



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:25 AM GMT

PDB ID : 3EHK  
Title : Crystal structure of Pru du amandin, an allergenic protein from prunus dulcis  
Authors : Gaur, V.; Salunke, D.M.  
Deposited on : 2008-09-13  
Resolution : 3.20 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

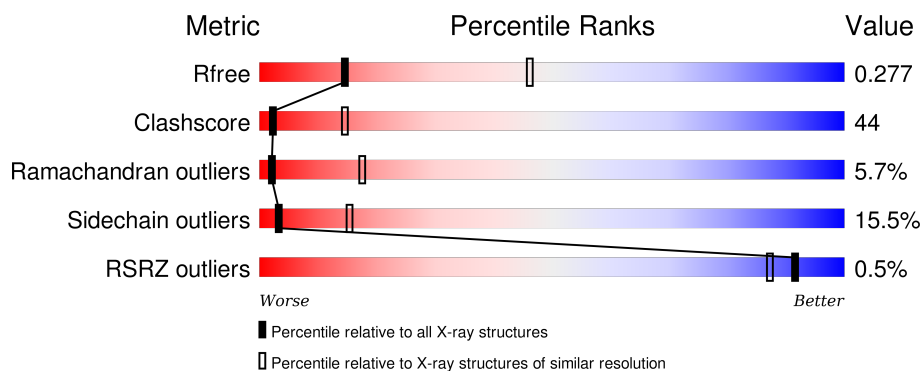
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 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	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)

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	531	
1	B	531	
1	C	531	
1	D	531	
1	E	531	

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Mol	Chain	Length	Quality of chain
1	F	531	<div><div><div><div><div>%</div><div></div></div><div><div></div><div>30%</div></div><div><div></div><div>33%</div></div><div><div></div><div>9%</div></div><div><div></div><div>28%</div></div></div><div></div></div></div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 18359 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 Prunin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	384	Total	C	N	O	S	0	0	0
			3042	1891	569	578	4			
1	B	384	Total	C	N	O	S	0	0	0
			3042	1891	569	578	4			
1	C	384	Total	C	N	O	S	0	0	0
			3042	1891	569	578	4			
1	D	384	Total	C	N	O	S	0	0	0
			3042	1891	569	578	4			
1	E	384	Total	C	N	O	S	0	0	0
			3042	1891	569	578	4			
1	F	384	Total	C	N	O	S	0	0	0
			3042	1891	569	578	4			

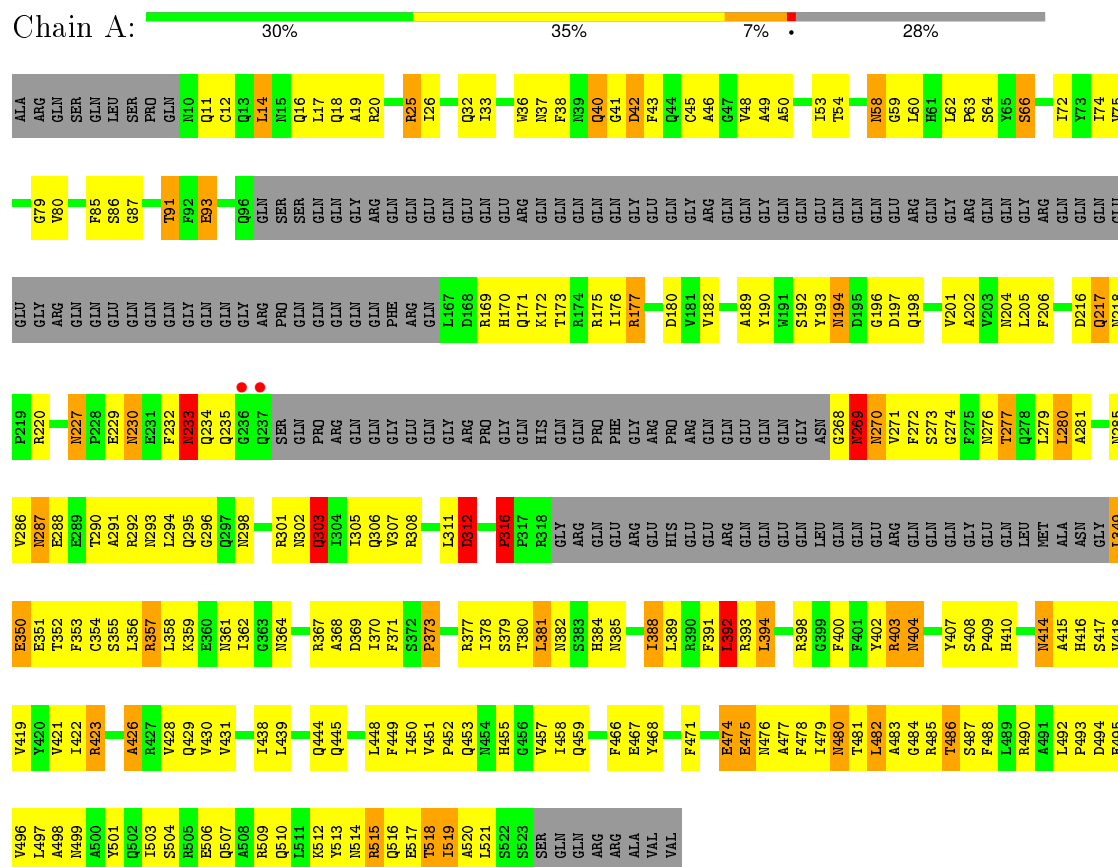
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	9	Total	O	0	0
			9	9		
2	C	80	Total	O	0	0
			80	80		
2	F	18	Total	O	0	0
			18	18		

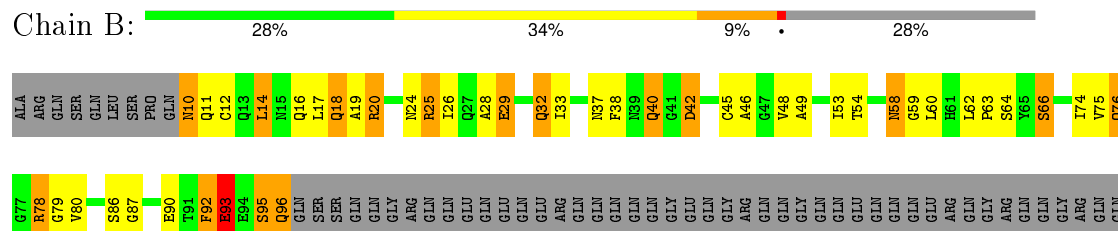
### 3 Residue-property plots

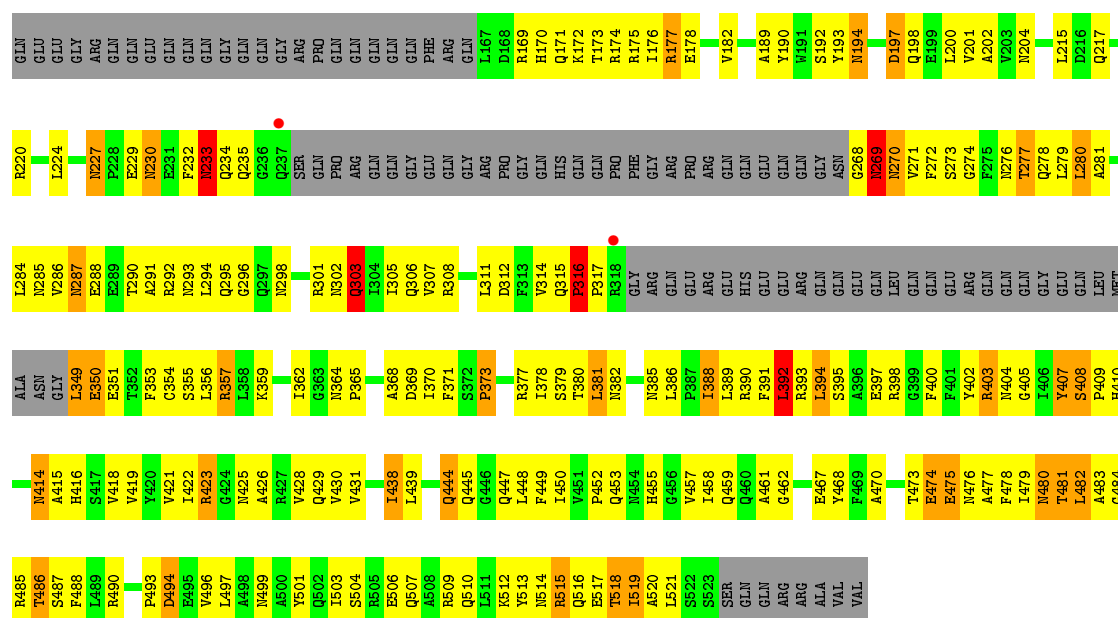
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

#### • Molecule 1: Prunin

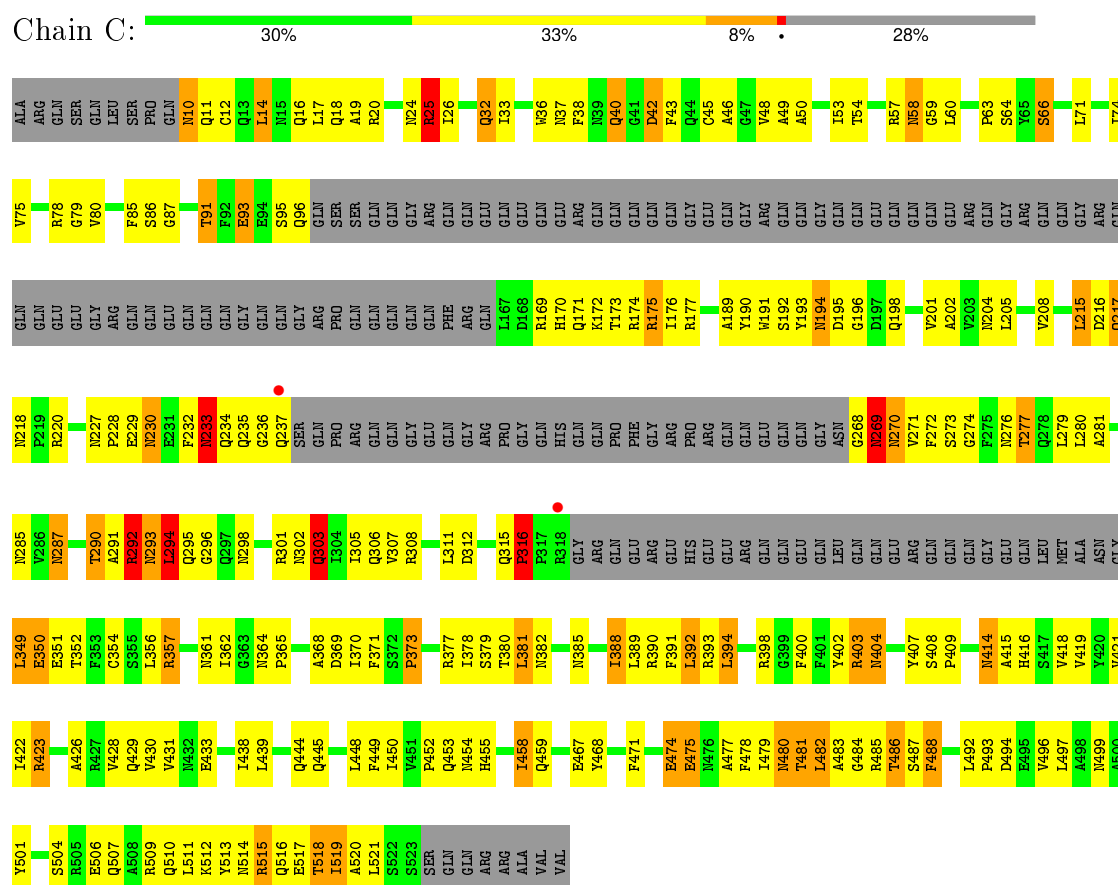


#### • Molecule 1: Prunin

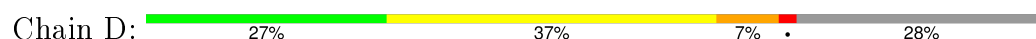




## • Molecule 1: Prunin



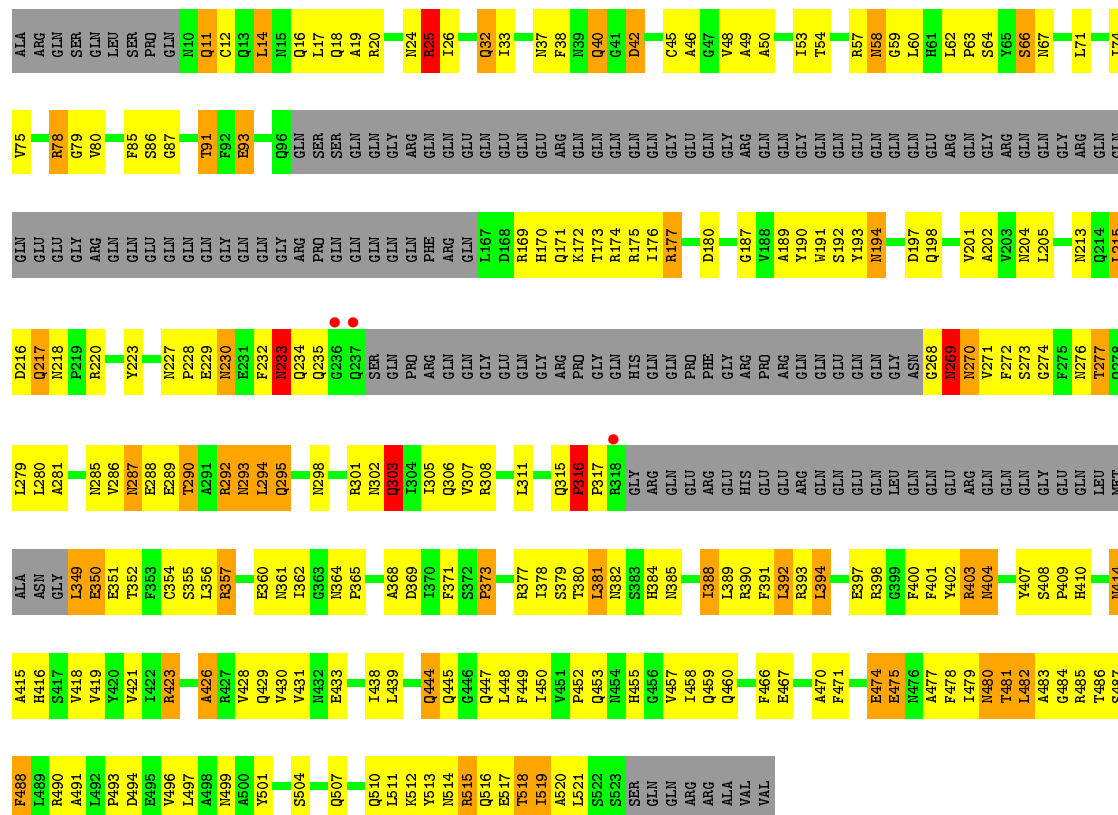
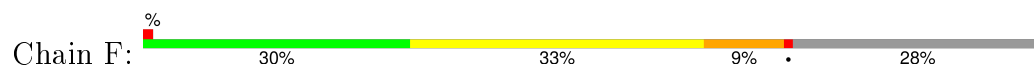
## • Molecule 1: Prunin







# Molecule 1: Prunin





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	151.10Å 151.10Å 164.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.31 – 3.20 33.31 – 3.20	Depositor EDS
% Data completeness (in resolution range)	78.7 (33.31-3.20) 78.6 (33.31-3.20)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.53 (at 3.18Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.254 , 0.279 0.254 , 0.277	Depositor DCC
$R_{free}$ test set	5971 reflections (13.88%)	DCC
Wilson B-factor (Å <sup>2</sup> )	42.7	Xtriage
Anisotropy	0.550	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 45.4	EDS
Estimated twinning fraction	0.397 for h,-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	2 of 58904 reflections (0.003%)	Xtriage
$F_o, F_c$ correlation	0.86	EDS
Total number of atoms	18359	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.54% 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	0.47	0/3099	0.77	1/4200 (0.0%)
1	B	0.58	2/3099 (0.1%)	0.81	3/4200 (0.1%)
1	C	0.52	0/3099	0.82	5/4200 (0.1%)
1	D	0.59	4/3099 (0.1%)	0.84	8/4200 (0.2%)
1	E	0.56	4/3099 (0.1%)	0.91	15/4200 (0.4%)
1	F	0.58	2/3099 (0.1%)	0.83	4/4200 (0.1%)
All	All	0.55	12/18594 (0.1%)	0.83	36/25200 (0.1%)

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	2

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	293	ASN	CB-CG	-8.59	1.31	1.51
1	D	290	THR	N-CA	-8.17	1.30	1.46
1	F	293	ASN	CA-C	-7.28	1.34	1.52
1	E	291	ALA	N-CA	-6.55	1.33	1.46
1	D	292	ARG	CG-CD	6.42	1.68	1.51
1	E	293	ASN	N-CA	6.35	1.59	1.46
1	B	78	ARG	CB-CG	-6.00	1.36	1.52
1	B	93	GLU	CG-CD	-5.92	1.43	1.51
1	E	292	ARG	CG-CD	5.49	1.65	1.51
1	D	291	ALA	CA-CB	-5.41	1.41	1.52
1	E	293	ASN	CB-CG	-5.05	1.39	1.51
1	D	289	GLU	C-O	5.03	1.32	1.23

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	292	ARG	CA-C-N	-15.41	83.30	117.20
1	E	292	ARG	CB-CA-C	10.11	130.61	110.40
1	E	293	ASN	N-CA-CB	-9.71	93.11	110.60
1	E	293	ASN	N-CA-C	9.19	135.82	111.00
1	F	290	THR	CA-CB-CG2	-8.78	100.10	112.40
1	C	292	ARG	N-CA-C	-8.72	87.45	111.00
1	E	292	ARG	C-N-CA	-8.53	100.37	121.70
1	E	293	ASN	CA-C-O	-8.12	103.05	120.10
1	B	78	ARG	NE-CZ-NH1	-8.10	116.25	120.30
1	E	292	ARG	CA-CB-CG	8.00	130.99	113.40
1	E	294	LEU	CA-CB-CG	-7.64	97.72	115.30
1	E	292	ARG	O-C-N	7.54	134.77	122.70
1	E	294	LEU	CB-CG-CD2	-7.17	98.81	111.00
1	D	294	LEU	CA-CB-CG	-7.08	99.03	115.30
1	F	293	ASN	CB-CA-C	-7.07	96.27	110.40
1	E	293	ASN	CB-CG-OD1	-7.02	107.56	121.60
1	F	292	ARG	NE-CZ-NH2	-7.00	116.80	120.30
1	D	312	ASP	N-CA-CB	-6.74	98.47	110.60
1	C	294	LEU	CB-CG-CD1	-6.52	99.92	111.00
1	E	291	ALA	O-C-N	-6.19	112.80	122.70
1	B	92	PHE	N-CA-C	-6.15	94.40	111.00
1	D	290	THR	CA-C-N	-6.09	103.81	117.20
1	E	293	ASN	CA-C-N	6.08	130.57	117.20
1	C	290	THR	CA-CB-CG2	-5.89	104.15	112.40
1	B	90	GLU	CA-CB-CG	-5.80	100.64	113.40
1	F	294	LEU	N-CA-C	-5.72	95.54	111.00
1	C	293	ASN	CB-CA-C	-5.64	99.11	110.40
1	E	292	ARG	CG-CD-NE	5.38	123.09	111.80
1	D	291	ALA	CB-CA-C	-5.35	102.08	110.10
1	D	78	ARG	N-CA-C	-5.34	96.58	111.00
1	C	294	LEU	N-CA-C	-5.31	96.67	111.00
1	D	289	GLU	CB-CA-C	-5.29	99.81	110.40
1	D	292	ARG	NE-CZ-NH2	-5.25	117.67	120.30
1	A	312	ASP	CB-CA-C	5.12	120.64	110.40
1	D	290	THR	CA-C-O	5.11	130.83	120.10
1	E	292	ARG	CA-C-O	-5.10	109.39	120.10

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	292	ARG	Mainchain,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	3042	0	2902	294	0
1	B	3042	0	2902	306	0
1	C	3042	0	2902	291	0
1	D	3042	0	2902	297	0
1	E	3042	0	2902	296	0
1	F	3042	0	2902	286	0
2	A	9	0	0	3	0
2	C	80	0	0	14	0
2	F	18	0	0	3	0
All	All	18359	0	17412	1553	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 44.

