



# Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 01:31 am BST

PDB ID : 2QVW  
Title : Structure of Giardia Dicer refined against twinned data  
Authors : Doudna, J.A.; MacRae, I.J.  
Deposited on : 2007-08-09  
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

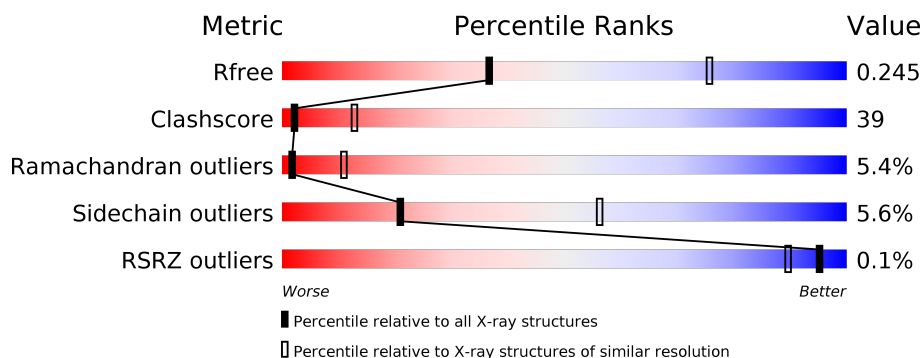
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	756	
1	B	756	
1	C	756	
1	D	756	

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

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	MN	D	759	-	-	-	X

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 22372 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called GLP\_546\_48378\_50642.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	732	Total	C	N	O	S	0	0	0
			5630	3614	957	1029	30			
1	B	726	Total	C	N	O	S	0	0	0
			5590	3589	950	1021	30			
1	C	718	Total	C	N	O	S	0	0	0
			5539	3560	941	1008	30			
1	D	720	Total	C	N	O	S	0	0	0
			5574	3586	942	1016	30			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	EXPRESSION TAG	UNP Q7R2M2
A	0	ALA	-	EXPRESSION TAG	UNP Q7R2M2
B	-1	GLY	-	EXPRESSION TAG	UNP Q7R2M2
B	0	ALA	-	EXPRESSION TAG	UNP Q7R2M2
C	-1	GLY	-	EXPRESSION TAG	UNP Q7R2M2
C	0	ALA	-	EXPRESSION TAG	UNP Q7R2M2
D	-1	GLY	-	EXPRESSION TAG	UNP Q7R2M2
D	0	ALA	-	EXPRESSION TAG	UNP Q7R2M2

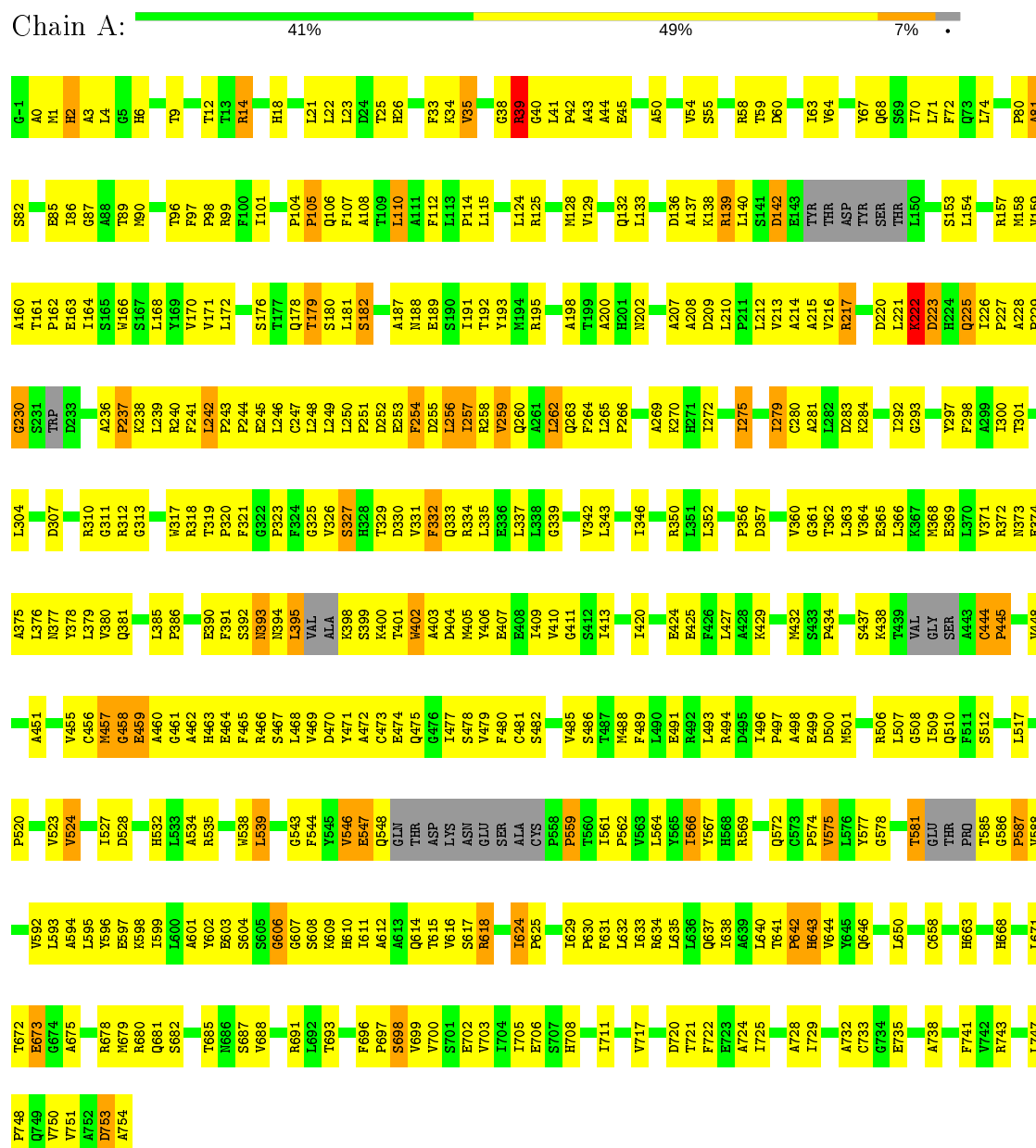
- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	9	Total	Mn	0	0
			9	9		
2	A	12	Total	Mn	0	0
			12	12		
2	D	9	Total	Mn	0	0
			9	9		
2	C	9	Total	Mn	0	0
			9	9		

### 3 Residue-property plots

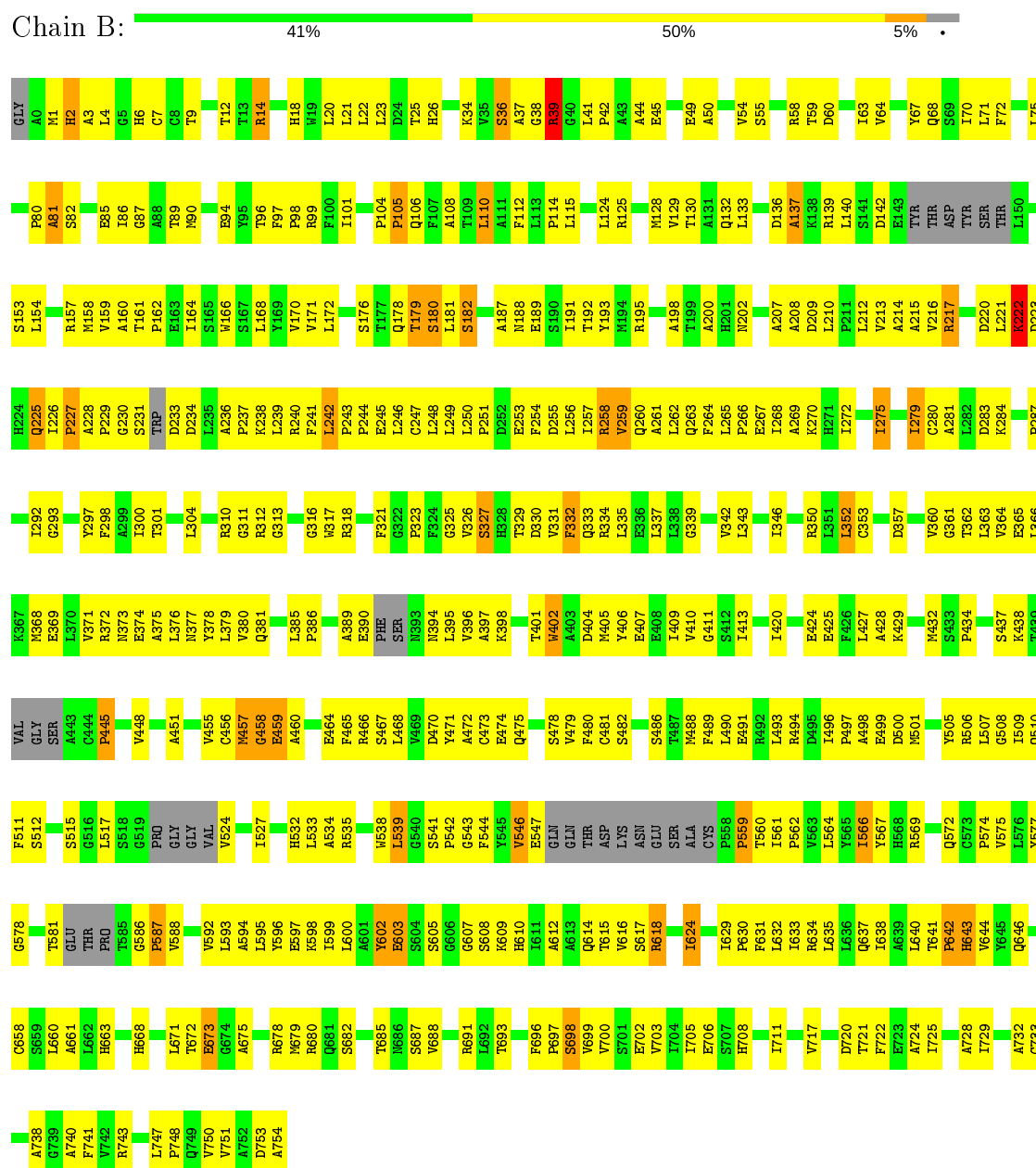
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

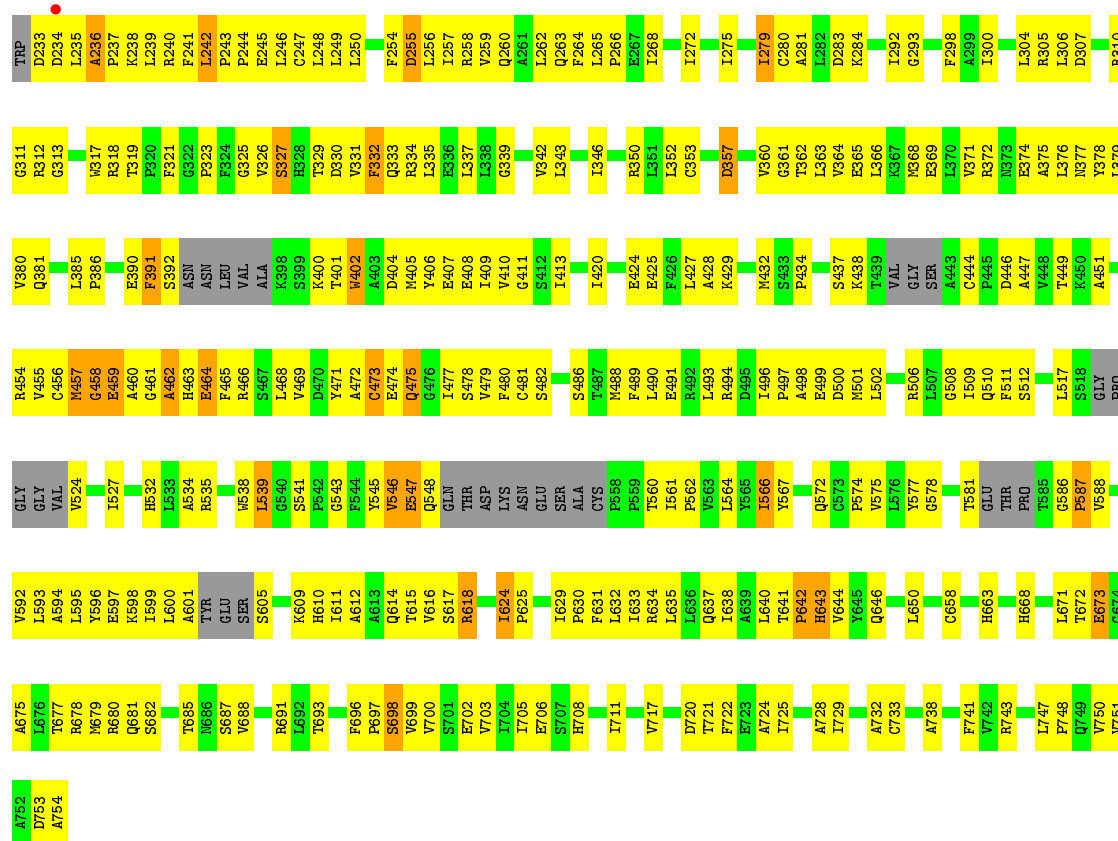
- Molecule 1: GLP\_546\_48378\_50642



- Molecule 1: GLP\_546\_48378\_50642

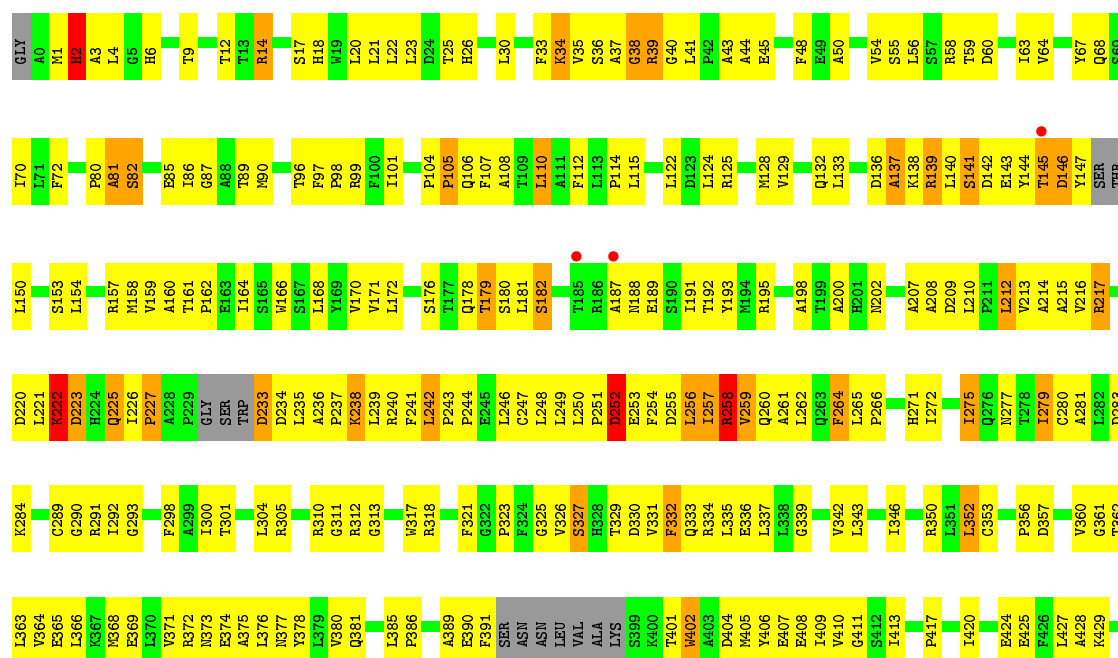
## Chain B:





• Molecule 1: GLP\_546\_48378\_50642

Chain D: 40% 47% 7% • 5%







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	155.41Å 173.49Å 155.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.00 49.16 – 3.00	Depositor EDS
% Data completeness (in resolution range)	95.9 (50.00-3.00) 97.8 (49.16-3.00)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.84 (at 3.01Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.221 , 0.263 0.216 , 0.245	Depositor DCC
$R_{free}$ test set	3938 reflections (4.76%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	53.2	Xtriage
Anisotropy	0.137	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 8.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.40$ , $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	0.478 for l,-k,h	Xtriage
Reported twinning fraction	0.500 for l,-k,h	Depositor
Outliers	0 of 82722 reflections	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	22372	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.94% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MN

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	0.37	0/5761	0.60	0/7836
1	B	0.36	0/5718	0.60	0/7777
1	C	0.36	0/5666	0.60	0/7704
1	D	0.36	0/5704	0.60	0/7759
All	All	0.36	0/22849	0.60	0/31076

There are no bond length outliers.

There are no bond angle outliers.

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	5630	0	5672	434	0
1	B	5590	0	5640	438	0
1	C	5539	0	5592	460	0
1	D	5574	0	5611	449	0
2	A	12	0	0	0	0
2	B	9	0	0	0	0
2	C	9	0	0	0	0
2	D	9	0	0	0	0
All	All	22372	0	22515	1769	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 39.

