



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:06 AM GMT

PDB ID : 1ZM3  
Title : Structure of the apo eEF2-ETA complex  
Authors : Joergensen, R.; Merrill, A.R.; Yates, S.P.; Marquez, V.E.; Schwan, A.L.; Boesen, T.; Andersen, G.R.  
Deposited on : 2005-05-10  
Resolution : 3.07 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

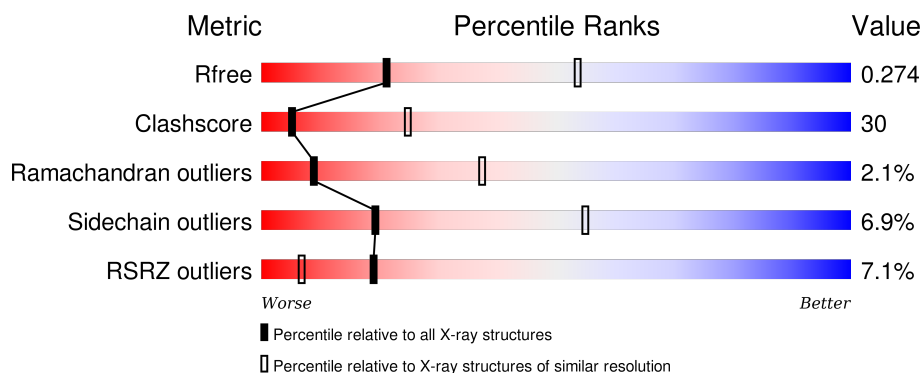
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.07 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))
$R_{free}$	91344	1119 (3.12-3.04)
Clashscore	102246	1098 (3.10-3.06)
Ramachandran outliers	100387	1057 (3.10-3.06)
Sidechain outliers	100360	1057 (3.10-3.06)
RSRZ outliers	91569	1001 (3.10-3.06)

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

Mol	Chain	Length	Quality of chain
1	A	842	<div> <div>2%</div> <div>54%</div> <div>40%</div> <div>• •</div> </div>
1	C	842	<div> <div>5%</div> <div>45%</div> <div>48%</div> <div>5%</div> <div>•</div> </div>
1	E	842	<div> <div>19%</div> <div>45%</div> <div>49%</div> <div>• •</div> </div>
2	B	207	<div> <div>%</div> <div>57%</div> <div>35%</div> <div>7%</div> </div>
2	D	207	<div> <div>55%</div> <div>42%</div> <div>•</div> </div>

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Mol	Chain	Length	Quality of chain
2	F	207	 A horizontal bar chart showing the quality of chain F. The bar is divided into three segments: green (57%), yellow (36%), and orange (6%). The percentages are labeled below the bar.

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 23979 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 Elongation factor 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	823	Total	C	N	O	S	0	0	0
			6405	4075	1093	1207	30			
1	C	823	Total	C	N	O	S	0	0	0
			6405	4075	1093	1207	30			
1	E	823	Total	C	N	O	S	0	0	0
			6405	4075	1093	1207	30			

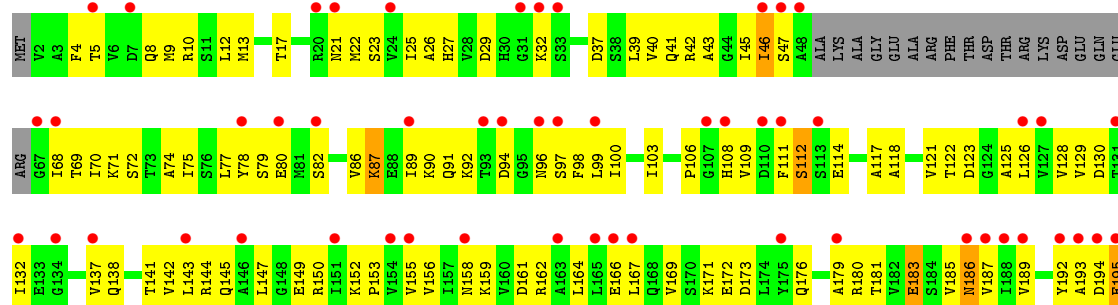
There are 3 discrepancies between the modelled and reference sequences:

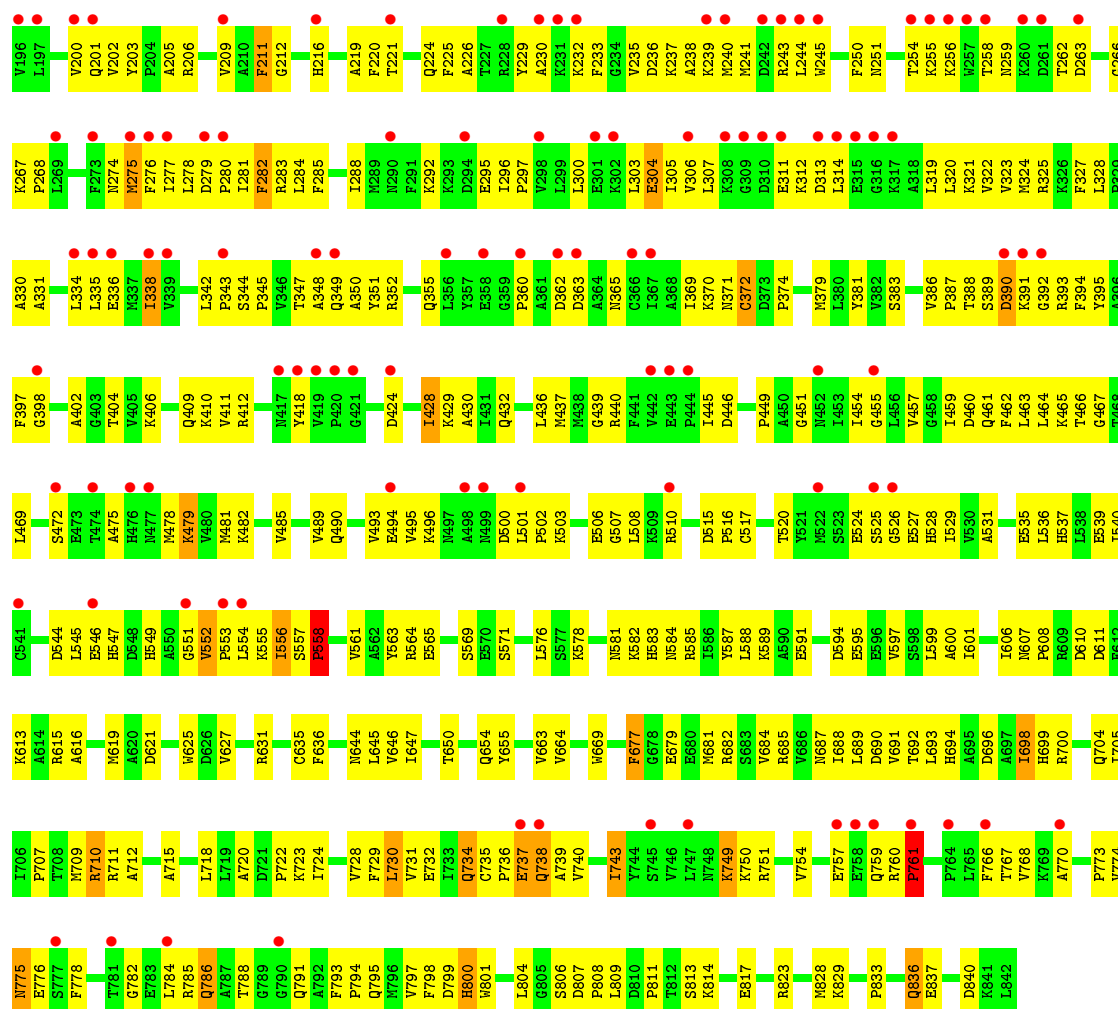
Chain	Residue	Modelled	Actual	Comment	Reference
A	699	DDE	HIS	MODIFIED RESIDUE	UNP P32324
C	699	DDE	HIS	MODIFIED RESIDUE	UNP P32324
E	699	DDE	HIS	MODIFIED RESIDUE	UNP P32324

- Molecule 2 is a protein called exotoxin A.

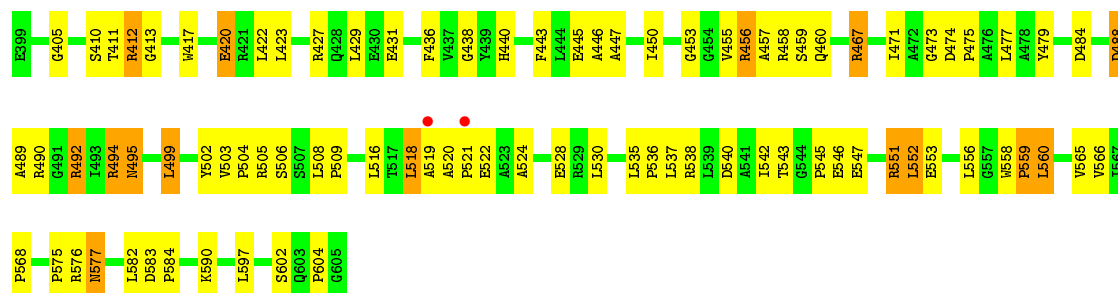
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	207	Total	C	N	O	0	0	0
			1588	1001	283	304			
2	D	207	Total	C	N	O	0	0	0
			1588	1001	283	304			
2	F	207	Total	C	N	O	0	0	0
			1588	1001	283	304			





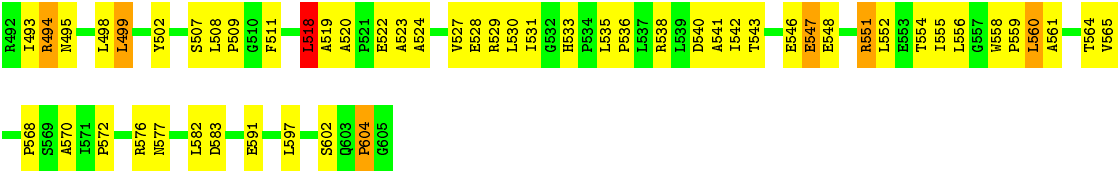


## • Molecule 2: exotoxin A

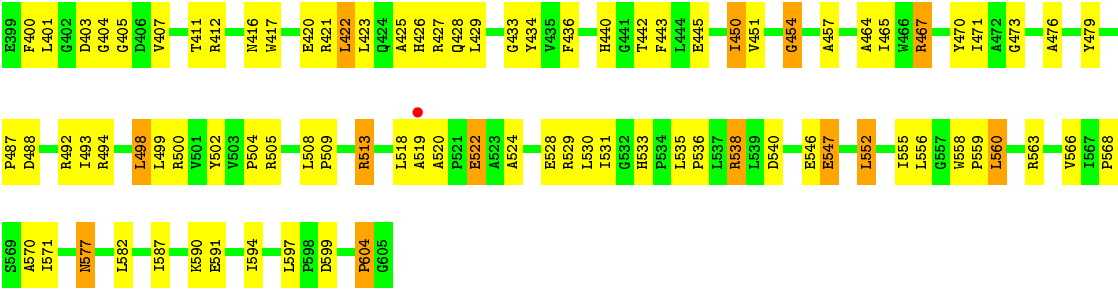


## • Molecule 2: exotoxin A





● Molecule 2: exotoxin A





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	329.43Å 69.09Å 190.80Å 90.00° 103.46° 90.00°	Depositor
Resolution (Å)	40.00 – 3.07 29.63 – 3.07	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-3.07) 97.9 (29.63-3.07)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.51 (at 3.06Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.249 , 0.282 0.243 , 0.274	Depositor DCC
$R_{free}$ test set	1536 reflections (1.99%)	DCC
Wilson B-factor (Å <sup>2</sup> )	54.3	Xtriage
Anisotropy	0.361	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 54.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	1 of 78889 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	23979	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 47.54 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 9.7793e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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, 0.375 respectively for untwinned datasets, and 0.333, 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: DDE

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	0.47	0/6517	0.68	1/8823 (0.0%)
1	C	0.49	1/6517 (0.0%)	0.71	1/8823 (0.0%)
1	E	0.44	1/6517 (0.0%)	0.65	1/8823 (0.0%)
2	B	0.64	0/1627	0.85	0/2216
2	D	0.66	0/1627	0.83	1/2216 (0.0%)
2	F	0.58	0/1627	0.83	0/2216
All	All	0.50	2/24432 (0.0%)	0.71	4/33117 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	195	GLU	CD-OE1	6.84	1.33	1.25
1	C	543	GLN	CG-CD	6.52	1.66	1.51

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	195	GLU	CG-CD-OE2	-7.76	102.77	118.30
1	A	236	ASP	N-CA-C	-5.55	96.01	111.00
1	C	554	LEU	N-CA-C	5.20	125.04	111.00
2	D	518	LEU	N-CA-C	5.04	124.61	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	195	GLU	Sidechain

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6405	0	6472	345	0
1	C	6405	0	6472	459	0
1	E	6405	0	6472	438	0
2	B	1588	0	1539	84	0
2	D	1588	0	1539	76	0
2	F	1588	0	1539	71	0
All	All	23979	0	24033	1462	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 30.

