



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:30 AM GMT

PDB ID : 3M6A  
Title : Crystal structure of Bacillus subtilis Lon C-terminal domain  
Authors : Duman, R.E.; Lowe, J.Y.  
Deposited on : 2010-03-15  
Resolution : 3.40 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

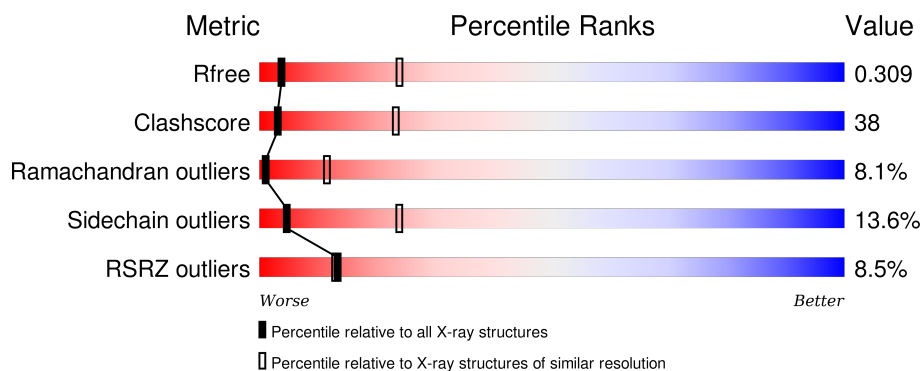
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.40 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	1476 (3.50-3.30)
Clashscore	102246	1611 (3.50-3.30)
Ramachandran outliers	100387	1571 (3.50-3.30)
Sidechain outliers	100360	1571 (3.50-3.30)
RSRZ outliers	91569	1485 (3.50-3.30)

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	543	<div> <div>5%</div> <div> <div>39%</div> <div>39%</div> <div>13%</div> <div>9%</div> </div> </div>
1	B	543	<div> <div>6%</div> <div> <div>39%</div> <div>38%</div> <div>13%</div> <div>9%</div> </div> </div>
1	C	543	<div> <div>8%</div> <div> <div>37%</div> <div>41%</div> <div>13%</div> <div>9%</div> </div> </div>
1	D	543	<div> <div>10%</div> <div> <div>37%</div> <div>42%</div> <div>12%</div> <div>9%</div> </div> </div>
1	E	543	<div> <div>11%</div> <div> <div>38%</div> <div>40%</div> <div>12%</div> <div>9%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	F	543	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ADP	D	783	-	-	X	-

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 23196 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 ATP-dependent protease La 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	496	Total	C	N	O	S	0	0	0
			3839	2427	666	736	10			
1	B	496	Total	C	N	O	S	0	0	0
			3839	2427	666	736	10			
1	C	496	Total	C	N	O	S	0	0	0
			3839	2427	666	736	10			
1	D	496	Total	C	N	O	S	0	0	0
			3839	2427	666	736	10			
1	E	496	Total	C	N	O	S	0	0	0
			3839	2427	666	736	10			
1	F	496	Total	C	N	O	S	0	0	0
			3839	2427	666	736	10			

There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	677	ALA	SER	ENGINEERED MUTATION	UNP P37945
A	775	LEU	-	EXPRESSION TAG	UNP P37945
A	776	GLU	-	EXPRESSION TAG	UNP P37945
A	777	HIS	-	EXPRESSION TAG	UNP P37945
A	778	HIS	-	EXPRESSION TAG	UNP P37945
A	779	HIS	-	EXPRESSION TAG	UNP P37945
A	780	HIS	-	EXPRESSION TAG	UNP P37945
A	781	HIS	-	EXPRESSION TAG	UNP P37945
A	782	HIS	-	EXPRESSION TAG	UNP P37945
B	677	ALA	SER	ENGINEERED MUTATION	UNP P37945
B	775	LEU	-	EXPRESSION TAG	UNP P37945
B	776	GLU	-	EXPRESSION TAG	UNP P37945
B	777	HIS	-	EXPRESSION TAG	UNP P37945
B	778	HIS	-	EXPRESSION TAG	UNP P37945
B	779	HIS	-	EXPRESSION TAG	UNP P37945
B	780	HIS	-	EXPRESSION TAG	UNP P37945
B	781	HIS	-	EXPRESSION TAG	UNP P37945

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Chain	Residue	Modelled	Actual	Comment	Reference
B	782	HIS	-	EXPRESSION TAG	UNP P37945
C	677	ALA	SER	ENGINEERED MUTATION	UNP P37945
C	775	LEU	-	EXPRESSION TAG	UNP P37945
C	776	GLU	-	EXPRESSION TAG	UNP P37945
C	777	HIS	-	EXPRESSION TAG	UNP P37945
C	778	HIS	-	EXPRESSION TAG	UNP P37945
C	779	HIS	-	EXPRESSION TAG	UNP P37945
C	780	HIS	-	EXPRESSION TAG	UNP P37945
C	781	HIS	-	EXPRESSION TAG	UNP P37945
C	782	HIS	-	EXPRESSION TAG	UNP P37945
D	677	ALA	SER	ENGINEERED MUTATION	UNP P37945
D	775	LEU	-	EXPRESSION TAG	UNP P37945
D	776	GLU	-	EXPRESSION TAG	UNP P37945
D	777	HIS	-	EXPRESSION TAG	UNP P37945
D	778	HIS	-	EXPRESSION TAG	UNP P37945
D	779	HIS	-	EXPRESSION TAG	UNP P37945
D	780	HIS	-	EXPRESSION TAG	UNP P37945
D	781	HIS	-	EXPRESSION TAG	UNP P37945
D	782	HIS	-	EXPRESSION TAG	UNP P37945
E	677	ALA	SER	ENGINEERED MUTATION	UNP P37945
E	775	LEU	-	EXPRESSION TAG	UNP P37945
E	776	GLU	-	EXPRESSION TAG	UNP P37945
E	777	HIS	-	EXPRESSION TAG	UNP P37945
E	778	HIS	-	EXPRESSION TAG	UNP P37945
E	779	HIS	-	EXPRESSION TAG	UNP P37945
E	780	HIS	-	EXPRESSION TAG	UNP P37945
E	781	HIS	-	EXPRESSION TAG	UNP P37945
E	782	HIS	-	EXPRESSION TAG	UNP P37945
F	677	ALA	SER	ENGINEERED MUTATION	UNP P37945
F	775	LEU	-	EXPRESSION TAG	UNP P37945
F	776	GLU	-	EXPRESSION TAG	UNP P37945
F	777	HIS	-	EXPRESSION TAG	UNP P37945
F	778	HIS	-	EXPRESSION TAG	UNP P37945
F	779	HIS	-	EXPRESSION TAG	UNP P37945
F	780	HIS	-	EXPRESSION TAG	UNP P37945
F	781	HIS	-	EXPRESSION TAG	UNP P37945
F	782	HIS	-	EXPRESSION TAG	UNP P37945

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).