All (1769) 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:B:465:PHE:HE2	1:B:533:LEU:HD21	1.23	1.03
1:C:597:GLU:HA	1:C:600:LEU:HD12	1.40	1.02
1:C:114:PRO:HA	1:C:258:ARG:HH12	1.21	1.01
1:C:465:PHE:HE1	1:C:502:LEU:HB2	1.29	0.97
1:B:373:ASN:HD21	1:B:401:THR:HG21	1.26	0.97
1:D:110:LEU:HD13	1:D:272:ILE:HD12	1.44	0.96
1:A:373:ASN:HD21	1:A:401:THR:HG21	1.32	0.94
1:B:99:ARG:HH12	1:B:390:GLU:C	1.70	0.94
1:B:466:ARG:NE	1:B:498:ALA:HB2	1.81	0.93
1:C:115:LEU:H	1:C:258:ARG:HH22	0.94	0.93
1:A:220:ASP:HB3	1:A:238:LYS:HD3	1.53	0.91
1:A:39:ARG:HD2	1:A:317:TRP:CZ2	2.06	0.91
1:A:104:PRO:HB3	1:A:280:CYS:SG	2.10	0.90
1:B:466:ARG:HH21	1:B:498:ALA:H	1.18	0.89
1:C:138:LYS:O	1:C:139:ARG:HD2	1.73	0.87
1:D:258:ARG:HH11	1:D:258:ARG:HA	1.40	0.87
1:C:110:LEU:HD13	1:C:272:ILE:HD12	1.57	0.87
1:C:115:LEU:H	1:C:258:ARG:NH2	1.73	0.86
1:A:743:ARG:HA	1:A:747:LEU:HB2	1.59	0.85
1:C:178:GLN:HE21	1:C:212:LEU:HD12	1.41	0.84
1:D:178:GLN:HE21	1:D:212:LEU:HD12	1.42	0.84
1:D:104:PRO:HB3	1:D:280:CYS:SG	2.17	0.84
1:D:279:ILE:O	1:D:283:ASP:HB2	1.77	0.84
1:B:377:ASN:HD21	1:B:395:LEU:HD21	1.42	0.84
1:C:743:ARG:HA	1:C:747:LEU:HB2	1.57	0.84
1:B:178:GLN:HE21	1:B:212:LEU:HD12	1.43	0.83
1:C:233:ASP:HB3	1:C:236:ALA:HB2	1.60	0.83
1:B:743:ARG:HA	1:B:747:LEU:HB2	1.61	0.83
1:D:743:ARG:HA	1:D:747:LEU:HB2	1.58	0.83
1:B:279:ILE:O	1:B:283:ASP:HB2	1.80	0.82
1:C:279:ILE:O	1:C:283:ASP:HB2	1.79	0.82
1:A:279:ILE:O	1:A:283:ASP:HB2	1.78	0.82
1:C:381:GLN:NE2	1:C:402:TRP:HD1	1.77	0.81
1:C:508:GLY:HA3	1:C:532:HIS:O	1.79	0.81
1:D:1:MET:HG3	1:D:55:SER:HB3	1.61	0.81
1:C:104:PRO:HB3	1:C:280:CYS:SG	2.21	0.81
1:B:220:ASP:HB3	1:B:238:LYS:HD3	1.61	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:350:ARG:HD3	1:C:538:TRP:O	1.81	0.81
1:B:36:SER:O	1:B:38:GLY:N	2.15	0.80
1:C:543:GLY:HA3	1:C:561:ILE:O	1.82	0.80
1:A:178:GLN:HE21	1:A:212:LEU:HD12	1.43	0.80
1:C:465:PHE:HA	1:C:468:LEU:HD12	1.64	0.79
1:D:543:GLY:HA3	1:D:561:ILE:O	1.82	0.79
1:A:39:ARG:HD2	1:A:317:TRP:CE2	2.17	0.79
1:D:508:GLY:HA3	1:D:532:HIS:O	1.82	0.79
1:C:305:ARG:HD2	1:C:390:GLU:HB3	1.64	0.79
1:D:333:GLN:NE2	1:D:672:THR:HB	1.98	0.79
1:D:747:LEU:O	1:D:750:VAL:HG12	1.83	0.79
1:D:362:THR:O	1:D:366:LEU:HG	1.83	0.79
1:A:110:LEU:HD13	1:A:272:ILE:HD12	1.64	0.78
1:B:85:GLU:O	1:B:89:THR:HG23	1.83	0.78
1:B:362:THR:O	1:B:366:LEU:HG	1.83	0.78
1:C:85:GLU:O	1:C:89:THR:HG23	1.83	0.78
1:A:609:LYS:HD3	1:A:641:THR:HG22	1.65	0.78
1:C:362:THR:O	1:C:366:LEU:HG	1.83	0.78
1:D:3:ALA:HB3	1:D:54:VAL:O	1.82	0.78
1:A:432:MET:HE2	1:A:534:ALA:HB1	1.66	0.78
1:A:85:GLU:O	1:A:89:THR:HG23	1.84	0.78
1:C:747:LEU:O	1:C:750:VAL:HG12	1.85	0.77
1:A:596:TYR:O	1:A:599:ILE:HG22	1.85	0.77
1:D:180:SER:HB2	1:D:208:ALA:O	1.84	0.77
1:A:362:THR:O	1:A:366:LEU:HG	1.84	0.77
1:B:747:LEU:O	1:B:750:VAL:HG12	1.84	0.77
1:A:399:SER:HA	1:B:395:LEU:HD12	1.66	0.77
1:D:38:GLY:H	1:D:41:LEU:HD12	1.49	0.77
1:D:172:LEU:HD12	1:D:239:LEU:HD13	1.67	0.77
1:C:471:TYR:O	1:C:475:GLN:HB2	1.85	0.77
1:B:465:PHE:HA	1:B:468:LEU:HD12	1.66	0.76
1:D:147:TYR:CG	1:D:150:LEU:HB2	2.20	0.76
1:C:205:LEU:HB3	1:C:245:GLU:OE2	1.86	0.76
1:D:139:ARG:NH1	1:D:162:PRO:HG3	2.00	0.76
1:A:508:GLY:HA3	1:A:532:HIS:O	1.85	0.76
1:D:369:GLU:HG2	1:D:485:VAL:HG23	1.66	0.76
1:D:337:LEU:HD22	1:D:673:GLU:HA	1.67	0.76
1:A:3:ALA:HB3	1:A:54:VAL:O	1.85	0.76
1:B:115:LEU:H	1:B:258:ARG:HH22	1.33	0.76
1:C:159:VAL:HG23	1:C:248:LEU:O	1.85	0.76
1:C:21:LEU:HD21	1:C:272:ILE:HD11	1.66	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:352:LEU:HD11	1:D:650:LEU:HD23	1.67	0.76
1:A:392:SER:O	1:A:394:ASN:N	2.17	0.76
1:C:596:TYR:O	1:C:599:ILE:HG22	1.85	0.76
1:D:160:ALA:HB2	1:D:168:LEU:HD23	1.68	0.76
1:D:1:MET:HG3	1:D:55:SER:CB	2.15	0.76
1:A:99:ARG:HH11	1:A:390:GLU:CD	1.89	0.76
1:A:310:ARG:HH22	1:A:392:SER:HB3	1.49	0.76
1:B:3:ALA:HB3	1:B:54:VAL:O	1.86	0.76
1:B:300:ILE:HG23	1:B:304:LEU:HD12	1.68	0.76
1:A:747:LEU:O	1:A:750:VAL:HG12	1.85	0.75
1:B:160:ALA:HB2	1:B:168:LEU:HD23	1.66	0.75
1:C:158:MET:HE3	1:C:256:LEU:HB2	1.68	0.75
1:C:465:PHE:CE1	1:C:502:LEU:HB2	2.19	0.75
1:D:300:ILE:HG23	1:D:304:LEU:HD12	1.69	0.75
1:A:300:ILE:HG23	1:A:304:LEU:HD12	1.68	0.75
1:C:160:ALA:HB2	1:C:168:LEU:HD23	1.67	0.75
1:C:705:ILE:HG12	1:C:711:ILE:HD11	1.69	0.75
1:C:180:SER:HB2	1:C:208:ALA:O	1.87	0.75
1:D:635:LEU:HD12	1:D:732:ALA:HB2	1.68	0.75
1:A:635:LEU:HD12	1:A:732:ALA:HB2	1.66	0.74
1:D:596:TYR:O	1:D:599:ILE:HG22	1.87	0.74
1:A:160:ALA:HB2	1:A:168:LEU:HD23	1.69	0.74
1:B:508:GLY:HA3	1:B:532:HIS:O	1.87	0.74
1:C:255:ASP:O	1:C:259:VAL:HG23	1.86	0.74
1:D:343:LEU:HD13	1:D:427:LEU:HD21	1.69	0.74
1:B:596:TYR:O	1:B:599:ILE:HG22	1.88	0.74
1:C:115:LEU:N	1:C:258:ARG:HH22	1.78	0.74
1:C:635:LEU:HD12	1:C:732:ALA:HB2	1.69	0.74
1:D:180:SER:HA	1:D:212:LEU:HD21	1.70	0.74
1:A:180:SER:HA	1:A:212:LEU:HD21	1.70	0.74
1:A:180:SER:HB2	1:A:208:ALA:O	1.88	0.74
1:C:180:SER:HA	1:C:212:LEU:HD21	1.70	0.74
1:B:466:ARG:CZ	1:B:498:ALA:HB2	2.17	0.74
1:B:180:SER:HB2	1:B:208:ALA:O	1.87	0.74
1:A:379:LEU:HD21	1:A:481:CYS:HB3	1.70	0.73
1:B:465:PHE:CE2	1:B:533:LEU:HD21	2.15	0.73
1:C:138:LYS:C	1:C:139:ARG:HD2	2.08	0.73
1:B:139:ARG:HG3	1:B:247:CYS:O	1.88	0.73
1:D:259:VAL:O	1:D:262:LEU:HB3	1.89	0.73
1:B:346:ILE:HG21	1:B:427:LEU:HD13	1.71	0.73
1:B:350:ARG:HD3	1:B:538:TRP:O	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:139:ARG:HG2	1:B:245:GLU:O	1.87	0.73
1:A:158:MET:HG3	1:A:259:VAL:HG21	1.70	0.73
1:B:39:ARG:HG3	1:B:317:TRP:CZ2	2.24	0.73
1:C:634:ARG:O	1:C:638:ILE:HG13	1.88	0.72
1:A:432:MET:HA	1:A:479:VAL:O	1.90	0.72
1:B:178:GLN:HB2	1:B:182:SER:OG	1.89	0.72
1:B:180:SER:HA	1:B:212:LEU:HD21	1.70	0.72
1:B:394:ASN:OD1	1:B:396:VAL:HG12	1.88	0.72
1:B:561:ILE:HD12	1:B:561:ILE:H	1.54	0.72
1:A:634:ARG:O	1:A:638:ILE:HG13	1.90	0.72
1:A:352:LEU:HD12	1:A:363:LEU:HD13	1.70	0.72
1:B:264:PHE:O	1:B:268:ILE:HG13	1.90	0.72
1:B:635:LEU:HD12	1:B:732:ALA:HB2	1.71	0.72
1:D:609:LYS:NZ	1:D:641:THR:HG21	2.05	0.72
1:C:14:ARG:NH2	1:C:224:HIS:O	2.22	0.72
1:A:310:ARG:HB2	1:A:310:ARG:NH1	2.05	0.72
1:D:342:VAL:HG12	1:D:658:CYS:SG	2.29	0.72
1:A:561:ILE:HD12	1:A:561:ILE:H	1.53	0.72
1:C:114:PRO:CA	1:C:258:ARG:HH12	2.01	0.72
1:C:14:ARG:HD2	1:C:260:GLN:OE1	1.89	0.72
1:B:602:TYR:HD2	1:B:634:ARG:NH1	1.86	0.71
1:C:133:LEU:O	1:C:137:ALA:N	2.23	0.71
1:D:705:ILE:HG12	1:D:711:ILE:HD11	1.72	0.71
1:A:705:ILE:HG12	1:A:711:ILE:HD11	1.72	0.71
1:A:228:ALA:O	1:A:230:GLY:N	2.23	0.71
1:A:624:ILE:HD13	1:A:624:ILE:H	1.55	0.71
1:C:178:GLN:HB2	1:C:182:SER:OG	1.90	0.71
1:C:310:ARG:HB2	1:C:310:ARG:NH1	2.05	0.71
1:D:624:ILE:H	1:D:624:ILE:HD13	1.54	0.71
1:B:705:ILE:HG12	1:B:711:ILE:HD11	1.73	0.71
1:D:448:VAL:HG13	1:D:468:LEU:HD23	1.72	0.71
1:A:41:LEU:O	1:A:41:LEU:HD12	1.90	0.71
1:A:98:PRO:HA	1:A:101:ILE:HD11	1.73	0.71
1:D:561:ILE:H	1:D:561:ILE:HD12	1.55	0.71
1:B:437:SER:HB3	1:B:478:SER:O	1.90	0.71
1:C:466:ARG:NH2	1:C:498:ALA:H	1.89	0.71
1:D:236:ALA:N	1:D:237:PRO:HD2	2.06	0.71
1:C:98:PRO:HA	1:C:101:ILE:HD11	1.73	0.70
1:B:634:ARG:O	1:B:638:ILE:HG13	1.90	0.70
1:B:98:PRO:HA	1:B:101:ILE:HD11	1.73	0.70
1:A:520:PRO:HD2	1:D:698:SER:OG	1.92	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:178:GLN:HB2	1:D:182:SER:OG	1.91	0.70
1:D:463:HIS:O	1:D:466:ARG:HB3	1.91	0.70
1:C:597:GLU:HA	1:C:600:LEU:CD1	2.19	0.70
1:C:596:TYR:O	1:C:600:LEU:HG	1.90	0.70
1:D:98:PRO:HA	1:D:101:ILE:HD11	1.73	0.70
1:B:21:LEU:HD21	1:B:272:ILE:HD11	1.72	0.70
1:D:310:ARG:NH1	1:D:310:ARG:HB2	2.07	0.70
1:D:37:ALA:HB2	1:D:43:ALA:HB2	1.72	0.70
1:D:85:GLU:O	1:D:89:THR:HG23	1.91	0.70
1:A:67:TYR:OH	1:A:114:PRO:HG3	1.92	0.70
1:B:129:VAL:O	1:B:133:LEU:HG	1.90	0.70
1:D:602:TYR:O	1:D:634:ARG:NH1	2.25	0.69
1:C:300:ILE:HG23	1:C:304:LEU:HD12	1.73	0.69
1:A:337:LEU:HD22	1:A:673:GLU:HA	1.74	0.69
1:A:137:ALA:CB	1:A:248:LEU:HD21	2.22	0.69
1:A:158:MET:HE1	1:A:256:LEU:HD13	1.73	0.69
1:B:352:LEU:HD12	1:B:363:LEU:HD13	1.73	0.69
1:B:432:MET:HE2	1:B:534:ALA:HB1	1.73	0.69
1:C:158:MET:HG3	1:C:259:VAL:HG21	1.74	0.69
1:B:466:ARG:NH2	1:B:498:ALA:H	1.89	0.69
1:C:343:LEU:HD13	1:C:427:LEU:HD21	1.75	0.69
1:C:624:ILE:HD13	1:C:624:ILE:H	1.56	0.69
1:D:352:LEU:HD12	1:D:363:LEU:HD13	1.75	0.69
1:B:310:ARG:HB2	1:B:310:ARG:NH1	2.07	0.69
1:C:129:VAL:O	1:C:133:LEU:HG	1.93	0.69
1:D:172:LEU:HB2	1:D:214:ALA:O	1.92	0.69
1:D:172:LEU:HD12	1:D:239:LEU:CD1	2.23	0.69
1:A:610:HIS:CD2	1:A:614:GLN:HE21	2.11	0.68
1:B:618:ARG:HH11	1:B:618:ARG:HB2	1.57	0.68
1:B:624:ILE:H	1:B:624:ILE:HD13	1.57	0.68
1:C:561:ILE:HD12	1:C:561:ILE:H	1.58	0.68
1:D:634:ARG:O	1:D:638:ILE:HG13	1.93	0.68
1:B:110:LEU:HD13	1:B:272:ILE:HD12	1.74	0.68
1:D:432:MET:HE2	1:D:534:ALA:HB1	1.76	0.68
1:A:138:LYS:HD3	1:A:142:ASP:HB3	1.73	0.68
1:C:36:SER:HB3	1:C:317:TRP:HB3	1.76	0.68
1:A:369:GLU:HG3	1:A:482:SER:OG	1.93	0.68
1:C:125:ARG:HG2	1:C:125:ARG:HH11	1.58	0.68
1:C:180:SER:O	1:C:193:TYR:HB2	1.93	0.68
1:C:284:LYS:HD2	1:C:284:LYS:H	1.58	0.68
1:D:609:LYS:HE3	1:D:637:GLN:HB3	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:GLN:HB2	1:A:182:SER:OG	1.93	0.68
1:B:333:GLN:HE21	1:B:673:GLU:HB3	1.58	0.68
1:C:198:ALA:O	1:C:202:ASN:HA	1.94	0.68
1:C:235:LEU:C	1:C:237:PRO:HD2	2.14	0.68
1:A:548:GLN:HA	1:A:548:GLN:HE21	1.57	0.68
1:B:139:ARG:HH21	1:B:162:PRO:HG3	1.58	0.68
1:A:307:ASP:HB3	1:A:391:PHE:HB2	1.75	0.68
1:C:420:ILE:O	1:C:424:GLU:HG3	1.94	0.68
1:D:602:TYR:CE1	1:D:603:GLU:HG2	2.28	0.68
1:C:67:TYR:OH	1:C:114:PRO:HG3	1.94	0.68
1:A:543:GLY:HA3	1:A:561:ILE:O	1.94	0.67
1:D:615:THR:HA	1:D:618:ARG:HH12	1.59	0.67
1:A:129:VAL:O	1:A:133:LEU:HG	1.94	0.67
1:A:618:ARG:HH11	1:A:618:ARG:HB2	1.58	0.67
1:D:139:ARG:HH12	1:D:162:PRO:HG3	1.54	0.67
1:B:377:ASN:HD21	1:B:395:LEU:CD2	2.05	0.67
1:C:114:PRO:HA	1:C:258:ARG:NH1	2.02	0.67
1:C:618:ARG:HB2	1:C:618:ARG:HH11	1.60	0.67
1:B:284:LYS:HD2	1:B:284:LYS:H	1.60	0.67
1:D:437:SER:HB3	1:D:478:SER:O	1.95	0.67
1:A:284:LYS:H	1:A:284:LYS:HD2	1.60	0.67
1:A:339:GLY:HA3	1:A:407:GLU:O	1.95	0.67
1:B:236:ALA:N	1:B:237:PRO:HD2	2.10	0.67
1:C:193:TYR:CE2	1:C:241:PHE:HB2	2.30	0.67
1:B:39:ARG:HD2	1:B:39:ARG:N	2.09	0.67
1:C:260:GLN:O	1:C:263:GLN:HG2	1.95	0.67
1:D:180:SER:O	1:D:193:TYR:HB2	1.95	0.67
1:D:608:SER:HA	1:D:611:ILE:HG12	1.77	0.67
1:A:523:VAL:HG11	1:D:618:ARG:HB2	1.77	0.67
1:B:373:ASN:ND2	1:B:401:THR:HG21	2.07	0.66
1:C:3:ALA:HB3	1:C:54:VAL:O	1.94	0.66
1:A:420:ILE:O	1:A:424:GLU:HG3	1.95	0.66
1:C:381:GLN:NE2	1:C:402:TRP:CD1	2.61	0.66
1:B:679:MET:O	1:B:750:VAL:HG23	1.96	0.66
1:C:466:ARG:NH1	1:C:501:MET:HE1	2.10	0.66
1:C:333:GLN:NE2	1:C:672:THR:HB	2.10	0.66
1:C:687:SER:O	1:C:691:ARG:HG3	1.95	0.66
1:D:527:ILE:H	1:D:527:ILE:HD12	1.59	0.66
1:A:527:ILE:H	1:A:527:ILE:HD12	1.61	0.66
1:A:432:MET:HE1	1:A:534:ALA:C	2.15	0.66
1:B:527:ILE:H	1:B:527:ILE:HD12	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:213:VAL:O	1:D:241:PHE:HA	1.95	0.66
1:C:337:LEU:HD22	1:C:673:GLU:HA	1.76	0.66
1:D:432:MET:HE1	1:D:534:ALA:C	2.15	0.66
1:C:305:ARG:CD	1:C:390:GLU:HG2	2.25	0.66
1:D:129:VAL:O	1:D:133:LEU:HG	1.95	0.66
1:B:180:SER:O	1:B:193:TYR:HB2	1.95	0.66
1:C:615:THR:HA	1:C:618:ARG:HH12	1.59	0.66
1:D:198:ALA:O	1:D:202:ASN:HA	1.95	0.66
1:D:610:HIS:CD2	1:D:614:GLN:HE21	2.13	0.66
1:B:172:LEU:HB2	1:B:214:ALA:O	1.96	0.66
1:D:67:TYR:OH	1:D:114:PRO:HG3	1.94	0.66
1:C:332:PHE:CZ	1:C:400:LYS:HE2	2.31	0.66
1:B:90:MET:CE	1:B:318:ARG:HH22	2.09	0.65
1:B:610:HIS:CD2	1:B:614:GLN:HE21	2.14	0.65
1:D:409:ILE:O	1:D:413:ILE:HG12	1.97	0.65
1:B:228:ALA:O	1:B:230:GLY:N	2.30	0.65
1:C:39:ARG:O	1:C:41:LEU:N	2.29	0.65
1:D:138:LYS:HD3	1:D:142:ASP:HB3	1.77	0.65
1:D:172:LEU:HD11	1:D:216:VAL:HG23	1.78	0.65
1:A:717:VAL:O	1:A:721:THR:HG23	1.97	0.65
1:C:610:HIS:CD2	1:C:614:GLN:HE21	2.13	0.65
1:D:14:ARG:HD3	1:D:257:ILE:HD13	1.76	0.65
1:B:420:ILE:O	1:B:424:GLU:HG3	1.95	0.65
1:C:172:LEU:HB2	1:C:214:ALA:O	1.97	0.65
1:A:180:SER:O	1:A:193:TYR:HB2	1.97	0.65
1:B:1:MET:HG3	1:B:55:SER:HB3	1.77	0.65
1:C:527:ILE:HD12	1:C:527:ILE:H	1.62	0.65
1:D:251:PRO:HG2	1:D:254:PHE:CD1	2.31	0.65
1:B:255:ASP:OD1	1:B:258:ARG:HB2	1.95	0.65
1:D:679:MET:O	1:D:750:VAL:HG23	1.97	0.65
1:A:629:ILE:O	1:A:633:ILE:HG12	1.96	0.65
1:B:615:THR:HA	1:B:618:ARG:HH12	1.62	0.65
1:A:469:VAL:O	1:A:473:CYS:HB2	1.96	0.65
1:D:125:ARG:HH11	1:D:125:ARG:HG2	1.62	0.65
1:A:642:PRO:O	1:A:644:VAL:N	2.30	0.65
1:A:226:ILE:N	1:A:226:ILE:HD12	2.12	0.64
1:A:1:MET:HG3	1:A:55:SER:HB3	1.80	0.64
1:B:140:LEU:HD21	1:B:249:LEU:HB2	1.77	0.64
1:B:629:ILE:O	1:B:633:ILE:HG12	1.97	0.64
1:C:137:ALA:CB	1:C:248:LEU:HD21	2.26	0.64
1:C:115:LEU:O	1:C:258:ARG:NH2	2.29	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:44:ALA:HB3	1:C:264:PHE:CE2	2.31	0.64
1:A:4:LEU:HD22	1:A:25:THR:O	1.97	0.64
1:A:60:ASP:O	1:A:64:VAL:HG23	1.97	0.64
1:B:225:GLN:H	1:B:225:GLN:NE2	1.95	0.64
1:C:466:ARG:NE	1:C:498:ALA:HB2	2.10	0.64
1:A:310:ARG:HB2	1:A:310:ARG:HH11	1.62	0.64
1:A:343:LEU:HD13	1:A:427:LEU:HD21	1.79	0.64
1:B:157:ARG:HE	1:B:249:LEU:HD21	1.62	0.64
1:B:198:ALA:O	1:B:202:ASN:HA	1.97	0.64
1:A:140:LEU:HB2	1:A:244:PRO:O	1.96	0.64
1:A:352:LEU:HD11	1:A:650:LEU:HD23	1.78	0.64
1:C:172:LEU:HD11	1:C:216:VAL:HG23	1.78	0.64
1:D:1:MET:HA	1:D:56:LEU:H	1.63	0.64
1:A:198:ALA:O	1:A:202:ASN:HA	1.97	0.64
1:C:352:LEU:HD12	1:C:363:LEU:HD13	1.78	0.64
1:A:444:CYS:SG	1:A:448:VAL:HB	2.36	0.64
1:C:381:GLN:HE21	1:C:402:TRP:HD1	1.43	0.64
1:D:140:LEU:HB3	1:D:144:TYR:HE2	1.63	0.64
1:B:139:ARG:NH2	1:B:162:PRO:HG3	2.13	0.64
1:C:82:SER:O	1:C:86:ILE:HG13	1.97	0.64
1:D:226:ILE:HD12	1:D:226:ILE:N	2.13	0.64
1:D:284:LYS:HD2	1:D:284:LYS:H	1.62	0.64
1:B:67:TYR:OH	1:B:114:PRO:HG3	1.97	0.64
1:D:420:ILE:O	1:D:424:GLU:HG3	1.96	0.64
1:D:191:ILE:HG23	1:D:195:ARG:HD3	1.79	0.64
1:D:4:LEU:HD22	1:D:25:THR:O	1.98	0.64
1:A:125:ARG:HG2	1:A:125:ARG:HH11	1.63	0.64
1:A:561:ILE:HD12	1:A:561:ILE:N	2.13	0.64
1:B:373:ASN:HD21	1:B:401:THR:CG2	2.08	0.64
1:B:409:ILE:O	1:B:413:ILE:HG12	1.98	0.64
1:D:637:GLN:O	1:D:641:THR:HG23	1.98	0.64
1:A:402:TRP:CH2	1:B:396:VAL:HG23	2.34	0.63
1:A:494:ARG:NH1	1:A:494:ARG:HG2	2.13	0.63
1:A:615:THR:HA	1:A:618:ARG:HH12	1.62	0.63
1:B:4:LEU:HD22	1:B:25:THR:O	1.98	0.63
1:C:4:LEU:HD22	1:C:25:THR:O	1.99	0.63
1:D:386:PRO:O	1:D:389:ALA:HB3	1.98	0.63
1:B:125:ARG:HG2	1:B:125:ARG:HH11	1.62	0.63
1:C:114:PRO:HB3	1:C:258:ARG:NH1	2.12	0.63
1:C:310:ARG:HB2	1:C:310:ARG:HH11	1.63	0.63
1:C:717:VAL:O	1:C:721:THR:HG23	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:679:MET:O	1:A:750:VAL:HG23	1.98	0.63
1:B:191:ILE:HG23	1:B:195:ARG:HD3	1.81	0.63
1:C:191:ILE:HG23	1:C:195:ARG:HD3	1.79	0.63
1:C:1:MET:HG3	1:C:55:SER:HB3	1.80	0.63
1:B:226:ILE:HD12	1:B:226:ILE:N	2.13	0.63
1:B:310:ARG:HB2	1:B:310:ARG:HH11	1.64	0.63
1:B:561:ILE:N	1:B:561:ILE:HD12	2.13	0.63
1:D:236:ALA:N	1:D:237:PRO:CD	2.62	0.63
1:D:159:VAL:HG23	1:D:248:LEU:C	2.19	0.63
1:B:687:SER:O	1:B:691:ARG:HG3	1.98	0.63
1:C:41:LEU:HD13	1:C:264:PHE:CE2	2.33	0.63
1:A:307:ASP:OD1	1:A:391:PHE:HA	1.97	0.63
1:B:265:LEU:N	1:B:266:PRO:CD	2.62	0.63
1:C:256:LEU:O	1:C:259:VAL:N	2.29	0.63
1:A:243:PRO:HD2	1:A:246:LEU:HD12	1.81	0.63
1:A:137:ALA:HB1	1:A:248:LEU:HD21	1.78	0.63
1:A:310:ARG:NH2	1:A:392:SER:HB3	2.14	0.63
1:D:687:SER:O	1:D:691:ARG:HG3	1.98	0.63
1:A:82:SER:O	1:A:86:ILE:HG13	1.99	0.62
1:C:226:ILE:HD12	1:C:226:ILE:N	2.14	0.62
1:D:494:ARG:HG2	1:D:494:ARG:HH11	1.64	0.62
1:A:472:ALA:HA	1:A:477:ILE:HD12	1.81	0.62
1:C:187:ALA:O	1:C:188:ASN:HB2	1.99	0.62
1:B:60:ASP:O	1:B:64:VAL:HG23	1.99	0.62
1:B:94:GLU:HG2	1:B:316:GLY:CA	2.29	0.62
1:B:90:MET:HE3	1:B:318:ARG:HH22	1.63	0.62
1:A:494:ARG:HG2	1:A:494:ARG:HH11	1.64	0.62
1:A:678:ARG:NH2	1:A:753:ASP:OD1	2.33	0.62
1:B:187:ALA:O	1:B:188:ASN:HB2	2.00	0.62
1:D:251:PRO:HG2	1:D:254:PHE:CE1	2.35	0.62
1:A:395:LEU:N	1:A:395:LEU:HD23	2.15	0.62
1:B:434:PRO:HA	1:B:527:ILE:CG2	2.28	0.62
1:D:225:GLN:H	1:D:225:GLN:NE2	1.97	0.62
1:A:705:ILE:HG23	1:A:711:ILE:HD11	1.82	0.62
1:B:717:VAL:O	1:B:721:THR:HG23	1.98	0.62
1:D:243:PRO:HD2	1:D:246:LEU:HD12	1.82	0.62
1:D:260:GLN:O	1:D:264:PHE:HE1	1.83	0.62
1:D:618:ARG:HH11	1:D:618:ARG:HB2	1.64	0.62
1:A:172:LEU:HD11	1:A:216:VAL:HG23	1.82	0.62
1:A:38:GLY:HA3	1:A:317:TRP:CZ3	2.35	0.62
1:B:434:PRO:HA	1:B:527:ILE:HG22	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:305:ARG:NE	1:C:390:GLU:HG2	2.15	0.62
1:C:679:MET:O	1:C:750:VAL:HG23	2.00	0.62
1:A:172:LEU:HB2	1:A:214:ALA:O	2.00	0.62
1:C:372:ARG:HD2	1:C:374:GLU:OE1	1.99	0.62
1:C:60:ASP:O	1:C:64:VAL:HG23	2.00	0.62
1:C:747:LEU:HB3	1:C:748:PRO:HD3	1.81	0.62
1:B:104:PRO:HB3	1:B:280:CYS:SG	2.40	0.62
1:B:394:ASN:O	1:B:395:LEU:HB2	1.98	0.62
1:C:346:ILE:HG21	1:C:427:LEU:HD13	1.80	0.62
1:C:629:ILE:O	1:C:633:ILE:HG12	1.99	0.62
1:A:225:GLN:NE2	1:A:225:GLN:H	1.98	0.61
1:D:494:ARG:NH1	1:D:494:ARG:HG2	2.14	0.61
1:A:405:MET:O	1:A:409:ILE:HD13	1.99	0.61
1:C:361:GLY:O	1:C:365:GLU:HG3	2.00	0.61
1:C:699:VAL:O	1:C:703:VAL:HG23	2.00	0.61
1:D:642:PRO:O	1:D:644:VAL:N	2.33	0.61
1:A:687:SER:O	1:A:691:ARG:HG3	2.01	0.61
1:B:721:THR:O	1:B:725:ILE:HG12	2.01	0.61
1:D:147:TYR:HB3	1:D:150:LEU:HD22	1.82	0.61
1:A:191:ILE:HG23	1:A:195:ARG:HD3	1.83	0.61
1:C:642:PRO:O	1:C:644:VAL:N	2.33	0.61
1:A:71:LEU:HD22	1:A:262:LEU:HD13	1.81	0.61
1:D:60:ASP:CG	1:D:124:LEU:HD13	2.21	0.61
1:A:747:LEU:HB3	1:A:748:PRO:HD3	1.81	0.61
1:C:178:GLN:HE21	1:C:212:LEU:CD1	2.14	0.61
1:B:139:ARG:HH21	1:B:162:PRO:CG	2.13	0.61
1:B:243:PRO:HD2	1:B:246:LEU:HD12	1.82	0.61
1:C:159:VAL:HG23	1:C:248:LEU:C	2.20	0.61
1:D:629:ILE:O	1:D:633:ILE:HG12	2.01	0.61
1:B:154:LEU:HA	1:B:157:ARG:HD3	1.83	0.61
1:C:262:LEU:HB3	1:C:263:GLN:NE2	2.16	0.61
1:D:717:VAL:O	1:D:721:THR:HG23	2.00	0.61
1:A:310:ARG:O	1:A:312:ARG:HG2	2.01	0.61
1:B:705:ILE:HG23	1:B:711:ILE:HD11	1.81	0.61
1:A:217:ARG:HB3	1:A:220:ASP:OD2	2.01	0.61
1:B:432:MET:HA	1:B:479:VAL:O	2.01	0.61
1:D:60:ASP:O	1:D:64:VAL:HG23	2.01	0.61
1:D:310:ARG:HH11	1:D:310:ARG:HB2	1.64	0.60
1:D:693:THR:OG1	1:D:722:PHE:HB2	2.01	0.60
1:A:489:PHE:CZ	1:A:534:ALA:HA	2.36	0.60
1:B:172:LEU:HD11	1:B:216:VAL:HG23	1.81	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:369:GLU:HG3	1:D:482:SER:CB	2.30	0.60
1:D:561:ILE:N	1:D:561:ILE:HD12	2.16	0.60
1:D:699:VAL:O	1:D:703:VAL:HG23	2.00	0.60
1:A:115:LEU:O	1:A:258:ARG:NH2	2.34	0.60
1:A:33:PHE:CD2	1:A:318:ARG:HB2	2.36	0.60
1:A:535:ARG:O	1:A:539:LEU:HD12	2.01	0.60
1:B:217:ARG:HB3	1:B:220:ASP:OD2	2.00	0.60
1:B:372:ARG:HD2	1:B:374:GLU:OE1	2.02	0.60
1:B:432:MET:HE1	1:B:534:ALA:C	2.22	0.60
1:A:346:ILE:HG21	1:A:427:LEU:HD13	1.81	0.60
1:B:564:LEU:HB3	1:B:592:VAL:HG11	1.83	0.60
1:B:437:SER:HB3	1:B:478:SER:H	1.65	0.60
1:C:605:SER:HB3	1:C:634:ARG:HH12	1.66	0.60
1:D:37:ALA:HB2	1:D:43:ALA:CA	2.31	0.60
1:D:41:LEU:O	1:D:41:LEU:HD12	2.00	0.60
1:A:12:THR:HG22	1:A:44:ALA:HB2	1.82	0.60
1:A:564:LEU:HB3	1:A:592:VAL:HG11	1.84	0.60
1:D:154:LEU:HA	1:D:157:ARG:HD3	1.84	0.60
1:D:567:TYR:HA	1:D:572:GLN:HE22	1.66	0.60
1:D:609:LYS:HZ3	1:D:641:THR:HG21	1.64	0.60
1:D:342:VAL:HA	1:D:658:CYS:SG	2.42	0.60
1:C:409:ILE:O	1:C:413:ILE:HG12	2.01	0.60
1:C:564:LEU:HB3	1:C:592:VAL:HG11	1.82	0.60
1:D:158:MET:HE1	1:D:256:LEU:HD13	1.84	0.60
1:D:310:ARG:O	1:D:312:ARG:HG2	2.02	0.60
1:D:369:GLU:CG	1:D:485:VAL:HG23	2.30	0.60
1:D:405:MET:O	1:D:409:ILE:HD13	2.02	0.60
1:B:535:ARG:O	1:B:539:LEU:HD12	2.01	0.60
1:B:699:VAL:O	1:B:703:VAL:HG23	2.02	0.60
1:D:678:ARG:NH2	1:D:753:ASP:OD1	2.34	0.60
1:D:80:PRO:O	1:D:82:SER:N	2.35	0.60
1:A:350:ARG:HD3	1:A:538:TRP:O	2.02	0.60
1:A:368:MET:O	1:A:372:ARG:HB2	2.02	0.60