All (1462) 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:C:391:LYS:HG2	1:C:392:GLY:H	1.13	1.11
1:E:71:LYS:HE3	1:E:387:PRO:HD2	1.32	1.11
1:E:556:ILE:HG22	1:E:557:SER:H	1.10	1.10
1:A:16:VAL:HG13	1:A:345:PRO:HG2	1.33	1.09
1:C:253:LYS:HA	1:C:253:LYS:HE3	1.35	1.06
1:E:552:VAL:HG22	1:E:553:PRO:HD3	1.36	1.05
1:E:68:ILE:HD12	1:E:390:ASP:HB2	1.37	1.03
1:C:231:LYS:HE3	1:C:232:LYS:HG3	1.40	1.02
1:E:10:ARG:HH12	1:E:449:PRO:CD	1.75	0.99
1:C:820:LEU:O	1:C:824:LYS:HG3	1.63	0.98
2:F:546:GLU:HG3	2:F:547:GLU:HG3	1.43	0.97
1:A:16:VAL:CG1	1:A:345:PRO:HG2	1.92	0.97
1:C:404:THR:HG22	1:C:449:PRO:HA	1.43	0.96
1:E:552:VAL:HG22	1:E:553:PRO:CD	1.94	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:737:GLU:HG3	1:A:766:PHE:CE2	2.01	0.94
1:E:694:HIS:HD2	1:E:696:ASP:H	1.06	0.94
1:C:265:GLU:HG3	1:C:266:GLY:H	1.29	0.94
1:E:535:GLU:OE2	1:E:778:PHE:HA	1.68	0.94
1:C:42:ARG:HG3	1:C:331:ALA:CB	1.98	0.93
1:A:627:VAL:HG12	2:F:405:GLY:HA2	1.51	0.93
1:C:552:VAL:HG22	1:C:553:PRO:CD	1.99	0.93
1:C:784:LEU:HD23	1:C:794:PRO:HG3	1.50	0.92
1:A:533:THR:H	1:A:537:HIS:CD2	1.88	0.92
1:A:533:THR:H	1:A:537:HIS:HD2	1.16	0.91
1:C:578:LYS:HE2	1:C:840:ASP:OD1	1.70	0.91
2:D:546:GLU:HG3	2:D:547:GLU:HG3	1.52	0.91
1:C:256:LYS:HA	1:C:256:LYS:HE2	1.51	0.90
1:C:256:LYS:HD3	1:C:257:TRP:H	1.36	0.90
1:E:91:GLN:HE22	1:E:344:SER:H	1.16	0.90
2:D:520:ALA:HB3	2:D:522:GLU:OE2	1.71	0.90
1:C:836:GLN:HE21	1:C:836:GLN:H	1.20	0.88
1:C:694:HIS:HD2	1:C:696:ASP:H	1.18	0.88
1:A:578:LYS:HE3	1:A:840:ASP:OD1	1.73	0.88
1:E:27:HIS:HD2	1:E:29:ASP:H	1.16	0.88
1:E:45:ILE:HD11	1:E:78:TYR:CB	2.04	0.87
1:C:506:GLU:HG3	1:C:510:ARG:NE	1.88	0.87
1:A:229:TYR:CE2	1:A:276:PHE:HB3	2.08	0.87
1:C:391:LYS:HG2	1:C:392:GLY:N	1.88	0.87
1:C:315:GLU:HA	1:C:319:LEU:HB2	1.56	0.87
1:C:379:MET:HB2	1:C:402:ALA:HB3	1.54	0.87
1:E:45:ILE:HD11	1:E:78:TYR:HB2	1.55	0.87
1:A:404:THR:HG22	1:A:449:PRO:HA	1.55	0.86
1:C:225:PHE:CD2	1:C:277:ILE:HG13	2.11	0.86
1:A:379:MET:HB2	1:A:402:ALA:HB3	1.58	0.85
1:E:404:THR:HG22	1:E:449:PRO:HA	1.56	0.85
1:E:147:LEU:HD13	1:E:192:TYR:HB2	1.58	0.85
1:E:546:GLU:HB3	1:E:554:LEU:HD12	1.56	0.85
1:A:694:HIS:HD2	1:A:696:ASP:H	1.18	0.85
1:A:71:LYS:HB3	1:A:386:VAL:HG23	1.60	0.84
1:E:694:HIS:O	1:E:700:ARG:HD3	1.77	0.84
1:C:545:LEU:O	1:C:550:ALA:HB3	1.77	0.84
1:A:584:ASN:HD22	1:A:693:LEU:HA	1.40	0.84
2:B:552:LEU:HD12	2:B:552:LEU:H	1.43	0.84
1:E:10:ARG:HH12	1:E:449:PRO:HD2	1.40	0.83
2:B:520:ALA:HB3	2:B:522:GLU:OE2	1.77	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:556:ILE:HG22	1:E:557:SER:N	1.92	0.83
2:D:531:ILE:HD11	2:D:533:HIS:O	1.77	0.83
1:E:784:LEU:HD23	1:E:794:PRO:HG3	1.59	0.83
2:D:488:ASP:OD2	2:D:490:ARG:HG2	1.79	0.83
1:C:504:LEU:O	1:C:508:LEU:HG	1.79	0.82
1:E:503:LYS:HB3	1:E:551:GLY:HA3	1.60	0.82
1:E:482:LYS:HD3	1:E:797:VAL:HG11	1.62	0.82
1:E:71:LYS:HE3	1:E:387:PRO:CD	2.09	0.82
1:C:296:ILE:HD13	1:C:319:LEU:HD21	1.61	0.82
1:E:694:HIS:CD2	1:E:696:ASP:H	1.95	0.82
1:C:314:LEU:HD11	1:C:318:ALA:HB1	1.62	0.82
1:A:132:ILE:HD12	1:A:162:ARG:HH11	1.44	0.82
1:A:737:GLU:HG3	1:A:766:PHE:HE2	1.41	0.81
2:D:546:GLU:CG	2:D:547:GLU:HG3	2.09	0.81
1:C:552:VAL:HG22	1:C:553:PRO:HD2	1.61	0.81
1:E:237:LYS:HA	1:E:240:MET:HB3	1.61	0.81
1:E:155:VAL:HG23	1:E:202:VAL:HG11	1.62	0.81
1:C:229:TYR:CE2	1:C:276:PHE:HB3	2.16	0.81
1:E:545:LEU:HD12	1:E:549:HIS:HB2	1.62	0.81
1:E:26:ALA:HB2	1:E:128:VAL:HB	1.61	0.81
1:A:27:HIS:HD2	1:A:29:ASP:H	1.27	0.80
1:A:820:LEU:HD11	1:A:830:GLU:HG2	1.64	0.80
1:A:500:ASP:HB2	1:A:552:VAL:HG11	1.64	0.80
1:A:694:HIS:O	1:A:700:ARG:HD3	1.82	0.80
1:A:132:ILE:HD12	1:A:162:ARG:CD	2.12	0.80
2:D:531:ILE:HD12	2:D:533:HIS:CE1	2.17	0.80
1:C:391:LYS:CG	1:C:392:GLY:H	1.94	0.79
1:E:147:LEU:CD1	1:E:192:TYR:HB2	2.12	0.79
1:C:191:THR:O	1:C:763:THR:HG22	1.80	0.79
1:A:45:ILE:HD12	1:A:76:SER:HB3	1.62	0.79
2:D:417:TRP:CE2	2:D:568:PRO:HB2	2.17	0.79
1:E:71:LYS:HB3	1:E:386:VAL:HG23	1.64	0.79
1:E:27:HIS:CD2	1:E:29:ASP:H	2.01	0.79
1:E:459:ILE:HG21	1:E:463:LEU:HD12	1.65	0.79
1:C:591:GLU:O	1:C:685:ARG:HB3	1.81	0.79
1:A:140:GLU:HG3	1:A:188:ILE:CD1	2.12	0.79
2:D:527:VAL:O	2:D:531:ILE:HG23	1.84	0.78
2:B:417:TRP:CE2	2:B:568:PRO:HB2	2.17	0.78
1:E:10:ARG:HH12	1:E:449:PRO:HD3	1.48	0.78
1:C:836:GLN:NE2	1:C:836:GLN:H	1.81	0.78
2:B:552:LEU:HD12	2:B:552:LEU:N	1.97	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:527:VAL:HG13	2:D:542:ILE:HD12	1.65	0.78
1:A:654:GLN:HG2	1:A:655:TYR:CD2	2.18	0.78
1:E:46:ILE:HG22	1:E:47:SER:H	1.49	0.78
1:C:157:ILE:CD1	1:C:181:THR:HG21	2.14	0.78
2:D:458:ARG:H	2:D:460:GLN:HE21	1.28	0.77
2:F:488:ASP:OD2	2:F:492:ARG:HB2	1.84	0.77
1:E:300:LEU:HG	1:E:305:ILE:HB	1.67	0.77
1:A:647:ILE:HG13	1:A:685:ARG:HE	1.49	0.77
1:C:544:ASP:HB3	1:C:549:HIS:CD2	2.20	0.77
1:C:258:THR:HG22	1:C:260:LYS:H	1.47	0.77
2:F:417:TRP:CE2	2:F:568:PRO:HB2	2.19	0.77
2:F:513:ARG:HH11	2:F:513:ARG:HB2	1.47	0.76
1:C:265:GLU:HG3	1:C:266:GLY:N	1.96	0.76
1:C:659:ILE:O	1:C:663:VAL:HG23	1.84	0.76
1:A:16:VAL:HG13	1:A:345:PRO:CG	2.14	0.76
1:C:2:VAL:HG22	1:C:3:ALA:H	1.51	0.76
1:E:495:VAL:HG12	1:E:554:LEU:HD23	1.67	0.76
1:E:238:ALA:O	1:E:241:MET:HG2	1.86	0.75
1:C:536:LEU:HD12	1:C:537:HIS:N	2.01	0.75
1:E:694:HIS:HD2	1:E:696:ASP:N	1.83	0.75
1:E:581:ASN:HD21	1:E:704:GLN:HG3	1.52	0.75
1:A:465:LYS:HD2	1:A:517:CYS:SG	2.27	0.75
1:C:584:ASN:HD22	1:C:693:LEU:HA	1.52	0.75
1:C:552:VAL:HG22	1:C:553:PRO:HD3	1.65	0.74
1:E:334:LEU:O	1:E:338:ILE:HG12	1.86	0.74
1:C:229:TYR:CZ	1:C:276:PHE:HB3	2.22	0.74
1:E:152:LYS:HD2	1:E:200:VAL:CG2	2.17	0.74
1:E:152:LYS:HD2	1:E:200:VAL:HG23	1.69	0.74
1:E:556:ILE:CG2	1:E:557:SER:H	1.94	0.74
1:A:533:THR:N	1:A:537:HIS:HD2	1.85	0.74
1:A:454:ILE:HG13	1:A:455:GLY:H	1.53	0.74
1:C:27:HIS:HD2	1:C:29:ASP:H	1.33	0.74
1:C:251:ASN:HB2	1:C:254:THR:OG1	1.88	0.74
1:C:584:ASN:HD21	1:C:694:HIS:H	1.32	0.74
1:E:546:GLU:HG3	1:E:547:HIS:CD2	2.23	0.74
1:A:140:GLU:HG3	1:A:188:ILE:HD13	1.68	0.74
1:A:321:LYS:O	1:A:325:ARG:HG3	1.86	0.74
1:C:494:GLU:O	1:C:555:LYS:HB3	1.87	0.74
1:A:235:VAL:HG21	1:A:240:MET:HB2	1.69	0.74
1:C:810:ASP:OD1	1:C:812:THR:HG22	1.88	0.74
1:E:338:ILE:HG23	1:E:342:LEU:HD12	1.70	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:316:GLY:N	1:C:319:LEU:HB2	2.02	0.74
1:A:132:ILE:HD12	1:A:162:ARG:HD3	1.70	0.74
1:C:533:THR:H	1:C:537:HIS:CD2	2.05	0.74
1:C:611:ASP:OD2	1:C:613:LYS:HB2	1.88	0.74
2:D:427:ARG:O	2:D:431:GLU:HG3	1.86	0.74
1:A:500:ASP:CB	1:A:552:VAL:HG11	2.18	0.73
1:E:734:GLN:N	1:E:734:GLN:HE21	1.86	0.73
1:E:26:ALA:CB	1:E:128:VAL:HB	2.17	0.73
2:B:495:ASN:N	2:B:495:ASN:HD22	1.84	0.73
1:A:561:VAL:HG21	1:A:775:ASN:HA	1.68	0.73
1:A:836:GLN:HE21	1:A:836:GLN:H	1.34	0.73
2:F:487:PRO:HA	2:F:492:ARG:O	1.89	0.73
1:C:2:VAL:HG22	1:C:3:ALA:N	2.02	0.73
1:E:158:ASN:ND2	1:E:159:LYS:HG3	2.04	0.73
1:E:500:ASP:OD2	1:E:552:VAL:HG21	1.87	0.73
2:B:427:ARG:O	2:B:431:GLU:HG3	1.88	0.73
1:C:523:SER:OG	1:C:527:GLU:HB2	1.88	0.72
1:E:74:ALA:O	1:E:439:GLY:HA2	1.89	0.72
1:C:472:SER:HB3	1:C:475:ALA:HB2	1.71	0.72
1:A:584:ASN:HD21	1:A:694:HIS:H	1.37	0.72
2:B:477:LEU:HD13	2:B:551:ARG:NH1	2.03	0.72
1:C:243:ARG:NH1	1:C:257:TRP:CG	2.57	0.72
1:A:464:LEU:HD21	1:A:485:VAL:HB	1.72	0.72
1:A:581:ASN:ND2	1:A:704:GLN:HG3	2.03	0.72
1:C:140:GLU:HG3	1:C:188:ILE:CD1	2.19	0.72
1:E:379:MET:HB2	1:E:402:ALA:HB3	1.72	0.72
1:C:25:ILE:HD12	1:C:125:ALA:HB1	1.71	0.72
1:E:69:THR:OG1	1:E:389:SER:HB3	1.90	0.72
1:E:581:ASN:ND2	1:E:704:GLN:HG3	2.05	0.71
1:A:627:VAL:CG1	2:F:405:GLY:HA2	2.20	0.71
1:E:236:ASP:OD1	1:E:238:ALA:HB3	1.90	0.71
1:A:27:HIS:CD2	1:A:29:ASP:H	2.09	0.71
2:B:455:VAL:O	2:B:456:ARG:HD2	1.91	0.71
1:E:288:ILE:HG23	1:E:319:LEU:HD23	1.72	0.71
1:E:87:LYS:HA	1:E:87:LYS:CE	2.20	0.71
1:C:454:ILE:HG13	1:C:455:GLY:H	1.54	0.71
1:C:694:HIS:O	1:C:700:ARG:HD3	1.91	0.71
1:E:155:VAL:HG21	1:E:202:VAL:HG21	1.72	0.71
1:C:171:LYS:HG2	1:C:282:PHE:CD1	2.25	0.71
1:A:32:LYS:NZ	1:A:105:SER:HB2	2.06	0.71
1:C:183:GLU:O	1:C:187:VAL:HG23	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:552:VAL:CG2	1:E:553:PRO:HD3	2.19	0.70
1:C:279:ASP:HB3	1:C:280:PRO:HD3	1.71	0.70
1:E:279:ASP:HB3	1:E:280:PRO:HD3	1.73	0.70
1:E:503:LYS:HB3	1:E:551:GLY:CA	2.22	0.70
1:C:484:SER:HB3	1:C:797:VAL:CG2	2.21	0.70
1:C:158:ASN:ND2	1:C:159:LYS:HG2	2.06	0.70
2:B:455:VAL:C	2:B:456:ARG:HD2	2.12	0.70
1:E:338:ILE:O	1:E:342:LEU:HB2	1.92	0.70
2:D:556:LEU:HD22	2:D:560:LEU:HD13	1.74	0.70
1:A:607:ASN:OD1	1:A:609:ARG:HG3	1.91	0.69
1:A:25:ILE:HD12	1:A:125:ALA:HB1	1.74	0.69
1:A:410:LYS:HA	1:A:430:ALA:HA	1.73	0.69
1:E:87:LYS:HE2	1:E:87:LYS:HA	1.73	0.69
1:C:263:ASP:O	1:C:265:GLU:N	2.25	0.69
1:E:331:ALA:O	1:E:335:LEU:HG	1.92	0.69
1:C:584:ASN:ND2	1:C:694:HIS:H	1.90	0.69
1:C:694:HIS:CD2	1:C:696:ASP:H	2.08	0.69
1:E:77:LEU:HB2	1:E:100:ILE:HB	1.74	0.69
1:A:35:LEU:HD22	1:A:334:LEU:HD11	1.75	0.69
1:E:496:LYS:HD3	1:E:555:LYS:HE2	1.74	0.69
2:D:477:LEU:HB2	2:D:551:ARG:HD2	1.75	0.69
1:C:140:GLU:HG3	1:C:188:ILE:HD13	1.74	0.69
1:E:464:LEU:HD21	1:E:485:VAL:HB	1.75	0.69
1:E:109:VAL:HG21	1:E:138:GLN:HG3	1.74	0.69
1:C:166:GLU:HB3	1:C:167:LEU:HD12	1.73	0.69
1:A:565:GLU:HG2	1:A:676:ILE:HD12	1.75	0.69
1:E:607:ASN:HB3	1:E:610:ASP:OD2	1.93	0.69
1:E:737:GLU:HG3	1:E:766:PHE:CE1	2.28	0.68
1:E:141:THR:HA	1:E:144:ARG:NH2	2.08	0.68
1:A:433:ARG:HH21	1:A:444:PRO:HB3	1.58	0.68
1:E:185:VAL:O	1:E:189:VAL:HG23	1.93	0.68
1:E:465:LYS:HD2	1:E:517:CYS:SG	2.32	0.68
1:A:277:ILE:O	1:A:280:PRO:HD2	1.93	0.68
1:C:501:LEU:C	1:C:501:LEU:HD23	2.14	0.68
2:D:473:GLY:HA3	2:D:597:LEU:HD11	1.76	0.68
1:C:253:LYS:HE3	1:C:253:LYS:CA	2.20	0.68
1:C:506:GLU:HG3	1:C:510:ARG:CZ	2.23	0.68
1:C:533:THR:H	1:C:537:HIS:HD2	1.42	0.68
1:C:734:GLN:HE21	1:C:734:GLN:N	1.92	0.68
1:C:10:ARG:HD3	1:C:445:ILE:HD11	1.76	0.67
1:A:459:ILE:HG21	1:A:463:LEU:HD12	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:260:LYS:HE3	1:A:262:THR:O	1.93	0.67
1:E:836:GLN:NE2	1:E:836:GLN:H	1.91	0.67
1:A:836:GLN:NE2	1:A:836:GLN:H	1.92	0.67
1:E:578:LYS:HE2	1:E:840:ASP:OD1	1.95	0.67
2:F:552:LEU:HD12	2:F:552:LEU:N	2.09	0.67
1:A:169:VAL:HG22	1:A:173:ASP:HB2	1.76	0.67
1:E:75:ILE:HD13	1:E:439:GLY:CA	2.24	0.67
1:E:589:LYS:HE3	1:E:689:LEU:HD11	1.76	0.67
1:C:189:VAL:CG1	1:C:200:VAL:HG12	2.24	0.67
1:E:490:GLN:HB3	1:E:531:ALA:HB2	1.76	0.67
1:A:132:ILE:CD1	1:A:162:ARG:HD3	2.25	0.67
1:A:591:GLU:O	1:A:685:ARG:HB3	1.94	0.67
1:E:496:LYS:HB2	1:E:555:LYS:HZ3	1.60	0.67
1:A:588:LEU:HD12	1:A:588:LEU:C	2.15	0.67
1:C:110:ASP:OD1	1:C:781:THR:HG21	1.95	0.67
1:E:836:GLN:HE21	1:E:836:GLN:H	1.42	0.66
1:C:103:ILE:HD11	1:C:453:ILE:HG12	1.78	0.66
1:C:535:GLU:O	1:C:539:GLU:HG3	1.95	0.66
1:C:166:GLU:C	1:C:167:LEU:HD12	2.14	0.66
2:B:467:ARG:HG3	2:B:558:TRP:CD1	2.31	0.66
1:E:91:GLN:NE2	1:E:344:SER:H	1.92	0.66
1:C:45:ILE:HD11	1:C:78:TYR:CB	2.25	0.66
2:D:486:GLU:OE1	2:D:487:PRO:HD2	1.95	0.66
1:C:315:GLU:CA	1:C:319:LEU:HB2	2.25	0.66
1:A:584:ASN:ND2	1:A:694:HIS:H	1.93	0.66
1:C:192:TYR:HA	1:C:763:THR:HG21	1.78	0.66
1:C:234:GLY:O	1:C:235:VAL:HG23	1.95	0.66
1:C:256:LYS:HA	1:C:256:LYS:CE	2.25	0.66
1:C:565:GLU:O	1:C:681:MET:HA	1.95	0.66
1:E:226:ALA:O	1:E:230:ALA:HB2	1.96	0.66
1:E:321:LYS:O	1:E:325:ARG:HG3	1.95	0.66
1:C:109:VAL:HG13	1:C:793:PHE:HE1	1.59	0.66
1:E:565:GLU:O	1:E:681:MET:HA	1.96	0.66
1:C:320:LEU:HD12	1:C:324:MET:HG3	1.77	0.66
1:E:142:VAL:O	1:E:145:GLN:HB2	1.96	0.66
1:A:288:ILE:HG23	1:A:319:LEU:HD23	1.77	0.66
1:E:584:ASN:ND2	1:E:694:HIS:H	1.93	0.66
2:B:417:TRP:NE1	2:B:568:PRO:HB2	2.10	0.66
1:A:392:GLY:HA2	1:A:513:LYS:HE2	1.76	0.66
1:C:288:ILE:HG23	1:C:319:LEU:HD23	1.77	0.65
1:A:644:ASN:HD22	1:A:684:VAL:HB	1.62	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:87:LYS:HE2	1:E:87:LYS:CA	2.26	0.65
2:F:465:ILE:HD12	2:F:535:LEU:HD12	1.77	0.65
1:E:654:GLN:HG2	1:E:655:TYR:CD2	2.31	0.65
1:A:581:ASN:ND2	1:A:699:DDE:O	2.28	0.65
1:C:162:ARG:HD2	1:C:166:GLU:OE2	1.97	0.65
1:C:703:GLY:HA2	2:D:493:ILE:HD13	1.78	0.65
1:E:536:LEU:HD11	1:E:540:ILE:HD11	1.77	0.65
1:E:45:ILE:HD11	1:E:78:TYR:HB3	1.78	0.65
1:E:279:ASP:O	1:E:283:ARG:HG2	1.97	0.65
1:C:284:LEU:O	1:C:288:ILE:HB	1.97	0.65
1:A:258:THR:HG22	1:A:259:ASN:N	2.12	0.65
2:B:537:LEU:O	2:B:538:ARG:HD3	1.96	0.65
2:B:490:ARG:N	2:B:490:ARG:HD2	2.12	0.65
1:E:292:LYS:HD3	1:E:295:GLU:OE2	1.96	0.64
1:C:243:ARG:NH1	1:C:257:TRP:CD1	2.65	0.64
1:A:220:PHE:HB3	1:A:328:LEU:HD13	1.78	0.64
1:E:211:PHE:HD2	1:E:220:PHE:CE1	2.15	0.64
1:A:373:ASP:OD2	1:A:376:ALA:HB2	1.98	0.64
1:C:685:ARG:HE	1:C:687:ASN:HD21	1.46	0.64
1:E:757:GLU:HG3	1:E:768:VAL:HG22	1.78	0.64
1:A:7:ASP:HA	1:A:10:ARG:HG2	1.79	0.64
1:E:391:LYS:HB3	1:E:393:ARG:HG2	1.80	0.64
1:A:103:ILE:HD11	1:A:453:ILE:HG12	1.80	0.64
2:B:473:GLY:HA3	2:B:597:LEU:HD11	1.78	0.64
1:C:588:LEU:C	1:C:588:LEU:HD12	2.18	0.64
1:C:545:LEU:O	1:C:550:ALA:CB	2.45	0.64
1:C:166:GLU:HB3	1:C:167:LEU:CD1	2.28	0.64
1:C:581:ASN:O	1:C:582:LYS:HB2	1.98	0.64
1:E:736:PRO:HB2	1:E:738:GLN:HG2	1.78	0.64
1:C:509:LYS:HD2	1:C:509:LYS:N	2.11	0.64
1:C:285:PHE:HE2	1:C:324:MET:SD	2.21	0.64
1:C:491:VAL:O	1:C:529:ILE:HA	1.97	0.64
1:C:492:ALA:HA	1:C:528:HIS:O	1.97	0.64
1:E:584:ASN:HD21	1:E:694:HIS:H	1.45	0.63
1:E:281:ILE:HG12	1:E:327:PHE:HE2	1.63	0.63
1:C:316:GLY:N	1:C:319:LEU:CB	2.61	0.63
1:C:157:ILE:HD12	1:C:181:THR:HG21	1.79	0.63
1:A:348:ALA:HA	1:A:351:TYR:CE2	2.33	0.63
1:C:757:GLU:HG3	1:C:768:VAL:HG22	1.79	0.63
1:C:192:TYR:HA	1:C:763:THR:CG2	2.29	0.63
1:A:580:PRO:O	1:A:582:LYS:HG2	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:410:LYS:HA	1:C:430:ALA:HA	1.81	0.63
1:C:239:LYS:O	1:C:243:ARG:HG3	1.99	0.63
1:A:454:ILE:HG13	1:A:455:GLY:N	2.11	0.63
1:C:38:SER:HA	1:C:41:GLN:HG2	1.80	0.63
1:A:222:ILE:HG22	1:A:241:MET:HB2	1.80	0.63
1:A:589:LYS:HE3	1:A:689:LEU:HD11	1.80	0.63
1:E:166:GLU:HB3	1:E:167:LEU:HD12	1.81	0.63
1:E:186:ASN:CG	1:E:201:GLN:HE21	2.03	0.62
1:C:220:PHE:HA	1:C:224:GLN:OE1	1.98	0.62
1:A:719:LEU:HD21	1:A:835:TRP:CD2	2.35	0.62
1:E:495:VAL:CG1	1:E:554:LEU:HD23	2.28	0.62
1:E:75:ILE:HD13	1:E:439:GLY:HA3	1.81	0.62
1:A:251:ASN:HB3	1:A:254:THR:OG1	1.99	0.62
2:B:524:ALA:O	2:B:528:GLU:HG3	1.99	0.62
1:E:704:GLN:O	1:E:707:PRO:HD2	1.99	0.62
1:C:256:LYS:HD3	1:C:257:TRP:N	2.11	0.62
1:A:568:GLU:HB3	1:A:721:ASP:OD2	1.99	0.62
1:C:157:ILE:HD11	1:C:181:THR:HG21	1.82	0.62
1:E:588:LEU:HD12	1:E:588:LEU:C	2.19	0.62
1:C:231:LYS:HE3	1:C:232:LYS:CG	2.23	0.62
1:C:277:ILE:O	1:C:280:PRO:HD2	1.99	0.62
1:E:307:LEU:HD13	1:E:312:LYS:HA	1.82	0.62
1:C:784:LEU:HD23	1:C:794:PRO:CG	2.26	0.62
2:B:551:ARG:HH11	2:B:551:ARG:HG3	1.65	0.62
1:E:635:CYS:SG	1:E:664:VAL:HG13	2.40	0.62
1:A:694:HIS:CD2	1:A:696:ASP:H	2.09	0.62
1:C:522:MET:HA	1:C:527:GLU:O	2.00	0.62
1:A:581:ASN:HD21	1:A:704:GLN:HG3	1.64	0.62
2:F:524:ALA:O	2:F:528:GLU:HG3	1.98	0.62
1:E:311:GLU:HB3	1:E:322:VAL:HG11	1.82	0.62
1:A:647:ILE:HG13	1:A:685:ARG:NE	2.13	0.61
1:A:183:GLU:O	1:A:187:VAL:HG23	1.99	0.61
2:B:440:HIS:HB2	2:B:471:ILE:HG22	1.82	0.61
2:B:495:ASN:ND2	2:B:495:ASN:H	1.97	0.61
1:A:32:LYS:HZ1	1:A:105:SER:HB2	1.63	0.61
1:A:2:VAL:HG22	1:A:3:ALA:N	2.14	0.61
1:E:285:PHE:CE2	1:E:320:LEU:HD11	2.35	0.61
1:A:321:LYS:NZ	1:A:325:ARG:HD3	2.15	0.61
1:A:591:GLU:HG2	1:A:685:ARG:HG2	1.81	0.61
1:E:496:LYS:HD3	1:E:555:LYS:CE	2.30	0.61
1:C:4:PHE:HD1	1:C:8:GLN:OE1	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:354:GLU:OE2	1:C:361:ALA:HB1	2.00	0.61
1:E:472:SER:HB3	1:E:475:ALA:HB2	1.80	0.61
1:C:348:ALA:HA	1:C:351:TYR:CE2	2.35	0.61
1:E:91:GLN:HE22	1:E:344:SER:N	1.94	0.61
1:E:203:TYR:HD2	1:E:206:ARG:HD2	1.64	0.61
1:E:89:ILE:C	1:E:91:GLN:H	2.03	0.61
1:C:316:GLY:H	1:C:319:LEU:HB2	1.64	0.61
1:A:391:LYS:HG3	1:A:392:GLY:H	1.65	0.61
1:E:132:ILE:N	1:E:132:ILE:HD12	2.15	0.61
1:C:288:ILE:HG23	1:C:319:LEU:CD2	2.31	0.61
1:E:759:GLN:HB2	1:E:766:PHE:CE2	2.35	0.61
1:C:72:SER:HA	1:C:439:GLY:O	2.00	0.61
1:A:30:HIS:HA	1:A:159:LYS:CE	2.31	0.61
1:E:591:GLU:O	1:E:685:ARG:HB3	2.01	0.61
1:A:186:ASN:HB3	1:A:201:GLN:HG2	1.81	0.61
1:E:78:TYR:HE1	1:E:97:SER:HB3	1.65	0.61
2:D:417:TRP:NE1	2:D:568:PRO:HB2	2.15	0.61
1:A:594:ASP:HB2	1:A:597:VAL:HG23	1.83	0.61
1:E:552:VAL:HG22	1:E:553:PRO:HD2	1.82	0.60
1:A:411:VAL:HG12	1:A:412:ARG:N	2.15	0.60
1:C:5:THR:OG1	1:C:8:GLN:HG3	2.00	0.60
2:B:457:ALA:HB2	2:B:558:TRP:CD2	2.36	0.60
