:E:249:ILE:HG13	1.81	0.62
1:B:144:ILE:HG23	1:B:403:THR:HG21	1.80	0.62
1:D:346:VAL:HG11	1:D:373:ALA:HB2	1.81	0.62
1:E:144:ILE:HG23	1:E:403:THR:HG21	1.80	0.62
1:B:476:TYR:CE1	1:B:485:TYR:HB3	2.35	0.62
1:D:476:TYR:CE1	1:D:485:TYR:HB3	2.35	0.62
1:E:476:TYR:CE1	1:E:485:TYR:HB3	2.35	0.62
1:B:346:VAL:HG11	1:B:373:ALA:HB2	1.81	0.62
1:F:247:LEU:HD21	1:F:249:ILE:HG13	1.81	0.62
1:A:171:LYS:HB3	1:A:407:VAL:HG11	1.80	0.62
1:C:144:ILE:HG23	1:C:403:THR:HG21	1.80	0.62
1:G:476:TYR:CE1	1:G:485:TYR:HB3	2.35	0.62
1:C:476:TYR:CE1	1:C:485:TYR:HB3	2.35	0.62
1:G:77:VAL:HG11	1:G:510:VAL:HG22	1.81	0.62
1:A:346:VAL:HG11	1:A:373:ALA:HB2	1.81	0.62
1:D:77:VAL:HG11	1:D:510:VAL:HG22	1.81	0.62
1:A:386:GLU:HA	1:G:281:PHE:CE2	2.34	0.62
1:F:144:ILE:HG23	1:F:403:THR:HG21	1.80	0.62
1:C:144:ILE:HD13	1:C:166:MET:SD	2.40	0.62
1:F:476:TYR:CE1	1:F:485:TYR:HB3	2.35	0.62
1:A:476:TYR:CE1	1:A:485:TYR:HB3	2.35	0.62
1:G:346:VAL:HG11	1:G:373:ALA:HB2	1.81	0.62
1:D:144:ILE:HD13	1:D:166:MET:SD	2.39	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:144:ILE:HD13	1:B:166:MET:SD	2.40	0.62
1:F:77:VAL:HG11	1:F:510:VAL:HG22	1.81	0.62
1:D:247:LEU:HD21	1:D:249:ILE:HG13	1.81	0.62
1:A:144:ILE:HG23	1:A:403:THR:HG21	1.80	0.62
1:C:171:LYS:HB3	1:C:407:VAL:HG11	1.80	0.62
1:C:346:VAL:HG11	1:C:373:ALA:HB2	1.81	0.62
1:E:346:VAL:HG11	1:E:373:ALA:HB2	1.81	0.62
1:D:391:GLU:O	1:D:395:ARG:HG3	2.00	0.62
1:F:346:VAL:HG11	1:F:373:ALA:HB2	1.81	0.62
1:A:391:GLU:O	1:A:395:ARG:HG3	2.00	0.62
1:G:281:PHE:HA	1:G:285:ARG:CG	2.29	0.62
1:B:247:LEU:HD21	1:B:249:ILE:HG13	1.81	0.62
1:E:171:LYS:HB3	1:E:407:VAL:HG11	1.80	0.62
1:G:144:ILE:HD13	1:G:166:MET:SD	2.40	0.62
1:G:144:ILE:HG23	1:G:403:THR:HG21	1.80	0.62
1:B:436:GLN:O	1:B:440:ILE:HG13	2.00	0.62
1:D:436:GLN:O	1:D:440:ILE:HG13	2.00	0.62
1:E:391:GLU:O	1:E:395:ARG:HG3	2.00	0.62
1:A:40:LEU:HD23	1:G:521:VAL:HB	1.82	0.62
1:C:247:LEU:HD21	1:C:249:ILE:HG13	1.81	0.61
1:A:144:ILE:HD13	1:A:166:MET:SD	2.40	0.61
1:G:436:GLN:O	1:G:440:ILE:HG13	2.00	0.61
1:C:281:PHE:HA	1:C:285:ARG:CG	2.29	0.61
1:B:281:PHE:HA	1:B:285:ARG:CG	2.29	0.61
1:E:436:GLN:O	1:E:440:ILE:HG13	2.00	0.61
1:E:184:GLN:O	1:E:185:ASP:HB2	2.00	0.61
1:C:77:VAL:HG11	1:C:510:VAL:HG22	1.81	0.61
1:G:391:GLU:O	1:G:395:ARG:HG3	2.00	0.61
1:A:247:LEU:HD21	1:A:249:ILE:HG13	1.81	0.61
1:G:247:LEU:HD21	1:G:249:ILE:HG13	1.81	0.61
1:B:171:LYS:HB3	1:B:407:VAL:HG11	1.80	0.61
1:C:436:GLN:O	1:C:440:ILE:HG13	2.00	0.61
1:F:144:ILE:HD13	1:F:166:MET:SD	2.40	0.61
1:B:391:GLU:O	1:B:395:ARG:HG3	2.00	0.61
1:C:184:GLN:O	1:C:185:ASP:HB2	2.00	0.61
1:E:144:ILE:HD13	1:E:166:MET:SD	2.40	0.61
1:C:391:GLU:O	1:C:395:ARG:HG3	2.00	0.61
1:C:501:ARG:NH1	1:C:505:GLN:HE22	1.99	0.61
1:E:501:ARG:NH1	1:E:505:GLN:HE22	1.99	0.61
1:A:436:GLN:O	1:A:440:ILE:HG13	2.00	0.61
1:F:436:GLN:O	1:F:440:ILE:HG13	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:281:PHE:HA	1:E:285:ARG:CG	2.29	0.61
1:A:501:ARG:NH1	1:A:505:GLN:HE22	1.99	0.61
1:A:362:ARG:HD2	1:A:366:GLN:HB3	1.83	0.61
1:B:362:ARG:HD2	1:B:366:GLN:HB3	1.83	0.61
1:B:281:PHE:CE2	1:C:386:GLU:CA	2.81	0.61
1:D:281:PHE:HA	1:D:285:ARG:CG	2.29	0.61
1:D:114:MET:HG3	1:E:34:LYS:HG3	1.83	0.61
1:B:184:GLN:O	1:B:185:ASP:HB2	2.00	0.61
1:D:184:GLN:O	1:D:185:ASP:HB2	2.00	0.61
1:C:362:ARG:HD2	1:C:366:GLN:HB3	1.83	0.61
1:A:281:PHE:HA	1:A:285:ARG:CG	2.29	0.61
1:D:429:LEU:C	1:D:430:ARG:HD2	2.21	0.61
1:G:429:LEU:C	1:G:430:ARG:HD2	2.21	0.61
1:G:362:ARG:HD2	1:G:366:GLN:HB3	1.83	0.61
1:F:362:ARG:HD2	1:F:366:GLN:HB3	1.83	0.61
1:G:501:ARG:NH1	1:G:505:GLN:HE22	1.99	0.61
1:C:69:MET:HE2	1:D:39:VAL:HG12	1.82	0.61
1:F:281:PHE:HA	1:F:285:ARG:CG	2.29	0.60
1:F:501:ARG:NH1	1:F:505:GLN:HE22	1.99	0.60
1:B:429:LEU:C	1:B:430:ARG:HD2	2.21	0.60
1:C:429:LEU:C	1:C:430:ARG:HD2	2.21	0.60
1:E:100:ILE:HD13	1:E:514:MET:SD	2.41	0.60
1:A:184:GLN:O	1:A:185:ASP:HB2	2.00	0.60
1:F:391:GLU:O	1:F:395:ARG:HG3	2.00	0.60
1:E:288:MET:HG3	1:E:368:ARG:CD	2.29	0.60
1:A:429:LEU:C	1:A:430:ARG:HD2	2.21	0.60
1:A:517:THR:CG2	1:B:39:VAL:HG23	2.30	0.60
1:G:100:ILE:HD13	1:G:514:MET:SD	2.41	0.60
1:A:100:ILE:HD13	1:A:514:MET:SD	2.41	0.60
1:C:100:ILE:HD13	1:C:514:MET:SD	2.41	0.60
1:E:362:ARG:HD2	1:E:366:GLN:HB3	1.83	0.60
1:D:362:ARG:HD2	1:D:366:GLN:HB3	1.83	0.60
1:F:200:LEU:HD13	1:F:276:VAL:HA	1.82	0.60
1:E:429:LEU:C	1:E:430:ARG:HD2	2.21	0.60
1:A:281:PHE:HE2	1:B:386:GLU:N	2.00	0.60
1:E:281:PHE:CE2	1:F:386:GLU:CA	2.83	0.60
1:G:200:LEU:HD13	1:G:276:VAL:HA	1.82	0.60
1:B:200:LEU:HD13	1:B:276:VAL:HA	1.82	0.60
1:C:487:ASN:O	1:C:491:MET:HG3	2.01	0.60
1:F:184:GLN:O	1:F:185:ASP:HB2	2.00	0.60
1:B:100:ILE:HD13	1:B:514:MET:SD	2.41	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:100:ILE:HD13	1:F:514:MET:SD	2.41	0.60
1:C:222:LEU:H	1:C:300:VAL:HG11	1.67	0.60
1:B:487:ASN:O	1:B:491:MET:HG3	2.01	0.60
1:D:487:ASN:O	1:D:491:MET:HG3	2.01	0.60
1:B:222:LEU:H	1:B:300:VAL:HG11	1.67	0.60
1:A:200:LEU:HD13	1:A:276:VAL:HA	1.82	0.60
1:C:200:LEU:HD13	1:C:276:VAL:HA	1.82	0.60
1:D:501:ARG:NH1	1:D:505:GLN:HE22	1.99	0.60
1:F:429:LEU:C	1:F:430:ARG:HD2	2.21	0.60
1:E:487:ASN:O	1:E:491:MET:HG3	2.01	0.60
1:C:214:GLU:CG	1:C:324:VAL:HG13	2.26	0.60
1:D:222:LEU:H	1:D:300:VAL:HG11	1.67	0.60
1:E:200:LEU:HD13	1:E:276:VAL:HA	1.82	0.60
1:G:184:GLN:O	1:G:185:ASP:HB2	2.00	0.60
1:D:100:ILE:HD13	1:D:514:MET:SD	2.41	0.60
1:D:101:THR:O	1:D:105:LYS:HG3	2.02	0.60
1:B:501:ARG:NH1	1:B:505:GLN:HE22	1.99	0.60
1:D:200:LEU:HD13	1:D:276:VAL:HA	1.82	0.59
1:E:101:THR:O	1:E:105:LYS:HG3	2.02	0.59
1:F:487:ASN:O	1:F:491:MET:HG3	2.01	0.59
1:A:487:ASN:O	1:A:491:MET:HG3	2.01	0.59
1:B:214:GLU:CG	1:B:324:VAL:HG13	2.26	0.59
1:D:214:GLU:CG	1:D:324:VAL:HG13	2.26	0.59
1:C:101:THR:O	1:C:105:LYS:HG3	2.02	0.59
1:B:160:LYS:O	1:B:164:GLU:HG3	2.02	0.59
1:B:300:VAL:CG2	1:B:317:LEU:HA	2.32	0.59
1:F:160:LYS:O	1:F:164:GLU:HG3	2.02	0.59
1:A:214:GLU:CG	1:A:324:VAL:HG13	2.26	0.59
1:D:288:MET:HG3	1:D:368:ARG:CD	2.29	0.59
1:D:360:TYR:OH	1:E:183:LEU:HD13	2.03	0.59
1:A:222:LEU:H	1:A:300:VAL:HG11	1.67	0.59
1:G:487:ASN:O	1:G:491:MET:HG3	2.01	0.59
1:C:300:VAL:CG2	1:C:317:LEU:HA	2.33	0.59
1:G:160:LYS:O	1:G:164:GLU:HG3	2.03	0.59
1:B:101:THR:O	1:B:105:LYS:HG3	2.02	0.59
1:A:300:VAL:CG2	1:A:317:LEU:HA	2.33	0.59
1:D:340:ALA:CA	1:D:343:GLN:HG3	2.33	0.59
1:A:340:ALA:CA	1:A:343:GLN:HG3	2.33	0.59
1:B:14:VAL:O	1:B:18:ARG:HD3	2.03	0.59
1:E:160:LYS:O	1:E:164:GLU:HG3	2.02	0.59
1:F:300:VAL:CG2	1:F:317:LEU:HD23	2.31	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:300:VAL:CG2	1:D:317:LEU:HA	2.33	0.59
1:A:160:LYS:O	1:A:164:GLU:HG3	2.02	0.59
1:E:222:LEU:H	1:E:300:VAL:HG11	1.67	0.59
1:G:340:ALA:CA	1:G:343:GLN:HG3	2.33	0.59
1:D:160:LYS:O	1:D:164:GLU:HG3	2.03	0.59
1:G:14:VAL:O	1:G:18:ARG:HD3	2.03	0.58
1:F:101:THR:O	1:F:105:LYS:HG3	2.02	0.58
1:B:360:TYR:CE1	1:C:183:LEU:CD2	2.85	0.58
1:E:300:VAL:CG2	1:E:317:LEU:HA	2.33	0.58
1:G:222:LEU:H	1:G:300:VAL:HG11	1.67	0.58
1:G:300:VAL:CG2	1:G:317:LEU:HA	2.33	0.58
1:C:340:ALA:CA	1:C:343:GLN:HG3	2.33	0.58
1:C:160:LYS:O	1:C:164:GLU:HG3	2.03	0.58
1:D:14:VAL:O	1:D:18:ARG:HD3	2.03	0.58
1:G:281:PHE:CA	1:G:285:ARG:HG2	2.32	0.58
1:C:82:ASN:ND2	1:C:89:THR:N	2.52	0.58
1:F:222:LEU:H	1:F:300:VAL:HG11	1.67	0.58
1:G:342:ILE:HG23	1:G:372:LEU:HD22	1.85	0.58
1:B:342:ILE:HG23	1:B:372:LEU:HD22	1.85	0.58
1:A:342:ILE:HG23	1:A:372:LEU:HD22	1.85	0.58
1:E:214:GLU:CG	1:E:324:VAL:HG13	2.26	0.58
1:F:342:ILE:HG23	1:F:372:LEU:HD22	1.85	0.58
1:E:14:VAL:O	1:E:18:ARG:HD3	2.03	0.58
1:E:340:ALA:CA	1:E:343:GLN:HG3	2.33	0.58
1:G:101:THR:O	1:G:105:LYS:HG3	2.02	0.58
1:C:281:PHE:CA	1:C:285:ARG:HG2	2.32	0.58
1:F:14:VAL:O	1:F:18:ARG:HD3	2.03	0.58
1:D:16:MET:HA	1:D:70:GLY:HA3	1.86	0.58
1:A:282:GLY:HA2	1:B:181:THR:O	1.95	0.58
1:G:214:GLU:CG	1:G:324:VAL:HG13	2.26	0.58
1:F:300:VAL:CG2	1:F:317:LEU:HA	2.32	0.58
1:C:342:ILE:HG23	1:C:372:LEU:HD22	1.85	0.58
1:A:101:THR:O	1:A:105:LYS:HG3	2.02	0.58
1:D:82:ASN:ND2	1:D:89:THR:N	2.52	0.58
1:B:340:ALA:CA	1:B:343:GLN:HG3	2.33	0.58
1:F:157:THR:O	1:F:160:LYS:HB2	2.04	0.58
1:E:16:MET:HA	1:E:70:GLY:HA3	1.86	0.58
1:C:219:PHE:HD2	1:C:317:LEU:HD12	1.69	0.58
1:A:213:VAL:HG22	1:A:325:ILE:HB	1.85	0.58
1:E:342:ILE:HG23	1:E:372:LEU:HD22	1.85	0.58
1:F:340:ALA:CA	1:F:343:GLN:HG3	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:16:MET:HA	1:C:70:GLY:HA3	1.86	0.58
1:F:281:PHE:CA	1:F:285:ARG:HG2	2.32	0.57
1:C:288:MET:HG3	1:C:368:ARG:CD	2.29	0.57
1:A:219:PHE:HD2	1:A:317:LEU:HD12	1.69	0.57
1:G:219:PHE:HD2	1:G:317:LEU:HD12	1.69	0.57
1:E:82:ASN:ND2	1:E:89:THR:N	2.51	0.57
1:F:82:ASN:ND2	1:F:89:THR:N	2.51	0.57
1:G:213:VAL:HG22	1:G:325:ILE:HB	1.85	0.57
1:A:14:VAL:O	1:A:18:ARG:HD3	2.03	0.57
1:E:281:PHE:CA	1:E:285:ARG:HG2	2.32	0.57
1:E:219:PHE:HD2	1:E:317:LEU:HD12	1.69	0.57
1:A:157:THR:O	1:A:160:LYS:HB2	2.04	0.57
1:D:157:THR:O	1:D:160:LYS:HB2	2.04	0.57
1:C:14:VAL:O	1:C:18:ARG:HD3	2.03	0.57
1:B:213:VAL:HG22	1:B:325:ILE:HB	1.85	0.57
1:D:213:VAL:HG22	1:D:325:ILE:HB	1.85	0.57
1:C:213:VAL:HG22	1:C:325:ILE:HB	1.85	0.57
1:F:213:VAL:HG22	1:F:325:ILE:HB	1.85	0.57
1:B:16:MET:HA	1:B:70:GLY:HA3	1.86	0.57
1:A:281:PHE:CA	1:A:285:ARG:HG2	2.32	0.57
1:C:288:MET:O	1:C:292:ILE:HG13	2.05	0.57
1:D:342:ILE:HG23	1:D:372:LEU:HD22	1.85	0.57
1:B:157:THR:O	1:B:160:LYS:HB2	2.04	0.57
1:A:288:MET:O	1:A:292:ILE:HG13	2.05	0.57
1:E:213:VAL:HG22	1:E:325:ILE:HB	1.85	0.57
1:F:16:MET:HA	1:F:70:GLY:HA3	1.86	0.57
1:F:219:PHE:HD2	1:F:317:LEU:HD12	1.69	0.57
1:D:206:ASN:HB3	1:D:213:VAL:CA	2.32	0.57
1:F:281:PHE:HE2	1:G:385:THR:O	1.88	0.57
1:C:206:ASN:HB3	1:C:213:VAL:CA	2.32	0.57
1:C:157:THR:O	1:C:160:LYS:HB2	2.04	0.57
1:B:219:PHE:HD2	1:B:317:LEU:HD12	1.69	0.57
1:F:433:ASN:ND2	1:F:436:GLN:HG3	2.20	0.57
1:A:386:GLU:CA	1:G:281:PHE:CD2	2.87	0.56
1:B:281:PHE:HD2	1:C:386:GLU:CA	2.18	0.56
1:E:288:MET:O	1:E:292:ILE:HG13	2.05	0.56
1:G:288:MET:O	1:G:292:ILE:HG13	2.05	0.56
1:F:288:MET:O	1:F:292:ILE:HG13	2.05	0.56
1:B:433:ASN:ND2	1:B:436:GLN:HG3	2.20	0.56
1:C:433:ASN:ND2	1:C:436:GLN:HG3	2.20	0.56
1:G:433:ASN:ND2	1:G:436:GLN:HG3	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:433:ASN:ND2	1:D:436:GLN:HG3	2.20	0.56
1:G:157:THR:O	1:G:160:LYS:HB2	2.04	0.56
1:E:157:THR:O	1:E:160:LYS:HB2	2.04	0.56
1:E:73:MET:HG2	1:F:49:ILE:HD11	1.87	0.56
1:A:281:PHE:CE2	1:B:386:GLU:CA	2.89	0.56
1:B:288:MET:HG3	1:B:368:ARG:CD	2.29	0.56
1:B:206:ASN:HB3	1:B:213:VAL:CA	2.32	0.56
1:A:433:ASN:ND2	1:A:436:GLN:HG3	2.20	0.56
1:E:433:ASN:ND2	1:E:436:GLN:HG3	2.20	0.56
1:F:281:PHE:CE2	1:G:386:GLU:HA	2.41	0.56
1:G:82:ASN:ND2	1:G:89:THR:N	2.52	0.56
1:D:219:PHE:HD2	1:D:317:LEU:HD12	1.69	0.56
1:D:327:LYS:HG3	1:D:327:LYS:O	2.06	0.56
1:G:252:GLU:O	1:G:254:VAL:N	2.39	0.56
1:F:252:GLU:O	1:F:254:VAL:N	2.39	0.56
1:G:206:ASN:HB3	1:G:213:VAL:CA	2.32	0.56
1:A:327:LYS:O	1:A:327:LYS:HG3	2.06	0.56
1:B:288:MET:O	1:B:292:ILE:HG13	2.05	0.56
1:E:300:VAL:HG23	1:E:317:LEU:H	1.71	0.56
1:G:300:VAL:HG23	1:G:317:LEU:H	1.71	0.56
1:B:300:VAL:HG23	1:B:317:LEU:H	1.71	0.56
1:A:206:ASN:HB3	1:A:213:VAL:CA	2.32	0.56
1:E:206:ASN:HB3	1:E:213:VAL:CA	2.32	0.56
1:F:320:ALA:HA	1:F:334:ASP:O	2.06	0.56
1:A:502:SER:O	1:A:506:TYR:HD2	1.88	0.56
1:G:16:MET:HA	1:G:70:GLY:HA3	1.86	0.56
1:A:16:MET:HA	1:A:70:GLY:HA3	1.86	0.56
1:D:502:SER:O	1:D:506:TYR:HD2	1.88	0.56
1:F:214:GLU:CG	1:F:324:VAL:HG13	2.26	0.56
1:E:281:PHE:CE1	1:F:389:MET:HG3	2.41	0.56
1:G:193:MET:SD	1:G:292:ILE:HG12	2.46	0.56
1:G:421:ARG:NH2	1:G:470:LYS:O	2.39	0.56
1:C:502:SER:O	1:C:506:TYR:HD2	1.88	0.56
1:C:281:PHE:HZ	1:D:384:ALA:C	2.09	0.56
1:D:193:MET:SD	1:D:292:ILE:HG12	2.46	0.56
1:A:193:MET:SD	1:A:292:ILE:HG12	2.46	0.56
1:D:298:GLY:C	1:D:300:VAL:H	2.10	0.56
1:E:252:GLU:O	1:E:254:VAL:N	2.39	0.56
1:A:252:GLU:O	1:A:254:VAL:N	2.39	0.56
1:F:206:ASN:HB3	1:F:213:VAL:CA	2.32	0.56
1:C:320:ALA:HA	1:C:334:ASP:O	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:502:SER:O	1:F:506:TYR:HD2	1.88	0.56
1:B:327:LYS:O	1:B:327:LYS:HG3	2.06	0.56
1:E:327:LYS:O	1:E:327:LYS:HG3	2.06	0.56
1:D:223:ALA:HB3	1:D:251:ALA:HB2	1.88	0.56
1:D:288:MET:O	1:D:292:ILE:HG13	2.05	0.56
1:D:300:VAL:HG23	1:D:317:LEU:H	1.71	0.56
1:C:421:ARG:NH2	1:C:470:LYS:O	2.39	0.56
1:G:320:ALA:HA	1:G:334:ASP:O	2.06	0.56
1:D:421:ARG:NH2	1:D:470:LYS:O	2.39	0.56
1:D:281:PHE:CA	1:D:285:ARG:HG2	2.32	0.56
1:E:421:ARG:NH2	1:E:470:LYS:O	2.39	0.56
1:E:320:ALA:HA	1:E:334:ASP:O	2.06	0.56
1:G:502:SER:O	1:G:506:TYR:HD2	1.88	0.56
1:D:338:GLU:O	1:D:341:ALA:N	2.39	0.56
1:B:193:MET:SD	1:B:292:ILE:HG12	2.46	0.55
1:E:193:MET:SD	1:E:292:ILE:HG12	2.46	0.55
1:F:193:MET:SD	1:F:292:ILE:HG12	2.46	0.55
1:A:421:ARG:NH2	1:A:470:LYS:O	2.39	0.55
1:E:186:GLU:HB2	1:E:380:LYS:HB2	1.89	0.55
1:G:338:GLU:O	1:G:341:ALA:N	2.39	0.55
1:C:193:MET:SD	1:C:292:ILE:HG12	2.46	0.55
1:F:298:GLY:C	1:F:300:VAL:H	2.10	0.55
1:A:320:ALA:HA	1:A:334:ASP:O	2.06	0.55
1:E:223:ALA:HB3	1:E:251:ALA:HB2	1.88	0.55
1:A:223:ALA:HB3	1:A:251:ALA:HB2	1.88	0.55
1:C:186:GLU:HB2	1:C:380:LYS:HB2	1.89	0.55
1:D:186:GLU:HB2	1:D:380:LYS:HB2	1.89	0.55
1:B:298:GLY:C	1:B:300:VAL:H	2.10	0.55
1:B:252:GLU:O	1:B:254:VAL:N	2.39	0.55
1:D:252:GLU:O	1:D:254:VAL:N	2.39	0.55
1:B:320:ALA:HA	1:B:334:ASP:O	2.06	0.55
1:B:502:SER:O	1:B:506:TYR:HD2	1.88	0.55
1:C:338:GLU:O	1:C:341:ALA:N	2.39	0.55
1:E:502:SER:O	1:E:506:TYR:HD2	1.88	0.55
1:G:298:GLY:C	1:G:300:VAL:H	2.10	0.55
1:C:252:GLU:O	1:C:254:VAL:N	2.39	0.55
1:D:320:ALA:HA	1:D:334:ASP:O	2.06	0.55
1:G:327:LYS:HG3	1:G:327:LYS:O	2.06	0.55
1:G:223:ALA:HB3	1:G:251:ALA:HB2	1.88	0.55
1:B:186:GLU:HB2	1:B:380:LYS:HB2	1.89	0.55
1:F:281:PHE:CE2	1:G:386:GLU:CA	2.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:281:PHE:CD2	1:G:386:GLU:N	2.74	0.55
1:A:298:GLY:C	1:A:300:VAL:H	2.10	0.55
1:F:338:GLU:O	1:F:341:ALA:N	2.39	0.55
1:F:186:GLU:HB2	1:F:380:LYS:HB2	1.89	0.55
1:B:223:ALA:HB3	1:B:251:ALA:HB2	1.88	0.55
1:A:186:GLU:HB2	1:A:380:LYS:HB2	1.89	0.55
1:E:338:GLU:O	1:E:341:ALA:N	2.39	0.55
1:E:362:ARG:HD2	1:E:362:ARG:O	2.07	0.55
1:A:338:GLU:O	1:A:341:ALA:N	2.39	0.55
1:G:362:ARG:HD2	1:G:362:ARG:O	2.07	0.55
1:A:362:ARG:HD2	1:A:362:ARG:O	2.07	0.55
1:D:213:VAL:HG23	1:D:213:VAL:O	2.06	0.55
1:E:213:VAL:HG23	1:E:213:VAL:O	2.06	0.55
1:E:465:VAL:O	1:E:469:VAL:HG23	2.07	0.55
1:G:186:GLU:HB2	1:G:380:LYS:HB2	1.89	0.55
1:A:465:VAL:O	1:A:469:VAL:HG23	2.07	0.55
1:A:288:MET:HG3	1:A:368:ARG:CD	2.29	0.55
1:G:82:ASN:H	1:G:82:ASN:HD22	1.54	0.55
1:C:298:GLY:C	1:C:300:VAL:H	2.10	0.55
1:C:362:ARG:HD2	1:C:362:ARG:O	2.07	0.55
1:F:362:ARG:HD2	1:F:362:ARG:O	2.06	0.55
1:B:362:ARG:O	1:B:362:ARG:HD2	2.06	0.55
1:D:362:ARG:O	1:D:362:ARG:HD2	2.06	0.55
1:F:300:VAL:HG23	1:F:317:LEU:H	1.71	0.55
1:C:300:VAL:HG23	1:C:317:LEU:H	1.71	0.55
1:F:421:ARG:NH2	1:F:470:LYS:O	2.39	0.55
1:C:327:LYS:O	1:C:327:LYS:HG3	2.06	0.55
1:E:12:ALA:HB1	1:E:520:MET:HG3	1.89	0.55
1:C:82:ASN:H	1:C:82:ASN:HD22	1.54	0.55
1:A:82:ASN:H	1:A:82:ASN:HD22	1.55	0.55
1:A:82:ASN:ND2	1:A:89:THR:N	2.51	0.55
1:D:360:TYR:C	1:D:360:TYR:CD1	2.80	0.55
1:A:300:VAL:HG23	1:A:317:LEU:H	1.71	0.55
1:A:191:GLU:O	1:A:334:ASP:HA	2.07	0.55
1:A:12:ALA:HB1	1:A:520:MET:HG3	1.89	0.55
1:C:223:ALA:HB3	1:C:251:ALA:HB2	1.88	0.55
1:B:465:VAL:O	1:B:469:VAL:HG23	2.07	0.55
1:D:7:LYS:NZ	1:D:15:LYS:HE3	2.22	0.55
1:F:82:ASN:H	1:F:82:ASN:HD22	1.55	0.54
1:B:421:ARG:NH2	1:B:470:LYS:O	2.39	0.54
1:B:191:GLU:O	1:B:334:ASP:HA	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:223:ALA:HB3	1:F:251:ALA:HB2	1.88	0.54
1:F:327:LYS:HG3	1:F:327:LYS:O	2.06	0.54
1:A:281:PHE:CE2	1:B:386:GLU:N	2.76	0.54
1:C:191:GLU:O	1:C:334:ASP:HA	2.07	0.54
1:D:465:VAL:O	1:D:469:VAL:HG23	2.07	0.54
1:E:7:LYS:NZ	1:E:15:LYS:HE3	2.22	0.54
1:F:360:TYR:C	1:F:360:TYR:CD1	2.80	0.54
1:B:281:PHE:CA	1:B:285:ARG:HG2	2.32	0.54
1:B:82:ASN:HD22	1:B:82:ASN:H	1.55	0.54
1:C:213:VAL:HG23	1:C:213:VAL:O	2.06	0.54
1:E:140:ASP:OD1	1:E:143:ALA:HB2	2.07	0.54
1:G:360:TYR:CD1	1:G:360:TYR:C	2.80	0.54
1:F:300:VAL:HG21	1:F:317:LEU:HA	1.90	0.54
1:F:213:VAL:HG23	1:F:213:VAL:O	2.06	0.54
1:A:517:THR:HA	1:B:37:ASN:HB2	1.89	0.54
1:C:7:LYS:NZ	1:C:15:LYS:HE3	2.22	0.54
1:F:465:VAL:O	1:F:469:VAL:HG23	2.07	0.54
1:F:140:ASP:OD1	1:F:143:ALA:HB2	2.07	0.54
1:E:360:TYR:CD1	1:E:360:TYR:C	2.80	0.54
1:G:300:VAL:HG21	1:G:317:LEU:HA	1.90	0.54
1:C:300:VAL:HG21	1:C:317:LEU:HA	1.90	0.54
1:G:191:GLU:O	1:G:334:ASP:HA	2.07	0.54
1:B:12:ALA:HB1	1:B:520:MET:HG3	1.89	0.54
1:D:12:ALA:HB1	1:D:520:MET:HG3	1.89	0.54
1:C:360:TYR:CD1	1:C:360:TYR:C	2.80	0.54
1:E:360:TYR:CE1	1:F:183:LEU:CD2	2.85	0.54
1:D:82:ASN:H	1:D:82:ASN:HD22	1.55	0.54
1:B:300:VAL:HG21	1:B:317:LEU:HA	1.90	0.54
1:G:213:VAL:O	1:G:213:VAL:HG23	2.06	0.54
1:E:191:GLU:O	1:E:334:ASP:HA	2.07	0.54
1:B:140:ASP:OD1	1:B:143:ALA:HB2	2.07	0.54
1:C:140:ASP:OD1	1:C:143:ALA:HB2	2.07	0.54
1:B:338:GLU:O	1:B:341:ALA:N	2.40	0.54
1:G:465:VAL:O	1:G:469:VAL:HG23	2.07	0.54
1:D:140:ASP:OD1	1:D:143:ALA:HB2	2.07	0.54
1:B:7:LYS:NZ	1:B:15:LYS:HE3	2.22	0.54
1:A:386:GLU:N	1:G:281:PHE:CE2	2.76	0.54
1:A:360:TYR:C	1:A:360:TYR:CD1	2.80	0.54
1:D:82:ASN:HD21	1:D:89:THR:N	1.97	0.54
1:E:300:VAL:HG21	1:E:317:LEU:HA	1.90	0.54
1:E:82:ASN:HD22	1:E:82:ASN:H	1.55	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:176:THR:HG21	1:F:333:ILE:HD11	1.90	0.54
1:G:140:ASP:OD1	1:G:143:ALA:HB2	2.07	0.54
1:F:12:ALA:HB1	1:F:520:MET:HG3	1.89	0.54
1:E:298:GLY:C	1:E:300:VAL:H	2.10	0.54
1:B:213:VAL:HG23	1:B:213:VAL:O	2.06	0.54
1:G:176:THR:HG21	1:G:333:ILE:HD11	1.90	0.54
1:A:300:VAL:HG21	1:A:317:LEU:HA	1.90	0.54
1:E:132:LYS:HE3	1:E:409:GLU:HB3	1.90	0.54