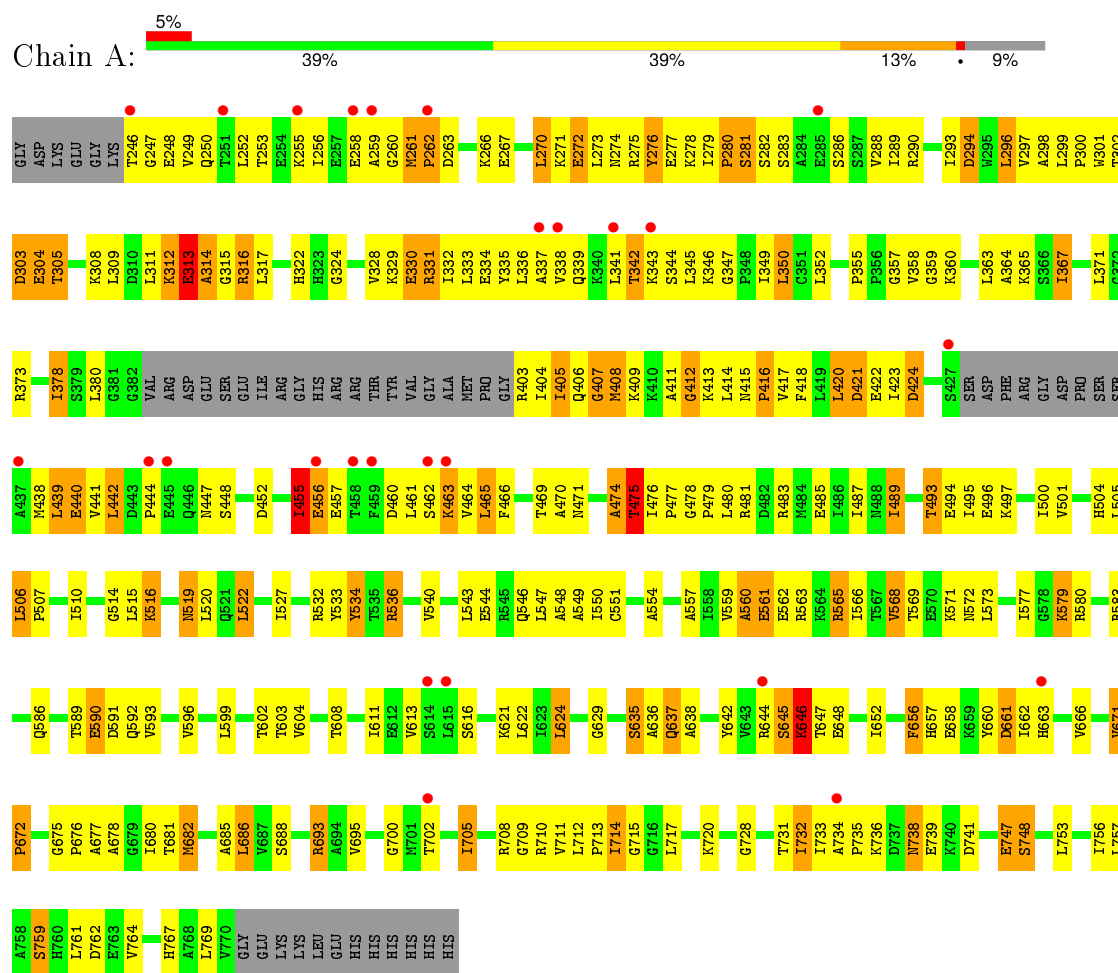


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	F	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

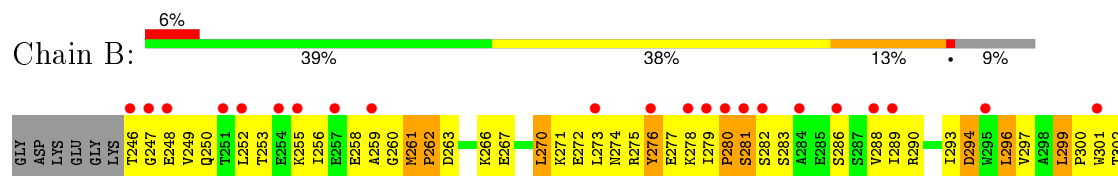
### 3 Residue-property plots

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: ATP-dependent protease La 1



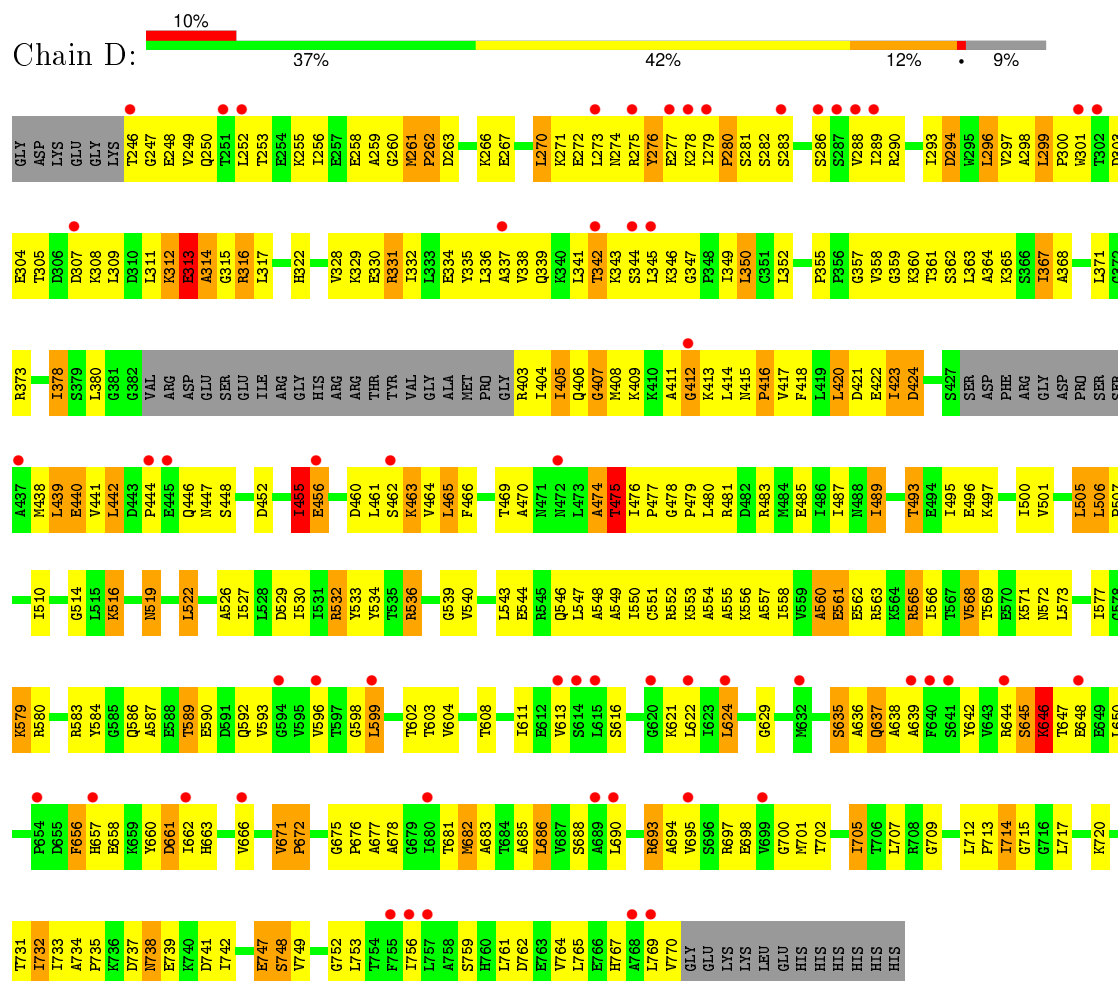
#### • Molecule 1: ATP-dependent protease La 1