1:E:412:ARG:HH12	1:E:428:ILE:HD11	1.66	0.60
1:C:707:PRO:O	1:C:711:ARG:HG3	2.00	0.60
1:E:211:PHE:CD2	1:E:220:PHE:CE1	2.89	0.60
1:E:536:LEU:O	1:E:539:GLU:N	2.34	0.60
1:A:823:ARG:NH1	1:A:829:LYS:O	2.34	0.60
1:A:501:LEU:HB3	1:A:502:PRO:HD3	1.84	0.60
1:A:485:VAL:O	1:A:487:PRO:HD3	2.01	0.60
1:E:69:THR:O	1:E:389:SER:N	2.34	0.60
1:C:221:THR:OG1	1:C:224:GLN:HG3	2.01	0.60
1:E:728:VAL:HB	1:E:800:HIS:CD2	2.36	0.60
1:E:381:TYR:O	1:E:398:GLY:HA3	2.01	0.60
1:E:43:ALA:HB1	1:E:78:TYR:O	2.02	0.60
1:C:591:GLU:CG	1:C:685:ARG:HG2	2.32	0.60
1:A:186:ASN:HB3	1:A:201:GLN:HE21	1.67	0.60
1:E:126:LEU:HD11	1:E:156:VAL:CG2	2.32	0.60
1:E:221:THR:OG1	1:E:224:GLN:HG3	2.02	0.60
1:C:3:ALA:HA	1:C:46:ILE:O	2.02	0.60
1:C:171:LYS:HG2	1:C:282:PHE:CE1	2.37	0.60
1:A:459:ILE:HD11	1:A:469:LEU:HD21	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172:GLU:OE2	1:A:271:ARG:NH2	2.35	0.60
1:C:384:LYS:HB2	1:C:465:LYS:NZ	2.16	0.60
1:C:500:ASP:OD2	1:C:552:VAL:HG21	2.02	0.59
2:D:551:ARG:HG3	2:D:551:ARG:HH11	1.67	0.59
2:D:477:LEU:HD13	2:D:551:ARG:NH1	2.17	0.59
1:A:690:ASP:OD1	1:A:691:VAL:N	2.30	0.59
1:C:581:ASN:HB3	1:C:583:HIS:HB2	1.84	0.59
1:C:581:ASN:ND2	1:C:699:DDE:O	2.35	0.59
1:A:544:ASP:O	1:A:549:HIS:HD2	1.85	0.59
1:E:730:LEU:HB2	1:E:799:ASP:HB2	1.84	0.59
1:E:212:GLY:HA3	1:E:219:ALA:HA	1.84	0.59
1:A:258:THR:HG22	1:A:259:ASN:H	1.67	0.59
1:E:303:LEU:O	1:E:304:GLU:HB2	2.03	0.59
1:E:71:LYS:O	1:E:386:VAL:HG21	2.03	0.59
1:A:321:LYS:HZ2	1:A:325:ARG:HD3	1.67	0.59
1:E:176:GLN:O	1:E:180:ARG:HG3	2.02	0.59
2:D:455:VAL:O	2:D:456:ARG:HG3	2.03	0.59
1:C:404:THR:HG22	1:C:449:PRO:CA	2.27	0.59
1:C:784:LEU:CD2	1:C:794:PRO:HG3	2.26	0.59
1:C:316:GLY:H	1:C:319:LEU:CB	2.15	0.59
1:C:685:ARG:NE	1:C:687:ASN:HD21	1.99	0.59
1:A:591:GLU:CG	1:A:685:ARG:HG2	2.32	0.59
1:A:545:LEU:HD12	1:A:549:HIS:HB2	1.84	0.59
1:E:690:ASP:OD1	1:E:691:VAL:N	2.35	0.59
1:E:10:ARG:NH1	1:E:449:PRO:HD3	2.16	0.59
1:E:581:ASN:O	1:E:582:LYS:HB2	2.01	0.59
1:C:644:ASN:ND2	1:C:684:VAL:H	2.00	0.59
1:A:258:THR:HG22	1:A:260:LYS:H	1.67	0.59
1:A:381:TYR:O	1:A:398:GLY:HA3	2.02	0.59
1:C:497:ASN:N	1:C:497:ASN:ND2	2.50	0.59
2:B:551:ARG:NH1	2:B:551:ARG:HG3	2.17	0.59
1:C:35:LEU:HD22	1:C:334:LEU:HD11	1.84	0.59
1:E:410:LYS:HA	1:E:430:ALA:HA	1.84	0.59
1:E:255:LYS:O	1:E:256:LYS:HG2	2.03	0.59
1:A:30:HIS:HA	1:A:159:LYS:HE3	1.84	0.58
1:C:454:ILE:HG13	1:C:455:GLY:N	2.18	0.58
1:E:183:GLU:OE1	1:E:186:ASN:ND2	2.36	0.58
1:C:10:ARG:NH2	1:C:449:PRO:HD3	2.18	0.58
1:E:219:ALA:HB3	1:E:330:ALA:HA	1.85	0.58
2:B:420:GLU:N	2:B:420:GLU:OE1	2.35	0.58
1:A:406:LYS:O	1:A:409:GLN:HB3	2.01	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:258:THR:HG22	1:E:259:ASN:H	1.68	0.58
1:C:226:ALA:O	1:C:230:ALA:HB2	2.04	0.58
1:C:614:ALA:O	1:C:618:ILE:HG12	2.03	0.58
1:C:314:LEU:HD21	1:C:318:ALA:O	2.03	0.58
1:C:258:THR:HG22	1:C:259:ASN:N	2.18	0.58
1:C:654:GLN:HG2	1:C:655:TYR:CD2	2.38	0.58
1:A:758:GLU:O	1:A:766:PHE:HD1	1.86	0.58
1:A:520:THR:HA	1:A:529:ILE:O	2.03	0.58
2:B:477:LEU:HD22	2:B:551:ARG:HB2	1.86	0.58
1:C:515:ASP:HB3	1:C:518:VAL:HG12	1.86	0.58
1:A:763:THR:HB	1:A:764:PRO:HD2	1.84	0.58
1:C:9:MET:O	1:C:13:MET:HG3	2.04	0.58
1:C:236:ASP:OD2	1:C:239:LYS:HE2	2.04	0.57
1:E:391:LYS:HG3	1:E:392:GLY:H	1.69	0.57
1:C:529:ILE:N	1:C:529:ILE:HD12	2.19	0.57
1:A:561:VAL:HG21	1:A:775:ASN:CA	2.34	0.57
2:F:520:ALA:HB1	2:F:522:GLU:OE2	2.05	0.57
1:E:145:GLN:NE2	1:E:793:PHE:CZ	2.72	0.57
1:E:685:ARG:HE	1:E:687:ASN:HD21	1.53	0.57
1:E:126:LEU:HD11	1:E:156:VAL:HG21	1.86	0.57
1:E:412:ARG:HG2	1:E:412:ARG:HH11	1.69	0.57
2:F:433:GLY:O	2:F:505:ARG:HB2	2.04	0.57
1:C:414:GLN:HB3	1:C:418:TYR:CD2	2.39	0.57
1:A:132:ILE:HD12	1:A:162:ARG:HD2	1.84	0.57
1:A:7:ASP:O	1:A:10:ARG:HG2	2.05	0.57
1:E:561:VAL:HG21	1:E:775:ASN:CB	2.34	0.57
1:A:493:VAL:HG12	1:A:554:LEU:HD22	1.86	0.57
2:D:445:GLU:OE1	2:D:494:ARG:NH2	2.38	0.57
1:E:556:ILE:HD12	1:E:556:ILE:N	2.20	0.57
1:E:736:PRO:HB2	1:E:738:GLN:CG	2.35	0.57
1:E:284:LEU:HD13	1:E:324:MET:HE3	1.87	0.57
1:C:644:ASN:HD22	1:C:684:VAL:H	1.53	0.57
1:E:365:ASN:O	1:E:369:ILE:HG12	2.05	0.57
1:A:784:LEU:HD23	1:A:794:PRO:HG3	1.86	0.57
1:C:251:ASN:OD1	1:C:269:LEU:HD11	2.05	0.57
1:C:509:LYS:O	1:C:513:LYS:HE3	2.05	0.57
1:E:591:GLU:CG	1:E:685:ARG:HG2	2.35	0.57
1:C:231:LYS:HG2	1:C:232:LYS:N	2.19	0.56
1:C:546:GLU:HG3	1:C:553:PRO:HA	1.87	0.56
1:E:258:THR:HG22	1:E:259:ASN:N	2.20	0.56
1:C:627:VAL:HG21	1:C:631:ARG:NH2	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:521:TYR:CE1	1:A:529:ILE:HD12	2.40	0.56
1:C:732:GLU:OE1	1:C:769:LYS:HE3	2.04	0.56
1:E:71:LYS:HB3	1:E:386:VAL:CG2	2.33	0.56
1:C:493:VAL:HG21	1:C:545:LEU:HD21	1.86	0.56
1:C:220:PHE:HB3	1:C:328:LEU:HD13	1.87	0.56
1:C:497:ASN:N	1:C:497:ASN:HD22	2.04	0.56
1:C:594:ASP:HB2	1:C:597:VAL:HG23	1.87	0.56
2:D:438:GLY:HA3	2:D:471:ILE:HD12	1.86	0.56
1:E:749:LYS:O	1:E:750:LYS:HD2	2.05	0.56
1:C:251:ASN:H	1:C:251:ASN:HD22	1.54	0.56
1:C:550:ALA:O	1:C:552:VAL:N	2.38	0.56
1:A:647:ILE:HB	1:A:687:ASN:HD22	1.70	0.56
1:C:494:GLU:OE1	1:C:494:GLU:HA	2.04	0.56
1:A:156:VAL:HG21	1:A:334:LEU:CD2	2.35	0.56
1:A:156:VAL:HG21	1:A:334:LEU:HD22	1.88	0.56
1:C:155:VAL:HG12	1:C:156:VAL:N	2.19	0.56
1:E:722:PRO:O	1:E:723:LYS:HD2	2.04	0.56
1:C:730:LEU:HB2	1:C:799:ASP:HB2	1.86	0.56
2:B:484:ASP:OD2	2:B:494:ARG:HG2	2.05	0.56
1:A:162:ARG:O	1:A:166:GLU:HB2	2.06	0.56
1:A:550:ALA:O	1:A:552:VAL:HG23	2.05	0.56
2:F:488:ASP:OD2	2:F:492:ARG:HD3	2.05	0.56
1:E:37:ASP:O	1:E:41:GLN:HG3	2.05	0.56
1:A:111:PHE:HB3	1:A:114:GLU:HG2	1.87	0.56
2:D:432:ARG:HA	2:D:432:ARG:CZ	2.35	0.56
1:E:225:PHE:CD2	1:E:277:ILE:HD12	2.41	0.56
1:A:734:GLN:HE21	1:A:734:GLN:N	2.04	0.56
1:E:158:ASN:HD22	1:E:159:LYS:HG3	1.70	0.56
2:F:473:GLY:HA3	2:F:597:LEU:HD11	1.88	0.56
1:E:240:MET:O	1:E:244:LEU:HG	2.05	0.56
1:C:484:SER:HB3	1:C:797:VAL:HG22	1.88	0.56
1:C:240:MET:O	1:C:244:LEU:HG	2.05	0.56
2:B:405:GLY:HA2	1:C:627:VAL:HG12	1.88	0.56
1:C:42:ARG:HG3	1:C:331:ALA:HB3	1.85	0.56
1:C:538:LEU:O	1:C:542:LEU:HG	2.06	0.55
1:A:220:PHE:HA	1:A:224:GLN:OE1	2.04	0.55
1:E:432:GLN:HB2	1:E:457:VAL:O	2.06	0.55
1:E:707:PRO:O	1:E:711:ARG:HG3	2.06	0.55
1:E:114:GLU:O	1:E:117:ALA:HB3	2.06	0.55
1:A:486:SER:O	1:A:488:VAL:HG13	2.05	0.55
2:B:495:ASN:N	2:B:495:ASN:ND2	2.47	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172:GLU:HA	1:A:274:ASN:HD21	1.70	0.55
1:E:150:ARG:CZ	1:E:355:GLN:OE1	2.55	0.55
1:E:26:ALA:O	1:E:32:LYS:HD2	2.06	0.55
1:C:27:HIS:CD2	1:C:29:ASP:H	2.20	0.55
1:C:607:ASN:HB3	1:C:610:ASP:CG	2.26	0.55
1:A:140:GLU:HG3	1:A:188:ILE:HD11	1.85	0.55
2:B:495:ASN:HD22	2:B:495:ASN:H	1.53	0.55
1:C:155:VAL:HG21	1:C:185:VAL:HG11	1.88	0.55
1:C:675:PRO:HD3	1:C:714:TYR:CE1	2.41	0.55
1:A:229:TYR:HE2	1:A:276:PHE:HB3	1.68	0.55
1:A:3:ALA:HA	1:A:46:ILE:O	2.07	0.55
1:A:4:PHE:HA	1:A:8:GLN:OE1	2.07	0.55
1:C:585:ARG:HD2	1:C:692:THR:OG1	2.07	0.55
1:A:820:LEU:CD1	1:A:830:GLU:HG2	2.34	0.55
1:E:496:LYS:HD3	1:E:555:LYS:NZ	2.20	0.55
2:F:500:ARG:O	2:F:566:VAL:HG13	2.06	0.55
1:C:89:ILE:HG22	1:C:91:GLN:HG2	1.89	0.55
2:B:518:LEU:H	2:B:518:LEU:HD22	1.72	0.55
1:C:563:TYR:O	1:C:564:ARG:HD2	2.07	0.55
2:D:546:GLU:HG3	2:D:547:GLU:CG	2.33	0.55
2:D:527:VAL:HG22	2:D:542:ILE:CD1	2.37	0.55
1:A:166:GLU:HB3	1:A:167:LEU:HD12	1.88	0.55
1:C:200:VAL:O	1:C:200:VAL:CG1	2.55	0.55
1:E:454:ILE:HG13	1:E:455:GLY:N	2.22	0.55
1:E:9:MET:O	1:E:12:LEU:HB3	2.07	0.55
1:A:306:VAL:O	1:A:306:VAL:HG23	2.07	0.55
1:A:737:GLU:HG3	1:A:766:PHE:CD2	2.41	0.55
1:E:225:PHE:CG	1:E:277:ILE:HD12	2.42	0.55
1:E:179:ALA:O	1:E:183:GLU:HB2	2.07	0.55
1:E:429:LYS:HG3	1:E:462:PHE:CZ	2.41	0.55
2:F:420:GLU:H	2:F:420:GLU:CD	2.10	0.55
1:C:25:ILE:CD1	1:C:125:ALA:HB1	2.37	0.54
1:E:167:LEU:H	1:E:167:LEU:HD12	1.71	0.54
2:F:467:ARG:HG3	2:F:558:TRP:CD1	2.43	0.54
1:C:406:LYS:HB3	1:C:447:ASP:HB3	1.88	0.54
1:C:288:ILE:HG23	1:C:319:LEU:HG	1.90	0.54
2:B:552:LEU:CD1	2:B:552:LEU:H	2.18	0.54
1:C:157:ILE:HD11	1:C:181:THR:CG2	2.37	0.54
1:A:155:VAL:HG12	1:A:156:VAL:N	2.21	0.54
2:B:488:ASP:OD1	2:B:489:ALA:N	2.40	0.54
1:A:223:ARG:HH11	1:A:223:ARG:HG2	1.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:690:ASP:O	1:A:691:VAL:HG23	2.08	0.54
1:C:314:LEU:HG	1:C:319:LEU:HA	1.89	0.54
2:D:458:ARG:H	2:D:460:GLN:NE2	2.04	0.54
1:E:669:TRP:CZ2	2:F:492:ARG:HG2	2.42	0.54
1:E:348:ALA:O	1:E:352:ARG:HB2	2.06	0.54
1:E:80:GLU:HA	1:E:96:ASN:O	2.06	0.54
2:D:529:ARG:NH1	2:D:604:PRO:HG2	2.21	0.54
1:C:288:ILE:HG23	1:C:319:LEU:CG	2.37	0.54
1:E:251:ASN:HB3	1:E:254:THR:OG1	2.07	0.54
1:C:77:LEU:HB2	1:C:100:ILE:HB	1.88	0.54
1:E:68:ILE:HG23	1:E:390:ASP:HB2	1.90	0.54
1:A:737:GLU:CG	1:A:766:PHE:HE2	2.19	0.54
1:E:411:VAL:HG11	1:E:469:LEU:HB3	1.89	0.54
1:C:490:GLN:O	1:C:491:VAL:HG13	2.07	0.54
1:C:584:ASN:ND2	1:C:693:LEU:HA	2.20	0.54
1:C:126:LEU:HD11	1:C:156:VAL:CG2	2.37	0.54
1:C:543:GLN:O	1:C:546:GLU:N	2.41	0.54
1:C:348:ALA:O	1:C:352:ARG:HB2	2.08	0.54
1:E:278:LEU:O	1:E:282:PHE:HB2	2.08	0.54
1:A:388:THR:HG21	1:A:395:TYR:CD1	2.43	0.54
1:C:365:ASN:O	1:C:369:ILE:HG12	2.08	0.54
1:C:316:GLY:O	1:C:319:LEU:HB3	2.07	0.54
2:B:477:LEU:HD11	2:B:546:GLU:OE1	2.08	0.54
1:E:109:VAL:CG2	1:E:138:GLN:HG3	2.38	0.54
2:F:505:ARG:NH1	2:F:505:ARG:HG3	2.23	0.54
1:A:466:THR:HG22	1:A:467:GLY:N	2.23	0.54
1:C:10:ARG:CZ	1:C:449:PRO:HD3	2.38	0.54
1:A:501:LEU:HD23	1:A:501:LEU:C	2.29	0.54
1:A:285:PHE:CE2	1:A:320:LEU:HD11	2.43	0.54
2:D:447:ALA:HA	2:D:499:LEU:HD21	1.89	0.54
1:A:459:ILE:CD1	1:A:469:LEU:HD21	2.37	0.53
1:C:200:VAL:O	1:C:200:VAL:HG13	2.08	0.53
1:E:150:ARG:NH1	1:E:355:GLN:HB2	2.23	0.53
1:A:669:TRP:CZ2	2:B:492:ARG:HB3	2.43	0.53
1:A:710:ARG:HG3	1:A:710:ARG:HH11	1.72	0.53
1:C:750:LYS:O	1:C:751:ARG:HB2	2.08	0.53
1:C:836:GLN:N	1:C:836:GLN:HE21	1.98	0.53
1:C:45:ILE:HD11	1:C:78:TYR:N	2.24	0.53
1:E:739:ALA:HB2	1:E:791:GLN:OE1	2.07	0.53
2:F:529:ARG:NH1	2:F:604:PRO:HG2	2.24	0.53
2:F:530:LEU:HA	2:F:604:PRO:HG3	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:311:GLU:OE2	1:C:322:VAL:HG11	2.09	0.53
2:B:505:ARG:NH1	2:B:505:ARG:HG3	2.22	0.53
1:E:75:ILE:HD13	1:E:439:GLY:HA2	1.89	0.53
1:A:447:ASP:CG	1:A:448:CYS:N	2.61	0.53
1:C:109:VAL:HG13	1:C:793:PHE:CE1	2.42	0.53
2:B:445:GLU:OE1	2:B:494:ARG:NH2	2.37	0.53
1:A:117:ALA:HA	1:A:481:MET:SD	2.48	0.53
1:A:89:ILE:HG22	1:A:91:GLN:HG2	1.91	0.53
1:C:569:SER:O	1:C:720:ALA:HB1	2.08	0.53
1:A:235:VAL:CG2	1:A:240:MET:HB2	2.39	0.53
1:C:466:THR:HG22	1:C:467:GLY:N	2.24	0.53
2:F:440:HIS:HB2	2:F:471:ILE:HG22	1.90	0.53
1:E:576:LEU:HD13	1:E:587:TYR:CE1	2.44	0.53
1:A:189:VAL:CG1	1:A:200:VAL:HG12	2.39	0.53
1:A:25:ILE:CD1	1:A:125:ALA:HB1	2.38	0.53
1:E:478:MET:O	1:E:479:LYS:C	2.47	0.53
1:C:132:ILE:HG23	1:C:133:GLU:N	2.24	0.53
2:D:551:ARG:HG3	2:D:551:ARG:NH1	2.23	0.53
1:C:509:LYS:O	1:C:513:LYS:HG3	2.09	0.53
1:C:116:THR:HB	1:C:481:MET:HE3	1.90	0.53
1:C:782:GLY:O	1:C:785:ARG:HB3	2.09	0.53
1:A:472:SER:HB3	1:A:475:ALA:HB2	1.91	0.53
2:D:457:ALA:HB2	2:D:558:TRP:CD2	2.44	0.53
1:E:70:ILE:HG22	1:E:388:THR:HG22	1.89	0.53
2:F:488:ASP:CG	2:F:492:ARG:HB2	2.28	0.53
1:C:45:ILE:HG12	1:C:76:SER:O	2.09	0.53
1:A:348:ALA:HA	1:A:351:TYR:CZ	2.44	0.53
2:F:522:GLU:CD	2:F:522:GLU:H	2.12	0.53
1:E:152:LYS:CD	1:E:200:VAL:HG23	2.38	0.53
1:E:307:LEU:HD12	1:E:312:LYS:HD3	1.91	0.53
1:A:200:VAL:O	1:A:200:VAL:HG13	2.07	0.53
1:C:132:ILE:HG23	1:C:133:GLU:HG3	1.91	0.53
1:C:129:VAL:HG13	1:C:134:GLY:O	2.09	0.52
1:E:644:ASN:HD22	1:E:684:VAL:HB	1.74	0.52
1:C:429:LYS:HG3	1:C:462:PHE:CZ	2.43	0.52
1:C:291:PHE:HE1	1:C:315:GLU:HB2	1.74	0.52
1:E:508:LEU:HD22	1:E:520:THR:HB	1.91	0.52
1:C:391:LYS:HD3	1:C:393:ARG:HG3	1.91	0.52
1:A:70:ILE:HG22	1:A:388:THR:HG22	1.90	0.52
1:A:71:LYS:HB3	1:A:386:VAL:CG2	2.38	0.52
1:C:647:ILE:HB	1:C:687:ASN:HD22	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:647:ILE:HG13	1:C:685:ARG:HE	1.73	0.52
1:C:544:ASP:O	1:C:549:HIS:HB2	2.10	0.52
1:A:797:VAL:HG22	1:A:798:PHE:N	2.24	0.52
1:E:17:THR:HB	1:E:92:LYS:O	2.09	0.52
2:F:505:ARG:HH11	2:F:505:ARG:HG3	1.75	0.52
1:E:646:VAL:HG13	1:E:688:ILE:CD1	2.40	0.52
2:D:508:LEU:N	2:D:509:PRO:CD	2.73	0.52
1:C:436:LEU:HD23	1:C:454:ILE:CD1	2.40	0.52
1:E:171:LYS:NZ	1:E:283:ARG:NH2	2.57	0.52
1:A:186:ASN:CB	1:A:201:GLN:HG2	2.40	0.52
1:C:155:VAL:CG1	1:C:156:VAL:N	2.72	0.52
1:A:72:SER:HA	1:A:439:GLY:O	2.10	0.52
1:C:26:ALA:HB2	1:C:128:VAL:HB	1.91	0.52
1:E:694:HIS:CE1	1:E:699:DDE:HD2	2.45	0.52
1:C:258:THR:HG22	1:C:259:ASN:H	1.74	0.52
1:C:126:LEU:HD11	1:C:156:VAL:HG21	1.92	0.52
2:B:530:LEU:HD23	2:B:604:PRO:HD3	1.92	0.52
1:C:742:GLY:O	1:C:745:SER:HB3	2.10	0.52
1:C:743:ILE:HD13	1:C:784:LEU:HD11	1.91	0.52
1:C:384:LYS:HB2	1:C:465:LYS:HE3	1.92	0.52
2:B:429:LEU:HD21	2:B:565:VAL:HG11	1.91	0.52
1:E:493:VAL:HG12	1:E:494:GLU:N	2.25	0.52
1:A:478:MET:O	1:A:479:LYS:C	2.48	0.52
1:E:103:ILE:HD12	1:E:103:ILE:N	2.23	0.52
1:A:172:GLU:CD	1:A:271:ARG:HH21	2.13	0.51
1:A:335:LEU:O	1:A:339:VAL:HG23	2.10	0.51
1:A:673:GLU:HG2	1:A:678:GLY:O	2.10	0.51
1:A:759:GLN:HB2	1:A:766:PHE:CE1	2.45	0.51
1:A:581:ASN:N	1:A:704:GLN:OE1	2.35	0.51
1:A:155:VAL:HG21	1:A:185:VAL:HG11	1.92	0.51
1:C:384:LYS:CB	1:C:465:LYS:HE3	2.40	0.51
1:E:9:MET:HE2	1:E:436:LEU:HD13	1.91	0.51
1:E:13:MET:SD	1:E:436:LEU:HD21	2.50	0.51
1:E:155:VAL:CG2	1:E:202:VAL:HG21	2.38	0.51
1:C:524:GLU:C	1:C:526:GLY:H	2.14	0.51
1:A:493:VAL:CG1	1:A:554:LEU:HD22	2.40	0.51
2:F:426:HIS:NE2	2:F:594:ILE:HB	2.25	0.51
1:C:529:ILE:HG22	1:C:530:VAL:N	2.25	0.51
1:A:707:PRO:O	1:A:711:ARG:HG3	2.10	0.51
1:A:273:PHE:CD1	1:A:277:ILE:HD12	2.45	0.51
1:E:750:LYS:O	1:E:751:ARG:HB2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:571:SER:HB2	1:C:589:LYS:HG2	1.91	0.51
1:A:809:LEU:O	1:A:811:PRO:HD3	2.11	0.51
2:B:575:PRO:HG2	2:B:576:ARG:NH1	2.26	0.51
1:E:229:TYR:CE2	1:E:276:PHE:HB3	2.45	0.51
1:E:387:PRO:HG3	1:E:394:PHE:CE1	2.45	0.51
1:E:500:ASP:O	1:E:503:LYS:HB2	2.10	0.51
1:E:395:TYR:CE1	1:E:457:VAL:HG13	2.45	0.51
1:C:335:LEU:O	1:C:339:VAL:HG23	2.10	0.51
1:E:186:ASN:OD1	1:E:186:ASN:C	2.49	0.51
1:A:279:ASP:HB3	1:A:280:PRO:HD3	1.91	0.51
1:C:226:ALA:CB	1:C:241:MET:HB3	2.41	0.51
1:C:544:ASP:O	1:C:549:HIS:N	2.44	0.51
2:B:460:GLN:HB3	2:B:467:ARG:HD3	1.92	0.51
1:A:155:VAL:CG1	1:A:156:VAL:N	2.74	0.51
2:F:442:THR:OG1	2:F:443:PHE:N	2.42	0.51
1:C:265:GLU:CG	1:C:266:GLY:H	2.14	0.51
2:B:457:ALA:O	2:B:458:ARG:HG3	2.10	0.51
1:A:7:ASP:CA	1:A:10:ARG:HG2	2.40	0.51
1:C:91:GLN:O	1:C:93:THR:HG23	2.10	0.51
1:E:627:VAL:O	1:E:631:ARG:HG3	2.11	0.51
2:F:407:VAL:HG22	2:F:416:ASN:O	2.11	0.51
1:A:9:MET:O	1:A:13:MET:HG3	2.11	0.51
1:E:307:LEU:HB2	1:E:312:LYS:HE2	1.93	0.51
1:A:223:ARG:NH1	1:A:223:ARG:HG2	2.26	0.51
1:A:68:ILE:HG23	1:A:390:ASP:HB2	1.93	0.51
1:A:644:ASN:ND2	1:A:684:VAL:H	2.09	0.51
1:A:110:ASP:C	1:A:112:SER:H	2.14	0.51
2:D:548:GLU:O	2:D:548:GLU:HG3	2.11	0.51
1:E:10:ARG:HD3	1:E:445:ILE:HD11	1.92	0.50
1:C:262:THR:HA	1:C:269:LEU:HG	1.93	0.50
1:C:578:LYS:HA	1:C:584:ASN:O	2.11	0.50
1:E:43:ALA:O	1:E:77:LEU:HA	2.11	0.50
1:C:3:ALA:HA	1:C:46:ILE:HG22	1.93	0.50
1:A:231:LYS:C	1:A:233:PHE:H	2.15	0.50
1:C:208:THR:HG22	1:C:341:HIS:CG	2.46	0.50
1:E:454:ILE:HG13	1:E:455:GLY:H	1.75	0.50
2:F:426:HIS:CE1	2:F:594:ILE:HB	2.46	0.50
1:A:423:LYS:HG2	1:A:423:LYS:O	2.11	0.50
1:E:693:LEU:HB3	1:E:700:ARG:HD2	1.94	0.50
1:E:482:LYS:HB3	1:E:797:VAL:HG21	1.94	0.50
1:A:581:ASN:O	1:A:582:LYS:HG3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:22:MET:HA	1:E:122:THR:HB	1.92	0.50
2:D:546:GLU:HG2	2:D:547:GLU:HG3	1.91	0.50
1:C:132:ILE:HG23	1:C:133:GLU:H	1.77	0.50
2:D:552:LEU:HD12	2:D:552:LEU:N	2.27	0.50
1:E:809:LEU:O	1:E:811:PRO:HD3	2.12	0.50
1:E:39:LEU:CD1	1:E:334:LEU:HD12	2.42	0.50
1:A:406:LYS:HG3	1:A:409:GLN:HB2	1.94	0.50
1:E:495:VAL:HA	1:E:554:LEU:HA	1.93	0.50
1:E:524:GLU:HA	2:F:492:ARG:HH12	1.76	0.50
1:A:226:ALA:CB	1:A:241:MET:HB3	2.41	0.50
2:B:508:LEU:N	2:B:509:PRO:CD	2.74	0.50
1:A:429:LYS:HG3	1:A:462:PHE:CZ	2.47	0.50
1:A:447:ASP:CG	1:A:448:CYS:H	2.15	0.50
1:A:29:ASP:O	1:A:159:LYS:NZ	2.29	0.50
1:C:129:VAL:HG12	1:C:130:ASP:N	2.27	0.50
1:A:485:VAL:HG22	1:A:485:VAL:O	2.12	0.50
1:A:7:ASP:HA	1:A:10:ARG:CG	2.42	0.50
2:D:484:ASP:OD2	2:D:494:ARG:HD3	2.12	0.50
2:D:524:ALA:O	2:D:528:GLU:HG3	2.11	0.50
1:E:597:VAL:O	1:E:601:ILE:HG13	2.11	0.50
2:F:513:ARG:CB	2:F:513:ARG:HH11	2.22	0.50
1:A:3:ALA:HA	1:A:46:ILE:HG22	1.92	0.50