1:A:523:VAL:C	1:A:524:VAL:HG23	2.20	0.60
1:B:225:GLN:H	1:B:225:GLN:CD	2.05	0.60
1:B:361:GLY:O	1:B:365:GLU:HG3	2.02	0.60
1:B:458:GLY:C	1:B:460:ALA:H	2.06	0.60
1:C:259:VAL:O	1:C:263:GLN:NE2	2.35	0.60
1:C:284:LYS:N	1:C:284:LYS:HD2	2.17	0.60
1:C:561:ILE:HD12	1:C:561:ILE:N	2.17	0.60
1:C:705:ILE:HG23	1:C:711:ILE:HD11	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:327:SER:O	1:D:331:VAL:HG23	2.02	0.60
1:A:158:MET:CE	1:A:256:LEU:HD13	2.32	0.59
1:A:409:ILE:O	1:A:413:ILE:HG12	2.02	0.59
1:B:642:PRO:O	1:B:644:VAL:N	2.35	0.59
1:C:161:THR:OG1	1:C:164:ILE:HB	2.01	0.59
1:C:139:ARG:HG3	1:C:247:CYS:O	2.02	0.59
1:C:140:LEU:HD23	1:C:249:LEU:HB2	1.84	0.59
1:C:36:SER:HB2	1:C:312:ARG:O	2.03	0.59
1:D:217:ARG:HB3	1:D:220:ASP:OD2	2.00	0.59
1:D:747:LEU:HB3	1:D:748:PRO:HD3	1.84	0.59
1:A:567:TYR:HA	1:A:572:GLN:HE22	1.68	0.59
1:C:693:THR:OG1	1:C:722:PHE:HB2	2.02	0.59
1:C:432:MET:HE2	1:C:534:ALA:HB1	1.84	0.59
1:C:612:ALA:O	1:C:616:VAL:HG23	2.02	0.59
1:D:187:ALA:O	1:D:188:ASN:HB2	2.02	0.59
1:D:261:ALA:O	1:D:264:PHE:HD1	1.84	0.59
1:A:34:LYS:HB3	1:A:45:GLU:HG3	1.82	0.59
1:B:693:THR:OG1	1:B:722:PHE:HB2	2.03	0.59
1:C:21:LEU:HD11	1:C:110:LEU:HB2	1.84	0.59
1:C:171:VAL:HA	1:C:215:ALA:HB2	1.84	0.59
1:A:458:GLY:C	1:A:460:ALA:H	2.06	0.59
1:A:523:VAL:HB	1:A:528:ASP:OD2	2.02	0.59
1:A:420:ILE:HD13	1:A:569:ARG:NH2	2.17	0.59
1:B:494:ARG:NH1	1:B:494:ARG:HG2	2.17	0.59
1:B:71:LEU:HD22	1:B:262:LEU:CD1	2.33	0.59
1:A:256:LEU:O	1:A:257:ILE:C	2.41	0.59
1:B:448:VAL:HG13	1:B:468:LEU:HD23	1.84	0.59
1:C:14:ARG:HH12	1:C:223:ASP:HA	1.67	0.59
1:C:154:LEU:HA	1:C:157:ARG:HD3	1.83	0.59
1:C:39:ARG:C	1:C:41:LEU:H	2.06	0.59
1:D:82:SER:O	1:D:86:ILE:HG13	2.02	0.59
1:B:559:PRO:CG	1:B:599:ILE:HG13	2.33	0.59
1:B:599:ILE:HG21	1:B:631:PHE:CE1	2.38	0.59
1:B:637:GLN:O	1:B:641:THR:HG23	2.02	0.59
1:A:187:ALA:O	1:A:188:ASN:HB2	2.03	0.59
1:B:497:PRO:HG2	1:B:500:ASP:OD2	2.03	0.59
1:B:333:GLN:NE2	1:B:672:THR:HB	2.18	0.59
1:C:327:SER:O	1:C:331:VAL:HG23	2.02	0.59
1:C:458:GLY:C	1:C:460:ALA:H	2.05	0.59
1:D:144:TYR:CE2	1:D:244:PRO:HB3	2.38	0.59
1:D:548:GLN:HE21	1:D:548:GLN:HA	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:697:PRO:O	1:B:699:VAL:N	2.36	0.59
1:B:94:GLU:HG2	1:B:316:GLY:HA3	1.84	0.59
1:C:225:GLN:NE2	1:C:225:GLN:H	2.00	0.59
1:C:391:PHE:O	1:C:392:SER:HB3	2.03	0.59
1:C:605:SER:CB	1:C:634:ARG:HH12	2.16	0.59
1:D:171:VAL:HA	1:D:215:ALA:HB2	1.84	0.59
1:D:612:ALA:HB2	1:D:703:VAL:HG21	1.85	0.59
1:D:705:ILE:HG23	1:D:711:ILE:HD11	1.85	0.59
1:A:432:MET:HE1	1:A:534:ALA:O	2.03	0.58
1:B:473:CYS:HA	1:B:490:LEU:HD13	1.84	0.58
1:C:217:ARG:HB3	1:C:220:ASP:OD2	2.02	0.58
1:C:494:ARG:NH1	1:C:494:ARG:HG2	2.17	0.58
1:D:458:GLY:C	1:D:460:ALA:H	2.06	0.58
1:A:266:PRO:O	1:A:270:LYS:HG3	2.04	0.58
1:A:535:ARG:HH11	1:A:535:ARG:HG3	1.69	0.58
1:A:80:PRO:O	1:A:82:SER:N	2.35	0.58
1:B:310:ARG:O	1:B:312:ARG:HG2	2.03	0.58
1:C:310:ARG:O	1:C:312:ARG:HG2	2.03	0.58
1:D:457:MET:O	1:D:459:GLU:N	2.36	0.58
1:D:564:LEU:HB3	1:D:592:VAL:HG11	1.84	0.58
1:A:372:ARG:HD2	1:A:374:GLU:OE1	2.02	0.58
1:D:401:THR:HG22	1:D:402:TRP:N	2.17	0.58
1:A:253:GLU:O	1:A:255:ASP:N	2.35	0.58
1:A:373:ASN:ND2	1:A:401:THR:HG21	2.13	0.58
1:A:457:MET:O	1:A:459:GLU:N	2.36	0.58
1:B:678:ARG:NH2	1:B:753:ASP:OD1	2.35	0.58
1:B:82:SER:O	1:B:86:ILE:HG13	2.03	0.58
1:C:193:TYR:HE2	1:C:241:PHE:HB2	1.66	0.58
1:A:445:PRO:HG2	1:A:448:VAL:HG23	1.85	0.58
1:B:159:VAL:HG23	1:B:248:LEU:O	2.02	0.58
1:C:335:LEU:O	1:C:411:GLY:HA3	2.03	0.58
1:C:432:MET:HE1	1:C:534:ALA:C	2.23	0.58
1:C:535:ARG:O	1:C:539:LEU:HD12	2.03	0.58
1:A:699:VAL:O	1:A:703:VAL:HG23	2.02	0.58
1:A:693:THR:OG1	1:A:722:PHE:HB2	2.04	0.58
1:B:327:SER:O	1:B:331:VAL:HG23	2.03	0.58
1:C:159:VAL:HA	1:C:250:LEU:HG	1.86	0.58
1:D:139:ARG:HG3	1:D:247:CYS:O	2.03	0.58
1:D:225:GLN:CD	1:D:225:GLN:H	2.07	0.58
1:D:137:ALA:HB2	1:D:251:PRO:HD3	1.85	0.58
1:D:612:ALA:O	1:D:616:VAL:HG23	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:721:THR:O	1:D:725:ILE:HG12	2.01	0.58
1:B:284:LYS:N	1:B:284:LYS:HD2	2.18	0.58
1:C:137:ALA:HB3	1:C:248:LEU:HD21	1.84	0.58
1:D:472:ALA:CB	1:D:477:ILE:HD12	2.33	0.58
1:A:154:LEU:HA	1:A:157:ARG:HD3	1.84	0.58
1:A:456:CYS:SG	1:A:524:VAL:HA	2.44	0.58
1:B:213:VAL:O	1:B:241:PHE:HA	2.04	0.58
1:B:321:PHE:CD2	1:B:325:GLY:HA2	2.39	0.58
1:C:310:ARG:O	1:C:312:ARG:N	2.37	0.58
1:C:494:ARG:HH11	1:C:494:ARG:HG2	1.68	0.58
1:C:497:PRO:HG2	1:C:500:ASP:OD2	2.04	0.58
1:A:523:VAL:HG13	1:D:619:SER:OG	2.03	0.58
1:B:360:VAL:O	1:B:364:VAL:HG23	2.04	0.58
1:B:343:LEU:HD13	1:B:427:LEU:HD21	1.85	0.58
1:C:114:PRO:O	1:C:115:LEU:HD23	2.03	0.58
1:C:327:SER:OG	1:C:329:THR:HB	2.04	0.58
1:C:612:ALA:HB2	1:C:703:VAL:HG21	1.85	0.58
1:D:310:ARG:O	1:D:312:ARG:N	2.37	0.58
1:D:527:ILE:N	1:D:527:ILE:HD12	2.19	0.58
1:A:721:THR:O	1:A:725:ILE:HG12	2.03	0.58
1:B:337:LEU:HD22	1:B:673:GLU:HA	1.84	0.58
1:C:21:LEU:HD13	1:C:112:PHE:CE1	2.38	0.58
1:C:405:MET:O	1:C:409:ILE:HD13	2.04	0.58
1:C:80:PRO:O	1:C:82:SER:N	2.35	0.58
1:D:361:GLY:O	1:D:365:GLU:HG3	2.03	0.58
1:A:401:THR:HG22	1:A:403:ALA:N	2.19	0.57
1:A:327:SER:OG	1:A:329:THR:HB	2.04	0.57
1:A:376:LEU:O	1:A:380:VAL:HG23	2.04	0.57
1:B:159:VAL:HG23	1:B:248:LEU:C	2.23	0.57
1:B:599:ILE:HG21	1:B:631:PHE:HE1	1.69	0.57
1:C:125:ARG:NH1	1:C:125:ARG:HG2	2.18	0.57
1:C:243:PRO:HD2	1:C:246:LEU:HD12	1.85	0.57
1:C:564:LEU:HD23	1:C:592:VAL:HG12	1.85	0.57
1:D:161:THR:OG1	1:D:164:ILE:HB	2.04	0.57
1:A:298:PHE:CZ	1:A:331:VAL:HG21	2.40	0.57
1:A:310:ARG:O	1:A:312:ARG:N	2.37	0.57
1:B:71:LEU:HD22	1:B:262:LEU:HD13	1.86	0.57
1:B:112:PHE:CG	1:B:265:LEU:HD22	2.40	0.57
1:C:675:ALA:O	1:C:679:MET:HG3	2.04	0.57
1:D:372:ARG:HD2	1:D:374:GLU:OE1	2.04	0.57
1:D:4:LEU:HD21	1:D:26:HIS:ND1	2.20	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:497:PRO:HG2	1:A:500:ASP:OD2	2.04	0.57
1:A:637:GLN:O	1:A:641:THR:HG23	2.05	0.57
1:C:473:CYS:C	1:C:475:GLN:H	2.08	0.57
1:C:567:TYR:HA	1:C:572:GLN:HE22	1.69	0.57
1:D:37:ALA:HB2	1:D:43:ALA:CB	2.35	0.57
1:A:161:THR:OG1	1:A:164:ILE:HB	2.04	0.57
1:A:284:LYS:HD2	1:A:284:LYS:N	2.18	0.57
1:B:747:LEU:HB3	1:B:748:PRO:HD3	1.85	0.57
1:D:227:PRO:HG3	1:D:234:ASP:OD2	2.05	0.57
1:D:637:GLN:HA	1:D:640:LEU:HD12	1.85	0.57
1:A:60:ASP:CG	1:A:124:LEU:HD13	2.24	0.57
1:A:507:LEU:HD22	1:A:588:VAL:HG21	1.85	0.57
1:B:251:PRO:HG2	1:B:254:PHE:CD1	2.40	0.57
1:D:178:GLN:HE21	1:D:212:LEU:CD1	2.14	0.57
1:D:497:PRO:HG2	1:D:500:ASP:OD2	2.04	0.57
1:A:470:ASP:O	1:A:474:GLU:HG2	2.04	0.57
1:B:310:ARG:O	1:B:312:ARG:N	2.38	0.57
1:C:140:LEU:HD12	1:C:213:VAL:HG21	1.87	0.57
1:A:112:PHE:CD2	1:A:265:LEU:HD13	2.40	0.57
1:C:33:PHE:CD2	1:C:318:ARG:HB2	2.40	0.57
1:C:321:PHE:CD2	1:C:325:GLY:HA2	2.40	0.57
1:C:462:ALA:O	1:C:465:PHE:N	2.36	0.57
1:C:721:THR:O	1:C:725:ILE:HG12	2.05	0.57
1:D:34:LYS:HB3	1:D:45:GLU:HG3	1.85	0.57
1:B:60:ASP:CG	1:B:124:LEU:HD13	2.25	0.57
1:B:612:ALA:O	1:B:616:VAL:HG23	2.04	0.57
1:B:494:ARG:HH11	1:B:494:ARG:HG2	1.69	0.56
1:C:527:ILE:HD12	1:C:527:ILE:N	2.20	0.56
1:D:37:ALA:HB2	1:D:43:ALA:N	2.20	0.56
1:C:685:THR:HG22	1:D:487:THR:HG21	1.87	0.56
1:C:708:HIS:HB3	1:C:711:ILE:HG21	1.87	0.56
1:C:678:ARG:NH2	1:C:753:ASP:OD1	2.38	0.56
1:D:145:THR:O	1:D:147:TYR:N	2.38	0.56
1:A:225:GLN:CD	1:A:225:GLN:H	2.07	0.56
1:A:327:SER:O	1:A:331:VAL:HG23	2.05	0.56
1:B:236:ALA:N	1:B:237:PRO:CD	2.68	0.56
1:C:637:GLN:O	1:C:641:THR:HG23	2.05	0.56
1:A:97:PHE:HZ	1:A:301:THR:HA	1.71	0.56
1:A:4:LEU:HD21	1:A:26:HIS:ND1	2.20	0.56
1:A:612:ALA:HB2	1:A:703:VAL:HG21	1.87	0.56
1:B:112:PHE:CE2	1:B:265:LEU:HB3	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:172:LEU:HD12	1:B:239:LEU:HD13	1.87	0.56
1:B:14:ARG:HB2	1:B:257:ILE:HD12	1.87	0.56
1:C:60:ASP:CG	1:C:124:LEU:HD13	2.25	0.56
1:C:437:SER:HB3	1:C:478:SER:O	2.06	0.56
1:D:462:ALA:HA	1:D:498:ALA:HB1	1.86	0.56
1:A:321:PHE:CD2	1:A:325:GLY:HA2	2.41	0.56
1:B:242:LEU:N	1:B:242:LEU:HD23	2.20	0.56
1:B:711:ILE:O	1:B:711:ILE:HD12	2.06	0.56
1:D:136:ASP:O	1:D:137:ALA:C	2.44	0.56
1:D:327:SER:OG	1:D:329:THR:HB	2.05	0.56
1:D:369:GLU:CG	1:D:482:SER:OG	2.54	0.56
1:A:512:SER:HA	1:A:517:LEU:HD11	1.88	0.56
1:B:527:ILE:N	1:B:527:ILE:HD12	2.19	0.56
1:B:680:ARG:HH11	1:B:680:ARG:HG3	1.71	0.56
1:D:262:LEU:HD12	1:D:262:LEU:O	2.05	0.56
1:D:725:ILE:HG22	1:D:729:ILE:HD11	1.88	0.56
1:B:339:GLY:HA3	1:B:407:GLU:O	2.06	0.56
1:B:432:MET:HE1	1:B:534:ALA:O	2.06	0.56
1:C:432:MET:HA	1:C:479:VAL:O	2.06	0.56
1:C:547:GLU:HG2	1:C:548:GLN:N	2.21	0.56
1:D:23:LEU:CD2	1:D:110:LEU:HB3	2.36	0.56
1:D:512:SER:HA	1:D:517:LEU:HD11	1.88	0.56
1:A:624:ILE:CD1	1:A:624:ILE:H	2.19	0.56
1:B:80:PRO:O	1:B:82:SER:N	2.38	0.56
1:C:262:LEU:C	1:C:264:PHE:H	2.10	0.56
1:D:369:GLU:HG3	1:D:482:SER:HB2	1.87	0.56
1:B:178:GLN:HE21	1:B:212:LEU:CD1	2.16	0.55
1:B:457:MET:O	1:B:459:GLU:N	2.38	0.55
1:B:612:ALA:HB2	1:B:703:VAL:HG21	1.87	0.55
1:D:143:GLU:O	1:D:146:ASP:N	2.39	0.55
1:D:376:LEU:O	1:D:380:VAL:HG23	2.06	0.55
1:A:464:GLU:O	1:A:468:LEU:HG	2.06	0.55
1:B:191:ILE:HG22	1:B:192:THR:N	2.21	0.55
1:B:394:ASN:HD21	1:B:396:VAL:HB	1.71	0.55
1:C:489:PHE:CZ	1:C:534:ALA:HA	2.41	0.55
1:D:235:LEU:C	1:D:237:PRO:HD2	2.26	0.55
1:D:342:VAL:HG23	1:D:343:LEU:N	2.20	0.55
1:D:711:ILE:O	1:D:711:ILE:HD12	2.05	0.55
1:A:361:GLY:O	1:A:365:GLU:HG3	2.07	0.55
1:B:603:GLU:HA	1:B:634:ARG:HH22	1.70	0.55
1:B:738:ALA:O	1:B:741:PHE:HB3	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:637:GLN:HA	1:C:640:LEU:HD12	1.87	0.55
1:D:292:ILE:HD12	1:D:292:ILE:C	2.26	0.55
1:D:360:VAL:O	1:D:364:VAL:HG23	2.06	0.55
1:A:207:ALA:HB1	1:A:210:LEU:HG	1.88	0.55
1:A:23:LEU:HD21	1:A:272:ILE:HD13	1.89	0.55
1:B:171:VAL:HA	1:B:215:ALA:HB2	1.87	0.55
1:D:708:HIS:HB3	1:D:711:ILE:HG21	1.89	0.55
1:B:140:LEU:C	1:B:142:ASP:H	2.09	0.55
1:D:145:THR:C	1:D:147:TYR:H	2.08	0.55
1:D:207:ALA:HB1	1:D:210:LEU:HG	1.87	0.55
1:D:21:LEU:HD13	1:D:112:PHE:CE1	2.41	0.55
1:A:527:ILE:N	1:A:527:ILE:HD12	2.22	0.55
1:B:342:VAL:HG12	1:B:658:CYS:SG	2.46	0.55
1:C:235:LEU:C	1:C:237:PRO:CD	2.75	0.55
1:C:457:MET:O	1:C:459:GLU:N	2.38	0.55
1:C:725:ILE:HG22	1:C:729:ILE:HD11	1.89	0.55
1:D:221:LEU:O	1:D:222:LYS:C	2.45	0.55
1:D:242:LEU:N	1:D:242:LEU:HD23	2.21	0.55
1:D:284:LYS:N	1:D:284:LYS:HD2	2.20	0.55
1:D:471:TYR:CZ	1:D:475:GLN:HG3	2.42	0.55
1:D:663:HIS:CD2	1:D:743:ARG:HB3	2.41	0.55
1:A:171:VAL:HA	1:A:215:ALA:HB2	1.88	0.55
1:A:298:PHE:HZ	1:A:331:VAL:HG21	1.72	0.55
1:A:725:ILE:HG22	1:A:729:ILE:HD11	1.89	0.55
1:B:114:PRO:O	1:B:115:LEU:HD23	2.06	0.55
1:B:4:LEU:HD21	1:B:26:HIS:ND1	2.22	0.55
1:B:708:HIS:HB3	1:B:711:ILE:HG21	1.88	0.55
1:B:725:ILE:HG22	1:B:729:ILE:HD11	1.89	0.55
1:C:225:GLN:H	1:C:225:GLN:CD	2.08	0.55
1:C:298:PHE:CZ	1:C:331:VAL:HG21	2.42	0.55
1:C:342:VAL:HG23	1:C:343:LEU:N	2.21	0.55
1:C:697:PRO:O	1:C:699:VAL:N	2.39	0.55
1:D:114:PRO:O	1:D:115:LEU:HD23	2.07	0.55
1:D:375:ALA:O	1:D:378:TYR:HB3	2.06	0.55
1:A:462:ALA:HB1	1:A:498:ALA:HB3	1.88	0.55
1:B:564:LEU:HD23	1:B:592:VAL:HG12	1.88	0.55
1:C:42:PRO:HB3	1:C:223:ASP:HB3	1.88	0.55
1:D:110:LEU:HD13	1:D:272:ILE:CD1	2.29	0.55
1:D:158:MET:HE1	1:D:170:VAL:HB	1.89	0.55
1:A:178:GLN:HE21	1:A:212:LEU:CD1	2.15	0.55
1:B:489:PHE:CZ	1:B:534:ALA:HA	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:543:GLY:HA3	1:B:561:ILE:O	2.06	0.55
1:B:562:PRO:HB3	1:B:595:LEU:HB2	1.89	0.55
1:C:360:VAL:O	1:C:364:VAL:HG23	2.07	0.55
1:C:306:LEU:HD22	1:C:400:LYS:NZ	2.22	0.55
1:A:437:SER:HB3	1:A:478:SER:O	2.07	0.55
1:B:425:GLU:HG2	1:B:429:LYS:HE3	1.89	0.55
1:D:191:ILE:HG22	1:D:192:THR:N	2.22	0.55
1:D:350:ARG:HD3	1:D:538:TRP:O	2.05	0.55
1:A:637:GLN:HA	1:A:640:LEU:HD12	1.89	0.54
1:B:161:THR:OG1	1:B:164:ILE:HB	2.06	0.54
1:B:179:THR:HG22	1:B:181:LEU:H	1.72	0.54
1:B:327:SER:OG	1:B:329:THR:HB	2.06	0.54
1:B:637:GLN:HA	1:B:640:LEU:HD12	1.89	0.54
1:B:680:ARG:NH1	1:B:680:ARG:HG3	2.21	0.54
1:C:305:ARG:HD2	1:C:390:GLU:CB	2.37	0.54
1:D:369:GLU:HG3	1:D:482:SER:OG	2.07	0.54
1:A:711:ILE:HD12	1:A:711:ILE:O	2.06	0.54
1:B:428:ALA:HB3	1:B:511:PHE:CZ	2.42	0.54
1:D:147:TYR:HB3	1:D:150:LEU:HB2	1.90	0.54
1:D:675:ALA:O	1:D:679:MET:HG3	2.07	0.54
1:A:738:ALA:O	1:A:741:PHE:HB3	2.07	0.54
1:B:14:ARG:HD3	1:B:257:ILE:HD13	1.90	0.54
1:B:333:GLN:HE21	1:B:673:GLU:CB	2.21	0.54
1:C:164:ILE:HG22	1:C:164:ILE:O	2.07	0.54
1:C:191:ILE:HG22	1:C:192:THR:N	2.22	0.54
1:C:375:ALA:O	1:C:378:TYR:HB3	2.07	0.54
1:C:663:HIS:CD2	1:C:743:ARG:HB3	2.42	0.54
1:D:335:LEU:O	1:D:411:GLY:HA3	2.08	0.54
1:A:21:LEU:HD21	1:A:272:ILE:HD11	1.88	0.54
1:A:265:LEU:N	1:A:266:PRO:CD	2.70	0.54
1:B:20:LEU:HB2	1:B:115:LEU:HD11	1.90	0.54
1:B:567:TYR:HA	1:B:572:GLN:HE22	1.71	0.54
1:B:663:HIS:CD2	1:B:743:ARG:HB3	2.43	0.54
1:C:265:LEU:HB2	1:C:266:PRO:HD3	1.89	0.54
1:D:128:MET:O	1:D:132:GLN:HG3	2.07	0.54
1:D:327:SER:HG	1:D:329:THR:HB	1.73	0.54
1:D:432:MET:HE1	1:D:534:ALA:O	2.08	0.54
1:A:697:PRO:O	1:A:699:VAL:N	2.40	0.54
1:B:136:ASP:O	1:B:137:ALA:C	2.46	0.54
1:C:105:PRO:HG2	1:C:106:GLN:H	1.73	0.54
1:C:23:LEU:HD21	1:C:272:ILE:HD13	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:298:PHE:HZ	1:C:331:VAL:HG21	1.73	0.54
1:C:624:ILE:H	1:C:624:ILE:CD1	2.21	0.54
1:D:141:SER:C	1:D:143:GLU:H	2.11	0.54
1:D:170:VAL:HG11	1:D:221:LEU:HD22	1.87	0.54
1:D:564:LEU:HD23	1:D:592:VAL:HG12	1.88	0.54
1:C:158:MET:HG3	1:C:259:VAL:CG2	2.37	0.54
1:C:546:VAL:HB	1:C:644:VAL:HG13	1.89	0.54
1:C:596:TYR:CE2	1:C:600:LEU:HD11	2.42	0.54
1:D:489:PHE:CZ	1:D:534:ALA:HA	2.42	0.54
1:A:708:HIS:HB3	1:A:711:ILE:HG21	1.90	0.54
1:B:230:GLY:HA2	1:B:233:ASP:OD2	2.07	0.54
1:B:376:LEU:O	1:B:380:VAL:HG23	2.08	0.54
1:C:451:ALA:O	1:C:455:VAL:HG23	2.08	0.54
1:A:125:ARG:HG2	1:A:125:ARG:NH1	2.23	0.54
1:A:159:VAL:HG21	1:A:247:CYS:HB3	1.90	0.54
1:A:164:ILE:HG22	1:A:164:ILE:O	2.08	0.54
1:A:172:LEU:HD12	1:A:239:LEU:HD13	1.89	0.54
1:A:342:VAL:HG23	1:A:343:LEU:N	2.23	0.54
1:B:266:PRO:O	1:B:270:LYS:HG3	2.08	0.54
1:B:600:LEU:HD21	1:B:631:PHE:HA	1.89	0.54
1:C:4:LEU:HD21	1:C:26:HIS:ND1	2.22	0.54
1:D:321:PHE:CD2	1:D:325:GLY:HA2	2.42	0.54
1:A:564:LEU:HD23	1:A:592:VAL:HG12	1.88	0.54
1:A:680:ARG:HG3	1:A:680:ARG:HH11	1.73	0.54
1:B:125:ARG:NH1	1:B:125:ARG:HG2	2.22	0.54
1:B:207:ALA:HB1	1:B:210:LEU:HG	1.89	0.54
1:B:456:CYS:SG	1:B:524:VAL:HG13	2.47	0.54
1:C:242:LEU:HD23	1:C:242:LEU:N	2.23	0.54
1:C:535:ARG:HG3	1:C:535:ARG:HH11	1.73	0.54
1:A:221:LEU:O	1:A:222:LYS:C	2.47	0.54
1:C:353:CYS:HB3	1:C:541:SER:HB2	1.90	0.54
1:C:12:THR:HG22	1:C:44:ALA:HB2	1.89	0.54
1:C:497:PRO:HB2	1:C:499:GLU:OE2	2.07	0.54
1:B:172:LEU:HD12	1:B:239:LEU:CD1	2.38	0.53
1:B:23:LEU:HD21	1:B:272:ILE:HD13	1.90	0.53
1:B:512:SER:HA	1:B:517:LEU:HD11	1.89	0.53
1:C:160:ALA:HB2	1:C:168:LEU:CD2	2.37	0.53
1:C:207:ALA:HB1	1:C:210:LEU:HG	1.89	0.53
1:A:292:ILE:C	1:A:292:ILE:HD12	2.28	0.53
1:A:342:VAL:HG12	1:A:658:CYS:SG	2.48	0.53
1:A:369:GLU:CG	1:A:482:SER:OG	2.55	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:375:ALA:O	1:A:378:TYR:HB3	2.07	0.53
1:A:602:TYR:O	1:A:634:ARG:NH2	2.41	0.53
1:B:256:LEU:O	1:B:257:ILE:C	2.47	0.53
1:C:140:LEU:CD2	1:C:249:LEU:HD12	2.37	0.53
1:C:463:HIS:O	1:C:464:GLU:C	2.46	0.53
1:D:220:ASP:HB3	1:D:238:LYS:HD3	1.90	0.53
1:D:608:SER:C	1:D:610:HIS:H	2.11	0.53
1:A:159:VAL:HG23	1:A:248:LEU:C	2.28	0.53
1:B:342:VAL:O	1:B:346:ILE:HG12	2.08	0.53
1:C:292:ILE:C	1:C:292:ILE:HD12	2.28	0.53
1:C:339:GLY:HA3	1:C:407:GLU:O	2.08	0.53
1:C:376:LEU:O	1:C:380:VAL:HG23	2.08	0.53
1:C:390:GLU:O	1:C:391:PHE:HB3	2.07	0.53
1:D:125:ARG:NH1	1:D:125:ARG:HG2	2.23	0.53
1:A:342:VAL:O	1:A:346:ILE:HG12	2.07	0.53
1:A:594:ALA:O	1:A:598:LYS:HG3	2.09	0.53
1:A:612:ALA:O	1:A:616:VAL:HG23	2.08	0.53
1:B:405:MET:O	1:B:409:ILE:HD13	2.07	0.53
1:C:391:PHE:CE2	1:C:402:TRP:HH2	2.27	0.53
1:A:548:GLN:HA	1:A:548:GLN:NE2	2.23	0.53
1:A:725:ILE:O	1:A:728:ALA:N	2.41	0.53
1:B:292:ILE:HD12	1:B:292:ILE:C	2.28	0.53
1:B:298:PHE:CZ	1:B:331:VAL:HG21	2.43	0.53
1:C:221:LEU:O	1:C:222:LYS:C	2.45	0.53
1:C:562:PRO:HB3	1:C:595:LEU:HB2	1.89	0.53
1:D:255:ASP:O	1:D:256:LEU:C	2.46	0.53
1:D:546:VAL:HB	1:D:644:VAL:HG13	1.91	0.53
1:A:160:ALA:HB2	1:A:168:LEU:CD2	2.39	0.53
1:B:39:ARG:NH2	1:B:267:GLU:OE2	2.41	0.53
1:B:375:ALA:O	1:B:378:TYR:HB3	2.08	0.53
1:C:90:MET:HE3	1:C:318:ARG:HH22	1.74	0.53
1:C:425:GLU:HG2	1:C:429:LYS:HE3	1.90	0.53
1:D:262:LEU:HA	1:D:265:LEU:HD12	1.89	0.53
1:A:172:LEU:HD12	1:A:239:LEU:CD1	2.39	0.53
1:A:437:SER:HB3	1:A:478:SER:H	1.74	0.53
1:A:680:ARG:HG3	1:A:680:ARG:NH1	2.23	0.53
1:B:170:VAL:HG11	1:B:221:LEU:HD22	1.91	0.53
1:B:497:PRO:HB2	1:B:499:GLU:OE2	2.09	0.53
1:C:512:SER:HA	1:C:517:LEU:HD11	1.90	0.53
1:D:697:PRO:O	1:D:699:VAL:N	2.41	0.53
1:A:675:ALA:O	1:A:679:MET:HG3	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:42:PRO:HD3	1:C:222:LYS:O	2.08	0.53
1:C:402:TRP:CE3	1:C:405:MET:CE	2.92	0.53
1:D:298:PHE:CZ	1:D:331:VAL:HG21	2.44	0.53
1:A:663:HIS:CD2	1:A:743:ARG:HB3	2.43	0.53
1:B:221:LEU:O	1:B:222:LYS:C	2.47	0.52
1:D:290:GLY:HA3	1:D:417:PRO:HG2	1.90	0.52
1:D:390:GLU:O	1:D:391:PHE:HB3	2.10	0.52
1:A:360:VAL:O	1:A:364:VAL:HG23	2.09	0.52
1:A:392:SER:C	1:A:394:ASN:H	2.10	0.52
1:A:369:GLU:HG3	1:A:482:SER:CB	2.40	0.52
1:A:497:PRO:HB2	1:A:499:GLU:OE2	2.09	0.52
1:C:170:VAL:O	1:C:215:ALA:HB1	2.09	0.52
1:C:236:ALA:C	1:C:238:LYS:H	2.13	0.52
1:C:614:GLN:O	1:C:617:SER:HB3	2.09	0.52
1:C:72:PHE:CG	1:C:81:ALA:HA	2.44	0.52
1:D:451:ALA:O	1:D:455:VAL:HG23	2.08	0.52
1:D:535:ARG:O	1:D:539:LEU:HD12	2.09	0.52
1:A:523:VAL:HG21	1:D:618:ARG:NH1	2.24	0.52
1:B:353:CYS:HB3	1:B:541:SER:HB2	1.91	0.52
1:C:170:VAL:HG11	1:C:221:LEU:HD22	1.91	0.52
1:C:629:ILE:N	1:C:630:PRO:HD2	2.24	0.52
1:C:738:ALA:O	1:C:741:PHE:HB3	2.09	0.52
1:A:179:THR:HG22	1:A:181:LEU:H	1.73	0.52
1:A:99:ARG:NH1	1:A:390:GLU:CD	2.60	0.52
1:B:261:ALA:C	1:B:263:GLN:H	2.13	0.52
1:C:306:LEU:HD22	1:C:400:LYS:HZ3	1.73	0.52
1:D:147:TYR:CB	1:D:150:LEU:HB2	2.39	0.52
1:D:172:LEU:CD1	1:D:239:LEU:HD13	2.39	0.52
1:D:425:GLU:HG2	1:D:429:LYS:HE3	1.91	0.52
1:A:191:ILE:HG22	1:A:192:THR:N	2.24	0.52
1:A:562:PRO:HB3	1:A:595:LEU:HB2	1.90	0.52
1:A:603:GLU:N	1:A:603:GLU:CD	2.62	0.52
1:B:160:ALA:HB2	1:B:168:LEU:CD2	2.37	0.52
1:B:4:LEU:CD2	1:B:26:HIS:HA	2.40	0.52
1:C:456:CYS:HB2	1:C:457:MET:HE2	1.92	0.52
1:C:682:SER:HB2	1:C:751:VAL:HG12	1.91	0.52
1:A:599:ILE:HG21	1:A:631:PHE:HE1	1.75	0.52
1:A:643:HIS:O	1:A:646:GLN:HG2	2.09	0.52
1:B:298:PHE:HZ	1:B:331:VAL:HG21	1.75	0.52
1:B:99:ARG:NH1	1:B:390:GLU:O	2.42	0.52
1:C:160:ALA:CB	1:C:168:LEU:HD23	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:36:SER:HB3	1:C:317:TRP:HE3	1.74	0.52
1:D:90:MET:HE1	1:D:318:ARG:NH2	2.24	0.52
1:A:259:VAL:O	1:A:262:LEU:HB3	2.09	0.52
1:A:466:ARG:O	1:A:470:ASP:OD1	2.28	0.52
1:B:594:ALA:O	1:B:598:LYS:HG3	2.10	0.52
1:B:682:SER:HB2	1:B:751:VAL:HG12	1.92	0.52
1:D:20:LEU:HD23	1:D:122:LEU:HD13	1.92	0.52
1:D:227:PRO:CB	1:D:233:ASP:N	2.73	0.52
1:D:298:PHE:HZ	1:D:331:VAL:HG21	1.75	0.52
1:D:562:PRO:HB3	1:D:595:LEU:HB2	1.91	0.52
1:D:356:PRO:O	1:D:647:LYS:NZ	2.43	0.52
1:A:260:GLN:HA	1:A:263:GLN:HG2	1.92	0.52
1:A:379:LEU:HD21	1:A:481:CYS:CB	2.38	0.52
1:B:164:ILE:O	1:B:164:ILE:HG22	2.09	0.52
1:C:307:ASP:OD1	1:C:391:PHE:HA	2.10	0.52
1:D:264:PHE:CD1	1:D:264:PHE:N	2.77	0.52
1:D:38:GLY:N	1:D:41:LEU:HD12	2.24	0.52
1:D:456:CYS:HB2	1:D:457:MET:HE2	1.92	0.52
1:D:594:ALA:O	1:D:598:LYS:HG3	2.10	0.52
1:D:624:ILE:H	1:D:624:ILE:CD1	2.20	0.52
1:A:300:ILE:CG2	1:A:304:LEU:HD12	2.39	0.52
1:A:35:VAL:O	1:A:43:ALA:HA	2.10	0.52
1:A:462:ALA:HA	1:A:498:ALA:HB1	1.91	0.52
1:A:729:ILE:HD12	1:A:729:ILE:N	2.25	0.52