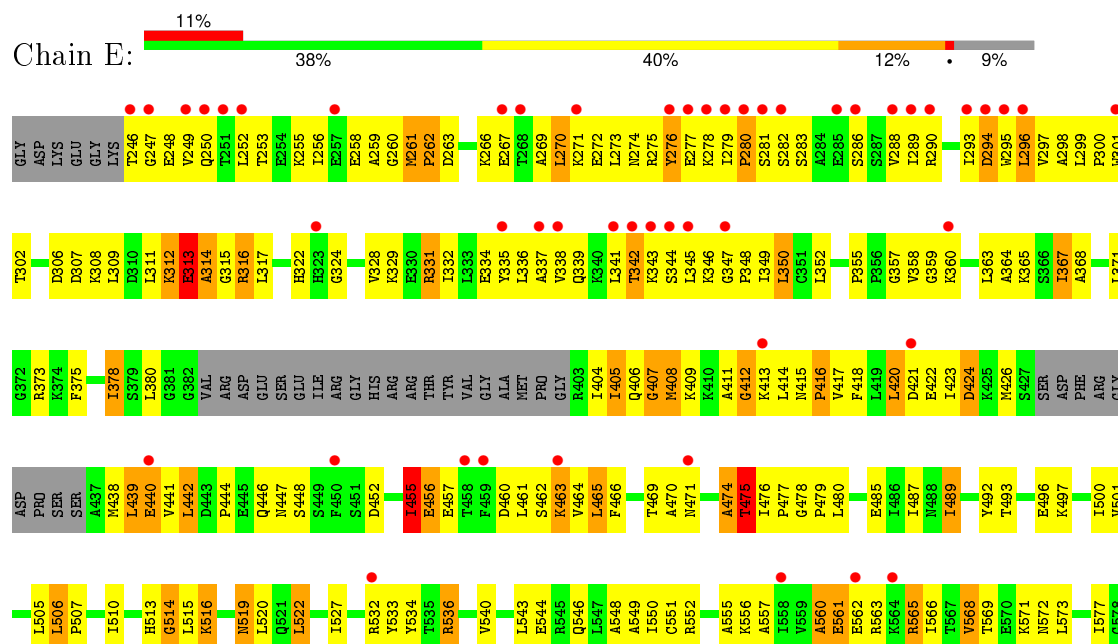


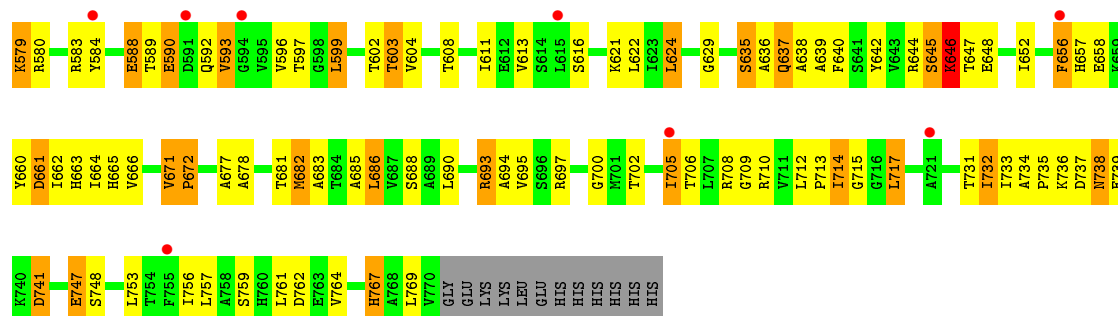


- Molecule 1: ATP-dependent protease La 1

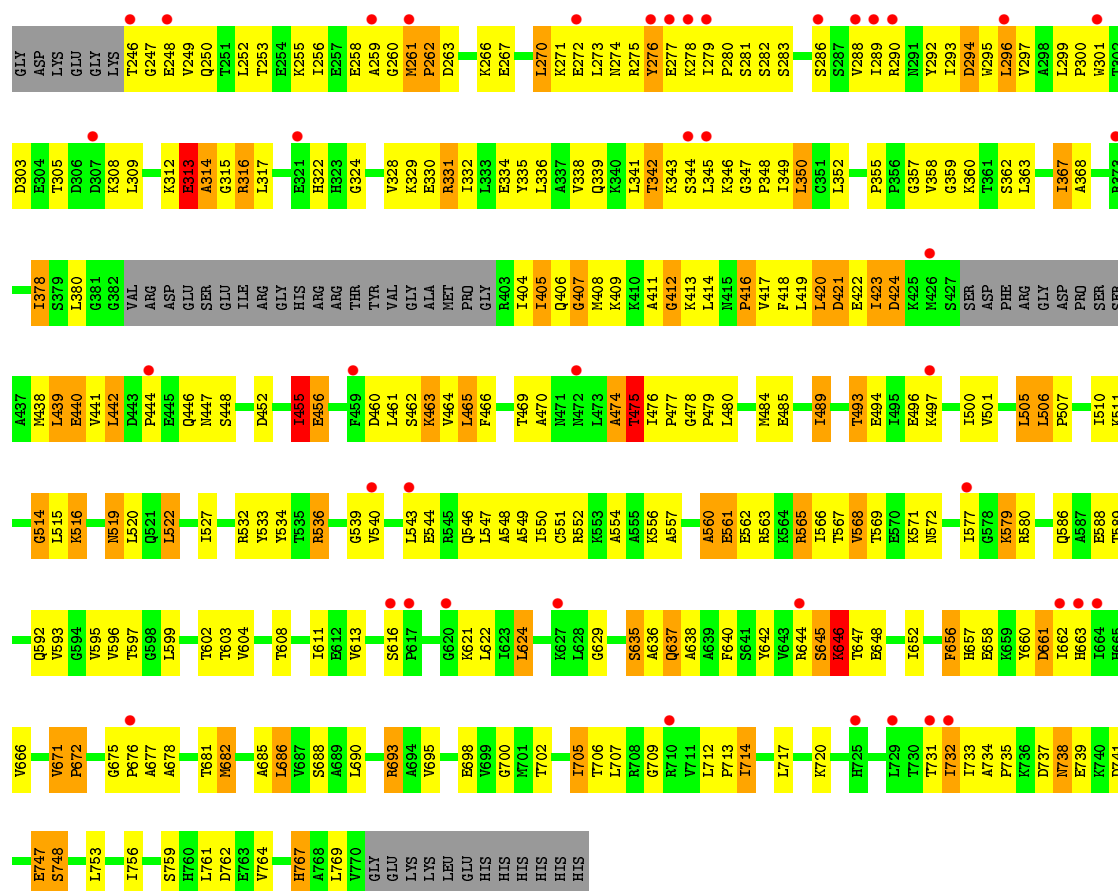


- Molecule 1: ATP-dependent protease La 1





• Molecule 1: ATP-dependent protease La 1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	103.38 Å 127.40 Å 148.99 Å 90.00° 100.50° 90.00°	Depositor
Resolution (Å)	29.91 – 3.40 58.42 – 3.40	Depositor EDS
% Data completeness (in resolution range)	98.7 (29.91-3.40) 99.6 (58.42-3.40)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.09 (at 3.40 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.1_357)	Depositor
R, $R_{free}$	0.265 , 0.313 0.261 , 0.309	Depositor DCC
$R_{free}$ test set	2605 reflections (5.25%)	DCC
Wilson B-factor (Å <sup>2</sup> )	117.1	Xtriage
Anisotropy	0.202	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.22 , 131.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 52254 reflections	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	23196	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	194.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.59% 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 [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.49	0/3892	0.63	0/5246
1	B	0.47	0/3892	0.64	0/5246
1	C	0.45	0/3892	0.62	0/5246
1	D	0.51	0/3892	0.64	1/5246 (0.0%)
1	E	0.46	0/3892	0.63	0/5246
1	F	0.44	0/3892	0.63	1/5246 (0.0%)
All	All	0.47	0/23352	0.63	2/31476 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	505	LEU	CB-CG-CD2	-5.66	101.37	111.00
1	F	505	LEU	CB-CG-CD2	-5.54	101.58	111.00

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	3839	0	3968	297	0
1	B	3839	0	3968	324	0
1	C	3839	0	3968	317	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	3839	0	3968	300	1
1	E	3839	0	3968	308	0
1	F	3839	0	3968	287	1
2	A	27	0	12	7	0
2	B	27	0	12	7	0
2	C	27	0	12	6	0
2	D	27	0	12	11	0
2	E	27	0	12	6	0
2	F	27	0	12	7	0
All	All	23196	0	23880	1793	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 38.