1:A:819:VAL:O	1:A:823:ARG:HG3	2.11	0.50
2:D:507:SER:C	2:D:509:PRO:HD2	2.32	0.50
2:F:426:HIS:O	2:F:429:LEU:HB2	2.11	0.50
1:E:729:PHE:CE2	1:E:774:VAL:HG22	2.47	0.50
1:A:16:VAL:HG12	1:A:346:VAL:HG23	1.94	0.50
1:C:578:LYS:HG2	1:C:585:ARG:HG2	1.94	0.50
1:C:506:GLU:HG3	1:C:510:ARG:HE	1.75	0.50
1:A:693:LEU:HB3	1:A:700:ARG:HD2	1.94	0.50
1:E:784:LEU:HD23	1:E:794:PRO:CG	2.38	0.50
1:E:39:LEU:HB3	1:E:77:LEU:HD21	1.92	0.50
1:E:39:LEU:HD11	1:E:334:LEU:CD1	2.42	0.50
1:C:167:LEU:N	1:C:167:LEU:HD12	2.25	0.50
1:C:627:VAL:O	1:C:631:ARG:HG3	2.12	0.50
1:A:388:THR:HG21	1:A:395:TYR:CG	2.46	0.50
1:A:153:PRO:HD2	1:A:200:VAL:HG13	1.94	0.50
1:C:106:PRO:HG3	1:C:114:GLU:HG3	1.93	0.50
1:E:235:VAL:HG11	1:E:239:LYS:HD3	1.94	0.50
1:A:581:ASN:C	1:A:582:LYS:CG	2.81	0.49
1:A:411:VAL:CG1	1:A:412:ARG:N	2.74	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:384:LYS:HB2	1:C:465:LYS:CE	2.42	0.49
1:C:601:ILE:HG12	1:C:606:ILE:HB	1.94	0.49
1:C:39:LEU:HB3	1:C:77:LEU:HD21	1.93	0.49
1:A:730:LEU:CD2	1:A:730:LEU:C	2.81	0.49
1:C:823:ARG:NH1	1:C:828:MET:HB2	2.26	0.49
1:E:585:ARG:HD2	1:E:692:THR:OG1	2.12	0.49
1:C:669:TRP:HE1	1:C:710:ARG:HH21	1.59	0.49
1:E:563:TYR:O	1:E:564:ARG:HD2	2.12	0.49
1:A:584:ASN:ND2	1:A:693:LEU:HA	2.17	0.49
1:E:183:GLU:O	1:E:187:VAL:HG23	2.12	0.49
1:E:571:SER:HB2	1:E:589:LYS:HG2	1.93	0.49
2:D:485:GLN:O	2:D:486:GLU:HG2	2.12	0.49
1:E:581:ASN:HB3	1:E:583:HIS:HD2	1.77	0.49
1:A:132:ILE:HD12	1:A:162:ARG:NH1	2.22	0.49
2:B:411:THR:OG1	2:B:495:ASN:ND2	2.43	0.49
2:B:410:SER:HB3	2:B:413:GLY:O	2.13	0.49
1:A:26:ALA:HB2	1:A:128:VAL:HB	1.94	0.49
1:A:677:PHE:CZ	1:A:679:GLU:HG3	2.47	0.49
1:A:129:VAL:HG13	1:A:134:GLY:C	2.32	0.49
1:A:374:PRO:O	1:A:404:THR:HG23	2.12	0.49
2:D:447:ALA:O	2:D:448:GLN:C	2.50	0.49
1:A:129:VAL:HG13	1:A:134:GLY:O	2.13	0.49
1:E:823:ARG:NH1	1:E:828:MET:HB2	2.27	0.49
1:C:478:MET:O	1:C:479:LYS:C	2.50	0.49
1:E:754:VAL:HA	1:E:770:ALA:HB2	1.94	0.49
1:E:296:ILE:O	1:E:300:LEU:HB2	2.12	0.49
1:C:2:VAL:CG2	1:C:3:ALA:H	2.19	0.49
1:E:650:THR:CG2	1:E:688:ILE:HG22	2.42	0.49
2:F:504:PRO:HD3	2:F:563:ARG:O	2.11	0.49
2:F:552:LEU:H	2:F:552:LEU:HD12	1.75	0.49
1:C:703:GLY:HA2	2:D:493:ILE:CD1	2.42	0.49
1:E:167:LEU:HD12	1:E:167:LEU:N	2.28	0.49
1:E:284:LEU:HD11	1:E:303:LEU:CD1	2.41	0.49
2:D:488:ASP:CG	2:D:489:ALA:N	2.66	0.49
1:A:27:HIS:HD2	1:A:29:ASP:N	2.01	0.49
1:E:200:VAL:O	1:E:200:VAL:HG22	2.13	0.49
1:E:162:ARG:O	1:E:166:GLU:HB2	2.13	0.49
1:A:594:ASP:O	1:A:597:VAL:HG23	2.12	0.49
2:F:451:VAL:CG1	2:F:451:VAL:O	2.59	0.49
1:A:344:SER:C	1:A:346:VAL:H	2.15	0.49
1:C:729:PHE:CE2	1:C:774:VAL:HG22	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:153:PRO:HD2	1:E:200:VAL:HG22	1.95	0.49
2:B:453:GLY:O	2:B:456:ARG:HD3	2.12	0.49
1:A:191:THR:O	1:A:763:THR:HG22	2.13	0.49
1:E:749:LYS:HG3	1:E:749:LYS:O	2.13	0.49
1:C:729:PHE:O	1:C:771:TYR:HA	2.13	0.49
1:C:148:GLY:HA2	1:C:760:ARG:NH2	2.28	0.49
1:C:792:ALA:O	1:C:794:PRO:HD3	2.13	0.49
1:C:296:ILE:CD1	1:C:319:LEU:HD21	2.38	0.49
1:A:125:ALA:HB2	1:A:151:ILE:HG21	1.95	0.49
2:D:484:ASP:OD2	2:D:494:ARG:CD	2.60	0.49
1:A:109:VAL:CG2	1:A:138:GLN:HG3	2.43	0.49
1:E:710:ARG:NH1	1:E:710:ARG:HG3	2.28	0.49
1:E:503:LYS:CB	1:E:551:GLY:HA3	2.38	0.48
2:D:518:LEU:H	2:D:518:LEU:HD22	1.77	0.48
1:A:230:ALA:O	1:A:235:VAL:HG22	2.12	0.48
1:E:171:LYS:NZ	1:E:283:ARG:HH21	2.11	0.48
1:A:106:PRO:HG3	1:A:114:GLU:HG3	1.95	0.48
1:C:459:ILE:HG21	1:C:463:LEU:HD12	1.94	0.48
2:B:436:PHE:HB2	2:B:502:TYR:CE2	2.48	0.48
2:D:451:VAL:O	2:D:451:VAL:HG12	2.13	0.48
2:B:479:TYR:CG	2:B:582:LEU:HB2	2.48	0.48
1:C:390:ASP:O	1:C:391:LYS:HB3	2.13	0.48
1:E:374:PRO:O	1:E:404:THR:HG23	2.13	0.48
1:C:681:MET:CE	1:C:717:PHE:CD1	2.97	0.48
1:C:607:ASN:HB3	1:C:610:ASP:OD2	2.13	0.48
1:A:615:ARG:HG2	1:A:619:MET:HE1	1.95	0.48
1:A:175:TYR:HD2	1:A:176:GLN:HE21	1.61	0.48
2:F:556:LEU:HD22	2:F:560:LEU:HD13	1.95	0.48
1:A:45:ILE:HB	1:A:76:SER:HB2	1.94	0.48
1:C:2:VAL:CG2	1:C:3:ALA:N	2.71	0.48
2:B:551:ARG:CG	2:B:551:ARG:HH11	2.27	0.48
1:A:126:LEU:HD11	1:A:156:VAL:CG2	2.43	0.48
1:C:211:PHE:O	1:C:219:ALA:HA	2.13	0.48
1:E:606:ILE:HD12	1:E:619:MET:CG	2.43	0.48
2:F:427:ARG:HG2	2:F:428:GLN:N	2.28	0.48
1:E:348:ALA:HA	1:E:351:TYR:CE2	2.49	0.48
1:E:646:VAL:HG13	1:E:688:ILE:HD12	1.95	0.48
1:A:77:LEU:HB2	1:A:100:ILE:HB	1.95	0.48
1:C:314:LEU:CD2	1:C:318:ALA:O	2.61	0.48
1:E:186:ASN:HB2	1:E:201:GLN:HG2	1.96	0.48
1:C:580:PRO:HD2	1:C:704:GLN:CD	2.34	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:504:LEU:HD13	1:A:554:LEU:HD21	1.96	0.48
1:A:100:ILE:HD13	1:A:338:ILE:HG21	1.94	0.48
1:C:712:ALA:O	1:C:715:ALA:HB3	2.13	0.48
1:A:307:LEU:HD13	1:A:312:LYS:HA	1.96	0.48
1:E:536:LEU:CD1	1:E:540:ILE:HD11	2.42	0.48
1:A:2:VAL:CG2	1:A:3:ALA:N	2.77	0.48
1:E:644:ASN:ND2	1:E:684:VAL:H	2.11	0.48
1:E:144:ARG:HG2	1:E:192:TYR:CD2	2.48	0.48
1:A:387:PRO:HG3	1:A:394:PHE:CE1	2.47	0.48
1:E:237:LYS:HA	1:E:240:MET:CB	2.38	0.48
1:E:220:PHE:HA	1:E:224:GLN:OE1	2.12	0.48
1:E:607:ASN:HB3	1:E:610:ASP:CG	2.34	0.48
2:B:438:GLY:HA3	2:B:471:ILE:CD1	2.43	0.48
1:E:527:GLU:HB3	1:E:529:ILE:HD11	1.95	0.48
1:E:569:SER:O	1:E:720:ALA:HB1	2.14	0.48
1:C:344:SER:C	1:C:346:VAL:H	2.17	0.48
1:C:647:ILE:HG13	1:C:685:ARG:NE	2.28	0.48
1:E:647:ILE:HG13	1:E:685:ARG:HE	1.78	0.48
1:E:685:ARG:NE	1:E:687:ASN:HD21	2.11	0.48
1:A:521:TYR:CZ	1:A:529:ILE:HD12	2.48	0.48
1:C:120:ARG:NH1	1:C:479:LYS:HG3	2.29	0.48
2:D:465:ILE:HG13	2:D:466:TRP:CD1	2.49	0.48
2:F:508:LEU:N	2:F:509:PRO:CD	2.77	0.48
1:C:172:GLU:HA	1:C:274:ASN:HD21	1.79	0.48
1:A:167:LEU:N	1:A:167:LEU:HD12	2.28	0.48
1:E:220:PHE:HB3	1:E:328:LEU:HD13	1.95	0.48
1:A:130:ASP:OD1	1:A:159:LYS:HD2	2.14	0.48
1:E:325:ARG:HH11	1:E:325:ARG:HG2	1.79	0.48
2:D:476:ALA:HA	2:D:582:LEU:HD23	1.95	0.48
1:E:677:PHE:CZ	1:E:679:GLU:HG3	2.49	0.48
1:C:468:THR:C	1:C:469:LEU:HD12	2.34	0.48
2:B:450:ILE:HG23	2:B:455:VAL:HG23	1.96	0.48
2:B:438:GLY:HA3	2:B:471:ILE:HD13	1.96	0.48
1:E:412:ARG:HG2	1:E:412:ARG:NH1	2.29	0.48
1:E:528:HIS:O	1:E:529:ILE:HD13	2.14	0.48
1:C:571:SER:HB2	1:C:589:LYS:CG	2.43	0.48
1:C:42:ARG:HG3	1:C:331:ALA:HB1	1.93	0.47
1:C:647:ILE:HB	1:C:687:ASN:ND2	2.29	0.47
1:C:385:MET:SD	1:C:396:ALA:HA	2.54	0.47
1:A:91:GLN:HE22	1:A:343:PRO:HA	1.79	0.47
1:A:636:PHE:CE1	1:A:645:LEU:HD21	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:181:THR:O	1:E:185:VAL:HG23	2.15	0.47
1:C:189:VAL:HG13	1:C:200:VAL:HG12	1.96	0.47
1:E:203:TYR:CD2	1:E:206:ARG:HD2	2.46	0.47
1:E:606:ILE:HD12	1:E:619:MET:HG2	1.96	0.47
1:A:806:SER:HB2	1:A:813:SER:HB2	1.97	0.47
1:E:82:SER:O	1:E:86:VAL:HG23	2.14	0.47
1:E:262:THR:CG2	1:E:266:GLY:HA2	2.44	0.47
1:A:647:ILE:CG1	1:A:685:ARG:HE	2.25	0.47
1:A:225:PHE:CE2	1:A:277:ILE:HG23	2.49	0.47
1:A:719:LEU:HD21	1:A:835:TRP:CE2	2.48	0.47
1:A:81:MET:O	1:A:96:ASN:HB3	2.14	0.47
1:C:488:VAL:HG23	1:C:489:VAL:HG22	1.95	0.47
2:F:470:TYR:CE2	2:F:555:ILE:HG12	2.50	0.47
1:E:129:VAL:HG12	1:E:130:ASP:N	2.28	0.47
1:C:386:VAL:HG11	1:C:437:MET:CE	2.45	0.47
1:E:10:ARG:NH1	1:E:449:PRO:HD2	2.20	0.47
2:D:488:ASP:OD1	2:D:489:ALA:N	2.47	0.47
1:C:581:ASN:O	1:C:582:LYS:CB	2.62	0.47
1:E:436:LEU:HD23	1:E:454:ILE:CD1	2.44	0.47
1:A:569:SER:O	1:A:592:PRO:HD3	2.14	0.47
1:E:172:GLU:HA	1:E:274:ASN:HD21	1.79	0.47
1:E:807:ASP:OD2	1:E:809:LEU:N	2.33	0.47
2:D:570:ALA:HB3	2:D:591:GLU:OE1	2.15	0.47
2:B:560:LEU:HD22	2:B:560:LEU:O	2.14	0.47
2:F:493:ILE:HG22	2:F:493:ILE:O	2.14	0.47
1:C:43:ALA:HB1	1:C:78:TYR:O	2.13	0.47
1:C:116:THR:HB	1:C:481:MET:CE	2.45	0.47
2:F:422:LEU:HD13	2:F:594:ILE:HD11	1.97	0.47
2:B:542:ILE:HD12	2:B:543:THR:H	1.80	0.47
1:A:83:ASP:O	1:A:87:LYS:HG3	2.14	0.47
1:E:503:LYS:HB3	1:E:551:GLY:N	2.30	0.47
1:C:231:LYS:CG	1:C:232:LYS:N	2.77	0.47
1:E:581:ASN:ND2	1:E:699:DDE:O	2.48	0.47
1:C:268:PRO:O	1:C:269:LEU:HD23	2.15	0.47
1:C:256:LYS:CA	1:C:256:LYS:HE2	2.24	0.47
1:C:411:VAL:HG12	1:C:412:ARG:N	2.29	0.47
1:E:155:VAL:HB	1:E:209:VAL:HG22	1.97	0.47
1:E:734:GLN:N	1:E:734:GLN:NE2	2.58	0.47
2:B:457:ALA:HB2	2:B:558:TRP:CE3	2.49	0.47
2:B:490:ARG:N	2:B:490:ARG:CD	2.77	0.47
1:E:411:VAL:HG12	1:E:412:ARG:N	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:615:ARG:HG2	1:E:619:MET:HE2	1.97	0.47
1:C:186:ASN:HB3	1:C:201:GLN:HG2	1.97	0.47
2:D:429:LEU:HD21	2:D:565:VAL:HG11	1.96	0.47
1:C:283:ARG:HB3	1:C:299:LEU:HD21	1.96	0.47
1:E:147:LEU:HD12	1:E:192:TYR:HB2	1.92	0.47
1:C:484:SER:HB3	1:C:797:VAL:HG23	1.97	0.47
1:E:739:ALA:HB1	1:E:788:THR:HB	1.97	0.47
2:F:556:LEU:HD22	2:F:560:LEU:CD1	2.45	0.47
1:C:638:PRO:HB3	1:C:672:LYS:HG2	1.96	0.47
1:C:681:MET:HE1	1:C:717:PHE:CD1	2.50	0.47
1:C:384:LYS:HB2	1:C:465:LYS:HZ2	1.79	0.47
1:C:729:PHE:CD2	1:C:774:VAL:HG22	2.50	0.47
2:D:465:ILE:HD12	2:D:535:LEU:HD12	1.97	0.47
1:E:773:PRO:HB2	1:E:776:GLU:HB2	1.97	0.47
2:B:552:LEU:CD1	2:B:552:LEU:N	2.70	0.47
2:B:546:GLU:HG3	2:B:553:GLU:OE1	2.15	0.47
1:A:348:ALA:O	1:A:352:ARG:HB2	2.15	0.47
1:E:285:PHE:CD2	1:E:320:LEU:HD11	2.50	0.47
1:E:284:LEU:HD13	1:E:324:MET:CE	2.45	0.47
2:F:427:ARG:CG	2:F:428:GLN:N	2.78	0.47
1:C:809:LEU:O	1:C:811:PRO:HD3	2.14	0.47
1:C:223:ARG:HH11	1:C:223:ARG:HG2	1.80	0.47
1:E:386:VAL:HG11	1:E:437:MET:CE	2.44	0.46
1:A:386:VAL:HA	1:A:387:PRO:HD3	1.78	0.46
1:C:45:ILE:HG12	1:C:76:SER:C	2.36	0.46
1:A:112:SER:CB	1:A:794:PRO:O	2.63	0.46
1:C:546:GLU:HB2	1:C:554:LEU:HD12	1.98	0.46
1:C:275:MET:HE1	1:C:276:PHE:CZ	2.50	0.46
1:E:607:ASN:HA	1:E:608:PRO:HD3	1.87	0.46
1:A:118:ALA:O	1:A:122:THR:HG23	2.14	0.46
2:B:556:LEU:HD22	2:B:560:LEU:CD1	2.45	0.46
1:A:16:VAL:HG21	1:A:450:ALA:O	2.14	0.46
1:E:552:VAL:CG2	1:E:553:PRO:CD	2.80	0.46
1:C:140:GLU:HG3	1:C:188:ILE:HD11	1.93	0.46
1:E:307:LEU:HB2	1:E:312:LYS:CE	2.45	0.46
1:A:495:VAL:HA	1:A:554:LEU:HD23	1.97	0.46
1:A:620:ALA:HA	1:A:625:TRP:O	2.15	0.46
1:E:829:LYS:N	1:E:829:LYS:HD2	2.30	0.46
1:C:539:GLU:HA	1:C:542:LEU:HD12	1.98	0.46
1:A:386:VAL:HG11	1:A:437:MET:CE	2.46	0.46
1:C:147:LEU:HD11	1:C:189:VAL:HA	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:ILE:HD12	1:A:122:THR:HG22	1.96	0.46
1:E:132:ILE:HD12	1:E:132:ILE:H	1.79	0.46
1:C:706:ILE:HB	1:C:707:PRO:HD3	1.97	0.46
1:C:385:MET:H	1:C:465:LYS:HD2	1.79	0.46
2:B:420:GLU:CD	2:B:420:GLU:N	2.69	0.46
1:C:131:THR:HG21	1:C:163:ALA:HB2	1.96	0.46
1:E:506:GLU:O	1:E:510:ARG:HG2	2.15	0.46
2:F:538:ARG:HD2	2:F:538:ARG:HA	1.49	0.46
1:E:581:ASN:HB3	1:E:583:HIS:CD2	2.51	0.46
1:E:39:LEU:HD11	1:E:334:LEU:CB	2.46	0.46
1:E:39:LEU:HD11	1:E:334:LEU:HD12	1.98	0.46
1:E:740:VAL:HG21	1:E:766:PHE:CD1	2.49	0.46
1:A:7:ASP:HA	1:A:10:ARG:CD	2.44	0.46
2:F:518:LEU:O	2:F:520:ALA:N	2.49	0.46
1:C:391:LYS:CG	1:C:392:GLY:N	2.61	0.46
1:C:253:LYS:CE	1:C:253:LYS:HA	2.23	0.46
1:E:784:LEU:CD2	1:E:794:PRO:HG3	2.38	0.46
1:C:589:LYS:HE3	1:C:689:LEU:HD11	1.97	0.46
1:E:807:ASP:C	1:E:807:ASP:OD2	2.53	0.46
1:C:669:TRP:C	1:C:669:TRP:CD1	2.88	0.46
1:E:710:ARG:HH11	1:E:710:ARG:HG3	1.81	0.46
1:E:829:LYS:H	1:E:829:LYS:HD2	1.81	0.46
1:E:595:GLU:OE2	1:E:682:ARG:NH2	2.41	0.46
1:C:306:VAL:HG23	1:C:306:VAL:O	2.15	0.46
1:C:374:PRO:O	1:C:404:THR:HG23	2.15	0.46
1:C:235:VAL:CG1	1:C:236:ASP:N	2.79	0.46
1:A:365:ASN:O	1:A:369:ILE:HG12	2.16	0.46
1:E:137:VAL:CG1	1:E:785:ARG:NH2	2.78	0.46
1:E:557:SER:O	1:E:558:PRO:O	2.33	0.46
1:C:552:VAL:CG2	1:C:553:PRO:CD	2.83	0.46
1:C:580:PRO:HD2	1:C:704:GLN:NE2	2.31	0.46
1:C:222:ILE:HG22	1:C:241:MET:HB2	1.98	0.46
1:E:647:ILE:HG13	1:E:685:ARG:NE	2.31	0.46
1:E:528:HIS:C	1:E:529:ILE:HD13	2.35	0.46
1:C:262:THR:OG1	1:C:263:ASP:N	2.49	0.46
1:C:156:VAL:HG22	1:C:210:ALA:HB3	1.98	0.46
1:E:493:VAL:CG1	1:E:494:GLU:N	2.79	0.46
1:E:345:PRO:HG2	1:E:451:GLY:O	2.16	0.46
1:A:41:GLN:O	1:A:41:GLN:HG2	2.16	0.46
1:C:331:ALA:O	1:C:335:LEU:HG	2.16	0.46
1:C:520:THR:HG22	1:C:530:VAL:HG22	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:545:LEU:HD12	1:E:549:HIS:CB	2.41	0.46
1:A:436:LEU:HD23	1:A:454:ILE:CD1	2.46	0.46
1:A:228:ARG:C	1:A:230:ALA:H	2.17	0.46
1:C:228:ARG:C	1:C:230:ALA:H	2.20	0.46
1:C:89:ILE:CG2	1:C:91:GLN:HG2	2.45	0.46
1:A:757:GLU:HG3	1:A:768:VAL:HG22	1.97	0.46
1:E:705:ILE:HD12	1:E:705:ILE:N	2.31	0.45
2:D:542:ILE:HG12	2:D:543:THR:N	2.31	0.45
1:A:565:GLU:O	1:A:681:MET:HA	2.16	0.45
1:A:411:VAL:HG11	1:A:469:LEU:HB3	1.97	0.45
1:E:654:GLN:HG2	1:E:655:TYR:CG	2.52	0.45
1:A:231:LYS:C	1:A:233:PHE:N	2.70	0.45
2:F:436:PHE:HB2	2:F:502:TYR:CE2	2.50	0.45
2:B:423:LEU:HD11	2:B:590:LYS:HD3	1.98	0.45
1:C:216:HIS:NE2	1:C:317:LYS:NZ	2.62	0.45
1:C:315:GLU:C	1:C:319:LEU:HB2	2.36	0.45
1:E:202:VAL:O	1:E:202:VAL:HG23	2.16	0.45
1:C:45:ILE:HD11	1:C:78:TYR:HB3	1.95	0.45
2:B:490:ARG:HD2	2:B:490:ARG:H	1.82	0.45
1:E:348:ALA:HA	1:E:351:TYR:CZ	2.51	0.45
1:A:710:ARG:NH1	1:A:710:ARG:HG3	2.32	0.45
1:A:730:LEU:HB2	1:A:799:ASP:HB2	1.98	0.45
1:E:501:LEU:HB3	1:E:502:PRO:HD3	1.98	0.45
1:E:732:GLU:N	1:E:795:GLN:O	2.46	0.45
1:E:10:ARG:NH1	1:E:449:PRO:CD	2.59	0.45
1:C:816:GLY:O	1:C:820:LEU:HB3	2.16	0.45
1:C:493:VAL:HG21	1:C:545:LEU:CD2	2.45	0.45
1:C:685:ARG:HE	1:C:687:ASN:ND2	2.13	0.45
1:E:117:ALA:HA	1:E:481:MET:SD	2.57	0.45
1:C:515:ASP:HB3	1:C:518:VAL:CG1	2.47	0.45
1:E:150:ARG:HH12	1:E:355:GLN:HB2	1.81	0.45
2:F:400:PHE:CD1	2:F:429:LEU:HD23	2.51	0.45
1:C:558:PRO:HA	1:C:559:PRO:HD3	1.79	0.45
1:E:466:THR:HG22	1:E:467:GLY:N	2.32	0.45
1:C:277:ILE:HG22	1:C:278:LEU:N	2.31	0.45
1:E:143:LEU:O	1:E:147:LEU:HG	2.16	0.45
2:B:417:TRP:CD1	2:B:568:PRO:HB2	2.51	0.45
1:A:220:PHE:C	1:A:220:PHE:CD1	2.90	0.45
1:E:735:CYS:HA	1:E:736:PRO:HD3	1.81	0.45
1:C:311:GLU:OE2	1:C:322:VAL:CG1	2.64	0.45
1:E:137:VAL:HG13	1:E:785:ARG:NH2	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:LEU:HG	1:A:99:LEU:HB2	1.96	0.45
1:A:296:ILE:N	1:A:297:PRO:HD2	2.31	0.45
1:C:733:ILE:HG21	1:C:743:ILE:CD1	2.47	0.45
1:C:291:PHE:O	1:C:293:LYS:N	2.50	0.45
1:E:32:LYS:NZ	1:E:106:PRO:O	2.49	0.45
1:E:485:VAL:HG22	1:E:485:VAL:O	2.17	0.45
1:C:675:PRO:HD3	1:C:714:TYR:CD1	2.52	0.45
1:E:12:LEU:HG	1:E:99:LEU:HB2	1.98	0.45
1:E:743:ILE:HD13	1:E:784:LEU:HD11	1.98	0.45
1:A:647:ILE:HB	1:A:687:ASN:ND2	2.30	0.45
1:A:454:ILE:CG1	1:A:455:GLY:H	2.27	0.45
1:A:126:LEU:HD11	1:A:156:VAL:HG23	1.99	0.45
1:C:38:SER:CA	1:C:41:GLN:HG2	2.46	0.45
1:E:360:PRO:HB2	1:E:363:ASP:HB2	1.99	0.45
1:E:371:ASN:O	1:E:372:CYS:C	2.54	0.45
1:E:611:ASP:OD2	1:E:613:LYS:HB2	2.17	0.45
1:C:164:LEU:HD21	1:C:174:LEU:HD22	1.98	0.45
1:E:507:GLY:CA	1:E:549:HIS:HB3	2.46	0.45
1:C:129:VAL:HG13	1:C:134:GLY:C	2.37	0.45
1:A:561:VAL:HG21	1:A:775:ASN:CB	2.46	0.45
1:A:258:THR:HG21	1:A:260:LYS:HG2	1.97	0.45
1:C:581:ASN:ND2	1:C:704:GLN:HG3	2.32	0.45
1:E:635:CYS:CB	1:E:664:VAL:HG13	2.46	0.45
1:C:348:ALA:HA	1:C:351:TYR:CZ	2.52	0.45
1:E:823:ARG:NH2	1:E:833:PRO:HD3	2.31	0.45
1:A:338:ILE:O	1:A:342:LEU:HB2	2.17	0.45
1:C:45:ILE:HB	1:C:76:SER:HB2	1.99	0.45
2:B:420:GLU:CD	2:B:420:GLU:H	2.19	0.45
2:B:484:ASP:OD2	2:B:494:ARG:N	2.50	0.45
1:E:508:LEU:HD22	1:E:520:THR:CG2	2.47	0.45
1:C:464:LEU:HD12	1:C:483:PHE:CZ	2.52	0.45
1:C:82:SER:O	1:C:86:VAL:HG23	2.17	0.45
2:B:474:ASP:OD1	2:B:475:PRO:HD2	2.16	0.45
1:E:712:ALA:O	1:E:715:ALA:HB3	2.17	0.45
1:C:523:SER:O	1:C:526:GLY:N	2.50	0.45
1:E:149:GLU:O	1:E:150:ARG:HB2	2.16	0.45
1:C:111:PHE:HB3	1:C:114:GLU:HG2	1.99	0.45
2:F:451:VAL:HG12	2:F:451:VAL:O	2.17	0.45
1:C:729:PHE:HB2	1:C:772:LEU:O	2.17	0.45
2:D:535:LEU:HB3	2:D:536:PRO:HA	1.99	0.45
2:D:561:ALA:O	2:D:564:THR:HG23	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:450:ILE:O	2:F:454:GLY:N	2.50	0.45
1:C:542:LEU:O	1:C:545:LEU:HB3	2.17	0.45
1:C:693:LEU:HB3	1:C:700:ARG:HD2	1.99	0.45
2:D:541:ALA:HB2	2:D:556:LEU:HD23	1.99	0.45
1:A:7:ASP:O	1:A:10:ARG:CG	2.65	0.45
2:D:471:ILE:HG13	2:D:554:THR:HB	1.97	0.45
1:E:520:THR:HA	1:E:529:ILE:O	2.17	0.45
2:F:443:PHE:CE2	2:F:445:GLU:HB2	2.52	0.45
1:E:306:VAL:O	1:E:306:VAL:HG23	2.17	0.45
2:F:498:LEU:HD23	2:F:498:LEU:HA	1.72	0.45
1:C:552:VAL:CG2	1:C:553:PRO:HD3	2.39	0.44
1:C:567:VAL:HG23	1:C:592:PRO:HG3	1.99	0.44
1:E:72:SER:HA	1:E:439:GLY:O	2.18	0.44
1:A:690:ASP:O	1:A:691:VAL:CG2	2.65	0.44
1:A:200:VAL:O	1:A:200:VAL:CG1	2.65	0.44
2:D:558:TRP:O	2:D:559:PRO:C	2.55	0.44
1:A:43:ALA:HB1	1:A:78:TYR:O	2.17	0.44
1:E:386:VAL:HA	1:E:387:PRO:HD3	1.79	0.44
1:C:251:ASN:HA	1:C:252:PRO:HD3	1.64	0.44
1:C:490:GLN:HB2	1:C:529:ILE:CG2	2.47	0.44
1:C:507:GLY:O	1:C:511:LEU:HB2	2.17	0.44
1:E:89:ILE:C	1:E:91:GLN:N	2.69	0.44