1:B:139:ARG:N	1:B:142:ASP:OD2	2.42	0.52
1:B:258:ARG:C	1:B:260:GLN:H	2.13	0.52
1:C:42:PRO:CB	1:C:223:ASP:HB3	2.40	0.52
1:D:160:ALA:HB2	1:D:168:LEU:CD2	2.39	0.52
1:A:606:GLY:HA2	1:A:610:HIS:CB	2.39	0.51
1:B:38:GLY:HA3	1:B:41:LEU:HD11	1.90	0.51
1:C:342:VAL:O	1:C:346:ILE:HG12	2.10	0.51
1:D:101:ILE:HG23	1:D:277:ASN:HD21	1.76	0.51
1:D:300:ILE:CG2	1:D:304:LEU:HD12	2.38	0.51
1:D:368:MET:O	1:D:372:ARG:HB2	2.09	0.51
1:D:72:PHE:CG	1:D:81:ALA:HA	2.45	0.51
1:D:738:ALA:O	1:D:741:PHE:HB3	2.10	0.51
1:A:242:LEU:HD23	1:A:242:LEU:N	2.25	0.51
1:A:395:LEU:O	1:A:398:LYS:N	2.43	0.51
1:B:251:PRO:HG2	1:B:254:PHE:HD1	1.75	0.51
1:C:112:PHE:CD2	1:C:265:LEU:HD13	2.45	0.51
1:C:18:HIS:O	1:C:258:ARG:NH2	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:725:ILE:O	1:C:728:ALA:N	2.43	0.51
1:A:157:ARG:HH21	1:A:249:LEU:HD21	1.75	0.51
1:A:425:GLU:HG2	1:A:429:LYS:HE3	1.92	0.51
1:B:624:ILE:H	1:B:624:ILE:CD1	2.21	0.51
1:C:236:ALA:N	1:C:237:PRO:CD	2.73	0.51
1:C:357:ASP:OD1	1:D:716:LYS:NZ	2.38	0.51
1:C:594:ALA:O	1:C:598:LYS:HG3	2.10	0.51
1:A:451:ALA:O	1:A:455:VAL:HG23	2.10	0.51
1:D:172:LEU:HD11	1:D:216:VAL:CG2	2.40	0.51
1:B:258:ARG:O	1:B:260:GLN:N	2.44	0.51
1:B:1:MET:HG3	1:B:55:SER:CB	2.40	0.51
1:B:507:LEU:HD22	1:B:588:VAL:HG21	1.92	0.51
1:B:72:PHE:CG	1:B:81:ALA:HA	2.46	0.51
1:A:587:PRO:HG2	1:A:588:VAL:H	1.76	0.51
1:C:212:LEU:HD13	1:C:241:PHE:HB3	1.92	0.51
1:D:170:VAL:O	1:D:215:ALA:HB1	2.11	0.51
1:D:401:THR:HG22	1:D:402:TRP:H	1.76	0.51
1:A:4:LEU:CD2	1:A:26:HIS:HA	2.41	0.51
1:A:698:SER:O	1:A:702:GLU:HG3	2.11	0.51
1:B:39:ARG:H	1:B:39:ARG:CD	2.23	0.51
1:B:559:PRO:HG3	1:B:599:ILE:HG13	1.92	0.51
1:D:251:PRO:O	1:D:252:ASP:C	2.48	0.51
1:D:463:HIS:HA	1:D:466:ARG:HB3	1.91	0.51
1:D:535:ARG:HG3	1:D:535:ARG:HH11	1.75	0.51
1:D:614:GLN:O	1:D:617:SER:HB3	2.11	0.51
1:A:41:LEU:HD13	1:A:264:PHE:CE2	2.46	0.51
1:D:587:PRO:HG2	1:D:588:VAL:H	1.76	0.51
1:A:434:PRO:HA	1:A:527:ILE:HG22	1.92	0.51
1:B:368:MET:O	1:B:372:ARG:HB2	2.11	0.51
1:C:366:LEU:O	1:C:369:GLU:HB3	2.10	0.51
1:D:373:ASN:HD21	1:D:401:THR:HG21	1.75	0.51
1:A:614:GLN:O	1:A:617:SER:HB3	2.11	0.51
1:D:456:CYS:HB2	1:D:457:MET:CE	2.41	0.51
1:A:179:THR:HG23	1:A:180:SER:N	2.27	0.50
1:B:614:GLN:O	1:B:617:SER:HB3	2.11	0.50
1:C:179:THR:HG22	1:C:181:LEU:H	1.75	0.50
1:C:434:PRO:HA	1:C:527:ILE:CG2	2.41	0.50
1:C:446:ASP:HA	1:C:449:THR:HB	1.92	0.50
1:D:497:PRO:HB2	1:D:499:GLU:OE2	2.11	0.50
1:D:725:ILE:HG22	1:D:729:ILE:CD1	2.42	0.50
1:A:213:VAL:O	1:A:241:PHE:HA	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:366:LEU:O	1:D:369:GLU:HB3	2.10	0.50
1:D:36:SER:HB3	1:D:317:TRP:HE3	1.75	0.50
1:D:99:ARG:NH1	1:D:390:GLU:OE2	2.44	0.50
1:B:105:PRO:HG2	1:B:106:GLN:H	1.76	0.50
1:B:429:LYS:O	1:B:432:MET:O	2.29	0.50
1:D:4:LEU:CD2	1:D:26:HIS:HA	2.42	0.50
1:A:455:VAL:HG21	1:A:468:LEU:CD1	2.42	0.50
1:B:342:VAL:HG23	1:B:343:LEU:N	2.27	0.50
1:B:39:ARG:HD2	1:B:39:ARG:H	1.75	0.50
1:B:629:ILE:N	1:B:630:PRO:HD2	2.27	0.50
1:D:179:THR:HG22	1:D:181:LEU:H	1.76	0.50
1:B:377:ASN:ND2	1:B:395:LEU:HD11	2.26	0.50
1:C:172:LEU:HD11	1:C:216:VAL:CG2	2.39	0.50
1:D:144:TYR:OH	1:D:213:VAL:HG22	2.11	0.50
1:A:21:LEU:HD11	1:A:110:LEU:HB2	1.93	0.50
1:A:1:MET:HG3	1:A:55:SER:CB	2.41	0.50
1:A:682:SER:HB2	1:A:751:VAL:HG12	1.93	0.50
1:B:602:TYR:O	1:B:603:GLU:HB2	2.11	0.50
1:D:105:PRO:HG2	1:D:106:GLN:H	1.77	0.50
1:D:498:ALA:HA	1:D:501:MET:HE3	1.94	0.50
1:D:609:LYS:NZ	1:D:641:THR:CG2	2.74	0.50
1:D:632:LEU:HD22	1:D:733:CYS:SG	2.52	0.50
1:A:96:THR:HG21	1:A:301:THR:HG23	1.94	0.50
1:A:72:PHE:CG	1:A:81:ALA:HA	2.47	0.50
1:B:160:ALA:CB	1:B:168:LEU:HD23	2.38	0.50
1:B:603:GLU:CA	1:B:634:ARG:HH22	2.24	0.50
1:C:41:LEU:HD13	1:C:264:PHE:CZ	2.47	0.50
1:C:327:SER:HG	1:C:329:THR:HB	1.76	0.50
1:D:147:TYR:CD2	1:D:150:LEU:HB2	2.47	0.50
1:D:463:HIS:HA	1:D:466:ARG:CB	2.42	0.50
1:A:105:PRO:HG2	1:A:106:GLN:H	1.76	0.50
1:A:434:PRO:HA	1:A:527:ILE:CG2	2.42	0.50
1:A:569:ARG:NE	1:A:735:GLU:OE1	2.44	0.50
1:B:685:THR:OG1	1:B:688:VAL:HG23	2.12	0.50
1:C:350:ARG:HD2	1:C:539:LEU:HA	1.94	0.50
1:D:227:PRO:HB2	1:D:233:ASP:N	2.26	0.50
1:D:261:ALA:O	1:D:264:PHE:CD1	2.62	0.50
1:D:60:ASP:HA	1:D:63:ILE:HD12	1.93	0.50
1:A:172:LEU:HD11	1:A:216:VAL:CG2	2.42	0.50
1:A:255:ASP:O	1:A:258:ARG:HB2	2.12	0.50
1:B:179:THR:HG23	1:B:180:SER:N	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:172:LEU:HD11	1:B:216:VAL:CG2	2.42	0.50
1:B:603:GLU:CA	1:B:634:ARG:HH12	2.23	0.50
1:B:94:GLU:HG2	1:B:316:GLY:HA2	1.92	0.50
1:C:385:LEU:N	1:C:386:PRO:CD	2.75	0.50
1:C:4:LEU:CD2	1:C:26:HIS:HA	2.42	0.50
1:A:561:ILE:CD1	1:A:561:ILE:H	2.24	0.49
1:A:593:LEU:O	1:A:597:GLU:HG3	2.12	0.49
1:B:170:VAL:O	1:B:215:ALA:HB1	2.12	0.49
1:B:258:ARG:C	1:B:260:GLN:N	2.65	0.49
1:B:377:ASN:ND2	1:B:395:LEU:HD21	2.21	0.49
1:B:486:SER:O	1:B:489:PHE:HB3	2.12	0.49
1:B:559:PRO:HG2	1:B:599:ILE:HG13	1.93	0.49
1:C:114:PRO:CB	1:C:258:ARG:NH1	2.75	0.49
1:C:368:MET:O	1:C:372:ARG:HB2	2.12	0.49
1:C:456:CYS:HB2	1:C:457:MET:CE	2.42	0.49
1:C:643:HIS:O	1:C:646:GLN:HG2	2.11	0.49
1:C:711:ILE:O	1:C:711:ILE:HD12	2.11	0.49
1:D:402:TRP:HA	1:D:402:TRP:CE3	2.47	0.49
1:D:564:LEU:C	1:D:566:ILE:H	2.15	0.49
1:A:158:MET:HE3	1:A:256:LEU:HB2	1.94	0.49
1:A:708:HIS:O	1:A:711:ILE:HG13	2.12	0.49
1:B:396:VAL:HG13	1:B:396:VAL:O	2.11	0.49
1:B:39:ARG:NH1	1:B:41:LEU:HD21	2.27	0.49
1:B:459:GLU:O	1:B:459:GLU:HG2	2.12	0.49
1:C:333:GLN:HE21	1:C:673:GLU:HB3	1.76	0.49
1:D:259:VAL:O	1:D:262:LEU:N	2.39	0.49
1:A:34:LYS:HA	1:A:45:GLU:HA	1.93	0.49
1:A:366:LEU:O	1:A:369:GLU:HB3	2.12	0.49
1:B:451:ALA:O	1:B:455:VAL:HG23	2.11	0.49
1:C:14:ARG:NH1	1:C:223:ASP:HA	2.26	0.49
1:C:21:LEU:HD12	1:C:22:LEU:N	2.26	0.49
1:C:456:CYS:SG	1:C:524:VAL:HG13	2.52	0.49
1:C:434:PRO:HA	1:C:527:ILE:HG22	1.94	0.49
1:D:160:ALA:CB	1:D:168:LEU:HD23	2.40	0.49
1:D:608:SER:C	1:D:610:HIS:N	2.62	0.49
1:A:310:ARG:NH2	1:A:392:SER:CB	2.75	0.49
1:A:369:GLU:HG2	1:A:485:VAL:HG23	1.93	0.49
1:A:604:SER:N	1:A:634:ARG:HH12	2.10	0.49
1:A:87:GLY:O	1:A:90:MET:HG3	2.13	0.49
1:B:663:HIS:NE2	1:B:743:ARG:HB3	2.27	0.49
1:D:164:ILE:O	1:D:164:ILE:HG22	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:261:ALA:HA	1:D:264:PHE:CE1	2.47	0.49
1:D:377:ASN:O	1:D:381:GLN:HG2	2.13	0.49
1:C:465:PHE:O	1:C:468:LEU:N	2.46	0.49
1:C:353:CYS:HB3	1:C:541:SER:CB	2.41	0.49
1:D:401:THR:H	1:D:404:ASP:CG	2.15	0.49
1:D:629:ILE:N	1:D:630:PRO:HD2	2.28	0.49
1:A:170:VAL:HG11	1:A:221:LEU:HD22	1.93	0.49
1:A:523:VAL:O	1:A:524:VAL:HG23	2.13	0.49
1:B:292:ILE:HD12	1:B:292:ILE:O	2.13	0.49
1:B:535:ARG:HG3	1:B:535:ARG:HH11	1.77	0.49
1:B:703:VAL:O	1:B:706:GLU:HB3	2.13	0.49
1:C:708:HIS:O	1:C:711:ILE:HG13	2.13	0.49
1:D:643:HIS:O	1:D:646:GLN:HG2	2.13	0.49
1:A:406:TYR:O	1:A:410:VAL:HG23	2.12	0.49
1:A:399:SER:CA	1:B:395:LEU:HD12	2.40	0.49
1:C:172:LEU:HD12	1:C:239:LEU:HD13	1.93	0.49
1:C:332:PHE:C	1:C:332:PHE:CD2	2.86	0.49
1:C:698:SER:O	1:C:702:GLU:HG3	2.13	0.49
1:C:725:ILE:HG22	1:C:729:ILE:CD1	2.43	0.49
1:D:110:LEU:HD23	1:D:110:LEU:N	2.28	0.49
1:D:90:MET:CE	1:D:318:ARG:HH22	2.26	0.49
1:D:725:ILE:O	1:D:728:ALA:N	2.44	0.49
1:B:115:LEU:N	1:B:258:ARG:HH22	2.07	0.49
1:B:110:LEU:HD11	1:B:269:ALA:HA	1.95	0.49
1:B:643:HIS:O	1:B:646:GLN:HG2	2.12	0.49
1:B:333:GLN:HG2	1:B:673:GLU:HB2	1.95	0.49
1:C:136:ASP:O	1:C:138:LYS:HG3	2.13	0.49
1:C:459:GLU:HG2	1:C:459:GLU:O	2.12	0.49
1:C:721:THR:O	1:C:724:ALA:HB3	2.13	0.49
1:D:336:GLU:HG3	1:D:407:GLU:HB2	1.95	0.49
1:D:38:GLY:H	1:D:41:LEU:CD1	2.23	0.49
1:D:472:ALA:HA	1:D:477:ILE:HD12	1.94	0.49
1:D:682:SER:HB2	1:D:751:VAL:HG12	1.94	0.49
1:B:39:ARG:HG3	1:B:317:TRP:CE2	2.47	0.49
1:C:352:LEU:HD11	1:C:650:LEU:HD23	1.95	0.49
1:D:36:SER:HB2	1:D:312:ARG:O	2.13	0.49
1:D:698:SER:O	1:D:702:GLU:HG3	2.13	0.49
1:A:110:LEU:HD11	1:A:269:ALA:HA	1.95	0.49
1:A:624:ILE:N	1:A:624:ILE:HD13	2.26	0.49
1:B:546:VAL:HB	1:B:644:VAL:HG13	1.94	0.49
1:C:179:THR:HG23	1:C:180:SER:N	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:466:ARG:NH2	1:C:498:ALA:N	2.59	0.49
1:C:473:CYS:HA	1:C:490:LEU:HD13	1.95	0.49
1:C:729:ILE:N	1:C:729:ILE:HD12	2.28	0.49
1:D:138:LYS:CD	1:D:142:ASP:HB3	2.42	0.49
1:D:624:ILE:N	1:D:624:ILE:HD13	2.27	0.49
1:A:332:PHE:CD2	1:A:332:PHE:C	2.86	0.48
1:A:455:VAL:HG21	1:A:468:LEU:HD11	1.95	0.48
1:A:471:TYR:O	1:A:475:GLN:HB2	2.13	0.48
1:B:128:MET:O	1:B:132:GLN:HG3	2.13	0.48
1:C:703:VAL:O	1:C:706:GLU:HB3	2.13	0.48
1:D:140:LEU:HB3	1:D:144:TYR:CE2	2.46	0.48
1:D:461:GLY:H	1:D:464:GLU:CD	2.16	0.48
1:D:609:LYS:HZ2	1:D:641:THR:HG21	1.77	0.48
1:D:696:PHE:HB3	1:D:700:VAL:HG21	1.95	0.48
1:A:114:PRO:O	1:A:115:LEU:HD23	2.13	0.48
1:B:21:LEU:HD12	1:B:22:LEU:N	2.28	0.48
1:B:725:ILE:HG22	1:B:729:ILE:CD1	2.43	0.48
1:C:220:ASP:HB3	1:C:238:LYS:HD3	1.94	0.48
1:C:708:HIS:HB3	1:C:711:ILE:CG2	2.43	0.48
1:D:30:LEU:O	1:D:48:PHE:HB2	2.13	0.48
1:A:390:GLU:OE1	1:A:390:GLU:HA	2.13	0.48
1:A:599:ILE:HG21	1:A:631:PHE:CE1	2.47	0.48
1:A:609:LYS:CD	1:A:641:THR:HG22	2.41	0.48
1:C:446:ASP:O	1:C:447:ALA:C	2.51	0.48
1:B:675:ALA:O	1:B:679:MET:HG3	2.14	0.48
1:C:460:ALA:HA	1:C:464:GLU:HG2	1.94	0.48
1:C:663:HIS:NE2	1:C:743:ARG:HB3	2.27	0.48
1:D:179:THR:HG23	1:D:180:SER:N	2.27	0.48
1:D:599:ILE:HG21	1:D:631:PHE:HE1	1.78	0.48
1:B:99:ARG:NH2	1:B:390:GLU:O	2.46	0.48
1:C:546:VAL:O	1:C:547:GLU:O	2.31	0.48
1:D:145:THR:C	1:D:147:TYR:N	2.67	0.48
1:D:271:HIS:O	1:D:275:ILE:HG13	2.13	0.48
1:D:39:ARG:C	1:D:41:LEU:N	2.66	0.48
1:D:663:HIS:NE2	1:D:743:ARG:HB3	2.28	0.48
1:A:459:GLU:O	1:A:459:GLU:HG2	2.12	0.48
1:B:323:PRO:O	1:B:326:VAL:HG23	2.13	0.48
1:B:561:ILE:H	1:B:561:ILE:CD1	2.25	0.48
1:C:346:ILE:HD12	1:C:424:GLU:HG2	1.95	0.48
1:D:159:VAL:HG23	1:D:248:LEU:O	2.13	0.48
1:A:6:HIS:HB2	1:A:21:LEU:HB3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:601:ALA:O	1:A:603:GLU:OE2	2.31	0.48
1:C:310:ARG:HH11	1:C:310:ARG:CB	2.27	0.48
1:D:469:VAL:C	1:D:471:TYR:H	2.16	0.48
1:D:680:ARG:HG3	1:D:680:ARG:NH1	2.29	0.48
1:A:564:LEU:C	1:A:566:ILE:H	2.17	0.48
1:B:12:THR:HG22	1:B:44:ALA:HB2	1.94	0.48
1:B:472:ALA:O	1:B:475:GLN:N	2.41	0.48
1:D:753:ASP:O	1:D:754:ALA:C	2.52	0.48
1:A:432:MET:CE	1:A:534:ALA:HB1	2.41	0.48
1:A:356:PRO:CB	1:A:544:PHE:HA	2.44	0.48
1:A:629:ILE:N	1:A:630:PRO:HD2	2.29	0.48
1:A:753:ASP:O	1:A:754:ALA:C	2.52	0.48
1:B:110:LEU:HD23	1:B:110:LEU:N	2.29	0.48
1:B:725:ILE:O	1:B:728:ALA:N	2.47	0.48
1:C:238:LYS:O	1:C:240:ARG:HG3	2.14	0.48
1:C:168:LEU:HD13	1:C:259:VAL:CG1	2.42	0.48
1:C:342:VAL:HG12	1:C:658:CYS:SG	2.54	0.48
1:D:459:GLU:O	1:D:459:GLU:HG2	2.13	0.48
1:D:548:GLN:O	1:D:643:HIS:HB3	2.14	0.48
1:A:377:ASN:O	1:A:381:GLN:HG2	2.13	0.48
1:B:157:ARG:HH21	1:B:249:LEU:HD21	1.77	0.48
1:B:366:LEU:O	1:B:369:GLU:HB3	2.14	0.48
1:B:420:ILE:HD13	1:B:569:ARG:NH2	2.28	0.48
1:B:353:CYS:HB3	1:B:541:SER:CB	2.44	0.48
1:B:708:HIS:O	1:B:711:ILE:HG13	2.13	0.48
1:C:377:ASN:O	1:C:381:GLN:HG2	2.13	0.48
1:C:401:THR:H	1:C:404:ASP:CG	2.17	0.48
1:C:473:CYS:O	1:C:475:GLN:N	2.47	0.48
1:C:432:MET:HE1	1:C:534:ALA:O	2.13	0.48
1:C:624:ILE:N	1:C:624:ILE:HD13	2.28	0.48
1:C:680:ARG:NH1	1:C:680:ARG:HG3	2.29	0.48
1:D:332:PHE:CD2	1:D:332:PHE:C	2.87	0.48
1:D:708:HIS:HB3	1:D:711:ILE:CG2	2.44	0.48
1:A:67:TYR:CZ	1:A:114:PRO:HG3	2.48	0.47
1:B:729:ILE:N	1:B:729:ILE:HD12	2.28	0.47
1:C:306:LEU:HB2	1:C:391:PHE:HB3	1.95	0.47
1:D:39:ARG:HE	1:D:41:LEU:HD21	1.79	0.47
1:D:635:LEU:HA	1:D:638:ILE:HD12	1.96	0.47
1:D:67:TYR:CZ	1:D:114:PRO:HG3	2.49	0.47
1:B:377:ASN:O	1:B:381:GLN:HG2	2.13	0.47
1:B:708:HIS:HB3	1:B:711:ILE:CG2	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:535:ARG:O	1:C:538:TRP:HB3	2.14	0.47
1:D:260:GLN:O	1:D:264:PHE:CE1	2.66	0.47
1:A:128:MET:O	1:A:132:GLN:HG3	2.13	0.47
1:B:332:PHE:CD2	1:B:332:PHE:C	2.88	0.47
1:C:254:PHE:O	1:C:255:ASP:O	2.32	0.47
1:D:323:PRO:O	1:D:326:VAL:HG23	2.14	0.47
1:A:248:LEU:C	1:A:248:LEU:HD23	2.35	0.47
1:A:249:LEU:HD23	1:A:250:LEU:O	2.14	0.47
1:A:310:ARG:CB	1:A:310:ARG:HH11	2.27	0.47
1:B:248:LEU:HD23	1:B:248:LEU:C	2.35	0.47
1:B:96:THR:HG21	1:B:301:THR:HG23	1.96	0.47
1:B:546:VAL:O	1:B:547:GLU:C	2.51	0.47
1:C:139:ARG:HB3	1:C:141:SER:H	1.79	0.47
1:C:564:LEU:C	1:C:566:ILE:H	2.17	0.47
1:C:87:GLY:O	1:C:90:MET:HG3	2.15	0.47
1:D:471:TYR:CE1	1:D:475:GLN:HG3	2.49	0.47
1:D:602:TYR:O	1:D:603:GLU:C	2.53	0.47
1:D:67:TYR:O	1:D:70:ILE:HB	2.15	0.47
1:A:395:LEU:HD23	1:A:395:LEU:H	1.76	0.47
1:B:632:LEU:HD22	1:B:733:CYS:SG	2.54	0.47
1:C:406:TYR:O	1:C:410:VAL:HG23	2.15	0.47
1:C:67:TYR:CZ	1:C:114:PRO:HG3	2.48	0.47
1:D:140:LEU:HD21	1:D:249:LEU:HD12	1.95	0.47
1:D:342:VAL:O	1:D:346:ILE:HG12	2.13	0.47
1:A:369:GLU:CG	1:A:485:VAL:HG23	2.45	0.47
1:A:395:LEU:CD2	1:A:395:LEU:N	2.78	0.47
1:A:535:ARG:NH1	1:A:535:ARG:HG3	2.29	0.47
1:B:21:LEU:HD13	1:B:112:PHE:CE1	2.49	0.47
1:B:593:LEU:O	1:B:597:GLU:HG3	2.15	0.47
1:C:249:LEU:HD23	1:C:250:LEU:O	2.15	0.47
1:D:292:ILE:HD12	1:D:292:ILE:O	2.14	0.47
1:D:593:LEU:O	1:D:597:GLU:HG3	2.15	0.47
1:D:609:LYS:HD3	1:D:641:THR:HG22	1.95	0.47
1:A:445:PRO:HG2	1:A:448:VAL:CG2	2.44	0.47
1:A:486:SER:O	1:A:489:PHE:HB3	2.14	0.47
1:B:259:VAL:O	1:B:259:VAL:HG12	2.15	0.47
1:B:371:VAL:O	1:B:371:VAL:HG12	2.15	0.47
1:C:114:PRO:CA	1:C:258:ARG:NH1	2.69	0.47
1:C:429:LYS:O	1:C:432:MET:O	2.33	0.47
1:C:462:ALA:O	1:C:465:PHE:HB2	2.15	0.47
1:D:406:TYR:O	1:D:410:VAL:HG23	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:527:ILE:H	1:D:527:ILE:CD1	2.27	0.47
1:D:596:TYR:CE2	1:D:600:LEU:HD11	2.49	0.47
1:A:41:LEU:HD23	1:A:263:GLN:HB3	1.95	0.47
1:D:703:VAL:O	1:D:706:GLU:HB3	2.14	0.47
1:D:729:ILE:N	1:D:729:ILE:HD12	2.30	0.47
1:A:160:ALA:CB	1:A:168:LEU:HD23	2.40	0.47
1:A:546:VAL:O	1:A:547:GLU:O	2.33	0.47
1:A:721:THR:O	1:A:724:ALA:HB3	2.14	0.47
1:C:486:SER:O	1:C:489:PHE:HB3	2.14	0.47
1:C:587:PRO:HG2	1:C:588:VAL:H	1.79	0.47
1:D:87:GLY:O	1:D:90:MET:HG3	2.14	0.47
1:A:472:ALA:CB	1:A:477:ILE:HD12	2.45	0.47
1:B:406:TYR:O	1:B:410:VAL:HG23	2.15	0.47
1:B:4:LEU:HD12	1:B:4:LEU:N	2.29	0.47
1:C:6:HIS:HB2	1:C:21:LEU:HB3	1.97	0.47
1:D:385:LEU:N	1:D:386:PRO:CD	2.78	0.47
1:D:668:HIS:CB	1:D:671:LEU:HD12	2.45	0.47
1:A:385:LEU:N	1:A:386:PRO:CD	2.78	0.47
1:A:399:SER:HA	1:B:395:LEU:CD1	2.39	0.47
1:B:157:ARG:NE	1:B:249:LEU:HD21	2.26	0.47
1:B:381:GLN:NE2	1:B:402:TRP:HD1	2.13	0.47
1:B:38:GLY:HA3	1:B:41:LEU:CD1	2.45	0.47
1:B:456:CYS:HB2	1:B:457:MET:CE	2.45	0.47
1:B:721:THR:O	1:B:724:ALA:HB3	2.15	0.47
1:C:461:GLY:O	1:C:462:ALA:O	2.33	0.47
1:A:137:ALA:HB1	1:A:248:LEU:CD2	2.45	0.46
1:A:139:ARG:CG	1:A:245:GLU:O	2.63	0.46
1:A:725:ILE:HG22	1:A:729:ILE:CD1	2.45	0.46
1:B:624:ILE:HD13	1:B:624:ILE:N	2.28	0.46
1:B:698:SER:O	1:B:702:GLU:HG3	2.14	0.46
1:C:128:MET:O	1:C:129:VAL:C	2.53	0.46
1:C:35:VAL:HG12	1:C:318:ARG:HB3	1.98	0.46
1:C:696:PHE:HB3	1:C:700:VAL:HG21	1.96	0.46
1:D:128:MET:O	1:D:129:VAL:C	2.54	0.46
1:D:6:HIS:HB2	1:D:21:LEU:HB3	1.97	0.46
1:D:609:LYS:CE	1:D:637:GLN:HB3	2.42	0.46
1:A:429:LYS:O	1:A:432:MET:O	2.33	0.46
1:B:602:TYR:C	1:B:634:ARG:NH2	2.68	0.46
1:D:238:LYS:O	1:D:240:ARG:HG3	2.14	0.46
1:A:110:LEU:HD23	1:A:110:LEU:N	2.30	0.46
1:A:179:THR:HG21	1:A:209:ASP:HA	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:GLY:O	1:A:41:LEU:O	2.33	0.46
1:A:535:ARG:O	1:A:538:TRP:HB3	2.14	0.46
1:A:632:LEU:HD22	1:A:733:CYS:SG	2.55	0.46
1:B:238:LYS:O	1:B:240:ARG:HG3	2.14	0.46
1:B:465:PHE:HZ	1:B:505:TYR:CG	2.33	0.46
1:C:300:ILE:CG2	1:C:304:LEU:HD12	2.43	0.46
1:C:386:PRO:HB3	1:C:402:TRP:NE1	2.31	0.46
1:C:4:LEU:N	1:C:4:LEU:HD12	2.30	0.46
1:C:597:GLU:O	1:C:600:LEU:HB2	2.16	0.46
1:A:323:PRO:O	1:A:326:VAL:HG23	2.16	0.46
1:A:402:TRP:CE3	1:A:405:MET:CE	2.98	0.46
1:A:34:LYS:CB	1:A:45:GLU:HG3	2.46	0.46
1:B:39:ARG:HH22	1:B:267:GLU:CD	2.19	0.46
1:B:300:ILE:CG2	1:B:304:LEU:HD12	2.40	0.46
1:B:587:PRO:HG2	1:B:588:VAL:H	1.79	0.46
1:C:599:ILE:HG21	1:C:631:PHE:HE1	1.80	0.46
1:D:20:LEU:HB2	1:D:115:LEU:HD11	1.96	0.46
1:A:587:PRO:HG2	1:A:588:VAL:N	2.30	0.46
1:B:6:HIS:HB2	1:B:21:LEU:HB3	1.96	0.46
1:C:153:SER:O	1:C:157:ARG:HD2	2.15	0.46
1:C:465:PHE:CZ	1:C:502:LEU:HD13	2.50	0.46
1:C:82:SER:HB3	1:C:85:GLU:HB3	1.98	0.46
1:D:33:PHE:CD2	1:D:318:ARG:HB2	2.51	0.46
1:A:96:THR:CG2	1:A:301:THR:HG23	2.45	0.46
1:A:90:MET:CE	1:A:318:ARG:HH22	2.29	0.46
1:A:494:ARG:HH11	1:A:494:ARG:CG	2.29	0.46
1:A:708:HIS:HB3	1:A:711:ILE:CG2	2.46	0.46
1:B:59:THR:O	1:B:63:ILE:HG13	2.16	0.46
1:D:142:ASP:O	1:D:143:GLU:HG3	2.16	0.46
1:D:21:LEU:HD12	1:D:22:LEU:N	2.31	0.46
1:D:248:LEU:HD23	1:D:248:LEU:C	2.36	0.46
1:D:680:ARG:HG3	1:D:680:ARG:HH11	1.80	0.46
1:A:280:CYS:O	1:A:280:CYS:SG	2.74	0.46
1:A:335:LEU:O	1:A:411:GLY:HA3	2.15	0.46
1:A:456:CYS:HB2	1:A:457:MET:CE	2.45	0.46
1:A:4:LEU:N	1:A:4:LEU:HD12	2.31	0.46
1:A:663:HIS:NE2	1:A:743:ARG:HB3	2.30	0.46
1:B:39:ARG:N	1:B:39:ARG:CD	2.75	0.46
1:D:153:SER:O	1:D:157:ARG:HD2	2.16	0.46
1:D:352:LEU:CD1	1:D:363:LEU:HD13	2.45	0.46
1:D:546:VAL:O	1:D:547:GLU:O	2.33	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:401:THR:HB	1:A:404:ASP:OD2	2.15	0.46
1:B:261:ALA:C	1:B:263:GLN:N	2.69	0.46
1:B:564:LEU:C	1:B:566:ILE:H	2.18	0.46
1:C:161:THR:CB	1:C:164:ILE:HB	2.46	0.46
1:D:265:LEU:N	1:D:266:PRO:CD	2.79	0.46
1:D:708:HIS:O	1:D:711:ILE:HG13	2.15	0.46
1:A:292:ILE:O	1:A:292:ILE:HD12	2.15	0.46
1:A:685:THR:OG1	1:A:688:VAL:HG23	2.15	0.46
1:B:493:LEU:HD23	1:B:496:ILE:HD12	1.98	0.46
1:C:685:THR:OG1	1:C:688:VAL:HG23	2.16	0.46
1:D:708:HIS:CB	1:D:711:ILE:HG21	2.46	0.46
1:B:517:LEU:C	1:B:517:LEU:HD12	2.36	0.46
1:B:574:PRO:O	1:B:575:VAL:C	2.54	0.46
1:B:7:CYS:HB2	1:B:49:GLU:HG3	1.96	0.46
1:C:90:MET:CE	1:C:318:ARG:HH22	2.28	0.46
1:D:494:ARG:CG	1:D:494:ARG:HH11	2.29	0.46
1:A:189:GLU:OE2	1:A:191:ILE:HD11	2.16	0.45
1:A:458:GLY:O	1:A:460:ALA:N	2.49	0.45
1:C:248:LEU:C	1:C:248:LEU:HD23	2.36	0.45
1:D:189:GLU:OE2	1:D:191:ILE:HD11	2.16	0.45
1:D:685:THR:OG1	1:D:688:VAL:HG23	2.17	0.45
1:A:170:VAL:O	1:A:215:ALA:HB1	2.15	0.45
1:A:371:VAL:O	1:A:371:VAL:HG12	2.15	0.45
1:A:604:SER:HB3	1:A:634:ARG:NH1	2.32	0.45
1:C:680:ARG:HH11	1:C:680:ARG:HG3	1.81	0.45
1:C:632:LEU:HD22	1:C:733:CYS:SG	2.57	0.45
1:D:330:ASP:O	1:D:334:ARG:HG2	2.16	0.45
1:D:39:ARG:O	1:D:41:LEU:N	2.49	0.45
1:D:9:THR:HG23	1:D:18:HIS:CE1	2.51	0.45
1:C:323:PRO:O	1:C:326:VAL:HG23	2.16	0.45
1:C:593:LEU:O	1:C:597:GLU:HG3	2.17	0.45
1:D:235:LEU:HA	1:D:235:LEU:HD23	1.75	0.45
1:D:339:GLY:HA3	1:D:407:GLU:O	2.16	0.45
1:D:332:PHE:CD1	1:D:408:GLU:HG3	2.51	0.45
1:D:4:LEU:N	1:D:4:LEU:HD12	2.32	0.45
1:D:535:ARG:O	1:D:538:TRP:HB3	2.15	0.45
1:B:154:LEU:HD22	1:B:249:LEU:CD1	2.47	0.45
1:B:465:PHE:CZ	1:B:505:TYR:HB2	2.52	0.45
1:B:67:TYR:CZ	1:B:114:PRO:HG3	2.51	0.45
1:C:110:LEU:N	1:C:110:LEU:HD23	2.32	0.45
1:D:371:VAL:HG12	1:D:371:VAL:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:381:GLN:NE2	1:D:402:TRP:HD1	2.15	0.45
1:D:446:ASP:O	1:D:447:ALA:C	2.55	0.45
1:A:524:VAL:O	1:A:524:VAL:HG12	2.16	0.45
1:B:287:PRO:HG2	1:B:409:ILE:HG12	1.99	0.45
1:B:96:THR:CG2	1:B:301:THR:HG23	2.47	0.45
1:B:385:LEU:N	1:B:386:PRO:CD	2.79	0.45
1:B:535:ARG:O	1:B:538:TRP:HB3	2.17	0.45
1:B:635:LEU:HA	1:B:638:ILE:HD12	1.97	0.45
1:C:22:LEU:O	1:C:110:LEU:HA	2.16	0.45
1:C:279:ILE:HD11	1:C:293:GLY:O	2.17	0.45
1:C:454:ARG:HE	1:C:464:GLU:CD	2.20	0.45
1:D:429:LYS:O	1:D:432:MET:O	2.34	0.45
1:D:498:ALA:HA	1:D:501:MET:CE	2.47	0.45
1:D:506:ARG:O	1:D:510:GLN:HB2	2.16	0.45
1:D:574:PRO:O	1:D:575:VAL:C	2.55	0.45
1:D:334:ARG:NH2	1:D:669:PRO:HA	2.32	0.45
1:D:682:SER:CB	1:D:751:VAL:HG12	2.47	0.45
1:A:251:PRO:O	1:A:252:ASP:C	2.55	0.45
1:A:90:MET:HE1	1:A:318:ARG:NH2	2.31	0.45
1:A:703:VAL:O	1:A:706:GLU:HB3	2.17	0.45