All (1793) 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:F:493:THR:HG21	1:F:748:SER:HB2	1.26	1.08
1:B:552:ARG:HG3	1:E:338:VAL:HG21	1.31	1.08
1:C:350:LEU:HD12	1:C:350:LEU:H	1.18	1.02
1:B:337:ALA:CB	1:F:556:LYS:HA	1.89	1.02
1:A:501:VAL:HG11	1:A:527:ILE:HD13	1.39	1.01
1:F:501:VAL:HG11	1:F:527:ILE:HD13	1.42	0.97
1:B:350:LEU:H	1:B:350:LEU:HD12	1.28	0.96
1:B:501:VAL:HG11	1:B:527:ILE:HD13	1.48	0.95
1:D:501:VAL:HG11	1:D:527:ILE:HD13	1.49	0.95
1:F:586:GLN:HG2	1:F:698:GLU:HG2	1.46	0.93
1:C:569:THR:HG23	1:C:571:LYS:H	1.33	0.93
1:A:350:LEU:HD12	1:A:350:LEU:H	1.31	0.93
1:A:378:ILE:O	1:A:378:ILE:HG12	1.69	0.93
1:A:596:VAL:HG22	1:A:695:VAL:HG21	1.48	0.92
1:E:671:VAL:HG22	1:E:672:PRO:HD2	1.51	0.91
1:F:671:VAL:HG22	1:F:672:PRO:HD2	1.49	0.91
1:B:493:THR:HG21	1:B:748:SER:HB2	1.50	0.91
1:E:501:VAL:HG11	1:E:527:ILE:HD13	1.51	0.91
1:B:378:ILE:O	1:B:378:ILE:HG12	1.69	0.91
1:E:350:LEU:HD12	1:E:350:LEU:H	1.32	0.91
1:F:586:GLN:HE21	1:F:698:GLU:HA	1.38	0.89
1:E:536:ARG:HH11	1:E:536:ARG:HG3	1.35	0.89
1:D:350:LEU:H	1:D:350:LEU:HD12	1.36	0.88
1:C:501:VAL:HG11	1:C:527:ILE:HD13	1.55	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:404:ILE:HG23	1:D:418:PHE:CE2	2.08	0.88
1:C:536:ARG:HG3	1:C:536:ARG:HH11	1.37	0.88
1:C:671:VAL:HG22	1:C:672:PRO:HD2	1.55	0.88
1:A:569:THR:HG23	1:A:571:LYS:H	1.37	0.88
1:C:337:ALA:CB	1:E:556:LYS:HA	2.03	0.87
1:C:596:VAL:HG22	1:C:695:VAL:HG21	1.56	0.87
1:D:359:GLY:HA2	2:D:783:ADP:C5'	2.04	0.87
1:B:536:ARG:HH11	1:B:536:ARG:HG3	1.40	0.87
1:F:569:THR:HG23	1:F:571:LYS:H	1.37	0.87
1:D:688:SER:HB2	1:D:769:LEU:HD21	1.55	0.87
1:E:569:THR:HG23	1:E:571:LYS:H	1.39	0.87
1:D:671:VAL:HG22	1:D:672:PRO:HD2	1.57	0.86
1:A:536:ARG:HG3	1:A:536:ARG:HH11	1.40	0.86
1:B:569:THR:HG23	1:B:571:LYS:H	1.39	0.86
1:D:536:ARG:HH11	1:D:536:ARG:HG3	1.39	0.86
1:D:378:ILE:HG12	1:D:378:ILE:O	1.74	0.86
1:D:493:THR:HG21	1:D:748:SER:HB2	1.58	0.85
1:E:688:SER:HB2	1:E:769:LEU:HD21	1.56	0.85
1:F:536:ARG:HG3	1:F:536:ARG:HH11	1.42	0.85
1:F:596:VAL:HG22	1:F:695:VAL:HG21	1.58	0.85
1:E:378:ILE:HG12	1:E:378:ILE:O	1.77	0.84
1:B:522:LEU:HD12	1:B:527:ILE:HG12	1.60	0.84
1:D:596:VAL:HG22	1:D:695:VAL:HG21	1.60	0.84
1:D:569:THR:HG23	1:D:571:LYS:H	1.40	0.83
1:A:671:VAL:HG22	1:A:672:PRO:HD2	1.60	0.83
1:C:688:SER:HB2	1:C:769:LEU:HD21	1.59	0.83
1:E:596:VAL:HG22	1:E:695:VAL:HG21	1.60	0.83
1:F:516:LYS:HA	1:F:516:LYS:NZ	1.93	0.83
1:F:360:LYS:HD2	1:F:469:THR:HG23	1.60	0.83
1:B:733:ILE:HG21	1:B:764:VAL:HG13	1.58	0.82
1:A:733:ILE:HG21	1:A:764:VAL:HG13	1.62	0.82
1:D:733:ILE:HG21	1:D:764:VAL:HG13	1.62	0.81
1:F:378:ILE:HG12	1:F:378:ILE:O	1.80	0.81
1:B:516:LYS:O	1:B:519:ASN:HB2	1.80	0.81
1:C:536:ARG:HH11	1:C:536:ARG:CG	1.93	0.81
1:F:688:SER:HB2	1:F:769:LEU:HD21	1.63	0.81
1:F:404:ILE:HG23	1:F:418:PHE:CE2	2.16	0.81
1:A:411:ALA:O	1:A:413:LYS:N	2.14	0.81
1:C:501:VAL:HA	1:C:505:LEU:HB2	1.62	0.81
1:F:516:LYS:O	1:F:519:ASN:HB2	1.81	0.80
1:A:522:LEU:HD12	1:A:527:ILE:HG12	1.60	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:522:LEU:HB3	1:F:568:VAL:HG13	1.64	0.80
1:C:522:LEU:HB3	1:C:568:VAL:HG13	1.62	0.80
1:F:733:ILE:HG21	1:F:764:VAL:HG13	1.63	0.80
1:E:439:LEU:H	1:E:439:LEU:HD22	1.44	0.79
1:F:522:LEU:HD12	1:F:527:ILE:HG12	1.65	0.79
1:F:506:LEU:HD21	1:F:522:LEU:HD21	1.65	0.79
1:D:536:ARG:HH11	1:D:536:ARG:CG	1.96	0.79
1:C:506:LEU:HD21	1:C:522:LEU:HD21	1.65	0.79
1:A:337:ALA:CB	1:C:556:LYS:HA	2.12	0.79
1:C:404:ILE:HG23	1:C:418:PHE:CE2	2.17	0.79
1:C:439:LEU:H	1:C:439:LEU:HD22	1.47	0.79
1:D:522:LEU:HD12	1:D:527:ILE:HG12	1.65	0.79
1:E:536:ARG:HH11	1:E:536:ARG:CG	1.96	0.79
