



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:24 AM GMT

PDB ID : 3EIQ  
Title : Crystal structure of Pdcd4-eIF4A  
Authors : Loh, P.G.; Cheng, Z.; Song, H.  
Deposited on : 2008-09-17  
Resolution : 3.50 Å(reported)

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

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 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

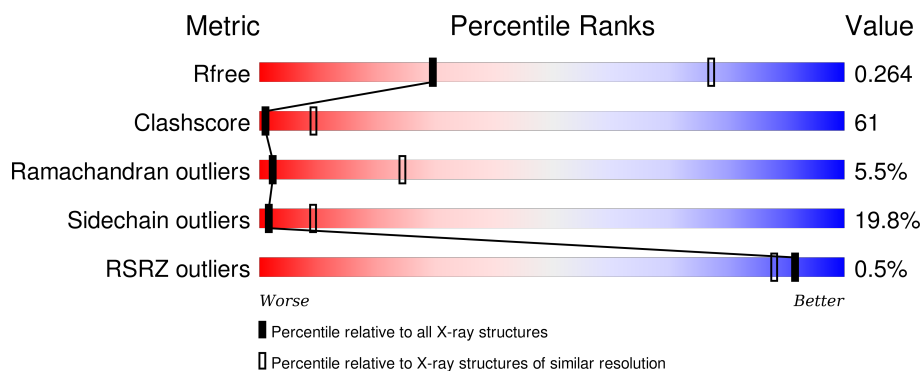
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	1051 (3.60-3.40)
Clashscore	102246	1157 (3.60-3.40)
Ramachandran outliers	100387	1120 (3.60-3.40)
Sidechain outliers	100360	1121 (3.60-3.40)
RSRZ outliers	91569	1058 (3.60-3.40)

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

Mol	Chain	Length	Quality of chain
1	A	414	<div> <div></div> <div>35% 37% 14% • 12%</div> </div>
1	D	414	<div> <div>%</div> <div>35% 38% 14% • 10%</div> </div>
2	C	358	<div> <div></div> <div>25% 42% 9% • 22%</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8080 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 Eukaryotic initiation factor 4A-I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	364	Total	C	N	O	S	0	0	0
			2923	1853	497	554	19			
1	D	371	Total	C	N	O	S	0	0	0
			2979	1887	511	562	19			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	GLY	-	EXPRESSION TAG	UNP P60842
A	-6	PRO	-	EXPRESSION TAG	UNP P60842
A	-5	LEU	-	EXPRESSION TAG	UNP P60842
A	-4	GLY	-	EXPRESSION TAG	UNP P60842
A	-3	SER	-	EXPRESSION TAG	UNP P60842
A	-2	PRO	-	EXPRESSION TAG	UNP P60842
A	-1	GLU	-	EXPRESSION TAG	UNP P60842
A	0	PHE	-	EXPRESSION TAG	UNP P60842
D	-7	GLY	-	EXPRESSION TAG	UNP P60842
D	-6	PRO	-	EXPRESSION TAG	UNP P60842
D	-5	LEU	-	EXPRESSION TAG	UNP P60842
D	-4	GLY	-	EXPRESSION TAG	UNP P60842
D	-3	SER	-	EXPRESSION TAG	UNP P60842
D	-2	PRO	-	EXPRESSION TAG	UNP P60842
D	-1	GLU	-	EXPRESSION TAG	UNP P60842
D	0	PHE	-	EXPRESSION TAG	UNP P60842

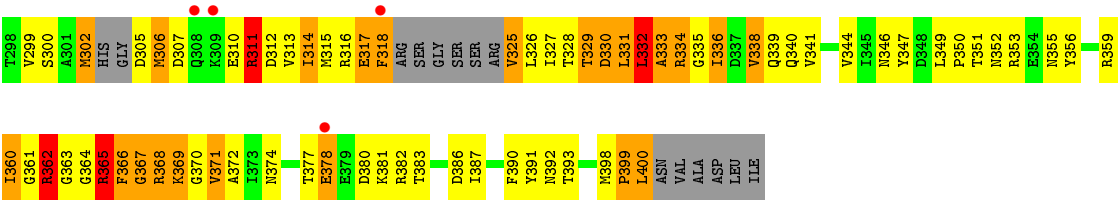
- Molecule 2 is a protein called Programmed cell death protein 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	278	Total	C	N	O	S	0	0	0
			2178	1380	359	424	15			

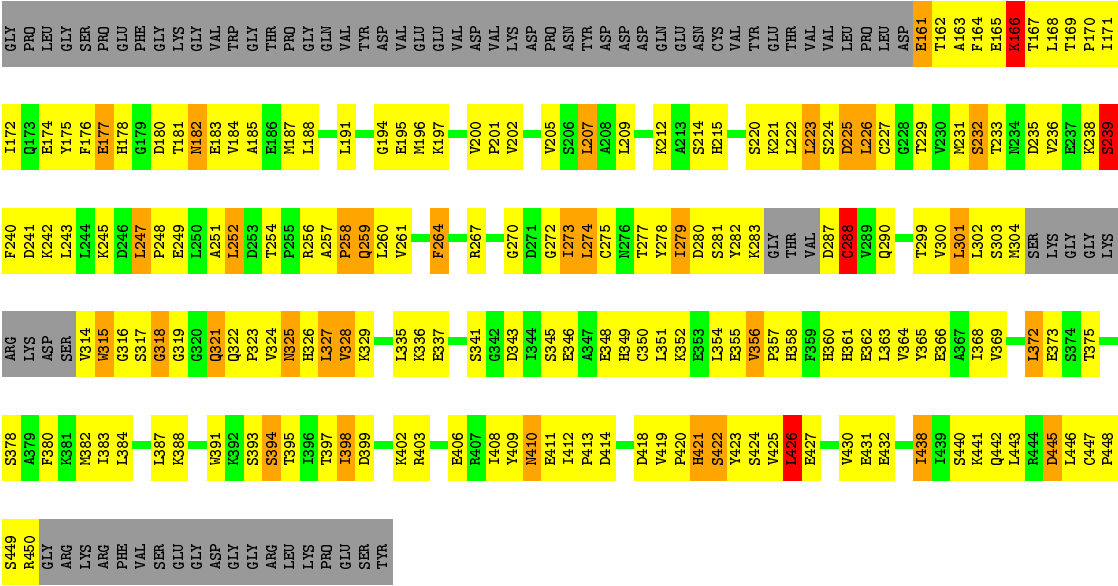
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	112	GLY	-	EXPRESSION TAG	UNP Q61823
C	113	PRO	-	EXPRESSION TAG	UNP Q61823
C	114	LEU	-	EXPRESSION TAG	UNP Q61823
C	115	GLY	-	EXPRESSION TAG	UNP Q61823
C	116	SER	-	EXPRESSION TAG	UNP Q61823
C	117	PRO	-	EXPRESSION TAG	UNP Q61823
C	118	GLU	-	EXPRESSION TAG	UNP Q61823
C	119	PHE	-	EXPRESSION TAG	UNP Q61823





● Molecule 2: Programmed cell death protein 4



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	198.36Å 198.36Å 198.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.91 – 3.50 29.90 – 3.50	Depositor EDS
% Data completeness (in resolution range)	99.8 (29.91-3.50) 100.0 (29.90-3.50)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.44 (at 3.47Å)	Xtriage
Refinement program	REFMAC 5.5.0066	Depositor
R, $R_{free}$	0.220 , 0.269 0.217 , 0.264	Depositor DCC
$R_{free}$ test set	1670 reflections (5.34%)	DCC
Wilson B-factor (Å <sup>2</sup> )	93.8	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 60.9	EDS
Estimated twinning fraction	0.029 for l,-k,h	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 32972 reflections (0.003%)	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	8080	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.07% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	0.95	3/2963 (0.1%)	1.01	8/3998 (0.2%)
1	D	0.96	1/3022 (0.0%)	1.07	11/4077 (0.3%)
2	C	0.72	0/2213	0.91	4/2989 (0.1%)
All	All	0.90	4/8198 (0.0%)	1.01	23/11064 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	D	0	1
All	All	0	3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	80	THR	CA-CB	5.42	1.67	1.53
1	A	200	PHE	CE1-CZ	5.40	1.47	1.37
1	A	66	CYS	CB-SG	-5.35	1.73	1.81
1	A	200	PHE	CG-CD2	5.04	1.46	1.38

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	365	ARG	NE-CZ-NH1	-13.21	113.69	120.30
1	D	365	ARG	NE-CZ-NH2	10.91	125.75	120.30
1	A	137	GLY	N-CA-C	-8.85	90.99	113.10
2	C	351	LEU	CA-CB-CG	-8.29	96.23	115.30
1	A	58	ILE	CG1-CB-CG2	-7.30	95.34	111.40
1	D	362	ARG	CB-CA-C	-7.05	96.30	110.40
1	D	137	GLY	N-CA-C	-7.05	95.47	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	148	GLN	N-CA-C	-6.80	92.63	111.00
1	A	165	MET	CG-SD-CE	-6.07	90.49	100.20
1	D	90	ILE	CG1-CB-CG2	-6.02	98.16	111.40
2	C	327	LEU	CB-CG-CD2	-5.95	100.88	111.00
1	D	332	LEU	CA-CB-CG	-5.83	101.89	115.30
1	A	362	ARG	CB-CG-CD	-5.76	96.62	111.60
1	D	29	GLU	N-CA-C	-5.62	95.83	111.00
1	D	58	ILE	CG1-CB-CG2	-5.60	99.09	111.40
1	D	165	MET	CG-SD-CE	-5.58	91.28	100.20
1	A	148	GLN	N-CA-C	-5.44	96.31	111.00
1	A	80	THR	N-CA-C	-5.44	96.32	111.00
2	C	446	LEU	CA-CB-CG	5.33	127.55	115.30
1	A	230	ASP	CB-CA-C	-5.30	99.80	110.40
1	A	371	VAL	CB-CA-C	-5.11	101.70	111.40
1	D	80	THR	N-CA-CB	5.05	119.90	110.30
2	C	267	ARG	NE-CZ-NH2	-5.03	117.78	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	329	THR	Peptide
1	A	370	GLY	Peptide
1	D	150	GLU	Peptide

## 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	2923	0	2962	368	1
1	D	2979	0	3020	380	1
2	C	2178	0	2183	267	0
All	All	8080	0	8165	985	1

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 61.