All (1553) 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:507:GLN:NE2	1:F:290:THR:HG21	1.59	1.15
1:E:290:THR:HG23	1:F:507:GLN:NE2	1.61	1.14
1:F:423:ARG:HB3	1:F:423:ARG:HH11	1.10	1.13
1:D:507:GLN:HE21	1:F:290:THR:HG21	1.05	1.11
1:E:290:THR:HG23	1:F:507:GLN:HE21	1.00	1.11
1:D:507:GLN:NE2	1:F:290:THR:CG2	2.13	1.10
1:D:423:ARG:HH11	1:D:423:ARG:HB3	1.10	1.09
1:B:290:THR:HG22	1:C:507:GLN:NE2	1.68	1.09
1:A:423:ARG:HH11	1:A:423:ARG:HB3	1.07	1.08
1:C:423:ARG:HH11	1:C:423:ARG:HB3	1.19	1.07
1:A:423:ARG:NH1	1:A:423:ARG:HB3	1.69	1.06
1:B:423:ARG:HB3	1:B:423:ARG:HH11	1.12	1.05
1:E:290:THR:O	1:E:293:ASN:HB3	1.56	1.05
1:B:290:THR:HG22	1:C:507:GLN:HE21	0.89	1.05
1:A:290:THR:HG22	1:B:507:GLN:HE21	1.17	1.04
1:D:423:ARG:HB3	1:D:423:ARG:NH1	1.72	1.04
1:A:302:ASN:HB3	1:A:303:GLN:HE21	1.22	1.03
1:D:507:GLN:HE21	1:F:290:THR:CG2	1.72	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:423:ARG:HB3	1:B:423:ARG:NH1	1.74	1.02
1:E:423:ARG:HB3	1:E:423:ARG:HH11	1.21	1.00
1:A:517:GLU:HB2	1:D:93:GLU:CD	1.83	0.99
1:F:423:ARG:HB3	1:F:423:ARG:NH1	1.76	0.99
1:D:302:ASN:HB3	1:D:303:GLN:HE21	1.28	0.97
1:C:423:ARG:NH1	1:C:423:ARG:HB3	1.79	0.97
1:C:93:GLU:CD	1:E:517:GLU:HB2	1.85	0.97
1:F:302:ASN:HB3	1:F:303:GLN:HE21	1.31	0.96
1:B:302:ASN:HB3	1:B:303:GLN:HE21	1.26	0.96
1:A:93:GLU:CD	1:D:517:GLU:HB2	1.86	0.96
1:E:302:ASN:HB3	1:E:303:GLN:HE21	1.27	0.96
1:C:349:LEU:HG	1:C:350:GLU:H	1.32	0.95
1:C:302:ASN:HB3	1:C:303:GLN:HE21	1.32	0.95
1:F:349:LEU:HG	1:F:350:GLU:H	1.30	0.94
1:C:349:LEU:CG	1:C:350:GLU:H	1.81	0.94
1:C:414:ASN:HD22	1:C:414:ASN:H	1.16	0.93
1:E:423:ARG:HB3	1:E:423:ARG:NH1	1.83	0.93
1:D:349:LEU:CG	1:D:350:GLU:H	1.80	0.93
1:B:517:GLU:HB2	1:F:93:GLU:CD	1.89	0.93
1:A:290:THR:HG22	1:B:507:GLN:NE2	1.84	0.93
1:A:517:GLU:HB2	1:D:93:GLU:OE2	1.67	0.93
1:F:414:ASN:HD22	1:F:414:ASN:H	1.17	0.92
1:A:409:PRO:HG3	1:A:458:ILE:CD1	2.00	0.92
1:D:493:PRO:HB3	1:F:170:HIS:CD2	2.05	0.92
1:D:409:PRO:HG3	1:D:458:ILE:CD1	2.00	0.92
1:B:349:LEU:HG	1:B:350:GLU:H	1.35	0.91
1:C:293:ASN:O	1:C:295:GLN:N	2.03	0.91
1:F:349:LEU:CG	1:F:350:GLU:H	1.82	0.91
1:A:388:ILE:N	1:A:388:ILE:HD13	1.85	0.90
1:F:382:ASN:H	1:F:385:ASN:HD22	1.19	0.90
1:A:479:ILE:O	1:D:349:LEU:HD22	1.71	0.90
1:A:349:LEU:CG	1:A:350:GLU:H	1.83	0.90
1:B:93:GLU:OE1	1:F:517:GLU:HB2	1.72	0.90
1:B:93:GLU:OE2	1:F:485:ARG:NH1	2.04	0.90
1:B:290:THR:CG2	1:C:507:GLN:HE21	1.82	0.89
1:A:388:ILE:H	1:A:388:ILE:HD13	1.36	0.89
1:B:93:GLU:OE1	1:F:517:GLU:CB	2.20	0.89
1:A:414:ASN:HD22	1:A:414:ASN:H	1.20	0.89
1:D:349:LEU:HG	1:D:350:GLU:H	1.34	0.89
1:C:229:GLU:H	1:C:303:GLN:HE22	1.20	0.89
1:E:388:ILE:N	1:E:388:ILE:HD13	1.85	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:229:GLU:H	1:D:303:GLN:HE22	1.22	0.88
1:A:409:PRO:HG3	1:A:458:ILE:HD12	1.54	0.88
1:E:382:ASN:H	1:E:385:ASN:HD22	1.19	0.88
1:F:25:ARG:HH11	1:F:32:GLN:HE21	1.21	0.88
1:A:493:PRO:HB3	1:C:170:HIS:CD2	2.09	0.88
1:C:409:PRO:HG3	1:C:458:ILE:HD12	1.56	0.88
1:A:349:LEU:HG	1:A:350:GLU:H	1.36	0.87
1:E:290:THR:O	1:E:293:ASN:CB	2.22	0.87
1:B:409:PRO:HD2	1:B:483:ALA:HB3	1.57	0.86
1:C:388:ILE:HD13	1:C:388:ILE:N	1.90	0.86
1:F:273:SER:HA	1:F:295:GLN:CG	2.06	0.86
1:E:273:SER:HA	1:E:295:GLN:HB3	1.57	0.86
1:B:349:LEU:CG	1:B:350:GLU:H	1.87	0.86
1:B:172:LYS:HE3	1:F:368:ALA:O	1.76	0.86
1:B:76:GLN:O	1:B:76:GLN:HG3	1.74	0.86
1:D:409:PRO:HG3	1:D:458:ILE:HD12	1.57	0.85
1:D:388:ILE:HD13	1:D:388:ILE:N	1.90	0.85
1:C:368:ALA:O	1:E:172:LYS:HE3	1.76	0.85
1:C:517:GLU:HB2	1:E:93:GLU:OE2	1.75	0.85
1:C:291:ALA:O	1:C:295:GLN:HG3	1.75	0.85
1:C:409:PRO:HD2	1:C:483:ALA:HB3	1.59	0.85
1:C:517:GLU:HB2	1:E:93:GLU:CD	1.96	0.85
1:B:414:ASN:H	1:B:414:ASN:HD22	1.20	0.85
1:E:349:LEU:CG	1:E:350:GLU:H	1.89	0.85
1:D:382:ASN:H	1:D:385:ASN:HD22	1.25	0.84
1:A:349:LEU:HD12	1:A:350:GLU:N	1.91	0.84
1:E:414:ASN:HD22	1:E:414:ASN:H	1.20	0.84
1:C:382:ASN:H	1:C:385:ASN:HD22	1.24	0.84
1:F:229:GLU:H	1:F:303:GLN:HE22	1.26	0.84
1:E:388:ILE:H	1:E:388:ILE:HD13	1.39	0.84
1:A:229:GLU:H	1:A:303:GLN:HE22	1.26	0.84
1:C:291:ALA:C	1:C:292:ARG:O	2.06	0.84
1:D:349:LEU:HD13	1:D:351:GLU:OE1	1.78	0.84
1:E:349:LEU:HG	1:E:350:GLU:H	1.43	0.83
1:B:18:GLN:HE21	1:B:20:ARG:HG2	1.43	0.83
1:C:370:ILE:HA	1:E:91:THR:OG1	1.79	0.83
1:B:290:THR:O	1:B:293:ASN:HB2	1.78	0.83
1:F:409:PRO:HD2	1:F:483:ALA:HB3	1.61	0.83
1:D:414:ASN:HD22	1:D:414:ASN:H	1.24	0.83
1:E:409:PRO:HD2	1:E:483:ALA:HB3	1.60	0.83
1:A:349:LEU:HD22	1:D:479:ILE:O	1.79	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:25:ARG:HH11	1:F:32:GLN:NE2	1.76	0.82
1:E:349:LEU:HD12	1:E:350:GLU:N	1.94	0.82
1:F:388:ILE:HD13	1:F:388:ILE:N	1.94	0.82
1:D:349:LEU:HD12	1:D:350:GLU:N	1.93	0.82
1:D:388:ILE:HD13	1:D:388:ILE:H	1.43	0.82
1:C:10:ASN:HD22	1:C:10:ASN:N	1.78	0.82
1:D:418:VAL:HG22	1:D:450:ILE:HG12	1.60	0.82
1:C:409:PRO:HG3	1:C:458:ILE:CD1	2.10	0.81
1:B:382:ASN:H	1:B:385:ASN:HD22	1.26	0.81
1:C:349:LEU:HD12	1:C:350:GLU:N	1.94	0.81
1:A:486:THR:HG21	1:C:87:GLY:HA2	1.62	0.81
1:C:277:THR:HG21	1:C:292:ARG:HG3	1.61	0.81
1:A:370:ILE:HA	1:D:91:THR:OG1	1.81	0.81
1:A:93:GLU:OE2	1:D:517:GLU:HB2	1.78	0.81
1:E:287:ASN:ND2	1:E:290:THR:OG1	2.14	0.80
1:A:423:ARG:HH11	1:A:423:ARG:CB	1.92	0.80
1:A:431:VAL:HG11	1:C:274:GLY:HA3	1.62	0.80
1:D:290:THR:O	1:D:293:ASN:HB3	1.82	0.80
1:E:77:GLY:C	1:E:78:ARG:HG3	2.00	0.80
1:B:10:ASN:N	1:B:10:ASN:HD22	1.79	0.80
1:A:513:TYR:OH	1:C:169:ARG:HG2	1.82	0.80
1:B:510:GLN:O	1:B:514:ASN:HB2	1.82	0.80
1:A:381:LEU:HD13	1:A:389:LEU:HD11	1.64	0.80
1:B:388:ILE:N	1:B:388:ILE:HD13	1.97	0.80
1:C:388:ILE:HD13	1:C:388:ILE:H	1.47	0.79
1:D:66:SER:HB2	1:D:220:ARG:O	1.81	0.79
1:C:486:THR:H	1:C:518:THR:HB	1.47	0.79
1:E:409:PRO:HG3	1:E:458:ILE:HD12	1.64	0.79
2:C:609:HOH:O	1:D:169:ARG:HG3	1.83	0.79
1:B:229:GLU:H	1:B:303:GLN:HE22	1.30	0.79
1:F:409:PRO:HG3	1:F:458:ILE:HD12	1.65	0.79
1:A:274:GLY:HA3	1:B:431:VAL:HG11	1.63	0.79
1:F:349:LEU:HD12	1:F:350:GLU:N	1.98	0.79
1:D:423:ARG:HH11	1:D:423:ARG:CB	1.94	0.79
1:B:517:GLU:HB2	1:F:93:GLU:OE2	1.83	0.78
1:C:25:ARG:HH11	1:C:32:GLN:HE21	1.31	0.78
1:B:349:LEU:HD12	1:B:350:GLU:N	1.97	0.78
1:C:292:ARG:O	1:C:293:ASN:HB2	1.83	0.78
1:E:409:PRO:HG3	1:E:458:ILE:CD1	2.14	0.78
1:F:493:PRO:O	1:F:496:VAL:HG12	1.83	0.78
1:D:409:PRO:HD2	1:D:483:ALA:HB3	1.65	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:486:THR:HB	1:F:518:THR:HG21	1.66	0.77
1:B:80:VAL:CG1	1:B:173:THR:HG23	2.15	0.77
1:B:349:LEU:HD22	1:F:479:ILE:O	1.84	0.77
1:F:486:THR:H	1:F:518:THR:HB	1.49	0.77
1:F:388:ILE:H	1:F:388:ILE:HD13	1.49	0.77
1:B:493:PRO:O	1:B:496:VAL:HG12	1.84	0.77
1:A:277:THR:HG21	1:A:292:ARG:HG2	1.65	0.77
1:A:382:ASN:H	1:A:385:ASN:HD22	1.31	0.77
1:B:17:LEU:HB2	1:B:439:LEU:HB2	1.66	0.77
1:D:381:LEU:HD13	1:D:389:LEU:HD11	1.67	0.77
1:D:64:SER:O	1:D:189:ALA:HA	1.84	0.76
1:C:479:ILE:O	1:E:349:LEU:HD22	1.86	0.76
1:A:486:THR:H	1:A:518:THR:HB	1.51	0.76
1:A:517:GLU:CB	1:D:93:GLU:CD	2.54	0.76
1:D:431:VAL:HG11	1:F:274:GLY:HA3	1.64	0.76
1:D:25:ARG:HH11	1:D:32:GLN:HE21	1.34	0.76
1:A:66:SER:HB2	1:A:220:ARG:O	1.84	0.76
1:A:418:VAL:HG22	1:A:450:ILE:HG12	1.66	0.75
1:C:93:GLU:OE2	1:E:517:GLU:HB2	1.85	0.75
1:A:510:GLN:O	1:A:514:ASN:HB2	1.86	0.75
1:C:493:PRO:O	1:C:496:VAL:HG12	1.86	0.75
1:C:64:SER:O	1:C:189:ALA:HA	1.86	0.75
1:A:91:THR:OG1	1:D:370:ILE:HA	1.86	0.75
1:F:409:PRO:HG3	1:F:458:ILE:CD1	2.16	0.75
1:D:274:GLY:HA3	1:E:431:VAL:HG11	1.67	0.75
1:B:370:ILE:HA	1:F:91:THR:OG1	1.86	0.75
1:B:277:THR:HG21	1:B:292:ARG:HG2	1.68	0.75
1:F:423:ARG:HH11	1:F:423:ARG:CB	1.96	0.74
1:C:290:THR:HA	1:C:293:ASN:HD22	1.52	0.74
1:B:25:ARG:HH11	1:B:32:GLN:HE21	1.35	0.74
1:A:349:LEU:HD13	1:A:351:GLU:OE1	1.87	0.74
1:D:493:PRO:O	1:D:496:VAL:HG12	1.88	0.74
1:A:495:GLU:CD	1:C:312:ASP:OD2	2.26	0.74
1:E:80:VAL:CG1	1:E:173:THR:HG23	2.17	0.74
1:D:350:GLU:OE2	1:D:350:GLU:HA	1.87	0.74
1:B:17:LEU:HG	1:B:438:ILE:HG12	1.69	0.74
1:B:409:PRO:HG3	1:B:458:ILE:CD1	2.18	0.74
1:C:349:LEU:CG	1:C:350:GLU:N	2.51	0.74
1:F:11:GLN:HG3	2:F:545:HOH:O	1.86	0.74
1:F:349:LEU:CG	1:F:350:GLU:N	2.51	0.74
1:C:414:ASN:ND2	1:C:414:ASN:H	1.85	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:518:THR:HG23	1:B:519:ILE:HG13	1.69	0.74
1:D:486:THR:HG21	1:F:87:GLY:HA2	1.70	0.74
1:D:409:PRO:HB2	1:D:482:LEU:HD12	1.69	0.73
1:C:381:LEU:HD13	1:C:389:LEU:HD11	1.70	0.73
1:A:175:ARG:NH2	1:A:177:ARG:HD3	2.03	0.73
1:C:418:VAL:HG22	1:C:450:ILE:HG12	1.70	0.73
1:A:409:PRO:HD2	1:A:483:ALA:HB3	1.69	0.73
1:A:25:ARG:HH11	1:A:32:GLN:HE21	1.35	0.73
1:B:504:SER:HB2	1:B:507:GLN:H	1.52	0.73
1:C:91:THR:OG1	1:E:370:ILE:HA	1.87	0.73
1:A:64:SER:O	1:A:189:ALA:HA	1.88	0.73
1:F:66:SER:HB2	1:F:220:ARG:O	1.88	0.73
1:E:25:ARG:HH11	1:E:32:GLN:HE21	1.36	0.73
1:D:486:THR:H	1:D:518:THR:HB	1.54	0.73
1:A:170:HIS:CD2	1:B:493:PRO:HB3	2.24	0.73
1:E:381:LEU:HD13	1:E:389:LEU:HD11	1.70	0.73
1:E:273:SER:CA	1:E:295:GLN:HB3	2.18	0.72
1:C:518:THR:HG23	1:C:519:ILE:HG13	1.70	0.72
1:F:518:THR:HG23	1:F:519:ILE:HG13	1.70	0.72
1:F:350:GLU:OE2	1:F:350:GLU:HA	1.89	0.72
1:D:349:LEU:CG	1:D:350:GLU:N	2.52	0.72
1:F:273:SER:HA	1:F:295:GLN:HG3	1.68	0.72
1:A:414:ASN:H	1:A:414:ASN:ND2	1.87	0.72
1:C:287:ASN:HD21	1:C:290:THR:HG23	1.55	0.72
1:F:349:LEU:HD13	1:F:351:GLU:OE1	1.88	0.72
1:A:290:THR:O	1:A:293:ASN:CB	2.38	0.72
1:B:349:LEU:HD13	1:B:351:GLU:OE1	1.89	0.72
1:E:78:ARG:NH1	1:E:198:GLN:HG2	2.04	0.72
1:C:208:VAL:HG21	2:C:569:HOH:O	1.89	0.72
1:A:486:THR:HB	1:A:518:THR:HG21	1.71	0.72
1:A:349:LEU:CG	1:A:350:GLU:N	2.53	0.72
1:B:66:SER:HB2	1:B:220:ARG:O	1.90	0.72
1:C:369:ASP:OD2	1:E:355:SER:HB3	1.89	0.72
1:D:270:ASN:ND2	1:D:273:SER:H	1.88	0.72
1:C:510:GLN:O	1:C:514:ASN:HB2	1.90	0.72
1:C:25:ARG:HH11	1:C:32:GLN:NE2	1.87	0.71
1:D:414:ASN:ND2	1:D:414:ASN:H	1.88	0.71
1:E:78:ARG:HH12	1:E:198:GLN:HG2	1.54	0.71
1:B:169:ARG:HG2	1:C:513:TYR:OH	1.90	0.71
1:F:510:GLN:O	1:F:514:ASN:HB2	1.90	0.71
1:E:414:ASN:ND2	1:E:414:ASN:H	1.88	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:93:GLU:HG3	1:B:93:GLU:O	1.90	0.71
1:B:25:ARG:HH11	1:B:32:GLN:NE2	1.88	0.71
1:B:423:ARG:HH11	1:B:423:ARG:CB	1.96	0.71
1:B:350:GLU:HA	1:B:350:GLU:OE2	1.90	0.71
1:C:356:LEU:HD12	1:C:388:ILE:HD12	1.71	0.71
1:F:349:LEU:HD12	1:F:351:GLU:H	1.56	0.70
1:A:480:ASN:ND2	1:C:86:SER:HB3	2.06	0.70
1:B:287:ASN:HD21	1:B:290:THR:HG23	1.54	0.70
1:A:302:ASN:HB3	1:A:303:GLN:NE2	2.03	0.70
1:B:87:GLY:HA2	1:C:486:THR:HG21	1.73	0.70
1:E:493:PRO:O	1:E:496:VAL:HG12	1.90	0.70
1:F:381:LEU:HD13	1:F:389:LEU:HD11	1.71	0.70
1:A:493:PRO:O	1:A:496:VAL:HG12	1.92	0.70
1:E:518:THR:HG23	1:E:519:ILE:HG13	1.72	0.70
1:D:349:LEU:HD12	1:D:351:GLU:H	1.55	0.70
1:F:293:ASN:O	1:F:294:LEU:C	2.28	0.70
1:B:349:LEU:CG	1:B:350:GLU:N	2.54	0.70
1:F:414:ASN:H	1:F:414:ASN:ND2	1.88	0.70
1:C:293:ASN:O	1:C:296:GLY:N	2.23	0.70
1:F:272:PHE:O	1:F:295:GLN:NE2	2.24	0.70
1:B:414:ASN:H	1:B:414:ASN:ND2	1.89	0.70
1:E:504:SER:HB2	1:E:507:GLN:H	1.55	0.70
1:C:93:GLU:CD	1:E:517:GLU:CB	2.60	0.70
1:F:356:LEU:HD12	1:F:388:ILE:HD12	1.74	0.70
1:C:486:THR:HB	1:C:518:THR:HG21	1.74	0.70
1:A:80:VAL:HG13	1:A:173:THR:HG23	1.73	0.70
1:F:421:VAL:HG12	1:F:445:GLN:HA	1.72	0.69
1:C:66:SER:HB2	1:C:220:ARG:O	1.92	0.69
1:E:350:GLU:OE2	1:E:350:GLU:HA	1.92	0.69
1:C:172:LYS:HE3	1:E:368:ALA:O	1.92	0.69
1:B:486:THR:H	1:B:518:THR:HB	1.56	0.69
1:F:409:PRO:HB2	1:F:482:LEU:HD12	1.72	0.69
1:F:409:PRO:HB2	1:F:482:LEU:CD1	2.23	0.69
1:A:87:GLY:HA2	1:B:486:THR:HG21	1.75	0.69
1:D:409:PRO:HB2	1:D:482:LEU:CD1	2.22	0.69
1:E:270:ASN:ND2	1:E:273:SER:H	1.90	0.69
1:D:419:VAL:O	1:D:448:LEU:HD22	1.92	0.69
1:B:357:ARG:O	1:B:388:ILE:HD11	1.92	0.69
1:D:25:ARG:HH11	1:D:32:GLN:NE2	1.91	0.69
1:D:60:LEU:HD12	1:D:192:SER:O	1.93	0.69
1:D:486:THR:HB	1:D:518:THR:HG21	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:349:LEU:CD1	1:D:350:GLU:H	2.06	0.69
1:E:170:HIS:CD2	1:F:493:PRO:HB3	2.27	0.69
1:B:95:SER:O	1:B:96:GLN:O	2.10	0.69
1:B:302:ASN:HB3	1:B:303:GLN:NE2	2.05	0.69
1:C:291:ALA:O	1:C:295:GLN:CG	2.40	0.69
1:A:349:LEU:CD1	1:A:350:GLU:N	2.56	0.69
1:C:63:PRO:HA	1:C:190:TYR:O	1.93	0.69
1:A:287:ASN:HD21	1:A:290:THR:HG23	1.56	0.69
2:C:589:HOH:O	1:D:351:GLU:OE2	2.10	0.69
1:C:269:ASN:HB3	1:C:273:SER:OG	1.93	0.69
1:D:513:TYR:OH	1:F:169:ARG:HG2	1.93	0.69
1:F:78:ARG:NH1	1:F:175:ARG:NH1	2.41	0.69
1:B:479:ILE:O	1:F:349:LEU:HD22	1.93	0.68
1:E:175:ARG:NH2	1:E:177:ARG:HD3	2.08	0.68
1:A:388:ILE:H	1:A:388:ILE:CD1	1.99	0.68
1:A:349:LEU:HD12	1:A:351:GLU:H	1.58	0.68
1:B:368:ALA:O	1:F:172:LYS:HE3	1.93	0.68
1:B:409:PRO:HG3	1:B:458:ILE:HD12	1.76	0.68
1:A:409:PRO:HB2	1:A:482:LEU:CD1	2.24	0.68
1:B:388:ILE:HD13	1:B:388:ILE:H	1.56	0.68
1:B:80:VAL:HG13	1:B:173:THR:HG23	1.74	0.68
1:D:349:LEU:CD1	1:D:350:GLU:N	2.57	0.68
1:F:269:ASN:HB3	1:F:273:SER:OG	1.94	0.68
1:A:349:LEU:CD1	1:A:350:GLU:H	2.07	0.68
1:A:93:GLU:CD	1:D:517:GLU:CB	2.61	0.68
1:C:452:PRO:HB2	1:C:455:HIS:CD2	2.29	0.68
1:B:14:LEU:CD1	1:B:17:LEU:HD21	2.23	0.68
1:E:302:ASN:HB3	1:E:303:GLN:NE2	2.05	0.67
1:E:409:PRO:HB2	1:E:482:LEU:CD1	2.24	0.67
1:B:270:ASN:ND2	1:B:273:SER:H	1.92	0.67
1:D:415:ALA:HB2	1:D:474:GLU:HB2	1.75	0.67
1:D:497:LEU:HD12	1:D:512:LYS:HE3	1.77	0.67
1:A:63:PRO:HA	1:A:190:TYR:O	1.94	0.67
1:B:414:ASN:HD21	1:B:478:PHE:H	1.42	0.67
1:E:87:GLY:HA2	1:F:486:THR:HG21	1.75	0.67
1:A:368:ALA:O	1:D:172:LYS:HE3	1.93	0.67
1:A:80:VAL:CG1	1:A:173:THR:HG23	2.25	0.67
1:C:414:ASN:HD22	1:C:414:ASN:N	1.85	0.67
1:D:452:PRO:HB2	1:D:455:HIS:CD2	2.28	0.67
1:B:418:VAL:HG22	1:B:450:ILE:HG12	1.77	0.67
1:E:486:THR:H	1:E:518:THR:HB	1.57	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:388:ILE:H	1:D:388:ILE:CD1	2.02	0.67
1:B:381:LEU:HD13	1:B:389:LEU:HD11	1.76	0.67
1:E:357:ARG:O	1:E:388:ILE:HD11	1.95	0.66
1:D:510:GLN:O	1:D:514:ASN:HB2	1.94	0.66
1:A:75:VAL:HG23	1:A:202:ALA:HA	1.76	0.66
1:D:290:THR:HG23	1:E:507:GLN:NE2	2.09	0.66
1:F:63:PRO:HA	1:F:190:TYR:O	1.95	0.66
1:D:518:THR:HG23	1:D:519:ILE:HG13	1.76	0.66
1:C:415:ALA:HB2	1:C:474:GLU:HB2	1.76	0.66
1:A:409:PRO:HB2	1:A:482:LEU:HD12	1.76	0.66
1:E:349:LEU:CG	1:E:350:GLU:N	2.58	0.66
1:F:64:SER:O	1:F:189:ALA:HA	1.95	0.66
1:E:350:GLU:OE2	1:E:350:GLU:CA	2.44	0.66
1:B:409:PRO:HB2	1:B:482:LEU:CD1	2.26	0.66
1:B:409:PRO:HB2	1:B:482:LEU:HD12	1.76	0.66
1:C:409:PRO:HB2	1:C:482:LEU:CD1	2.26	0.66
1:E:452:PRO:HB2	1:E:455:HIS:CD2	2.31	0.66
1:E:229:GLU:H	1:E:303:GLN:HE22	1.43	0.66
1:C:349:LEU:CD1	1:C:350:GLU:N	2.57	0.66
1:B:517:GLU:CB	1:F:93:GLU:CD	2.64	0.66
1:E:290:THR:CG2	1:F:507:GLN:HE21	1.92	0.66
1:C:350:GLU:OE2	1:C:350:GLU:HA	1.94	0.66
1:E:486:THR:HB	1:E:518:THR:HG21	1.76	0.66
1:C:349:LEU:HD12	1:C:351:GLU:H	1.60	0.66
1:C:292:ARG:O	1:C:293:ASN:C	2.30	0.66
1:B:350:GLU:OE2	1:B:350:GLU:CA	2.44	0.66
1:E:54:THR:HG23	1:E:201:VAL:HG22	1.77	0.66
1:D:170:HIS:CD2	1:E:493:PRO:HB3	2.31	0.65
1:F:452:PRO:HB2	1:F:455:HIS:CD2	2.31	0.65
1:B:269:ASN:HB3	1:B:273:SER:OG	1.96	0.65
1:C:290:THR:O	1:C:293:ASN:HB2	1.96	0.65
1:B:415:ALA:HB2	1:B:474:GLU:HB2	1.79	0.65
1:D:350:GLU:CA	1:D:350:GLU:OE2	2.44	0.65
1:A:25:ARG:HH11	1:A:32:GLN:NE2	1.95	0.65
1:D:175:ARG:NH2	1:D:177:ARG:HD3	2.12	0.65
1:C:293:ASN:O	1:C:295:GLN:CA	2.44	0.65
1:F:418:VAL:HG22	1:F:450:ILE:HG12	1.78	0.65
1:C:388:ILE:H	1:C:388:ILE:CD1	2.07	0.65
1:B:452:PRO:HB2	1:B:455:HIS:CD2	2.32	0.65
1:C:423:ARG:HH11	1:C:423:ARG:CB	2.03	0.65
1:C:349:LEU:HD22	1:E:479:ILE:O	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:349:LEU:CD1	1:E:350:GLU:N	2.60	0.65
1:E:80:VAL:HG13	1:E:173:THR:HG23	1.78	0.65
1:B:93:GLU:CD	1:F:517:GLU:HB2	2.18	0.65
1:E:419:VAL:O	1:E:448:LEU:HD22	1.97	0.65
1:C:421:VAL:HG12	1:C:445:GLN:HA	1.77	0.65
1:A:270:ASN:ND2	1:A:273:SER:H	1.95	0.65
1:A:350:GLU:OE2	1:A:350:GLU:HA	1.96	0.65
1:D:391:PHE:O	1:D:392:LEU:HB2	1.96	0.65
1:B:274:GLY:HA3	1:C:431:VAL:HG11	1.79	0.65
1:F:54:THR:HG23	1:F:201:VAL:HG22	1.78	0.65
1:C:270:ASN:ND2	1:C:273:SER:H	1.95	0.65
1:A:452:PRO:HB2	1:A:455:HIS:CD2	2.31	0.65
1:B:476:ASN:HB3	1:F:352:THR:HG22	1.79	0.65
1:A:12:CYS:C	1:A:14:LEU:H	1.99	0.65
1:F:350:GLU:OE2	1:F:350:GLU:CA	2.44	0.64
1:E:66:SER:HB2	1:E:220:ARG:O	1.97	0.64
1:A:33:ILE:HG12	1:A:53:ILE:HD13	1.79	0.64
1:F:378:ILE:HD12	1:F:519:ILE:CG2	2.26	0.64
1:E:510:GLN:O	1:E:514:ASN:HB2	1.97	0.64
1:D:12:CYS:HA	1:D:14:LEU:HD23	1.78	0.64
1:B:170:HIS:CD2	1:C:493:PRO:HB3	2.31	0.64
1:D:12:CYS:C	1:D:14:LEU:H	2.00	0.64
1:C:350:GLU:HB3	1:C:354:CYS:HB2	1.79	0.64
1:F:349:LEU:CD1	1:F:350:GLU:N	2.59	0.64
1:F:270:ASN:ND2	1:F:273:SER:H	1.96	0.64
1:B:382:ASN:HB3	2:C:547:HOH:O	1.98	0.64
1:E:25:ARG:HH11	1:E:32:GLN:NE2	1.96	0.64
1:E:169:ARG:HG2	1:F:513:TYR:OH	1.96	0.64
1:D:429:GLN:HE22	1:F:276:ASN:H	1.45	0.64
1:C:370:ILE:HA	1:E:91:THR:HG1	1.60	0.64
1:A:12:CYS:HA	1:A:14:LEU:HD23	1.78	0.64
1:A:497:LEU:HD12	1:A:512:LYS:HE3	1.79	0.64
1:B:429:GLN:HB2	1:B:458:ILE:HG22	1.79	0.64
1:A:290:THR:CG2	1:B:507:GLN:HE21	2.01	0.64
1:B:301:ARG:O	1:B:302:ASN:HB2	1.98	0.63
1:C:17:LEU:HB2	1:C:439:LEU:HB2	1.80	0.63
1:E:290:THR:CG2	1:F:507:GLN:NE2	2.51	0.63
1:A:518:THR:HG23	1:A:519:ILE:HG13	1.78	0.63
1:A:429:GLN:HE22	1:C:276:ASN:H	1.45	0.63
1:B:349:LEU:CD1	1:B:350:GLU:N	2.60	0.63