1:C:129:VAL:HB	1:C:157:ILE:HD13	1.98	0.44
1:E:109:VAL:O	1:E:109:VAL:HG12	2.16	0.44
1:E:536:LEU:O	1:E:537:HIS:C	2.55	0.44
1:A:7:ASP:HA	1:A:10:ARG:HD3	1.99	0.44
1:C:211:PHE:CD2	1:C:211:PHE:N	2.85	0.44
1:A:249:PHE:CD2	1:A:249:PHE:N	2.85	0.44
1:C:735:CYS:SG	1:C:739:ALA:HB3	2.58	0.44
1:C:225:PHE:CE2	1:C:277:ILE:HG23	2.51	0.44
1:E:225:PHE:CZ	1:E:328:LEU:HD11	2.53	0.44
1:E:158:ASN:HA	1:E:212:GLY:O	2.17	0.44
2:F:420:GLU:N	2:F:420:GLU:CD	2.71	0.44
1:C:381:TYR:O	1:C:398:GLY:HA3	2.18	0.44
1:C:371:ASN:O	1:C:372:CYS:C	2.55	0.44
1:C:218:TRP:CA	1:C:330:ALA:HB2	2.47	0.44
2:F:570:ALA:HB3	2:F:591:GLU:OE1	2.18	0.44
1:E:4:PHE:HA	1:E:8:GLN:OE1	2.18	0.44
1:A:582:LYS:HE3	1:A:582:LYS:HB3	1.49	0.44
1:E:25:ILE:HG12	1:E:125:ALA:HB1	1.99	0.44
1:C:644:ASN:HD22	1:C:684:VAL:HB	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:413:ILE:HD13	1:C:459:ILE:HG23	1.98	0.44
1:C:301:GLU:HG3	1:C:301:GLU:O	2.18	0.44
1:E:500:ASP:HA	1:E:503:LYS:HD2	1.98	0.44
1:C:42:ARG:HG3	1:C:331:ALA:HB2	1.90	0.44
1:A:30:HIS:HA	1:A:159:LYS:NZ	2.32	0.44
1:A:581:ASN:HB3	1:A:583:HIS:ND1	2.33	0.44
1:A:32:LYS:HZ2	1:A:105:SER:HB2	1.79	0.44
1:C:501:LEU:CD2	1:C:501:LEU:C	2.86	0.44
1:E:571:SER:HB2	1:E:589:LYS:CG	2.47	0.44
1:C:110:ASP:C	1:C:112:SER:H	2.20	0.44
1:C:109:VAL:CG1	1:C:793:PHE:CE1	3.01	0.44
1:C:223:ARG:HG2	1:C:223:ARG:NH1	2.33	0.44
1:E:663:VAL:HG13	1:E:709:MET:SD	2.57	0.44
1:E:109:VAL:HG23	1:E:138:GLN:CD	2.38	0.44
2:F:518:LEU:HD22	2:F:518:LEU:N	2.32	0.44
1:E:644:ASN:HD22	1:E:684:VAL:H	1.66	0.44
1:A:782:GLY:O	1:A:785:ARG:HB3	2.17	0.44
1:E:349:GLN:O	1:E:370:LYS:HA	2.17	0.44
1:E:503:LYS:HB3	1:E:551:GLY:H	1.83	0.44
1:C:251:ASN:H	1:C:251:ASN:ND2	2.14	0.44
1:C:500:ASP:HB3	1:C:552:VAL:HG11	2.00	0.44
1:C:296:ILE:N	1:C:297:PRO:HD2	2.33	0.44
2:B:490:ARG:CD	2:B:490:ARG:H	2.31	0.44
1:A:112:SER:HB3	1:A:794:PRO:O	2.18	0.44
1:C:344:SER:C	1:C:346:VAL:N	2.70	0.44
1:E:700:ARG:O	1:E:705:ILE:HD13	2.17	0.44
1:E:338:ILE:HA	1:E:342:LEU:HG	1.99	0.44
2:D:531:ILE:CD1	2:D:533:HIS:CE1	2.94	0.44
1:C:108:HIS:HD2	1:C:110:ASP:H	1.65	0.44
1:C:45:ILE:HD11	1:C:78:TYR:HB2	1.98	0.44
1:A:589:LYS:HE3	1:A:689:LEU:CD1	2.45	0.44
1:C:224:GLN:O	1:C:228:ARG:HG3	2.18	0.44
1:E:613:LYS:O	1:E:616:ALA:HB3	2.18	0.44
1:A:357:TYR:CE2	1:A:359:GLY:HA3	2.53	0.44
1:E:79:SER:O	1:E:98:PHE:N	2.50	0.44
2:B:447:ALA:HA	2:B:499:LEU:HD21	2.00	0.44
1:E:274:ASN:O	1:E:279:ASP:HB2	2.17	0.44
1:A:258:THR:CG2	1:A:260:LYS:HG2	2.48	0.44
1:E:735:CYS:SG	1:E:739:ALA:HB3	2.57	0.44
1:E:685:ARG:HE	1:E:687:ASN:ND2	2.15	0.44
1:E:118:ALA:O	1:E:122:THR:HG23	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:626:ASP:C	1:A:628:THR:N	2.71	0.44
1:A:491:VAL:HG13	1:A:538:LEU:HD21	2.00	0.44
1:E:694:HIS:NE2	1:E:699:DDE:HD2	2.33	0.43
1:C:411:VAL:HG12	1:C:412:ARG:O	2.17	0.43
1:E:389:SER:O	1:E:391:LYS:N	2.51	0.43
1:A:488:VAL:HG23	1:A:489:VAL:CG2	2.48	0.43
2:B:479:TYR:CD2	2:B:582:LEU:HB2	2.53	0.43
1:A:39:LEU:HB3	1:A:77:LEU:HD21	2.00	0.43
1:C:317:LYS:HD2	1:C:317:LYS:HA	1.28	0.43
1:E:250:PHE:HD2	1:E:275:MET:HE1	1.83	0.43
1:E:40:VAL:C	1:E:42:ARG:H	2.21	0.43
2:F:479:TYR:CG	2:F:582:LEU:HB2	2.53	0.43
2:B:516:LEU:O	2:B:545:PRO:HD2	2.18	0.43
1:E:68:ILE:HG21	1:E:395:TYR:OH	2.18	0.43
1:C:521:TYR:CD1	1:C:529:ILE:HD13	2.52	0.43
1:C:494:GLU:OE1	1:C:494:GLU:CA	2.66	0.43
1:C:734:GLN:HE21	1:C:734:GLN:CA	2.29	0.43
1:E:381:TYR:OH	1:E:481:MET:HG3	2.18	0.43
2:F:467:ARG:HG3	2:F:558:TRP:NE1	2.33	0.43
1:A:19:VAL:HA	1:A:99:LEU:O	2.18	0.43
1:E:296:ILE:N	1:E:297:PRO:HD2	2.34	0.43
1:A:690:ASP:C	1:A:691:VAL:HG23	2.38	0.43
1:C:606:ILE:HD12	1:C:619:MET:CG	2.48	0.43
1:C:16:VAL:HG12	1:C:346:VAL:HG23	2.00	0.43
1:A:19:VAL:HG22	1:A:99:LEU:HB3	2.00	0.43
2:F:476:ALA:HA	2:F:582:LEU:HD23	2.01	0.43
1:A:414:GLN:HB3	1:A:418:TYR:CD2	2.52	0.43
1:A:558:PRO:HA	1:A:559:PRO:HD3	1.92	0.43
1:E:4:PHE:CE2	1:E:45:ILE:HD12	2.53	0.43
1:A:654:GLN:HG2	1:A:655:TYR:CG	2.54	0.43
1:E:153:PRO:HD2	1:E:200:VAL:CG2	2.48	0.43
1:C:156:VAL:HG21	1:C:334:LEU:HD22	2.00	0.43
2:D:436:PHE:CE1	2:D:438:GLY:O	2.71	0.43
1:E:749:LYS:HG3	1:E:750:LYS:HD2	1.98	0.43
1:E:461:GLN:NE2	1:E:462:PHE:CE2	2.87	0.43
1:C:411:VAL:HG13	1:C:470:THR:O	2.19	0.43
2:F:443:PHE:CD2	2:F:445:GLU:HB2	2.53	0.43
2:D:437:VAL:HG11	2:D:511:PHE:CE2	2.54	0.43
1:C:262:THR:CA	1:C:269:LEU:HG	2.48	0.43
1:C:659:ILE:HD13	1:C:693:LEU:HD21	2.00	0.43
1:C:288:ILE:CG2	1:C:319:LEU:HG	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:411:VAL:CG1	1:C:412:ARG:N	2.81	0.43
2:B:489:ALA:HB3	2:B:490:ARG:HH11	1.82	0.43
1:A:549:HIS:H	1:A:549:HIS:CD2	2.35	0.43
1:C:387:PRO:HG3	1:C:394:PHE:CE1	2.54	0.43
1:A:733:ILE:O	1:A:767:THR:HA	2.19	0.43
2:D:470:TYR:CE2	2:D:555:ILE:HD11	2.54	0.43
1:A:580:PRO:HB2	1:A:704:GLN:HE22	1.83	0.43
2:D:541:ALA:CB	2:D:556:LEU:HD23	2.49	0.43
1:E:490:GLN:HA	1:E:531:ALA:HA	2.01	0.43
1:E:229:TYR:CD1	1:E:232:LYS:HD2	2.54	0.43
1:A:569:SER:O	1:A:720:ALA:HB1	2.18	0.43
1:E:350:ALA:O	1:E:370:LYS:HG2	2.18	0.43
1:E:782:GLY:O	1:E:786:GLN:NE2	2.52	0.43
1:A:824:LYS:HE3	1:A:830:GLU:OE2	2.19	0.43
1:A:504:LEU:HD22	1:A:554:LEU:CD2	2.49	0.43
1:A:522:MET:CE	1:A:526:GLY:O	2.66	0.43
1:E:209:VAL:HG12	1:E:211:PHE:CE1	2.53	0.43
1:A:240:MET:O	1:A:244:LEU:HG	2.18	0.43
1:A:704:GLN:O	1:A:707:PRO:HD2	2.19	0.43
1:E:171:LYS:HZ3	1:E:283:ARG:HH21	1.67	0.43
1:C:497:ASN:H	1:C:497:ASN:HD22	1.67	0.43
1:C:459:ILE:O	1:C:462:PHE:N	2.48	0.43
1:C:186:ASN:CB	1:C:201:GLN:HG2	2.49	0.43
1:C:216:HIS:CE1	1:C:317:LYS:HZ1	2.36	0.43
1:C:253:LYS:HG3	1:C:253:LYS:O	2.19	0.43
1:E:4:PHE:CD2	1:E:45:ILE:HD12	2.54	0.43
1:A:408:GLY:O	1:A:409:GLN:C	2.57	0.43
1:A:591:GLU:OE2	1:A:685:ARG:NH1	2.52	0.43
1:A:411:VAL:HG13	1:A:470:THR:O	2.19	0.43
1:C:655:TYR:O	1:C:656:LEU:C	2.57	0.43
1:C:749:LYS:O	1:C:750:LYS:HD2	2.19	0.43
2:F:427:ARG:O	2:F:428:GLN:C	2.55	0.43
2:B:499:LEU:HB3	2:B:566:VAL:CG1	2.49	0.43
1:C:587:TYR:CD2	1:C:690:ASP:HB3	2.53	0.43
2:B:583:ASP:HA	2:B:584:PRO:HD2	1.86	0.43
1:C:646:VAL:HG13	1:C:688:ILE:HD13	2.01	0.43
1:C:694:HIS:HD2	1:C:696:ASP:N	2.00	0.42
2:B:520:ALA:HB1	2:B:521:PRO:CD	2.48	0.42
1:E:737:GLU:HG3	1:E:766:PHE:CZ	2.53	0.42
1:C:760:ARG:O	1:C:761:PRO:C	2.58	0.42
2:B:503:VAL:HB	2:B:504:PRO:CD	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:VAL:HG12	1:A:345:PRO:HG2	1.94	0.42
1:A:711:ARG:HH11	2:B:577:ASN:HD21	1.67	0.42
1:A:588:LEU:CD1	1:A:588:LEU:C	2.86	0.42
1:C:285:PHE:CE2	1:C:324:MET:SD	3.09	0.42
1:A:597:VAL:O	1:A:601:ILE:HG13	2.20	0.42
1:C:515:ASP:HA	1:C:516:PRO:HD3	1.85	0.42
2:B:518:LEU:H	2:B:518:LEU:CD2	2.33	0.42
1:E:21:ASN:ND2	1:E:345:PRO:HG3	2.34	0.42
1:C:236:ASP:OD1	1:C:238:ALA:HB3	2.19	0.42
1:C:158:ASN:HD22	1:C:159:LYS:HG2	1.78	0.42
2:B:458:ARG:O	2:B:459:SER:HB2	2.18	0.42
1:E:800:HIS:N	1:E:800:HIS:CD2	2.87	0.42
1:E:814:LYS:O	1:E:817:GLU:HB3	2.20	0.42
1:A:729:PHE:CD2	1:A:774:VAL:HG22	2.54	0.42
1:A:576:LEU:HD13	1:A:587:TYR:CE1	2.54	0.42
1:A:591:GLU:HG2	1:A:685:ARG:CG	2.46	0.42
1:C:494:GLU:HG2	1:C:528:HIS:HE1	1.85	0.42
1:C:565:GLU:CD	1:C:676:ILE:HB	2.40	0.42
1:A:488:VAL:HG23	1:A:489:VAL:HG23	2.01	0.42
2:F:401:LEU:O	2:F:421:ARG:NE	2.48	0.42
1:C:522:MET:SD	1:C:528:HIS:HA	2.59	0.42
1:C:410:LYS:HE2	1:C:430:ALA:HB2	2.02	0.42
1:E:564:ARG:HD3	1:E:801:TRP:CH2	2.55	0.42
1:A:626:ASP:O	1:A:628:THR:N	2.53	0.42
1:C:690:ASP:OD1	1:C:691:VAL:N	2.47	0.42
1:C:650:THR:CG2	1:C:688:ILE:HG22	2.50	0.42
1:E:698:ILE:HD13	1:E:698:ILE:N	2.35	0.42
1:E:89:ILE:HG22	1:E:91:GLN:HB3	2.01	0.42
1:E:202:VAL:HB	1:E:209:VAL:CG2	2.49	0.42
1:C:525:SER:OG	1:C:527:GLU:HG3	2.20	0.42
1:A:580:PRO:HD2	1:A:704:GLN:CD	2.40	0.42
1:C:4:PHE:HD2	1:C:45:ILE:HG23	1.84	0.42
1:A:644:ASN:HD22	1:A:684:VAL:H	1.68	0.42
2:B:410:SER:OG	2:B:412:ARG:HB3	2.19	0.42
1:E:108:HIS:O	1:E:111:PHE:HD2	2.01	0.42
2:D:498:LEU:HA	2:D:498:LEU:HD23	1.69	0.42
1:E:25:ILE:HD12	1:E:142:VAL:CG1	2.50	0.42
1:E:25:ILE:HD12	1:E:142:VAL:HG12	2.02	0.42
1:E:132:ILE:CD1	1:E:132:ILE:N	2.82	0.42
2:D:582:LEU:HD12	2:D:583:ASP:N	2.35	0.42
2:F:531:ILE:HG22	2:F:533:HIS:H	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:636:PHE:CE1	1:E:645:LEU:HD21	2.54	0.42
1:A:556:ILE:HG22	1:A:557:SER:O	2.19	0.42
1:A:760:ARG:O	1:A:761:PRO:C	2.58	0.42
1:C:569:SER:O	1:C:592:PRO:HD3	2.20	0.42
1:A:607:ASN:HA	1:A:608:PRO:HD3	1.82	0.42
1:C:501:LEU:O	1:C:501:LEU:HD23	2.17	0.42
1:A:46:ILE:HD12	1:A:46:ILE:HA	1.91	0.42
2:B:484:ASP:OD2	2:B:494:ARG:CG	2.68	0.42
2:D:523:ALA:O	2:D:524:ALA:C	2.57	0.42
1:A:144:ARG:NH2	1:A:791:GLN:O	2.53	0.42
1:E:525:SER:O	2:F:412:ARG:CZ	2.67	0.42
1:E:121:VAL:HG11	1:E:383:SER:HB3	2.01	0.42
1:E:418:TYR:HD1	1:E:424:ASP:O	2.02	0.42
1:E:694:HIS:CE1	1:E:699:DDE:CD2	3.03	0.42
1:E:89:ILE:O	1:E:91:GLN:N	2.53	0.42
1:E:78:TYR:CE1	1:E:97:SER:HB3	2.48	0.42
1:A:590:ALA:HA	1:A:685:ARG:O	2.20	0.42
1:E:740:VAL:HG21	1:E:766:PHE:HD1	1.85	0.42
2:B:443:PHE:CD2	2:B:445:GLU:HB2	2.55	0.42
1:C:828:MET:CE	2:D:576:ARG:HE	2.32	0.42
2:F:470:TYR:CD2	2:F:555:ILE:HG12	2.55	0.42
1:C:487:PRO:HB3	1:C:531:ALA:HB1	2.02	0.42
2:D:518:LEU:CD2	2:D:518:LEU:H	2.33	0.42
1:C:46:ILE:HD12	1:C:46:ILE:HA	1.92	0.42
1:A:607:ASN:HB3	1:A:610:ASP:CG	2.40	0.42
2:B:558:TRP:O	2:B:559:PRO:C	2.55	0.42
1:E:536:LEU:O	1:E:539:GLU:HB3	2.20	0.42
1:C:237:LYS:O	1:C:241:MET:HG2	2.20	0.42
1:A:154:VAL:CG1	1:A:337:MET:HE3	2.50	0.42
1:C:543:GLN:O	1:C:547:HIS:N	2.46	0.41
1:C:511:LEU:HD22	1:C:545:LEU:HD13	2.02	0.41
2:D:518:LEU:HD11	2:D:542:ILE:HD13	2.02	0.41
1:E:237:LYS:O	1:E:241:MET:HE2	2.19	0.41
1:A:10:ARG:HG3	1:A:11:SER:N	2.35	0.41
1:A:380:LEU:HD23	1:A:381:TYR:N	2.35	0.41
2:F:457:ALA:HB2	2:F:558:TRP:CD2	2.55	0.41
1:A:600:ALA:HB1	1:A:606:ILE:HG12	2.00	0.41
1:E:600:ALA:HB1	1:E:606:ILE:HG12	2.01	0.41
2:D:570:ALA:O	2:D:572:PRO:HD3	2.20	0.41
1:C:739:ALA:HB2	1:C:791:GLN:OE1	2.20	0.41
1:C:426:LEU:O	1:C:427:PHE:CD1	2.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:515:ASP:HA	1:E:516:PRO:HD3	1.80	0.41
1:E:584:ASN:HD22	1:E:693:LEU:HA	1.84	0.41
1:E:524:GLU:C	1:E:526:GLY:H	2.24	0.41
1:E:305:ILE:HG21	1:E:323:VAL:HG13	2.02	0.41
1:A:258:THR:CG2	1:A:259:ASN:N	2.79	0.41
1:C:646:VAL:HG13	1:C:688:ILE:CD1	2.50	0.41
1:A:515:ASP:HA	1:A:516:PRO:HD3	1.89	0.41
1:E:123:ASP:HB3	1:E:343:PRO:HG2	2.00	0.41
1:E:406:LYS:O	1:E:409:GLN:HB3	2.19	0.41
1:C:19:VAL:HG12	1:C:20:ARG:N	2.35	0.41
1:E:804:LEU:N	1:E:804:LEU:HD23	2.35	0.41
1:C:73:THR:HG22	1:C:73:THR:O	2.21	0.41
1:C:530:VAL:O	1:C:538:LEU:HD11	2.21	0.41
1:E:144:ARG:HG2	1:E:192:TYR:CG	2.55	0.41
1:C:192:TYR:HA	1:C:763:THR:HG22	2.02	0.41
1:E:314:LEU:C	1:E:319:LEU:HB2	2.40	0.41
1:E:314:LEU:O	1:E:319:LEU:HB2	2.20	0.41
1:C:38:SER:HA	1:C:41:GLN:CG	2.49	0.41
1:E:164:LEU:HD12	1:E:285:PHE:CE1	2.56	0.41
1:A:395:TYR:CE1	1:A:457:VAL:HG13	2.55	0.41
1:A:556:ILE:N	1:A:556:ILE:HD12	2.35	0.41
1:E:760:ARG:O	1:E:761:PRO:C	2.59	0.41
2:B:535:LEU:HB3	2:B:536:PRO:HA	2.02	0.41
1:C:609:ARG:NH1	1:C:609:ARG:HG3	2.35	0.41
1:C:274:ASN:HA	1:C:278:LEU:HB2	2.02	0.41
1:A:503:LYS:HB2	1:A:552:VAL:HG21	2.01	0.41
1:C:192:TYR:HE1	1:C:765:LEU:HB2	1.86	0.41
1:E:46:ILE:HG22	1:E:47:SER:N	2.27	0.41
1:A:221:THR:OG1	1:A:224:GLN:HG3	2.20	0.41
2:B:518:LEU:N	2:B:518:LEU:HD22	2.34	0.41
1:E:239:LYS:NZ	1:E:243:ARG:NH2	2.69	0.41
1:C:740:VAL:HG21	1:C:766:PHE:HB2	2.01	0.41
1:C:485:VAL:O	1:C:485:VAL:HG22	2.19	0.41
1:A:406:LYS:HB3	1:A:447:ASP:HB2	2.03	0.41
1:E:734:GLN:H	1:E:734:GLN:HE21	1.65	0.41
1:C:501:LEU:N	1:C:502:PRO:CD	2.83	0.41
1:A:103:ILE:HD13	1:A:121:VAL:HG23	2.01	0.41
1:C:418:TYR:HB3	1:C:477:ASN:HD21	1.85	0.41
1:C:600:ALA:HB1	1:C:606:ILE:HG12	2.00	0.41
2:B:484:ASP:OD2	2:B:494:ARG:CD	2.69	0.41
2:D:530:LEU:HD23	2:D:604:PRO:HD3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:758:GLU:O	1:C:759:GLN:HB3	2.19	0.41
2:D:518:LEU:N	2:D:518:LEU:HD22	2.35	0.41
1:C:523:SER:HG	1:C:527:GLU:HB2	1.85	0.41
1:E:807:ASP:HA	1:E:808:PRO:HD2	1.95	0.41
2:D:451:VAL:O	2:D:451:VAL:CG1	2.68	0.41
2:B:446:ALA:O	2:B:447:ALA:C	2.59	0.41
1:A:634:TRP:O	1:A:635:CYS:HB3	2.20	0.41
1:C:124:GLY:HA3	1:C:342:LEU:HD22	2.01	0.41
2:F:571:ILE:HD11	2:F:587:ILE:HD12	2.02	0.41
2:F:423:LEU:HD11	2:F:590:LYS:HD3	2.03	0.41
1:A:654:GLN:HG2	1:A:655:TYR:CE2	2.54	0.41
1:C:167:LEU:N	1:C:167:LEU:CD1	2.84	0.41
1:E:126:LEU:HD11	1:E:156:VAL:HG23	2.00	0.41
1:A:606:ILE:HD12	1:A:619:MET:HG3	2.01	0.41
1:C:397:PHE:HD1	1:C:437:MET:HG3	1.86	0.41
1:C:218:TRP:C	1:C:330:ALA:HB2	2.41	0.41
1:A:239:LYS:HG2	1:A:239:LYS:O	2.20	0.41
1:C:804:LEU:N	1:C:804:LEU:HD23	2.35	0.41
1:E:10:ARG:HA	1:E:10:ARG:HD2	1.91	0.41
1:A:27:HIS:CD2	1:A:29:ASP:HB2	2.56	0.41
2:B:450:ILE:HG23	2:B:455:VAL:CG2	2.51	0.41
1:A:124:GLY:HA3	1:A:342:LEU:HD22	2.02	0.41
1:A:512:SER:HA	1:A:518:VAL:CG1	2.51	0.41
1:E:397:PHE:HD1	1:E:437:MET:HG3	1.85	0.41
1:A:71:LYS:O	1:A:386:VAL:HG21	2.21	0.41
1:E:221:THR:HG21	1:E:336:GLU:OE1	2.21	0.41
1:E:186:ASN:HA	1:E:189:VAL:HB	2.03	0.41
1:C:152:LYS:HD2	1:C:200:VAL:HG22	2.03	0.41
2:B:467:ARG:HG3	2:B:558:TRP:HD1	1.84	0.41
1:A:254:THR:O	1:A:255:LYS:HB2	2.21	0.41
1:E:303:LEU:O	1:E:304:GLU:CB	2.69	0.41
2:D:445:GLU:CD	2:D:494:ARG:HH22	2.23	0.41
1:C:597:VAL:O	1:C:601:ILE:HG13	2.20	0.41
1:E:594:ASP:HB2	1:E:597:VAL:HG23	2.03	0.41
1:C:338:ILE:O	1:C:342:LEU:HB2	2.21	0.41
1:E:806:SER:HB2	1:E:813:SER:HB2	2.02	0.41
1:A:363:ASP:O	1:A:367:ILE:HG13	2.21	0.41
2:D:495:ASN:OD1	2:D:495:ASN:N	2.53	0.41
1:C:169:VAL:HG13	1:C:169:VAL:O	2.21	0.41
1:E:70:ILE:HA	1:E:388:THR:HA	2.03	0.41
1:C:521:TYR:O	1:C:529:ILE:HD12	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:39:LEU:HD11	1:E:334:LEU:HB2	2.03	0.41
1:E:5:THR:OG1	1:E:8:GLN:HG3	2.21	0.41
1:C:291:PHE:CE1	1:C:315:GLU:HB2	2.52	0.41
1:C:316:GLY:O	1:C:319:LEU:N	2.54	0.41
1:A:784:LEU:CD2	1:A:794:PRO:HG3	2.50	0.41
2:F:464:ALA:O	2:F:467:ARG:HB3	2.21	0.41
2:D:448:GLN:HB2	2:D:448:GLN:HE21	1.71	0.41
1:E:262:THR:HG21	1:E:266:GLY:HA2	2.02	0.41
1:A:729:PHE:CE2	1:A:774:VAL:HG22	2.56	0.41
1:C:495:VAL:CG1	1:C:554:LEU:HD23	2.50	0.40
1:C:379:MET:SD	1:C:470:THR:HG22	2.61	0.40
1:E:797:VAL:HG22	1:E:798:PHE:N	2.35	0.40
1:C:611:ASP:O	1:C:612:PHE:C	2.59	0.40
1:C:588:LEU:CD1	1:C:588:LEU:C	2.87	0.40
1:C:799:ASP:OD1	1:C:800:HIS:HD2	2.04	0.40
2:F:558:TRP:O	2:F:559:PRO:C	2.57	0.40
2:F:400:PHE:O	2:F:425:ALA:HB1	2.20	0.40
1:E:731:VAL:HG13	1:E:731:VAL:O	2.20	0.40
1:E:500:ASP:O	1:E:503:LYS:N	2.50	0.40
1:C:550:ALA:C	1:C:552:VAL:H	2.24	0.40
1:A:700:ARG:HB2	1:A:700:ARG:HE	1.49	0.40
1:E:391:LYS:CG	1:E:392:GLY:H	2.34	0.40
1:E:189:VAL:O	1:E:193:ALA:CB	2.69	0.40
1:A:91:GLN:O	1:A:93:THR:HG23	2.21	0.40
2:F:429:LEU:O	2:F:434:TYR:HB2	2.22	0.40
1:E:823:ARG:HG2	1:E:823:ARG:NH1	2.36	0.40
1:A:576:LEU:HD13	1:A:587:TYR:CD1	2.56	0.40
1:E:205:ALA:HB2	1:E:245:TRP:HB3	2.02	0.40
1:E:267:LYS:HA	1:E:268:PRO:HD3	1.86	0.40
1:E:388:THR:HG21	1:E:395:TYR:CD1	2.56	0.40
1:A:404:THR:HB	1:A:447:ASP:OD2	2.21	0.40
1:A:694:HIS:HD2	1:A:696:ASP:N	1.99	0.40
1:E:74:ALA:O	1:E:439:GLY:CA	2.67	0.40
1:E:167:LEU:CD1	1:E:167:LEU:H	2.34	0.40
1:C:237:LYS:HA	1:C:240:MET:HB3	2.04	0.40
1:A:26:ALA:CB	1:A:128:VAL:HB	2.51	0.40
1:E:108:HIS:HB2	1:E:111:PHE:CE2	2.57	0.40
1:E:68:ILE:HG23	1:E:390:ASP:CB	2.50	0.40
1:C:411:VAL:HG11	1:C:469:LEU:HB3	2.04	0.40
1:C:591:GLU:OE2	1:C:685:ARG:NH1	2.55	0.40
1:C:454:ILE:CG1	1:C:455:GLY:N	2.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:116:THR:CB	1:C:481:MET:HE3	2.52	0.40
1:C:360:PRO:C	1:C:362:ASP:H	2.24	0.40
1:E:169:VAL:CG2	1:E:173:ASP:HB2	2.51	0.40
1:C:319:LEU:O	1:C:323:VAL:HG23	2.20	0.40
1:C:591:GLU:HA	1:C:592:PRO:HD3	1.84	0.40
1:A:644:ASN:ND2	1:A:684:VAL:HB	2.31	0.40
2:F:535:LEU:HB3	2:F:536:PRO:HA	2.04	0.40
2:D:436:PHE:HB2	2:D:502:TYR:CE2	2.56	0.40
2:D:479:TYR:CD2	2:D:582:LEU:HB2	2.56	0.40
1:C:736:PRO:O	1:C:739:ALA:N	2.52	0.40
1:E:111:PHE:O	1:E:112:SER:C	2.59	0.40
1:A:512:SER:HA	1:A:518:VAL:HG13	2.04	0.40
1:C:146:ALA:O	1:C:151:ILE:HG12	2.22	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	818/842 (97%)	729 (89%)	75 (9%)	14 (2%)	11	43
1	C	818/842 (97%)	716 (88%)	80 (10%)	22 (3%)	6	31
1	E	818/842 (97%)	712 (87%)	90 (11%)	16 (2%)	9	38
2	B	205/207 (99%)	181 (88%)	22 (11%)	2 (1%)	19	58
2	D	205/207 (99%)	182 (89%)	17 (8%)	6 (3%)	6	29
2	F	205/207 (99%)	179 (87%)	21 (10%)	5 (2%)	7	33
All	All	3069/3147 (98%)	2699 (88%)	305 (10%)	65 (2%)	9	37