All (985) 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:D:367:GLY:HA2	1:D:368:ARG:CG	1.27	1.62
1:D:338:VAL:CG2	1:D:362:ARG:HH22	1.19	1.54
1:D:135:ILE:CG2	1:D:136:GLY:HA3	1.34	1.54
1:A:135:ILE:CG2	1:A:136:GLY:HA3	1.40	1.51
1:A:338:VAL:CG2	1:A:362:ARG:HH22	1.19	1.51
1:A:338:VAL:C	1:A:362:ARG:HH12	1.14	1.50
1:A:150:GLU:CB	1:A:151:ALA:HB2	1.44	1.48
1:D:135:ILE:HG22	1:D:136:GLY:CA	1.43	1.44
1:D:367:GLY:CA	1:D:368:ARG:HG3	1.46	1.44
1:D:338:VAL:C	1:D:362:ARG:HH12	1.17	1.43
1:D:339:GLN:HG2	1:D:362:ARG:CZ	1.51	1.40
1:A:135:ILE:HG22	1:A:136:GLY:CA	1.50	1.39
1:A:150:GLU:HB2	1:A:151:ALA:CB	1.55	1.34
1:D:367:GLY:CA	1:D:368:ARG:CG	1.99	1.34
1:A:339:GLN:OE1	1:A:362:ARG:HD3	1.16	1.33
1:A:338:VAL:HG23	1:A:362:ARG:NH2	0.98	1.29
1:D:338:VAL:HG23	1:D:362:ARG:NH2	0.95	1.28
1:A:339:GLN:HG2	1:A:362:ARG:NE	1.50	1.25
1:A:339:GLN:HG2	1:A:362:ARG:CZ	1.66	1.24
1:A:339:GLN:CA	1:A:362:ARG:NH1	2.01	1.24
2:C:223:LEU:O	2:C:273:ILE:CD1	1.86	1.24
1:A:339:GLN:N	1:A:362:ARG:NH1	1.86	1.24
1:A:118:LYS:HD3	1:A:307:ASP:OD2	1.34	1.23
1:D:339:GLN:HG2	1:D:362:ARG:NE	1.24	1.22
1:A:339:GLN:CA	1:A:362:ARG:HH11	1.51	1.22
1:D:338:VAL:C	1:D:362:ARG:NH1	1.89	1.21
1:D:150:GLU:HB2	1:D:151:ALA:CB	1.69	1.21
2:C:321:GLN:OE1	2:C:321:GLN:N	1.72	1.21
1:D:339:GLN:CG	1:D:362:ARG:NE	2.02	1.21
1:A:134:CYS:O	1:A:135:ILE:HG12	1.38	1.20
1:A:338:VAL:C	1:A:362:ARG:NH1	1.94	1.18
1:D:235:LEU:O	1:D:235:LEU:HD13	1.41	1.17
2:C:164:PHE:CE1	2:C:168:LEU:HD13	1.79	1.17
1:D:240:GLU:HA	1:D:241:LEU:HB2	1.27	1.16
1:A:339:GLN:HA	1:A:362:ARG:NH1	1.57	1.15
1:D:99:LYS:HD3	1:D:150:GLU:OE1	1.45	1.13
1:A:137:GLY:HA2	1:A:140:VAL:HG23	1.29	1.13
1:A:332:LEU:N	1:A:332:LEU:HD12	1.59	1.12
1:D:367:GLY:HA2	1:D:368:ARG:HG2	1.16	1.12
1:D:332:LEU:N	1:D:332:LEU:HD12	1.58	1.12
2:C:317:SER:HB2	2:C:318:GLY:HA3	1.24	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:365:ARG:HA	1:D:367:GLY:N	1.63	1.11
1:A:311:ARG:HH11	1:A:311:ARG:CG	1.63	1.11
1:D:313:VAL:O	1:D:317:GLU:HB2	1.49	1.10
1:D:339:GLN:N	1:D:362:ARG:NH1	2.00	1.09
1:D:150:GLU:HB2	1:D:151:ALA:HB2	1.11	1.09
1:D:314:ILE:HG22	1:D:336:ILE:HG22	1.32	1.09
1:D:339:GLN:HA	1:D:362:ARG:HH11	1.04	1.08
1:D:367:GLY:HA3	1:D:368:ARG:HG3	1.17	1.08
1:A:354:GLU:OE2	2:C:357:PRO:HD2	1.51	1.08
2:C:161:GLU:HG3	2:C:162:THR:N	1.46	1.08
1:D:361:GLY:O	1:D:362:ARG:HG2	1.50	1.07
1:A:110:ARG:HD3	1:A:135:ILE:HG23	1.11	1.07
2:C:317:SER:HB2	2:C:318:GLY:CA	1.82	1.07
1:D:236:VAL:HG22	1:D:236:VAL:O	1.54	1.07
1:D:134:CYS:O	1:D:135:ILE:HG12	1.54	1.07
1:A:311:ARG:HH11	1:A:311:ARG:HG3	0.98	1.07
1:D:338:VAL:CG2	1:D:362:ARG:NH2	1.87	1.07
1:D:241:LEU:O	1:D:242:THR:HG22	1.52	1.07
1:D:314:ILE:CG2	1:D:336:ILE:HG22	1.85	1.06
2:C:287:ASP:O	2:C:288:CYS:HB3	1.52	1.06
1:D:339:GLN:CA	1:D:362:ARG:NH1	2.19	1.05
1:A:136:GLY:H	1:A:137:GLY:CA	1.68	1.05
1:D:339:GLN:HA	1:D:362:ARG:NH1	1.70	1.05
1:D:136:GLY:H	1:D:137:GLY:CA	1.69	1.05
1:A:22:VAL:CG1	1:A:75:GLN:OE1	2.05	1.05
1:D:110:ARG:CD	1:D:135:ILE:HG23	1.86	1.04
1:D:237:LYS:HG2	1:D:238:LYS:H	1.20	1.04
1:D:101:THR:HB	1:D:152:PRO:O	1.57	1.04
1:D:360:ILE:HG23	1:D:361:GLY:H	1.21	1.04
1:A:339:GLN:CD	1:A:362:ARG:HD3	1.79	1.03
1:D:311:ARG:HG3	1:D:311:ARG:HH11	1.21	1.03
1:A:101:THR:HB	1:A:152:PRO:O	1.55	1.03
1:D:267:TYR:CD2	1:D:297:PHE:CD2	2.47	1.03
1:D:110:ARG:HD3	1:D:135:ILE:HG23	1.07	1.03
1:A:267:TYR:CD2	1:A:297:PHE:CD2	2.45	1.03
1:A:267:TYR:CD2	1:A:297:PHE:HD2	1.75	1.03
1:D:240:GLU:HA	1:D:241:LEU:CB	1.88	1.03
1:A:110:ARG:HD3	1:A:135:ILE:CG2	1.88	1.02
1:A:269:THR:O	1:A:270:LEU:HD12	1.58	1.02
1:D:110:ARG:HD3	1:D:135:ILE:CG2	1.88	1.02
1:D:150:GLU:CB	1:D:151:ALA:HB2	1.89	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:314:ILE:O	1:D:318:PHE:HB2	1.57	1.02
1:D:267:TYR:CD2	1:D:297:PHE:HD2	1.77	1.01
2:C:426:LEU:O	2:C:430:VAL:HG23	1.60	1.01
1:A:339:GLN:HG2	1:A:362:ARG:CD	1.91	1.01
1:A:338:VAL:CG2	1:A:362:ARG:NH2	1.95	1.01
1:D:311:ARG:HH11	1:D:311:ARG:CG	1.71	1.01
1:D:368:ARG:O	1:D:369:LYS:HB2	1.58	1.00
1:A:110:ARG:CD	1:A:135:ILE:HG23	1.91	1.00
1:A:339:GLN:OE1	1:A:362:ARG:CD	2.10	0.99
1:D:367:GLY:HA2	1:D:368:ARG:CB	1.87	0.99
1:A:361:GLY:O	1:A:362:ARG:HG2	1.61	0.99
2:C:420:PRO:O	2:C:421:HIS:HB2	1.63	0.99
1:A:302:MET:CE	1:A:310:GLU:HG2	1.93	0.99
1:D:237:LYS:HG2	1:D:238:LYS:N	1.75	0.98
1:D:147:LEU:HD13	1:D:165:MET:HE3	1.45	0.98
1:A:314:ILE:CG2	1:A:336:ILE:HG22	1.92	0.98
1:D:302:MET:HG3	1:D:328:THR:HG22	1.45	0.98
1:D:137:GLY:HA2	1:D:140:VAL:HG23	1.44	0.98
1:D:65:PRO:HB3	1:D:232:ILE:HD11	1.45	0.97
2:C:161:GLU:CG	2:C:162:THR:N	2.25	0.97
1:A:311:ARG:HG3	1:A:311:ARG:NH1	1.65	0.97
1:D:339:GLN:CG	1:D:362:ARG:CZ	2.40	0.97
2:C:402:LYS:HE2	2:C:406:GLU:OE2	1.66	0.96
1:D:362:ARG:HG3	1:D:369:LYS:HG3	1.46	0.96
2:C:372:LEU:HD21	2:C:426:LEU:HB2	1.48	0.96
1:A:339:GLN:N	1:A:362:ARG:HH12	1.53	0.95
1:A:22:VAL:HG12	1:A:75:GLN:NE2	1.80	0.95
2:C:227:CYS:CB	2:C:273:ILE:HD11	1.97	0.95
1:D:57:ALA:HB1	1:D:236:VAL:HG21	1.48	0.95
1:D:243:LEU:HD12	1:D:243:LEU:H	1.30	0.95
2:C:349:HIS:CE1	1:D:283:ARG:HH22	1.85	0.95
1:A:378:GLU:HA	1:A:378:GLU:OE1	1.67	0.95
1:D:22:VAL:HG12	1:D:75:GLN:NE2	1.79	0.95
2:C:384:LEU:CD2	2:C:432:GLU:HB3	1.97	0.95
1:A:339:GLN:HA	1:A:362:ARG:HH11	0.80	0.94
1:A:23:ILE:HG23	1:A:216:MET:HG3	1.49	0.94
1:A:95:GLU:H	1:A:102:GLN:HE22	1.15	0.94
1:A:302:MET:O	1:A:332:LEU:HD21	1.66	0.94
2:C:402:LYS:O	2:C:406:GLU:HG3	1.67	0.94
2:C:164:PHE:CD2	2:C:196:MET:CE	2.51	0.94
1:A:79:GLY:HA2	1:A:82:LYS:HB3	1.50	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:VAL:HG12	1:A:75:GLN:HE22	1.30	0.93
2:C:442:GLN:HA	2:C:445:ASP:HB2	1.50	0.93
1:D:134:CYS:C	1:D:135:ILE:HG12	1.87	0.92
2:C:325:ASN:HA	2:C:328:VAL:HG23	1.49	0.92
2:C:227:CYS:HB2	2:C:273:ILE:HD11	1.52	0.92
2:C:212:LYS:H	2:C:215:HIS:HD2	1.14	0.92
1:A:136:GLY:H	1:A:137:GLY:HA2	1.34	0.92
1:A:339:GLN:CG	1:A:362:ARG:CD	2.47	0.92
1:A:314:ILE:O	1:A:318:PHE:HB2	1.69	0.92
2:C:178:HIS:HD2	2:C:180:ASP:H	1.16	0.91
1:A:360:ILE:HG23	1:A:361:GLY:H	1.35	0.91
1:D:314:ILE:HG21	1:D:335:GLY:O	1.69	0.91
1:D:378:GLU:HA	1:D:378:GLU:OE1	1.70	0.91
1:D:136:GLY:N	1:D:137:GLY:CA	2.31	0.91
1:A:307:ASP:O	1:A:311:ARG:HB2	1.71	0.91
1:A:134:CYS:C	1:A:135:ILE:CG1	2.40	0.91
1:A:302:MET:HE1	1:A:310:GLU:HG2	1.53	0.91
1:A:329:THR:HG21	2:C:174:GLU:OE1	1.71	0.91
1:D:23:ILE:HG23	1:D:216:MET:HG3	1.51	0.90
1:D:235:LEU:O	1:D:235:LEU:CD1	2.20	0.90
2:C:321:GLN:OE1	2:C:321:GLN:CA	2.19	0.90
2:C:223:LEU:O	2:C:273:ILE:HD11	1.69	0.90
1:D:22:VAL:HG12	1:D:75:GLN:HE22	1.35	0.90
1:D:353:ARG:HG2	1:D:387:ILE:HD13	1.54	0.90
1:D:242:THR:O	1:D:363:GLY:HA2	1.71	0.89
1:D:311:ARG:HG3	1:D:311:ARG:NH1	1.79	0.89
1:D:95:GLU:H	1:D:102:GLN:HE22	1.19	0.89
1:A:236:VAL:HG12	1:A:236:VAL:O	1.72	0.89
1:A:136:GLY:N	1:A:137:GLY:CA	2.30	0.89
1:D:79:GLY:HA2	1:D:82:LYS:HB3	1.54	0.89
1:D:367:GLY:CA	1:D:368:ARG:CB	2.42	0.89
1:D:368:ARG:O	1:D:369:LYS:CB	2.21	0.89
2:C:384:LEU:HD21	2:C:432:GLU:HB3	1.53	0.89
1:D:136:GLY:H	1:D:137:GLY:HA2	1.34	0.89
1:A:272:ILE:HD12	1:A:273:THR:H	1.36	0.89
1:D:338:VAL:HG23	1:D:362:ARG:CZ	2.03	0.89
1:A:314:ILE:HG22	1:A:336:ILE:HG22	1.52	0.88
1:A:267:TYR:CE2	1:A:297:PHE:HD2	1.91	0.88
1:D:272:ILE:HD12	1:D:273:THR:H	1.35	0.88
1:D:332:LEU:N	1:D:332:LEU:CD1	2.32	0.88
1:D:267:TYR:CE2	1:D:297:PHE:HD2	1.92	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:269:THR:O	1:D:270:LEU:HD12	1.73	0.88
1:D:135:ILE:CB	1:D:136:GLY:HA3	1.97	0.87
1:A:380:ASP:O	1:A:383:THR:HG22	1.73	0.87
1:A:307:ASP:O	1:A:311:ARG:CB	2.23	0.87
1:A:99:LYS:HD3	1:A:150:GLU:OE1	1.73	0.87
1:D:241:LEU:O	1:D:242:THR:CG2	2.23	0.86
2:C:164:PHE:CE1	2:C:168:LEU:CD1	2.59	0.85
1:A:137:GLY:CA	1:A:140:VAL:HG23	2.05	0.85
1:A:241:LEU:N	1:A:241:LEU:HD23	1.90	0.85
1:A:134:CYS:C	1:A:135:ILE:HG12	1.96	0.85
1:D:380:ASP:O	1:D:383:THR:HG22	1.76	0.85
1:D:22:VAL:CG1	1:D:75:GLN:OE1	2.24	0.85
2:C:248:PRO:HA	2:C:290:GLN:OE1	1.77	0.85
1:D:77:GLN:OE1	1:D:77:GLN:HA	1.76	0.84
2:C:224:SER:HA	2:C:273:ILE:HD12	1.58	0.84
2:C:301:LEU:HA	2:C:304:MET:HE1	1.59	0.84
1:A:134:CYS:O	1:A:135:ILE:CG1	2.23	0.84
1:A:77:GLN:HA	1:A:77:GLN:OE1	1.77	0.84
1:A:302:MET:CE	1:A:310:GLU:CG	2.56	0.84
1:D:239:GLU:C	1:D:241:LEU:HG	1.99	0.83
1:A:354:GLU:CD	2:C:357:PRO:HD2	1.99	0.83
2:C:247:LEU:HD11	2:C:258:PRO:HA	1.57	0.83
2:C:398:ILE:HG12	2:C:399:ASP:N	1.86	0.83
1:D:364:GLY:O	1:D:365:ARG:C	2.17	0.83
2:C:449:SER:O	2:C:450:ARG:HB3	1.77	0.83
1:A:242:THR:O	1:A:242:THR:CG2	2.26	0.83
2:C:380:PHE:HE1	2:C:432:GLU:HG3	1.42	0.82
1:A:306:MET:O	1:A:306:MET:HG2	1.77	0.82
1:A:339:GLN:CG	1:A:362:ARG:NE	2.40	0.82
2:C:223:LEU:O	2:C:273:ILE:HD12	1.78	0.82
2:C:164:PHE:CD2	2:C:196:MET:HE1	2.12	0.82