1:A:140:ASP:OD1	1:A:143:ALA:HB2	2.07	0.54
1:A:176:THR:HG21	1:A:333:ILE:HD11	1.90	0.54
1:G:12:ALA:HB1	1:G:520:MET:HG3	1.89	0.54
1:F:7:LYS:NZ	1:F:15:LYS:HE3	2.22	0.54
1:B:82:ASN:ND2	1:B:89:THR:N	2.51	0.54
1:D:191:GLU:O	1:D:334:ASP:HA	2.07	0.54
1:D:132:LYS:HE3	1:D:409:GLU:HB3	1.90	0.54
1:F:132:LYS:HE3	1:F:409:GLU:HB3	1.90	0.54
1:B:360:TYR:C	1:B:360:TYR:CD1	2.80	0.53
1:D:300:VAL:HG21	1:D:317:LEU:HA	1.90	0.53
1:E:176:THR:HG21	1:E:333:ILE:HD11	1.90	0.53
1:B:176:THR:HG21	1:B:333:ILE:HD11	1.90	0.53
1:A:7:LYS:NZ	1:A:15:LYS:HE3	2.22	0.53
1:C:176:THR:HG21	1:C:333:ILE:HD11	1.90	0.53
1:A:378:VAL:HG12	1:A:380:LYS:HD2	1.90	0.53
1:A:360:TYR:HD1	1:A:361:ASP:N	2.07	0.53
1:F:360:TYR:HD1	1:F:361:ASP:N	2.07	0.53
1:A:213:VAL:HG23	1:A:213:VAL:O	2.06	0.53
1:F:191:GLU:O	1:F:334:ASP:HA	2.07	0.53
1:C:521:VAL:N	1:D:39:VAL:O	2.25	0.53
1:G:378:VAL:HG12	1:G:380:LYS:HD2	1.90	0.53
1:C:465:VAL:O	1:C:469:VAL:HG23	2.07	0.53
1:G:360:TYR:HD1	1:G:361:ASP:N	2.07	0.53
1:C:360:TYR:HD1	1:C:361:ASP:N	2.07	0.53
1:B:360:TYR:HD1	1:B:361:ASP:N	2.07	0.53
1:E:360:TYR:HD1	1:E:361:ASP:N	2.07	0.53
1:D:360:TYR:HD1	1:D:361:ASP:N	2.07	0.53
1:G:132:LYS:HE3	1:G:409:GLU:HB3	1.90	0.53
1:A:517:THR:HG21	1:B:39:VAL:CG2	2.38	0.53
1:C:378:VAL:HG12	1:C:380:LYS:HD2	1.90	0.53
1:D:176:THR:HG21	1:D:333:ILE:HD11	1.90	0.53
1:E:463:SER:O	1:E:467:ASN:HB2	2.09	0.53
1:F:34:LYS:O	1:F:457:ASN:HB3	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:386:GLU:N	1:G:281:PHE:HE2	2.07	0.53
1:G:288:MET:HG3	1:G:368:ARG:CD	2.29	0.53
1:C:132:LYS:HE3	1:C:409:GLU:HB3	1.90	0.53
1:G:34:LYS:O	1:G:457:ASN:HB3	2.09	0.53
1:A:386:GLU:CA	1:G:281:PHE:CE2	2.92	0.53
1:F:463:SER:O	1:F:467:ASN:HB2	2.09	0.53
1:G:7:LYS:NZ	1:G:15:LYS:HE3	2.22	0.53
1:A:300:VAL:CG2	1:A:317:LEU:HD23	2.31	0.53
1:E:34:LYS:O	1:E:457:ASN:HB3	2.09	0.53
1:F:378:VAL:HG12	1:F:380:LYS:HD2	1.90	0.53
1:C:518:GLU:HG3	1:D:36:ARG:HG3	1.89	0.53
1:A:34:LYS:O	1:A:457:ASN:HB3	2.09	0.53
1:F:288:MET:HG3	1:F:368:ARG:CD	2.29	0.53
1:A:132:LYS:HE3	1:A:409:GLU:HB3	1.90	0.53
1:C:12:ALA:HB1	1:C:520:MET:HG3	1.89	0.53
1:D:378:VAL:HG12	1:D:380:LYS:HD2	1.90	0.53
1:B:378:VAL:HG12	1:B:380:LYS:HD2	1.90	0.53
1:D:463:SER:O	1:D:467:ASN:HB2	2.09	0.53
1:D:34:LYS:O	1:D:457:ASN:HB3	2.09	0.53
1:C:463:SER:O	1:C:467:ASN:HB2	2.09	0.52
1:B:281:PHE:CZ	1:C:389:MET:CG	2.92	0.52
1:B:132:LYS:HE3	1:B:409:GLU:HB3	1.90	0.52
1:A:362:ARG:CZ	1:A:366:GLN:NE2	2.72	0.52
1:B:362:ARG:CZ	1:B:366:GLN:NE2	2.72	0.52
1:A:82:ASN:HD21	1:A:89:THR:N	1.97	0.52
1:C:300:VAL:CG2	1:C:317:LEU:HD23	2.31	0.52
1:F:325:ILE:HG22	1:F:326:ASN:H	1.74	0.52
1:G:321:LYS:HE3	1:G:321:LYS:HA	1.91	0.52
1:E:378:VAL:HG12	1:E:380:LYS:HD2	1.90	0.52
1:A:36:ARG:HG3	1:G:518:GLU:HG3	1.91	0.52
1:A:288:MET:HA	1:A:291:ASP:OD2	2.10	0.52
1:F:288:MET:HA	1:F:291:ASP:OD2	2.10	0.52
1:B:300:VAL:CG2	1:B:317:LEU:HD23	2.31	0.52
1:F:321:LYS:HA	1:F:321:LYS:HE3	1.91	0.52
1:B:321:LYS:HA	1:B:321:LYS:HE3	1.91	0.52
1:G:463:SER:O	1:G:467:ASN:HB2	2.09	0.52
1:D:300:VAL:CG2	1:D:317:LEU:HD23	2.31	0.52
1:A:501:ARG:NH1	1:A:505:GLN:OE1	2.43	0.52
1:D:183:LEU:HD12	1:D:383:ALA:O	2.10	0.52
1:C:362:ARG:CZ	1:C:366:GLN:NE2	2.73	0.52
1:E:362:ARG:CZ	1:E:366:GLN:NE2	2.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:288:MET:HA	1:D:291:ASP:OD2	2.10	0.52
1:A:321:LYS:HE3	1:A:321:LYS:HA	1.92	0.52
1:E:501:ARG:NH1	1:E:505:GLN:NE2	2.58	0.52
1:C:34:LYS:O	1:C:457:ASN:HB3	2.09	0.52
1:B:288:MET:HA	1:B:291:ASP:OD2	2.10	0.52
1:D:362:ARG:CZ	1:D:366:GLN:NE2	2.72	0.52
1:C:501:ARG:NH1	1:C:505:GLN:OE1	2.43	0.52
1:G:501:ARG:NH1	1:G:505:GLN:OE1	2.43	0.52
1:D:517:THR:HA	1:E:37:ASN:HB2	1.91	0.52
1:C:183:LEU:HD12	1:C:383:ALA:O	2.10	0.52
1:C:288:MET:HA	1:C:291:ASP:OD2	2.10	0.52
1:E:325:ILE:HG22	1:E:326:ASN:H	1.74	0.52
1:E:321:LYS:HE3	1:E:321:LYS:HA	1.92	0.52
1:F:521:VAL:HB	1:G:40:LEU:HD23	1.90	0.52
1:B:463:SER:O	1:B:467:ASN:HB2	2.09	0.52
1:B:34:LYS:O	1:B:457:ASN:HB3	2.09	0.52
1:E:288:MET:HA	1:E:291:ASP:OD2	2.10	0.52
1:C:321:LYS:HE3	1:C:321:LYS:HA	1.91	0.52
1:E:501:ARG:NH1	1:E:505:GLN:OE1	2.43	0.52
1:B:183:LEU:HD12	1:B:383:ALA:O	2.10	0.52
1:G:362:ARG:CZ	1:G:366:GLN:NE2	2.72	0.51
1:B:281:PHE:CE2	1:C:389:MET:HB3	2.43	0.51
1:D:501:ARG:NH1	1:D:505:GLN:OE1	2.43	0.51
1:F:501:ARG:NH1	1:F:505:GLN:OE1	2.43	0.51
1:B:501:ARG:NH1	1:B:505:GLN:OE1	2.43	0.51
1:A:183:LEU:HD12	1:A:383:ALA:O	2.10	0.51
1:E:183:LEU:HD12	1:E:383:ALA:O	2.10	0.51
1:G:501:ARG:NH1	1:G:505:GLN:NE2	2.58	0.51
1:G:288:MET:HA	1:G:291:ASP:OD2	2.10	0.51
1:B:501:ARG:NH1	1:B:505:GLN:NE2	2.58	0.51
1:G:183:LEU:HD12	1:G:383:ALA:O	2.10	0.51
1:F:362:ARG:CZ	1:F:366:GLN:NE2	2.73	0.51
1:B:353:ILE:HG12	1:B:365:LEU:HB3	1.93	0.51
1:D:453:GLN:O	1:D:456:LEU:N	2.44	0.51
1:C:353:ILE:HG12	1:C:365:LEU:HB3	1.93	0.51
1:D:325:ILE:HG22	1:D:326:ASN:H	1.74	0.51
1:E:453:GLN:O	1:E:456:LEU:N	2.44	0.51
1:A:353:ILE:HG12	1:A:365:LEU:HB3	1.93	0.51
1:E:107:VAL:HG21	1:E:515:ILE:HG23	1.93	0.51
1:A:463:SER:O	1:A:467:ASN:HB2	2.09	0.51
1:A:107:VAL:HG21	1:A:515:ILE:HG23	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:183:LEU:HD12	1:F:383:ALA:O	2.10	0.51
1:G:300:VAL:CG2	1:G:317:LEU:HD23	2.31	0.51
1:E:82:ASN:HD21	1:E:89:THR:N	1.97	0.51
1:D:16:MET:O	1:D:20:VAL:HG23	2.11	0.51
1:E:16:MET:O	1:E:20:VAL:HG23	2.11	0.51
1:G:7:LYS:HZ2	1:G:15:LYS:HE3	1.76	0.51
1:C:107:VAL:HG21	1:C:515:ILE:HG23	1.93	0.51
1:G:146:GLN:HE21	1:G:146:GLN:HA	1.75	0.51
1:G:124:VAL:HG13	1:G:504:LEU:HD13	1.93	0.51
1:B:107:VAL:HG21	1:B:515:ILE:HG23	1.93	0.51
1:A:453:GLN:O	1:A:456:LEU:N	2.44	0.51
1:D:107:VAL:HG21	1:D:515:ILE:HG23	1.93	0.51
1:G:107:VAL:HG21	1:G:515:ILE:HG23	1.93	0.51
1:E:146:GLN:HA	1:E:146:GLN:HE21	1.75	0.51
1:D:327:LYS:O	1:D:328:ASP:HB2	2.11	0.51
1:E:12:ALA:O	1:E:520:MET:HE1	2.11	0.51
1:F:453:GLN:O	1:F:456:LEU:N	2.44	0.51
1:G:453:GLN:O	1:G:456:LEU:N	2.44	0.51
1:D:321:LYS:HE3	1:D:321:LYS:HA	1.91	0.51
1:G:16:MET:O	1:G:20:VAL:HG23	2.11	0.51
1:D:12:ALA:O	1:D:520:MET:HE1	2.11	0.51
1:A:146:GLN:HE21	1:A:146:GLN:HA	1.75	0.51
1:F:124:VAL:HG13	1:F:504:LEU:HD13	1.93	0.51
1:C:146:GLN:HA	1:C:146:GLN:HE21	1.75	0.51
1:A:39:VAL:HG12	1:G:69:MET:CE	2.40	0.51
1:F:16:MET:O	1:F:20:VAL:HG23	2.11	0.51
1:C:327:LYS:O	1:C:328:ASP:HB2	2.11	0.51
1:F:12:ALA:O	1:F:520:MET:HE1	2.11	0.51
1:A:103:GLY:O	1:A:107:VAL:HG23	2.11	0.51
1:C:124:VAL:HG13	1:C:504:LEU:HD13	1.93	0.51
1:G:353:ILE:HG12	1:G:365:LEU:HB3	1.93	0.50
1:B:281:PHE:CG	1:C:389:MET:CE	2.91	0.50
1:E:349:ILE:HG23	1:E:365:LEU:HG	1.93	0.50
1:D:501:ARG:NH1	1:D:505:GLN:NE2	2.58	0.50
1:C:12:ALA:O	1:C:520:MET:HE1	2.11	0.50
1:A:197:ARG:CG	1:A:197:ARG:HH11	2.23	0.50
1:A:16:MET:O	1:A:20:VAL:HG23	2.11	0.50
1:E:327:LYS:O	1:E:328:ASP:HB2	2.11	0.50
1:C:196:ASP:HA	1:C:328:ASP:O	2.12	0.50
1:A:12:ALA:O	1:A:520:MET:HE1	2.11	0.50
1:B:124:VAL:HG13	1:B:504:LEU:HD13	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:73:MET:HG2	1:C:49:ILE:HD11	1.93	0.50
1:C:453:GLN:O	1:C:456:LEU:N	2.44	0.50
1:F:107:VAL:HG21	1:F:515:ILE:HG23	1.93	0.50
1:D:197:ARG:HH11	1:D:197:ARG:CG	2.23	0.50
1:C:197:ARG:HH11	1:C:197:ARG:CG	2.23	0.50
1:F:417:VAL:HG21	1:F:477:GLY:HA3	1.94	0.50
1:G:196:ASP:HA	1:G:328:ASP:O	2.12	0.50
1:C:140:ASP:OD2	1:C:142:LYS:HB2	2.11	0.50
1:G:103:GLY:O	1:G:107:VAL:HG23	2.10	0.50
1:F:146:GLN:HA	1:F:146:GLN:HE21	1.75	0.50
1:B:453:GLN:O	1:B:456:LEU:N	2.44	0.50
1:C:325:ILE:HG22	1:C:326:ASN:H	1.74	0.50
1:B:197:ARG:CG	1:B:197:ARG:HH11	2.23	0.50
1:G:417:VAL:HG21	1:G:477:GLY:HA3	1.94	0.50
1:B:16:MET:O	1:B:20:VAL:HG23	2.11	0.50
1:D:251:ALA:O	1:D:277:LYS:HA	2.12	0.50
1:F:196:ASP:HA	1:F:328:ASP:O	2.12	0.50
1:B:140:ASP:OD2	1:B:142:LYS:HB2	2.11	0.50
1:G:12:ALA:O	1:G:520:MET:HE1	2.11	0.50
1:D:35:GLY:O	1:D:51:LYS:HE2	2.11	0.50
1:F:35:GLY:O	1:F:51:LYS:HE2	2.11	0.50
1:A:124:VAL:HG13	1:A:504:LEU:HD13	1.93	0.50
1:B:35:GLY:O	1:B:51:LYS:HE2	2.12	0.50
1:D:353:ILE:HG12	1:D:365:LEU:HB3	1.93	0.50
1:G:197:ARG:CG	1:G:197:ARG:HH11	2.23	0.50
1:C:16:MET:O	1:C:20:VAL:HG23	2.11	0.50
1:E:251:ALA:O	1:E:277:LYS:HA	2.12	0.50
1:F:327:LYS:O	1:F:328:ASP:HB2	2.11	0.50
1:A:140:ASP:OD2	1:A:142:LYS:HB2	2.11	0.50
1:C:103:GLY:O	1:C:107:VAL:HG23	2.10	0.50
1:B:103:GLY:O	1:B:107:VAL:HG23	2.11	0.50
1:F:413:ALA:HB2	1:F:475:ASN:HB3	1.93	0.50
1:E:124:VAL:HG13	1:E:504:LEU:HD13	1.93	0.50
1:D:349:ILE:HG23	1:D:365:LEU:HG	1.93	0.50
1:E:221:LEU:HD12	1:E:300:VAL:CG1	2.39	0.50
1:B:82:ASN:HD22	1:B:82:ASN:N	2.09	0.50
1:B:327:LYS:O	1:B:328:ASP:HB2	2.12	0.50
1:D:124:VAL:HG13	1:D:504:LEU:HD13	1.93	0.50
1:G:35:GLY:O	1:G:51:LYS:HE2	2.11	0.50
1:D:281:PHE:CD2	1:E:386:GLU:HA	2.47	0.50
1:C:66:PHE:HB3	1:C:520:MET:HE3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:35:GLY:O	1:E:51:LYS:HE2	2.11	0.50
1:A:66:PHE:HB3	1:A:520:MET:HE3	1.93	0.50
1:C:251:ALA:O	1:C:277:LYS:HA	2.12	0.50
1:G:413:ALA:HB2	1:G:475:ASN:HB3	1.93	0.50
1:B:146:GLN:HA	1:B:146:GLN:HE21	1.75	0.50
1:D:146:GLN:HA	1:D:146:GLN:HE21	1.75	0.50
1:F:353:ILE:HG12	1:F:365:LEU:HB3	1.93	0.50
1:C:82:ASN:HD22	1:C:82:ASN:N	2.09	0.50
1:D:82:ASN:O	1:D:86:GLY:N	2.43	0.50
1:E:513:LEU:HD22	1:F:49:ILE:HG21	1.94	0.50
1:B:66:PHE:HB3	1:B:520:MET:HE3	1.93	0.50
1:D:140:ASP:OD2	1:D:142:LYS:HB2	2.11	0.50
1:A:413:ALA:HB2	1:A:475:ASN:HB3	1.93	0.50
1:E:417:VAL:HG21	1:E:477:GLY:HA3	1.94	0.50
1:B:300:VAL:HG21	1:B:317:LEU:CD2	2.34	0.50
1:F:82:ASN:N	1:F:82:ASN:HD22	2.09	0.50
1:E:197:ARG:CG	1:E:197:ARG:HH11	2.23	0.50
1:B:196:ASP:HA	1:B:328:ASP:O	2.12	0.50
1:E:196:ASP:HA	1:E:328:ASP:O	2.12	0.50
1:F:176:THR:HG21	1:F:333:ILE:CD1	2.42	0.50
1:G:140:ASP:OD2	1:G:142:LYS:HB2	2.11	0.50
1:D:103:GLY:O	1:D:107:VAL:HG23	2.10	0.50
1:E:413:ALA:HB2	1:E:475:ASN:HB3	1.93	0.50
1:A:349:ILE:HG23	1:A:365:LEU:HG	1.93	0.50
1:F:349:ILE:HG23	1:F:365:LEU:HG	1.93	0.50
1:B:349:ILE:HG23	1:B:365:LEU:HG	1.92	0.50
1:E:353:ILE:HG12	1:E:365:LEU:HB3	1.93	0.50
1:E:300:VAL:CG2	1:E:317:LEU:HD23	2.31	0.50
1:F:197:ARG:CG	1:F:197:ARG:HH11	2.23	0.50
1:A:35:GLY:O	1:A:51:LYS:HE2	2.12	0.50
1:C:349:ILE:HG23	1:C:365:LEU:HG	1.93	0.49
1:A:361:ASP:O	1:A:365:LEU:HB2	2.12	0.49
1:B:222:LEU:HD22	1:B:289:LEU:O	2.12	0.49
1:E:82:ASN:HD22	1:E:82:ASN:N	2.09	0.49
1:A:348:GLN:O	1:A:352:GLN:HG3	2.12	0.49
1:G:348:GLN:O	1:G:352:GLN:HG3	2.12	0.49
1:D:517:THR:CG2	1:E:39:VAL:HG23	2.42	0.49
1:G:327:LYS:O	1:G:328:ASP:HB2	2.12	0.49
1:D:66:PHE:HB3	1:D:520:MET:HE3	1.93	0.49
1:F:103:GLY:O	1:F:107:VAL:HG23	2.11	0.49
1:B:413:ALA:HB2	1:B:475:ASN:HB3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:413:ALA:HB2	1:C:475:ASN:HB3	1.93	0.49
1:A:417:VAL:HG21	1:A:477:GLY:HA3	1.94	0.49
1:G:361:ASP:O	1:G:365:LEU:HB2	2.12	0.49
1:G:349:ILE:HG23	1:G:365:LEU:HG	1.93	0.49
1:C:361:ASP:O	1:C:365:LEU:HB2	2.12	0.49
1:D:348:GLN:O	1:D:352:GLN:HG3	2.12	0.49
1:C:348:GLN:O	1:C:352:GLN:HG3	2.12	0.49
1:A:327:LYS:O	1:A:328:ASP:HB2	2.11	0.49
1:B:251:ALA:O	1:B:277:LYS:HA	2.12	0.49
1:F:251:ALA:O	1:F:277:LYS:HA	2.12	0.49
1:B:12:ALA:O	1:B:520:MET:HE1	2.11	0.49
1:B:176:THR:HG21	1:B:333:ILE:CD1	2.42	0.49
1:C:35:GLY:O	1:C:51:LYS:HE2	2.11	0.49
1:C:455:VAL:O	1:C:458:CYS:HB2	2.13	0.49
1:A:386:GLU:OE2	1:G:285:ARG:CZ	2.51	0.49
1:G:82:ASN:HD22	1:G:82:ASN:N	2.09	0.49
1:D:222:LEU:HD22	1:D:289:LEU:O	2.12	0.49
1:C:222:LEU:HD22	1:C:289:LEU:O	2.12	0.49
1:F:348:GLN:O	1:F:352:GLN:HG3	2.12	0.49
1:E:455:VAL:O	1:E:458:CYS:HB2	2.13	0.49
1:D:196:ASP:HA	1:D:328:ASP:O	2.12	0.49
1:A:196:ASP:HA	1:A:328:ASP:O	2.12	0.49
1:G:66:PHE:HB3	1:G:520:MET:HE3	1.93	0.49
1:D:417:VAL:HG21	1:D:477:GLY:HA3	1.94	0.49
1:G:455:VAL:O	1:G:458:CYS:HB2	2.12	0.49
1:A:364:LYS:NZ	1:A:365:LEU:HD13	2.22	0.49
1:D:82:ASN:N	1:D:82:ASN:HD22	2.09	0.49
1:A:222:LEU:HD22	1:A:289:LEU:O	2.12	0.49
1:D:162:ILE:O	1:D:166:MET:HB2	2.13	0.49
1:E:348:GLN:O	1:E:352:GLN:HG3	2.12	0.49
1:B:348:GLN:O	1:B:352:GLN:HG3	2.12	0.49
1:D:176:THR:HG21	1:D:333:ILE:CD1	2.42	0.49
1:G:251:ALA:O	1:G:277:LYS:HA	2.12	0.49
1:G:176:THR:HG21	1:G:333:ILE:CD1	2.42	0.49
1:D:413:ALA:HB2	1:D:475:ASN:HB3	1.93	0.49
1:E:361:ASP:O	1:E:365:LEU:HB2	2.12	0.49
1:C:82:ASN:O	1:C:86:GLY:N	2.43	0.49
1:G:300:VAL:HG21	1:G:317:LEU:CD2	2.34	0.49
1:E:82:ASN:O	1:E:86:GLY:N	2.43	0.49
1:B:325:ILE:HG22	1:B:326:ASN:H	1.74	0.49
1:C:162:ILE:O	1:C:166:MET:HB2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:132:LYS:HD2	1:G:497:THR:HG21	1.95	0.49
1:D:132:LYS:HD2	1:D:497:THR:HG21	1.95	0.49
1:A:132:LYS:HD2	1:A:497:THR:HG21	1.95	0.49
1:E:140:ASP:OD2	1:E:142:LYS:HB2	2.11	0.49
1:D:441:LYS:HE3	1:D:445:ARG:NH1	2.28	0.49
1:C:349:ILE:O	1:C:353:ILE:HG13	2.13	0.49
1:E:281:PHE:CZ	1:F:389:MET:CG	2.96	0.49
1:A:82:ASN:N	1:A:82:ASN:HD22	2.09	0.49
1:D:300:VAL:HG21	1:D:317:LEU:CD2	2.34	0.49
1:C:132:LYS:HD2	1:C:497:THR:HG21	1.95	0.49
1:E:132:LYS:HD2	1:E:497:THR:HG21	1.95	0.49
1:F:66:PHE:HB3	1:F:520:MET:HE3	1.93	0.49
1:E:103:GLY:O	1:E:107:VAL:HG23	2.10	0.49
1:A:455:VAL:O	1:A:458:CYS:HB2	2.13	0.49
1:G:353:ILE:O	1:G:356:ALA:HB3	2.13	0.49
1:A:349:ILE:O	1:A:353:ILE:HG13	2.13	0.49
1:F:361:ASP:O	1:F:365:LEU:HB2	2.12	0.49
1:E:349:ILE:O	1:E:353:ILE:HG13	2.13	0.49
1:B:162:ILE:O	1:B:166:MET:HB2	2.13	0.49
1:F:132:LYS:HD2	1:F:497:THR:HG21	1.95	0.49
1:F:441:LYS:HE3	1:F:445:ARG:NH1	2.28	0.49
1:C:281:PHE:CD2	1:D:386:GLU:CA	2.96	0.49
1:B:353:ILE:O	1:B:356:ALA:HB3	2.13	0.49
1:B:281:PHE:HE2	1:C:385:THR:C	2.16	0.49
1:B:132:LYS:HD2	1:B:497:THR:HG21	1.95	0.49
1:E:66:PHE:HB3	1:E:520:MET:HE3	1.93	0.49
1:A:176:THR:HG21	1:A:333:ILE:CD1	2.42	0.49
1:D:85:ALA:HB1	1:D:499:VAL:HG12	1.94	0.49
1:C:417:VAL:HG21	1:C:477:GLY:HA3	1.94	0.49
1:B:441:LYS:HE3	1:B:445:ARG:NH1	2.28	0.49
1:A:389:MET:HB2	1:G:281:PHE:CZ	2.48	0.49
1:B:361:ASP:O	1:B:365:LEU:HB2	2.12	0.49
1:E:353:ILE:O	1:E:356:ALA:HB3	2.13	0.49
1:E:222:LEU:HD22	1:E:289:LEU:O	2.12	0.49
1:A:300:VAL:HG21	1:A:317:LEU:CD2	2.34	0.49
1:B:82:ASN:O	1:B:86:GLY:N	2.43	0.49
1:E:162:ILE:O	1:E:166:MET:HB2	2.13	0.49
1:D:69:MET:HE1	1:E:39:VAL:HG12	1.95	0.49
1:F:140:ASP:OD2	1:F:142:LYS:HB2	2.11	0.49
1:F:165:ALA:HB2	1:F:379:ILE:HD11	1.94	0.49
1:B:455:VAL:O	1:B:458:CYS:HB2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:349:ILE:O	1:G:353:ILE:HG13	2.13	0.49
1:B:284:ARG:NH2	1:B:360:TYR:HH	2.11	0.49
1:D:353:ILE:O	1:D:356:ALA:HB3	2.13	0.49
1:G:222:LEU:HD22	1:G:289:LEU:O	2.12	0.49
1:C:300:VAL:HG21	1:C:317:LEU:CD2	2.34	0.49
1:G:441:LYS:HE3	1:G:445:ARG:NH1	2.28	0.49
1:E:281:PHE:CG	1:F:389:MET:CE	2.96	0.48
1:F:222:LEU:HD22	1:F:289:LEU:O	2.12	0.48
1:F:27:VAL:HG21	1:F:57:ALA:HB2	1.95	0.48
1:A:441:LYS:HE3	1:A:445:ARG:NH1	2.28	0.48
1:E:85:ALA:HB1	1:E:499:VAL:HG12	1.94	0.48
1:B:417:VAL:HG21	1:B:477:GLY:HA3	1.94	0.48
1:E:165:ALA:HB2	1:E:379:ILE:HD11	1.95	0.48
1:D:282:GLY:HA2	1:E:181:THR:O	1.94	0.48
1:C:353:ILE:O	1:C:356:ALA:HB3	2.13	0.48
1:A:353:ILE:O	1:A:356:ALA:HB3	2.13	0.48
1:B:349:ILE:O	1:B:353:ILE:HG13	2.13	0.48
1:A:325:ILE:HG22	1:A:326:ASN:H	1.74	0.48
1:F:162:ILE:O	1:F:166:MET:HB2	2.13	0.48
1:C:27:VAL:HG21	1:C:57:ALA:HB2	1.96	0.48
1:B:85:ALA:HB1	1:B:499:VAL:HG12	1.94	0.48
1:G:130:GLU:OE2	1:G:425:LYS:HD3	2.13	0.48
1:A:85:ALA:HB1	1:A:499:VAL:HG12	1.94	0.48
1:C:85:ALA:HB1	1:C:499:VAL:HG12	1.94	0.48
1:E:281:PHE:HD2	1:F:386:GLU:CA	2.26	0.48
1:F:501:ARG:NH1	1:F:505:GLN:NE2	2.58	0.48
1:E:27:VAL:HG21	1:E:57:ALA:HB2	1.95	0.48
1:A:501:ARG:NH1	1:A:505:GLN:NE2	2.58	0.48
1:B:27:VAL:HG21	1:B:57:ALA:HB2	1.96	0.48
1:A:251:ALA:O	1:A:277:LYS:HA	2.12	0.48
1:F:455:VAL:O	1:F:458:CYS:HB2	2.12	0.48
1:C:522:THR:HA	1:D:41:ASP:HB2	1.96	0.48
1:G:85:ALA:HB1	1:G:499:VAL:HG12	1.94	0.48
1:A:324:VAL:CG1	1:A:324:VAL:O	2.62	0.48
1:A:162:ILE:O	1:A:166:MET:HB2	2.13	0.48
1:F:111:MET:HG2	1:F:435:ASP:OD1	2.13	0.48
1:E:176:THR:HG21	1:E:333:ILE:CD1	2.42	0.48
1:B:130:GLU:OE2	1:B:425:LYS:HD3	2.14	0.48
1:F:85:ALA:HB1	1:F:499:VAL:HG12	1.94	0.48
1:D:455:VAL:O	1:D:458:CYS:HB2	2.13	0.48
1:G:324:VAL:O	1:G:324:VAL:CG1	2.62	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:221:LEU:HD12	1:C:300:VAL:CG1	2.39	0.48
1:C:176:THR:HG21	1:C:333:ILE:CD1	2.42	0.48
1:E:146:GLN:O	1:E:150:ILE:HG13	2.14	0.48
1:C:441:LYS:HE3	1:C:445:ARG:NH1	2.28	0.48
1:C:364:LYS:NZ	1:C:365:LEU:HD13	2.22	0.48
1:F:349:ILE:O	1:F:353:ILE:HG13	2.13	0.48
1:F:353:ILE:O	1:F:356:ALA:HB3	2.13	0.48
1:G:82:ASN:O	1:G:86:GLY:N	2.43	0.48
1:A:82:ASN:O	1:A:86:GLY:N	2.43	0.48
1:E:111:MET:HG2	1:E:435:ASP:OD1	2.13	0.48
1:G:111:MET:HG2	1:G:435:ASP:OD1	2.13	0.48
1:D:128:VAL:HG22	1:D:501:ARG:HG3	1.96	0.48
1:B:128:VAL:HG22	1:B:501:ARG:HG3	1.96	0.48
1:E:128:VAL:HG22	1:E:501:ARG:HG3	1.96	0.48
1:D:346:VAL:HG21	1:D:373:ALA:HB2	1.96	0.48
1:C:327:LYS:O	1:C:328:ASP:CB	2.62	0.48
1:A:165:ALA:HB2	1:A:379:ILE:HD11	1.94	0.48
1:D:349:ILE:O	1:D:353:ILE:HG13	2.13	0.48
1:D:361:ASP:O	1:D:365:LEU:HB2	2.12	0.48
1:F:82:ASN:O	1:F:86:GLY:N	2.43	0.48
1:A:111:MET:HG2	1:A:435:ASP:OD1	2.13	0.48
1:C:128:VAL:HG22	1:C:501:ARG:HG3	1.96	0.48
1:F:128:VAL:HG22	1:F:501:ARG:HG3	1.96	0.48
1:C:346:VAL:HG21	1:C:373:ALA:HB2	1.96	0.48
1:D:327:LYS:O	1:D:328:ASP:CB	2.62	0.48
1:F:146:GLN:O	1:F:150:ILE:HG13	2.14	0.48
1:D:130:GLU:OE2	1:D:425:LYS:HD3	2.13	0.48
1:B:165:ALA:HB2	1:B:379:ILE:HD11	1.95	0.48
1:D:165:ALA:HB2	1:D:379:ILE:HD11	1.95	0.48
1:B:346:VAL:HG21	1:B:373:ALA:HB2	1.96	0.48
1:G:325:ILE:HG22	1:G:326:ASN:H	1.74	0.48
1:G:27:VAL:HG21	1:G:57:ALA:HB2	1.96	0.48
1:B:327:LYS:O	1:B:328:ASP:CB	2.62	0.48
1:F:413:ALA:HA	1:F:489:ILE:HD11	1.96	0.48
1:D:146:GLN:O	1:D:150:ILE:HG13	2.14	0.48
1:D:521:VAL:HB	1:E:40:LEU:CD2	2.43	0.48
1:C:165:ALA:HB2	1:C:379:ILE:HD11	1.94	0.48
1:D:32:GLY:HA2	1:D:454:ILE:HG12	1.96	0.48
1:G:162:ILE:O	1:G:166:MET:HB2	2.13	0.48