1:B:153:SER:O	1:B:157:ARG:HD2	2.16	0.45
1:B:602:TYR:C	1:B:634:ARG:HH22	2.20	0.45
1:B:708:HIS:CB	1:B:711:ILE:HG21	2.46	0.45
1:B:753:ASP:O	1:B:754:ALA:C	2.55	0.45
1:C:137:ALA:HB1	1:C:248:LEU:HD21	1.98	0.45
1:C:154:LEU:HD22	1:C:249:LEU:HD11	1.98	0.45
1:C:708:HIS:CB	1:C:711:ILE:HG21	2.45	0.45
1:A:608:SER:O	1:A:611:ILE:N	2.50	0.45
1:A:682:SER:CB	1:A:751:VAL:HG12	2.47	0.45
1:B:178:GLN:NE2	1:B:212:LEU:HD12	2.23	0.45
1:B:243:PRO:HA	1:B:244:PRO:HD3	1.89	0.45
1:B:429:LYS:HE2	1:B:515:SER:HB3	1.99	0.45
1:A:574:PRO:O	1:A:575:VAL:C	2.55	0.45
1:A:74:LEU:HD11	1:A:254:PHE:CE2	2.52	0.45
1:B:524:VAL:O	1:B:524:VAL:HG12	2.17	0.45
1:C:601:ALA:O	1:C:634:ARG:NH2	2.49	0.45
1:A:21:LEU:HD12	1:A:22:LEU:N	2.32	0.45
1:A:258:ARG:HA	1:A:258:ARG:HD3	1.78	0.45
1:B:352:LEU:CD1	1:B:363:LEU:HD13	2.44	0.45
1:B:542:PRO:HA	1:B:592:VAL:HG22	1.98	0.45
1:B:696:PHE:HB3	1:B:700:VAL:HG21	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:222:LYS:O	1:C:260:GLN:NE2	2.50	0.45
1:C:262:LEU:HB3	1:C:263:GLN:HE21	1.81	0.45
1:C:574:PRO:O	1:C:575:VAL:C	2.55	0.45
1:C:682:SER:CB	1:C:751:VAL:HG12	2.47	0.45
1:D:21:LEU:HD11	1:D:110:LEU:HB2	1.98	0.45
1:D:14:ARG:HH12	1:D:223:ASP:HA	1.80	0.45
1:D:310:ARG:CB	1:D:310:ARG:HH11	2.29	0.45
1:D:448:VAL:HG13	1:D:468:LEU:CD2	2.43	0.45
1:A:330:ASP:O	1:A:334:ARG:HG2	2.17	0.45
1:B:401:THR:O	1:B:404:ASP:CG	2.55	0.45
1:C:330:ASP:O	1:C:334:ARG:HG2	2.17	0.45
1:C:535:ARG:HG3	1:C:535:ARG:NH1	2.32	0.45
1:C:635:LEU:HA	1:C:638:ILE:HD12	1.98	0.45
1:D:176:SER:C	1:D:178:GLN:N	2.69	0.45
1:D:428:ALA:HB3	1:D:511:PHE:CZ	2.52	0.45
1:A:128:MET:O	1:A:129:VAL:C	2.55	0.44
1:A:139:ARG:NH2	1:A:163:GLU:OE2	2.49	0.44
1:A:368:MET:HG3	1:B:368:MET:HG3	1.99	0.44
1:B:330:ASP:O	1:B:334:ARG:HG2	2.16	0.44
1:B:458:GLY:O	1:B:460:ALA:N	2.50	0.44
1:B:498:ALA:HA	1:B:501:MET:CE	2.46	0.44
1:B:90:MET:CE	1:B:318:ARG:NH2	2.79	0.44
1:C:179:THR:HG21	1:C:209:ASP:HA	1.98	0.44
1:C:292:ILE:O	1:C:292:ILE:HD12	2.16	0.44
1:C:472:ALA:CB	1:C:477:ILE:HD12	2.46	0.44
1:D:178:GLN:NE2	1:D:212:LEU:HD12	2.22	0.44
1:D:524:VAL:O	1:D:524:VAL:HG12	2.17	0.44
1:D:574:PRO:HA	1:D:578:GLY:H	1.83	0.44
1:D:587:PRO:HG2	1:D:588:VAL:N	2.32	0.44
1:A:312:ARG:HG3	1:A:313:GLY:N	2.32	0.44
1:B:170:VAL:HG12	1:B:216:VAL:O	2.17	0.44
1:C:517:LEU:HD12	1:C:517:LEU:C	2.38	0.44
1:C:609:LYS:HD3	1:C:641:THR:HG22	1.99	0.44
1:C:753:ASP:O	1:C:754:ALA:C	2.55	0.44
1:D:243:PRO:HA	1:D:244:PRO:HD3	1.91	0.44
1:D:256:LEU:O	1:D:257:ILE:C	2.56	0.44
1:D:402:TRP:HE3	1:D:402:TRP:HA	1.82	0.44
1:A:390:GLU:O	1:A:391:PHE:HB3	2.16	0.44
1:A:391:PHE:CE1	1:A:393:ASN:HA	2.52	0.44
1:B:189:GLU:OE2	1:B:191:ILE:HD11	2.17	0.44
1:B:14:ARG:HD3	1:B:257:ILE:CD1	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:312:ARG:HG3	1:C:313:GLY:N	2.32	0.44
1:C:566:ILE:HD11	1:C:577:TYR:CE2	2.53	0.44
1:C:705:ILE:HG12	1:C:711:ILE:CD1	2.44	0.44
1:D:312:ARG:HG3	1:D:313:GLY:N	2.33	0.44
1:D:353:CYS:SG	1:D:563:VAL:HG21	2.58	0.44
1:A:238:LYS:O	1:A:240:ARG:HG3	2.17	0.44
1:B:115:LEU:H	1:B:258:ARG:NH2	2.09	0.44
1:B:67:TYR:O	1:B:70:ILE:HB	2.18	0.44
1:C:11:VAL:O	1:C:44:ALA:HB1	2.17	0.44
1:D:159:VAL:HG21	1:D:247:CYS:HB3	1.99	0.44
1:A:21:LEU:HD13	1:A:112:PHE:CE1	2.52	0.44
1:B:312:ARG:HG3	1:B:313:GLY:N	2.31	0.44
1:C:1:MET:O	1:C:3:ALA:N	2.51	0.44
1:C:205:LEU:HD22	1:C:245:GLU:CD	2.38	0.44
1:C:371:VAL:O	1:C:371:VAL:HG12	2.17	0.44
1:C:458:GLY:O	1:C:460:ALA:N	2.50	0.44
1:C:527:ILE:CD1	1:C:527:ILE:H	2.29	0.44
1:D:280:CYS:SG	1:D:280:CYS:O	2.75	0.44
1:D:12:THR:HG22	1:D:44:ALA:HB2	1.98	0.44
1:D:486:SER:O	1:D:489:PHE:HB3	2.18	0.44
1:D:517:LEU:HD12	1:D:517:LEU:C	2.38	0.44
1:D:599:ILE:HG21	1:D:631:PHE:CE1	2.52	0.44
1:A:159:VAL:HG23	1:A:248:LEU:O	2.17	0.44
1:A:259:VAL:O	1:A:262:LEU:N	2.44	0.44
1:A:668:HIS:CB	1:A:671:LEU:HD12	2.48	0.44
1:A:9:THR:HG23	1:A:18:HIS:CE1	2.53	0.44
1:B:327:SER:HG	1:B:329:THR:HB	1.82	0.44
1:C:189:GLU:OE2	1:C:191:ILE:HD11	2.17	0.44
1:C:480:PHE:C	1:C:482:SER:H	2.20	0.44
1:C:512:SER:HG	1:C:532:HIS:CE1	2.36	0.44
1:C:642:PRO:HB2	1:C:643:HIS:H	1.63	0.44
1:D:104:PRO:HG2	1:D:107:PHE:CE1	2.52	0.44
1:A:158:MET:HE1	1:A:170:VAL:HB	2.00	0.44
1:A:170:VAL:HG12	1:A:216:VAL:O	2.18	0.44
1:B:1:MET:O	1:B:3:ALA:N	2.51	0.44
1:B:527:ILE:H	1:B:527:ILE:CD1	2.28	0.44
1:B:75:LEU:HD21	1:B:262:LEU:O	2.18	0.44
1:C:34:LYS:NZ	1:C:319:THR:HB	2.32	0.44
1:C:39:ARG:C	1:C:41:LEU:N	2.71	0.44
1:C:446:ASP:O	1:C:449:THR:HB	2.18	0.44
1:D:170:VAL:HG12	1:D:216:VAL:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:33:PHE:N	1:D:321:PHE:CE1	2.85	0.44
1:D:465:PHE:O	1:D:466:ARG:C	2.55	0.44
1:D:82:SER:HB3	1:D:85:GLU:HB3	1.99	0.44
1:A:139:ARG:HG3	1:A:245:GLU:O	2.18	0.44
1:A:498:ALA:HA	1:A:501:MET:CE	2.47	0.44
1:A:506:ARG:O	1:A:510:GLN:HB2	2.18	0.44
1:B:90:MET:HE1	1:B:318:ARG:NH2	2.32	0.44
1:C:176:SER:C	1:C:178:GLN:N	2.71	0.44
1:C:256:LEU:C	1:C:256:LEU:HD12	2.37	0.44
1:C:599:ILE:HG21	1:C:631:PHE:CE1	2.53	0.44
1:D:158:MET:CE	1:D:170:VAL:HB	2.47	0.44
1:A:226:ILE:N	1:A:226:ILE:CD1	2.81	0.44
1:A:574:PRO:HA	1:A:578:GLY:H	1.83	0.44
1:B:279:ILE:HD11	1:B:293:GLY:O	2.18	0.44
1:C:178:GLN:NE2	1:C:212:LEU:HD12	2.21	0.44
1:C:465:PHE:O	1:C:466:ARG:C	2.56	0.44
1:C:473:CYS:C	1:C:475:GLN:N	2.70	0.44
1:A:527:ILE:CD1	1:A:527:ILE:H	2.29	0.43
1:A:587:PRO:CG	1:A:588:VAL:H	2.31	0.43
1:B:179:THR:HG21	1:B:209:ASP:HA	2.00	0.43
1:B:21:LEU:HD11	1:B:110:LEU:HB2	1.99	0.43
1:B:264:PHE:N	1:B:264:PHE:CD1	2.86	0.43
1:C:465:PHE:CE1	1:C:502:LEU:CB	2.98	0.43
1:C:428:ALA:HB3	1:C:511:PHE:CZ	2.52	0.43
1:A:1:MET:O	1:A:3:ALA:N	2.51	0.43
1:A:38:GLY:O	1:A:40:GLY:N	2.51	0.43
1:A:461:GLY:H	1:A:464:GLU:CD	2.21	0.43
1:A:696:PHE:HB3	1:A:700:VAL:HG21	1.99	0.43
1:B:310:ARG:CB	1:B:310:ARG:HH11	2.29	0.43
1:B:445:PRO:HD2	1:B:471:TYR:CE1	2.53	0.43
1:B:618:ARG:HH11	1:B:618:ARG:CB	2.30	0.43
1:B:698:SER:O	1:B:699:VAL:C	2.57	0.43
1:B:682:SER:CB	1:B:751:VAL:HG12	2.48	0.43
1:C:280:CYS:SG	1:C:280:CYS:O	2.76	0.43
1:C:306:LEU:HB3	1:C:400:LYS:HZ3	1.82	0.43
1:A:517:LEU:C	1:A:517:LEU:HD12	2.39	0.43
1:A:59:THR:O	1:A:63:ILE:HG13	2.18	0.43
1:B:249:LEU:HD23	1:B:250:LEU:O	2.18	0.43
1:B:97:PHE:HZ	1:B:301:THR:HA	1.83	0.43
1:C:158:MET:HE3	1:C:256:LEU:CB	2.42	0.43
1:D:279:ILE:HD11	1:D:293:GLY:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:ASP:O	1:A:256:LEU:C	2.57	0.43
1:A:402:TRP:HE3	1:A:402:TRP:HA	1.83	0.43
1:B:41:LEU:HB2	1:B:42:PRO:HD2	1.99	0.43
1:C:498:ALA:HA	1:C:501:MET:CE	2.48	0.43
1:C:564:LEU:HD23	1:C:592:VAL:CG1	2.48	0.43
1:D:39:ARG:O	1:D:40:GLY:C	2.55	0.43
1:A:14:ARG:HH12	1:A:223:ASP:HA	1.83	0.43
1:A:402:TRP:CE3	1:A:402:TRP:HA	2.53	0.43
1:A:708:HIS:CB	1:A:711:ILE:HG21	2.47	0.43
1:B:87:GLY:O	1:B:90:MET:HG3	2.19	0.43
1:B:566:ILE:HD11	1:B:577:TYR:CD2	2.54	0.43
1:C:264:PHE:O	1:C:268:ILE:HG13	2.18	0.43
1:D:179:THR:HG21	1:D:209:ASP:HA	2.00	0.43
1:D:566:ILE:HD11	1:D:577:TYR:CE2	2.54	0.43
1:D:641:THR:O	1:D:642:PRO:O	2.36	0.43
1:A:635:LEU:HA	1:A:638:ILE:HD12	2.01	0.43
1:B:130:THR:HG23	1:B:253:GLU:OE1	2.19	0.43
1:B:280:CYS:SG	1:B:280:CYS:O	2.76	0.43
1:B:90:MET:HE1	1:B:318:ARG:HH22	1.83	0.43
1:B:480:PHE:C	1:B:482:SER:H	2.22	0.43
1:C:545:TYR:HD1	1:C:560:THR:HG1	1.64	0.43
1:C:561:ILE:CD1	1:C:561:ILE:H	2.29	0.43
1:D:161:THR:CB	1:D:164:ILE:HB	2.48	0.43
1:D:34:LYS:CB	1:D:45:GLU:HG3	2.48	0.43
1:D:721:THR:O	1:D:724:ALA:HB3	2.19	0.43
1:A:161:THR:CB	1:A:164:ILE:HB	2.48	0.43
1:A:265:LEU:H	1:A:266:PRO:CD	2.31	0.43
1:A:275:ILE:HG23	1:A:297:TYR:HB2	1.99	0.43
1:A:566:ILE:HD11	1:A:577:TYR:CD2	2.54	0.43
1:A:333:GLN:NE2	1:A:672:THR:HB	2.34	0.43
1:C:235:LEU:O	1:C:237:PRO:HD2	2.18	0.43
1:C:27:LEU:HA	1:C:293:GLY:HA3	2.00	0.43
1:C:326:VAL:HG12	1:C:330:ASP:HB2	2.01	0.43
1:D:1:MET:CE	1:D:55:SER:HB3	2.48	0.43
1:D:463:HIS:O	1:D:464:GLU:C	2.56	0.43
1:D:472:ALA:HB1	1:D:477:ILE:HB	2.00	0.43
1:A:178:GLN:NE2	1:A:212:LEU:HD12	2.23	0.43
1:A:470:ASP:O	1:A:474:GLU:N	2.51	0.43
1:B:228:ALA:HB3	1:B:231:SER:HB3	2.01	0.43
1:B:566:ILE:HD11	1:B:577:TYR:CE2	2.54	0.43
1:D:237:PRO:O	1:D:238:LYS:HG3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:249:LEU:HD23	1:D:250:LEU:O	2.19	0.43
1:D:457:MET:C	1:D:459:GLU:H	2.20	0.43
1:D:535:ARG:HG3	1:D:535:ARG:NH1	2.34	0.43
1:D:59:THR:O	1:D:63:ILE:HG13	2.19	0.43
1:A:279:ILE:HD11	1:A:293:GLY:O	2.19	0.43
1:A:523:VAL:O	1:A:524:VAL:CB	2.66	0.43
1:A:60:ASP:HB3	1:A:124:LEU:HD13	2.00	0.43
1:B:178:GLN:NE2	1:B:193:TYR:OH	2.49	0.43
1:B:457:MET:C	1:B:459:GLU:H	2.22	0.43
1:B:660:LEU:O	1:B:661:ALA:C	2.57	0.43
1:B:668:HIS:CB	1:B:671:LEU:HD12	2.49	0.43
1:C:140:LEU:CD1	1:C:213:VAL:HG21	2.48	0.43
1:C:60:ASP:HA	1:C:63:ILE:HD12	1.99	0.43
1:C:698:SER:O	1:C:699:VAL:C	2.56	0.43
1:D:564:LEU:HD23	1:D:592:VAL:CG1	2.49	0.43
1:A:137:ALA:HB3	1:A:248:LEU:HD21	1.99	0.42
1:A:352:LEU:CD1	1:A:363:LEU:HD13	2.43	0.42
1:B:506:ARG:O	1:B:510:GLN:HB2	2.19	0.42
1:B:559:PRO:HB2	1:B:560:THR:H	1.69	0.42
1:C:466:ARG:NH1	1:C:501:MET:CE	2.80	0.42
1:D:143:GLU:O	1:D:146:ASP:HB2	2.19	0.42
1:D:346:ILE:HG21	1:D:427:LEU:HD13	2.00	0.42
1:D:460:ALA:HA	1:D:464:GLU:OE2	2.18	0.42
1:A:462:ALA:HB1	1:A:498:ALA:CB	2.47	0.42
1:A:566:ILE:HD11	1:A:577:TYR:CE2	2.54	0.42
1:B:254:PHE:CD1	1:B:254:PHE:N	2.86	0.42
1:B:256:LEU:O	1:B:258:ARG:N	2.53	0.42
1:B:381:GLN:HE21	1:B:402:TRP:HD1	1.66	0.42
1:C:205:LEU:HA	1:C:245:GLU:OE1	2.18	0.42
1:C:465:PHE:HZ	1:C:502:LEU:HD13	1.84	0.42
1:C:611:ILE:O	1:C:615:THR:HG23	2.19	0.42
1:C:624:ILE:HB	1:C:625:PRO:HD2	2.01	0.42
1:D:261:ALA:HA	1:D:264:PHE:CD1	2.54	0.42
1:D:566:ILE:HD11	1:D:577:TYR:CD2	2.54	0.42
1:D:668:HIS:HB3	1:D:671:LEU:HD12	2.00	0.42
1:A:176:SER:C	1:A:178:GLN:N	2.70	0.42
1:A:326:VAL:HG12	1:A:330:ASP:HB2	2.01	0.42
1:B:128:MET:O	1:B:129:VAL:C	2.57	0.42
1:B:379:LEU:HD21	1:B:481:CYS:HB3	2.01	0.42
1:B:494:ARG:HH11	1:B:494:ARG:CG	2.33	0.42
1:C:33:PHE:HD2	1:C:318:ARG:HB2	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:402:TRP:CE3	1:C:402:TRP:HA	2.55	0.42
1:C:41:LEU:HD12	1:C:42:PRO:O	2.20	0.42
1:C:350:ARG:CD	1:C:539:LEU:HA	2.50	0.42
1:D:14:ARG:HD3	1:D:257:ILE:CD1	2.47	0.42
1:D:158:MET:CE	1:D:256:LEU:HD13	2.49	0.42
1:D:1:MET:O	1:D:3:ALA:N	2.52	0.42
1:D:97:PHE:HZ	1:D:301:THR:HA	1.84	0.42
1:A:327:SER:HG	1:A:329:THR:HB	1.82	0.42
1:A:67:TYR:O	1:A:70:ILE:HB	2.19	0.42
1:A:747:LEU:N	1:A:748:PRO:CD	2.82	0.42
1:B:176:SER:C	1:B:178:GLN:N	2.70	0.42
1:B:603:GLU:N	1:B:634:ARG:HH22	2.17	0.42
1:C:170:VAL:HG12	1:C:216:VAL:O	2.19	0.42
1:C:36:SER:CB	1:C:317:TRP:HE3	2.33	0.42
1:C:494:ARG:HH11	1:C:494:ARG:CG	2.32	0.42
1:D:561:ILE:H	1:D:561:ILE:CD1	2.27	0.42
1:D:587:PRO:CG	1:D:588:VAL:H	2.32	0.42
1:D:60:ASP:HB3	1:D:124:LEU:HD13	2.01	0.42
1:A:236:ALA:N	1:A:237:PRO:HD3	2.34	0.42
1:A:493:LEU:HD23	1:A:496:ILE:HD12	2.02	0.42
1:B:191:ILE:CG2	1:B:195:ARG:HD3	2.49	0.42
1:B:437:SER:CB	1:B:478:SER:O	2.64	0.42
1:C:466:ARG:HD3	1:C:466:ARG:HA	1.84	0.42
1:D:609:LYS:CD	1:D:641:THR:HG22	2.49	0.42
1:A:0:ALA:O	1:A:1:MET:C	2.55	0.42
1:A:153:SER:O	1:A:157:ARG:HD2	2.19	0.42
1:A:217:ARG:NH1	1:A:217:ARG:HG2	2.34	0.42
1:A:457:MET:C	1:A:459:GLU:H	2.21	0.42
1:A:480:PHE:C	1:A:482:SER:H	2.21	0.42
1:B:9:THR:HG23	1:B:18:HIS:CE1	2.54	0.42
1:B:326:VAL:HG12	1:B:330:ASP:HB2	2.02	0.42
1:C:307:ASP:CG	1:C:391:PHE:HA	2.39	0.42
1:C:596:TYR:CD2	1:C:600:LEU:HD11	2.54	0.42
1:D:226:ILE:CD1	1:D:226:ILE:N	2.82	0.42
1:D:96:THR:HG21	1:D:301:THR:HG23	2.00	0.42
1:A:381:GLN:NE2	1:A:402:TRP:CD1	2.88	0.42
1:B:465:PHE:CD2	1:B:501:MET:HB3	2.55	0.42
1:B:638:ILE:HG13	1:B:638:ILE:H	1.60	0.42
1:B:82:SER:HB3	1:B:85:GLU:HB3	2.02	0.42
1:C:668:HIS:CB	1:C:671:LEU:HD12	2.49	0.42
1:D:259:VAL:O	1:D:260:GLN:C	2.56	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:458:GLY:C	1:A:460:ALA:N	2.72	0.42
1:B:161:THR:CB	1:B:164:ILE:HB	2.49	0.42
1:B:470:ASP:O	1:B:474:GLU:HG3	2.20	0.42
1:C:242:LEU:HA	1:C:243:PRO:HD3	1.89	0.42
1:C:480:PHE:C	1:C:482:SER:N	2.72	0.42
1:C:62:THR:O	1:C:66:VAL:HG23	2.19	0.42
1:D:242:LEU:HD12	1:D:247:CYS:SG	2.59	0.42
1:A:342:VAL:CG2	1:A:410:VAL:HG12	2.49	0.42
1:A:548:GLN:CA	1:A:548:GLN:NE2	2.83	0.42
1:B:110:LEU:HD11	1:B:269:ALA:CB	2.50	0.42
1:B:574:PRO:HA	1:B:578:GLY:H	1.83	0.42
1:C:20:LEU:HB2	1:C:115:LEU:HD11	2.02	0.42
1:C:265:LEU:N	1:C:266:PRO:CD	2.83	0.42
1:C:506:ARG:O	1:C:510:GLN:HB2	2.20	0.42
1:C:566:ILE:HD11	1:C:577:TYR:CD2	2.55	0.42
1:D:251:PRO:HG2	1:D:254:PHE:HD1	1.82	0.42
1:D:289:CYS:SG	1:D:291:ARG:HG3	2.60	0.42
1:D:602:TYR:CD1	1:D:603:GLU:HG2	2.55	0.42
1:A:39:ARG:CD	1:A:317:TRP:CE2	2.97	0.42
1:A:445:PRO:CG	1:A:448:VAL:HG23	2.49	0.42
1:A:698:SER:O	1:A:699:VAL:C	2.58	0.42
1:B:265:LEU:N	1:B:266:PRO:HD3	2.35	0.42
1:C:401:THR:O	1:C:404:ASP:N	2.43	0.42
1:C:458:GLY:C	1:C:460:ALA:N	2.71	0.42
1:C:493:LEU:HD23	1:C:496:ILE:HD12	2.01	0.42
1:C:747:LEU:N	1:C:748:PRO:CD	2.83	0.42
1:D:162:PRO:HA	1:D:166:TRP:CD1	2.55	0.42
1:D:458:GLY:O	1:D:460:ALA:N	2.51	0.42
1:A:110:LEU:HD12	1:A:112:PHE:CZ	2.55	0.41
1:A:402:TRP:CE3	1:A:405:MET:HE3	2.55	0.41
1:A:444:CYS:SG	1:A:445:PRO:HD2	2.60	0.41
1:A:480:PHE:C	1:A:482:SER:N	2.73	0.41
1:A:668:HIS:HB3	1:A:671:LEU:HD12	2.01	0.41
1:A:747:LEU:HD23	1:A:747:LEU:O	2.19	0.41
1:B:158:MET:HE1	1:B:170:VAL:HB	2.02	0.41
1:B:226:ILE:CD1	1:B:226:ILE:N	2.82	0.41
1:B:41:LEU:HD13	1:B:42:PRO:O	2.20	0.41
1:B:432:MET:CE	1:B:538:TRP:HB2	2.50	0.41
1:B:587:PRO:HG2	1:B:588:VAL:N	2.35	0.41
1:C:466:ARG:HH21	1:C:498:ALA:H	1.65	0.41
1:C:524:VAL:O	1:C:524:VAL:HG12	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:631:PHE:CZ	1:C:635:LEU:HD11	2.55	0.41
1:D:67:TYR:CZ	1:D:114:PRO:CG	3.03	0.41
1:D:141:SER:HB3	1:D:210:LEU:CD1	2.50	0.41
1:D:312:ARG:O	1:D:317:TRP:HA	2.19	0.41
1:A:587:PRO:CG	1:A:588:VAL:N	2.83	0.41
1:B:226:ILE:HA	1:B:227:PRO:HD3	1.97	0.41
1:C:158:MET:CE	1:C:170:VAL:HB	2.50	0.41
1:C:137:ALA:HB1	1:C:248:LEU:CD2	2.49	0.41
1:D:608:SER:O	1:D:611:ILE:N	2.53	0.41
1:A:97:PHE:CZ	1:A:301:THR:HA	2.52	0.41
1:B:377:ASN:HD21	1:B:395:LEU:HD11	1.84	0.41
1:C:210:LEU:HB3	1:C:244:PRO:HG2	2.02	0.41
1:D:23:LEU:HD23	1:D:110:LEU:HB3	2.02	0.41
1:D:462:ALA:O	1:D:464:GLU:N	2.52	0.41
1:A:23:LEU:HD21	1:A:272:ILE:CD1	2.49	0.41
1:A:564:LEU:C	1:A:566:ILE:N	2.74	0.41
1:D:1:MET:HE2	1:D:55:SER:HB3	2.03	0.41
1:D:305:ARG:HA	1:D:305:ARG:HD2	1.92	0.41
1:C:685:THR:CG2	1:D:487:THR:HG21	2.50	0.41
1:C:545:TYR:CD1	1:C:560:THR:OG1	2.73	0.41
1:C:677:THR:O	1:C:681:GLN:HG3	2.21	0.41
1:D:142:ASP:C	1:D:143:GLU:HG3	2.40	0.41
1:B:162:PRO:HA	1:B:166:TRP:CD1	2.56	0.41
1:B:217:ARG:HG2	1:B:217:ARG:NH1	2.35	0.41
1:B:445:PRO:HD2	1:B:471:TYR:CZ	2.56	0.41
1:B:747:LEU:N	1:B:748:PRO:CD	2.83	0.41
1:C:262:LEU:C	1:C:264:PHE:N	2.73	0.41
1:C:332:PHE:CD1	1:C:408:GLU:HG3	2.56	0.41
1:C:333:GLN:HE21	1:C:673:GLU:CB	2.34	0.41
1:D:178:GLN:HG3	1:D:212:LEU:HD12	2.03	0.41
1:D:480:PHE:C	1:D:482:SER:H	2.23	0.41
1:D:564:LEU:C	1:D:566:ILE:N	2.73	0.41
1:D:342:VAL:CG1	1:D:658:CYS:SG	3.06	0.41
1:A:243:PRO:HA	1:A:244:PRO:HD3	1.90	0.41
1:B:179:THR:HG23	1:B:208:ALA:O	2.21	0.41
1:B:275:ILE:HG23	1:B:297:TYR:HB2	2.02	0.41
1:B:331:VAL:O	1:B:335:LEU:HG	2.21	0.41
1:B:335:LEU:O	1:B:411:GLY:HA3	2.21	0.41
1:B:480:PHE:C	1:B:482:SER:N	2.73	0.41
1:C:227:PRO:HG3	1:C:234:ASP:OD2	2.20	0.41
1:C:564:LEU:HD12	1:C:564:LEU:C	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:217:ARG:HG2	1:D:217:ARG:NH1	2.35	0.41
1:A:158:MET:CE	1:A:170:VAL:HB	2.51	0.41
1:A:179:THR:HG23	1:A:208:ALA:O	2.21	0.41
1:A:319:THR:HA	1:A:320:PRO:HD3	1.84	0.41
1:A:463:HIS:CD2	1:A:464:GLU:HG3	2.56	0.41
1:A:60:ASP:HA	1:A:63:ILE:HD12	2.03	0.41
1:B:257:ILE:O	1:B:260:GLN:HB3	2.21	0.41
1:B:261:ALA:HA	1:B:264:PHE:CD1	2.55	0.41
1:B:39:ARG:NH2	1:B:267:GLU:CD	2.74	0.41
1:B:607:GLY:C	1:B:609:LYS:H	2.24	0.41
1:B:71:LEU:HD22	1:B:262:LEU:HD11	2.02	0.41
1:C:23:LEU:CD2	1:C:110:LEU:HB3	2.51	0.41
1:C:254:PHE:C	1:C:255:ASP:O	2.58	0.41
1:C:379:LEU:HD21	1:C:481:CYS:HB3	2.02	0.41
1:C:9:THR:HG23	1:C:18:HIS:CE1	2.56	0.41
1:D:381:GLN:NE2	1:D:402:TRP:CD1	2.89	0.41
1:D:458:GLY:C	1:D:460:ALA:N	2.72	0.41
1:D:456:CYS:SG	1:D:524:VAL:HG13	2.60	0.41
1:A:138:LYS:HD3	1:A:142:ASP:CB	2.45	0.41
1:A:455:VAL:HA	1:A:460:ALA:CB	2.51	0.41
1:A:465:PHE:O	1:A:468:LEU:HB2	2.20	0.41
1:A:680:ARG:HG3	1:A:681:GLN:N	2.35	0.41
1:A:750:VAL:HG13	1:A:750:VAL:O	2.20	0.41
1:B:34:LYS:HG3	1:B:321:PHE:CD1	2.55	0.41
1:B:544:PHE:O	1:B:560:THR:HG23	2.21	0.41
1:C:34:LYS:HZ3	1:C:319:THR:CG2	2.33	0.41
1:C:455:VAL:HG21	1:C:468:LEU:HD11	2.03	0.41
1:C:455:VAL:HA	1:C:460:ALA:HB3	2.03	0.41
1:C:463:HIS:HA	1:C:466:ARG:HB2	2.02	0.41
1:D:698:SER:O	1:D:699:VAL:C	2.59	0.41
1:A:469:VAL:O	1:A:473:CYS:N	2.53	0.41
1:A:546:VAL:HB	1:A:644:VAL:HG13	2.03	0.41
1:B:140:LEU:CD2	1:B:249:LEU:HB2	2.47	0.41
1:B:668:HIS:HB3	1:B:671:LEU:HD12	2.03	0.41
1:C:136:ASP:O	1:C:138:LYS:N	2.54	0.41
1:C:380:VAL:HG21	1:C:402:TRP:O	2.21	0.41
1:C:574:PRO:HA	1:C:578:GLY:H	1.85	0.41
1:C:587:PRO:HG2	1:C:588:VAL:N	2.35	0.41
1:C:67:TYR:O	1:C:70:ILE:HB	2.21	0.41
1:D:221:LEU:O	1:D:223:ASP:N	2.54	0.41
1:D:461:GLY:O	1:D:462:ALA:O	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:624:ILE:HB	1:A:625:PRO:HD2	2.03	0.41
1:B:4:LEU:HD21	1:B:26:HIS:HA	2.02	0.41
1:B:460:ALA:HA	1:B:464:GLU:HG2	2.02	0.41
1:C:191:ILE:CG2	1:C:195:ARG:HD3	2.48	0.41
1:C:352:LEU:CD1	1:C:363:LEU:HD13	2.50	0.41
1:C:455:VAL:HA	1:C:460:ALA:CB	2.51	0.41
1:C:67:TYR:CZ	1:C:114:PRO:CG	3.04	0.41
1:D:747:LEU:N	1:D:748:PRO:CD	2.84	0.41
1:A:104:PRO:HG2	1:A:107:PHE:CE1	2.56	0.40
1:A:258:ARG:O	1:A:259:VAL:O	2.38	0.40
1:B:140:LEU:C	1:B:142:ASP:N	2.74	0.40
1:B:39:ARG:HH12	1:B:41:LEU:HD21	1.86	0.40
1:B:434:PRO:CA	1:B:527:ILE:HG22	2.49	0.40
1:C:128:MET:O	1:C:132:GLN:HG3	2.21	0.40
1:C:115:LEU:N	1:C:258:ARG:NH2	2.50	0.40
1:D:60:ASP:CB	1:D:124:LEU:HD13	2.52	0.40
1:D:631:PHE:CE2	1:D:635:LEU:HD11	2.56	0.40
1:A:312:ARG:O	1:A:317:TRP:HA	2.22	0.40
1:B:455:VAL:HA	1:B:460:ALA:CB	2.51	0.40
1:B:432:MET:CE	1:B:534:ALA:HB1	2.48	0.40
1:C:1:MET:O	1:C:2:HIS:C	2.60	0.40
1:C:235:LEU:HD23	1:C:235:LEU:HA	1.88	0.40
1:C:609:LYS:CD	1:C:641:THR:HG22	2.52	0.40
1:A:162:PRO:HA	1:A:166:TRP:CD1	2.56	0.40
1:A:581:THR:O	1:A:585:THR:HG22	2.21	0.40
1:A:67:TYR:CZ	1:A:114:PRO:CG	3.04	0.40
1:B:394:ASN:ND2	1:B:396:VAL:HB	2.34	0.40
1:B:642:PRO:HB2	1:B:643:HIS:H	1.64	0.40
1:B:740:ALA:HA	1:B:743:ARG:HG2	2.04	0.40
1:C:57:SER:O	1:C:59:THR:N	2.54	0.40
1:D:150:LEU:HD12	1:D:153:SER:OG	2.20	0.40
1:D:17:SER:OG	1:D:258:ARG:NH1	2.54	0.40
1:D:1:MET:O	1:D:2:HIS:C	2.60	0.40
1:D:469:VAL:C	1:D:471:TYR:N	2.75	0.40
1:A:258:ARG:O	1:A:259:VAL:C	2.60	0.40
1:B:157:ARG:NH2	1:B:249:LEU:HD21	2.36	0.40
1:B:34:LYS:HA	1:B:45:GLU:HA	2.03	0.40
1:B:564:LEU:HD12	1:B:564:LEU:C	2.42	0.40
1:C:36:SER:HB3	1:C:317:TRP:CE3	2.55	0.40
1:C:543:GLY:CA	1:C:561:ILE:O	2.63	0.40
1:C:587:PRO:CG	1:C:588:VAL:H	2.35	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:480:PHE:C	1:D:482:SER:N	2.74	0.40
1:D:609:LYS:HZ2	1:D:641:THR:CG2	2.32	0.40
1:A:221:LEU:O	1:A:223:ASP:N	2.55	0.40
1:A:368:MET:O	1:A:372:ARG:CB	2.68	0.40
1:A:82:SER:HB3	1:A:85:GLU:HB3	2.04	0.40
1:B:158:MET:CE	1:B:170:VAL:HB	2.51	0.40
1:C:12:THR:OG1	1:C:14:ARG:HG3	2.22	0.40
1:C:210:LEU:HA	1:C:211:PRO:HD3	1.92	0.40
1:C:401:THR:O	1:C:402:TRP:C	2.59	0.40
1:C:342:VAL:CG2	1:C:410:VAL:HG12	2.50	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	718/756 (95%)	593 (83%)	87 (12%)	38 (5%)	2	11
1	B	710/756 (94%)	580 (82%)	91 (13%)	39 (6%)	2	10
1	C	700/756 (93%)	578 (83%)	87 (12%)	35 (5%)	2	12
1	D	702/756 (93%)	578 (82%)	82 (12%)	42 (6%)	1	9
All	All	2830/3024 (94%)	2329 (82%)	347 (12%)	154 (5%)	2	11