1:D:311:ARG:HH11	1:D:311:ARG:CB	1.91	0.82
1:D:23:ILE:CG2	1:D:216:MET:HG3	2.09	0.82
1:D:147:LEU:HD13	1:D:165:MET:CE	2.10	0.82
1:D:237:LYS:CG	1:D:238:LYS:H	1.91	0.82
2:C:168:LEU:HD22	2:C:200:VAL:HG22	1.58	0.81
1:D:353:ARG:HE	1:D:386:ASP:HB3	1.45	0.81
1:A:332:LEU:H	1:A:332:LEU:HD12	1.41	0.81
1:D:317:GLU:OE2	1:D:317:GLU:HA	1.79	0.81
1:D:149:MET:HA	1:D:150:GLU:HB3	1.63	0.81
1:D:105:VAL:HB	1:D:180:VAL:HG13	1.61	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:338:VAL:HG23	1:D:362:ARG:HH21	1.45	0.81
1:A:151:ALA:H	1:A:152:PRO:CD	1.91	0.81
1:A:135:ILE:CB	1:A:136:GLY:HA3	2.02	0.80
1:D:267:TYR:CE2	1:D:297:PHE:CD2	2.69	0.80
1:D:255:ARG:HG3	1:D:258:TRP:CE3	2.16	0.80
1:A:242:THR:HG23	1:A:244:GLU:HB2	1.63	0.80
1:A:147:LEU:CD1	1:A:165:MET:CE	2.59	0.80
2:C:337:GLU:OE1	1:D:282:ARG:HD3	1.82	0.80
1:A:22:VAL:HG12	1:A:75:GLN:CD	2.02	0.80
2:C:164:PHE:CD2	2:C:196:MET:HE2	2.15	0.80
1:D:241:LEU:C	1:D:242:THR:CG2	2.50	0.80
1:D:307:ASP:O	1:D:311:ARG:CB	2.30	0.79
1:D:314:ILE:CG2	1:D:336:ILE:CG2	2.59	0.79
1:D:332:LEU:H	1:D:332:LEU:HD12	1.45	0.79
1:D:91:LEU:HD22	1:D:127:MET:CE	2.12	0.79
1:A:22:VAL:HG12	1:A:75:GLN:OE1	1.81	0.79
1:A:168:ARG:O	1:A:169:ARG:HB2	1.83	0.79
1:A:314:ILE:HG23	1:A:336:ILE:HG22	1.64	0.79
1:D:147:LEU:CD1	1:D:165:MET:CE	2.60	0.79
1:D:307:ASP:O	1:D:311:ARG:N	2.15	0.79
2:C:164:PHE:CD1	2:C:168:LEU:HD13	2.18	0.79
1:D:332:LEU:O	1:D:335:GLY:N	2.16	0.79
2:C:164:PHE:CE2	2:C:196:MET:HE2	2.18	0.79
1:A:317:GLU:OE2	1:A:321:GLY:O	2.00	0.79
1:A:105:VAL:HB	1:A:180:VAL:HG13	1.63	0.79
1:D:360:ILE:HG23	1:D:361:GLY:N	1.98	0.78
1:D:134:CYS:C	1:D:135:ILE:CG1	2.52	0.78
1:A:278:PHE:HE1	1:A:333:ALA:HB2	1.48	0.78
2:C:164:PHE:HE1	2:C:168:LEU:HD13	1.45	0.78
1:D:307:ASP:O	1:D:311:ARG:HB2	1.84	0.78
1:D:302:MET:CA	1:D:305:ASP:OD2	2.32	0.78
2:C:168:LEU:CD2	2:C:200:VAL:HG22	2.14	0.78
1:D:278:PHE:HE1	1:D:333:ALA:HB2	1.47	0.78
1:A:302:MET:HE2	1:A:310:GLU:CG	2.14	0.77
1:A:22:VAL:HG11	1:A:75:GLN:OE1	1.82	0.77
2:C:325:ASN:HA	2:C:328:VAL:CG2	2.13	0.77
1:D:338:VAL:O	1:D:362:ARG:NH1	2.09	0.77
1:D:149:MET:HA	1:D:150:GLU:CB	2.15	0.77
2:C:380:PHE:CE1	2:C:432:GLU:HG3	2.19	0.77
1:A:360:ILE:HG13	1:A:372:ALA:CB	2.14	0.77
1:A:86:PHE:O	1:A:90:ILE:HG12	1.84	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:349:HIS:CD2	1:D:283:ARG:HH12	2.03	0.77
1:D:242:THR:O	1:D:242:THR:OG1	1.99	0.77
1:A:353:ARG:HG2	1:A:387:ILE:HD13	1.67	0.77
2:C:420:PRO:O	2:C:421:HIS:CB	2.29	0.76
2:C:349:HIS:CG	1:D:283:ARG:HH12	2.03	0.76
1:A:58:ILE:HG12	1:A:236:VAL:HG21	1.65	0.76
1:A:295:ARG:O	1:A:296:ASP:HB2	1.85	0.76
1:D:147:LEU:CD1	1:D:165:MET:HE1	2.15	0.76
1:D:82:LYS:HD3	1:D:212:LEU:HD22	1.68	0.76
1:D:365:ARG:HA	1:D:367:GLY:H	1.50	0.76
1:A:92:GLN:HG3	1:A:92:GLN:O	1.85	0.76
1:D:136:GLY:N	1:D:137:GLY:HA2	1.99	0.75
2:C:164:PHE:HE1	2:C:168:LEU:CD1	1.97	0.75
1:D:339:GLN:HG2	1:D:362:ARG:NH1	2.01	0.75
1:A:151:ALA:H	1:A:152:PRO:HD3	1.50	0.75
2:C:414:ASP:OD1	1:D:161:ARG:NH2	2.18	0.75
1:A:267:TYR:CE2	1:A:297:PHE:CD2	2.71	0.75
1:A:147:LEU:HD13	1:A:165:MET:HE3	1.66	0.75
1:A:200:PHE:CD1	1:A:227:PHE:CD1	2.75	0.75
1:D:22:VAL:HG12	1:D:75:GLN:CD	2.06	0.75
2:C:227:CYS:HB3	2:C:273:ILE:HD11	1.67	0.74
2:C:212:LYS:H	2:C:215:HIS:CD2	2.04	0.74
1:A:217:PRO:HD2	1:A:220:VAL:HB	1.69	0.74
1:D:399:PRO:O	1:D:400:LEU:CD1	2.36	0.74
2:C:431:GLU:OE1	2:C:431:GLU:HA	1.87	0.74
1:A:361:GLY:C	1:A:362:ARG:HG2	2.08	0.73
2:C:238:LYS:O	2:C:241:ASP:N	2.21	0.73
1:D:101:THR:CB	1:D:152:PRO:O	2.36	0.73
1:D:150:GLU:HB2	1:D:151:ALA:HB3	1.68	0.73
1:A:147:LEU:CD1	1:A:165:MET:HE1	2.19	0.73
1:D:332:LEU:H	1:D:332:LEU:CD1	2.00	0.73
1:A:339:GLN:CG	1:A:362:ARG:CZ	2.58	0.73
1:D:135:ILE:HA	1:D:161:ARG:NH1	2.04	0.73
1:D:346:ASN:HD22	1:D:374:ASN:HD21	1.36	0.72
1:A:361:GLY:O	1:A:362:ARG:CG	2.36	0.72
1:D:353:ARG:O	1:D:391:TYR:OH	2.07	0.72
1:A:23:ILE:CG2	1:A:216:MET:HG3	2.18	0.72
1:D:255:ARG:HD3	1:D:257:GLU:OE1	1.89	0.72
2:C:178:HIS:CD2	2:C:180:ASP:H	2.06	0.72
1:A:200:PHE:CE2	1:A:227:PHE:CD2	2.78	0.72
1:A:204:ASN:C	1:A:206:ASN:H	1.93	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:314:ILE:HG23	1:D:336:ILE:HG22	1.72	0.72
1:A:22:VAL:CG1	1:A:75:GLN:CD	2.57	0.72
2:C:319:GLY:H	2:C:322:GLN:HG3	1.55	0.72
2:C:180:ASP:OD1	2:C:182:ASN:HB3	1.90	0.72
1:D:253:VAL:HG12	1:D:262:THR:HG21	1.73	0.71
1:A:200:PHE:CE1	1:A:227:PHE:HB3	2.25	0.71
1:D:338:VAL:CB	1:D:362:ARG:HH22	2.02	0.71
1:A:302:MET:HG3	1:A:328:THR:HG22	1.73	0.71
1:D:240:GLU:N	1:D:241:LEU:HG	2.05	0.71
2:C:176:PHE:HB3	2:C:215:HIS:ND1	2.04	0.71
1:D:105:VAL:HG22	1:D:156:VAL:HG13	1.71	0.71
1:D:204:ASN:C	1:D:206:ASN:H	1.93	0.71
1:A:339:GLN:CG	1:A:362:ARG:HD3	2.18	0.71
1:A:267:TYR:HE1	1:A:325:VAL:HG11	1.56	0.71
1:A:302:MET:HE2	1:A:310:GLU:HG2	1.72	0.70
1:D:314:ILE:HG23	1:D:336:ILE:CG2	2.21	0.70
1:A:200:PHE:CZ	1:A:227:PHE:CG	2.78	0.70
1:D:365:ARG:NH2	1:D:366:PHE:CZ	2.60	0.70
1:D:255:ARG:HG3	1:D:258:TRP:CZ3	2.27	0.70
1:A:317:GLU:OE2	1:A:317:GLU:HA	1.91	0.70
1:A:333:ALA:O	1:A:336:ILE:HD13	1.91	0.70
2:C:223:LEU:O	2:C:273:ILE:HD13	1.89	0.70
1:A:338:VAL:HG23	1:A:362:ARG:HH21	1.46	0.70
1:A:319:ARG:O	1:A:320:SER:HB3	1.92	0.70
1:A:255:ARG:HG3	1:A:258:TRP:CE3	2.26	0.70
1:A:333:ALA:HA	1:A:336:ILE:CD1	2.22	0.70
1:A:339:GLN:HG2	1:A:362:ARG:NH1	2.05	0.70
1:D:302:MET:O	1:D:332:LEU:HD21	1.91	0.70
1:D:365:ARG:NH2	1:D:366:PHE:CE1	2.60	0.69
1:A:272:ILE:HD12	1:A:273:THR:N	2.07	0.69
1:A:242:THR:CG2	1:A:244:GLU:HB2	2.21	0.69
1:A:251:ILE:HD13	1:A:398:MET:HB3	1.74	0.69
2:C:384:LEU:HD22	2:C:432:GLU:HB3	1.74	0.69
1:D:377:THR:H	1:D:380:ASP:HB2	1.57	0.69
1:D:217:PRO:HD2	1:D:220:VAL:HB	1.73	0.69
1:D:269:THR:C	1:D:270:LEU:HD12	2.12	0.69
2:C:365:TYR:O	2:C:369:VAL:HG23	1.92	0.69
1:A:161:ARG:NH2	2:C:249:GLU:OE2	2.26	0.69
1:A:56:SER:O	1:A:60:GLN:HG3	1.92	0.69
1:D:168:ARG:O	1:D:169:ARG:HB2	1.91	0.69
2:C:411:GLU:C	2:C:413:PRO:HD2	2.13	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:ILE:HA	1:A:161:ARG:NH1	2.07	0.69
1:D:221:LEU:O	1:D:224:THR:HB	1.93	0.69
1:D:311:ARG:O	1:D:315:MET:HB2	1.92	0.69
1:D:272:ILE:HD12	1:D:273:THR:N	2.07	0.69
2:C:161:GLU:O	2:C:164:PHE:CB	2.41	0.68
1:A:23:ILE:H	1:A:75:GLN:HE22	1.40	0.68
1:A:360:ILE:HG23	1:A:361:GLY:N	2.07	0.68
1:D:136:GLY:H	1:D:137:GLY:HA3	1.58	0.68
2:C:346:GLU:HG2	1:D:281:THR:HG21	1.75	0.68
1:A:147:LEU:CD1	1:A:165:MET:HE3	2.22	0.68
1:A:339:GLN:OE1	1:A:362:ARG:HB2	1.92	0.68
1:A:101:THR:CB	1:A:152:PRO:O	2.38	0.68
1:A:105:VAL:HG22	1:A:156:VAL:HG13	1.76	0.68
1:A:267:TYR:CD2	1:A:297:PHE:CE2	2.80	0.68
1:A:311:ARG:CB	1:A:311:ARG:HH11	2.07	0.68
2:C:317:SER:CB	2:C:318:GLY:HA3	2.14	0.68
1:A:276:VAL:HG23	1:A:341:VAL:HG11	1.75	0.68
1:A:134:CYS:C	1:A:135:ILE:HG13	2.14	0.68
1:D:302:MET:C	1:D:305:ASP:OD2	2.32	0.68
2:C:319:GLY:HA3	2:C:354:LEU:O	1.94	0.68
1:A:390:PHE:HZ	2:C:356:VAL:HG12	1.59	0.67
1:D:313:VAL:CG1	1:D:326:LEU:HD11	2.24	0.67
2:C:222:LEU:O	2:C:226:LEU:HB2	1.95	0.67
1:D:302:MET:CE	1:D:310:GLU:HG2	2.25	0.67
1:D:276:VAL:HG23	1:D:341:VAL:HG11	1.77	0.67
1:A:333:ALA:HA	1:A:336:ILE:HD11	1.76	0.67
1:A:311:ARG:O	1:A:315:MET:HB2	1.95	0.66
1:D:241:LEU:C	1:D:242:THR:HG23	2.15	0.66
1:D:236:VAL:O	1:D:236:VAL:CG2	2.29	0.66
1:D:295:ARG:O	1:D:296:ASP:HB2	1.93	0.66
1:D:229:ARG:O	1:D:230:ASP:C	2.34	0.66
1:A:150:GLU:HB2	1:A:151:ALA:HB2	0.71	0.66
1:A:82:LYS:HD3	1:A:212:LEU:HD22	1.76	0.66
1:A:377:THR:H	1:A:380:ASP:HB2	1.58	0.66
2:C:202:VAL:HG11	2:C:242:LYS:HD3	1.77	0.66
1:D:149:MET:CA	1:D:150:GLU:CB	2.74	0.66
2:C:419:VAL:HB	2:C:422:SER:HB3	1.77	0.66
2:C:426:LEU:C	2:C:426:LEU:HD13	2.16	0.66
1:A:332:LEU:CD1	1:A:332:LEU:H	2.00	0.66
2:C:364:VAL:O	2:C:368:ILE:HG12	1.96	0.66
1:D:174:LYS:HE3	1:D:175:TYR:CE2	2.31	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:56:SER:O	1:D:60:GLN:HG3	1.94	0.66
1:D:366:PHE:O	1:D:367:GLY:O	2.13	0.66
2:C:317:SER:CB	2:C:318:GLY:CA	2.57	0.66
1:A:338:VAL:O	1:A:362:ARG:NH1	2.27	0.66
2:C:258:PRO:O	2:C:259:GLN:C	2.35	0.65
1:A:209:VAL:HG12	1:A:228:MET:CE	2.25	0.65
1:A:151:ALA:N	1:A:152:PRO:CD	2.57	0.65
2:C:161:GLU:CG	2:C:162:THR:H	2.09	0.65
1:A:200:PHE:CG	1:A:227:PHE:CE1	2.85	0.65
1:A:399:PRO:O	1:A:400:LEU:CD1	2.45	0.65
1:D:267:TYR:CD2	1:D:297:PHE:CE2	2.84	0.65
1:D:80:THR:H	1:D:82:LYS:H	1.44	0.65
1:A:269:THR:C	1:A:270:LEU:HD12	2.17	0.65
1:A:242:THR:O	1:A:242:THR:HG22	1.96	0.65
1:D:181:LEU:N	1:D:181:LEU:HD12	2.09	0.65
1:D:399:PRO:O	1:D:400:LEU:HD12	1.96	0.65
1:A:118:LYS:CD	1:A:307:ASP:OD2	2.28	0.65
2:C:418:ASP:OD2	1:D:161:ARG:HG3	1.96	0.64
2:C:222:LEU:HG	2:C:226:LEU:HD22	1.77	0.64
2:C:214:SER:OG	2:C:355:GLU:OE2	2.15	0.64
1:A:150:GLU:HB3	1:A:151:ALA:HB2	1.71	0.64
1:A:181:LEU:HD12	1:A:181:LEU:N	2.11	0.64
1:D:137:GLY:CA	1:D:140:VAL:HG23	2.22	0.64