1:B:111:MET:HG2	1:B:435:ASP:OD1	2.13	0.48
1:C:501:ARG:NH1	1:C:505:GLN:NE2	2.58	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:195:PHE:HZ	1:D:250:ILE:HD11	1.79	0.48
1:E:413:ALA:HA	1:E:489:ILE:HD11	1.96	0.48
1:E:441:LYS:HE3	1:E:445:ARG:NH1	2.28	0.48
1:G:165:ALA:HB2	1:G:379:ILE:HD11	1.95	0.48
1:C:353:ILE:CG2	1:C:362:ARG:HG2	2.44	0.48
1:B:353:ILE:CG2	1:B:362:ARG:HG2	2.44	0.48
1:F:324:VAL:O	1:F:324:VAL:CG1	2.62	0.48
1:E:300:VAL:HG21	1:E:317:LEU:CD2	2.34	0.48
1:F:300:VAL:HG21	1:F:317:LEU:CD2	2.34	0.48
1:A:128:VAL:HG22	1:A:501:ARG:HG3	1.96	0.48
1:F:49:ILE:HD12	1:F:49:ILE:N	2.29	0.48
1:A:146:GLN:O	1:A:150:ILE:HG13	2.14	0.48
1:E:32:GLY:HA2	1:E:454:ILE:HG12	1.96	0.48
1:G:221:LEU:HD12	1:G:300:VAL:CG1	2.39	0.47
1:E:195:PHE:CE2	1:E:197:ARG:HB2	2.49	0.47
1:B:195:PHE:HZ	1:B:250:ILE:HD11	1.79	0.47
1:F:195:PHE:HZ	1:F:250:ILE:HD11	1.79	0.47
1:A:346:VAL:HG21	1:A:373:ALA:HB2	1.96	0.47
1:E:346:VAL:HG21	1:E:373:ALA:HB2	1.96	0.47
1:A:327:LYS:O	1:A:328:ASP:CB	2.62	0.47
1:C:146:GLN:O	1:C:150:ILE:HG13	2.14	0.47
1:C:49:ILE:HD12	1:C:49:ILE:N	2.29	0.47
1:G:413:ALA:HA	1:G:489:ILE:HD11	1.96	0.47
1:F:32:GLY:HA2	1:F:454:ILE:HG12	1.96	0.47
1:C:32:GLY:HA2	1:C:454:ILE:HG12	1.96	0.47
1:G:49:ILE:HD12	1:G:49:ILE:N	2.29	0.47
1:B:49:ILE:N	1:B:49:ILE:HD12	2.29	0.47
1:G:346:VAL:HG21	1:G:373:ALA:HB2	1.96	0.47
1:F:353:ILE:CG2	1:F:362:ARG:HG2	2.44	0.47
1:E:218:PRO:O	1:E:319:GLN:O	2.32	0.47
1:G:128:VAL:HG22	1:G:501:ARG:HG3	1.96	0.47
1:E:49:ILE:HD12	1:E:49:ILE:N	2.29	0.47
1:G:146:GLN:O	1:G:150:ILE:HG13	2.14	0.47
1:A:49:ILE:HD12	1:A:49:ILE:N	2.29	0.47
1:E:130:GLU:OE2	1:E:425:LYS:HD3	2.13	0.47
1:C:111:MET:HG2	1:C:435:ASP:OD1	2.13	0.47
1:A:195:PHE:CE2	1:A:197:ARG:HB2	2.49	0.47
1:E:195:PHE:HZ	1:E:250:ILE:HD11	1.79	0.47
1:F:195:PHE:CE2	1:F:197:ARG:HB2	2.49	0.47
1:F:346:VAL:HG21	1:F:373:ALA:HB2	1.96	0.47
1:D:521:VAL:HB	1:E:40:LEU:HD23	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:32:GLY:HA2	1:G:454:ILE:HG12	1.96	0.47
1:C:130:GLU:OE2	1:C:425:LYS:HD3	2.14	0.47
1:D:49:ILE:N	1:D:49:ILE:HD12	2.29	0.47
1:F:130:GLU:OE2	1:F:425:LYS:HD3	2.13	0.47
1:B:82:ASN:HD21	1:B:89:THR:N	1.97	0.47
1:D:27:VAL:HG21	1:D:57:ALA:HB2	1.95	0.47
1:A:195:PHE:HZ	1:A:250:ILE:HD11	1.79	0.47
1:C:195:PHE:HZ	1:C:250:ILE:HD11	1.79	0.47
1:E:327:LYS:O	1:E:328:ASP:CB	2.62	0.47
1:B:32:GLY:HA2	1:B:454:ILE:HG12	1.96	0.47
1:G:325:ILE:CG2	1:G:326:ASN:N	2.77	0.47
1:G:218:PRO:O	1:G:319:GLN:O	2.32	0.47
1:A:27:VAL:HG21	1:A:57:ALA:HB2	1.95	0.47
1:G:195:PHE:CE2	1:G:197:ARG:HB2	2.49	0.47
1:C:195:PHE:CE2	1:C:197:ARG:HB2	2.49	0.47
1:B:146:GLN:O	1:B:150:ILE:HG13	2.14	0.47
1:A:32:GLY:HA2	1:A:454:ILE:HG12	1.96	0.47
1:B:286:LYS:HB3	1:B:286:LYS:HE2	1.77	0.47
1:A:353:ILE:CG2	1:A:362:ARG:HG2	2.44	0.47
1:F:218:PRO:O	1:F:319:GLN:O	2.32	0.47
1:D:111:MET:HG2	1:D:435:ASP:OD1	2.13	0.47
1:G:376:VAL:HG12	1:G:377:ALA:N	2.29	0.47
1:A:376:VAL:HG12	1:A:377:ALA:N	2.29	0.47
1:F:376:VAL:HG12	1:F:377:ALA:N	2.29	0.47
1:A:130:GLU:OE2	1:A:425:LYS:HD3	2.13	0.47
1:E:332:ILE:HG22	1:E:332:ILE:O	2.14	0.47
1:A:284:ARG:NH2	1:A:360:TYR:OH	2.48	0.47
1:B:281:PHE:HE2	1:C:385:THR:O	1.97	0.47
1:E:324:VAL:CG1	1:E:324:VAL:O	2.62	0.47
1:D:353:ILE:CG2	1:D:362:ARG:HG2	2.44	0.47
1:F:82:ASN:HD21	1:F:89:THR:N	1.97	0.47
1:D:218:PRO:O	1:D:319:GLN:O	2.32	0.47
1:C:218:PRO:O	1:C:319:GLN:O	2.32	0.47
1:B:376:VAL:HG12	1:B:377:ALA:N	2.29	0.47
1:A:395:ARG:O	1:A:398:ASP:HB3	2.15	0.47
1:D:395:ARG:O	1:D:398:ASP:HB3	2.15	0.47
1:F:395:ARG:O	1:F:398:ASP:HB3	2.15	0.47
1:G:327:LYS:O	1:G:328:ASP:CB	2.62	0.47
1:F:327:LYS:O	1:F:328:ASP:CB	2.62	0.47
1:A:413:ALA:HA	1:A:489:ILE:HD11	1.96	0.47
1:D:413:ALA:HA	1:D:489:ILE:HD11	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:297:GLY:O	1:E:299:THR:HG23	2.15	0.47
1:C:286:LYS:HE2	1:C:286:LYS:HB3	1.77	0.47
1:F:332:ILE:O	1:F:332:ILE:HG22	2.14	0.47
1:A:332:ILE:O	1:A:332:ILE:HG22	2.14	0.47
1:D:297:GLY:O	1:D:299:THR:HG23	2.15	0.47
1:F:297:GLY:O	1:F:299:THR:HG23	2.15	0.47
1:G:353:ILE:CG2	1:G:362:ARG:HG2	2.44	0.47
1:B:284:ARG:NH2	1:B:360:TYR:OH	2.48	0.47
1:B:218:PRO:O	1:B:319:GLN:O	2.32	0.47
1:G:195:PHE:HZ	1:G:250:ILE:HD11	1.79	0.47
1:C:395:ARG:O	1:C:398:ASP:HB3	2.15	0.47
1:E:284:ARG:NH2	1:E:360:TYR:OH	2.48	0.47
1:E:353:ILE:CG2	1:E:362:ARG:HG2	2.44	0.47
1:D:217:SER:N	1:D:321:LYS:O	2.48	0.47
1:A:218:PRO:O	1:A:319:GLN:O	2.32	0.47
1:E:376:VAL:HG12	1:E:377:ALA:N	2.29	0.47
1:D:332:ILE:O	1:D:332:ILE:HG22	2.14	0.47
1:G:284:ARG:NH2	1:G:360:TYR:OH	2.48	0.47
1:C:284:ARG:NH2	1:C:360:TYR:OH	2.48	0.47
1:F:284:ARG:NH2	1:F:360:TYR:OH	2.48	0.47
1:A:221:LEU:HD12	1:A:300:VAL:CG1	2.39	0.47
1:B:217:SER:N	1:B:321:LYS:O	2.48	0.47
1:B:195:PHE:CE2	1:B:197:ARG:HB2	2.49	0.47
1:B:395:ARG:O	1:B:398:ASP:HB3	2.15	0.47
1:E:217:SER:N	1:E:321:LYS:O	2.48	0.46
1:D:319:GLN:HB2	1:D:336:VAL:HG21	1.97	0.46
1:C:319:GLN:HB2	1:C:336:VAL:HG21	1.97	0.46
1:E:352:GLN:O	1:E:355:GLU:HG2	2.15	0.46
1:E:395:ARG:O	1:E:398:ASP:HB3	2.15	0.46
1:G:297:GLY:O	1:G:299:THR:HG23	2.15	0.46
1:C:217:SER:N	1:C:321:LYS:O	2.48	0.46
1:A:319:GLN:HB2	1:A:336:VAL:HG21	1.97	0.46
1:B:174:VAL:O	1:B:174:VAL:HG13	2.16	0.46
1:C:376:VAL:HG12	1:C:377:ALA:N	2.29	0.46
1:F:479:ASN:O	1:F:483:GLU:N	2.49	0.46
1:C:479:ASN:O	1:C:483:GLU:N	2.49	0.46
1:E:281:PHE:CE2	1:F:389:MET:HB3	2.50	0.46
1:B:319:GLN:HB2	1:B:336:VAL:HG21	1.97	0.46
1:D:376:VAL:HG12	1:D:377:ALA:N	2.29	0.46
1:C:174:VAL:HG13	1:C:174:VAL:O	2.16	0.46
1:D:195:PHE:CE2	1:D:197:ARG:HB2	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:100:ILE:CD1	1:F:514:MET:SD	3.03	0.46
1:A:479:ASN:O	1:A:483:GLU:N	2.49	0.46
1:B:332:ILE:HG22	1:B:332:ILE:O	2.14	0.46
1:C:297:GLY:O	1:C:299:THR:HG23	2.15	0.46
1:B:325:ILE:CG2	1:B:326:ASN:N	2.77	0.46
1:F:217:SER:N	1:F:321:LYS:O	2.48	0.46
1:G:217:SER:N	1:G:321:LYS:O	2.48	0.46
1:G:319:GLN:HB2	1:G:336:VAL:HG21	1.97	0.46
1:D:174:VAL:O	1:D:174:VAL:HG13	2.16	0.46
1:D:100:ILE:CD1	1:D:514:MET:SD	3.03	0.46
1:E:432:GLN:HB2	1:E:436:GLN:CD	2.36	0.46
1:G:499:VAL:O	1:G:503:ALA:HB2	2.16	0.46
1:F:499:VAL:O	1:F:503:ALA:HB2	2.16	0.46
1:E:479:ASN:O	1:E:483:GLU:N	2.49	0.46
1:C:332:ILE:HG22	1:C:332:ILE:O	2.14	0.46
1:G:364:LYS:NZ	1:G:365:LEU:HD13	2.22	0.46
1:D:324:VAL:CG1	1:D:324:VAL:O	2.62	0.46
1:D:284:ARG:NH2	1:D:360:TYR:OH	2.48	0.46
1:B:293:ALA:O	1:B:298:GLY:N	2.49	0.46
1:C:293:ALA:O	1:C:298:GLY:N	2.49	0.46
1:F:325:ILE:CG2	1:F:326:ASN:N	2.77	0.46
1:A:217:SER:N	1:A:321:LYS:O	2.48	0.46
1:D:352:GLN:O	1:D:355:GLU:HG2	2.15	0.46
1:B:413:ALA:HA	1:B:489:ILE:HD11	1.96	0.46
1:E:499:VAL:O	1:E:503:ALA:HB2	2.16	0.46
1:F:69:MET:CE	1:G:39:VAL:HG12	2.45	0.46
1:A:297:GLY:O	1:A:299:THR:HG23	2.15	0.46
1:A:116:LEU:O	1:A:120:ILE:HG13	2.15	0.46
1:F:281:PHE:CZ	1:G:389:MET:HB2	2.50	0.46
1:F:221:LEU:HD12	1:F:300:VAL:CG1	2.39	0.46
1:A:174:VAL:HG13	1:A:174:VAL:O	2.16	0.46
1:C:100:ILE:CD1	1:C:514:MET:SD	3.03	0.46
1:B:499:VAL:O	1:B:503:ALA:HB2	2.16	0.46
1:D:222:LEU:H	1:D:300:VAL:CG1	2.29	0.46
1:D:293:ALA:O	1:D:298:GLY:N	2.49	0.46
1:G:205:ILE:HD13	1:G:205:ILE:HA	1.61	0.46
1:B:352:GLN:O	1:B:355:GLU:HG2	2.15	0.46
1:F:432:GLN:HB2	1:F:436:GLN:CD	2.36	0.46
1:G:395:ARG:O	1:G:398:ASP:HB3	2.15	0.46
1:C:413:ALA:HA	1:C:489:ILE:HD11	1.96	0.46
1:G:116:LEU:O	1:G:120:ILE:HG13	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:479:ASN:O	1:D:483:GLU:N	2.49	0.46
1:A:281:PHE:CD2	1:B:386:GLU:HA	2.50	0.46
1:F:362:ARG:CZ	1:F:366:GLN:HE22	2.29	0.46
1:C:222:LEU:H	1:C:300:VAL:CG1	2.29	0.46
1:F:319:GLN:HB2	1:F:336:VAL:HG21	1.97	0.46
1:A:352:GLN:O	1:A:355:GLU:HG2	2.15	0.46
1:F:340:ALA:HA	1:F:343:GLN:CG	2.42	0.46
1:D:432:GLN:HB2	1:D:436:GLN:CD	2.36	0.46
1:B:100:ILE:CD1	1:B:514:MET:SD	3.03	0.46
1:A:499:VAL:O	1:A:503:ALA:HB2	2.16	0.46
1:F:281:PHE:CE2	1:G:385:THR:O	2.67	0.46
1:B:364:LYS:NZ	1:B:365:LEU:HD13	2.22	0.46
1:C:324:VAL:CG1	1:C:324:VAL:O	2.62	0.46
1:A:293:ALA:O	1:A:298:GLY:N	2.49	0.46
1:G:174:VAL:HG13	1:G:174:VAL:O	2.16	0.46
1:E:100:ILE:CD1	1:E:514:MET:SD	3.03	0.46
1:B:479:ASN:O	1:B:483:GLU:N	2.49	0.46
1:F:286:LYS:HB3	1:F:286:LYS:HE2	1.77	0.46
1:D:221:LEU:HD12	1:D:300:VAL:CG1	2.39	0.46
1:E:319:GLN:HB2	1:E:336:VAL:HG21	1.97	0.46
1:C:116:LEU:O	1:C:120:ILE:HG13	2.15	0.46
1:D:116:LEU:O	1:D:120:ILE:HG13	2.15	0.46
1:B:297:GLY:O	1:B:299:THR:HG23	2.15	0.46
1:G:332:ILE:O	1:G:332:ILE:HG22	2.14	0.46
1:B:116:LEU:O	1:B:120:ILE:HG13	2.15	0.46
1:G:362:ARG:CZ	1:G:366:GLN:HE22	2.29	0.45
1:F:364:LYS:NZ	1:F:365:LEU:HD13	2.22	0.45
1:B:362:ARG:CZ	1:B:366:GLN:HE22	2.29	0.45
1:G:352:GLN:O	1:G:355:GLU:HG2	2.15	0.45
1:F:174:VAL:O	1:F:174:VAL:HG13	2.16	0.45
1:A:100:ILE:CD1	1:A:514:MET:SD	3.03	0.45
1:C:499:VAL:O	1:C:503:ALA:HB2	2.16	0.45
1:G:479:ASN:O	1:G:483:GLU:N	2.49	0.45
1:A:286:LYS:HE2	1:A:286:LYS:HB3	1.77	0.45
1:E:350:ARG:HA	1:E:353:ILE:HD12	1.98	0.45
1:D:362:ARG:CZ	1:D:366:GLN:HE22	2.29	0.45
1:B:222:LEU:H	1:B:300:VAL:CG1	2.29	0.45
1:G:195:PHE:O	1:G:330:THR:HG22	2.17	0.45
1:C:432:GLN:HB2	1:C:436:GLN:CD	2.36	0.45
1:D:499:VAL:O	1:D:503:ALA:HB2	2.16	0.45
1:E:116:LEU:O	1:E:120:ILE:HG13	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:116:LEU:O	1:F:120:ILE:HG13	2.15	0.45
1:G:286:LYS:HE2	1:G:286:LYS:HB3	1.77	0.45
1:D:360:TYR:CZ	1:E:183:LEU:HD22	2.51	0.45
1:E:293:ALA:O	1:E:298:GLY:N	2.49	0.45
1:G:293:ALA:O	1:G:298:GLY:N	2.49	0.45
1:D:325:ILE:CG2	1:D:326:ASN:N	2.77	0.45
1:D:205:ILE:HD11	1:D:211:GLY:C	2.37	0.45
1:G:432:GLN:HB2	1:G:436:GLN:CD	2.36	0.45
1:F:77:VAL:CG1	1:F:510:VAL:HG22	2.46	0.45
1:F:350:ARG:HA	1:F:353:ILE:HD12	1.98	0.45
1:B:205:ILE:HD11	1:B:211:GLY:C	2.37	0.45
1:E:174:VAL:HG13	1:E:174:VAL:O	2.16	0.45
1:E:195:PHE:O	1:E:330:THR:HG22	2.17	0.45
1:E:77:VAL:CG1	1:E:510:VAL:HG22	2.46	0.45
1:D:114:MET:HG3	1:E:34:LYS:HB3	1.99	0.45
1:B:7:LYS:HZ1	1:B:15:LYS:HE3	1.81	0.45
1:D:423:ALA:HB2	1:D:447:MET:SD	2.56	0.45
1:D:420:ILE:HG13	1:D:448:GLU:HG2	1.99	0.45
1:A:222:LEU:H	1:A:300:VAL:CG1	2.29	0.45
1:D:298:GLY:C	1:D:300:VAL:N	2.70	0.45
1:C:352:GLN:O	1:C:355:GLU:HG2	2.15	0.45
1:B:195:PHE:O	1:B:330:THR:HG22	2.17	0.45
1:C:195:PHE:O	1:C:330:THR:HG22	2.17	0.45
1:D:165:ALA:HB1	1:D:175:ILE:CG2	2.47	0.45
1:E:423:ALA:HB2	1:E:447:MET:SD	2.56	0.45
1:E:420:ILE:HG13	1:E:448:GLU:HG2	1.99	0.45
1:A:423:ALA:HB2	1:A:447:MET:SD	2.56	0.45
1:C:420:ILE:HG13	1:C:448:GLU:HG2	1.99	0.45
1:A:362:ARG:CZ	1:A:366:GLN:HE22	2.29	0.45
1:A:281:PHE:CD2	1:B:386:GLU:CA	3.00	0.45
1:E:194:GLN:CD	1:E:331:THR:HG22	2.37	0.45
1:F:194:GLN:CD	1:F:331:THR:HG22	2.37	0.45
1:E:319:GLN:O	1:E:320:ALA:HB3	2.17	0.45
1:F:352:GLN:O	1:F:355:GLU:HG2	2.15	0.45
1:C:69:MET:CE	1:D:39:VAL:CG1	2.92	0.45
1:D:77:VAL:CG1	1:D:510:VAL:HG22	2.47	0.45
1:F:168:LYS:HD3	1:F:189:VAL:HG23	1.98	0.45
1:G:168:LYS:HD3	1:G:189:VAL:HG23	1.98	0.45
1:A:168:LYS:HD3	1:A:189:VAL:HG23	1.98	0.45
1:F:165:ALA:HB1	1:F:175:ILE:CG2	2.47	0.45
1:E:165:ALA:HB1	1:E:175:ILE:CG2	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:165:ALA:HB1	1:C:175:ILE:CG2	2.47	0.45
1:G:165:ALA:HB1	1:G:175:ILE:CG2	2.47	0.45
1:G:420:ILE:HG13	1:G:448:GLU:HG2	1.99	0.45
1:G:423:ALA:HB2	1:G:447:MET:SD	2.56	0.45
1:F:423:ALA:HB2	1:F:447:MET:SD	2.56	0.45
1:C:423:ALA:HB2	1:C:447:MET:SD	2.56	0.45
1:B:420:ILE:HG13	1:B:448:GLU:HG2	1.99	0.45
1:C:194:GLN:CD	1:C:331:THR:HG22	2.36	0.45
1:B:194:GLN:CD	1:B:331:THR:HG22	2.36	0.45
1:D:194:GLN:CD	1:D:331:THR:HG22	2.36	0.45
1:E:362:ARG:CZ	1:E:366:GLN:HE22	2.29	0.45
1:E:364:LYS:NZ	1:E:365:LEU:HD13	2.22	0.45
1:D:350:ARG:HA	1:D:353:ILE:HD12	1.99	0.45
1:F:293:ALA:O	1:F:298:GLY:N	2.49	0.45
1:G:319:GLN:O	1:G:320:ALA:HB3	2.17	0.45
1:A:346:VAL:HG11	1:A:373:ALA:CB	2.46	0.45
1:A:7:LYS:HZ1	1:A:15:LYS:HE3	1.81	0.45
1:A:49:ILE:HG12	1:G:73:MET:HE3	1.99	0.45
1:G:194:GLN:CD	1:G:331:THR:HG22	2.37	0.45
1:E:321:LYS:HB3	1:E:334:ASP:HB3	1.99	0.45
1:B:432:GLN:HB2	1:B:436:GLN:CD	2.36	0.45
1:B:168:LYS:HD3	1:B:189:VAL:HG23	1.98	0.45
1:C:168:LYS:HD3	1:C:189:VAL:HG23	1.99	0.45
1:F:420:ILE:HG13	1:F:448:GLU:HG2	1.99	0.45
1:G:350:ARG:HA	1:G:353:ILE:HD12	1.98	0.45
1:D:364:LYS:NZ	1:D:365:LEU:HD13	2.22	0.45
1:G:205:ILE:HD11	1:G:211:GLY:C	2.37	0.45
1:D:319:GLN:O	1:D:320:ALA:HB3	2.17	0.45
1:F:321:LYS:HB3	1:F:334:ASP:HB3	1.99	0.45
1:E:197:ARG:NH2	1:E:280:GLY:H	2.15	0.45
1:A:420:ILE:HG13	1:A:448:GLU:HG2	1.99	0.45
1:B:423:ALA:HB2	1:B:447:MET:SD	2.56	0.45
1:C:350:ARG:HA	1:C:353:ILE:HD12	1.98	0.45
1:A:194:GLN:CD	1:A:331:THR:HG22	2.36	0.45
1:D:168:LYS:HD3	1:D:189:VAL:HG23	1.98	0.45
1:A:165:ALA:HB1	1:A:175:ILE:CG2	2.47	0.45
1:B:165:ALA:HB1	1:B:175:ILE:CG2	2.47	0.45
1:G:346:VAL:HG11	1:G:373:ALA:CB	2.46	0.44
1:A:362:ARG:NE	1:A:366:GLN:NE2	2.65	0.44
1:B:346:VAL:HG11	1:B:373:ALA:CB	2.46	0.44
1:B:362:ARG:NE	1:B:366:GLN:NE2	2.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:324:VAL:O	1:B:324:VAL:CG1	2.62	0.44
1:G:222:LEU:H	1:G:300:VAL:CG1	2.29	0.44
1:B:298:GLY:C	1:B:300:VAL:N	2.70	0.44
1:F:205:ILE:HD11	1:F:211:GLY:C	2.37	0.44
1:G:213:VAL:O	1:G:215:LEU:N	2.50	0.44
1:C:319:GLN:O	1:C:320:ALA:HB3	2.17	0.44
1:D:195:PHE:O	1:D:330:THR:HG22	2.17	0.44
1:A:195:PHE:O	1:A:330:THR:HG22	2.17	0.44
1:C:77:VAL:CG1	1:C:510:VAL:HG22	2.47	0.44
1:D:114:MET:HE2	1:E:35:GLY:O	2.17	0.44
1:E:168:LYS:HD3	1:E:189:VAL:HG23	1.98	0.44
1:A:34:LYS:HG3	1:G:114:MET:HG3	1.98	0.44
1:D:146:GLN:HE21	1:D:146:GLN:CA	2.31	0.44
1:A:350:ARG:HA	1:A:353:ILE:HD12	1.98	0.44
1:E:205:ILE:HD11	1:E:211:GLY:C	2.37	0.44
1:A:213:VAL:O	1:A:215:LEU:N	2.50	0.44
1:A:325:ILE:CG2	1:A:326:ASN:N	2.77	0.44
1:A:319:GLN:O	1:A:320:ALA:HB3	2.17	0.44
1:F:197:ARG:NH2	1:F:280:GLY:H	2.15	0.44
1:A:432:GLN:HB2	1:A:436:GLN:CD	2.36	0.44
1:G:100:ILE:CD1	1:G:514:MET:SD	3.03	0.44
1:E:146:GLN:HE21	1:E:146:GLN:CA	2.31	0.44
1:B:146:GLN:CA	1:B:146:GLN:HE21	2.31	0.44
1:E:413:ALA:HA	1:E:489:ILE:CD1	2.48	0.44
1:G:362:ARG:NE	1:G:366:GLN:NE2	2.65	0.44
1:C:362:ARG:NE	1:C:366:GLN:NE2	2.65	0.44
1:C:362:ARG:CZ	1:C:366:GLN:HE22	2.29	0.44
1:B:350:ARG:HA	1:B:353:ILE:HD12	1.98	0.44
1:D:362:ARG:NE	1:D:366:GLN:NE2	2.65	0.44
1:F:298:GLY:C	1:F:300:VAL:N	2.70	0.44
1:C:298:GLY:C	1:C:300:VAL:N	2.70	0.44
1:F:213:VAL:O	1:F:215:LEU:N	2.50	0.44
1:D:413:ALA:HA	1:D:489:ILE:CD1	2.48	0.44
1:A:298:GLY:C	1:A:300:VAL:N	2.70	0.44
1:D:213:VAL:O	1:D:215:LEU:N	2.51	0.44
1:D:321:LYS:HB3	1:D:334:ASP:HB3	1.99	0.44
1:B:319:GLN:O	1:B:320:ALA:HB3	2.17	0.44
1:G:197:ARG:NH2	1:G:280:GLY:H	2.15	0.44
1:B:197:ARG:NH2	1:B:280:GLY:H	2.15	0.44
1:F:146:GLN:CA	1:F:146:GLN:HE21	2.31	0.44
1:F:413:ALA:HA	1:F:489:ILE:CD1	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:281:PHE:HD2	1:C:386:GLU:CB	2.30	0.44
1:G:321:LYS:HB3	1:G:334:ASP:HB3	1.99	0.44
1:B:321:LYS:HB3	1:B:334:ASP:HB3	1.99	0.44
1:D:197:ARG:NH2	1:D:280:GLY:H	2.15	0.44
1:B:433:ASN:HD21	1:B:436:GLN:HG3	1.82	0.44
1:C:346:VAL:HG11	1:C:373:ALA:CB	2.46	0.44
1:F:277:LYS:HG2	1:F:278:ALA:N	2.32	0.44
1:C:413:ALA:HA	1:C:489:ILE:CD1	2.48	0.44
1:E:282:GLY:HA2	1:F:181:THR:HA	1.73	0.44
1:A:205:ILE:HD11	1:A:211:GLY:C	2.37	0.44
1:B:213:VAL:O	1:B:215:LEU:N	2.50	0.44
1:C:321:LYS:HB3	1:C:334:ASP:HB3	1.99	0.44
1:A:321:LYS:HB3	1:A:334:ASP:HB3	1.99	0.44
1:E:16:MET:HG2	1:E:70:GLY:HA2	1.99	0.44
1:G:413:ALA:HA	1:G:489:ILE:CD1	2.48	0.44
1:F:362:ARG:NE	1:F:366:GLN:NE2	2.65	0.44
1:B:360:TYR:HE1	1:C:183:LEU:HD22	1.72	0.44
1:C:205:ILE:HD11	1:C:211:GLY:C	2.37	0.44
1:C:213:VAL:O	1:C:215:LEU:N	2.50	0.44
1:E:213:VAL:O	1:E:215:LEU:N	2.51	0.44
1:F:339:GLU:O	1:F:343:GLN:HG3	2.18	0.44
1:G:339:GLU:O	1:G:343:GLN:HG3	2.18	0.44
1:F:195:PHE:O	1:F:330:THR:HG22	2.17	0.44
1:F:433:ASN:HD21	1:F:436:GLN:HG3	1.82	0.44
1:B:77:VAL:CG1	1:B:510:VAL:HG22	2.47	0.44
1:E:277:LYS:HG2	1:E:278:ALA:N	2.32	0.44
1:G:277:LYS:HG2	1:G:278:ALA:N	2.32	0.44
1:B:277:LYS:HG2	1:B:278:ALA:N	2.32	0.44
1:G:146:GLN:HE21	1:G:146:GLN:CA	2.30	0.44
1:A:146:GLN:HE21	1:A:146:GLN:CA	2.30	0.44
1:B:340:ALA:O	1:B:343:GLN:HB2	2.18	0.44
1:C:197:ARG:NH2	1:C:280:GLY:H	2.15	0.44
1:A:433:ASN:HD21	1:A:436:GLN:HG3	1.82	0.44
1:E:346:VAL:HG11	1:E:373:ALA:CB	2.46	0.44
1:D:16:MET:HG2	1:D:70:GLY:HA2	2.00	0.44
1:E:298:GLY:C	1:E:300:VAL:N	2.70	0.44
1:G:298:GLY:C	1:G:300:VAL:N	2.70	0.44
1:F:319:GLN:O	1:F:320:ALA:HB3	2.17	0.44
1:C:340:ALA:O	1:C:343:GLN:HB2	2.18	0.44
1:A:339:GLU:O	1:A:343:GLN:HG3	2.18	0.44
1:D:277:LYS:HG2	1:D:278:ALA:N	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:357:THR:OG1	1:D:358:SER:N	2.50	0.44
1:C:281:PHE:CE2	1:D:385:THR:N	2.85	0.43
1:E:362:ARG:NE	1:E:366:GLN:NE2	2.65	0.43
1:E:339:GLU:O	1:E:343:GLN:HG3	2.18	0.43
1:A:105:LYS:HE2	1:A:105:LYS:HB3	1.80	0.43
1:D:149:THR:HG22	1:D:156:GLU:HA	2.00	0.43
1:B:285:ARG:NH1	1:C:386:GLU:OE2	2.50	0.43
1:F:222:LEU:H	1:F:300:VAL:CG1	2.29	0.43
1:F:351:GLN:O	1:F:354:GLU:N	2.52	0.43
1:A:340:ALA:O	1:A:343:GLN:HB2	2.18	0.43
1:G:433:ASN:HD21	1:G:436:GLN:HG3	1.82	0.43
1:A:277:LYS:HG2	1:A:278:ALA:N	2.32	0.43
1:C:146:GLN:CA	1:C:146:GLN:HE21	2.30	0.43
1:A:413:ALA:HA	1:A:489:ILE:CD1	2.48	0.43
1:B:413:ALA:HA	1:B:489:ILE:CD1	2.48	0.43
1:A:521:VAL:HB	1:B:40:LEU:HD23	2.00	0.43
1:F:346:VAL:HG11	1:F:373:ALA:CB	2.46	0.43
1:B:16:MET:HG2	1:B:70:GLY:HA2	1.99	0.43
1:F:16:MET:HG2	1:F:70:GLY:HA2	1.99	0.43
1:D:417:VAL:HG21	1:D:488:MET:HG3	2.00	0.43
1:D:518:GLU:HB3	1:E:29:VAL:HG21	2.01	0.43
1:E:302:SER:O	1:E:303:GLU:CA	2.64	0.43
1:D:363:GLU:CA	1:D:366:GLN:HE21	2.24	0.43
1:E:205:ILE:HA	1:E:205:ILE:HD13	1.61	0.43
1:D:340:ALA:O	1:D:343:GLN:HB2	2.18	0.43
1:B:339:GLU:O	1:B:343:GLN:HG3	2.18	0.43
1:A:197:ARG:NH2	1:A:280:GLY:H	2.15	0.43
1:C:16:MET:HG2	1:C:70:GLY:HA2	1.99	0.43
1:C:7:LYS:HZ2	1:C:15:LYS:HE3	1.83	0.43