All (65) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	112	SER
1	A	761	PRO
2	B	518	LEU
2	B	519	ALA
1	C	235	VAL
1	C	264	ALA
1	C	761	PRO
2	D	518	LEU
2	D	519	ALA
1	E	112	SER
1	E	558	PRO
1	E	761	PRO
2	F	519	ALA
1	A	309	GLY
1	A	390	ASP
1	A	498	ALA
1	C	112	SER
1	C	309	GLY
1	C	460	ASP
1	C	549	HIS
1	C	551	GLY
1	C	737	GLU
2	D	491	GLY
1	E	304	GLU
1	E	390	ASP
1	E	479	LYS
2	F	454	GLY
1	A	111	PHE
1	A	237	LYS
1	A	479	LYS
1	C	266	GLY
1	C	479	LYS
1	E	90	LYS
1	E	233	PHE
2	F	577	ASN
1	A	460	ASP
1	A	677	PHE
1	C	265	GLU
1	C	314	LEU
1	C	558	PRO
1	C	743	ILE
1	C	785	ARG
1	E	372	CYS

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Mol	Chain	Res	Type
1	E	621	ASP
1	A	446	ASP
1	C	120	ARG
1	C	329	PRO
1	C	446	ASP
1	C	525	SER
2	D	604	PRO
1	E	446	ASP
1	E	737	GLU
1	E	743	ILE
2	F	404	GLY
1	A	621	ASP
1	E	428	ILE
2	D	404	GLY
2	D	405	GLY
1	E	338	ILE
2	F	450	ILE
1	C	491	VAL
1	A	604	GLY
1	A	329	PRO
1	E	556	ILE
1	C	604	GLY