2:C:288:CYS:SG	2:C:288:CYS:O	2.54	0.64
1:A:229:ARG:O	1:A:230:ASP:C	2.34	0.64
1:D:267:TYR:O	1:D:271:THR:HA	1.98	0.64
1:D:23:ILE:H	1:D:75:GLN:HE22	1.43	0.64
1:D:22:VAL:HG12	1:D:75:GLN:OE1	1.96	0.64
1:A:255:ARG:HG3	1:A:258:TRP:CZ3	2.32	0.64
1:D:302:MET:HE1	1:D:310:GLU:HG2	1.81	0.63
2:C:326:HIS:C	2:C:326:HIS:ND1	2.51	0.63
1:A:282:ARG:HH12	2:C:171:ILE:HG12	1.63	0.63
1:A:188:LEU:HD13	1:A:219:ASP:HB3	1.80	0.63
1:A:136:GLY:N	1:A:137:GLY:HA2	2.02	0.63
1:A:146:LYS:O	1:A:148:GLN:N	2.32	0.63
2:C:165:GLU:C	2:C:167:THR:H	2.01	0.63
2:C:270:GLY:C	2:C:272:GLY:H	2.01	0.63
1:D:311:ARG:HA	1:D:314:ILE:HG13	1.80	0.63
1:A:255:ARG:HD3	1:A:257:GLU:OE1	1.99	0.63
1:A:137:GLY:HA2	1:A:140:VAL:CG2	2.18	0.63
1:D:302:MET:CB	1:D:305:ASP:OD2	2.47	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:391:TYR:O	1:D:393:THR:N	2.31	0.63
1:D:334:ARG:HH11	1:D:334:ARG:HG2	1.64	0.63
2:C:275:CYS:HB3	2:C:278:TYR:HB2	1.80	0.62
1:D:253:VAL:HG23	1:D:253:VAL:O	1.99	0.62
1:A:64:LEU:CB	1:A:65:PRO:CD	2.77	0.62
2:C:402:LYS:HE2	2:C:406:GLU:CD	2.20	0.62
1:A:311:ARG:HA	1:A:314:ILE:HG13	1.81	0.62
1:A:114:GLN:O	1:A:114:GLN:HG3	1.99	0.62
1:A:174:LYS:HB3	1:A:175:TYR:CD2	2.35	0.62
1:D:150:GLU:CB	1:D:151:ALA:CB	2.60	0.62
1:D:360:ILE:HG13	1:D:372:ALA:CB	2.29	0.62
1:D:22:VAL:CG1	1:D:75:GLN:CD	2.68	0.62
1:D:188:LEU:HD13	1:D:219:ASP:HB3	1.82	0.62
1:A:200:PHE:CG	1:A:227:PHE:CD1	2.88	0.62
1:A:64:LEU:CB	1:A:65:PRO:HD3	2.30	0.62
1:A:92:GLN:O	1:A:92:GLN:CG	2.47	0.61
1:A:150:GLU:CA	1:A:151:ALA:HB2	2.28	0.61
1:A:109:THR:OG1	1:A:112:LEU:HB2	1.99	0.61
1:A:136:GLY:H	1:A:137:GLY:HA3	1.60	0.61
1:D:174:LYS:HB3	1:D:175:TYR:CD2	2.36	0.61
1:D:110:ARG:CD	1:D:135:ILE:CG2	2.62	0.61
2:C:227:CYS:CB	2:C:273:ILE:CD1	2.75	0.61
2:C:393:SER:HG	2:C:395:THR:HG1	1.48	0.61
1:A:314:ILE:HG23	1:A:336:ILE:CG2	2.30	0.61
2:C:426:LEU:HD22	2:C:426:LEU:O	2.01	0.61
1:A:110:ARG:CD	1:A:135:ILE:CG2	2.65	0.61
2:C:349:HIS:ND1	1:D:283:ARG:NH2	2.47	0.61
1:D:74:ALA:O	1:D:212:LEU:HA	2.01	0.61
1:A:253:VAL:O	1:A:253:VAL:HG23	2.00	0.61
1:A:314:ILE:CG2	1:A:336:ILE:CG2	2.75	0.61
1:D:267:TYR:HE1	1:D:325:VAL:HG11	1.65	0.61
1:A:209:VAL:HG12	1:A:228:MET:HE2	1.82	0.61
1:D:365:ARG:HA	1:D:366:PHE:C	2.19	0.61
1:D:146:LYS:O	1:D:148:GLN:N	2.34	0.61
2:C:409:TYR:CE1	2:C:447:CYS:HA	2.35	0.60
2:C:426:LEU:O	2:C:430:VAL:CG2	2.44	0.60
1:A:22:VAL:CG1	1:A:75:GLN:NE2	2.61	0.60
1:A:391:TYR:O	1:A:393:THR:N	2.34	0.60
1:D:175:TYR:N	1:D:175:TYR:CD2	2.69	0.60
1:D:302:MET:HA	1:D:305:ASP:OD2	2.01	0.60
1:A:95:GLU:H	1:A:102:GLN:NE2	1.92	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:236:VAL:CG1	1:A:236:VAL:O	2.48	0.60
1:D:346:ASN:HD22	1:D:374:ASN:ND2	1.99	0.60
1:A:242:THR:HG23	1:A:242:THR:O	1.98	0.60
1:A:313:VAL:O	1:A:317:GLU:HB2	2.01	0.60
1:A:353:ARG:HE	1:A:386:ASP:HB3	1.65	0.60
1:D:235:LEU:CG	1:D:235:LEU:O	2.49	0.60
1:A:313:VAL:CG1	1:A:326:LEU:HD11	2.32	0.60
2:C:321:GLN:H	2:C:321:GLN:CD	1.98	0.60
1:D:166:LEU:HD21	1:D:171:LEU:HD23	1.82	0.60
2:C:423:TYR:C	2:C:425:VAL:H	2.04	0.59
1:A:278:PHE:HE1	1:A:333:ALA:CB	2.14	0.59
1:A:135:ILE:CG2	1:A:136:GLY:CA	2.37	0.59
2:C:349:HIS:CE1	1:D:283:ARG:NH2	2.65	0.59
1:D:164:ASP:OD2	1:D:168:ARG:NH1	2.34	0.59
2:C:423:TYR:O	2:C:425:VAL:N	2.36	0.59
1:A:300:SER:HB2	1:A:326:LEU:HD12	1.83	0.59
1:D:361:GLY:C	1:D:362:ARG:HG2	2.23	0.59
1:D:306:MET:O	1:D:310:GLU:HB2	2.01	0.59
1:D:399:PRO:O	1:D:400:LEU:HD13	2.03	0.59
1:A:112:LEU:O	1:A:116:ILE:HD12	2.03	0.59
2:C:183:GLU:HG3	2:C:187:MET:HE2	1.84	0.59
1:D:240:GLU:CA	1:D:241:LEU:CB	2.73	0.59
1:A:149:MET:HA	1:A:150:GLU:CB	2.28	0.59
1:D:209:VAL:HG12	1:D:228:MET:HE3	1.84	0.59
1:D:314:ILE:CG2	1:D:335:GLY:O	2.47	0.59
1:A:246:ILE:HA	1:A:370:GLY:HA3	1.84	0.59
1:A:80:THR:H	1:A:82:LYS:H	1.51	0.58
2:C:354:LEU:O	2:C:355:GLU:HB2	2.02	0.58
1:A:399:PRO:O	1:A:400:LEU:HD12	2.02	0.58
1:D:251:ILE:HD13	1:D:398:MET:HB3	1.84	0.58
1:A:346:ASN:HD22	1:A:374:ASN:HD21	1.50	0.58
1:A:149:MET:HA	1:A:150:GLU:HB3	1.85	0.58
2:C:362:GLU:OE2	2:C:366:GLU:CG	2.51	0.58
2:C:317:SER:HB2	2:C:318:GLY:HA2	1.80	0.58
2:C:409:TYR:OH	2:C:430:VAL:HG11	2.03	0.58
1:D:95:GLU:H	1:D:102:GLN:NE2	1.96	0.58
2:C:410:ASN:O	2:C:413:PRO:HD3	2.03	0.58
1:A:339:GLN:OE1	1:A:362:ARG:CB	2.51	0.58
1:D:378:GLU:O	1:D:381:LYS:HB2	2.03	0.58
1:D:135:ILE:CG2	1:D:136:GLY:CA	2.29	0.58
2:C:302:LEU:C	2:C:304:MET:H	2.06	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:300:SER:HB2	1:D:326:LEU:HD12	1.86	0.57
2:C:349:HIS:CG	1:D:283:ARG:NH1	2.71	0.57
1:A:95:GLU:N	1:A:102:GLN:HE22	1.94	0.57
1:A:200:PHE:CE1	1:A:227:PHE:CG	2.92	0.57
2:C:182:ASN:O	2:C:185:ALA:N	2.37	0.57
1:A:307:ASP:O	1:A:311:ARG:N	2.33	0.57
2:C:161:GLU:O	2:C:164:PHE:HB2	2.04	0.57
1:D:311:ARG:O	1:D:315:MET:N	2.38	0.57
1:A:353:ARG:O	1:A:391:TYR:OH	2.14	0.57
1:A:331:LEU:C	1:A:331:LEU:HD12	2.25	0.57
2:C:169:THR:HG23	2:C:207:LEU:HD21	1.85	0.57
2:C:165:GLU:O	2:C:167:THR:N	2.37	0.57
1:D:311:ARG:O	1:D:315:MET:CB	2.53	0.57
2:C:423:TYR:O	2:C:427:GLU:HG2	2.04	0.57
1:A:150:GLU:CB	1:A:151:ALA:CB	2.39	0.57
1:D:302:MET:CE	1:D:310:GLU:CG	2.83	0.57
1:D:133:ALA:HA	1:D:156:VAL:O	2.05	0.57
2:C:384:LEU:HD22	2:C:432:GLU:CB	2.35	0.57
1:A:135:ILE:HG22	1:A:136:GLY:HA3	0.62	0.56
1:A:148:GLN:HE21	1:A:170:TYR:HA	1.70	0.56
1:A:166:LEU:HD21	1:A:171:LEU:HD23	1.87	0.56
1:D:361:GLY:O	1:D:362:ARG:CG	2.41	0.56
1:D:148:GLN:HE21	1:D:170:TYR:HA	1.70	0.56
2:C:449:SER:O	2:C:450:ARG:CB	2.50	0.56
1:D:209:VAL:HG12	1:D:228:MET:CE	2.36	0.56
1:A:360:ILE:HG13	1:A:372:ALA:HB2	1.87	0.56
1:D:57:ALA:HB1	1:D:236:VAL:CG2	2.31	0.56
1:D:91:LEU:HD13	1:D:127:MET:HE2	1.87	0.56
1:D:155:ILE:HG13	1:D:155:ILE:O	2.05	0.56
1:A:278:PHE:CD1	1:A:359:ARG:HG2	2.41	0.56
2:C:236:VAL:HG11	2:C:273:ILE:HG23	1.88	0.56
1:D:99:LYS:CD	1:D:150:GLU:OE1	2.38	0.56
2:C:178:HIS:HD2	2:C:180:ASP:N	1.95	0.56
1:A:200:PHE:CZ	1:A:227:PHE:CB	2.89	0.56
1:D:242:THR:OG1	1:D:244:GLU:HG3	2.06	0.56
1:A:204:ASN:C	1:A:206:ASN:N	2.60	0.56
1:D:212:LEU:HD12	1:D:212:LEU:H	1.71	0.55
1:D:204:ASN:C	1:D:206:ASN:N	2.60	0.55
1:D:175:TYR:N	1:D:175:TYR:HD2	2.05	0.55
1:A:302:MET:CE	1:A:310:GLU:HG3	2.36	0.55
2:C:442:GLN:CA	2:C:445:ASP:HB2	2.31	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:319:ARG:O	1:A:320:SER:CB	2.55	0.55
1:D:135:ILE:HG22	1:D:136:GLY:HA3	0.59	0.55
2:C:277:THR:O	2:C:280:ASP:HB2	2.05	0.55
2:C:249:GLU:HA	2:C:249:GLU:OE1	2.06	0.55
2:C:165:GLU:C	2:C:167:THR:N	2.60	0.55
1:D:352:ASN:HB3	1:D:355:ASN:HB2	1.89	0.55
1:A:329:THR:OG1	1:A:332:LEU:HD11	2.07	0.55
2:C:412:ILE:HD12	2:C:426:LEU:HG	1.88	0.55
2:C:383:ILE:HG23	2:C:387:LEU:HD12	1.88	0.55
1:A:174:LYS:HB3	1:A:175:TYR:CE2	2.40	0.55
2:C:299:THR:HG22	2:C:300:VAL:N	2.22	0.55
1:A:135:ILE:CB	1:A:136:GLY:CA	2.77	0.54
1:D:151:ALA:N	1:D:152:PRO:CD	2.71	0.54
2:C:317:SER:CB	2:C:318:GLY:HA2	2.37	0.54
1:D:181:LEU:CD1	1:D:181:LEU:N	2.70	0.54
1:D:28:ASN:OD1	1:D:28:ASN:O	2.25	0.54
1:D:109:THR:OG1	1:D:112:LEU:HB2	2.06	0.54
1:A:353:ARG:HG2	1:A:387:ILE:CD1	2.36	0.54
1:D:339:GLN:CA	1:D:362:ARG:HH11	1.83	0.54
1:A:371:VAL:HG23	1:A:372:ALA:N	2.23	0.54
2:C:227:CYS:SG	2:C:273:ILE:HG12	2.47	0.54
1:D:278:PHE:CG	1:D:359:ARG:HG2	2.42	0.54
1:D:243:LEU:HD22	1:D:248:GLN:NE2	2.22	0.54
1:D:43:LEU:O	1:D:47:ILE:HG23	2.07	0.54
1:D:302:MET:HE2	1:D:310:GLU:CG	2.38	0.54
2:C:423:TYR:HD1	2:C:450:ARG:NH2	2.05	0.54
1:A:147:LEU:HD12	1:A:165:MET:HE1	1.90	0.54
1:A:91:LEU:HB3	1:A:127:MET:CE	2.37	0.54
1:D:65:PRO:HB3	1:D:232:ILE:CD1	2.27	0.54
1:A:74:ALA:O	1:A:212:LEU:HA	2.08	0.54
1:A:43:LEU:O	1:A:47:ILE:HG23	2.08	0.54
2:C:426:LEU:HD13	2:C:427:GLU:N	2.23	0.54
1:A:168:ARG:HD3	1:A:170:TYR:CE2	2.43	0.54
1:A:181:LEU:N	1:A:181:LEU:CD1	2.70	0.54
2:C:282:TYR:O	2:C:282:TYR:CD2	2.61	0.54
1:A:267:TYR:O	1:A:271:THR:HA	2.08	0.54
1:D:253:VAL:CG1	1:D:262:THR:HG21	2.37	0.54
1:A:168:ARG:O	1:A:169:ARG:CB	2.53	0.53
2:C:238:LYS:O	2:C:239:SER:C	2.47	0.53
1:A:242:THR:HG23	1:A:244:GLU:H	1.73	0.53
1:D:179:PHE:CE2	1:D:181:LEU:HD11	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:TYR:N	1:A:175:TYR:CD2	2.74	0.53
1:D:212:LEU:HD12	1:D:212:LEU:N	2.23	0.53
1:A:382:ARG:HG3	1:A:383:THR:H	1.73	0.53
1:D:39:LEU:O	1:D:40:SER:C	2.47	0.53
1:A:149:MET:CA	1:A:150:GLU:CB	2.86	0.53
1:D:306:MET:O	1:D:306:MET:HG2	2.09	0.53
1:D:344:VAL:O	1:D:372:ALA:HA	2.08	0.53
2:C:227:CYS:HB2	2:C:273:ILE:CD1	2.30	0.53
1:A:311:ARG:O	1:A:315:MET:N	2.41	0.53
1:A:336:ILE:O	1:A:336:ILE:HG12	2.09	0.53
1:D:149:MET:CA	1:D:150:GLU:HB3	2.32	0.53
2:C:161:GLU:O	2:C:164:PHE:HB3	2.08	0.53
1:D:336:ILE:HG12	1:D:336:ILE:O	2.08	0.53
1:A:23:ILE:H	1:A:75:GLN:NE2	2.07	0.53
1:A:79:GLY:HA2	1:A:82:LYS:CB	2.32	0.53
2:C:316:GLY:O	2:C:317:SER:HB3	2.08	0.53