1:B:351:GLU:O	1:F:380:THR:HG21	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:429:GLN:HB2	1:D:458:ILE:HG22	1.80	0.63
1:A:350:GLU:OE2	1:A:350:GLU:CA	2.46	0.63
1:C:391:PHE:O	1:C:392:LEU:HB2	1.99	0.63
1:B:28:ALA:O	1:B:29:GLU:C	2.37	0.63
1:F:301:ARG:O	1:F:302:ASN:HB2	1.97	0.63
1:F:415:ALA:HB2	1:F:474:GLU:HB2	1.79	0.63
1:E:269:ASN:HB3	1:E:273:SER:OG	1.99	0.63
1:C:517:GLU:CB	1:E:93:GLU:CD	2.65	0.63
1:C:380:THR:HG21	1:E:351:GLU:O	1.98	0.63
1:A:269:ASN:HB3	1:A:273:SER:OG	1.97	0.63
1:F:78:ARG:CZ	1:F:175:ARG:NH1	2.62	0.63
1:C:350:GLU:CA	1:C:350:GLU:OE2	2.47	0.63
1:F:272:PHE:C	1:F:295:GLN:HE21	2.01	0.63
1:D:269:ASN:HB3	1:D:273:SER:OG	1.98	0.63
1:C:378:ILE:HD12	1:C:519:ILE:CG2	2.29	0.63
1:E:63:PRO:HA	1:E:190:TYR:O	1.99	0.63
1:A:391:PHE:O	1:A:392:LEU:HB2	1.98	0.63
1:A:378:ILE:HD12	1:A:519:ILE:CG2	2.29	0.62
1:F:504:SER:HB2	1:F:507:GLN:H	1.64	0.62
1:E:268:GLY:O	1:E:269:ASN:HB2	1.99	0.62
1:D:280:LEU:HD12	1:D:280:LEU:O	1.99	0.62
1:A:290:THR:O	1:A:293:ASN:HB3	2.00	0.62
1:C:349:LEU:HD13	1:C:351:GLU:OE1	1.98	0.62
1:C:80:VAL:HG13	1:C:173:THR:HG23	1.80	0.62
1:C:268:GLY:O	1:C:269:ASN:HB2	1.98	0.62
1:F:17:LEU:HB2	1:F:439:LEU:HB2	1.81	0.62
1:E:429:GLN:HB2	1:E:458:ILE:HG22	1.81	0.62
1:E:12:CYS:C	1:E:14:LEU:H	2.03	0.62
1:E:349:LEU:CD1	1:E:350:GLU:H	2.11	0.62
1:A:430:VAL:O	1:A:438:ILE:HG22	2.00	0.62
1:A:60:LEU:HD12	1:A:192:SER:O	1.99	0.62
1:D:276:ASN:H	1:E:429:GLN:HE22	1.48	0.62
1:C:232:PHE:O	1:C:234:GLN:N	2.33	0.62
1:D:87:GLY:HA2	1:E:486:THR:HG21	1.81	0.62
1:B:349:LEU:HD12	1:B:351:GLU:H	1.64	0.62
1:F:12:CYS:C	1:F:14:LEU:H	2.03	0.62
1:B:54:THR:HG23	1:B:201:VAL:HG22	1.81	0.62
1:E:409:PRO:HB2	1:E:482:LEU:HD12	1.82	0.62
1:E:77:GLY:O	1:E:78:ARG:HG3	2.00	0.62
1:C:349:LEU:CD1	1:C:350:GLU:H	2.10	0.62
1:D:291:ALA:C	1:D:293:ASN:N	2.44	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:175:ARG:NH2	1:B:177:ARG:HD3	2.14	0.62
1:C:60:LEU:HD12	1:C:192:SER:O	2.00	0.62
1:F:414:ASN:HD21	1:F:478:PHE:H	1.48	0.61
1:F:268:GLY:O	1:F:269:ASN:HB2	1.98	0.61
1:D:268:GLY:O	1:D:269:ASN:HB2	1.99	0.61
1:A:301:ARG:O	1:A:302:ASN:HB2	1.99	0.61
1:F:486:THR:CB	1:F:518:THR:HG21	2.30	0.61
1:F:175:ARG:NH2	1:F:177:ARG:HD3	2.15	0.61
1:D:194:ASN:HD22	1:D:194:ASN:C	2.02	0.61
1:A:393:ARG:HB2	2:A:539:HOH:O	2.00	0.61
1:C:305:ILE:HG22	1:C:306:GLN:N	2.16	0.61
1:A:268:GLY:O	1:A:269:ASN:HB2	1.99	0.61
1:F:516:GLN:HG3	1:F:517:GLU:N	2.15	0.61
1:E:305:ILE:HG22	1:E:306:GLN:N	2.16	0.61
1:E:388:ILE:CD1	1:E:388:ILE:H	1.97	0.61
1:D:75:VAL:HG23	1:D:202:ALA:HA	1.81	0.61
1:F:391:PHE:O	1:F:392:LEU:HB2	2.01	0.61
1:B:75:VAL:O	1:B:76:GLN:HB3	2.01	0.61
1:E:12:CYS:HA	1:E:14:LEU:HD23	1.82	0.61
1:F:80:VAL:HG13	1:F:173:THR:HG23	1.82	0.61
1:D:504:SER:HB2	1:D:507:GLN:H	1.65	0.61
1:B:398:ARG:HH12	1:B:467:GLU:HG2	1.65	0.61
1:C:93:GLU:OE1	1:E:517:GLU:CB	2.49	0.61
1:E:301:ARG:O	1:E:302:ASN:HB2	2.01	0.61
1:C:290:THR:O	1:C:292:ARG:O	2.18	0.61
1:E:19:ALA:HB2	1:E:449:PHE:HB3	1.82	0.61
1:A:429:GLN:HB2	1:A:458:ILE:HG22	1.83	0.61
1:D:414:ASN:HD21	1:D:478:PHE:H	1.49	0.61
1:B:10:ASN:N	1:B:10:ASN:ND2	2.48	0.61
1:F:60:LEU:HD12	1:F:192:SER:O	2.01	0.61
1:D:63:PRO:HA	1:D:190:TYR:O	2.00	0.61
1:E:423:ARG:CB	1:E:423:ARG:HH11	2.06	0.61
1:A:415:ALA:HB2	1:A:474:GLU:HB2	1.82	0.61
1:B:305:ILE:HG22	1:B:306:GLN:N	2.16	0.61
1:D:232:PHE:O	1:D:234:GLN:N	2.33	0.61
1:A:93:GLU:HG3	1:D:485:ARG:HH22	1.66	0.60
1:A:517:GLU:OE2	1:A:518:THR:HG22	2.01	0.60
1:E:516:GLN:HG3	1:E:517:GLU:N	2.16	0.60
1:A:504:SER:HB2	1:A:507:GLN:H	1.66	0.60
1:B:391:PHE:O	1:B:392:LEU:HB2	2.01	0.60
1:B:62:LEU:HG	1:B:303:GLN:O	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:268:GLY:O	1:B:269:ASN:HB2	2.01	0.60
1:C:301:ARG:O	1:C:302:ASN:HB2	2.01	0.60
1:A:414:ASN:HD22	1:A:414:ASN:N	1.88	0.60
1:E:391:PHE:O	1:E:392:LEU:HB2	2.01	0.60
1:C:409:PRO:HB2	1:C:482:LEU:HD12	1.82	0.60
1:B:355:SER:HB3	1:F:369:ASP:OD2	2.01	0.60
1:F:80:VAL:CG1	1:F:173:THR:HG23	2.31	0.60
1:B:64:SER:O	1:B:189:ALA:HA	2.01	0.60
1:F:421:VAL:CG1	1:F:445:GLN:HA	2.31	0.60
1:E:87:GLY:HA2	1:F:486:THR:CG2	2.32	0.60
1:E:64:SER:O	1:E:189:ALA:HA	2.02	0.60
1:A:370:ILE:HA	1:D:91:THR:HG1	1.63	0.59
1:B:12:CYS:C	1:B:14:LEU:H	2.05	0.59
1:A:414:ASN:HD21	1:A:478:PHE:H	1.50	0.59
1:A:419:VAL:O	1:A:448:LEU:HD22	2.02	0.59
1:C:516:GLN:HG3	1:C:517:GLU:N	2.16	0.59
1:E:350:GLU:HB3	1:E:354:CYS:HB2	1.84	0.59
1:D:291:ALA:HA	1:D:294:LEU:HD12	1.83	0.59
1:D:290:THR:HG23	1:E:507:GLN:HE21	1.67	0.59
1:A:480:ASN:CG	1:C:86:SER:HB3	2.22	0.59
1:D:480:ASN:ND2	1:F:86:SER:HB3	2.17	0.59
1:C:54:THR:HG23	1:C:201:VAL:HG22	1.83	0.59
1:F:357:ARG:O	1:F:388:ILE:HD11	2.01	0.59
1:C:91:THR:HG1	1:E:370:ILE:HA	1.66	0.59
1:D:517:GLU:OE2	1:D:518:THR:HG22	2.02	0.59
1:E:415:ALA:HB2	1:E:474:GLU:HB2	1.84	0.59
1:F:388:ILE:CD1	1:F:388:ILE:N	2.64	0.59
1:D:273:SER:HA	1:D:295:GLN:HG2	1.84	0.59
1:D:54:THR:HG23	1:D:201:VAL:HG22	1.83	0.59
1:A:172:LYS:HE3	1:D:368:ALA:O	2.02	0.59
1:F:232:PHE:O	1:F:234:GLN:N	2.36	0.59
1:B:193:TYR:CZ	1:B:311:LEU:HB3	2.37	0.59
1:F:515:ARG:NH1	1:F:516:GLN:OE1	2.36	0.59
1:F:368:ALA:HA	1:F:379:SER:OG	2.03	0.59
1:A:516:GLN:HG3	1:A:517:GLU:N	2.17	0.59
1:F:293:ASN:C	1:F:295:GLN:N	2.45	0.59
1:B:516:GLN:HG3	1:B:517:GLU:N	2.18	0.58
1:E:220:ARG:HD3	1:F:433:GLU:OE1	2.03	0.58
1:D:80:VAL:HG13	1:D:173:THR:HG23	1.84	0.58
1:B:287:ASN:ND2	1:B:290:THR:HG23	2.18	0.58
1:B:93:GLU:H	1:B:314:VAL:HG11	1.67	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:12:CYS:HA	1:F:14:LEU:HD23	1.84	0.58
1:D:414:ASN:HD22	1:D:414:ASN:N	1.89	0.58
1:C:80:VAL:CG1	1:C:173:THR:HG23	2.32	0.58
1:C:293:ASN:O	1:C:295:GLN:HB2	2.03	0.58
1:C:12:CYS:C	1:C:14:LEU:H	2.05	0.58
1:E:79:GLY:O	1:E:176:ILE:HG12	2.03	0.58
1:A:486:THR:CG2	1:C:87:GLY:HA2	2.31	0.58
1:F:389:LEU:HB3	1:F:394:LEU:O	2.04	0.58
1:B:419:VAL:O	1:B:448:LEU:HD22	2.04	0.58
1:A:232:PHE:O	1:A:234:GLN:N	2.35	0.58
1:F:517:GLU:OE2	1:F:518:THR:HG22	2.04	0.58
1:C:414:ASN:HD21	1:C:478:PHE:H	1.52	0.58
1:C:74:ILE:CD1	1:C:176:ILE:HB	2.34	0.58
1:C:316:PRO:HB3	1:E:371:PHE:CD2	2.38	0.58
1:A:54:THR:HG23	1:A:201:VAL:HG22	1.84	0.58
1:D:301:ARG:O	1:D:302:ASN:HB2	2.02	0.58
1:A:172:LYS:HB3	2:A:538:HOH:O	2.03	0.58
1:B:378:ILE:HD12	1:B:519:ILE:CG2	2.34	0.58
1:A:17:LEU:HB2	1:A:439:LEU:HB2	1.86	0.58
1:A:455:HIS:HE1	2:C:532:HOH:O	1.86	0.58
1:A:507:GLN:NE2	1:C:290:THR:HG22	2.19	0.58
1:F:14:LEU:HD12	1:F:438:ILE:HD11	1.86	0.58
1:B:29:GLU:OE2	1:B:306:GLN:HB3	2.04	0.58
1:F:230:ASN:HB3	1:F:233:ASN:ND2	2.18	0.58
1:E:382:ASN:N	1:E:385:ASN:HD22	1.96	0.57
1:A:194:ASN:HD22	1:A:194:ASN:C	2.05	0.57
1:B:12:CYS:HA	1:B:14:LEU:HD23	1.85	0.57
1:F:382:ASN:N	1:F:385:ASN:HD22	1.97	0.57
1:C:12:CYS:HA	1:C:14:LEU:HD23	1.85	0.57
1:F:230:ASN:HB3	1:F:233:ASN:HD22	1.70	0.57
1:B:38:PHE:CE2	1:B:232:PHE:HB3	2.40	0.57
1:F:493:PRO:HG2	1:F:496:VAL:CG1	2.34	0.57
1:F:305:ILE:HG22	1:F:306:GLN:N	2.20	0.57
1:C:504:SER:HB2	1:C:507:GLN:H	1.70	0.57
1:D:382:ASN:N	1:D:385:ASN:HD22	1.99	0.57
1:A:495:GLU:OE1	1:C:312:ASP:OD2	2.23	0.57
1:C:194:ASN:HD22	1:C:194:ASN:C	2.06	0.57
1:B:194:ASN:C	1:B:194:ASN:HD22	2.06	0.57
1:A:485:ARG:HH22	1:D:93:GLU:HG3	1.69	0.57
1:A:388:ILE:N	1:A:388:ILE:CD1	2.56	0.57
1:E:220:ARG:HD3	1:F:433:GLU:CD	2.25	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:92:PHE:O	1:B:93:GLU:HB3	2.03	0.57
1:B:93:GLU:OE1	1:F:517:GLU:HG2	2.04	0.57
1:C:515:ARG:HD3	1:C:516:GLN:H	1.69	0.57
1:C:517:GLU:OE2	1:C:518:THR:HG22	2.04	0.57
1:D:291:ALA:O	1:D:295:GLN:OE1	2.23	0.57
1:C:287:ASN:ND2	1:C:290:THR:HG23	2.19	0.57
1:C:515:ARG:NH1	1:C:516:GLN:OE1	2.38	0.57
1:B:370:ILE:HA	1:F:91:THR:HG1	1.69	0.57
1:E:349:LEU:HD13	1:E:351:GLU:OE1	2.03	0.57
1:B:388:ILE:CD1	1:B:388:ILE:N	2.65	0.57
1:E:274:GLY:HA3	1:F:431:VAL:HG11	1.85	0.57
1:D:448:LEU:HD13	1:D:449:PHE:N	2.19	0.57
1:D:307:VAL:HG13	1:E:499:ASN:CG	2.25	0.57
1:A:62:LEU:HG	1:A:303:GLN:O	2.04	0.56
1:D:486:THR:CG2	1:F:87:GLY:HA2	2.34	0.56
1:B:60:LEU:HD12	1:B:192:SER:O	2.05	0.56
1:A:517:GLU:CB	1:D:93:GLU:OE1	2.54	0.56
1:E:33:ILE:HG12	1:E:53:ILE:HD13	1.86	0.56
1:B:389:LEU:HB3	1:B:394:LEU:O	2.05	0.56
1:B:486:THR:HB	1:B:518:THR:HG21	1.87	0.56
1:F:273:SER:CA	1:F:295:GLN:HG3	2.35	0.56
1:B:349:LEU:CD1	1:B:350:GLU:H	2.16	0.56
1:B:93:GLU:OE1	1:F:517:GLU:CG	2.53	0.56
1:C:486:THR:CB	1:C:518:THR:HG21	2.35	0.56
1:F:429:GLN:HB2	1:F:458:ILE:HG22	1.87	0.56
1:D:80:VAL:CG1	1:D:173:THR:HG23	2.35	0.56
1:A:380:THR:HG21	1:D:351:GLU:O	2.06	0.56
1:B:517:GLU:CB	1:F:93:GLU:OE1	2.54	0.56
1:E:78:ARG:NH1	1:E:198:GLN:CG	2.68	0.56
1:B:414:ASN:HD22	1:B:414:ASN:N	1.89	0.56
1:B:286:VAL:HG22	1:B:290:THR:OG1	2.06	0.56
1:E:515:ARG:HD3	1:E:516:GLN:H	1.71	0.56
1:A:428:VAL:HG22	1:A:459:GLN:HG2	1.88	0.56
1:D:357:ARG:O	1:D:388:ILE:HD11	2.05	0.56
1:B:277:THR:CG2	1:B:292:ARG:HG2	2.34	0.56
1:C:230:ASN:HB3	1:C:233:ASN:ND2	2.20	0.56
1:B:515:ARG:NH1	1:B:521:LEU:HB3	2.21	0.56
1:A:305:ILE:HG22	1:A:306:GLN:N	2.20	0.56
1:A:506:GLU:HA	1:A:509:ARG:HD3	1.88	0.56
1:B:92:PHE:C	1:B:93:GLU:HG2	2.26	0.56
1:E:414:ASN:HD22	1:E:414:ASN:N	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:316:PRO:HB3	1:D:371:PHE:CD2	2.41	0.56
1:C:291:ALA:O	1:C:292:ARG:O	2.23	0.56
1:B:87:GLY:HA2	1:C:486:THR:CG2	2.36	0.56
1:A:410:HIS:CE1	1:A:457:VAL:HG13	2.41	0.56
1:B:33:ILE:HG12	1:B:53:ILE:HD13	1.87	0.56
1:F:78:ARG:HD3	1:F:175:ARG:HH11	1.69	0.56
1:F:497:LEU:HD12	1:F:512:LYS:HE3	1.88	0.56
1:E:232:PHE:O	1:E:234:GLN:N	2.38	0.56
1:D:516:GLN:HG3	1:D:517:GLU:N	2.21	0.55
1:D:378:ILE:HD12	1:D:519:ILE:CG2	2.36	0.55
1:F:349:LEU:CD1	1:F:350:GLU:H	2.15	0.55
1:C:270:ASN:ND2	1:C:272:PHE:HB2	2.21	0.55
1:B:350:GLU:HB3	1:B:354:CYS:HB2	1.87	0.55
1:E:414:ASN:HD21	1:E:478:PHE:H	1.54	0.55
1:B:63:PRO:HA	1:B:190:TYR:O	2.06	0.55
1:C:349:LEU:HD12	1:C:350:GLU:CA	2.35	0.55
1:D:349:LEU:HD12	1:D:351:GLU:N	2.21	0.55
1:E:268:GLY:O	1:E:269:ASN:CB	2.55	0.55
1:B:78:ARG:HG2	1:B:79:GLY:N	2.22	0.55
1:E:17:LEU:HB2	1:E:439:LEU:HB2	1.88	0.55
1:C:230:ASN:HB3	1:C:233:ASN:HD22	1.72	0.55
1:B:280:LEU:O	1:B:280:LEU:HD12	2.06	0.55
1:B:371:PHE:CD2	1:F:316:PRO:HB3	2.42	0.55
1:B:76:GLN:CG	1:B:76:GLN:O	2.51	0.55
1:E:60:LEU:HD12	1:E:192:SER:O	2.07	0.55
1:C:352:THR:HG22	1:E:476:ASN:HB3	1.87	0.55
1:A:290:THR:O	1:A:293:ASN:HB2	2.05	0.55
1:C:475:GLU:O	1:C:477:ALA:N	2.39	0.55
1:F:515:ARG:HD3	1:F:516:GLN:H	1.71	0.55
1:C:368:ALA:HA	1:C:379:SER:OG	2.07	0.55
1:B:270:ASN:ND2	1:B:272:PHE:HB2	2.19	0.55
1:A:494:ASP:O	1:A:497:LEU:HB2	2.07	0.55
1:A:398:ARG:HH12	1:A:467:GLU:HG2	1.70	0.55
1:B:515:ARG:HD3	1:B:516:GLN:H	1.72	0.55
1:D:493:PRO:HG2	1:D:496:VAL:CG1	2.36	0.55
1:A:33:ILE:HG12	1:A:53:ILE:CD1	2.37	0.55
1:D:205:LEU:HG	1:D:471:PHE:HB2	1.87	0.55
1:B:517:GLU:OE2	1:B:518:THR:HG22	2.06	0.55
1:F:14:LEU:CD1	1:F:438:ILE:HD11	2.37	0.55
1:D:169:ARG:HG2	1:E:513:TYR:OH	2.06	0.55
1:E:170:HIS:HB3	1:F:493:PRO:HA	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:220:ARG:HD3	1:C:433:GLU:OE1	2.07	0.55
1:B:497:LEU:HD12	1:B:512:LYS:HE3	1.88	0.55
1:C:390:ARG:O	1:C:393:ARG:HD3	2.06	0.55
1:F:485:ARG:HD3	2:F:546:HOH:O	2.07	0.55
1:A:391:PHE:O	1:A:392:LEU:CB	2.55	0.55
1:E:193:TYR:CZ	1:E:311:LEU:HB3	2.42	0.55
1:A:270:ASN:ND2	1:A:272:PHE:HB2	2.22	0.55
1:A:350:GLU:HB3	1:A:354:CYS:HB2	1.88	0.55
1:B:232:PHE:O	1:B:234:GLN:N	2.39	0.55
1:A:355:SER:HB3	1:D:369:ASP:OD2	2.07	0.55
1:D:507:GLN:NE2	1:F:290:THR:HG22	2.18	0.55
1:C:292:ARG:O	1:C:293:ASN:CB	2.45	0.55
1:B:276:ASN:HD22	1:B:279:LEU:H	1.53	0.55
1:D:356:LEU:HD12	1:D:388:ILE:HD12	1.88	0.55
1:C:518:THR:O	1:C:519:ILE:HB	2.07	0.55
1:D:286:VAL:HG22	1:D:290:THR:OG1	2.06	0.55
1:E:418:VAL:HG22	1:E:450:ILE:HG12	1.88	0.55
1:F:194:ASN:HD22	1:F:194:ASN:C	2.09	0.55
1:C:423:ARG:NH1	1:C:467:GLU:OE1	2.40	0.54
1:F:486:THR:N	1:F:518:THR:HB	2.20	0.54
1:A:479:ILE:O	1:D:349:LEU:CD2	2.51	0.54
1:D:515:ARG:NH1	1:D:521:LEU:HB3	2.22	0.54
1:E:270:ASN:ND2	1:E:272:PHE:HB2	2.20	0.54
1:B:268:GLY:O	1:B:269:ASN:CB	2.56	0.54
1:E:288:GLU:O	1:E:292:ARG:HB3	2.08	0.54
1:F:388:ILE:CD1	1:F:388:ILE:H	2.11	0.54
1:D:391:PHE:O	1:D:392:LEU:CB	2.56	0.54
1:E:38:PHE:CE2	1:E:232:PHE:HB3	2.43	0.54
1:D:79:GLY:O	1:D:176:ILE:HG12	2.08	0.54
1:C:19:ALA:HB2	1:C:449:PHE:HB3	1.90	0.54
1:F:33:ILE:HG12	1:F:53:ILE:HD13	1.88	0.54
1:D:484:GLY:N	1:D:487:SER:HB3	2.23	0.54
1:B:78:ARG:O	1:B:200:LEU:HD22	2.08	0.54
1:F:48:VAL:HG12	1:F:49:ALA:N	2.22	0.54
1:A:93:GLU:OE1	1:D:517:GLU:CB	2.56	0.54
1:A:349:LEU:HD12	1:A:350:GLU:CA	2.37	0.54
1:E:398:ARG:HH12	1:E:467:GLU:HG2	1.73	0.54
1:F:350:GLU:HB3	1:F:354:CYS:HB2	1.89	0.54
1:F:268:GLY:O	1:F:269:ASN:CB	2.55	0.54
1:A:91:THR:HG1	1:D:370:ILE:HA	1.70	0.54
1:F:419:VAL:O	1:F:448:LEU:HD22	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:48:VAL:HG12	1:E:49:ALA:N	2.22	0.54
1:A:169:ARG:HG2	1:B:513:TYR:OH	2.08	0.54
1:A:281:ALA:O	1:A:285:ASN:N	2.40	0.54
1:C:268:GLY:O	1:C:269:ASN:CB	2.55	0.54
1:C:293:ASN:O	1:C:294:LEU:C	2.47	0.54
1:C:429:GLN:HB2	1:C:458:ILE:HG22	1.89	0.54
1:D:293:ASN:O	1:D:294:LEU:C	2.44	0.54
1:B:393:ARG:H	1:B:393:ARG:HD3	1.73	0.54
1:F:38:PHE:CE2	1:F:232:PHE:HB3	2.43	0.54
1:D:410:HIS:CE1	1:D:457:VAL:HG13	2.43	0.54
1:E:378:ILE:HD12	1:E:519:ILE:CG2	2.37	0.53
1:A:277:THR:CG2	1:A:292:ARG:HG2	2.38	0.53
1:F:302:ASN:HB3	1:F:303:GLN:NE2	2.13	0.53
1:C:393:ARG:H	1:C:393:ARG:HD3	1.74	0.53
1:D:305:ILE:HG22	1:D:306:GLN:N	2.22	0.53
1:F:423:ARG:HG3	1:F:445:GLN:NE2	2.23	0.53
1:C:398:ARG:HH12	1:C:467:GLU:HG2	1.73	0.53
1:B:93:GLU:HA	1:B:314:VAL:HG21	1.90	0.53
1:D:388:ILE:N	1:D:388:ILE:CD1	2.59	0.53
1:C:421:VAL:CG1	1:C:445:GLN:HA	2.38	0.53
1:E:517:GLU:OE2	1:E:518:THR:HG22	2.07	0.53
1:B:14:LEU:CD1	1:B:438:ILE:HD11	2.37	0.53
1:E:414:ASN:HA	1:E:453:GLN:HE21	1.74	0.53
1:B:86:SER:HB3	1:C:480:ASN:CG	2.29	0.53
1:A:391:PHE:O	1:A:392:LEU:HD13	2.09	0.53
1:C:362:ILE:HD12	1:C:398:ARG:HB3	1.90	0.53
1:B:423:ARG:HG3	1:B:445:GLN:NE2	2.24	0.53
1:A:287:ASN:ND2	1:A:290:THR:HG23	2.22	0.53
1:A:517:GLU:CB	1:D:93:GLU:OE2	2.51	0.53
1:A:276:ASN:H	1:B:429:GLN:HE22	1.54	0.53
1:C:423:ARG:HG3	1:C:445:GLN:NE2	2.24	0.53
1:D:17:LEU:HB2	1:D:439:LEU:HB2	1.91	0.53
1:C:486:THR:N	1:C:518:THR:HB	2.21	0.53
1:F:393:ARG:HD3	1:F:393:ARG:H	1.74	0.53
1:F:75:VAL:HG23	1:F:202:ALA:HA	1.91	0.53
1:D:193:TYR:CZ	1:D:311:LEU:HB3	2.44	0.53
1:D:515:ARG:HD3	1:D:516:GLN:H	1.74	0.53
1:D:349:LEU:HD12	1:D:350:GLU:CA	2.37	0.53
1:C:276:ASN:HD22	1:C:279:LEU:H	1.57	0.53
1:A:79:GLY:O	1:A:176:ILE:HG12	2.09	0.53
1:E:280:LEU:HD12	1:E:280:LEU:O	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:516:GLN:CG	1:A:517:GLU:N	2.72	0.53
1:F:349:LEU:HD12	1:F:350:GLU:CA	2.39	0.53
1:B:79:GLY:O	1:B:176:ILE:HG12	2.09	0.52
1:E:428:VAL:HG22	1:E:459:GLN:HG2	1.90	0.52
1:A:352:THR:HG22	1:D:476:ASN:HB3	1.90	0.52
1:C:357:ARG:O	1:C:388:ILE:HD11	2.09	0.52
1:F:24:ASN:O	1:F:25:ARG:CB	2.58	0.52
1:E:276:ASN:H	1:F:429:GLN:HE22	1.58	0.52
1:D:475:GLU:O	1:D:477:ALA:N	2.42	0.52
1:D:268:GLY:O	1:D:269:ASN:CB	2.57	0.52
1:D:480:ASN:CG	1:F:86:SER:HB3	2.30	0.52
1:B:293:ASN:O	1:B:296:GLY:N	2.38	0.52
1:D:294:LEU:HD23	1:E:501:TYR:CE2	2.44	0.52
1:E:74:ILE:CD1	1:E:176:ILE:HB	2.39	0.52
1:D:302:ASN:HB3	1:D:303:GLN:NE2	2.10	0.52
1:F:349:LEU:HD12	1:F:351:GLU:N	2.22	0.52
1:D:14:LEU:HD12	1:D:438:ILE:HD11	1.91	0.52
1:A:38:PHE:CE2	1:A:232:PHE:HB3	2.44	0.52
1:A:369:ASP:OD2	1:D:355:SER:HB3	2.09	0.52
1:C:273:SER:HA	1:C:295:GLN:NE2	2.25	0.52
1:E:75:VAL:HG23	1:E:202:ALA:HA	1.91	0.52
1:E:497:LEU:HD12	1:E:512:LYS:HE3	1.91	0.52
1:A:26:ILE:O	1:A:26:ILE:HG13	2.09	0.52
1:D:418:VAL:HG13	1:D:448:LEU:HD11	1.92	0.52
1:C:480:ASN:HD22	1:C:481:THR:N	2.08	0.52
1:C:53:ILE:HG12	1:C:204:ASN:ND2	2.25	0.52
1:A:268:GLY:O	1:A:269:ASN:CB	2.57	0.52
1:F:19:ALA:HB2	1:F:449:PHE:HB3	1.92	0.52
1:A:515:ARG:HD3	1:A:516:GLN:H	1.75	0.52
1:F:429:GLN:HA	1:F:439:LEU:O	2.09	0.52
1:C:316:PRO:HB3	1:E:371:PHE:CE2	2.45	0.52
1:A:205:LEU:HG	1:A:471:PHE:HB2	1.92	0.52
1:A:280:LEU:HD12	1:A:280:LEU:O	2.10	0.52
1:D:423:ARG:HG3	1:D:445:GLN:NE2	2.25	0.52
1:B:14:LEU:HD12	1:B:438:ILE:HD11	1.91	0.52
1:C:10:ASN:ND2	1:C:10:ASN:N	2.47	0.52
1:D:413:VAL:HG21	1:D:478:PHE:CE1	2.45	0.51
1:C:281:ALA:O	1:C:285:ASN:N	2.43	0.51
1:A:356:LEU:HD12	1:A:388:ILE:HD12	1.91	0.51
1:B:170:HIS:HB3	1:C:493:PRO:HA	1.92	0.51
1:C:497:LEU:HD12	1:C:512:LYS:HE3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:602:HOH:O	1:E:385:ASN:ND2	2.42	0.51
1:C:493:PRO:HG2	1:C:496:VAL:CG1	2.39	0.51
1:D:12:CYS:SG	1:F:215:LEU:O	2.68	0.51
1:F:280:LEU:HD12	1:F:280:LEU:O	2.10	0.51
1:E:516:GLN:HG3	1:E:517:GLU:H	1.74	0.51
1:E:349:LEU:HD12	1:E:351:GLU:H	1.74	0.51
1:D:391:PHE:O	1:D:392:LEU:HD13	2.10	0.51
1:A:12:CYS:SG	1:C:215:LEU:O	2.68	0.51
1:C:371:PHE:CE2	1:E:316:PRO:HB3	2.45	0.51
1:C:293:ASN:O	1:C:295:GLN:CB	2.58	0.51
1:C:85:PHE:CZ	1:C:356:LEU:HD21	2.45	0.51
1:B:75:VAL:HG23	1:B:202:ALA:HA	1.93	0.51
1:D:430:VAL:O	1:D:438:ILE:HG22	2.10	0.51
1:E:293:ASN:O	1:E:294:LEU:C	2.45	0.51
1:E:485:ARG:HB2	1:E:516:GLN:O	2.10	0.51
1:B:493:PRO:HG2	1:B:496:VAL:CG1	2.41	0.51
1:A:414:ASN:HA	1:A:453:GLN:HE21	1.76	0.51
1:E:40:GLN:C	1:E:42:ASP:N	2.62	0.51
1:C:14:LEU:HD12	1:C:438:ILE:HD11	1.93	0.51
1:A:516:GLN:HG3	1:A:517:GLU:H	1.74	0.51