1:A:32:GLY:CA	1:A:454:ILE:HG12	2.49	0.43
1:B:282:GLY:HA2	1:C:181:THR:HA	1.64	0.43
1:A:351:GLN:O	1:A:354:GLU:N	2.52	0.43
1:D:351:GLN:O	1:D:354:GLU:N	2.52	0.43
1:F:488:MET:HE2	1:F:493:ILE:HB	1.99	0.43
1:G:107:VAL:CG2	1:G:515:ILE:HG23	2.49	0.43
1:C:32:GLY:CA	1:C:454:ILE:HG12	2.49	0.43
1:E:149:THR:HG22	1:E:156:GLU:HA	2.00	0.43
1:C:281:PHE:HE2	1:D:385:THR:N	2.13	0.43
1:F:349:ILE:CG2	1:F:365:LEU:HG	2.49	0.43
1:F:353:ILE:HG23	1:F:362:ARG:HG2	2.01	0.43
1:E:183:LEU:HA	1:E:383:ALA:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:300:VAL:CG1	1:E:301:ILE:N	2.82	0.43
1:D:300:VAL:CG1	1:D:301:ILE:N	2.82	0.43
1:C:325:ILE:CG2	1:C:326:ASN:N	2.77	0.43
1:C:351:GLN:O	1:C:354:GLU:N	2.52	0.43
1:G:340:ALA:O	1:G:343:GLN:HB2	2.18	0.43
1:G:16:MET:HG2	1:G:70:GLY:HA2	1.99	0.43
1:C:277:LYS:HG2	1:C:278:ALA:N	2.32	0.43
1:C:353:ILE:HG23	1:C:362:ARG:HG2	2.01	0.43
1:F:365:LEU:HD12	1:F:365:LEU:HA	1.86	0.43
1:C:183:LEU:HA	1:C:383:ALA:O	2.19	0.43
1:B:281:PHE:HZ	1:C:389:MET:HB2	1.71	0.43
1:G:302:SER:O	1:G:303:GLU:CA	2.64	0.43
1:D:302:SER:O	1:D:303:GLU:CA	2.64	0.43
1:D:349:ILE:CG2	1:D:365:LEU:HG	2.49	0.43
1:F:300:VAL:CG1	1:F:301:ILE:N	2.82	0.43
1:A:352:GLN:HA	1:A:355:GLU:HG2	2.01	0.43
1:B:351:GLN:O	1:B:354:GLU:N	2.52	0.43
1:E:27:VAL:HG13	1:E:53:GLY:O	2.19	0.43
1:D:27:VAL:HG13	1:D:53:GLY:O	2.19	0.43
1:D:339:GLU:O	1:D:343:GLN:HG3	2.18	0.43
1:C:433:ASN:HD21	1:C:436:GLN:HG3	1.82	0.43
1:D:346:VAL:HG11	1:D:373:ALA:CB	2.46	0.43
1:C:107:VAL:CG2	1:C:515:ILE:HG23	2.49	0.43
1:C:417:VAL:HG21	1:C:488:MET:HG3	2.00	0.43
1:F:357:THR:OG1	1:F:358:SER:N	2.50	0.43
1:C:149:THR:HG22	1:C:156:GLU:HA	2.00	0.43
1:F:302:SER:O	1:F:303:GLU:CA	2.64	0.43
1:B:302:SER:O	1:B:303:GLU:CA	2.64	0.43
1:F:340:ALA:O	1:F:343:GLN:HB2	2.18	0.43
1:E:433:ASN:HD21	1:E:436:GLN:HG3	1.82	0.43
1:A:77:VAL:CG1	1:A:510:VAL:HG22	2.46	0.43
1:G:183:LEU:HA	1:G:383:ALA:O	2.19	0.43
1:D:107:VAL:CG2	1:D:515:ILE:HG23	2.49	0.43
1:E:417:VAL:HG21	1:E:488:MET:HG3	2.00	0.43
1:F:32:GLY:CA	1:F:454:ILE:HG12	2.49	0.43
1:F:149:THR:HG22	1:F:156:GLU:HA	2.00	0.43
1:G:149:THR:HG22	1:G:156:GLU:HA	2.00	0.43
1:B:149:THR:HG22	1:B:156:GLU:HA	2.00	0.43
1:A:46:ALA:HA	1:A:47:PRO:HD2	1.86	0.43
1:C:349:ILE:CG2	1:C:365:LEU:HG	2.49	0.43
1:A:349:ILE:CG2	1:A:365:LEU:HG	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:353:ILE:HG23	1:B:362:ARG:HG2	2.01	0.43
1:E:281:PHE:HE2	1:F:385:THR:C	2.21	0.43
1:G:345:ARG:O	1:G:348:GLN:HB3	2.19	0.43
1:G:351:GLN:O	1:G:354:GLU:N	2.52	0.43
1:C:345:ARG:O	1:C:348:GLN:HB3	2.19	0.43
1:F:164:GLU:O	1:F:168:LYS:HB2	2.19	0.43
1:C:164:GLU:O	1:C:168:LYS:HB2	2.19	0.43
1:A:16:MET:HG2	1:A:70:GLY:CA	2.49	0.43
1:A:16:MET:HG2	1:A:70:GLY:HA2	1.99	0.43
1:A:39:VAL:HG12	1:G:69:MET:HE1	2.01	0.43
1:B:417:VAL:HG21	1:B:488:MET:HG3	2.00	0.43
1:E:112:ASN:ND2	1:F:458:CYS:O	2.45	0.43
1:E:40:LEU:HD13	1:E:59:GLU:HG3	2.01	0.43
1:D:406:ALA:HB2	1:D:496:PRO:HG3	2.01	0.43
1:F:40:LEU:HD13	1:F:59:GLU:HG3	2.01	0.43
1:D:324:VAL:HB	1:D:331:THR:OG1	2.19	0.43
1:A:302:SER:O	1:A:303:GLU:CA	2.64	0.43
1:C:300:VAL:CG1	1:C:301:ILE:N	2.82	0.43
1:B:352:GLN:HA	1:B:355:GLU:HG2	2.01	0.43
1:F:27:VAL:HG13	1:F:53:GLY:O	2.19	0.43
1:D:352:GLN:HA	1:D:355:GLU:HG2	2.01	0.43
1:C:69:MET:HE1	1:D:39:VAL:CG1	2.46	0.43
1:C:16:MET:HG2	1:C:70:GLY:CA	2.49	0.43
1:G:40:LEU:HD13	1:G:59:GLU:HG3	2.01	0.43
1:E:107:VAL:CG2	1:E:515:ILE:HG23	2.49	0.43
1:D:32:GLY:CA	1:D:454:ILE:HG12	2.49	0.43
1:B:40:LEU:HD13	1:B:59:GLU:HG3	2.01	0.43
1:C:40:LEU:HD13	1:C:59:GLU:HG3	2.01	0.43
1:E:406:ALA:HB2	1:E:496:PRO:HG3	2.01	0.43
1:A:406:ALA:HB2	1:A:496:PRO:HG3	2.01	0.43
1:G:353:ILE:HG23	1:G:362:ARG:HG2	2.01	0.42
1:G:364:LYS:HG3	1:G:365:LEU:N	2.34	0.42
1:C:281:PHE:CE2	1:D:385:THR:O	2.66	0.42
1:A:363:GLU:CA	1:A:366:GLN:HE21	2.24	0.42
1:B:324:VAL:HB	1:B:331:THR:OG1	2.19	0.42
1:D:281:PHE:O	1:D:284:ARG:HB2	2.19	0.42
1:E:351:GLN:O	1:E:354:GLU:N	2.52	0.42
1:G:27:VAL:HG13	1:G:53:GLY:O	2.19	0.42
1:C:27:VAL:HG13	1:C:53:GLY:O	2.19	0.42
1:D:40:LEU:HD13	1:D:59:GLU:HG3	2.01	0.42
1:C:339:GLU:O	1:C:343:GLN:HG3	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:340:ALA:O	1:E:343:GLN:HB2	2.18	0.42
1:A:340:ALA:HA	1:A:343:GLN:CG	2.42	0.42
1:G:197:ARG:HA	1:G:197:ARG:HD3	1.80	0.42
1:E:7:LYS:HZ2	1:E:15:LYS:HE3	1.84	0.42
1:C:17:LEU:HD13	1:C:104:LEU:HD12	2.01	0.42
1:A:149:THR:HG22	1:A:156:GLU:HA	2.00	0.42
1:B:406:ALA:HB2	1:B:496:PRO:HG3	2.01	0.42
1:F:406:ALA:HB2	1:F:496:PRO:HG3	2.01	0.42
1:G:406:ALA:HB2	1:G:496:PRO:HG3	2.01	0.42
1:B:349:ILE:CG2	1:B:365:LEU:HG	2.49	0.42
1:G:324:VAL:HB	1:G:331:THR:OG1	2.19	0.42
1:E:349:ILE:CG2	1:E:365:LEU:HG	2.49	0.42
1:C:82:ASN:HD21	1:C:89:THR:N	1.97	0.42
1:G:218:PRO:HG3	1:G:323:VAL:HG23	2.02	0.42
1:A:218:PRO:HG3	1:A:323:VAL:HG23	2.02	0.42
1:B:218:PRO:HG3	1:B:323:VAL:HG23	2.01	0.42
1:G:352:GLN:HA	1:G:355:GLU:HG2	2.01	0.42
1:C:352:GLN:HA	1:C:355:GLU:HG2	2.01	0.42
1:B:164:GLU:O	1:B:168:LYS:HB2	2.19	0.42
1:G:164:GLU:O	1:G:168:LYS:HB2	2.19	0.42
1:E:164:GLU:O	1:E:168:LYS:HB2	2.19	0.42
1:A:183:LEU:HA	1:A:383:ALA:O	2.19	0.42
1:A:417:VAL:HG21	1:A:488:MET:HG3	2.00	0.42
1:F:17:LEU:HD13	1:F:104:LEU:HD12	2.01	0.42
1:C:406:ALA:HB2	1:C:496:PRO:HG3	2.01	0.42
1:A:357:THR:OG1	1:A:358:SER:N	2.50	0.42
1:E:17:LEU:HD13	1:E:104:LEU:HD12	2.01	0.42
1:G:349:ILE:CG2	1:G:365:LEU:HG	2.49	0.42
1:C:281:PHE:O	1:C:284:ARG:HB2	2.19	0.42
1:E:353:ILE:HG23	1:E:362:ARG:HG2	2.01	0.42
1:G:300:VAL:CG1	1:G:301:ILE:N	2.82	0.42
1:A:27:VAL:HG13	1:A:53:GLY:O	2.19	0.42
1:C:430:ARG:HD2	1:C:430:ARG:N	2.35	0.42
1:G:417:VAL:HG21	1:G:488:MET:HG3	2.00	0.42
1:A:40:LEU:HD13	1:A:59:GLU:HG3	2.01	0.42
1:F:430:ARG:N	1:F:430:ARG:HD2	2.35	0.42
1:A:107:VAL:CG2	1:A:515:ILE:HG23	2.49	0.42
1:G:32:GLY:CA	1:G:454:ILE:HG12	2.49	0.42
1:A:94:VAL:HG12	1:A:449:ALA:HB1	2.01	0.42
1:B:17:LEU:HD13	1:B:104:LEU:HD12	2.01	0.42
1:E:286:LYS:HE2	1:E:286:LYS:HB3	1.77	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:364:LYS:HG3	1:A:365:LEU:N	2.34	0.42
1:B:360:TYR:CZ	1:C:183:LEU:HD13	2.52	0.42
1:C:302:SER:O	1:C:303:GLU:CA	2.64	0.42
1:B:300:VAL:CG1	1:B:301:ILE:N	2.82	0.42
1:F:205:ILE:HD13	1:F:205:ILE:HA	1.61	0.42
1:E:325:ILE:CG2	1:E:326:ASN:N	2.77	0.42
1:E:352:GLN:HA	1:E:355:GLU:HG2	2.01	0.42
1:D:345:ARG:O	1:D:348:GLN:HB3	2.19	0.42
1:D:340:ALA:HA	1:D:343:GLN:CG	2.42	0.42
1:B:340:ALA:HA	1:B:343:GLN:CG	2.42	0.42
1:F:417:VAL:HG21	1:F:488:MET:HG3	2.00	0.42
1:F:16:MET:HG2	1:F:70:GLY:CA	2.49	0.42
1:G:16:MET:HG2	1:G:70:GLY:CA	2.49	0.42
1:E:32:GLY:CA	1:E:454:ILE:HG12	2.49	0.42
1:G:17:LEU:HD13	1:G:104:LEU:HD12	2.01	0.42
1:G:46:ALA:HA	1:G:47:PRO:HD2	1.86	0.42
1:D:94:VAL:HG12	1:D:449:ALA:HB1	2.01	0.42
1:F:324:VAL:HB	1:F:331:THR:OG1	2.19	0.42
1:F:252:GLU:O	1:F:253:ASP:C	2.58	0.42
1:F:218:PRO:HG3	1:F:323:VAL:HG23	2.01	0.42
1:A:345:ARG:O	1:A:348:GLN:HB3	2.19	0.42
1:F:352:GLN:HA	1:F:355:GLU:HG2	2.01	0.42
1:E:16:MET:HG2	1:E:70:GLY:CA	2.49	0.42
1:B:183:LEU:HA	1:B:383:ALA:O	2.19	0.42
1:B:107:VAL:CG2	1:B:515:ILE:HG23	2.49	0.42
1:F:107:VAL:CG2	1:F:515:ILE:HG23	2.49	0.42
1:B:32:GLY:CA	1:B:454:ILE:HG12	2.49	0.42
1:C:61:GLU:HA	1:C:68:ASN:ND2	2.35	0.42
1:D:17:LEU:HD13	1:D:104:LEU:HD12	2.01	0.42
1:G:94:VAL:HG12	1:G:449:ALA:HB1	2.01	0.42
1:B:94:VAL:HG12	1:B:449:ALA:HB1	2.01	0.42
1:A:61:GLU:HA	1:A:68:ASN:ND2	2.35	0.42
1:C:364:LYS:HG3	1:C:365:LEU:N	2.34	0.42
1:B:281:PHE:O	1:B:284:ARG:HB2	2.19	0.42
1:F:183:LEU:HA	1:F:383:ALA:O	2.19	0.42
1:D:281:PHE:CZ	1:E:389:MET:HB2	2.55	0.42
1:E:222:LEU:H	1:E:300:VAL:CG1	2.29	0.42
1:G:293:ALA:HB1	1:G:298:GLY:HA3	2.02	0.42
1:C:340:ALA:HA	1:C:343:GLN:CG	2.42	0.42
1:D:487:ASN:HB3	1:D:490:ASP:HB2	2.02	0.42
1:A:17:LEU:HD13	1:A:104:LEU:HD12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:434:GLU:O	1:E:437:ASN:N	2.50	0.42
1:C:94:VAL:HG12	1:C:449:ALA:HB1	2.01	0.42
1:B:61:GLU:HA	1:B:68:ASN:ND2	2.35	0.42
1:G:281:PHE:O	1:G:284:ARG:HB2	2.19	0.42
1:A:281:PHE:O	1:A:284:ARG:HB2	2.19	0.42
1:F:214:GLU:HA	1:F:324:VAL:HA	2.01	0.42
1:E:281:PHE:HD2	1:F:386:GLU:CB	2.32	0.42
1:E:293:ALA:HB1	1:E:298:GLY:HA3	2.02	0.42
1:F:293:ALA:HB1	1:F:298:GLY:HA3	2.02	0.42
1:B:221:LEU:HD12	1:B:300:VAL:CG1	2.39	0.42
1:B:300:VAL:C	1:B:301:ILE:HG13	2.39	0.42
1:D:300:VAL:C	1:D:301:ILE:HG13	2.39	0.42
1:C:252:GLU:O	1:C:253:ASP:C	2.58	0.42
1:B:27:VAL:HG13	1:B:53:GLY:O	2.19	0.42
1:E:487:ASN:HB3	1:E:490:ASP:HB2	2.02	0.42
1:F:487:ASN:HB3	1:F:490:ASP:HB2	2.02	0.42
1:D:183:LEU:HA	1:D:383:ALA:O	2.19	0.42
1:E:94:VAL:HG12	1:E:449:ALA:HB1	2.01	0.42
1:D:21:ASN:O	1:D:25:ASP:HB2	2.20	0.42
1:C:46:ALA:HA	1:C:47:PRO:HD2	1.86	0.42
1:B:364:LYS:HG3	1:B:365:LEU:N	2.34	0.42
1:E:214:GLU:HA	1:E:324:VAL:HA	2.01	0.42
1:E:324:VAL:HB	1:E:331:THR:OG1	2.19	0.42
1:E:281:PHE:O	1:E:284:ARG:HB2	2.19	0.42
1:A:300:VAL:C	1:A:301:ILE:HG13	2.39	0.42
1:C:218:PRO:HG3	1:C:323:VAL:HG23	2.02	0.42
1:B:345:ARG:O	1:B:348:GLN:HB3	2.19	0.42
1:B:351:GLN:O	1:B:352:GLN:C	2.58	0.42
1:F:345:ARG:O	1:F:348:GLN:HB3	2.19	0.42
1:D:433:ASN:HD21	1:D:436:GLN:HG3	1.82	0.42
1:G:430:ARG:HD2	1:G:430:ARG:N	2.35	0.42
1:C:487:ASN:HB3	1:C:490:ASP:HB2	2.02	0.42
1:D:164:GLU:O	1:D:168:LYS:HB2	2.19	0.42
1:A:21:ASN:O	1:A:25:ASP:HB2	2.20	0.42
1:B:21:ASN:O	1:B:25:ASP:HB2	2.20	0.42
1:C:21:ASN:O	1:C:25:ASP:HB2	2.20	0.42
1:A:353:ILE:HG23	1:A:362:ARG:HG2	2.01	0.42
1:D:353:ILE:HG23	1:D:362:ARG:HG2	2.01	0.42
1:F:300:VAL:C	1:F:301:ILE:HG13	2.39	0.42
1:D:293:ALA:HB1	1:D:298:GLY:HA3	2.02	0.42
1:D:16:MET:HG2	1:D:70:GLY:CA	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:16:MET:HG2	1:B:70:GLY:CA	2.49	0.42
1:A:39:VAL:HG12	1:G:69:MET:HE2	2.01	0.42
1:F:94:VAL:HG12	1:F:449:ALA:HB1	2.01	0.42
1:F:281:PHE:O	1:F:284:ARG:HB2	2.19	0.42
1:F:364:LYS:HG3	1:F:365:LEU:N	2.34	0.42
1:C:324:VAL:HB	1:C:331:THR:OG1	2.19	0.42
1:D:364:LYS:HG3	1:D:365:LEU:N	2.34	0.42
1:E:300:VAL:HG23	1:E:317:LEU:HA	2.02	0.42
1:A:293:ALA:HB1	1:A:298:GLY:HA3	2.02	0.42
1:C:293:ALA:HB1	1:C:298:GLY:HA3	2.02	0.42
1:C:300:VAL:HG23	1:C:317:LEU:HA	2.02	0.42
1:G:252:GLU:O	1:G:253:ASP:C	2.58	0.42
1:D:351:GLN:O	1:D:352:GLN:C	2.58	0.42
1:C:214:GLU:HA	1:C:324:VAL:HA	2.01	0.41
1:A:324:VAL:HB	1:A:331:THR:OG1	2.19	0.41
1:A:300:VAL:CG1	1:A:301:ILE:N	2.82	0.41
1:B:293:ALA:HB1	1:B:298:GLY:HA3	2.02	0.41
1:C:351:GLN:O	1:C:352:GLN:C	2.58	0.41
1:E:430:ARG:N	1:E:430:ARG:HD2	2.35	0.41
1:B:487:ASN:HB3	1:B:490:ASP:HB2	2.02	0.41
1:C:105:LYS:HE2	1:C:105:LYS:HB3	1.80	0.41
1:E:21:ASN:O	1:E:25:ASP:HB2	2.20	0.41
1:F:434:GLU:O	1:F:437:ASN:N	2.50	0.41
1:G:434:GLU:O	1:G:437:ASN:N	2.50	0.41
1:D:61:GLU:HA	1:D:68:ASN:ND2	2.35	0.41
1:G:21:ASN:O	1:G:25:ASP:HB2	2.20	0.41
1:B:214:GLU:HA	1:B:324:VAL:HA	2.01	0.41
1:G:214:GLU:HA	1:G:324:VAL:HA	2.01	0.41
1:D:214:GLU:HA	1:D:324:VAL:HA	2.01	0.41
1:F:300:VAL:HG12	1:F:301:ILE:N	2.35	0.41
1:G:300:VAL:C	1:G:301:ILE:HG13	2.39	0.41
1:G:300:VAL:HG23	1:G:317:LEU:HA	2.02	0.41
1:C:300:VAL:C	1:C:301:ILE:HG13	2.39	0.41
1:E:252:GLU:O	1:E:253:ASP:C	2.58	0.41
1:E:218:PRO:HG3	1:E:323:VAL:HG23	2.01	0.41
1:A:351:GLN:O	1:A:352:GLN:C	2.58	0.41
1:B:430:ARG:HD2	1:B:430:ARG:N	2.35	0.41
1:A:164:GLU:O	1:A:168:LYS:HB2	2.19	0.41
1:G:61:GLU:HA	1:G:68:ASN:ND2	2.35	0.41
1:D:300:VAL:HG12	1:D:301:ILE:N	2.35	0.41
1:E:345:ARG:O	1:E:348:GLN:HB3	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:61:GLU:HA	1:F:68:ASN:ND2	2.35	0.41
1:A:300:VAL:HG12	1:A:301:ILE:N	2.35	0.41
1:B:300:VAL:HG12	1:B:301:ILE:N	2.35	0.41
1:B:252:GLU:O	1:B:253:ASP:C	2.58	0.41
1:G:77:VAL:CG1	1:G:510:VAL:HG22	2.46	0.41
1:A:158:VAL:HG13	1:A:396:VAL:HG22	2.02	0.41
1:B:357:THR:OG1	1:B:358:SER:N	2.50	0.41
1:B:46:ALA:HA	1:B:47:PRO:HD2	1.86	0.41
1:A:214:GLU:HA	1:A:324:VAL:HA	2.01	0.41
1:E:364:LYS:HG3	1:E:365:LEU:N	2.34	0.41
1:E:360:TYR:CZ	1:F:183:LEU:HD22	2.53	0.41
1:G:82:ASN:HD21	1:G:89:THR:N	1.97	0.41
1:E:300:VAL:C	1:E:301:ILE:HG13	2.39	0.41
1:E:351:GLN:O	1:E:352:GLN:C	2.58	0.41
1:G:340:ALA:HA	1:G:343:GLN:CG	2.42	0.41
1:B:250:ILE:O	1:B:250:ILE:HG22	2.21	0.41
1:D:430:ARG:N	1:D:430:ARG:HD2	2.35	0.41
1:G:487:ASN:HB3	1:G:490:ASP:HB2	2.02	0.41
1:F:431:GLY:H	1:F:437:ASN:ND2	2.19	0.41
1:F:21:ASN:O	1:F:25:ASP:HB2	2.20	0.41
1:C:158:VAL:HG13	1:C:396:VAL:HG22	2.02	0.41
1:E:516:THR:O	1:F:36:ARG:HB3	2.20	0.41
1:G:365:LEU:HD12	1:G:365:LEU:HA	1.86	0.41
1:C:363:GLU:CA	1:C:366:GLN:HE21	2.24	0.41
1:D:218:PRO:HG3	1:D:323:VAL:HG23	2.02	0.41
1:A:250:ILE:HG22	1:A:250:ILE:O	2.21	0.41
1:G:250:ILE:HG22	1:G:250:ILE:O	2.21	0.41
1:G:431:GLY:H	1:G:437:ASN:ND2	2.19	0.41
1:E:61:GLU:HA	1:E:68:ASN:ND2	2.35	0.41
1:D:158:VAL:HG13	1:D:396:VAL:HG22	2.03	0.41
1:G:300:VAL:HG12	1:G:301:ILE:N	2.35	0.41
1:B:300:VAL:HG23	1:B:317:LEU:HA	2.02	0.41
1:A:252:GLU:O	1:A:253:ASP:C	2.58	0.41
1:G:351:GLN:O	1:G:352:GLN:C	2.58	0.41
1:E:488:MET:HE2	1:E:493:ILE:HB	2.02	0.41
1:E:187:LEU:HD13	1:E:379:ILE:HG12	2.03	0.41
1:E:357:THR:OG1	1:E:358:SER:N	2.50	0.41
1:C:126:VAL:HG11	1:C:426:LEU:HD22	2.03	0.41
1:B:158:VAL:HG13	1:B:396:VAL:HG22	2.03	0.41
1:D:126:VAL:HG11	1:D:426:LEU:HD22	2.03	0.41
1:C:250:ILE:HG22	1:C:250:ILE:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:430:ARG:HD2	1:A:430:ARG:N	2.35	0.41
1:A:413:ALA:HB2	1:A:475:ASN:CB	2.51	0.41
1:D:413:ALA:HB2	1:D:475:ASN:CB	2.51	0.41
1:E:443:ALA:O	1:E:446:ALA:HB3	2.20	0.41
1:A:431:GLY:H	1:A:437:ASN:ND2	2.19	0.41
1:G:443:ALA:O	1:G:446:ALA:HB3	2.20	0.41
1:E:158:VAL:HG13	1:E:396:VAL:HG22	2.02	0.41
1:B:434:GLU:O	1:B:437:ASN:N	2.50	0.41
1:B:431:GLY:H	1:B:437:ASN:ND2	2.19	0.41
1:F:386:GLU:HG3	1:F:389:MET:HE3	2.02	0.41
1:E:219:PHE:HA	1:E:318:GLY:O	2.21	0.41
1:D:219:PHE:HA	1:D:318:GLY:O	2.21	0.41
1:C:300:VAL:HG12	1:C:301:ILE:N	2.36	0.41
1:G:205:ILE:HD11	1:G:211:GLY:HA2	2.03	0.41
1:A:205:ILE:HD11	1:A:211:GLY:HA2	2.03	0.41
1:C:205:ILE:HD11	1:C:211:GLY:HA2	2.03	0.41
1:B:205:ILE:HD13	1:B:205:ILE:HA	1.61	0.41
1:B:205:ILE:HD11	1:B:211:GLY:HA2	2.03	0.41
1:F:205:ILE:HD11	1:F:211:GLY:HA2	2.03	0.41
1:D:205:ILE:HD11	1:D:211:GLY:HA2	2.03	0.41
1:F:250:ILE:HG22	1:F:250:ILE:O	2.21	0.41
1:B:513:LEU:HD22	1:C:49:ILE:HG21	2.02	0.41
1:F:413:ALA:HB2	1:F:475:ASN:CB	2.51	0.41
1:G:413:ALA:HB2	1:G:475:ASN:CB	2.51	0.41
1:E:413:ALA:HB2	1:E:475:ASN:CB	2.51	0.41
1:B:413:ALA:HB2	1:B:475:ASN:CB	2.51	0.41
1:A:187:LEU:HD13	1:A:379:ILE:HG12	2.03	0.41
1:D:187:LEU:HD13	1:D:379:ILE:HG12	2.03	0.41
1:B:187:LEU:HD13	1:B:379:ILE:HG12	2.03	0.41
1:C:187:LEU:HD13	1:C:379:ILE:HG12	2.03	0.41
1:A:49:ILE:HD11	1:G:73:MET:HG2	2.03	0.41
1:B:431:GLY:H	1:B:437:ASN:HD21	1.68	0.41
1:B:126:VAL:HG11	1:B:426:LEU:HD22	2.03	0.41
1:G:158:VAL:HG13	1:G:396:VAL:HG22	2.03	0.41
1:F:443:ALA:O	1:F:446:ALA:HB3	2.20	0.41
1:E:126:VAL:HG11	1:E:426:LEU:HD22	2.03	0.41
1:C:357:THR:OG1	1:C:358:SER:N	2.50	0.41
1:A:443:ALA:O	1:A:446:ALA:HB3	2.20	0.41
1:B:443:ALA:O	1:B:446:ALA:HB3	2.20	0.41
1:C:431:GLY:H	1:C:437:ASN:ND2	2.19	0.41
1:C:434:GLU:O	1:C:437:ASN:N	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:281:PHE:HD2	1:B:386:GLU:HB2	1.86	0.41
1:E:205:ILE:HD11	1:E:211:GLY:HA2	2.03	0.41
1:C:413:ALA:HB2	1:C:475:ASN:CB	2.51	0.41
1:D:488:MET:HE2	1:D:493:ILE:HB	2.02	0.41
1:F:187:LEU:HD13	1:F:379:ILE:HG12	2.03	0.41
1:E:431:GLY:H	1:E:437:ASN:ND2	2.19	0.41
1:C:431:GLY:H	1:C:437:ASN:HD21	1.69	0.41
1:F:158:VAL:HG13	1:F:396:VAL:HG22	2.03	0.41
1:D:443:ALA:O	1:D:446:ALA:HB3	2.20	0.41
1:F:126:VAL:HG11	1:F:426:LEU:HD22	2.03	0.41
1:C:219:PHE:HA	1:C:318:GLY:O	2.21	0.40
1:D:252:GLU:O	1:D:253:ASP:C	2.58	0.40
1:D:205:ILE:HA	1:D:205:ILE:HD13	1.61	0.40
1:C:520:MET:HA	1:D:39:VAL:HB	2.02	0.40
1:G:488:MET:HE2	1:G:493:ILE:HB	2.02	0.40
1:A:40:LEU:CD2	1:G:521:VAL:HB	2.48	0.40
1:D:46:ALA:HA	1:D:47:PRO:HD2	1.86	0.40
1:C:443:ALA:O	1:C:446:ALA:HB3	2.20	0.40
1:D:431:GLY:H	1:D:437:ASN:ND2	2.19	0.40
1:B:349:ILE:HG21	1:B:369:VAL:CG1	2.52	0.40
1:A:205:ILE:HA	1:A:205:ILE:HD13	1.61	0.40
1:A:487:ASN:HB3	1:A:490:ASP:HB2	2.02	0.40
1:E:176:THR:HB	1:E:378:VAL:HG22	2.03	0.40
1:F:35:GLY:O	1:F:51:LYS:NZ	2.53	0.40
1:G:187:LEU:HD13	1:G:379:ILE:HG12	2.03	0.40
1:F:431:GLY:H	1:F:437:ASN:HD21	1.68	0.40
1:F:219:PHE:HA	1:F:318:GLY:O	2.21	0.40
1:F:477:GLY:O	1:F:485:TYR:HA	2.22	0.40
1:C:123:ALA:HA	1:C:429:LEU:HD21	2.04	0.40
1:D:123:ALA:HA	1:D:429:LEU:HD21	2.04	0.40
1:F:176:THR:HB	1:F:378:VAL:HG22	2.03	0.40
1:G:176:THR:HB	1:G:378:VAL:HG22	2.03	0.40
1:C:404:ARG:HD2	1:C:404:ARG:HA	1.91	0.40
1:G:349:ILE:HG21	1:G:369:VAL:CG1	2.52	0.40
1:E:347:ALA:O	1:E:350:ARG:HB2	2.22	0.40
1:F:179:ASP:OD1	1:F:389:MET:SD	2.80	0.40
1:D:366:GLN:O	1:D:369:VAL:HG22	2.21	0.40
1:F:351:GLN:O	1:F:352:GLN:C	2.58	0.40
1:E:340:ALA:HA	1:E:343:GLN:CG	2.42	0.40
1:F:197:ARG:HA	1:F:197:ARG:HD3	1.81	0.40
1:G:477:GLY:O	1:G:485:TYR:HA	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:7:LYS:HZ1	1:D:15:LYS:HE3	1.84	0.40
1:A:35:GLY:O	1:A:51:LYS:NZ	2.53	0.40
1:A:126:VAL:HG11	1:A:426:LEU:HD22	2.03	0.40
1:B:179:ASP:OD1	1:B:389:MET:SD	2.80	0.40
1:A:179:ASP:OD1	1:A:389:MET:SD	2.80	0.40
1:G:347:ALA:O	1:G:350:ARG:HB2	2.22	0.40
1:G:346:VAL:HG13	1:G:369:VAL:HB	2.03	0.40
1:C:347:ALA:O	1:C:350:ARG:HB2	2.22	0.40
1:B:346:VAL:HG13	1:B:369:VAL:HB	2.03	0.40
1:D:353:ILE:HA	1:D:356:ALA:HB2	2.03	0.40
1:E:300:VAL:HG12	1:E:301:ILE:N	2.35	0.40
1:A:219:PHE:HA	1:A:318:GLY:O	2.21	0.40
1:G:219:PHE:HA	1:G:318:GLY:O	2.21	0.40
1:B:123:ALA:HA	1:B:429:LEU:HD21	2.04	0.40
1:A:123:ALA:HA	1:A:429:LEU:HD21	2.04	0.40
1:A:346:VAL:HG13	1:A:369:VAL:HB	2.03	0.40
1:C:346:VAL:HG13	1:C:369:VAL:HB	2.03	0.40
1:D:176:THR:HB	1:D:378:VAL:HG22	2.03	0.40
1:F:46:ALA:HA	1:F:47:PRO:HD2	1.87	0.40
1:F:199:TYR:HD1	1:F:199:TYR:O	2.04	0.40