2:C:411:GLU:C	2:C:413:PRO:CD	2.77	0.53
1:D:360:ILE:HG12	1:D:361:GLY:N	2.23	0.53
1:A:212:LEU:N	1:A:212:LEU:HD12	2.24	0.53
1:A:360:ILE:HG13	1:A:372:ALA:HB3	1.91	0.53
1:D:272:ILE:CD1	1:D:273:THR:H	2.17	0.53
1:A:382:ARG:HG3	1:A:383:THR:N	2.23	0.53
1:D:91:LEU:HD22	1:D:127:MET:HE3	1.87	0.53
1:A:221:LEU:O	1:A:224:THR:HB	2.09	0.53
2:C:442:GLN:HA	2:C:445:ASP:CB	2.31	0.52
1:D:174:LYS:HB3	1:D:175:TYR:CE2	2.44	0.52
2:C:270:GLY:C	2:C:272:GLY:N	2.62	0.52
2:C:222:LEU:CD1	2:C:226:LEU:HD22	2.39	0.52
1:A:311:ARG:NH1	1:A:311:ARG:CG	2.35	0.52
1:D:311:ARG:CG	1:D:311:ARG:NH1	2.40	0.52
1:A:390:PHE:O	2:C:361:HIS:NE2	2.41	0.52
2:C:423:TYR:C	2:C:425:VAL:N	2.62	0.52
1:A:73:ILE:O	1:A:73:ILE:HG12	2.08	0.52
2:C:412:ILE:N	2:C:413:PRO:CD	2.72	0.52
2:C:321:GLN:C	2:C:321:GLN:OE1	2.48	0.52
2:C:372:LEU:HD21	2:C:426:LEU:CB	2.33	0.52
1:A:354:GLU:OE2	2:C:357:PRO:CD	2.42	0.52
1:D:339:GLN:CB	1:D:362:ARG:HD2	2.35	0.52
1:A:391:TYR:HB3	2:C:403:ARG:HH22	1.74	0.52
1:D:162:VAL:O	1:D:165:MET:HB2	2.10	0.52
1:A:306:MET:O	1:A:306:MET:CG	2.53	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:258:TRP:O	1:D:262:THR:HG23	2.10	0.52
1:A:200:PHE:CE1	1:A:227:PHE:CB	2.93	0.52
1:A:107:ALA:HB1	1:A:108:PRO:HD2	1.92	0.52
2:C:325:ASN:CA	2:C:328:VAL:HG23	2.32	0.51
2:C:393:SER:O	2:C:394:SER:C	2.47	0.51
1:A:338:VAL:CA	1:A:362:ARG:HH12	2.16	0.51
2:C:224:SER:O	2:C:226:LEU:N	2.44	0.51
1:A:360:ILE:CG2	1:A:361:GLY:H	2.16	0.51
1:A:330:ASP:OD2	1:A:359:ARG:HD2	2.09	0.51
2:C:361:HIS:H	2:C:361:HIS:CD2	2.29	0.51
1:A:306:MET:SD	1:A:309:LYS:HD2	2.51	0.51
1:A:311:ARG:O	1:A:315:MET:CB	2.59	0.51
1:D:92:GLN:O	1:D:92:GLN:HG3	2.08	0.51
1:D:33:SER:HB3	1:D:35:ASP:H	1.75	0.51
2:C:247:LEU:CD1	2:C:258:PRO:HG3	2.41	0.51
1:D:371:VAL:HG23	1:D:372:ALA:N	2.26	0.51
2:C:419:VAL:O	2:C:422:SER:HB3	2.11	0.51
1:A:155:ILE:HG13	1:A:155:ILE:O	2.11	0.51
1:D:135:ILE:CB	1:D:136:GLY:CA	2.73	0.51
1:D:101:THR:HA	1:D:152:PRO:O	2.10	0.51
2:C:384:LEU:CD2	2:C:432:GLU:CB	2.81	0.51
1:A:200:PHE:CE2	1:A:227:PHE:CG	2.98	0.51
2:C:194:GLY:O	2:C:197:LYS:HE2	2.11	0.51
1:D:110:ARG:NE	1:D:135:ILE:HG23	2.25	0.51
1:D:91:LEU:HB3	1:D:127:MET:CE	2.41	0.50
2:C:383:ILE:CG2	2:C:387:LEU:HD12	2.42	0.50
1:D:312:ASP:O	1:D:316:ARG:N	2.35	0.50
1:A:91:LEU:HD22	1:A:127:MET:CE	2.42	0.50
1:A:110:ARG:NE	1:A:135:ILE:HG23	2.26	0.50
1:A:134:CYS:HA	1:A:143:GLU:OE2	2.11	0.50
1:A:149:MET:C	1:A:150:GLU:HG3	2.31	0.50
1:D:377:THR:N	1:D:380:ASP:HB2	2.26	0.50
1:D:91:LEU:HB3	1:D:127:MET:HE1	1.92	0.50
2:C:175:TYR:CD2	2:C:222:LEU:HD22	2.46	0.50
1:D:77:GLN:NE2	1:D:239:GLU:OE1	2.43	0.50
2:C:227:CYS:HB3	2:C:273:ILE:CD1	2.38	0.50
1:A:79:GLY:CA	1:A:82:LYS:HB3	2.33	0.50
1:A:349:LEU:HD23	1:A:383:THR:HG23	1.94	0.50
1:A:138:THR:HG23	1:A:139:ASN:H	1.76	0.50
1:D:367:GLY:HA3	1:D:368:ARG:CG	1.99	0.49
1:A:377:THR:N	1:A:380:ASP:HB2	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:279:ILE:HD11	1:A:347:TYR:CD1	2.47	0.49
2:C:231:MET:HG3	2:C:235:ASP:OD2	2.12	0.49
1:D:90:ILE:O	1:D:94:ILE:HG12	2.12	0.49
2:C:373:GLU:OE2	1:D:110:ARG:NH1	2.45	0.49
2:C:304:MET:SD	1:D:290:GLU:HB3	2.52	0.49
1:A:339:GLN:HA	1:A:362:ARG:HD2	1.94	0.49
2:C:175:TYR:CE2	2:C:222:LEU:HD22	2.47	0.49
2:C:222:LEU:CG	2:C:226:LEU:HD22	2.43	0.49
1:A:50:TYR:HE1	1:A:311:ARG:NH2	2.10	0.49
1:D:350:PRO:HG3	1:D:359:ARG:NE	2.27	0.49
1:D:243:LEU:HD12	1:D:243:LEU:N	2.12	0.49
1:D:100:ALA:O	1:D:102:GLN:HG3	2.12	0.49
1:D:299:VAL:HG21	1:D:327:ILE:HD11	1.93	0.49
1:D:211:LEU:C	1:D:211:LEU:HD23	2.33	0.49
1:D:98:LEU:HD23	1:D:98:LEU:O	2.12	0.49
1:D:356:TYR:O	1:D:360:ILE:HG22	2.12	0.49
2:C:247:LEU:N	2:C:248:PRO:HD2	2.28	0.49
1:A:133:ALA:HA	1:A:156:VAL:O	2.13	0.49
1:D:311:ARG:CB	1:D:311:ARG:NH1	2.69	0.49
1:A:338:VAL:CB	1:A:362:ARG:HH22	2.11	0.49
1:D:353:ARG:HE	1:D:386:ASP:CB	2.21	0.49
2:C:304:MET:SD	1:D:290:GLU:CB	3.01	0.49
1:A:175:TYR:HD2	1:A:175:TYR:N	2.11	0.49
1:A:259:LYS:HB3	1:A:347:TYR:CZ	2.47	0.49
2:C:406:GLU:O	2:C:410:ASN:HB2	2.12	0.49
2:C:409:TYR:CD1	2:C:447:CYS:HA	2.48	0.49
2:C:224:SER:CA	2:C:273:ILE:HD12	2.38	0.49
1:D:239:GLU:OE2	1:D:241:LEU:HD11	2.13	0.49
1:D:314:ILE:HG22	1:D:336:ILE:CG2	2.21	0.49
2:C:432:GLU:OE2	2:C:432:GLU:HA	2.12	0.49
1:D:364:GLY:O	1:D:365:ARG:O	2.31	0.49
2:C:181:THR:OG1	2:C:225:ASP:HB2	2.13	0.49
1:D:297:PHE:CD1	1:D:297:PHE:N	2.81	0.49
1:D:151:ALA:H	1:D:152:PRO:CD	2.26	0.49
2:C:200:VAL:H	2:C:201:PRO:CD	2.26	0.49
2:C:363:LEU:HD13	2:C:363:LEU:C	2.32	0.49
2:C:224:SER:C	2:C:226:LEU:H	2.15	0.48
1:A:64:LEU:HB2	1:A:65:PRO:HD3	1.94	0.48
1:A:253:VAL:HG12	1:A:262:THR:HG21	1.93	0.48
1:A:32:ASP:O	1:A:55:PRO:HD2	2.13	0.48
1:D:173:PRO:HA	1:D:176:ILE:HD12	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:423:TYR:HD1	2:C:450:ARG:HH21	1.62	0.48
2:C:185:ALA:HB2	2:C:226:LEU:CD1	2.43	0.48
1:D:332:LEU:CD1	1:D:333:ALA:N	2.76	0.48
1:D:332:LEU:C	1:D:332:LEU:CD1	2.81	0.48
1:A:58:ILE:CG1	1:A:236:VAL:HG21	2.40	0.48
1:A:339:GLN:CG	1:A:362:ARG:NH1	2.73	0.48
2:C:388:LYS:HG2	2:C:438:ILE:HD11	1.94	0.48
1:D:380:ASP:C	1:D:383:THR:HG22	2.34	0.48
1:D:360:ILE:CG1	1:D:361:GLY:N	2.71	0.48
2:C:180:ASP:OD1	2:C:182:ASN:CB	2.58	0.48
1:A:302:MET:HE2	1:A:310:GLU:HG3	1.91	0.48
2:C:362:GLU:OE2	2:C:366:GLU:HG3	2.14	0.48
1:A:302:MET:O	1:A:332:LEU:CD2	2.50	0.48
1:D:328:THR:O	1:D:329:THR:O	2.32	0.48
1:D:353:ARG:NE	1:D:386:ASP:HB3	2.23	0.48
1:D:240:GLU:CA	1:D:241:LEU:HG	2.44	0.48
1:A:105:VAL:O	1:A:156:VAL:HA	2.14	0.48
1:A:64:LEU:HB3	1:A:65:PRO:HD3	1.96	0.48
1:D:360:ILE:CG2	1:D:361:GLY:N	2.67	0.48
1:A:91:LEU:HB3	1:A:127:MET:HE1	1.95	0.48
1:A:299:VAL:HA	1:A:325:VAL:HG23	1.95	0.47
1:A:100:ALA:O	1:A:102:GLN:HG3	2.14	0.47
1:D:237:LYS:CG	1:D:238:LYS:N	2.52	0.47
1:D:134:CYS:HA	1:D:143:GLU:OE2	2.15	0.47
1:A:278:PHE:CG	1:A:359:ARG:HG2	2.49	0.47
1:A:297:PHE:CD1	1:A:297:PHE:N	2.83	0.47
1:A:242:THR:HG23	1:A:244:GLU:N	2.28	0.47
1:A:101:THR:HA	1:A:152:PRO:O	2.15	0.47
1:A:250:TYR:CG	1:A:250:TYR:O	2.68	0.47
1:A:122:ALA:HB2	1:A:311:ARG:HH21	1.79	0.47
2:C:175:TYR:C	2:C:177:GLU:H	2.18	0.47
1:A:332:LEU:CD1	1:A:333:ALA:N	2.78	0.47
2:C:200:VAL:N	2:C:201:PRO:CD	2.77	0.47
2:C:349:HIS:CE1	1:D:283:ARG:HH12	2.33	0.47
1:A:212:LEU:H	1:A:212:LEU:HD12	1.79	0.47
1:D:382:ARG:HG3	1:D:383:THR:H	1.80	0.47
1:A:340:GLN:HB3	1:A:340:GLN:HE21	1.54	0.47
1:A:44:LEU:HA	1:A:44:LEU:HD12	1.74	0.47
1:D:365:ARG:CA	1:D:366:PHE:C	2.83	0.47
2:C:441:LYS:HG2	2:C:442:GLN:N	2.29	0.47
2:C:423:TYR:CD1	2:C:450:ARG:NH2	2.83	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:101:THR:CA	1:D:152:PRO:O	2.63	0.47
1:D:64:LEU:HD23	1:D:64:LEU:HA	1.68	0.47
2:C:169:THR:HB	2:C:170:PRO:HD3	1.97	0.47
2:C:166:LYS:HG2	2:C:166:LYS:O	2.15	0.47
1:A:328:THR:O	1:A:329:THR:O	2.33	0.46
1:D:353:ARG:HD2	1:D:390:PHE:CD2	2.50	0.46
1:A:346:ASN:HD22	1:A:374:ASN:ND2	2.13	0.46
1:D:331:LEU:HD12	1:D:331:LEU:C	2.36	0.46
1:A:164:ASP:OD2	1:A:168:ARG:NH1	2.48	0.46
1:D:272:ILE:CD1	1:D:273:THR:N	2.77	0.46
1:D:368:ARG:O	1:D:369:LYS:CG	2.62	0.46
1:A:332:LEU:HD13	1:A:333:ALA:N	2.31	0.46
1:D:79:GLY:CA	1:D:82:LYS:HB3	2.36	0.46
2:C:209:LEU:HA	2:C:209:LEU:HD23	1.54	0.46
2:C:247:LEU:HD13	2:C:258:PRO:HG3	1.98	0.46
1:D:334:ARG:CZ	1:D:334:ARG:HB2	2.46	0.46
1:D:360:ILE:CG2	1:D:361:GLY:H	2.03	0.46
1:D:365:ARG:HG3	1:D:366:PHE:N	2.26	0.46
2:C:391:TRP:CB	2:C:438:ILE:HG23	2.45	0.46
2:C:327:LEU:HD21	2:C:356:VAL:HG11	1.97	0.46
1:A:32:ASP:N	1:A:32:ASP:OD1	2.47	0.46
2:C:184:VAL:HG13	2:C:188:LEU:HD11	1.97	0.46
2:C:238:LYS:O	2:C:240:PHE:N	2.49	0.46
2:C:364:VAL:HG22	2:C:387:LEU:HD21	1.98	0.46
2:C:171:ILE:HG22	2:C:171:ILE:O	2.15	0.46
1:D:259:LYS:HB3	1:D:347:TYR:CZ	2.51	0.46
1:D:332:LEU:HD12	1:D:333:ALA:H	1.81	0.46
1:D:349:LEU:HD23	1:D:383:THR:HG23	1.98	0.46
1:A:27:TRP:HB2	1:A:232:ILE:CG2	2.46	0.46
1:D:369:LYS:HB3	1:D:370:GLY:H	1.66	0.46
1:D:149:MET:C	1:D:150:GLU:HG3	2.36	0.46
1:A:64:LEU:HB2	1:A:65:PRO:CD	2.46	0.46
2:C:183:GLU:O	2:C:187:MET:HE2	2.15	0.46
2:C:169:THR:N	2:C:170:PRO:HD2	2.31	0.46
2:C:343:ASP:CG	2:C:346:GLU:HB2	2.36	0.45
1:A:98:LEU:HD21	1:A:100:ALA:HB3	1.98	0.45
2:C:413:PRO:CD	2:C:414:ASP:H	2.29	0.45
1:A:330:ASP:OD2	1:A:359:ARG:NH1	2.41	0.45
1:A:272:ILE:CD1	1:A:273:THR:H	2.19	0.45
2:C:319:GLY:N	2:C:322:GLN:HG3	2.28	0.45
1:A:94:ILE:HG22	1:A:95:GLU:N	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:242:LYS:O	2:C:245:LYS:HB2	2.16	0.45
1:D:334:ARG:CG	1:D:334:ARG:HH11	2.27	0.45
1:D:86:PHE:O	1:D:90:ILE:HG12	2.17	0.45
1:A:312:ASP:O	1:A:316:ARG:N	2.39	0.45
2:C:421:HIS:O	2:C:423:TYR:N	2.49	0.45
1:A:90:ILE:O	1:A:94:ILE:HG12	2.16	0.45
2:C:247:LEU:HD11	2:C:258:PRO:CA	2.36	0.45
2:C:301:LEU:HA	2:C:304:MET:CE	2.38	0.45
2:C:251:ALA:HA	2:C:254:THR:O	2.17	0.45