1:B:76:GLN:HA	1:B:178:GLU:HG3	1.92	0.51
1:E:349:LEU:HD12	1:E:350:GLU:CA	2.41	0.51
1:A:274:GLY:CA	1:B:431:VAL:HG11	2.40	0.51
1:E:389:LEU:HB3	1:E:394:LEU:O	2.10	0.51
1:B:448:LEU:HD13	1:B:449:PHE:N	2.26	0.51
1:A:291:ALA:C	1:A:293:ASN:N	2.59	0.51
1:B:314:VAL:HG12	1:B:314:VAL:O	2.10	0.51
1:B:78:ARG:CG	1:B:79:GLY:N	2.74	0.51
1:C:305:ILE:CG2	1:C:306:GLN:N	2.74	0.51
1:B:391:PHE:O	1:B:392:LEU:HD13	2.11	0.51
1:C:419:VAL:O	1:C:448:LEU:HD22	2.11	0.51
1:C:174:ARG:HH11	1:C:174:ARG:HG3	1.76	0.51
1:A:423:ARG:HG3	1:A:445:GLN:NE2	2.26	0.50
1:D:14:LEU:CD1	1:D:438:ILE:HD11	2.41	0.50
1:A:294:LEU:HA	1:B:501:TYR:CD2	2.46	0.50
1:A:486:THR:CB	1:A:518:THR:HG21	2.41	0.50
1:A:517:GLU:HG3	1:A:518:THR:O	2.10	0.50
1:F:516:GLN:CG	1:F:517:GLU:N	2.71	0.50
1:B:74:ILE:CD1	1:B:176:ILE:HB	2.41	0.50
1:F:430:VAL:O	1:F:438:ILE:HG22	2.10	0.50
1:E:458:ILE:O	1:E:459:GLN:HG3	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:389:LEU:HB3	1:A:394:LEU:O	2.10	0.50
1:A:58:ASN:O	1:A:307:VAL:HG23	2.11	0.50
1:D:191:TRP:CD1	1:E:492:LEU:HD22	2.46	0.50
1:A:12:CYS:C	1:A:14:LEU:N	2.65	0.50
1:E:515:ARG:NH1	1:E:521:LEU:HB3	2.27	0.50
1:C:414:ASN:HA	1:C:453:GLN:HE21	1.77	0.50
1:B:485:ARG:NH1	1:F:93:GLU:OE2	2.45	0.50
1:C:517:GLU:CB	1:E:93:GLU:OE1	2.59	0.50
1:F:78:ARG:HD3	1:F:175:ARG:NH1	2.27	0.50
1:B:19:ALA:HB2	1:B:449:PHE:HB3	1.93	0.50
1:D:194:ASN:ND2	1:D:194:ASN:C	2.64	0.50
1:D:57:ARG:O	1:D:58:ASN:HB2	2.10	0.50
1:F:53:ILE:HG12	1:F:204:ASN:ND2	2.26	0.50
1:D:12:CYS:C	1:D:14:LEU:N	2.65	0.50
1:D:377:ARG:HH21	1:D:377:ARG:HG3	1.77	0.50
1:F:458:ILE:O	1:F:459:GLN:HG3	2.12	0.50
1:D:270:ASN:ND2	1:D:272:PHE:HB2	2.26	0.50
1:B:388:ILE:CD1	1:B:388:ILE:H	2.13	0.50
1:A:14:LEU:HD12	1:A:438:ILE:HD11	1.94	0.50
1:E:393:ARG:HD3	1:E:393:ARG:H	1.77	0.50
1:E:423:ARG:HG3	1:E:445:GLN:NE2	2.27	0.50
1:F:270:ASN:ND2	1:F:272:PHE:HB2	2.27	0.50
1:B:93:GLU:N	1:B:314:VAL:HG11	2.26	0.50
1:F:24:ASN:O	1:F:25:ARG:HB2	2.12	0.50
1:D:414:ASN:O	1:D:474:GLU:HG3	2.12	0.50
1:E:305:ILE:CG2	1:E:306:GLN:N	2.74	0.50
1:F:281:ALA:O	1:F:285:ASN:N	2.44	0.50
1:B:444:GLN:N	1:B:447:GLN:OE1	2.34	0.50
1:E:86:SER:HB3	1:F:480:ASN:ND2	2.27	0.50
1:C:280:LEU:O	1:C:280:LEU:HD12	2.11	0.50
1:B:291:ALA:C	1:B:293:ASN:N	2.64	0.50
1:D:486:THR:CB	1:D:518:THR:HG21	2.42	0.50
1:A:274:GLY:HA3	1:B:431:VAL:CG1	2.38	0.50
1:B:391:PHE:O	1:B:392:LEU:CB	2.60	0.50
1:C:272:PHE:O	1:C:295:GLN:NE2	2.45	0.50
1:A:455:HIS:CE1	2:C:532:HOH:O	2.62	0.50
1:B:414:ASN:ND2	1:B:414:ASN:N	2.54	0.50
1:C:24:ASN:O	1:C:25:ARG:CB	2.60	0.50
1:E:430:VAL:O	1:E:438:ILE:HG22	2.12	0.50
1:F:475:GLU:O	1:F:477:ALA:N	2.45	0.50
1:A:286:VAL:HG22	1:A:290:THR:OG1	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:515:ARG:NH1	1:A:521:LEU:HB3	2.27	0.49
1:D:350:GLU:HB3	1:D:354:CYS:HB2	1.92	0.49
1:D:393:ARG:HD3	1:D:393:ARG:H	1.77	0.49
1:A:393:ARG:HD3	1:A:393:ARG:H	1.78	0.49
1:D:74:ILE:CD1	1:D:176:ILE:HB	2.41	0.49
1:C:93:GLU:HG3	1:E:485:ARG:HH22	1.77	0.49
1:F:414:ASN:HD22	1:F:414:ASN:N	1.87	0.49
1:B:414:ASN:HA	1:B:453:GLN:HE21	1.77	0.49
1:E:493:PRO:HG2	1:E:496:VAL:CG1	2.42	0.49
1:E:220:ARG:NH1	1:F:433:GLU:OE2	2.44	0.49
1:F:46:ALA:HA	1:F:416:HIS:CD2	2.47	0.49
1:D:506:GLU:HA	1:D:509:ARG:HD3	1.94	0.49
1:A:517:GLU:CD	1:A:518:THR:N	2.65	0.49
1:E:515:ARG:NH1	1:E:516:GLN:OE1	2.45	0.49
1:E:368:ALA:HA	1:E:379:SER:OG	2.13	0.49
1:A:46:ALA:HA	1:A:416:HIS:CD2	2.48	0.49
1:F:423:ARG:NH1	1:F:467:GLU:OE1	2.45	0.49
1:A:485:ARG:HH21	1:A:516:GLN:HA	1.77	0.49
1:B:430:VAL:O	1:B:438:ILE:HG22	2.13	0.49
1:B:349:LEU:HD12	1:B:350:GLU:CA	2.42	0.49
1:B:74:ILE:HG22	1:B:178:GLU:HA	1.93	0.49
1:E:78:ARG:HH12	1:E:198:GLN:CG	2.22	0.49
1:B:28:ALA:O	1:B:29:GLU:O	2.30	0.49
1:B:284:LEU:HD13	1:C:511:LEU:CD2	2.43	0.49
1:D:74:ILE:HG22	1:D:178:GLU:HA	1.94	0.49
1:D:216:ASP:O	1:D:218:ASN:N	2.46	0.49
1:A:371:PHE:CD2	1:D:316:PRO:HB3	2.48	0.49
1:E:421:VAL:HG12	1:E:445:GLN:HA	1.93	0.49
1:A:349:LEU:HD12	1:A:351:GLU:N	2.25	0.49
1:B:276:ASN:H	1:C:429:GLN:HE22	1.61	0.49
1:D:291:ALA:C	1:D:293:ASN:H	2.09	0.49
1:D:497:LEU:CD1	1:D:512:LYS:HE3	2.43	0.49
1:F:286:VAL:HG22	1:F:290:THR:OG1	2.12	0.49
1:F:362:ILE:HD12	1:F:398:ARG:HB3	1.95	0.49
1:A:486:THR:N	1:A:518:THR:HB	2.23	0.49
1:E:272:PHE:O	1:E:295:GLN:NE2	2.45	0.49
1:E:276:ASN:HD22	1:E:279:LEU:H	1.60	0.49
1:B:311:LEU:HD12	1:B:312:ASP:H	1.77	0.49
1:A:492:LEU:HD22	1:C:191:TRP:NE1	2.27	0.49
1:C:78:ARG:HG2	1:C:175:ARG:HH12	1.77	0.49
1:E:194:ASN:C	1:E:194:ASN:HD22	2.14	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:423:ARG:NH1	1:D:467:GLU:OE1	2.46	0.49
1:C:349:LEU:HD12	1:C:351:GLU:N	2.26	0.49
1:F:276:ASN:HD22	1:F:279:LEU:H	1.60	0.49
2:C:581:HOH:O	1:F:233:ASN:HB2	2.12	0.49
1:D:516:GLN:HG3	1:D:517:GLU:H	1.76	0.49
1:F:518:THR:O	1:F:519:ILE:HB	2.13	0.49
1:C:409:PRO:CG	1:C:458:ILE:HD12	2.36	0.49
1:C:389:LEU:HB3	1:C:394:LEU:O	2.13	0.49
1:E:429:GLN:HB2	1:E:458:ILE:CG2	2.42	0.49
1:C:312:ASP:O	1:C:312:ASP:OD2	2.30	0.49
1:B:270:ASN:HD21	1:B:272:PHE:HB2	1.78	0.49
1:F:494:ASP:O	1:F:497:LEU:HB2	2.12	0.49
1:F:205:LEU:HG	1:F:471:PHE:HB2	1.94	0.49
2:C:597:HOH:O	1:E:90:GLU:HG2	2.12	0.49
1:C:14:LEU:CD1	1:C:438:ILE:HD11	2.43	0.49
1:C:450:ILE:O	1:C:452:PRO:HD3	2.12	0.49
1:B:54:THR:HG23	1:B:201:VAL:CG2	2.43	0.49
1:A:506:GLU:HA	1:A:509:ARG:CD	2.42	0.49
1:C:216:ASP:O	1:C:218:ASN:N	2.46	0.49
1:B:48:VAL:HG12	1:B:49:ALA:N	2.28	0.49
1:A:50:ALA:HA	1:A:204:ASN:O	2.13	0.49
1:E:425:ASN:HB2	1:E:462:GLY:HA3	1.94	0.49
1:E:314:VAL:O	1:E:314:VAL:HG12	2.12	0.49
1:A:230:ASN:HB3	1:A:233:ASN:ND2	2.28	0.49
1:F:519:ILE:O	1:F:520:ALA:HB3	2.12	0.48
1:D:12:CYS:CA	1:D:14:LEU:HD23	2.43	0.48
1:B:305:ILE:CG2	1:B:306:GLN:N	2.76	0.48
1:D:516:GLN:CG	1:D:517:GLU:N	2.76	0.48
1:A:276:ASN:HD22	1:A:279:LEU:H	1.61	0.48
1:B:486:THR:N	1:B:518:THR:HB	2.27	0.48
1:B:349:LEU:HD12	1:B:351:GLU:N	2.27	0.48
1:A:493:PRO:HG2	1:A:496:VAL:CG1	2.43	0.48
1:C:270:ASN:HD21	1:C:272:PHE:HB2	1.78	0.48
1:A:357:ARG:O	1:A:388:ILE:HD11	2.13	0.48
1:E:391:PHE:O	1:E:392:LEU:CB	2.62	0.48
1:B:485:ARG:HH22	1:F:93:GLU:HG3	1.78	0.48
1:C:519:ILE:O	1:C:520:ALA:HB3	2.13	0.48
1:B:382:ASN:N	1:B:385:ASN:HD22	2.03	0.48
1:E:494:ASP:O	1:E:497:LEU:HB2	2.12	0.48
1:C:494:ASP:O	1:C:497:LEU:HB2	2.13	0.48
1:B:429:GLN:HB2	1:B:458:ILE:CG2	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:517:GLU:OE2	1:C:518:THR:O	2.31	0.48
1:C:517:GLU:HB3	1:E:93:GLU:OE1	2.13	0.48
1:E:414:ASN:O	1:E:474:GLU:HG3	2.14	0.48
1:D:270:ASN:HD22	1:D:270:ASN:C	2.16	0.48
1:A:12:CYS:CA	1:A:14:LEU:HD23	2.44	0.48
1:A:492:LEU:HD22	1:C:191:TRP:CD1	2.48	0.48
1:D:230:ASN:HB3	1:D:233:ASN:ND2	2.29	0.48
1:B:26:ILE:HG13	1:B:26:ILE:O	2.13	0.48
1:A:485:ARG:NH1	1:D:93:GLU:OE2	2.46	0.48
1:B:380:THR:HG21	1:F:351:GLU:O	2.14	0.48
1:A:351:GLU:O	1:D:380:THR:HG21	2.14	0.48
1:D:281:ALA:O	1:D:285:ASN:N	2.46	0.48
1:B:288:GLU:O	1:B:292:ARG:HG3	2.13	0.48
1:B:270:ASN:HD22	1:B:272:PHE:N	2.12	0.48
1:C:230:ASN:HB3	1:C:233:ASN:O	2.13	0.48
1:C:217:GLN:HA	1:C:217:GLN:OE1	2.13	0.48
1:F:414:ASN:O	1:F:474:GLU:HG3	2.13	0.48
1:B:193:TYR:HE1	1:B:307:VAL:HG21	1.78	0.48
1:E:371:PHE:HD1	1:E:377:ARG:HB3	1.79	0.48
1:E:486:THR:N	1:E:518:THR:HB	2.26	0.48
1:D:517:GLU:CD	1:D:518:THR:N	2.67	0.48
1:D:19:ALA:HB2	1:D:449:PHE:HB3	1.96	0.48
1:C:38:PHE:CE2	1:C:232:PHE:HB3	2.48	0.48
1:A:40:GLN:C	1:A:42:ASP:N	2.66	0.48
1:A:421:VAL:HG12	1:A:445:GLN:HA	1.96	0.48
1:A:517:GLU:HB3	1:D:93:GLU:OE1	2.12	0.48
1:A:458:ILE:O	1:A:459:GLN:HG3	2.13	0.48
1:E:270:ASN:HD21	1:E:272:PHE:HB2	1.79	0.48
1:B:418:VAL:HG13	1:B:448:LEU:HD11	1.96	0.48
1:A:497:LEU:CD1	1:A:512:LYS:HE3	2.44	0.48
1:B:494:ASP:O	1:B:497:LEU:HB2	2.13	0.48
1:E:506:GLU:HA	1:E:509:ARG:HD3	1.96	0.48
1:C:303:GLN:NE2	1:C:303:GLN:H	2.11	0.48
1:A:429:GLN:HA	1:A:439:LEU:O	2.14	0.47
1:F:273:SER:HA	1:F:295:GLN:HG2	1.92	0.47
1:B:273:SER:HA	1:B:295:GLN:HB3	1.96	0.47
1:B:193:TYR:CE1	1:B:307:VAL:HG21	2.49	0.47
1:C:484:GLY:N	1:C:487:SER:HB3	2.29	0.47
1:D:486:THR:N	1:D:518:THR:HB	2.24	0.47
1:A:351:GLU:OE2	2:C:535:HOH:O	2.20	0.47
1:A:414:ASN:O	1:A:474:GLU:HG3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:458:ILE:O	1:C:459:GLN:HG3	2.14	0.47
1:A:14:LEU:CD1	1:A:438:ILE:HD11	2.44	0.47
1:C:79:GLY:O	1:C:176:ILE:HG12	2.15	0.47
1:F:305:ILE:CG2	1:F:306:GLN:N	2.76	0.47
1:A:353:PHE:CD2	1:D:384:HIS:CE1	3.02	0.47
1:B:402:TYR:O	1:B:403:ARG:C	2.52	0.47
1:C:14:LEU:CD1	1:C:17:LEU:HD21	2.44	0.47
1:B:414:ASN:O	1:B:474:GLU:HG3	2.15	0.47
1:D:414:ASN:HA	1:D:453:GLN:HE21	1.79	0.47
1:D:276:ASN:HD22	1:D:279:LEU:H	1.62	0.47
1:E:170:HIS:CG	1:F:493:PRO:HB3	2.49	0.47
1:C:53:ILE:HG12	1:C:204:ASN:HD21	1.79	0.47
1:F:71:LEU:HB2	1:F:471:PHE:CE1	2.49	0.47
1:A:353:PHE:HD2	1:D:384:HIS:CE1	2.33	0.47
1:B:230:ASN:HB3	1:B:233:ASN:O	2.14	0.47
1:C:414:ASN:O	1:C:474:GLU:HG3	2.14	0.47
1:A:507:GLN:HE21	1:C:290:THR:CG2	2.28	0.47
1:D:448:LEU:C	1:D:448:LEU:HD13	2.34	0.47
1:C:24:ASN:O	1:C:25:ARG:HB2	2.14	0.47
1:B:280:LEU:C	1:B:280:LEU:HD12	2.34	0.47
1:B:46:ALA:HA	1:B:416:HIS:CD2	2.49	0.47
1:A:362:ILE:HD12	1:A:398:ARG:HB3	1.97	0.47
1:E:516:GLN:CG	1:E:517:GLU:N	2.73	0.47
1:A:273:SER:HA	1:A:295:GLN:HG2	1.96	0.47
1:B:516:GLN:HG3	1:B:517:GLU:H	1.78	0.47
1:E:377:ARG:HH21	1:E:377:ARG:HG3	1.79	0.47
1:A:72:ILE:HG12	1:A:204:ASN:OD1	2.13	0.47
1:D:40:GLN:C	1:D:42:ASP:N	2.67	0.47
1:B:407:TYR:HE2	1:B:468:TYR:OH	1.98	0.47
1:D:428:VAL:HG22	1:D:459:GLN:HG2	1.97	0.47
1:E:78:ARG:NH1	1:E:198:GLN:OE1	2.46	0.47
1:D:280:LEU:C	1:D:280:LEU:HD12	2.34	0.47
1:D:217:GLN:HA	1:D:217:GLN:OE1	2.15	0.47
1:B:362:ILE:HD12	1:B:398:ARG:HB3	1.96	0.47
1:D:62:LEU:HG	1:D:303:GLN:O	2.15	0.47
1:C:93:GLU:OE1	1:E:517:GLU:HB3	2.15	0.47
1:C:93:GLU:OE2	1:E:485:ARG:NH1	2.48	0.47
1:D:485:ARG:HB2	1:D:516:GLN:O	2.14	0.47
1:D:493:PRO:HG2	1:D:496:VAL:HG12	1.97	0.47
1:A:350:GLU:OE2	1:A:350:GLU:N	2.48	0.47
1:C:516:GLN:CG	1:C:517:GLU:N	2.73	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:483:ALA:N	1:E:487:SER:HB2	2.30	0.47
1:D:453:GLN:O	1:D:455:HIS:HD2	1.98	0.47
1:B:385:ASN:O	1:F:357:ARG:HD3	2.15	0.47
1:D:291:ALA:O	1:D:292:ARG:C	2.50	0.47
1:B:357:ARG:O	1:B:388:ILE:CD1	2.60	0.47
1:D:58:ASN:O	1:D:307:VAL:HG23	2.15	0.47
1:F:490:ARG:HA	1:F:512:LYS:HG2	1.97	0.47
1:A:499:ASN:CG	1:C:307:VAL:HG13	2.35	0.47
1:E:227:ASN:HB2	1:E:296:GLY:O	2.15	0.47
1:E:284:LEU:HD13	1:F:511:LEU:CD2	2.44	0.47
1:B:421:VAL:HG12	1:B:445:GLN:HA	1.96	0.47
1:D:303:GLN:H	1:D:303:GLN:NE2	2.13	0.47
1:E:486:THR:CB	1:E:518:THR:HG21	2.45	0.47
1:A:19:ALA:HB2	1:A:449:PHE:HB3	1.97	0.47
1:B:78:ARG:N	1:B:200:LEU:HD13	2.29	0.47
1:C:485:ARG:HH21	1:C:516:GLN:HA	1.80	0.47
1:B:395:SER:HB2	2:C:547:HOH:O	2.15	0.47
1:D:270:ASN:HD22	1:D:272:PHE:N	2.12	0.47
1:C:46:ALA:HA	1:C:416:HIS:CD2	2.50	0.47
1:F:217:GLN:OE1	1:F:217:GLN:HA	2.15	0.47
1:E:33:ILE:HG12	1:E:53:ILE:CD1	2.44	0.47
1:F:25:ARG:HD3	1:F:32:GLN:HG3	1.97	0.47
1:A:194:ASN:C	1:A:194:ASN:ND2	2.68	0.47
1:C:422:ILE:HG13	1:C:468:TYR:HA	1.96	0.47
1:B:423:ARG:NH1	1:B:467:GLU:OE1	2.47	0.47
1:A:303:GLN:H	1:A:303:GLN:NE2	2.13	0.46
1:E:423:ARG:NH1	1:E:467:GLU:OE1	2.48	0.46
1:D:517:GLU:OE2	1:D:518:THR:O	2.33	0.46
1:F:414:ASN:HA	1:F:453:GLN:HE21	1.80	0.46
1:F:54:THR:HG23	1:F:201:VAL:CG2	2.45	0.46
1:E:14:LEU:HD12	1:E:438:ILE:HD11	1.97	0.46
1:E:14:LEU:CD1	1:E:438:ILE:HD11	2.45	0.46
1:A:316:PRO:HB3	1:D:371:PHE:CE2	2.50	0.46
1:F:287:ASN:HD22	1:F:289:GLU:H	1.63	0.46
1:F:57:ARG:O	1:F:58:ASN:HB2	2.14	0.46
1:D:398:ARG:HH12	1:D:467:GLU:HG2	1.79	0.46
1:D:517:GLU:HA	1:D:517:GLU:OE1	2.15	0.46
1:D:418:VAL:HG22	1:D:450:ILE:CG1	2.38	0.46
1:B:356:LEU:HD12	1:B:388:ILE:HD12	1.97	0.46
1:F:493:PRO:HG2	1:F:496:VAL:HG12	1.96	0.46
1:D:38:PHE:CE2	1:D:232:PHE:HB3	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:33:ILE:HG12	1:C:53:ILE:HD13	1.97	0.46
1:E:402:TYR:O	1:E:403:ARG:C	2.53	0.46
1:E:303:GLN:H	1:E:303:GLN:NE2	2.12	0.46
1:A:409:PRO:CG	1:A:458:ILE:HD12	2.34	0.46
1:C:516:GLN:HG3	1:C:517:GLU:H	1.80	0.46
1:E:350:GLU:OE2	1:E:350:GLU:N	2.49	0.46
1:E:414:ASN:ND2	1:E:414:ASN:N	2.53	0.46
1:B:307:VAL:HG12	1:B:308:ARG:N	2.31	0.46
1:B:371:PHE:CE2	1:F:316:PRO:HB3	2.51	0.46
1:B:403:ARG:H	1:B:403:ARG:HD2	1.81	0.46
1:E:230:ASN:HB3	1:E:233:ASN:ND2	2.31	0.46
1:D:33:ILE:HG12	1:D:53:ILE:HD13	1.97	0.46
1:D:53:ILE:HG12	1:D:204:ASN:ND2	2.30	0.46
1:B:293:ASN:O	1:B:294:LEU:C	2.54	0.46
1:F:485:ARG:HH21	1:F:516:GLN:HA	1.80	0.46
1:C:429:GLN:HA	1:C:439:LEU:O	2.15	0.46
1:E:12:CYS:CA	1:E:14:LEU:HD23	2.44	0.46
1:B:377:ARG:HG3	1:B:377:ARG:HH21	1.80	0.46
1:B:315:GLN:HG2	1:B:317:PRO:HD3	1.98	0.46
1:C:205:LEU:HG	1:C:471:PHE:HB2	1.97	0.46
1:E:294:LEU:HA	1:E:294:LEU:HD23	1.41	0.46
1:A:291:ALA:C	1:A:293:ASN:H	2.18	0.46
1:E:518:THR:O	1:E:519:ILE:HB	2.15	0.46
1:E:519:ILE:O	1:E:520:ALA:HB3	2.15	0.46
1:B:485:ARG:HB2	1:B:516:GLN:O	2.15	0.46
1:B:518:THR:O	1:B:519:ILE:HB	2.15	0.46
1:E:484:GLY:N	1:E:487:SER:HB3	2.30	0.46
1:A:305:ILE:CG2	1:A:306:GLN:N	2.78	0.46
1:F:50:ALA:HA	1:F:204:ASN:O	2.16	0.46
1:D:422:ILE:HG13	1:D:468:TYR:HA	1.98	0.46
1:B:428:VAL:HG22	1:B:459:GLN:HG2	1.96	0.46
1:F:26:ILE:O	1:F:32:GLN:HB2	2.15	0.46
1:B:453:GLN:O	1:B:455:HIS:HD2	1.98	0.46
1:D:220:ARG:HD3	1:E:433:GLU:OE1	2.15	0.46
1:A:307:VAL:HG12	1:A:308:ARG:N	2.30	0.46
1:C:193:TYR:CZ	1:C:311:LEU:HB3	2.51	0.46
1:F:397:GLU:HB3	1:F:470:ALA:HB3	1.97	0.46
1:D:499:ASN:CG	1:F:307:VAL:HG13	2.36	0.46
1:D:389:LEU:HB3	1:D:394:LEU:O	2.15	0.46
1:B:398:ARG:HH12	1:B:467:GLU:CG	2.27	0.46
1:E:517:GLU:CD	1:E:518:THR:N	2.69	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:517:GLU:CD	1:B:518:THR:N	2.69	0.46
1:D:458:ILE:O	1:D:459:GLN:HG3	2.16	0.46
1:F:85:PHE:CZ	1:F:356:LEU:HD21	2.50	0.46
1:B:59:GLY:HA2	1:B:305:ILE:O	2.16	0.46
1:A:426:ALA:HB2	1:A:466:PHE:CD1	2.51	0.46
1:B:353:PHE:CD2	1:F:384:HIS:CE1	3.04	0.46
1:C:48:VAL:HG12	1:C:49:ALA:N	2.30	0.46
1:A:402:TYR:O	1:A:403:ARG:C	2.54	0.46
1:A:485:ARG:HB2	1:A:516:GLN:O	2.15	0.46
1:A:507:GLN:HE21	1:C:290:THR:HG22	1.81	0.46
1:F:516:GLN:HG3	1:F:517:GLU:H	1.79	0.46
1:A:450:ILE:O	1:A:452:PRO:HD3	2.15	0.46
1:E:357:ARG:O	1:E:388:ILE:CD1	2.62	0.46
1:A:368:ALA:HA	1:A:379:SER:OG	2.16	0.46
1:E:74:ILE:HG22	1:E:178:GLU:HA	1.97	0.46
1:D:307:VAL:HG13	1:E:499:ASN:OD1	2.16	0.46
1:D:377:ARG:NH2	1:D:377:ARG:HG3	2.31	0.46
1:E:46:ALA:HA	1:E:416:HIS:CD2	2.51	0.46
1:A:475:GLU:O	1:A:477:ALA:N	2.49	0.46
1:F:428:VAL:HG22	1:F:459:GLN:HG2	1.98	0.46
1:A:431:VAL:CG1	1:C:274:GLY:HA3	2.40	0.46
1:E:12:CYS:C	1:E:14:LEU:N	2.69	0.46
1:D:421:VAL:HG12	1:D:445:GLN:HA	1.98	0.45
1:A:517:GLU:OE2	1:A:518:THR:O	2.34	0.45
1:A:519:ILE:O	1:A:520:ALA:HB3	2.16	0.45
1:E:485:ARG:HH21	1:E:516:GLN:HA	1.81	0.45
1:D:493:PRO:HA	1:F:170:HIS:HB3	1.97	0.45
1:F:12:CYS:C	1:F:14:LEU:N	2.68	0.45
1:B:25:ARG:HD3	1:B:32:GLN:HE21	1.81	0.45
1:C:194:ASN:ND2	1:C:194:ASN:C	2.70	0.45
1:C:480:ASN:HD22	1:C:480:ASN:C	2.19	0.45
1:F:390:ARG:O	1:F:393:ARG:HD3	2.16	0.45
1:A:230:ASN:HB3	1:A:233:ASN:HD22	1.81	0.45
1:F:40:GLN:C	1:F:42:ASP:N	2.69	0.45
1:B:475:GLU:O	1:B:477:ALA:N	2.49	0.45
1:D:314:VAL:O	1:D:314:VAL:HG12	2.16	0.45
1:A:227:ASN:HD22	1:A:227:ASN:C	2.19	0.45
1:E:410:HIS:CE1	1:E:457:VAL:HG13	2.51	0.45
1:B:517:GLU:OE2	1:B:518:THR:O	2.34	0.45
1:A:483:ALA:N	1:A:487:SER:HB2	2.31	0.45
1:D:493:PRO:HB3	1:F:170:HIS:CG	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:429:GLN:HA	1:D:439:LEU:O	2.17	0.45
1:D:483:ALA:N	1:D:487:SER:HB2	2.31	0.45
1:F:12:CYS:CA	1:F:14:LEU:HD23	2.46	0.45
1:C:26:ILE:O	1:C:32:GLN:HB2	2.16	0.45
1:B:448:LEU:HD13	1:B:448:LEU:C	2.36	0.45
1:D:401:PHE:HB2	1:D:466:PHE:HB3	1.98	0.45
1:A:287:ASN:ND2	1:A:290:THR:H	2.14	0.45
1:B:485:ARG:HH21	1:B:516:GLN:HA	1.81	0.45
1:E:270:ASN:HD22	1:E:272:PHE:N	2.15	0.45
1:C:486:THR:H	1:C:518:THR:CB	2.25	0.45
1:C:382:ASN:N	1:C:385:ASN:HD22	2.03	0.45
1:E:276:ASN:O	1:E:277:THR:C	2.55	0.45
1:B:33:ILE:HG12	1:B:53:ILE:CD1	2.46	0.45
1:B:230:ASN:HB3	1:B:233:ASN:ND2	2.31	0.45
1:A:193:TYR:CZ	1:A:311:LEU:HB3	2.52	0.45
1:E:303:GLN:CD	1:E:303:GLN:H	2.20	0.45
1:A:484:GLY:N	1:A:487:SER:HB3	2.32	0.45
1:E:86:SER:HB3	1:F:480:ASN:CG	2.37	0.45
1:E:230:ASN:HB3	1:E:233:ASN:O	2.16	0.45
1:B:397:GLU:HB3	1:B:470:ALA:HB3	1.97	0.45
1:F:303:GLN:H	1:F:303:GLN:NE2	2.14	0.45
1:B:484:GLY:N	1:B:487:SER:HB3	2.31	0.45
1:B:92:PHE:O	1:B:93:GLU:CB	2.64	0.45
1:C:485:ARG:HB2	1:C:516:GLN:O	2.16	0.45
1:F:448:LEU:HD13	1:F:448:LEU:C	2.37	0.45
1:B:410:HIS:CE1	1:B:457:VAL:HG13	2.51	0.45
1:D:485:ARG:HH21	1:D:516:GLN:HA	1.81	0.45
1:E:62:LEU:HG	1:E:303:GLN:O	2.17	0.45
1:B:516:GLN:CG	1:B:517:GLU:N	2.75	0.45
1:C:276:ASN:O	1:C:277:THR:C	2.55	0.45
1:C:17:LEU:HG	1:C:438:ILE:HG12	1.99	0.45
1:E:448:LEU:HD13	1:E:449:PHE:N	2.31	0.45
1:A:180:ASP:HA	1:A:361:ASN:HA	1.99	0.45
1:F:426:ALA:HB2	1:F:466:PHE:CD1	2.52	0.45
1:B:287:ASN:ND2	1:B:290:THR:H	2.14	0.45
1:A:370:ILE:HB	1:A:378:ILE:HB	1.99	0.45
1:B:519:ILE:O	1:B:520:ALA:HB3	2.16	0.45
1:A:501:TYR:CD2	1:C:294:LEU:HA	2.52	0.45
1:D:270:ASN:HD21	1:D:273:SER:H	1.59	0.45
1:E:418:VAL:HG13	1:E:448:LEU:HD11	1.99	0.45
1:F:391:PHE:O	1:F:392:LEU:CB	2.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:ILE:CD1	1:A:176:ILE:HB	2.46	0.45
1:D:492:LEU:HD22	1:F:191:TRP:CD1	2.51	0.45