1:F:411:ALA:O	1:F:413:LYS:N	2.17	0.78
1:C:337:ALA:HB1	1:E:556:LYS:HA	1.64	0.78
1:B:501:VAL:HA	1:B:505:LEU:HB2	1.65	0.78
1:A:536:ARG:CG	1:A:536:ARG:HH11	1.97	0.78
1:A:338:VAL:HG21	1:C:552:ARG:HG3	1.63	0.78
1:E:404:ILE:HG23	1:E:418:PHE:CE2	2.19	0.78
1:B:337:ALA:HB1	1:F:556:LYS:HA	1.63	0.78
1:B:536:ARG:HH11	1:B:536:ARG:CG	1.96	0.78
1:E:414:LEU:O	1:E:416:PRO:HD3	1.83	0.78
1:B:688:SER:HB2	1:B:769:LEU:HD21	1.64	0.78
1:F:359:GLY:HA2	2:F:783:ADP:O5'	1.84	0.78
1:E:411:ALA:O	1:E:413:LYS:N	2.18	0.77
1:D:411:ALA:O	1:D:413:LYS:N	2.18	0.77
1:B:282:SER:HB2	1:E:276:TYR:OH	1.82	0.77
1:E:584:TYR:O	1:E:584:TYR:CD1	2.37	0.77
1:B:671:VAL:HG22	1:B:672:PRO:HD2	1.66	0.77
1:B:411:ALA:O	1:B:413:LYS:N	2.17	0.77
1:D:522:LEU:HB3	1:D:568:VAL:HG13	1.65	0.77
1:C:414:LEU:O	1:C:416:PRO:HD3	1.85	0.77
1:A:456:GLU:CD	1:C:291:ASN:HD21	1.88	0.77
1:D:359:GLY:HA2	2:D:783:ADP:O5'	1.85	0.76
1:C:270:LEU:HD21	1:C:296:LEU:HD22	1.66	0.76
1:A:404:ILE:HG23	1:A:418:PHE:CE2	2.20	0.76
1:B:596:VAL:HG22	1:B:695:VAL:HG21	1.66	0.76
1:A:272:GLU:HB3	1:C:248:GLU:OE1	1.85	0.76
1:B:303:ASP:O	1:B:304:GLU:HB2	1.86	0.76
1:B:506:LEU:HB3	1:B:507:PRO:HD3	1.68	0.75
1:C:411:ALA:O	1:C:413:LYS:N	2.18	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:439:LEU:H	1:B:439:LEU:HD22	1.51	0.75
1:A:273:LEU:HD11	1:C:290:ARG:HH12	1.50	0.75
1:B:506:LEU:HD21	1:B:522:LEU:HD21	1.68	0.75
1:E:516:LYS:O	1:E:519:ASN:HB2	1.86	0.75
1:D:359:GLY:HA2	2:D:783:ADP:H5'2	1.69	0.75
1:E:733:ILE:HG21	1:E:764:VAL:HG13	1.67	0.75
1:D:439:LEU:HD22	1:D:439:LEU:H	1.50	0.75
1:A:439:LEU:H	1:A:439:LEU:HD22	1.51	0.74
1:C:733:ILE:HG21	1:C:764:VAL:HG13	1.68	0.74
1:F:350:LEU:H	1:F:350:LEU:HD12	1.51	0.74
1:F:439:LEU:H	1:F:439:LEU:HD22	1.53	0.74
1:D:505:LEU:HD22	1:D:544:GLU:HG3	1.70	0.74
1:F:536:ARG:CG	1:F:536:ARG:HH11	1.99	0.74
1:E:270:LEU:HD21	1:E:296:LEU:HD22	1.70	0.74
1:C:493:THR:HG21	1:C:748:SER:HB2	1.70	0.74
1:B:359:GLY:HA2	2:B:783:ADP:O5'	1.88	0.74
1:E:738:ASN:O	1:E:741:ASP:HB2	1.88	0.74
1:A:505:LEU:HD22	1:A:544:GLU:HG3	1.68	0.73
1:C:516:LYS:NZ	1:C:516:LYS:HA	2.02	0.73
1:C:522:LEU:HD12	1:C:527:ILE:HG12	1.70	0.73
1:A:688:SER:HB2	1:A:769:LEU:HD21	1.69	0.73
1:E:583:ARG:HD3	1:E:588:GLU:CD	2.08	0.73
1:E:506:LEU:HD21	1:E:522:LEU:HD21	1.70	0.73
1:D:404:ILE:HG23	1:D:418:PHE:HE2	1.53	0.73
1:A:516:LYS:O	1:A:519:ASN:HB2	1.89	0.73
1:A:270:LEU:HD21	1:A:296:LEU:HD22	1.70	0.73
1:C:602:THR:HG22	1:C:604:VAL:H	1.54	0.72
1:F:501:VAL:CG1	1:F:527:ILE:HD13	2.19	0.72
1:D:738:ASN:O	1:D:741:ASP:HB2	1.89	0.72
1:A:501:VAL:CG1	1:A:527:ILE:HD13	2.17	0.72
1:F:516:LYS:HA	1:F:516:LYS:CE	2.19	0.72
1:A:522:LEU:HB3	1:A:568:VAL:HG13	1.72	0.72
1:F:493:THR:HG21	1:F:748:SER:CB	2.15	0.72
1:B:420:LEU:H	1:B:420:LEU:HD22	1.54	0.72
1:B:347:GLY:HA3	1:B:444:PRO:HG3	1.72	0.72
1:C:332:ILE:HD12	1:C:367:ILE:HD11	1.72	0.72
1:B:404:ILE:HG23	1:B:418:PHE:CE2	2.25	0.72
1:C:359:GLY:HA2	2:C:783:ADP:O5'	1.90	0.72
1:E:501:VAL:HA	1:E:505:LEU:HB2	1.72	0.71
1:F:270:LEU:HD21	1:F:296:LEU:HD22	1.71	0.71
1:D:270:LEU:HD21	1:D:296:LEU:HD22	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:677:ALA:HA	1:D:714:ILE:HD11	1.72	0.71
1:A:677:ALA:HA	1:A:714:ILE:HD11	1.72	0.71
1:B:501:VAL:CG1	1:B:527:ILE:HD13	2.20	0.71
1:D:586:GLN:OE1	1:D:586:GLN:HA	1.90	0.71
1:C:677:ALA:HA	1:C:714:ILE:HD11	1.72	0.71
1:F:347:GLY:HA3	1:F:444:PRO:HG3	1.71	0.71
1:A:559:VAL:HG21	1:D:337:ALA:HB1	1.72	0.71
1:C:506:LEU:HB3	1:C:507:PRO:HD3	1.72	0.71
1:D:347:GLY:HA3	1:D:444:PRO:HG3	1.71	0.71
1:D:501:VAL:HA	1:D:505:LEU:HB2	1.71	0.71
1:E:300:PRO:HB2	1:E:414:LEU:HB3	1.71	0.71