2:C:409:TYR:OH	2:C:430:VAL:CG1	2.63	0.45
1:A:361:GLY:C	1:A:362:ARG:CG	2.77	0.45
2:C:180:ASP:OD1	2:C:182:ASN:N	2.50	0.45
1:A:332:LEU:CD1	1:A:333:ALA:H	2.29	0.45
1:A:22:VAL:HG11	1:A:75:GLN:CD	2.34	0.45
1:D:279:ILE:HG22	1:D:281:THR:H	1.81	0.45
1:D:188:LEU:HD23	1:D:188:LEU:HA	1.74	0.45
2:C:205:VAL:HG13	2:C:264:PHE:CE1	2.52	0.45
1:A:278:PHE:CE1	1:A:333:ALA:HB2	2.39	0.45
1:D:58:ILE:HG13	1:D:236:VAL:CG1	2.47	0.45
2:C:441:LYS:O	2:C:445:ASP:HB2	2.16	0.45
1:A:378:GLU:O	1:A:381:LYS:HB2	2.17	0.45
2:C:223:LEU:C	2:C:273:ILE:HD12	2.35	0.45
2:C:201:PRO:HD2	2:C:239:SER:OG	2.17	0.45
1:A:354:GLU:OE2	2:C:358:HIS:HB2	2.16	0.45
1:A:353:ARG:CZ	2:C:324:VAL:HG23	2.47	0.45
1:D:102:GLN:NE2	1:D:177:LYS:NZ	2.65	0.45
2:C:364:VAL:HG22	2:C:387:LEU:CD2	2.47	0.45
1:A:209:VAL:HG12	1:A:228:MET:HE3	1.96	0.45
1:D:58:ILE:HA	1:D:236:VAL:HG11	1.97	0.45
2:C:187:MET:O	2:C:191:LEU:HG	2.17	0.45
1:D:211:LEU:HD23	1:D:211:LEU:O	2.17	0.45
1:D:288:LEU:O	1:D:292:MET:HG3	2.17	0.45
1:D:360:ILE:HG13	1:D:372:ALA:HB3	1.97	0.45
2:C:164:PHE:CE2	2:C:196:MET:CE	2.88	0.45
1:D:229:ARG:O	1:D:231:PRO:N	2.50	0.45
1:D:138:THR:HG23	1:D:139:ASN:ND2	2.31	0.45
1:A:339:GLN:CD	1:A:362:ARG:CD	2.58	0.44
1:D:382:ARG:HG3	1:D:383:THR:N	2.32	0.44
2:C:431:GLU:OE1	2:C:431:GLU:CA	2.57	0.44
2:C:348:GLU:O	2:C:352:LYS:HB2	2.17	0.44
2:C:408:ILE:C	2:C:410:ASN:N	2.69	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:412:ILE:HG23	2:C:423:TYR:CZ	2.52	0.44
2:C:418:ASP:OD2	1:D:161:ARG:CG	2.65	0.44
1:A:361:GLY:O	1:A:362:ARG:CB	2.65	0.44
1:D:306:MET:O	1:D:310:GLU:N	2.50	0.44
1:A:299:VAL:HG23	1:A:325:VAL:HB	1.99	0.44
2:C:324:VAL:O	2:C:327:LEU:HB2	2.17	0.44
2:C:302:LEU:O	2:C:304:MET:N	2.50	0.44
1:A:138:THR:HG23	1:A:139:ASN:ND2	2.32	0.44
1:D:302:MET:HE2	1:D:310:GLU:HG3	1.98	0.44
2:C:440:SER:C	2:C:442:GLN:N	2.70	0.44
2:C:278:TYR:O	2:C:279:ILE:C	2.55	0.44
1:A:388:GLU:OE2	1:A:395:ILE:N	2.32	0.44
1:D:73:ILE:HG12	1:D:73:ILE:O	2.16	0.44
1:A:140:VAL:O	1:A:141:ARG:C	2.54	0.44
1:D:311:ARG:CA	1:D:314:ILE:HG13	2.46	0.44
2:C:383:ILE:O	2:C:387:LEU:HD12	2.17	0.44
1:A:73:ILE:HD13	1:A:73:ILE:HG21	1.52	0.44
2:C:227:CYS:HB3	2:C:273:ILE:CG1	2.47	0.44
1:D:164:ASP:O	1:D:168:ARG:HG3	2.18	0.44
1:A:209:VAL:CG1	1:A:228:MET:HE2	2.46	0.44
2:C:252:LEU:HA	2:C:252:LEU:HD12	1.82	0.44
1:A:173:PRO:HA	1:A:176:ILE:HD12	2.00	0.44
2:C:274:LEU:HA	2:C:274:LEU:HD23	1.70	0.44
2:C:409:TYR:CE1	2:C:447:CYS:CA	3.00	0.44
1:A:344:VAL:O	1:A:372:ALA:HA	2.18	0.44
2:C:236:VAL:HG11	2:C:273:ILE:O	2.18	0.44
2:C:349:HIS:ND1	2:C:349:HIS:O	2.49	0.44
1:D:90:ILE:HG21	1:D:90:ILE:HD12	1.58	0.44
2:C:443:LEU:HA	2:C:443:LEU:HD12	1.52	0.44
2:C:287:ASP:O	2:C:288:CYS:CB	2.37	0.44
1:D:364:GLY:C	1:D:365:ARG:O	2.49	0.43
2:C:175:TYR:C	2:C:177:GLU:N	2.70	0.43
1:D:302:MET:HB2	1:D:305:ASP:OD2	2.16	0.43
2:C:447:CYS:HA	2:C:448:PRO:HD3	1.80	0.43
1:D:330:ASP:OD2	1:D:359:ARG:NH1	2.43	0.43
2:C:343:ASP:OD1	2:C:346:GLU:HB2	2.17	0.43
2:C:222:LEU:HG	2:C:226:LEU:CD2	2.46	0.43
1:D:329:THR:OG1	1:D:332:LEU:HD11	2.18	0.43
1:D:147:LEU:HD11	1:D:165:MET:HE1	1.99	0.43
1:D:346:ASN:HB2	1:D:374:ASN:HD22	1.83	0.43
1:D:138:THR:HG23	1:D:139:ASN:H	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:SER:HB3	1:A:35:ASP:H	1.83	0.43
1:A:98:LEU:O	1:A:98:LEU:HD23	2.18	0.43
1:D:47:ILE:HD12	1:D:88:ILE:CD1	2.48	0.43
1:D:94:ILE:HA	1:D:94:ILE:HD13	1.81	0.43
1:A:272:ILE:CD1	1:A:273:THR:N	2.79	0.43
2:C:248:PRO:CA	2:C:290:GLN:OE1	2.58	0.43
1:D:110:ARG:NE	1:D:135:ILE:CG2	2.81	0.43
1:D:173:PRO:HA	1:D:176:ILE:CD1	2.49	0.43
1:D:64:LEU:CB	1:D:65:PRO:CD	2.96	0.43
1:A:199:ILE:O	1:A:200:PHE:C	2.56	0.43
1:A:200:PHE:CE1	1:A:227:PHE:CD1	3.06	0.43
1:A:91:LEU:HB3	1:A:127:MET:HE2	2.01	0.43
2:C:350:CYS:O	2:C:354:LEU:HG	2.19	0.43
1:A:399:PRO:O	1:A:400:LEU:HD13	2.15	0.43
1:A:28:ASN:O	1:A:28:ASN:OD1	2.37	0.43
2:C:243:LEU:HD23	2:C:243:LEU:HA	1.71	0.43
1:D:200:PHE:CG	1:D:227:PHE:CD1	3.06	0.43
1:A:188:LEU:HA	1:A:188:LEU:HD23	1.68	0.43
1:A:173:PRO:HA	1:A:176:ILE:CD1	2.49	0.43
1:A:249:PHE:HA	1:A:396:GLU:O	2.19	0.43
1:D:333:ALA:HA	1:D:336:ILE:CD1	2.49	0.42
1:A:180:VAL:HA	1:A:210:VAL:O	2.19	0.42
1:A:178:MET:HE3	1:A:178:MET:HB2	1.81	0.42
1:D:312:ASP:OD1	1:D:315:MET:CE	2.67	0.42
2:C:227:CYS:CB	2:C:273:ILE:CG1	2.97	0.42
2:C:164:PHE:HE1	2:C:168:LEU:HD11	1.81	0.42
1:D:332:LEU:HD12	1:D:333:ALA:N	2.33	0.42
1:A:354:GLU:CD	2:C:357:PRO:CD	2.81	0.42
1:D:232:ILE:HD13	1:D:232:ILE:HG23	1.80	0.42
1:D:164:ASP:OD1	1:D:168:ARG:NH1	2.52	0.42
2:C:183:GLU:HG3	2:C:187:MET:CE	2.48	0.42
1:A:232:ILE:HD13	1:A:232:ILE:HG23	1.83	0.42
1:A:339:GLN:CG	1:A:362:ARG:HD2	2.45	0.42
2:C:164:PHE:O	2:C:167:THR:N	2.51	0.42
1:D:332:LEU:HD13	1:D:333:ALA:N	2.35	0.42
1:D:27:TRP:CE2	1:D:65:PRO:HG3	2.54	0.42
1:A:353:ARG:HD2	1:A:390:PHE:CD2	2.54	0.42
1:A:58:ILE:HG23	1:A:58:ILE:HD13	1.31	0.42
1:D:34:PHE:CD1	1:D:47:ILE:HD11	2.54	0.42
2:C:314:VAL:HB	2:C:315:TRP:O	2.20	0.42
1:A:332:LEU:HD12	1:A:333:ALA:H	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:357:PRO:HA	2:C:360:HIS:CE1	2.55	0.42
1:A:95:GLU:O	1:A:96:LEU:C	2.58	0.42
2:C:341:SER:O	1:D:351:THR:HG21	2.18	0.42
1:A:24:GLU:O	1:A:233:ARG:HD2	2.18	0.42
1:D:306:MET:C	1:D:310:GLU:HB2	2.40	0.42
1:D:82:LYS:HD3	1:D:212:LEU:CD2	2.46	0.42
2:C:163:ALA:O	2:C:166:LYS:HD2	2.19	0.42
1:D:144:VAL:O	1:D:145:GLN:C	2.55	0.42
1:D:284:LYS:O	1:D:287:TRP:HB3	2.19	0.42
2:C:420:PRO:HG2	1:D:190:ARG:O	2.20	0.42
2:C:185:ALA:HB2	2:C:226:LEU:HD11	2.01	0.42
1:A:181:LEU:O	1:A:211:LEU:HA	2.19	0.42
2:C:326:HIS:ND1	2:C:326:HIS:O	2.52	0.42
1:A:81:GLY:HA2	1:A:84:ALA:HB3	2.00	0.42
1:D:151:ALA:H	1:D:152:PRO:HD2	1.84	0.42
1:A:94:ILE:HD12	1:A:94:ILE:HG23	1.70	0.42
2:C:232:SER:N	2:C:235:ASP:OD2	2.49	0.42
2:C:413:PRO:HD2	2:C:414:ASP:H	1.85	0.42
1:D:72:VAL:HG22	1:D:232:ILE:HD11	2.01	0.42
2:C:384:LEU:O	2:C:388:LYS:HG3	2.20	0.42
2:C:323:PRO:O	2:C:326:HIS:HB3	2.19	0.42
1:A:47:ILE:HG21	1:A:47:ILE:HD13	1.64	0.42
2:C:184:VAL:CG1	2:C:188:LEU:HD11	2.50	0.42
1:A:360:ILE:HG12	1:A:361:GLY:N	2.33	0.42
2:C:180:ASP:O	2:C:181:THR:C	2.58	0.42
2:C:302:LEU:C	2:C:304:MET:N	2.71	0.42
1:D:398:MET:HA	1:D:399:PRO:HD3	1.96	0.42
1:D:361:GLY:C	1:D:362:ARG:CG	2.87	0.41
1:A:267:TYR:HD2	1:A:297:PHE:CE2	2.32	0.41
1:D:64:LEU:CB	1:D:65:PRO:HD3	2.50	0.41
1:A:378:GLU:OE1	1:A:378:GLU:CA	2.51	0.41
1:A:200:PHE:CB	1:A:227:PHE:CE1	3.02	0.41
2:C:383:ILE:HG23	2:C:387:LEU:CD1	2.50	0.41
1:D:338:VAL:CA	1:D:362:ARG:HH22	2.32	0.41
1:D:58:ILE:HG21	1:D:58:ILE:HD13	1.55	0.41
1:D:163:PHE:C	1:D:165:MET:H	2.22	0.41
2:C:346:GLU:OE2	1:D:283:ARG:HD2	2.21	0.41
1:D:39:LEU:C	1:D:40:SER:O	2.59	0.41
1:D:235:LEU:O	1:D:235:LEU:HD22	2.19	0.41
1:A:93:GLN:HB3	1:A:178:MET:HE1	2.02	0.41
1:D:333:ALA:O	1:D:336:ILE:HD13	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:PHE:CD2	1:A:227:PHE:CZ	3.09	0.41
2:C:410:ASN:O	2:C:413:PRO:CD	2.68	0.41
2:C:257:ALA:N	2:C:258:PRO:CD	2.84	0.41
1:A:200:PHE:O	1:A:202:LYS:N	2.54	0.41
2:C:195:GLU:C	2:C:197:LYS:H	2.23	0.41
1:A:56:SER:O	1:A:57:ALA:C	2.58	0.41
1:A:140:VAL:HA	1:A:143:GLU:HB2	2.03	0.41
1:D:148:GLN:HA	1:D:149:MET:HA	1.82	0.41
2:C:196:MET:HE3	2:C:196:MET:HB2	1.98	0.41
1:A:91:LEU:HD13	1:A:127:MET:HE2	2.01	0.41
1:D:339:GLN:N	1:D:362:ARG:CZ	2.81	0.41
2:C:426:LEU:HD11	2:C:447:CYS:SG	2.61	0.41
1:A:267:TYR:CE1	1:A:325:VAL:HG11	2.45	0.41
1:D:232:ILE:HD12	1:D:232:ILE:HG21	1.74	0.41
1:A:83:THR:HA	1:A:86:PHE:CE2	2.56	0.41
1:A:200:PHE:CD2	1:A:227:PHE:CE2	3.09	0.41
1:A:81:GLY:HA2	1:A:84:ALA:CB	2.51	0.41
2:C:260:LEU:O	2:C:261:VAL:C	2.59	0.41
1:D:185:ASP:OD2	1:D:214:ALA:HB3	2.21	0.41
1:A:307:ASP:O	1:A:311:ARG:HB3	2.14	0.41
2:C:200:VAL:H	2:C:201:PRO:HD2	1.86	0.41
1:A:90:ILE:HG12	1:A:90:ILE:H	1.58	0.41
1:D:367:GLY:CA	1:D:368:ARG:HB2	2.43	0.40
2:C:412:ILE:HG21	2:C:423:TYR:CE2	2.55	0.40
1:D:278:PHE:CE1	1:D:333:ALA:HB2	2.39	0.40
2:C:442:GLN:O	2:C:442:GLN:HG2	2.21	0.40
1:A:148:GLN:HA	1:A:149:MET:HA	1.79	0.40
1:D:380:ASP:CA	1:D:383:THR:HG22	2.52	0.40
1:A:67:ILE:HG13	1:A:89:SER:HB3	2.03	0.40
1:A:110:ARG:NE	1:A:135:ILE:CG2	2.82	0.40
1:A:164:ASP:O	1:A:168:ARG:HG3	2.21	0.40
1:A:94:ILE:CG2	1:A:95:GLU:N	2.83	0.40
1:A:241:LEU:HB3	1:A:357:ILE:HD11	2.03	0.40
2:C:335:LEU:HA	2:C:335:LEU:HD23	1.87	0.40
2:C:161:GLU:HG3	2:C:162:THR:CA	2.42	0.40
1:D:310:GLU:O	1:D:312:ASP:N	2.54	0.40
2:C:324:VAL:O	2:C:328:VAL:HG23	2.20	0.40
1:D:185:ASP:N	1:D:185:ASP:OD1	2.55	0.40
1:D:140:VAL:O	1:D:141:ARG:C	2.57	0.40
1:A:278:PHE:CE1	1:A:333:ALA:CB	3.01	0.40
1:A:200:PHE:C	1:A:202:LYS:H	2.24	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:ILE:HG21	1:A:63:ILE:HD13	1.80	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:316:ARG:CD	1:D:99:LYS:CE[12_455]	1.94	0.26