All (75) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:358:SER:OG	1:G:169:VAL:CB[5_455]	0.65	1.55
1:C:358:SER:CB	1:G:169:VAL:CA[5_455]	0.74	1.46
1:C:358:SER:CA	1:G:169:VAL:CA[5_455]	0.89	1.31
1:C:359:ASP:N	1:G:170:GLY:H[5_455]	0.31	1.29
1:C:359:ASP:CB	1:G:167:ASP:CA[5_455]	0.97	1.23
1:E:338:GLU:CD	1:E:338:GLU:CD[3_454]	1.00	1.20
1:C:359:ASP:CG	1:G:167:ASP:N[5_455]	1.02	1.18
1:C:359:ASP:OD2	1:G:166:MET:C[5_455]	1.08	1.12
1:E:338:GLU:CD	1:E:338:GLU:OE1[3_454]	1.14	1.06
1:G:340:ALA:CB	1:G:340:ALA:CB[3_554]	1.15	1.05
1:E:338:GLU:CB	1:E:338:GLU:CB[3_454]	1.15	1.05
1:E:338:GLU:CG	1:E:338:GLU:CG[3_454]	1.20	1.00
1:C:358:SER:CB	1:G:169:VAL:N[5_455]	1.23	0.97
1:C:359:ASP:N	1:G:170:GLY:N[5_455]	1.26	0.94
1:C:359:ASP:CG	1:G:166:MET:C[5_455]	1.26	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:359:ASP:OD2	1:G:166:MET:CA[5_455]	1.27	0.93
1:C:359:ASP:OD2	1:G:167:ASP:N[5_455]	1.29	0.91
1:E:338:GLU:CB	1:E:338:GLU:CG[3_454]	1.32	0.88
1:C:358:SER:OG	1:G:169:VAL:CG1[5_455]	1.35	0.85
1:B:137:PRO:CD	1:E:132:LYS:O[5_555]	1.37	0.83
1:E:338:GLU:CG	1:E:338:GLU:CD[3_454]	1.42	0.78
1:C:359:ASP:CB	1:G:167:ASP:N[5_455]	1.46	0.74
1:C:359:ASP:OD1	1:G:165:ALA:O[5_455]	1.49	0.71
1:C:357:THR:OG1	1:G:168:LYS:O[5_455]	1.49	0.71
1:C:359:ASP:CA	1:G:166:MET:O[5_455]	1.52	0.68
1:C:359:ASP:OD2	1:G:166:MET:N[5_455]	1.55	0.65
1:C:359:ASP:OD1	1:G:168:LYS:N[5_455]	1.55	0.65
1:C:358:SER:N	1:G:168:LYS:O[5_455]	1.59	0.61
1:B:135:SER:O	1:E:133:ALA:CB[5_555]	1.60	0.60
1:E:338:GLU:OE1	1:E:338:GLU:OE1[3_454]	1.61	0.59
1:E:338:GLU:OE1	1:E:338:GLU:OE2[3_454]	1.61	0.59
1:C:358:SER:CB	1:G:169:VAL:CB[5_455]	1.62	0.58
1:C:358:SER:CA	1:G:169:VAL:C[5_455]	1.62	0.58
1:C:357:THR:O	1:G:169:VAL:CG2[5_455]	1.62	0.58
1:B:135:SER:O	1:E:133:ALA:CA[5_555]	1.65	0.55
1:C:358:SER:C	1:G:170:GLY:N[5_455]	1.65	0.55
1:C:358:SER:OG	1:G:169:VAL:CA[5_455]	1.66	0.54
1:C:359:ASP:H	1:G:170:GLY:H[5_455]	1.08	0.52
1:C:359:ASP:CB	1:G:167:ASP:C[5_455]	1.68	0.52
1:C:358:SER:CB	1:G:169:VAL:C[5_455]	1.71	0.49
1:B:473:ASP:O	1:E:425:LYS:O[5_555]	1.76	0.44
1:B:490:ASP:OD2	1:E:126:VAL:CG2[5_555]	1.77	0.43
1:C:359:ASP:CB	1:G:166:MET:O[5_455]	1.79	0.41
1:C:358:SER:HG	1:G:169:VAL:CG1[5_455]	1.20	0.40
1:C:358:SER:C	1:G:170:GLY:H[5_455]	1.21	0.39
1:C:359:ASP:CB	1:G:166:MET:C[5_455]	1.81	0.39
1:C:358:SER:CA	1:G:169:VAL:N[5_455]	1.82	0.38
1:C:357:THR:CB	1:G:168:LYS:O[5_455]	1.82	0.38
1:C:358:SER:N	1:G:169:VAL:CA[5_455]	1.88	0.32
1:C:359:ASP:CG	1:G:167:ASP:CA[5_455]	1.88	0.32
1:B:168:LYS:CG	1:E:362:ARG:NH2[5_555]	1.91	0.29
1:C:359:ASP:OD1	1:G:168:LYS:H[5_455]	1.34	0.26
1:E:338:GLU:CA	1:E:338:GLU:CG[3_454]	1.98	0.22
1:B:490:ASP:OD1	1:E:129:GLU:OE2[5_555]	1.99	0.21
1:C:359:ASP:H	1:G:170:GLY:N[5_455]	1.41	0.19
1:C:359:ASP:OD2	1:G:167:ASP:H[5_455]	1.41	0.19