All (154) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	HIS
1	A	39	ARG
1	A	81	ALA
1	A	182	SER
1	A	222	LYS

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Mol	Chain	Res	Type
1	A	259	VAL
1	A	393	ASN
1	A	524	VAL
1	A	547	GLU
1	A	642	PRO
1	A	643	HIS
1	A	698	SER
1	B	2	HIS
1	B	37	ALA
1	B	182	SER
1	B	222	LYS
1	B	234	ASP
1	B	398	LYS
1	B	642	PRO
1	B	643	HIS
1	B	698	SER
1	C	2	HIS
1	C	81	ALA
1	C	138	LYS
1	C	182	SER
1	C	222	LYS
1	C	255	ASP
1	C	462	ALA
1	C	547	GLU
1	C	642	PRO
1	C	643	HIS
1	C	698	SER
1	D	2	HIS
1	D	39	ARG
1	D	81	ALA
1	D	182	SER
1	D	222	LYS
1	D	256	LEU
1	D	445	PRO
1	D	462	ALA
1	D	463	HIS
1	D	547	GLU
1	D	642	PRO
1	D	643	HIS
1	D	698	SER
1	A	229	PRO
1	A	275	ILE

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Mol	Chain	Res	Type
1	A	281	ALA
1	A	311	GLY
1	A	458	GLY
1	A	586	GLY
1	A	606	GLY
1	B	39	ARG
1	B	81	ALA
1	B	275	ILE
1	B	311	GLY
1	B	458	GLY
1	B	586	GLY
1	B	602	TYR
1	B	603	GLU
1	B	605	SER
1	C	40	GLY
1	C	275	ILE
1	C	281	ALA
1	C	311	GLY
1	C	391	PHE
1	C	458	GLY
1	C	474	GLU
1	C	586	GLY
1	D	50	ALA
1	D	146	ASP
1	D	252	ASP
1	D	253	GLU
1	D	257	ILE
1	D	275	ILE
1	D	311	GLY
1	D	447	ALA
1	D	458	GLY
1	D	586	GLY
1	A	50	ALA
1	A	58	ARG
1	A	200	ALA
1	A	237	PRO
1	A	459	GLU
1	A	559	PRO
1	A	587	PRO
1	A	607	GLY
1	B	36	SER
1	B	58	ARG