## 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	354/414 (86%)	297 (84%)	38 (11%)	19 (5%)	2	25
1	D	365/414 (88%)	299 (82%)	45 (12%)	21 (6%)	2	23
2	C	272/358 (76%)	213 (78%)	44 (16%)	15 (6%)	2	24
All	All	991/1186 (84%)	809 (82%)	127 (13%)	55 (6%)	2	24

All (55) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	147	LEU
1	A	151	ALA
1	A	271	THR
1	A	320	SER
1	A	329	THR
1	A	392	ASN
1	D	147	LEU
1	D	151	ALA
1	D	271	THR
1	D	329	THR
1	D	362	ARG

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Mol	Chain	Res	Type
1	D	367	GLY
1	D	368	ARG
1	D	369	LYS
1	D	392	ASN
1	D	399	PRO
1	A	40	SER
1	A	237	LYS
1	A	311	ARG
1	A	330	ASP
1	A	399	PRO
2	C	166	LYS
2	C	225	ASP
2	C	239	SER
2	C	258	PRO
2	C	288	CYS
2	C	303	SER
2	C	394	SER
2	C	422	SER
2	C	426	LEU
1	D	40	SER
1	D	236	VAL
1	D	242	THR
1	D	311	ARG
1	D	330	ASP
1	D	333	ALA
1	A	27	TRP
1	A	57	ALA
1	A	318	PHE
1	A	331	LEU
2	C	233	THR
2	C	318	GLY
1	D	238	LYS
1	D	240	GLU
1	A	135	ILE
1	A	360	ILE
2	C	279	ILE
2	C	182	ASN
2	C	421	HIS
2	C	424	SER
1	D	137	GLY
1	D	366	PHE
1	A	236	VAL