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:358:SER:H	1:G:168:LYS:O[5_455]	1.41	0.19
1:A:315:GLU:OE1	1:A:338:GLU:OE2[3_554]	2.02	0.18
1:C:359:ASP:CG	1:G:166:MET:O[5_455]	2.02	0.18
1:E:338:GLU:CG	1:E:338:GLU:OE1[3_454]	2.04	0.16
1:B:434:GLU:OE2	1:F:434:GLU:OE2[4_555]	2.08	0.12
1:B:137:PRO:CG	1:E:132:LYS:O[5_555]	2.08	0.12
1:C:357:THR:C	1:G:168:LYS:O[5_455]	2.11	0.09
1:C:358:SER:C	1:G:169:VAL:C[5_455]	2.11	0.09
1:C:359:ASP:OD2	1:G:165:ALA:C[5_455]	2.12	0.08
1:C:358:SER:N	1:G:168:LYS:C[5_455]	2.14	0.06
1:C:359:ASP:OD1	1:G:167:ASP:C[5_455]	2.14	0.06
1:C:359:ASP:OD1	1:G:167:ASP:N[5_455]	2.14	0.06
1:C:358:SER:HG	1:G:169:VAL:CB[5_455]	1.55	0.05
1:C:359:ASP:CG	1:G:165:ALA:O[5_455]	2.16	0.04
1:C:359:ASP:N	1:G:166:MET:O[5_455]	2.16	0.04
1:C:359:ASP:CG	1:G:167:ASP:C[5_455]	2.17	0.03
1:C:358:SER:C	1:G:169:VAL:CA[5_455]	2.17	0.03
1:C:358:SER:OG	1:G:169:VAL:CG2[5_455]	2.17	0.03
1:C:359:ASP:CA	1:G:170:GLY:H[5_455]	1.60	0.00