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Mol	Chain	Res	Type
1	B	108	ALA
1	B	137	ALA
1	B	200	ALA
1	B	229	PRO
1	B	258	ARG
1	B	281	ALA
1	B	397	ALA
1	B	445	PRO
1	B	459	GLU
1	B	559	PRO
1	B	587	PRO
1	C	50	ALA
1	C	58	ARG
1	C	108	ALA
1	C	200	ALA
1	C	459	GLU
1	C	587	PRO
1	D	58	ARG
1	D	108	ALA
1	D	137	ALA
1	D	200	ALA
1	D	258	ARG
1	D	281	ALA
1	D	459	GLU
1	D	464	GLU
1	D	587	PRO
1	A	105	PRO
1	A	108	ALA
1	A	230	GLY
1	A	254	PHE
1	B	50	ALA
1	B	259	VAL
1	B	389	ALA
1	C	473	CYS
1	D	212	LEU
1	D	259	VAL
1	A	673	GLU
1	B	105	PRO
1	B	673	GLU
1	C	105	PRO
1	C	137	ALA
1	C	236	ALA

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Mol	Chain	Res	Type
1	C	257	ILE
1	C	673	GLU
1	D	105	PRO
1	D	238	LYS
1	D	673	GLU
1	A	256	LEU
1	A	257	ILE
1	B	180	SER
1	B	227	PRO
1	C	212	LEU
1	D	82	SER
1	A	227	PRO
1	A	445	PRO
1	C	227	PRO
1	D	227	PRO
1	B	279	ILE
1	D	38	GLY
1	C	279	ILE
1	C	469	VAL
1	A	279	ILE
1	A	575	VAL
1	D	279	ILE
1	D	575	VAL