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	699/714 (98%)	662 (95%)	37 (5%)	28	64
1	C	699/714 (98%)	649 (93%)	50 (7%)	18	53
1	E	699/714 (98%)	659 (94%)	40 (6%)	25	62
2	B	161/162 (99%)	142 (88%)	19 (12%)	6	25
2	D	161/162 (99%)	146 (91%)	15 (9%)	11	39
2	F	161/162 (99%)	144 (89%)	17 (11%)	8	32
All	All	2580/2628 (98%)	2402 (93%)	178 (7%)	19	55

All (178) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	ASP
1	A	15	LYS
1	A	36	THR
1	A	68	ILE
1	A	81	MET
1	A	83	ASP
1	A	91	GLN
1	A	113	SER
1	A	152	LYS
1	A	162	ARG
1	A	200	VAL
1	A	236	ASP
1	A	261	ASP
1	A	262	THR
1	A	275	MET
1	A	347	THR
1	A	352	ARG
1	A	362	ASP
1	A	460	ASP
1	A	489	VAL
1	A	536	LEU
1	A	544	ASP
1	A	582	LYS
1	A	597	VAL
1	A	599	LEU
1	A	609	ARG
1	A	677	PHE
1	A	710	ARG
1	A	718	LEU
1	A	724	ILE
1	A	730	LEU
1	A	734	GLN
1	A	738	GLN
1	A	767	THR
1	A	775	ASN
1	A	785	ARG
1	A	836	GLN
2	B	412	ARG
2	B	420	GLU
2	B	422	LEU
2	B	456	ARG
2	B	467	ARG