## 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	449/548 (82%)	358 (80%)	68 (15%)	23 (5%)	2	8
1	B	449/548 (82%)	359 (80%)	67 (15%)	23 (5%)	2	8
1	C	449/548 (82%)	358 (80%)	68 (15%)	23 (5%)	2	8
1	D	449/548 (82%)	358 (80%)	68 (15%)	23 (5%)	2	8
1	E	449/548 (82%)	358 (80%)	68 (15%)	23 (5%)	2	8
1	F	449/548 (82%)	358 (80%)	68 (15%)	23 (5%)	2	8
1	G	449/548 (82%)	358 (80%)	68 (15%)	23 (5%)	2	8

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	3143/3836 (82%)	2507 (80%)	475 (15%)	161 (5%)	2	8

All (161) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	184	GLN
1	A	185	ASP
1	A	214	GLU
1	A	253	ASP
1	A	301	ILE
1	A	325	ILE
1	A	359	ASP
1	A	360	TYR
1	B	184	GLN
1	B	185	ASP
1	B	214	GLU
1	B	253	ASP
1	B	301	ILE
1	B	325	ILE
1	B	359	ASP
1	B	360	TYR
1	C	184	GLN
1	C	185	ASP
1	C	214	GLU
1	C	253	ASP
1	C	301	ILE
1	C	325	ILE
1	C	359	ASP
1	C	360	TYR
1	D	184	GLN
1	D	185	ASP
1	D	214	GLU
1	D	253	ASP
1	D	301	ILE
1	D	325	ILE
1	D	359	ASP
1	D	360	TYR
1	E	184	GLN
1	E	185	ASP
1	E	214	GLU
1	E	253	ASP
1	E	301	ILE