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Mol	Chain	Res	Type
1	D	135	ILE
1	A	137	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	325/363 (90%)	260 (80%)	65 (20%)	1	9
1	D	329/363 (91%)	257 (78%)	72 (22%)	1	7
2	C	245/312 (78%)	204 (83%)	41 (17%)	3	16
All	All	899/1038 (87%)	721 (80%)	178 (20%)	1	9

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

Mol	Chain	Res	Type
1	A	22	VAL
1	A	28	ASN
1	A	33	SER
1	A	44	LEU
1	A	45	ARG
1	A	47	ILE
1	A	58	ILE
1	A	73	ILE
1	A	78	SER
1	A	82	LYS
1	A	90	ILE
1	A	97	ASP
1	A	101	THR
1	A	105	VAL
1	A	106	LEU
1	A	112	LEU
1	A	127	MET
1	A	130	SER
1	A	135	ILE
1	A	138	THR

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Mol	Chain	Res	Type
1	A	139	ASN
1	A	143	GLU
1	A	148	GLN
1	A	149	MET
1	A	150	GLU
1	A	156	VAL
1	A	161	ARG
1	A	167	ASN
1	A	169	ARG
1	A	175	TYR
1	A	178	MET
1	A	180	VAL
1	A	183	GLU
1	A	201	GLN
1	A	218	SER
1	A	221	LEU
1	A	222	GLU
1	A	232	ILE
1	A	241	LEU
1	A	242	THR
1	A	243	LEU
1	A	255	ARG
1	A	261	ASP
1	A	273	THR
1	A	292	MET
1	A	302	MET
1	A	306	MET
1	A	308	GLN
1	A	311	ARG
1	A	314	ILE
1	A	317	GLU
1	A	318	PHE
1	A	319	ARG
1	A	325	VAL
1	A	331	LEU
1	A	332	LEU
1	A	336	ILE
1	A	338	VAL
1	A	340	GLN
1	A	355	ASN
1	A	360	ILE
1	A	371	VAL

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Mol	Chain	Res	Type
1	A	378	GLU
1	A	393	THR
1	A	400	LEU
2	C	161	GLU
2	C	166	LYS
2	C	172	ILE
2	C	177	GLU
2	C	207	LEU
2	C	220	SER
2	C	221	LYS
2	C	223	LEU
2	C	226	LEU
2	C	229	THR
2	C	232	SER
2	C	239	SER
2	C	247	LEU
2	C	252	LEU
2	C	256	ARG
2	C	259	GLN
2	C	264	PHE
2	C	273	ILE
2	C	274	LEU
2	C	281	SER
2	C	283	LYS
2	C	288	CYS
2	C	301	LEU
2	C	315	TRP
2	C	321	GLN
2	C	325	ASN
2	C	328	VAL
2	C	329	LYS
2	C	336	LYS
2	C	345	SER
2	C	356	VAL
2	C	372	LEU
2	C	375	THR
2	C	378	SER
2	C	382	MET
2	C	397	THR
2	C	398	ILE
2	C	410	ASN
2	C	426	LEU

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Mol	Chain	Res	Type
2	C	438	ILE
2	C	445	ASP
1	D	22	VAL
1	D	28	ASN
1	D	33	SER
1	D	44	LEU
1	D	45	ARG
1	D	47	ILE
1	D	58	ILE
1	D	73	ILE
1	D	78	SER
1	D	82	LYS
1	D	90	ILE
1	D	97	ASP
1	D	101	THR
1	D	105	VAL
1	D	106	LEU
1	D	112	LEU
1	D	117	GLN
1	D	127	MET
1	D	130	SER
1	D	135	ILE
1	D	138	THR
1	D	139	ASN
1	D	143	GLU
1	D	148	GLN
1	D	149	MET
1	D	150	GLU
1	D	156	VAL
1	D	161	ARG
1	D	167	ASN
1	D	169	ARG
1	D	175	TYR
1	D	178	MET
1	D	180	VAL
1	D	201	GLN
1	D	212	LEU
1	D	218	SER
1	D	221	LEU
1	D	222	GLU
1	D	232	ILE
1	D	234	ILE

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Mol	Chain	Res	Type
1	D	235	LEU
1	D	237	LYS
1	D	238	LYS
1	D	239	GLU
1	D	240	GLU
1	D	242	THR
1	D	243	LEU
1	D	244	GLU
1	D	255	ARG
1	D	261	ASP
1	D	273	THR
1	D	280	ASN
1	D	297	PHE
1	D	302	MET
1	D	306	MET
1	D	311	ARG
1	D	314	ILE
1	D	317	GLU
1	D	318	PHE
1	D	325	VAL
1	D	331	LEU
1	D	332	LEU
1	D	334	ARG
1	D	336	ILE
1	D	338	VAL
1	D	340	GLN
1	D	360	ILE
1	D	362	ARG
1	D	365	ARG
1	D	371	VAL
1	D	378	GLU
1	D	400	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	ASN
1	A	75	GLN
1	A	93	GLN
1	A	102	GLN
1	A	148	GLN
1	A	206	ASN

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Mol	Chain	Res	Type
1	A	208	GLN
1	A	280	ASN
1	A	340	GLN
1	A	374	ASN
2	C	173	GLN
2	C	178	HIS
2	C	215	HIS
2	C	325	ASN
2	C	358	HIS
2	C	421	HIS
1	D	28	ASN
1	D	75	GLN
1	D	102	GLN
1	D	139	ASN
1	D	148	GLN
1	D	206	ASN
1	D	208	GLN
1	D	280	ASN
1	D	340	GLN
1	D	374	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

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

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

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	364/414 (87%)	-0.34	1 (0%) 94 91	46, 54, 74, 102	0
1	D	371/414 (89%)	-0.27	4 (1%) 82 73	35, 54, 73, 107	0
2	C	278/358 (77%)	-0.56	0 100 100	33, 56, 72, 80	4 (1%)
All	All	1013/1186 (85%)	-0.37	5 (0%) 91 88	33, 54, 73, 107	4 (0%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	318	PHE	3.3
1	D	378	GLU	3.1
1	D	309	LYS	2.9
1	D	308	GLN	2.2
1	A	307	ASP	2.0

### 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](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.