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Mol	Chain	Res	Type
2	B	488	ASP
2	B	492	ARG
2	B	494	ARG
2	B	495	ASN
2	B	499	LEU
2	B	506	SER
2	B	540	ASP
2	B	547	GLU
2	B	551	ARG
2	B	552	LEU
2	B	559	PRO
2	B	560	LEU
2	B	577	ASN
2	B	602	SER
1	C	14	ASP
1	C	36	THR
1	C	68	ILE
1	C	81	MET
1	C	83	ASP
1	C	94	ASP
1	C	113	SER
1	C	164	LEU
1	C	167	LEU
1	C	183	GLU
1	C	195	GLU
1	C	231	LYS
1	C	242	ASP
1	C	253	LYS
1	C	256	LYS
1	C	282	PHE
1	C	299	LEU
1	C	301	GLU
1	C	317	LYS
1	C	320	LEU
1	C	347	THR
1	C	362	ASP
1	C	432	GLN
1	C	460	ASP
1	C	461	GLN
1	C	489	VAL
1	C	494	GLU
1	C	495	VAL

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Mol	Chain	Res	Type
1	C	497	ASN
1	C	500	ASP
1	C	506	GLU
1	C	524	GLU
1	C	528	HIS
1	C	544	ASP
1	C	552	VAL
1	C	556	ILE
1	C	599	LEU
1	C	609	ARG
1	C	625	TRP
1	C	677	PHE
1	C	718	LEU
1	C	730	LEU
1	C	734	GLN
1	C	738	GLN
1	C	761	PRO
1	C	767	THR
1	C	775	ASN
1	C	820	LEU
1	C	836	GLN
1	C	837	GLU
2	D	403	ASP
2	D	410	SER
2	D	411	THR
2	D	422	LEU
2	D	483	GLN
2	D	488	ASP
2	D	494	ARG
2	D	499	LEU
2	D	538	ARG
2	D	540	ASP
2	D	547	GLU
2	D	551	ARG
2	D	560	LEU
2	D	577	ASN
2	D	602	SER
1	E	23	SER
1	E	46	ILE
1	E	87	LYS
1	E	94	ASP
1	E	161	ASP

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Mol	Chain	Res	Type
1	E	183	GLU
1	E	186	ASN
1	E	194	ASP
1	E	211	PHE
1	E	216	HIS
1	E	263	ASP
1	E	275	MET
1	E	282	PHE
1	E	313	ASP
1	E	347	THR
1	E	362	ASP
1	E	440	ARG
1	E	460	ASP
1	E	489	VAL
1	E	544	ASP
1	E	552	VAL
1	E	558	PRO
1	E	599	LEU
1	E	625	TRP
1	E	677	PHE
1	E	698	ILE
1	E	710	ARG
1	E	718	LEU
1	E	724	ILE
1	E	730	LEU
1	E	734	GLN
1	E	738	GLN
1	E	749	LYS
1	E	761	PRO
1	E	767	THR
1	E	775	ASN
1	E	786	GLN
1	E	800	HIS
1	E	836	GLN
1	E	837	GLU
2	F	403	ASP
2	F	411	THR
2	F	422	LEU
2	F	467	ARG
2	F	494	ARG
2	F	498	LEU
2	F	499	LEU

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Mol	Chain	Res	Type
2	F	513	ARG
2	F	522	GLU
2	F	538	ARG
2	F	540	ASP
2	F	547	GLU
2	F	552	LEU
2	F	560	LEU
2	F	577	ASN
2	F	599	ASP
2	F	604	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (80) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	HIS
1	A	30	HIS
1	A	91	GLN
1	A	101	ASN
1	A	108	HIS
1	A	138	GLN
1	A	176	GLN
1	A	201	GLN
1	A	274	ASN
1	A	371	ASN
1	A	537	HIS
1	A	547	HIS
1	A	549	HIS
1	A	581	ASN
1	A	584	ASN
1	A	644	ASN
1	A	654	GLN
1	A	687	ASN
1	A	694	HIS
1	A	734	GLN
1	A	738	GLN
1	A	753	GLN
1	A	800	HIS
1	A	836	GLN
2	B	428	GLN
2	B	448	GLN
2	B	495	ASN
2	B	577	ASN

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Mol	Chain	Res	Type
1	C	21	ASN
1	C	27	HIS
1	C	91	GLN
1	C	108	HIS
1	C	138	GLN
1	C	201	GLN
1	C	251	ASN
1	C	371	ASN
1	C	414	GLN
1	C	452	ASN
1	C	497	ASN
1	C	528	HIS
1	C	537	HIS
1	C	547	HIS
1	C	549	HIS
1	C	581	ASN
1	C	583	HIS
1	C	584	ASN
1	C	644	ASN
1	C	687	ASN
1	C	694	HIS
1	C	734	GLN
1	C	738	GLN
1	C	753	GLN
1	C	800	HIS
1	C	836	GLN
2	D	448	GLN
2	D	460	GLN
2	D	577	ASN
1	E	27	HIS
1	E	91	GLN
1	E	138	GLN
1	E	201	GLN
1	E	371	ASN
1	E	528	HIS
1	E	537	HIS
1	E	547	HIS
1	E	581	ASN
1	E	583	HIS
1	E	584	ASN
1	E	644	ASN
1	E	654	GLN

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Mol	Chain	Res	Type
1	E	687	ASN
1	E	694	HIS
1	E	734	GLN
1	E	753	GLN
1	E	800	HIS
1	E	836	GLN
2	F	428	GLN
2	F	448	GLN
2	F	460	GLN
2	F	577	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

3 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
1	DDE	A	699	1	5,10,21	0.57	0	3,12,30	1.88	2 (66%)
1	DDE	C	699	1	5,10,21	0.49	0	3,12,30	1.84	2 (66%)
1	DDE	E	699	1	5,10,21	0.53	0	3,12,30	1.74	2 (66%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	DDE	A	699	1	-	0/4/6/23	0/1/1/1
1	DDE	C	699	1	-	0/4/6/23	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	DDE	E	699	1	-	0/4/6/23	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	699	DDE	O-C-CA	-2.33	119.43	125.49
1	C	699	DDE	O-C-CA	-2.19	119.79	125.49
1	E	699	DDE	O-C-CA	-2.01	120.26	125.49
1	E	699	DDE	CD2-NE2-CE1	2.09	109.00	105.71
1	A	699	DDE	CD2-NE2-CE1	2.12	109.05	105.71
1	C	699	DDE	CD2-NE2-CE1	2.16	109.11	105.71

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	699	DDE	1	0
1	C	699	DDE	1	0
1	E	699	DDE	4	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	822/842 (97%)	-0.20	14 (1%) 73 51	8, 57, 85, 104	0
1	C	822/842 (97%)	0.12	40 (4%) 33 14	10, 69, 123, 135	0
1	E	822/842 (97%)	0.82	162 (19%) 1 0	6, 105, 128, 146	0
2	B	207/207 (100%)	-0.58	2 (0%) 84 68	5, 24, 57, 74	0
2	D	207/207 (100%)	-0.59	0 100 100	5, 23, 61, 76	0
2	F	207/207 (100%)	-0.52	1 (0%) 91 82	10, 31, 63, 82	0
All	All	3087/3147 (98%)	0.08	219 (7%) 19 7	5, 60, 123, 146	0

All (219) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	107	GLY	8.8
1	E	189	VAL	7.3
1	C	551	GLY	6.7
1	C	251	ASN	6.3
1	E	759	GLN	6.1
1	E	194	ASP	5.9
1	E	554	LEU	5.8
1	E	193	ALA	5.8
1	E	546	GLU	5.7
1	E	257	TRP	5.5
1	E	343	PRO	5.4
1	C	499	ASN	5.4
1	E	47	SER	5.3
1	E	97	SER	5.2
1	E	737	GLU	5.2
1	E	280	PRO	5.1
1	E	108	HIS	5.1
1	E	276	PHE	5.0
1	C	291	PHE	4.9

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Mol	Chain	Res	Type	RSRZ
1	C	296	ILE	4.9
1	E	33	SER	4.7
1	E	143	LEU	4.6
1	E	231	LYS	4.6
1	C	168	GLN	4.5
1	E	179	ALA	4.4
1	C	493	VAL	4.3
1	E	175	TYR	4.3
1	E	313	ASP	4.1
1	E	240	MET	4.1
1	E	256	LYS	4.1
1	E	110	ASP	4.1
1	E	146	ALA	4.1
1	E	67	GLY	4.1
1	E	314	LEU	4.0
1	E	245	TRP	3.9
1	E	525	SER	3.9
1	E	339	VAL	3.9
1	E	5	THR	3.9
1	C	552	VAL	3.8
1	C	108	HIS	3.8
1	E	155	VAL	3.8
1	E	89	ILE	3.8
1	E	167	LEU	3.7
1	E	335	LEU	3.7
1	E	80	GLU	3.7
1	C	307	LEU	3.7
1	E	310	ASP	3.7
1	E	279	ASP	3.6
1	E	99	LEU	3.6
1	E	551	GLY	3.5
1	E	317	LYS	3.5
1	C	544	ASP	3.4
1	E	398	GLY	3.4
1	E	269	LEU	3.4
1	E	348	ALA	3.4
1	C	306	VAL	3.4
1	E	501	LEU	3.4
1	A	47	SER	3.4
1	E	392	GLY	3.4
2	B	519	ALA	3.4
1	E	334	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
1	E	777	SER	3.3
1	E	349	GLN	3.3
1	C	549	HIS	3.3
1	E	201	GLN	3.3
1	E	499	ASN	3.3
1	C	264	ALA	3.3
1	E	444	PRO	3.3
1	E	510	ARG	3.2
1	C	547	HIS	3.2
1	C	300	LEU	3.2
1	E	311	GLU	3.1
1	E	134	GLY	3.1
1	E	78	TYR	3.1
1	E	273	PHE	3.1
1	E	290	ASN	3.1
1	C	555	LYS	3.1
1	A	398	GLY	3.1
1	E	553	PRO	3.1
1	E	243	ARG	3.1
1	E	166	GLU	3.1
1	E	242	ASP	3.1
1	E	96	ASN	3.0
1	C	323	VAL	3.0
1	E	132	ILE	3.0
1	C	29	ASP	3.0
1	E	200	VAL	3.0
1	E	494	GLU	3.0
1	E	784	LEU	3.0
1	A	33	SER	3.0
1	E	315	GLU	3.0
1	E	498	ALA	2.9
1	E	209	VAL	2.9
1	E	362	ASP	2.9
1	E	188	ILE	2.9
1	E	216	HIS	2.9
1	A	420	PRO	2.9
1	C	266	GLY	2.9
1	E	275	MET	2.9
1	E	766	PHE	2.9
1	E	302	LYS	2.9
1	E	258	THR	2.9
1	E	421	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	554	LEU	2.9
1	E	541	CYS	2.9
1	E	390	ASP	2.9
1	E	442	VAL	2.8
1	A	7	ASP	2.8
1	E	336	GLU	2.8
1	E	48	ALA	2.8
1	E	196	VAL	2.8
1	E	790	GLY	2.8
1	E	244	LEU	2.8
1	E	93	THR	2.8
1	E	745	SER	2.8
1	E	758	GLU	2.8
1	C	7	ASP	2.8
1	E	356	LEU	2.8
1	E	32	LYS	2.7
1	E	360	PRO	2.7
1	E	111	PHE	2.7
1	E	230	ALA	2.7
1	E	255	LYS	2.7
1	E	308	LYS	2.7
1	C	504	LEU	2.7
1	C	263	ASP	2.7
1	A	46	ILE	2.7
1	E	7	ASP	2.7
1	A	495	VAL	2.7
1	E	239	LYS	2.6
1	E	68	ILE	2.6
1	E	419	VAL	2.6
1	E	474	THR	2.6
1	E	472	SER	2.6
1	E	126	LEU	2.6
1	E	301	GLU	2.6
1	E	757	GLU	2.6
1	C	299	LEU	2.6
1	E	187	VAL	2.6
1	E	420	PRO	2.6
1	E	277	ILE	2.5
1	A	5	THR	2.5
1	E	316	GLY	2.5
1	E	197	LEU	2.5
1	E	522	MET	2.5

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Mol	Chain	Res	Type	RSRZ
1	E	391	LYS	2.5
1	E	781	THR	2.5
1	E	158	ASN	2.5
1	E	477	ASN	2.5
1	E	418	TYR	2.5
1	E	221	THR	2.5
1	A	107	GLY	2.4
1	E	761	PRO	2.4
1	E	367	ILE	2.4
1	E	452	ASN	2.4
1	E	260	LYS	2.4
1	A	392	GLY	2.4
1	E	770	ALA	2.4
1	E	82	SER	2.4
1	E	20	ARG	2.4
1	E	764	PRO	2.4
1	C	107	GLY	2.4
1	E	228	ARG	2.4
1	E	94	ASP	2.3
1	E	294	ASP	2.3
1	C	252	PRO	2.3
1	E	476	HIS	2.3
1	C	548	ASP	2.3
1	C	233	PHE	2.3
1	E	46	ILE	2.3
1	E	358	GLU	2.3
1	E	443	GLU	2.3
1	C	216	HIS	2.3
1	E	338	ILE	2.3
1	E	366	CYS	2.3
1	C	292	LYS	2.3
1	C	553	PRO	2.3
1	E	192	TYR	2.3
1	E	131	THR	2.3
1	C	236	ASP	2.3
1	E	738	GLN	2.3
1	E	195	GLU	2.3
1	E	254	THR	2.3
1	E	306	VAL	2.3
1	E	137	VAL	2.2
1	A	763	THR	2.2
1	E	163	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	309	GLY	2.2
1	C	270	GLU	2.2
1	C	362	ASP	2.2
1	C	513	LYS	2.2
1	E	232	LYS	2.2
1	A	361	ALA	2.2
1	E	113	SER	2.2
1	C	294	ASP	2.2
1	A	233	PHE	2.1
1	E	455	GLY	2.1
1	C	556	ILE	2.1
1	C	293	LYS	2.1
1	E	31	GLY	2.1
1	E	298	VAL	2.1
1	E	151	ILE	2.1
1	E	127	VAL	2.1
1	E	263	ASP	2.1
1	A	417	ASN	2.1
1	E	154	VAL	2.1
1	E	747	LEU	2.1
1	E	186	ASN	2.1
1	E	363	ASP	2.1
2	F	519	ALA	2.0
1	E	165	LEU	2.0
1	E	261	ASP	2.0
1	E	21	ASN	2.0
1	E	526	GLY	2.0
1	E	24	VAL	2.0
2	B	521	PRO	2.0
1	C	301	GLU	2.0
1	E	424	ASP	2.0
1	E	417	ASN	2.0

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

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
1	DDE	A	699	10/21	0.96	0.12	-	40,42,44,45	0
1	DDE	C	699	10/21	0.95	0.14	-	43,47,48,50	0
1	DDE	E	699	10/21	0.93	0.16	-	44,48,49,50	0

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

There are no ligands in this entry.

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

There are no such residues in this entry.