1:F:506:LEU:HB3	1:F:507:PRO:HD3	1.71	0.71
1:B:505:LEU:HD22	1:B:544:GLU:HG3	1.72	0.71
1:C:267:GLU:HA	1:C:270:LEU:HD12	1.73	0.70
1:D:506:LEU:HD21	1:D:522:LEU:HD21	1.72	0.70
1:E:506:LEU:HB3	1:E:507:PRO:HD3	1.72	0.70
1:B:274:ASN:C	1:B:276:TYR:H	1.94	0.70
1:E:352:LEU:HD22	1:E:489:ILE:HD11	1.73	0.70
1:E:522:LEU:HD12	1:E:527:ILE:HG12	1.73	0.70
1:A:271:LYS:HA	1:A:274:ASN:HB3	1.74	0.70
1:B:267:GLU:HA	1:B:270:LEU:HD12	1.72	0.70
1:E:271:LYS:HA	1:E:274:ASN:HB3	1.72	0.70
1:C:378:ILE:O	1:C:378:ILE:HG12	1.92	0.70
1:B:602:THR:HG22	1:B:604:VAL:H	1.56	0.70
1:D:506:LEU:HB3	1:D:507:PRO:HD3	1.74	0.70
1:D:602:THR:HG22	1:D:604:VAL:H	1.56	0.70
1:C:505:LEU:HD22	1:C:544:GLU:HG3	1.74	0.70
1:F:271:LYS:HA	1:F:274:ASN:HB3	1.73	0.70
1:D:420:LEU:HD22	1:D:420:LEU:H	1.57	0.70
1:A:347:GLY:HA3	1:A:444:PRO:HG3	1.73	0.70
1:D:271:LYS:HA	1:D:274:ASN:HB3	1.74	0.70
1:A:337:ALA:HB1	1:C:556:LYS:HA	1.71	0.70
1:D:702:THR:O	1:D:735:PRO:HD3	1.90	0.70
1:F:671:VAL:CG2	1:F:672:PRO:HD2	2.22	0.70
1:B:569:THR:H	1:B:572:ASN:HB2	1.56	0.70
1:F:441:VAL:HG13	1:F:442:LEU:HG	1.73	0.70
1:C:347:GLY:HA3	1:C:444:PRO:HG3	1.73	0.70
1:C:271:LYS:HA	1:C:274:ASN:HB3	1.74	0.70
1:C:350:LEU:N	1:C:350:LEU:HD12	1.98	0.69
1:D:266:LYS:HG3	1:D:267:GLU:N	2.07	0.69
1:F:501:VAL:HA	1:F:505:LEU:HB2	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:737:ASP:HB3	1:E:583:ARG:HH12	1.57	0.69
1:C:516:LYS:O	1:C:519:ASN:HB2	1.92	0.69
1:C:349:ILE:HD12	1:C:349:ILE:O	1.92	0.69
1:B:338:VAL:HG21	1:F:552:ARG:HG3	1.74	0.69
1:E:274:ASN:C	1:E:276:TYR:H	1.96	0.69
1:A:441:VAL:HG13	1:A:442:LEU:HG	1.75	0.69
1:B:421:ASP:O	1:B:469:THR:HB	1.92	0.69
1:B:271:LYS:HA	1:B:274:ASN:HB3	1.74	0.69
1:A:506:LEU:HD12	1:A:510:ILE:HG12	1.74	0.69
1:F:267:GLU:HA	1:F:270:LEU:HD12	1.75	0.69
1:B:677:ALA:HA	1:B:714:ILE:HD11	1.72	0.69
1:D:274:ASN:C	1:D:276:TYR:H	1.96	0.69
1:D:464:VAL:O	1:D:466:PHE:HD1	1.76	0.69
1:F:464:VAL:O	1:F:466:PHE:HD1	1.76	0.69
1:B:516:LYS:HA	1:B:516:LYS:NZ	2.08	0.69
1:C:266:LYS:HG3	1:C:267:GLU:N	2.08	0.69
1:D:516:LYS:NZ	1:D:516:LYS:HA	2.07	0.69
1:E:347:GLY:HA3	1:E:444:PRO:HG3	1.73	0.69
1:D:414:LEU:O	1:D:416:PRO:HD3	1.93	0.69
1:F:274:ASN:C	1:F:276:TYR:H	1.96	0.69
1:D:421:ASP:O	1:D:469:THR:HB	1.92	0.69
1:B:464:VAL:O	1:B:466:PHE:HD1	1.76	0.69
1:B:522:LEU:HB3	1:B:568:VAL:HG13	1.73	0.68
1:D:532:ARG:HG2	1:D:584:TYR:CE2	2.28	0.68
1:C:274:ASN:C	1:C:276:TYR:H	1.97	0.68
1:A:501:VAL:HA	1:A:505:LEU:HB2	1.74	0.68
1:C:256:ILE:HD11	1:C:293:ILE:HD11	1.76	0.68
1:E:516:LYS:NZ	1:E:516:LYS:HA	2.08	0.68
1:F:424:ASP:HB2	1:F:475:THR:HG23	1.76	0.68
1:B:556:LYS:HA	1:E:337:ALA:HB1	1.75	0.68
1:F:295:TRP:CZ3	1:F:405:ILE:HG21	2.28	0.68
1:F:266:LYS:HG3	1:F:267:GLU:N	2.08	0.68
1:B:337:ALA:HB3	1:F:556:LYS:HA	1.75	0.68
1:E:335:TYR:HE2	1:E:465:LEU:HD21	1.57	0.68
1:E:420:LEU:H	1:E:420:LEU:HD22	1.58	0.68
1:E:505:LEU:HD22	1:E:544:GLU:HG3	1.75	0.68
1:C:506:LEU:HD12	1:C:510:ILE:HG12	1.76	0.68
1:A:516:LYS:HA	1:A:516:LYS:NZ	2.09	0.68
1:F:738:ASN:O	1:F:741:ASP:HB2	1.94	0.67
1:E:421:ASP:O	1:E:469:THR:HB	1.94	0.67
1:E:646:LYS:H	1:E:646:LYS:HD2	1.58	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:702:THR:O	1:E:735:PRO:HD3	1.94	0.67
1:F:506:LEU:HD12	1:F:510:ILE:HG12	1.77	0.67
1:A:464:VAL:O	1:A:466:PHE:HD1	1.76	0.67
1:F:420:LEU:HD22	1:F:420:LEU:H	1.58	0.67
1:E:266:LYS:HG3	1:E:267:GLU:N	2.09	0.67
1:A:420:LEU:HD21	1:A:466:PHE:HD2	1.59	0.67
1:A:267:GLU:HA	1:A:270:LEU:HD12	1.75	0.67
1:A:274:ASN:C	1:A:276:TYR:H	1.96	0.67
1:F:505:LEU:HD22	1:F:544:GLU:HG3	1.77	0.67
1:A:266:LYS:HG3	1:A:267:GLU:N	2.09	0.67
1:C:317:LEU:HD23	1:C:317:LEU:O	1.94	0.67