### 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	611/632 (97%)	572 (94%)	39 (6%)	17	51
1	B	607/632 (96%)	577 (95%)	30 (5%)	25	61
1	C	602/632 (95%)	574 (95%)	28 (5%)	26	63
1	D	605/632 (96%)	566 (94%)	39 (6%)	17	51
All	All	2425/2528 (96%)	2289 (94%)	136 (6%)	21	56

All (136) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	HIS
1	A	14	ARG
1	A	35	VAL
1	A	39	ARG
1	A	42	PRO
1	A	68	GLN
1	A	110	LEU
1	A	136	ASP
1	A	139	ARG
1	A	142	ASP
1	A	179	THR
1	A	217	ARG
1	A	222	LYS
1	A	223	ASP
1	A	225	GLN
1	A	242	LEU
1	A	262	LEU
1	A	327	SER
1	A	332	PHE
1	A	357	ASP
1	A	395	LEU
1	A	400	LYS
1	A	402	TRP
1	A	438	LYS
1	A	444	CYS
1	A	457	MET
1	A	467	SER
1	A	488	MET
1	A	491	GLU
1	A	509	ILE
1	A	539	LEU
1	A	546	VAL
1	A	559	PRO
1	A	566	ILE
1	A	581	THR
1	A	618	ARG
1	A	624	ILE
1	A	720	ASP
1	A	753	ASP
1	B	2	HIS
1	B	14	ARG
1	B	39	ARG
1	B	68	GLN

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Mol	Chain	Res	Type
1	B	110	LEU
1	B	179	THR
1	B	217	ARG
1	B	222	LYS
1	B	223	ASP
1	B	225	GLN
1	B	242	LEU
1	B	327	SER
1	B	332	PHE
1	B	352	LEU
1	B	357	ASP
1	B	402	TRP
1	B	438	LYS
1	B	457	MET
1	B	467	SER
1	B	488	MET
1	B	491	GLU
1	B	509	ILE
1	B	539	LEU
1	B	546	VAL
1	B	566	ILE
1	B	581	THR
1	B	608	SER
1	B	618	ARG
1	B	624	ILE
1	B	720	ASP
1	C	2	HIS
1	C	14	ARG
1	C	110	LEU
1	C	179	THR
1	C	217	ARG
1	C	222	LYS
1	C	223	ASP
1	C	225	GLN
1	C	242	LEU
1	C	327	SER
1	C	332	PHE
1	C	357	ASP
1	C	402	TRP
1	C	438	LYS
1	C	444	CYS
1	C	457	MET

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Mol	Chain	Res	Type
1	C	464	GLU
1	C	475	GLN
1	C	488	MET
1	C	491	GLU
1	C	509	ILE
1	C	539	LEU
1	C	546	VAL
1	C	566	ILE
1	C	581	THR
1	C	618	ARG
1	C	624	ILE
1	C	720	ASP
1	D	2	HIS
1	D	14	ARG
1	D	34	LYS
1	D	35	VAL
1	D	68	GLN
1	D	110	LEU
1	D	139	ARG
1	D	141	SER
1	D	145	THR
1	D	179	THR
1	D	217	ARG
1	D	222	LYS
1	D	223	ASP
1	D	225	GLN
1	D	233	ASP
1	D	242	LEU
1	D	252	ASP
1	D	258	ARG
1	D	264	PHE
1	D	327	SER
1	D	332	PHE
1	D	352	LEU
1	D	357	ASP
1	D	402	TRP
1	D	438	LYS
1	D	457	MET
1	D	463	HIS
1	D	488	MET
1	D	491	GLU
1	D	509	ILE

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Mol	Chain	Res	Type
1	D	539	LEU
1	D	546	VAL
1	D	548	GLN
1	D	566	ILE
1	D	581	THR
1	D	618	ARG
1	D	624	ILE
1	D	720	ASP
1	D	753	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	GLN
1	A	132	GLN
1	A	178	GLN
1	A	202	ASN
1	A	225	GLN
1	A	260	GLN
1	A	333	GLN
1	A	373	ASN
1	A	418	ASN
1	A	463	HIS
1	A	548	GLN
1	A	572	GLN
1	A	610	HIS
1	A	637	GLN
1	A	745	HIS
1	B	68	GLN
1	B	132	GLN
1	B	178	GLN
1	B	202	ASN
1	B	225	GLN
1	B	333	GLN
1	B	373	ASN
1	B	377	ASN
1	B	381	GLN
1	B	572	GLN
1	B	610	HIS
1	B	745	HIS
1	C	68	GLN
1	C	132	GLN

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Mol	Chain	Res	Type
1	C	178	GLN
1	C	225	GLN
1	C	333	GLN
1	C	373	ASN
1	C	377	ASN
1	C	381	GLN
1	C	418	ASN
1	C	572	GLN
1	C	610	HIS
1	C	614	GLN
1	C	637	GLN
1	D	68	GLN
1	D	132	GLN
1	D	178	GLN
1	D	202	ASN
1	D	225	GLN
1	D	333	GLN
1	D	373	ASN
1	D	377	ASN
1	D	381	GLN
1	D	548	GLN
1	D	572	GLN
1	D	610	HIS
1	D	745	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

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

Of 39 ligands modelled in this entry, 39 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.



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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	732/756 (96%)	-0.32	0 <a href="#">100</a> <a href="#">100</a>	19, 36, 65, 92	1 (0%)
1	B	726/756 (96%)	-0.34	0 <a href="#">100</a> <a href="#">100</a>	21, 36, 67, 93	1 (0%)
1	C	718/756 (94%)	-0.39	1 (0%) <a href="#">95</a> <a href="#">89</a>	18, 36, 66, 92	1 (0%)
1	D	720/756 (95%)	-0.35	3 (0%) <a href="#">92</a> <a href="#">79</a>	20, 36, 65, 92	1 (0%)
All	All	2896/3024 (95%)	-0.35	4 (0%) <a href="#">95</a> <a href="#">89</a>	18, 36, 66, 93	4 (0%)

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	187	ALA	3.0
1	D	185	THR	2.5
1	D	145	THR	2.1
1	C	234	ASP	2.1

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

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	MN	C	759	1/1	0.55	0.26	113,113,113,113	0
2	MN	D	762	1/1	0.57	0.26	114,114,114,114	0
2	MN	C	757	1/1	0.61	0.12	100,100,100,100	0
2	MN	C	763	1/1	0.66	0.31	114,114,114,114	0
2	MN	D	759	1/1	0.69	0.54	107,107,107,107	0
2	MN	A	764	1/1	0.74	0.13	96,96,96,96	0
2	MN	C	758	1/1	0.75	0.20	85,85,85,85	0
2	MN	D	761	1/1	0.78	0.25	82,82,82,82	0
2	MN	B	758	1/1	0.83	0.23	97,97,97,97	0
2	MN	D	760	1/1	0.84	0.20	107,107,107,107	0
2	MN	D	755	1/1	0.84	0.12	39,39,39,39	0
2	MN	B	761	1/1	0.85	0.12	72,72,72,72	0
2	MN	C	760	1/1	0.86	0.33	92,92,92,92	0
2	MN	B	756	1/1	0.86	0.09	25,25,25,25	0
2	MN	A	759	1/1	0.88	0.26	49,49,49,49	0
2	MN	D	757	1/1	0.88	0.24	70,70,70,70	0
2	MN	B	759	1/1	0.89	0.19	49,49,49,49	0
2	MN	D	758	1/1	0.90	0.16	99,99,99,99	0
2	MN	A	761	1/1	0.90	0.31	63,63,63,63	0
2	MN	C	762	1/1	0.90	0.14	93,93,93,93	0
2	MN	B	762	1/1	0.91	0.08	61,61,61,61	0
2	MN	A	757	1/1	0.92	0.14	77,77,77,77	0
2	MN	B	760	1/1	0.93	0.18	49,49,49,49	0
2	MN	A	763	1/1	0.94	0.17	65,65,65,65	0
2	MN	B	763	1/1	0.94	0.10	48,48,48,48	0
2	MN	C	755	1/1	0.94	0.06	48,48,48,48	0
2	MN	D	763	1/1	0.95	0.30	86,86,86,86	0
2	MN	A	755	1/1	0.95	0.07	32,32,32,32	0
2	MN	B	757	1/1	0.95	0.34	79,79,79,79	0
2	MN	C	756	1/1	0.96	0.08	39,39,39,39	0
2	MN	D	756	1/1	0.96	0.07	34,34,34,34	0
2	MN	A	760	1/1	0.96	0.33	34,34,34,34	0
2	MN	A	758	1/1	0.97	0.05	68,68,68,68	0
2	MN	A	765	1/1	0.97	0.10	83,83,83,83	0
2	MN	A	762	1/1	0.97	0.10	50,50,50,50	0
2	MN	A	766	1/1	0.97	0.12	76,76,76,76	0
2	MN	C	761	1/1	0.97	0.18	78,78,78,78	0
2	MN	A	756	1/1	0.98	0.04	20,20,20,20	0
2	MN	B	755	1/1	0.99	0.03	38,38,38,38	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.