1:E:315:GLN:HG2	1:E:317:PRO:HD3	1.99	0.45
1:C:361:ASN:HD21	1:C:364:ASN:H	1.65	0.45
1:A:87:GLY:HA2	1:B:486:THR:CG2	2.44	0.45
1:A:288:GLU:O	1:A:292:ARG:HG3	2.17	0.45
1:B:392:LEU:O	1:B:393:ARG:C	2.55	0.45
1:B:425:ASN:HB2	1:B:462:GLY:HA3	1.98	0.45
1:F:74:ILE:CD1	1:F:176:ILE:HB	2.47	0.45
1:F:59:GLY:HA2	1:F:305:ILE:O	2.17	0.45
1:F:53:ILE:HG12	1:F:204:ASN:HD21	1.81	0.45
1:B:86:SER:HB3	1:C:480:ASN:ND2	2.32	0.45
1:C:371:PHE:CD2	1:E:316:PRO:HB3	2.51	0.45
1:A:48:VAL:HG12	1:A:49:ALA:N	2.31	0.45
1:A:384:HIS:CE1	1:D:353:PHE:CD2	3.05	0.45
1:C:75:VAL:HG23	1:C:202:ALA:HA	1.99	0.45
1:D:518:THR:O	1:D:519:ILE:HB	2.17	0.45
1:B:12:CYS:CA	1:B:14:LEU:HD23	2.46	0.45
1:B:515:ARG:NH1	1:B:516:GLN:OE1	2.50	0.45
1:D:273:SER:HA	1:D:295:GLN:CG	2.47	0.45
1:F:393:ARG:HD3	1:F:393:ARG:N	2.32	0.45
1:A:307:VAL:HG13	1:B:499:ASN:CG	2.37	0.45
1:F:480:ASN:HD22	1:F:481:THR:N	2.15	0.45
1:B:316:PRO:HB3	1:F:371:PHE:CE2	2.52	0.45
1:E:480:ASN:HD22	1:E:481:THR:N	2.14	0.45
1:B:182:VAL:HG22	1:B:359:LYS:HB3	1.98	0.45
1:B:40:GLN:C	1:B:42:ASP:N	2.69	0.45
1:D:429:GLN:HB2	1:D:458:ILE:CG2	2.46	0.44
1:F:25:ARG:HD3	1:F:32:GLN:HE21	1.80	0.44
1:E:429:GLN:HA	1:E:439:LEU:O	2.17	0.44
1:D:205:LEU:HG	1:D:471:PHE:CB	2.47	0.44
1:D:305:ILE:CG2	1:D:306:GLN:N	2.79	0.44
1:B:483:ALA:N	1:B:487:SER:HB2	2.32	0.44
1:F:486:THR:H	1:F:518:THR:CB	2.25	0.44
1:A:453:GLN:O	1:A:455:HIS:HD2	2.00	0.44
1:A:493:PRO:HA	1:C:170:HIS:HB3	1.99	0.44
1:C:25:ARG:HD3	1:C:32:GLN:HG3	1.99	0.44
1:F:381:LEU:CD1	1:F:389:LEU:HD11	2.42	0.44
1:C:497:LEU:HD23	1:C:501:TYR:HE1	1.82	0.44
1:D:50:ALA:HA	1:D:204:ASN:O	2.18	0.44
1:D:95:SER:C	1:D:96:GLN:HG2	2.38	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:174:ARG:HH11	1:D:174:ARG:HG3	1.83	0.44
1:D:36:TRP:HB3	1:D:43:PHE:CZ	2.52	0.44
1:E:390:ARG:O	1:E:393:ARG:HD3	2.17	0.44
1:F:194:ASN:ND2	1:F:194:ASN:C	2.71	0.44
1:C:175:ARG:HH22	1:C:195:ASP:HB3	1.83	0.44
1:E:290:THR:O	1:E:291:ALA:C	2.53	0.44
1:C:302:ASN:HB3	1:C:303:GLN:NE2	2.15	0.44
1:E:85:PHE:CZ	1:E:356:LEU:HD21	2.52	0.44
1:E:391:PHE:O	1:E:392:LEU:HD13	2.17	0.44
1:E:475:GLU:O	1:E:477:ALA:N	2.51	0.44
1:E:517:GLU:OE2	1:E:518:THR:O	2.36	0.44
1:F:62:LEU:HG	1:F:303:GLN:O	2.17	0.44
1:B:429:GLN:HA	1:B:439:LEU:O	2.17	0.44
1:A:85:PHE:CZ	1:A:356:LEU:HD21	2.51	0.44
1:D:450:ILE:O	1:D:452:PRO:HD3	2.17	0.44
1:A:382:ASN:N	1:A:385:ASN:HD22	2.08	0.44
1:B:493:PRO:HG2	1:B:496:VAL:HG12	2.00	0.44
1:B:58:ASN:O	1:B:307:VAL:HG23	2.18	0.44
1:B:377:ARG:NH2	1:B:377:ARG:HG3	2.33	0.44
1:C:193:TYR:CE1	1:C:307:VAL:HG21	2.53	0.44
1:E:230:ASN:HB3	1:E:233:ASN:HD22	1.81	0.44
1:D:417:SER:HB3	1:D:451:VAL:HB	1.98	0.44
1:E:307:VAL:HG12	1:E:308:ARG:N	2.33	0.44
1:E:290:THR:C	1:E:292:ARG:N	2.71	0.44
1:C:351:GLU:O	1:E:380:THR:HG21	2.18	0.44
1:C:428:VAL:HG22	1:C:459:GLN:HG2	2.00	0.44
1:D:24:ASN:O	1:D:25:ARG:CB	2.65	0.44
1:C:391:PHE:O	1:C:392:LEU:CB	2.63	0.44
1:B:193:TYR:CE2	1:B:311:LEU:HB3	2.53	0.44
1:A:180:ASP:OD1	1:A:361:ASN:HB2	2.18	0.44
1:F:371:PHE:HD1	1:F:377:ARG:HB3	1.82	0.44
1:A:182:VAL:HG22	1:A:359:LYS:HB3	2.00	0.44
1:F:484:GLY:N	1:F:487:SER:HB3	2.32	0.44
1:B:281:ALA:O	1:B:285:ASN:N	2.49	0.44
1:D:197:ASP:OD1	1:D:197:ASP:N	2.50	0.44
1:B:517:GLU:HB3	1:F:93:GLU:OE1	2.18	0.44
1:C:293:ASN:HB3	1:C:294:LEU:H	1.15	0.44
1:A:448:LEU:C	1:A:448:LEU:HD13	2.38	0.44
1:A:448:LEU:HD13	1:A:449:PHE:N	2.32	0.44
1:F:17:LEU:CB	1:F:439:LEU:HB2	2.47	0.44
1:D:474:GLU:O	1:D:475:GLU:O	2.36	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:24:ASN:O	1:B:25:ARG:CB	2.66	0.44
1:C:418:VAL:HG22	1:C:450:ILE:CG1	2.44	0.44
1:E:54:THR:HG23	1:E:201:VAL:CG2	2.44	0.44
1:C:193:TYR:HE1	1:C:307:VAL:HG21	1.81	0.44
1:E:50:ALA:HA	1:E:204:ASN:O	2.18	0.44
1:D:208:VAL:CG1	1:D:219:PRO:HB3	2.48	0.44
1:A:476:ASN:HB3	1:D:352:THR:HG22	1.98	0.44
1:D:46:ALA:HA	1:D:416:HIS:CD2	2.53	0.44
1:A:93:GLU:OE2	1:D:485:ARG:NH1	2.50	0.43
1:C:430:VAL:O	1:C:438:ILE:HG22	2.18	0.43
1:E:448:LEU:HD13	1:E:448:LEU:C	2.38	0.43
1:A:391:PHE:CD2	1:A:391:PHE:O	2.71	0.43
1:B:194:ASN:C	1:B:194:ASN:ND2	2.70	0.43
1:E:280:LEU:HD12	1:E:280:LEU:C	2.38	0.43
1:A:398:ARG:HH12	1:A:467:GLU:CG	2.31	0.43
1:A:518:THR:O	1:A:519:ILE:HB	2.18	0.43
1:B:493:PRO:HD2	1:B:496:VAL:HG11	2.00	0.43
2:C:599:HOH:O	1:E:393:ARG:NH2	2.50	0.43
1:F:33:ILE:HG12	1:F:53:ILE:CD1	2.47	0.43
1:E:307:VAL:HG13	1:F:499:ASN:CG	2.38	0.43
1:A:216:ASP:O	1:A:218:ASN:N	2.51	0.43
1:D:26:ILE:HG13	1:D:26:ILE:O	2.17	0.43
1:C:17:LEU:CB	1:C:439:LEU:HB2	2.47	0.43
1:E:507:GLN:O	1:E:510:GLN:HB2	2.18	0.43
1:B:368:ALA:HA	1:B:379:SER:OG	2.19	0.43
1:B:393:ARG:HD3	1:B:393:ARG:N	2.32	0.43
1:C:230:ASN:CB	1:C:233:ASN:O	2.66	0.43
1:A:371:PHE:HD1	1:A:377:ARG:HB3	1.83	0.43
1:C:40:GLN:C	1:C:42:ASP:N	2.69	0.43
1:E:224:LEU:HD13	1:F:488:PHE:CE2	2.53	0.43
1:B:227:ASN:HB2	1:B:296:GLY:O	2.19	0.43
1:D:515:ARG:NH1	1:D:516:GLN:OE1	2.52	0.43
1:D:409:PRO:CG	1:D:458:ILE:HD12	2.37	0.43
1:D:402:TYR:O	1:D:403:ARG:C	2.56	0.43
1:E:290:THR:O	1:E:293:ASN:HB2	2.13	0.43
1:A:270:ASN:HD21	1:A:272:PHE:HB2	1.84	0.43
1:C:12:CYS:C	1:C:14:LEU:N	2.70	0.43
1:C:492:LEU:HB3	1:C:496:VAL:CG1	2.48	0.43
1:F:307:VAL:HG12	1:F:308:ARG:N	2.33	0.43
1:F:180:ASP:HA	1:F:361:ASN:HA	2.01	0.43
1:A:285:ASN:HB3	1:B:514:ASN:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:17:LEU:HG	1:F:438:ILE:HG12	2.01	0.43
1:D:230:ASN:HB3	1:D:233:ASN:HD22	1.84	0.43
1:A:403:ARG:H	1:A:403:ARG:HD2	1.83	0.43
1:C:36:TRP:HB3	1:C:43:PHE:CZ	2.53	0.43
1:A:515:ARG:NH1	1:A:516:GLN:OE1	2.52	0.43
1:C:474:GLU:O	1:C:475:GLU:O	2.36	0.43
1:B:17:LEU:HG	1:B:438:ILE:CG1	2.45	0.43
1:F:450:ILE:O	1:F:452:PRO:HD3	2.18	0.43
1:D:24:ASN:O	1:D:25:ARG:HB2	2.18	0.43
1:D:54:THR:HG23	1:D:201:VAL:CG2	2.48	0.43
1:D:368:ALA:HA	1:D:379:SER:OG	2.18	0.43
1:C:448:LEU:HD13	1:C:448:LEU:C	2.39	0.43
1:C:371:PHE:HD1	1:C:377:ARG:HB3	1.83	0.43
1:E:281:ALA:O	1:E:285:ASN:N	2.50	0.43
1:A:486:THR:HG22	1:C:87:GLY:H	1.84	0.43
1:D:517:GLU:HG3	1:D:518:THR:O	2.19	0.43
1:F:78:ARG:CZ	1:F:175:ARG:HH12	2.31	0.43
1:B:390:ARG:O	1:B:393:ARG:HD3	2.18	0.43
1:E:377:ARG:NH2	1:E:377:ARG:HG3	2.34	0.43
1:E:490:ARG:HA	1:E:512:LYS:HG2	2.00	0.43
1:C:50:ALA:HA	1:C:204:ASN:O	2.19	0.43
1:E:284:LEU:CD1	1:E:294:LEU:CD1	2.97	0.43
1:A:280:LEU:C	1:A:280:LEU:HD12	2.39	0.43
1:D:498:ALA:HA	1:D:503:ILE:HG12	2.01	0.43
1:B:12:CYS:C	1:B:14:LEU:N	2.72	0.43
1:F:515:ARG:NH1	1:F:521:LEU:HB3	2.34	0.43
1:F:517:GLU:HB3	2:F:539:HOH:O	2.19	0.43
1:E:356:LEU:HD12	1:E:388:ILE:HD12	2.01	0.43
1:E:391:PHE:O	1:E:391:PHE:CD2	2.72	0.43
1:E:392:LEU:O	1:E:393:ARG:C	2.57	0.43
1:C:315:GLN:O	1:E:371:PHE:CE2	2.71	0.43
1:C:307:VAL:HG12	1:C:308:ARG:N	2.34	0.43
1:C:402:TYR:O	1:C:403:ARG:C	2.57	0.43
1:A:86:SER:HB3	1:B:480:ASN:CG	2.39	0.43
1:E:361:ASN:HD21	1:E:364:ASN:H	1.67	0.43
1:F:14:LEU:CD1	1:F:17:LEU:HD21	2.49	0.42
1:E:458:ILE:HG13	1:E:459:GLN:N	2.33	0.42
1:D:392:LEU:O	1:D:393:ARG:C	2.57	0.42
1:C:391:PHE:O	1:C:391:PHE:CD2	2.72	0.42
1:C:393:ARG:HD3	1:C:393:ARG:N	2.33	0.42
1:B:230:ASN:HB3	1:B:233:ASN:HD22	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:227:ASN:HD22	1:E:227:ASN:C	2.22	0.42
1:B:506:GLU:HA	1:B:509:ARG:HD3	2.01	0.42
1:F:193:TYR:CZ	1:F:311:LEU:HB3	2.54	0.42
1:D:361:ASN:HD21	1:D:364:ASN:H	1.67	0.42
1:B:197:ASP:OD1	1:B:197:ASP:N	2.52	0.42
1:E:193:TYR:CE2	1:E:311:LEU:HB3	2.54	0.42
1:D:315:GLN:HG2	1:D:317:PRO:HD3	2.00	0.42
1:A:422:ILE:HG13	1:A:468:TYR:HA	2.01	0.42
1:D:349:LEU:HG	1:D:350:GLU:N	2.16	0.42
1:A:273:SER:HA	1:A:295:GLN:CG	2.49	0.42
1:D:408:SER:HA	1:D:409:PRO:HD3	1.92	0.42
1:A:356:LEU:HG	1:A:358:LEU:CD1	2.49	0.42
1:B:18:GLN:HE21	1:B:20:ARG:CG	2.23	0.42
1:F:357:ARG:NH2	1:F:360:GLU:HB2	2.34	0.42
1:D:494:ASP:O	1:D:497:LEU:HB2	2.20	0.42
1:A:392:LEU:O	1:A:393:ARG:C	2.57	0.42
1:D:506:GLU:HA	1:D:509:ARG:CD	2.49	0.42
1:A:361:ASN:HD21	1:A:364:ASN:H	1.67	0.42
1:E:493:PRO:HG2	1:E:496:VAL:HG12	2.02	0.42
1:A:54:THR:HG23	1:A:201:VAL:CG2	2.48	0.42
1:F:426:ALA:HA	1:F:460:GLN:O	2.19	0.42
1:E:205:LEU:HG	1:E:471:PHE:HB2	2.02	0.42
1:E:361:ASN:ND2	1:E:363:GLY:H	2.18	0.42
1:F:288:GLU:O	1:F:292:ARG:HG3	2.19	0.42
1:C:398:ARG:HH12	1:C:467:GLU:CG	2.32	0.42
1:B:507:GLN:O	1:B:510:GLN:HB2	2.18	0.42
1:B:517:GLU:HG3	1:B:518:THR:O	2.19	0.42
1:D:85:PHE:CZ	1:D:356:LEU:HD21	2.53	0.42
1:C:312:ASP:N	1:C:312:ASP:OD2	2.48	0.42
1:D:390:ARG:O	1:D:393:ARG:HD3	2.19	0.42
1:C:59:GLY:HA2	1:C:305:ILE:O	2.19	0.42
1:A:205:LEU:HG	1:A:471:PHE:CB	2.49	0.42
1:F:364:ASN:HA	1:F:365:PRO:HD3	1.77	0.42
1:B:284:LEU:CD1	1:B:294:LEU:HD11	2.49	0.42
1:A:93:GLU:OE1	1:D:517:GLU:HB3	2.19	0.42
1:F:276:ASN:O	1:F:277:THR:C	2.58	0.42
1:B:220:ARG:HD3	1:C:433:GLU:CD	2.40	0.42
1:C:194:ASN:HD22	1:C:196:GLY:H	1.67	0.42
1:D:33:ILE:HG23	1:D:53:ILE:HD13	2.01	0.42
1:E:307:VAL:HG13	1:F:499:ASN:OD1	2.20	0.42
1:E:50:ALA:HB2	1:E:205:LEU:HD13	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:174:ARG:HH11	1:F:174:ARG:HG3	1.85	0.42
1:B:486:THR:CB	1:B:518:THR:HG21	2.49	0.42
1:C:270:ASN:HD22	1:C:270:ASN:C	2.23	0.42
1:A:474:GLU:O	1:A:475:GLU:O	2.38	0.42
1:C:381:LEU:CD1	1:C:389:LEU:HD11	2.45	0.42
1:D:66:SER:CB	1:D:220:ARG:O	2.62	0.42
1:E:24:ASN:O	1:E:25:ARG:CB	2.68	0.42
1:D:212:HIS:CE1	1:D:391:PHE:CE1	3.07	0.42
1:D:81:LEU:HB2	1:D:176:ILE:HD13	2.02	0.42
1:E:480:ASN:HD22	1:E:480:ASN:C	2.22	0.42
1:B:369:ASP:OD2	1:F:355:SER:HB3	2.20	0.42
1:E:174:ARG:HH11	1:E:174:ARG:HG3	1.84	0.42
1:C:71:LEU:HA	1:C:71:LEU:HD23	1.70	0.42
1:A:517:GLU:OE1	1:A:517:GLU:HA	2.20	0.42
1:B:407:TYR:HB3	1:B:459:GLN:HB2	2.00	0.42
1:F:270:ASN:C	1:F:270:ASN:HD22	2.23	0.42
1:A:418:VAL:HG13	1:A:448:LEU:HD11	2.02	0.42
1:F:66:SER:CB	1:F:220:ARG:O	2.64	0.42
1:C:305:ILE:HG22	1:C:306:GLN:O	2.20	0.42
1:F:287:ASN:ND2	1:F:289:GLU:CB	2.83	0.42
1:D:492:LEU:HD22	1:F:191:TRP:NE1	2.34	0.42
1:E:58:ASN:O	1:E:307:VAL:HG23	2.19	0.42
1:B:224:LEU:HD13	1:C:488:PHE:CE2	2.54	0.42
1:F:410:HIS:CE1	1:F:457:VAL:HG13	2.55	0.42
1:A:312:ASP:OD1	1:A:312:ASP:C	2.58	0.42
1:D:400:PHE:C	1:D:400:PHE:CD2	2.93	0.42
1:D:48:VAL:HG12	1:D:49:ALA:N	2.34	0.42
1:F:398:ARG:HH12	1:F:467:GLU:HG2	1.84	0.42
1:B:227:ASN:HD22	1:B:227:ASN:C	2.22	0.42
1:B:422:ILE:HG13	1:B:468:TYR:HA	2.01	0.42
1:C:294:LEU:HA	1:C:294:LEU:HD23	1.95	0.42
1:B:24:ASN:O	1:B:25:ARG:HB2	2.20	0.42
1:D:393:ARG:HD3	1:D:393:ARG:N	2.34	0.42
1:F:391:PHE:O	1:F:391:PHE:CD2	2.73	0.42
1:E:393:ARG:N	1:E:393:ARG:HD3	2.34	0.42
1:A:307:VAL:HG13	1:B:499:ASN:OD1	2.20	0.42
1:D:87:GLY:HA2	1:E:486:THR:CG2	2.47	0.42
1:B:407:TYR:O	1:B:408:SER:C	2.58	0.42
1:C:294:LEU:O	1:C:295:GLN:C	2.57	0.42
1:F:270:ASN:HD22	1:F:272:PHE:N	2.18	0.42
1:D:273:SER:HA	1:D:295:GLN:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:386:LEU:HG	1:B:388:ILE:HG12	2.02	0.42
1:E:40:GLN:O	1:E:42:ASP:N	2.53	0.42
1:D:191:TRP:NE1	1:E:492:LEU:HD22	2.35	0.42
1:A:384:HIS:CE1	1:D:353:PHE:HD2	2.37	0.42
1:E:364:ASN:HA	1:E:365:PRO:HD3	1.83	0.42
1:D:397:GLU:HB3	1:D:470:ALA:HB3	2.02	0.42
1:A:417:SER:HB3	1:A:451:VAL:HB	2.02	0.42
1:E:426:ALA:HB2	1:E:466:PHE:CD1	2.53	0.42
1:F:402:TYR:O	1:F:403:ARG:C	2.58	0.42
1:F:315:GLN:HG2	1:F:317:PRO:HD3	2.01	0.42
1:D:227:ASN:HB2	1:D:296:GLY:O	2.19	0.42
1:D:230:ASN:HB3	1:D:233:ASN:O	2.20	0.41
1:A:227:ASN:ND2	1:A:227:ASN:C	2.72	0.41
1:F:79:GLY:O	1:F:176:ILE:HG12	2.20	0.41
1:D:364:ASN:HA	1:D:365:PRO:HD3	1.81	0.41
2:C:579:HOH:O	1:D:490:ARG:NH2	2.53	0.41
1:A:490:ARG:NH2	2:A:536:HOH:O	2.52	0.41
1:E:33:ILE:HD12	1:E:303:GLN:HG3	2.02	0.41
1:A:429:GLN:HB2	1:A:458:ILE:CG2	2.49	0.41
1:E:386:LEU:HG	1:E:388:ILE:HG12	2.02	0.41
1:C:12:CYS:CA	1:C:14:LEU:HD23	2.49	0.41
1:E:453:GLN:O	1:E:454:ASN:HB2	2.19	0.41
1:E:437:ALA:O	1:E:439:LEU:N	2.54	0.41
1:A:230:ASN:HB3	1:A:233:ASN:O	2.20	0.41
1:F:361:ASN:HD21	1:F:364:ASN:H	1.68	0.41
1:C:408:SER:HB2	1:C:521:LEU:HD21	2.02	0.41
1:F:517:GLU:OE2	1:F:518:THR:O	2.37	0.41
1:E:414:ASN:HA	1:E:453:GLN:NE2	2.35	0.41
1:E:493:PRO:HD2	1:E:496:VAL:HG11	2.02	0.41
1:A:194:ASN:HD22	1:A:196:GLY:H	1.68	0.41
1:C:448:LEU:HD13	1:C:449:PHE:N	2.35	0.41
1:B:353:PHE:HD2	1:F:384:HIS:CE1	2.38	0.41
1:C:57:ARG:O	1:C:58:ASN:HB2	2.19	0.41
1:A:272:PHE:CE2	1:B:482:LEU:HD13	2.54	0.41
1:B:408:SER:HB2	1:B:521:LEU:HD21	2.01	0.41
1:D:177:ARG:O	1:D:180:ASP:HB2	2.20	0.41
1:E:58:ASN:HD22	1:E:58:ASN:HA	1.61	0.41
1:C:506:GLU:HA	1:C:509:ARG:HD3	2.00	0.41
1:A:367:ARG:NH2	2:C:582:HOH:O	2.48	0.41
1:A:270:ASN:C	1:A:270:ASN:HD22	2.23	0.41
1:B:350:GLU:N	1:B:350:GLU:OE2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:357:ARG:HD3	1:E:385:ASN:O	2.21	0.41
1:E:59:GLY:HA2	1:E:305:ILE:O	2.20	0.41
1:B:307:VAL:HG13	1:C:499:ASN:CG	2.41	0.41
1:E:74:ILE:HD11	1:E:176:ILE:HD12	2.02	0.41
1:E:40:GLN:C	1:E:42:ASP:H	2.24	0.41
1:C:95:SER:C	1:C:96:GLN:HG2	2.40	0.41
1:F:67:ASN:O	1:F:213:ASN:HB2	2.19	0.41
1:A:293:ASN:ND2	1:B:503:ILE:HG22	2.35	0.41
1:C:270:ASN:HD22	1:C:272:PHE:N	2.18	0.41
1:D:437:ALA:O	1:D:439:LEU:N	2.52	0.41
1:A:349:LEU:HG	1:A:350:GLU:N	2.18	0.41
1:C:391:PHE:O	1:C:391:PHE:CG	2.74	0.41
1:E:70:GLN:HA	1:E:205:LEU:O	2.20	0.41
1:B:217:GLN:OE1	1:B:217:GLN:HA	2.21	0.41
1:F:197:ASP:N	1:F:197:ASP:OD1	2.53	0.41
1:A:418:VAL:HG22	1:A:450:ILE:CG1	2.44	0.41
1:B:76:GLN:HA	1:B:178:GLU:CG	2.50	0.41
1:E:215:LEU:O	1:F:12:CYS:SG	2.78	0.41
1:B:457:VAL:HG13	1:B:457:VAL:O	2.21	0.41
1:C:364:ASN:HA	1:C:365:PRO:HD3	1.81	0.41
1:A:49:ALA:HB3	1:A:206:PHE:HB2	2.03	0.41
1:E:84:VAL:HG13	1:F:491:ALA:CB	2.51	0.41
1:B:458:ILE:O	1:B:459:GLN:HG3	2.21	0.41
1:C:485:ARG:HH22	1:E:93:GLU:HG3	1.85	0.41
1:D:413:VAL:HG13	1:F:187:GLY:O	2.21	0.41
1:D:293:ASN:C	1:D:293:ASN:OD1	2.57	0.41
1:A:33:ILE:HG23	1:A:53:ILE:HD13	2.03	0.41
1:A:40:GLN:O	1:A:41:GLY:C	2.59	0.41
1:E:57:ARG:O	1:E:58:ASN:HB2	2.20	0.41
1:C:362:ILE:CD1	1:C:398:ARG:HB3	2.51	0.41
1:C:414:ASN:HA	1:C:453:GLN:NE2	2.35	0.41
1:C:414:ASN:ND2	1:C:414:ASN:N	2.51	0.41
1:F:453:GLN:O	1:F:455:HIS:HD2	2.04	0.41
1:F:270:ASN:HD21	1:F:272:PHE:HB2	1.86	0.41
1:A:349:LEU:CD2	1:D:479:ILE:O	2.59	0.41
1:C:517:GLU:CB	1:E:93:GLU:OE2	2.58	0.41
1:F:483:ALA:N	1:F:487:SER:HB2	2.36	0.41
1:B:371:PHE:HD1	1:B:377:ARG:HB3	1.85	0.41
1:D:71:LEU:HB2	1:D:471:PHE:CE1	2.56	0.41
1:B:490:ARG:HA	1:B:512:LYS:HG2	2.02	0.41
1:D:33:ILE:HG12	1:D:53:ILE:CD1	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:400:PHE:HA	1:E:466:PHE:O	2.21	0.41
1:C:236:GLY:O	1:C:237:GLN:C	2.59	0.41
1:E:26:ILE:HG13	1:E:26:ILE:O	2.20	0.41
1:B:405:GLY:H	1:B:461:ALA:HB3	1.86	0.41
1:D:362:ILE:HD12	1:D:398:ARG:HB3	2.04	0.41
1:A:423:ARG:NH1	1:A:467:GLU:OE1	2.54	0.41
1:C:423:ARG:HA	1:C:445:GLN:HB2	2.03	0.41
1:D:482:LEU:HD13	1:F:272:PHE:CE2	2.56	0.41
1:D:290:THR:O	1:D:293:ASN:CB	2.61	0.41
1:B:53:ILE:HG12	1:B:204:ASN:ND2	2.36	0.41
1:F:401:PHE:HB2	1:F:466:PHE:HB3	2.03	0.41
1:A:270:ASN:HD22	1:A:272:PHE:N	2.18	0.40
1:F:53:ILE:CG1	1:F:204:ASN:HD21	2.34	0.40
1:E:194:ASN:C	1:E:194:ASN:ND2	2.74	0.40
1:E:227:ASN:C	1:E:227:ASN:ND2	2.74	0.40
1:E:426:ALA:HA	1:E:460:GLN:O	2.21	0.40
1:E:488:PHE:O	1:E:491:ALA:HB3	2.22	0.40
1:A:36:TRP:HB3	1:A:43:PHE:CZ	2.56	0.40
1:F:216:ASP:O	1:F:218:ASN:N	2.54	0.40
1:E:217:GLN:OE1	1:E:217:GLN:HA	2.21	0.40
1:B:276:ASN:HD21	1:B:278:GLN:HB3	1.86	0.40
1:C:381:LEU:HD22	1:C:385:ASN:HB2	2.02	0.40
1:F:429:GLN:HB2	1:F:458:ILE:CG2	2.50	0.40
1:D:270:ASN:HD21	1:D:272:PHE:HB2	1.87	0.40
1:D:391:PHE:O	1:D:391:PHE:CD2	2.74	0.40
1:B:58:ASN:HA	1:B:58:ASN:HD22	1.59	0.40
1:F:497:LEU:HD23	1:F:501:TYR:HE1	1.87	0.40
1:B:174:ARG:HH11	1:B:174:ARG:HG3	1.86	0.40
1:F:408:SER:HA	1:F:409:PRO:HD3	1.87	0.40
1:D:285:ASN:HB3	1:E:514:ASN:O	2.22	0.40
1:E:78:ARG:N	1:E:200:LEU:HD13	2.37	0.40
1:A:381:LEU:HD22	1:A:385:ASN:HB2	2.02	0.40
1:D:433:GLU:OE1	1:F:220:ARG:HD3	2.22	0.40
1:F:230:ASN:HB3	1:F:233:ASN:O	2.21	0.40
1:D:371:PHE:HD1	1:D:377:ARG:HB3	1.85	0.40
1:A:227:ASN:HB2	1:A:296:GLY:O	2.20	0.40
1:B:480:ASN:HD22	1:B:481:THR:N	2.19	0.40
1:F:444:GLN:N	1:F:447:GLN:OE1	2.33	0.40
1:B:364:ASN:HA	1:B:365:PRO:HD3	1.81	0.40
1:F:25:ARG:HG3	1:F:26:ILE:N	2.37	0.40
1:E:453:GLN:O	1:E:455:HIS:HD2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:391:PHE:O	1:A:391:PHE:CG	2.73	0.40
1:B:391:PHE:CD2	1:B:391:PHE:O	2.75	0.40
1:A:305:ILE:HG22	1:A:306:GLN:O	2.22	0.40
1:A:59:GLY:HA2	1:A:305:ILE:O	2.22	0.40
1:E:55:ILE:HG12	1:E:304:ILE:HD13	2.03	0.40
1:A:217:GLN:HA	1:A:217:GLN:OE1	2.21	0.40
1:A:197:ASP:N	1:A:197:ASP:OD1	2.54	0.40
1:E:421:VAL:CG1	1:E:445:GLN:HA	2.52	0.40
1:B:303:GLN:CD	1:B:303:GLN:H	2.25	0.40
1:C:349:LEU:CD2	1:D:86:SER:OG	2.70	0.40
1:C:453:GLN:O	1:C:454:ASN:HB2	2.21	0.40
1:D:291:ALA:O	1:D:293:ASN:N	2.54	0.40
1:E:24:ASN:O	1:E:25:ARG:HB2	2.22	0.40
1:C:54:THR:HG23	1:C:201:VAL:CG2	2.51	0.40
1:D:305:ILE:HG22	1:D:306:GLN:O	2.22	0.40
1:D:236:GLY:O	1:D:237:GLN:C	2.60	0.40
1:F:223:TYR:CD1	1:F:228:PRO:HG3	2.57	0.40
1:A:498:ALA:HA	1:A:503:ILE:HG12	2.03	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	376/531 (71%)	309 (82%)	48 (13%)	19 (5%)	2	20
1	B	376/531 (71%)	303 (81%)	48 (13%)	25 (7%)	1	12
1	C	376/531 (71%)	308 (82%)	47 (12%)	21 (6%)	2	18
1	D	376/531 (71%)	307 (82%)	47 (12%)	22 (6%)	2	16
1	E	376/531 (71%)	306 (81%)	48 (13%)	22 (6%)	2	16
1	F	376/531 (71%)	309 (82%)	48 (13%)	19 (5%)	2	20