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Mol	Chain	Res	Type
1	E	325	ILE
1	E	359	ASP
1	E	360	TYR
1	F	184	GLN
1	F	185	ASP
1	F	214	GLU
1	F	253	ASP
1	F	301	ILE
1	F	325	ILE
1	F	359	ASP
1	F	360	TYR
1	G	184	GLN
1	G	185	ASP
1	G	214	GLU
1	G	253	ASP
1	G	301	ILE
1	G	325	ILE
1	G	359	ASP
1	G	360	TYR
1	A	45	GLY
1	A	316	ASP
1	A	328	ASP
1	A	357	THR
1	B	45	GLY
1	B	316	ASP
1	B	328	ASP
1	B	357	THR
1	C	45	GLY
1	C	316	ASP
1	C	328	ASP
1	C	357	THR
1	D	45	GLY
1	D	316	ASP
1	D	328	ASP
1	D	357	THR
1	E	45	GLY
1	E	316	ASP
1	E	328	ASP
1	E	357	THR
1	F	45	GLY
1	F	316	ASP
1	F	328	ASP

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Mol	Chain	Res	Type
1	F	357	THR
1	G	45	GLY
1	G	316	ASP
1	G	328	ASP
1	G	357	THR
1	A	154	SER
1	A	194	GLN
1	A	358	SER
1	A	374	GLY
1	B	154	SER
1	B	194	GLN
1	B	358	SER
1	B	374	GLY
1	C	154	SER
1	C	194	GLN
1	C	358	SER
1	C	374	GLY
1	D	154	SER
1	D	194	GLN
1	D	358	SER
1	D	374	GLY
1	E	154	SER
1	E	194	GLN
1	E	358	SER
1	E	374	GLY
1	F	154	SER
1	F	194	GLN
1	F	358	SER
1	F	374	GLY
1	G	154	SER
1	G	194	GLN
1	G	358	SER
1	G	374	GLY
1	A	218	PRO
1	A	339	GLU
1	B	218	PRO
1	B	339	GLU
1	B	496	PRO
1	C	218	PRO
1	C	339	GLU
1	D	218	PRO
1	D	339	GLU

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Mol	Chain	Res	Type
1	E	218	PRO
1	E	339	GLU
1	E	496	PRO
1	F	218	PRO
1	F	339	GLU
1	G	218	PRO
1	G	339	GLU
1	A	217	SER
1	A	383	ALA
1	A	496	PRO
1	B	217	SER
1	B	383	ALA
1	C	217	SER
1	C	383	ALA
1	C	496	PRO
1	D	217	SER
1	D	383	ALA
1	D	496	PRO
1	E	217	SER
1	E	383	ALA
1	F	217	SER
1	F	383	ALA
1	F	496	PRO
1	G	217	SER
1	G	383	ALA
1	G	496	PRO
1	D	213	VAL
1	E	213	VAL
1	G	213	VAL
1	A	213	VAL
1	B	213	VAL
1	C	213	VAL
1	F	213	VAL
1	E	472	GLY
1	F	472	GLY
1	A	472	GLY
1	B	472	GLY
1	C	472	GLY
1	D	472	GLY
1	G	472	GLY

### 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	353/414 (85%)	300 (85%)	53 (15%)	3	11
1	B	353/414 (85%)	300 (85%)	53 (15%)	3	11
1	C	353/414 (85%)	300 (85%)	53 (15%)	3	11
1	D	353/414 (85%)	300 (85%)	53 (15%)	3	11
1	E	353/414 (85%)	300 (85%)	53 (15%)	3	11
1	F	353/414 (85%)	300 (85%)	53 (15%)	3	11
1	G	353/414 (85%)	300 (85%)	53 (15%)	3	11
All	All	2471/2898 (85%)	2100 (85%)	371 (15%)	3	11

All (371) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LYS
1	A	11	ASP
1	A	29	VAL
1	A	34	LYS
1	A	62	LEU
1	A	76	GLU
1	A	82	ASN
1	A	83	ASP
1	A	87	ASP
1	A	90	THR
1	A	118	ARG
1	A	122	LYS
1	A	139	SER
1	A	146	GLN
1	A	156	GLU
1	A	177	VAL
1	A	193	MET
1	A	194	GLN
1	A	197	ARG
1	A	199	TYR

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Mol	Chain	Res	Type
1	A	204	PHE
1	A	206	ASN
1	A	213	VAL
1	A	217	SER
1	A	218	PRO
1	A	247	LEU
1	A	248	LEU
1	A	250	ILE
1	A	276	VAL
1	A	283	ASP
1	A	284	ARG
1	A	285	ARG
1	A	286	LYS
1	A	288	MET
1	A	301	ILE
1	A	329	THR
1	A	334	ASP
1	A	336	VAL
1	A	338	GLU
1	A	339	GLU
1	A	355	GLU
1	A	360	TYR
1	A	362	ARG
1	A	365	LEU
1	A	380	LYS
1	A	385	THR
1	A	393	LYS
1	A	412	VAL
1	A	421	ARG
1	A	473	ASP
1	A	494	LEU
1	A	504	LEU
1	A	510	VAL
1	B	7	LYS
1	B	11	ASP
1	B	29	VAL
1	B	34	LYS
1	B	62	LEU
1	B	76	GLU
1	B	82	ASN
1	B	83	ASP
1	B	87	ASP

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Mol	Chain	Res	Type
1	B	90	THR
1	B	118	ARG
1	B	122	LYS
1	B	139	SER
1	B	146	GLN
1	B	156	GLU
1	B	177	VAL
1	B	193	MET
1	B	194	GLN
1	B	197	ARG
1	B	199	TYR
1	B	204	PHE
1	B	206	ASN
1	B	213	VAL
1	B	217	SER
1	B	218	PRO
1	B	247	LEU
1	B	248	LEU
1	B	250	ILE
1	B	276	VAL
1	B	283	ASP
1	B	284	ARG
1	B	285	ARG
1	B	286	LYS
1	B	288	MET
1	B	301	ILE
1	B	329	THR
1	B	334	ASP
1	B	336	VAL
1	B	338	GLU
1	B	339	GLU
1	B	355	GLU
1	B	360	TYR
1	B	362	ARG
1	B	365	LEU
1	B	380	LYS
1	B	385	THR
1	B	393	LYS
1	B	412	VAL
1	B	421	ARG
1	B	473	ASP
1	B	494	LEU

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Mol	Chain	Res	Type
1	B	504	LEU
1	B	510	VAL
1	C	7	LYS
1	C	11	ASP
1	C	29	VAL
1	C	34	LYS
1	C	62	LEU
1	C	76	GLU
1	C	82	ASN
1	C	83	ASP
1	C	87	ASP
1	C	90	THR
1	C	118	ARG
1	C	122	LYS
1	C	139	SER
1	C	146	GLN
1	C	156	GLU
1	C	177	VAL
1	C	193	MET
1	C	194	GLN
1	C	197	ARG
1	C	199	TYR
1	C	204	PHE
1	C	206	ASN
1	C	213	VAL
1	C	217	SER
1	C	218	PRO
1	C	247	LEU
1	C	248	LEU
1	C	250	ILE
1	C	276	VAL
1	C	283	ASP
1	C	284	ARG
1	C	285	ARG
1	C	286	LYS
1	C	288	MET
1	C	301	ILE
1	C	329	THR
1	C	334	ASP
1	C	336	VAL
1	C	338	GLU
1	C	339	GLU

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Mol	Chain	Res	Type
1	C	355	GLU
1	C	360	TYR
1	C	362	ARG
1	C	365	LEU
1	C	380	LYS
1	C	385	THR
1	C	393	LYS
1	C	412	VAL
1	C	421	ARG
1	C	473	ASP
1	C	494	LEU
1	C	504	LEU
1	C	510	VAL
1	D	7	LYS
1	D	11	ASP
1	D	29	VAL
1	D	34	LYS
1	D	62	LEU
1	D	76	GLU
1	D	82	ASN
1	D	83	ASP
1	D	87	ASP
1	D	90	THR
1	D	118	ARG
1	D	122	LYS
1	D	139	SER
1	D	146	GLN
1	D	156	GLU
1	D	177	VAL
1	D	193	MET
1	D	194	GLN
1	D	197	ARG
1	D	199	TYR
1	D	204	PHE
1	D	206	ASN
1	D	213	VAL
1	D	217	SER
1	D	218	PRO
1	D	247	LEU
1	D	248	LEU
1	D	250	ILE
1	D	276	VAL

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Mol	Chain	Res	Type
1	D	283	ASP
1	D	284	ARG
1	D	285	ARG
1	D	286	LYS
1	D	288	MET
1	D	301	ILE
1	D	329	THR
1	D	334	ASP
1	D	336	VAL
1	D	338	GLU
1	D	339	GLU
1	D	355	GLU
1	D	360	TYR
1	D	362	ARG
1	D	365	LEU
1	D	380	LYS
1	D	385	THR
1	D	393	LYS
1	D	412	VAL
1	D	421	ARG
1	D	473	ASP
1	D	494	LEU
1	D	504	LEU
1	D	510	VAL
1	E	7	LYS
1	E	11	ASP
1	E	29	VAL
1	E	34	LYS
1	E	62	LEU
1	E	76	GLU
1	E	82	ASN
1	E	83	ASP
1	E	87	ASP
1	E	90	THR
1	E	118	ARG
1	E	122	LYS
1	E	139	SER
1	E	146	GLN
1	E	156	GLU
1	E	177	VAL
1	E	193	MET
1	E	194	GLN

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Mol	Chain	Res	Type
1	E	197	ARG
1	E	199	TYR
1	E	204	PHE
1	E	206	ASN
1	E	213	VAL
1	E	217	SER
1	E	218	PRO
1	E	247	LEU
1	E	248	LEU
1	E	250	ILE
1	E	276	VAL
1	E	283	ASP
1	E	284	ARG
1	E	285	ARG
1	E	286	LYS
1	E	288	MET
1	E	301	ILE
1	E	329	THR
1	E	334	ASP
1	E	336	VAL
1	E	338	GLU
1	E	339	GLU
1	E	355	GLU
1	E	360	TYR
1	E	362	ARG
1	E	365	LEU
1	E	380	LYS
1	E	385	THR
1	E	393	LYS
1	E	412	VAL
1	E	421	ARG
1	E	473	ASP
1	E	494	LEU
1	E	504	LEU
1	E	510	VAL
1	F	7	LYS
1	F	11	ASP
1	F	29	VAL
1	F	34	LYS
1	F	62	LEU
1	F	76	GLU
1	F	82	ASN

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Mol	Chain	Res	Type
1	F	83	ASP
1	F	87	ASP
1	F	90	THR
1	F	118	ARG
1	F	122	LYS
1	F	139	SER
1	F	146	GLN
1	F	156	GLU
1	F	177	VAL
1	F	193	MET
1	F	194	GLN
1	F	197	ARG
1	F	199	TYR
1	F	204	PHE
1	F	206	ASN
1	F	213	VAL
1	F	217	SER
1	F	218	PRO
1	F	247	LEU
1	F	248	LEU
1	F	250	ILE
1	F	276	VAL
1	F	283	ASP
1	F	284	ARG
1	F	285	ARG
1	F	286	LYS
1	F	288	MET
1	F	301	ILE
1	F	329	THR
1	F	334	ASP
1	F	336	VAL
1	F	338	GLU
1	F	339	GLU
1	F	355	GLU
1	F	360	TYR
1	F	362	ARG
1	F	365	LEU
1	F	380	LYS
1	F	385	THR
1	F	393	LYS
1	F	412	VAL
1	F	421	ARG

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Mol	Chain	Res	Type
1	F	473	ASP
1	F	494	LEU
1	F	504	LEU
1	F	510	VAL
1	G	7	LYS
1	G	11	ASP
1	G	29	VAL
1	G	34	LYS
1	G	62	LEU
1	G	76	GLU
1	G	82	ASN
1	G	83	ASP
1	G	87	ASP
1	G	90	THR
1	G	118	ARG
1	G	122	LYS
1	G	139	SER
1	G	146	GLN
1	G	156	GLU
1	G	177	VAL
1	G	193	MET
1	G	194	GLN
1	G	197	ARG
1	G	199	TYR
1	G	204	PHE
1	G	206	ASN
1	G	213	VAL
1	G	217	SER
1	G	218	PRO
1	G	247	LEU
1	G	248	LEU
1	G	250	ILE
1	G	276	VAL
1	G	283	ASP
1	G	284	ARG
1	G	285	ARG
1	G	286	LYS
1	G	288	MET
1	G	301	ILE
1	G	329	THR
1	G	334	ASP
1	G	336	VAL

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Mol	Chain	Res	Type
1	G	338	GLU
1	G	339	GLU
1	G	355	GLU
1	G	360	TYR
1	G	362	ARG
1	G	365	LEU
1	G	380	LYS
1	G	385	THR
1	G	393	LYS
1	G	412	VAL
1	G	421	ARG
1	G	473	ASP
1	G	494	LEU
1	G	504	LEU
1	G	510	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (72) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
1	A	68	ASN
1	A	72	GLN
1	A	82	ASN
1	A	146	GLN
1	A	194	GLN
1	A	366	GLN
1	A	436	GLN
1	A	437	ASN
1	A	453	GLN
1	B	10	ASN
1	B	37	ASN
1	B	68	ASN
1	B	72	GLN
1	B	82	ASN
1	B	146	GLN
1	B	194	GLN
1	B	366	GLN
1	B	436	GLN
1	B	437	ASN
1	B	453	GLN
1	C	10	ASN
1	C	68	ASN

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Mol	Chain	Res	Type
1	C	72	GLN
1	C	82	ASN
1	C	146	GLN
1	C	194	GLN
1	C	366	GLN
1	C	436	GLN
1	C	437	ASN
1	C	453	GLN
1	D	10	ASN
1	D	68	ASN
1	D	72	GLN
1	D	82	ASN
1	D	146	GLN
1	D	194	GLN
1	D	366	GLN
1	D	436	GLN
1	D	437	ASN
1	D	453	GLN
1	E	10	ASN
1	E	37	ASN
1	E	68	ASN
1	E	72	GLN
1	E	82	ASN
1	E	146	GLN
1	E	194	GLN
1	E	366	GLN
1	E	436	GLN
1	E	437	ASN
1	E	453	GLN
1	F	10	ASN
1	F	68	ASN
1	F	72	GLN
1	F	82	ASN
1	F	146	GLN
1	F	194	GLN
1	F	366	GLN
1	F	436	GLN
1	F	437	ASN
1	F	453	GLN
1	G	10	ASN
1	G	68	ASN
1	G	72	GLN

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Mol	Chain	Res	Type
1	G	82	ASN
1	G	146	GLN
1	G	194	GLN
1	G	366	GLN
1	G	436	GLN
1	G	437	ASN
1	G	453	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

### 5.7 Other polymers ⓘ

There are no such residues in this entry.

### 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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

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

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

### 6.3 Carbohydrates [i](#)

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

### 6.4 Ligands [i](#)

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

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

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