1:B:556:LYS:HA	1:E:337:ALA:CB	2.24	0.67
1:B:270:LEU:HD21	1:B:296:LEU:HD22	1.75	0.67
1:E:464:VAL:O	1:E:466:PHE:HD1	1.77	0.67
1:E:671:VAL:CG2	1:E:672:PRO:HD2	2.23	0.67
1:E:267:GLU:HA	1:E:270:LEU:HD12	1.77	0.67
1:B:702:THR:O	1:B:735:PRO:HD3	1.94	0.67
1:D:441:VAL:HG13	1:D:442:LEU:HG	1.76	0.67
1:D:501:VAL:CG1	1:D:527:ILE:HD13	2.24	0.66
1:D:267:GLU:HA	1:D:270:LEU:HD12	1.76	0.66
1:A:506:LEU:HB3	1:A:507:PRO:HD3	1.75	0.66
1:C:702:THR:O	1:C:735:PRO:HD3	1.95	0.66
1:C:424:ASP:HB2	1:C:475:THR:HG23	1.77	0.66
1:E:441:VAL:HG13	1:E:442:LEU:HG	1.78	0.66
1:A:702:THR:O	1:A:735:PRO:HD3	1.96	0.66
1:F:702:THR:O	1:F:735:PRO:HD3	1.96	0.66
1:B:266:LYS:HG3	1:B:267:GLU:N	2.09	0.66
1:F:421:ASP:O	1:F:469:THR:HB	1.96	0.66
2:C:783:ADP:O1B	2:C:783:ADP:O1A	2.14	0.66
1:D:646:LYS:H	1:D:646:LYS:HD2	1.60	0.66
1:B:414:LEU:O	1:B:416:PRO:HD3	1.96	0.66
1:C:501:VAL:CG1	1:C:527:ILE:HD13	2.26	0.66
1:D:569:THR:H	1:D:572:ASN:HB2	1.61	0.66
1:F:677:ALA:HA	1:F:714:ILE:HD11	1.78	0.66
1:C:258:GLU:HG2	1:C:260:GLY:H	1.60	0.66
1:D:505:LEU:CD2	1:D:544:GLU:HG3	2.25	0.66
1:E:506:LEU:HD12	1:E:510:ILE:HG12	1.76	0.66
1:D:424:ASP:HB2	1:D:475:THR:HG23	1.77	0.65
1:F:474:ALA:O	1:F:476:ILE:N	2.29	0.65
1:A:252:LEU:O	1:A:256:ILE:HG13	1.97	0.65
1:A:258:GLU:HG2	1:A:260:GLY:H	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:345:LEU:HD23	1:B:346:LYS:N	2.12	0.65
1:A:644:ARG:HD2	1:C:616:SER:OG	1.96	0.65
1:E:522:LEU:HB3	1:E:568:VAL:HG13	1.77	0.65
1:E:345:LEU:HD11	1:E:465:LEU:HD22	1.78	0.65
1:E:677:ALA:HA	1:E:714:ILE:HD11	1.77	0.65
1:E:474:ALA:O	1:E:476:ILE:N	2.28	0.65
1:A:602:THR:HG22	1:A:604:VAL:H	1.61	0.65
1:F:292:TYR:CZ	1:F:455:ILE:HA	2.31	0.65
1:C:335:TYR:HE2	1:C:465:LEU:HD21	1.61	0.65
1:F:646:LYS:HD2	1:F:646:LYS:H	1.61	0.65
1:C:474:ALA:O	1:C:476:ILE:N	2.30	0.65
1:F:300:PRO:HB2	1:F:414:LEU:HB3	1.79	0.65
1:F:579:LYS:O	1:F:579:LYS:HE2	1.96	0.65
1:C:420:LEU:HD21	1:C:466:PHE:HD2	1.61	0.65
1:A:421:ASP:O	1:A:469:THR:HB	1.96	0.65
1:F:352:LEU:HD22	1:F:489:ILE:HD11	1.77	0.65
1:A:579:LYS:HE2	1:A:579:LYS:O	1.96	0.65
1:C:464:VAL:O	1:C:466:PHE:HD1	1.80	0.65
1:F:252:LEU:O	1:F:256:ILE:HG13	1.97	0.65
1:A:332:ILE:HD12	1:A:367:ILE:HD11	1.79	0.65
1:B:352:LEU:HD22	1:B:489:ILE:HD11	1.79	0.65
1:E:349:ILE:HD12	1:E:349:ILE:O	1.97	0.65
1:B:299:LEU:HD12	1:B:301:TRP:HE1	1.62	0.64
1:C:362:SER:HB2	2:C:783:ADP:H5'1	1.78	0.64
1:A:424:ASP:HB2	1:A:475:THR:HG23	1.77	0.64
1:C:646:LYS:HD2	1:C:646:LYS:H	1.61	0.64
1:A:414:LEU:O	1:A:416:PRO:HD3	1.96	0.64
1:E:252:LEU:O	1:E:256:ILE:HG13	1.98	0.64
1:C:599:LEU:HD22	1:C:599:LEU:H	1.62	0.64
1:F:345:LEU:HD11	1:F:465:LEU:HD22	1.79	0.64
1:A:506:LEU:HD21	1:A:522:LEU:HD21	1.78	0.64
1:F:569:THR:H	1:F:572:ASN:HB2	1.62	0.64
1:A:477:PRO:HB2	1:A:480:LEU:HD23	1.79	0.64
1:D:252:LEU:O	1:D:256:ILE:HG13	1.98	0.64
1:C:644:ARG:HE	1:C:657:HIS:CG	2.16	0.64
1:D:256:ILE:HD11	1:D:293:ILE:HD11	1.79	0.64
1:B:258:GLU:HG2	1:B:259:ALA:N	2.13	0.64
1:B:252:LEU:O	1:B:256:ILE:HG13	1.98	0.64
1:F:414:LEU:O	1:F:416:PRO:HD3	1.97	0.64
1:B:258:GLU:HG2	1:B:260:GLY:H	1.62	0.64
1:E:644:ARG:HE	1:E:657:HIS:CG	2.16	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:644:ARG:HE	1:F:657:HIS:CG	2.15	0.64
1:B:267:GLU:O	1:B:270:LEU:HB2	1.98	0.64
1:E:588:GLU:HG2	1:E:589:THR:N	2.13	0.64
1:B:424:ASP:HB2	1:B:475:THR:HG23	1.79	0.64
1:A:646:LYS:HD2	1:A:646:LYS:H	1.62	0.64
1:E:569:THR:H	1:E:572:ASN:HB2	1.62	0.64
1:F:258:GLU:HG2	1:F:260:GLY:H	1.61	0.64
1:B:493:THR:HG21	1:B:748:SER:CB	2.27	0.64
1:C:267:GLU:O	1:C:270:LEU:HB2	1.97	0.64
1:C:360:LYS:HD2	1:C:469:THR:HG23	1.80	0.64
1:D:506:LEU:HD12	1:D:510:ILE:HG12	1.79	0.63