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	2256/3186 (71%)	1842 (82%)	286 (13%)	128 (6%)	2	17

All (128) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	233	ASN
1	A	269	ASN
1	A	303	GLN
1	A	392	LEU
1	A	475	GLU
1	B	25	ARG
1	B	29	GLU
1	B	233	ASN
1	B	269	ASN
1	B	303	GLN
1	B	392	LEU
1	B	475	GLU
1	C	25	ARG
1	C	233	ASN
1	C	269	ASN
1	C	294	LEU
1	C	303	GLN
1	C	392	LEU
1	C	475	GLU
1	D	233	ASN
1	D	269	ASN
1	D	303	GLN
1	D	392	LEU
1	D	475	GLU
1	E	25	ARG
1	E	233	ASN
1	E	269	ASN
1	E	303	GLN
1	E	392	LEU
1	E	475	GLU
1	F	25	ARG
1	F	233	ASN
1	F	269	ASN
1	F	392	LEU
1	F	475	GLU
1	A	25	ARG
1	A	42	ASP

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Mol	Chain	Res	Type
1	B	11	GLN
1	B	76	GLN
1	B	93	GLU
1	B	287	ASN
1	B	316	PRO
1	C	11	GLN
1	C	316	PRO
1	D	25	ARG
1	D	42	ASP
1	D	217	GLN
1	D	316	PRO
1	E	316	PRO
1	F	303	GLN
1	F	316	PRO
1	A	217	GLN
1	A	235	GLN
1	A	287	ASN
1	A	316	PRO
1	A	403	ARG
1	A	404	ASN
1	B	42	ASP
1	B	235	GLN
1	B	277	THR
1	B	404	ASN
1	C	42	ASP
1	C	217	GLN
1	C	235	GLN
1	C	292	ARG
1	C	403	ARG
1	C	426	ALA
1	D	235	GLN
1	D	277	THR
1	D	287	ASN
1	D	403	ARG
1	D	404	ASN
1	E	42	ASP
1	E	235	GLN
1	E	277	THR
1	E	287	ASN
1	E	291	ALA
1	E	403	ARG
1	E	404	ASN

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Mol	Chain	Res	Type
1	F	42	ASP
1	F	235	GLN
1	F	277	THR
1	F	403	ARG
1	F	426	ALA
1	A	277	THR
1	A	426	ALA
1	A	519	ILE
1	B	215	LEU
1	B	403	ARG
1	B	426	ALA
1	B	519	ILE
1	C	519	ILE
1	D	426	ALA
1	D	519	ILE
1	E	215	LEU
1	E	217	GLN
1	E	426	ALA
1	E	438	ILE
1	E	519	ILE
1	F	215	LEU
1	F	217	GLN
1	F	287	ASN
1	F	404	ASN
1	A	373	PRO
1	B	473	THR
1	B	494	ASP
1	C	277	THR
1	C	287	ASN
1	C	373	PRO
1	C	404	ASN
1	D	215	LEU
1	D	295	GLN
1	D	373	PRO
1	E	11	GLN
1	E	296	GLY
1	F	11	GLN
1	F	519	ILE
1	A	11	GLN
1	C	215	LEU
1	D	11	GLN
1	D	435	GLY

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Mol	Chain	Res	Type
1	D	438	ILE
1	F	373	PRO
1	E	373	PRO
1	B	373	PRO
1	B	438	ILE
1	B	408	SER
1	A	408	SER

### 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	320/452 (71%)	272 (85%)	48 (15%)	3	17
1	B	320/452 (71%)	271 (85%)	49 (15%)	3	17
1	C	320/452 (71%)	269 (84%)	51 (16%)	3	14
1	D	320/452 (71%)	270 (84%)	50 (16%)	3	15
1	E	320/452 (71%)	269 (84%)	51 (16%)	3	14
1	F	320/452 (71%)	272 (85%)	48 (15%)	3	17
All	All	1920/2712 (71%)	1623 (84%)	297 (16%)	3	15

All (297) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	LEU
1	A	16	GLN
1	A	18	GLN
1	A	20	ARG
1	A	37	ASN
1	A	40	GLN
1	A	45	CYS
1	A	58	ASN
1	A	66	SER
1	A	91	THR
1	A	93	GLU

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Mol	Chain	Res	Type
1	A	171	GLN
1	A	177	ARG
1	A	194	ASN
1	A	198	GLN
1	A	227	ASN
1	A	230	ASN
1	A	233	ASN
1	A	269	ASN
1	A	270	ASN
1	A	271	VAL
1	A	280	LEU
1	A	298	ASN
1	A	303	GLN
1	A	312	ASP
1	A	316	PRO
1	A	349	LEU
1	A	350	GLU
1	A	357	ARG
1	A	373	PRO
1	A	381	LEU
1	A	388	ILE
1	A	392	LEU
1	A	394	LEU
1	A	400	PHE
1	A	404	ASN
1	A	407	TYR
1	A	414	ASN
1	A	423	ARG
1	A	444	GLN
1	A	474	GLU
1	A	480	ASN
1	A	481	THR
1	A	482	LEU
1	A	486	THR
1	A	488	PHE
1	A	515	ARG
1	A	518	THR
1	B	10	ASN
1	B	14	LEU
1	B	16	GLN
1	B	18	GLN
1	B	20	ARG

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Mol	Chain	Res	Type
1	B	32	GLN
1	B	37	ASN
1	B	40	GLN
1	B	45	CYS
1	B	58	ASN
1	B	66	SER
1	B	95	SER
1	B	96	GLN
1	B	171	GLN
1	B	177	ARG
1	B	194	ASN
1	B	197	ASP
1	B	198	GLN
1	B	227	ASN
1	B	230	ASN
1	B	233	ASN
1	B	269	ASN
1	B	270	ASN
1	B	271	VAL
1	B	280	LEU
1	B	298	ASN
1	B	303	GLN
1	B	316	PRO
1	B	349	LEU
1	B	350	GLU
1	B	357	ARG
1	B	373	PRO
1	B	381	LEU
1	B	388	ILE
1	B	392	LEU
1	B	394	LEU
1	B	400	PHE
1	B	407	TYR
1	B	414	ASN
1	B	423	ARG
1	B	444	GLN
1	B	474	GLU
1	B	480	ASN
1	B	481	THR
1	B	482	LEU
1	B	486	THR
1	B	488	PHE

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Mol	Chain	Res	Type
1	B	515	ARG
1	B	518	THR
1	C	10	ASN
1	C	14	LEU
1	C	16	GLN
1	C	18	GLN
1	C	20	ARG
1	C	25	ARG
1	C	32	GLN
1	C	37	ASN
1	C	40	GLN
1	C	45	CYS
1	C	58	ASN
1	C	66	SER
1	C	91	THR
1	C	93	GLU
1	C	171	GLN
1	C	175	ARG
1	C	177	ARG
1	C	194	ASN
1	C	198	GLN
1	C	227	ASN
1	C	228	PRO
1	C	230	ASN
1	C	233	ASN
1	C	269	ASN
1	C	270	ASN
1	C	271	VAL
1	C	298	ASN
1	C	303	GLN
1	C	316	PRO
1	C	349	LEU
1	C	350	GLU
1	C	357	ARG
1	C	373	PRO
1	C	381	LEU
1	C	388	ILE
1	C	394	LEU
1	C	400	PHE
1	C	404	ASN
1	C	407	TYR
1	C	414	ASN

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Mol	Chain	Res	Type
1	C	423	ARG
1	C	444	GLN
1	C	458	ILE
1	C	474	GLU
1	C	480	ASN
1	C	481	THR
1	C	482	LEU
1	C	486	THR
1	C	488	PHE
1	C	515	ARG
1	C	518	THR
1	D	14	LEU
1	D	16	GLN
1	D	18	GLN
1	D	20	ARG
1	D	25	ARG
1	D	37	ASN
1	D	40	GLN
1	D	45	CYS
1	D	58	ASN
1	D	66	SER
1	D	91	THR
1	D	93	GLU
1	D	171	GLN
1	D	177	ARG
1	D	194	ASN
1	D	198	GLN
1	D	227	ASN
1	D	230	ASN
1	D	233	ASN
1	D	269	ASN
1	D	270	ASN
1	D	271	VAL
1	D	280	LEU
1	D	290	THR
1	D	292	ARG
1	D	298	ASN
1	D	303	GLN
1	D	316	PRO
1	D	349	LEU
1	D	350	GLU
1	D	357	ARG

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Mol	Chain	Res	Type
1	D	373	PRO
1	D	381	LEU
1	D	388	ILE
1	D	392	LEU
1	D	394	LEU
1	D	400	PHE
1	D	404	ASN
1	D	407	TYR
1	D	414	ASN
1	D	423	ARG
1	D	444	GLN
1	D	474	GLU
1	D	480	ASN
1	D	481	THR
1	D	482	LEU
1	D	486	THR
1	D	488	PHE
1	D	515	ARG
1	D	518	THR
1	E	14	LEU
1	E	16	GLN
1	E	18	GLN
1	E	20	ARG
1	E	37	ASN
1	E	40	GLN
1	E	45	CYS
1	E	58	ASN
1	E	66	SER
1	E	78	ARG
1	E	91	THR
1	E	93	GLU
1	E	171	GLN
1	E	177	ARG
1	E	194	ASN
1	E	197	ASP
1	E	198	GLN
1	E	227	ASN
1	E	230	ASN
1	E	233	ASN
1	E	269	ASN
1	E	270	ASN
1	E	271	VAL

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Mol	Chain	Res	Type
1	E	280	LEU
1	E	290	THR
1	E	292	ARG
1	E	295	GLN
1	E	298	ASN
1	E	303	GLN
1	E	316	PRO
1	E	350	GLU
1	E	357	ARG
1	E	373	PRO
1	E	381	LEU
1	E	388	ILE
1	E	392	LEU
1	E	394	LEU
1	E	400	PHE
1	E	404	ASN
1	E	407	TYR
1	E	414	ASN
1	E	423	ARG
1	E	444	GLN
1	E	474	GLU
1	E	480	ASN
1	E	481	THR
1	E	482	LEU
1	E	486	THR
1	E	488	PHE
1	E	515	ARG
1	E	518	THR
1	F	14	LEU
1	F	16	GLN
1	F	18	GLN
1	F	20	ARG
1	F	25	ARG
1	F	32	GLN
1	F	37	ASN
1	F	40	GLN
1	F	45	CYS
1	F	58	ASN
1	F	66	SER
1	F	78	ARG
1	F	91	THR
1	F	93	GLU

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Mol	Chain	Res	Type
1	F	171	GLN
1	F	177	ARG
1	F	194	ASN
1	F	198	GLN
1	F	227	ASN
1	F	230	ASN
1	F	233	ASN
1	F	269	ASN
1	F	270	ASN
1	F	271	VAL
1	F	295	GLN
1	F	298	ASN
1	F	303	GLN
1	F	316	PRO
1	F	349	LEU
1	F	350	GLU
1	F	357	ARG
1	F	373	PRO
1	F	381	LEU
1	F	388	ILE
1	F	394	LEU
1	F	400	PHE
1	F	404	ASN
1	F	407	TYR
1	F	414	ASN
1	F	423	ARG
1	F	444	GLN
1	F	474	GLU
1	F	480	ASN
1	F	481	THR
1	F	482	LEU
1	F	488	PHE
1	F	515	ARG
1	F	518	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (136) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	GLN
1	A	58	ASN
1	A	194	ASN
1	A	198	GLN

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Mol	Chain	Res	Type
1	A	212	HIS
1	A	214	GLN
1	A	218	ASN
1	A	227	ASN
1	A	269	ASN
1	A	270	ASN
1	A	276	ASN
1	A	287	ASN
1	A	293	ASN
1	A	303	GLN
1	A	361	ASN
1	A	385	ASN
1	A	414	ASN
1	A	429	GLN
1	A	445	GLN
1	A	454	ASN
1	A	455	HIS
1	A	480	ASN
1	B	18	GLN
1	B	32	GLN
1	B	58	ASN
1	B	194	ASN
1	B	198	GLN
1	B	212	HIS
1	B	214	GLN
1	B	218	ASN
1	B	227	ASN
1	B	269	ASN
1	B	270	ASN
1	B	276	ASN
1	B	287	ASN
1	B	303	GLN
1	B	361	ASN
1	B	384	HIS
1	B	385	ASN
1	B	414	ASN
1	B	429	GLN
1	B	445	GLN
1	B	454	ASN
1	B	455	HIS
1	B	480	ASN
1	C	13	GLN

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Mol	Chain	Res	Type
1	C	32	GLN
1	C	58	ASN
1	C	194	ASN
1	C	198	GLN
1	C	212	HIS
1	C	214	GLN
1	C	218	ASN
1	C	227	ASN
1	C	269	ASN
1	C	270	ASN
1	C	276	ASN
1	C	287	ASN
1	C	293	ASN
1	C	303	GLN
1	C	361	ASN
1	C	364	ASN
1	C	385	ASN
1	C	414	ASN
1	C	429	GLN
1	C	445	GLN
1	C	455	HIS
1	C	480	ASN
1	C	507	GLN
1	D	32	GLN
1	D	58	ASN
1	D	194	ASN
1	D	198	GLN
1	D	212	HIS
1	D	214	GLN
1	D	218	ASN
1	D	227	ASN
1	D	269	ASN
1	D	270	ASN
1	D	276	ASN
1	D	287	ASN
1	D	295	GLN
1	D	303	GLN
1	D	361	ASN
1	D	385	ASN
1	D	414	ASN
1	D	429	GLN
1	D	445	GLN

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Mol	Chain	Res	Type
1	D	454	ASN
1	D	455	HIS
1	D	463	ASN
1	D	480	ASN
1	D	507	GLN
1	E	32	GLN
1	E	58	ASN
1	E	194	ASN
1	E	212	HIS
1	E	214	GLN
1	E	218	ASN
1	E	227	ASN
1	E	269	ASN
1	E	270	ASN
1	E	276	ASN
1	E	287	ASN
1	E	295	GLN
1	E	303	GLN
1	E	361	ASN
1	E	385	ASN
1	E	414	ASN
1	E	429	GLN
1	E	445	GLN
1	E	454	ASN
1	E	455	HIS
1	E	480	ASN
1	F	13	GLN
1	F	32	GLN
1	F	58	ASN
1	F	194	ASN
1	F	198	GLN
1	F	212	HIS
1	F	214	GLN
1	F	218	ASN
1	F	227	ASN
1	F	269	ASN
1	F	270	ASN
1	F	276	ASN
1	F	287	ASN
1	F	295	GLN
1	F	303	GLN
1	F	361	ASN

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Mol	Chain	Res	Type
1	F	385	ASN
1	F	414	ASN
1	F	429	GLN
1	F	445	GLN
1	F	455	HIS
1	F	480	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no 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 [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	384/531 (72%)	-0.31	2 (0%) 91 87	23, 48, 94, 133	0
1	B	384/531 (72%)	-0.28	2 (0%) 91 87	26, 54, 102, 139	0
1	C	384/531 (72%)	-0.27	2 (0%) 91 87	22, 47, 94, 138	0
1	D	384/531 (72%)	-0.31	1 (0%) 94 93	22, 48, 95, 133	0
1	E	384/531 (72%)	-0.27	2 (0%) 91 87	26, 54, 102, 140	0
1	F	384/531 (72%)	-0.29	3 (0%) 87 80	23, 47, 91, 132	0
All	All	2304/3186 (72%)	-0.29	12 (0%) 91 87	22, 49, 97, 140	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	237	GLN	3.4
1	A	237	GLN	3.3
1	C	318	ARG	3.1
1	B	237	GLN	2.9
1	F	236	GLY	2.7
1	B	318	ARG	2.4
1	A	236	GLY	2.4
1	F	237	GLN	2.4
1	D	236	GLY	2.3
1	F	318	ARG	2.2
1	E	318	ARG	2.1
1	C	237	GLN	2.1

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

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

There are no ligands in this entry.

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

There are no such residues in this entry.