1:C:671:VAL:CG2	1:C:672:PRO:HD2	2.26	0.63
1:E:258:GLU:HG2	1:E:260:GLY:H	1.62	0.63
1:B:644:ARG:HE	1:B:657:HIS:CG	2.16	0.63
1:D:345:LEU:HD11	1:D:465:LEU:HD22	1.79	0.63
1:D:258:GLU:HG2	1:D:260:GLY:H	1.61	0.63
1:E:253:THR:HA	1:E:256:ILE:HD12	1.79	0.63
1:E:256:ILE:HD11	1:E:293:ILE:HD11	1.80	0.63
1:E:501:VAL:CG1	1:E:527:ILE:HD13	2.26	0.63
1:E:249:VAL:HG12	1:E:278:LYS:HG2	1.81	0.63
1:B:296:LEU:HA	1:B:299:LEU:HD21	1.79	0.63
1:A:644:ARG:HE	1:A:657:HIS:CG	2.16	0.63
1:B:583:ARG:NH1	1:E:737:ASP:OD1	2.31	0.63
1:E:424:ASP:HB2	1:E:475:THR:HG23	1.81	0.63
1:A:493:THR:HG21	1:A:748:SER:HB2	1.81	0.63
1:A:412:GLY:O	1:A:413:LYS:HG2	1.98	0.63
1:B:412:GLY:O	1:B:413:LYS:HG2	1.99	0.63
1:C:420:LEU:H	1:C:420:LEU:HD22	1.64	0.63
1:B:444:PRO:HA	1:B:447:ASN:HD21	1.64	0.63
1:F:253:THR:HA	1:F:256:ILE:HD12	1.81	0.63
1:B:493:THR:CG2	1:B:748:SER:HB2	2.25	0.63
1:E:412:GLY:O	1:E:413:LYS:HG2	1.99	0.63
1:A:444:PRO:HA	1:A:447:ASN:HD21	1.64	0.63
1:F:412:GLY:O	1:F:413:LYS:HG2	1.98	0.63
1:D:300:PRO:HB3	1:D:412:GLY:C	2.20	0.63
1:F:256:ILE:HD11	1:F:293:ILE:HD11	1.80	0.63
1:C:421:ASP:O	1:C:469:THR:HB	1.98	0.63
1:C:350:LEU:CD1	1:C:350:LEU:H	1.98	0.62
1:A:256:ILE:HD11	1:A:293:ILE:HD11	1.81	0.62
1:C:258:GLU:HG2	1:C:259:ALA:N	2.14	0.62
1:A:317:LEU:O	1:A:317:LEU:HD23	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:THR:HA	1:A:256:ILE:HD12	1.80	0.62
1:A:360:LYS:HD2	1:A:469:THR:HG23	1.80	0.62
1:B:506:LEU:HD12	1:B:506:LEU:C	2.20	0.62
1:A:345:LEU:HD11	1:A:465:LEU:HD22	1.82	0.62
1:B:332:ILE:HD12	1:B:367:ILE:HD11	1.80	0.62
1:F:477:PRO:HB2	1:F:480:LEU:HD23	1.82	0.62
1:D:332:ILE:HD12	1:D:367:ILE:HD11	1.80	0.62
1:C:252:LEU:O	1:C:256:ILE:HG13	1.99	0.62
1:A:738:ASN:O	1:A:741:ASP:HB2	2.00	0.62
1:C:345:LEU:HD23	1:C:346:LYS:N	2.15	0.62
1:B:315:GLY:C	1:B:316:ARG:HD2	2.20	0.62
1:E:477:PRO:HB2	1:E:480:LEU:HD23	1.81	0.62
1:B:299:LEU:CD1	1:B:301:TRP:HE1	2.12	0.62
1:B:277:GLU:HB3	1:B:279:ILE:O	1.99	0.62
1:A:352:LEU:HD22	1:A:489:ILE:HD11	1.81	0.62
1:D:412:GLY:O	1:D:413:LYS:HG2	1.99	0.62
1:F:613:VAL:HA	1:F:663:HIS:O	2.00	0.62
1:D:345:LEU:HD23	1:D:346:LYS:N	2.15	0.62
1:D:249:VAL:HG12	1:D:278:LYS:HG2	1.81	0.62
1:C:253:THR:HA	1:C:256:ILE:HD12	1.82	0.62
1:B:256:ILE:HD11	1:B:293:ILE:HD11	1.82	0.61
1:A:569:THR:H	1:A:572:ASN:HB2	1.64	0.61
1:A:734:ALA:HB1	1:A:735:PRO:HD2	1.82	0.61
1:D:258:GLU:HG2	1:D:259:ALA:N	2.15	0.61
1:F:602:THR:HG22	1:F:604:VAL:H	1.64	0.61
1:A:315:GLY:C	1:A:316:ARG:HD2	2.20	0.61
1:D:671:VAL:CG2	1:D:672:PRO:HD2	2.28	0.61
1:C:412:GLY:O	1:C:413:LYS:HG2	1.99	0.61
1:F:444:PRO:HA	1:F:447:ASN:HD21	1.66	0.61
1:E:734:ALA:HB1	1:E:735:PRO:HD2	1.82	0.61
1:B:474:ALA:O	1:B:476:ILE:N	2.33	0.61
1:B:360:LYS:HD2	1:B:469:THR:HG23	1.82	0.61
1:D:644:ARG:HE	1:D:657:HIS:CG	2.17	0.61
1:B:646:LYS:HD2	1:B:646:LYS:H	1.64	0.61
1:F:368:ALA:HB2	1:F:417:VAL:HG21	1.82	0.61
1:B:441:VAL:HG13	1:B:442:LEU:HG	1.81	0.61
1:A:258:GLU:HG2	1:A:259:ALA:N	2.14	0.61
1:B:253:THR:HA	1:B:256:ILE:HD12	1.80	0.61
1:F:516:LYS:HA	1:F:516:LYS:HZ1	1.65	0.61
1:D:277:GLU:HB3	1:D:279:ILE:O	2.01	0.61
1:C:249:VAL:HG12	1:C:278:LYS:HG2	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:686:LEU:O	1:C:686:LEU:HD22	2.01	0.61
1:E:444:PRO:HA	1:E:447:ASN:HD21	1.66	0.61
1:D:565:ARG:HG2	1:D:566:ILE:N	2.14	0.61
1:D:315:GLY:C	1:D:316:ARG:HD2	2.21	0.61
1:A:474:ALA:O	1:A:476:ILE:N	2.33	0.61
1:B:506:LEU:HD12	1:B:510:ILE:HG12	1.81	0.61
1:C:277:GLU:HB3	1:C:279:ILE:O	2.01	0.61
1:A:249:VAL:HG12	1:A:278:LYS:HG2	1.82	0.61
1:B:565:ARG:HG2	1:B:566:ILE:N	2.14	0.61
1:E:533:TYR:HB3	1:E:580:ARG:HD2	1.83	0.61
1:B:613:VAL:HA	1:B:663:HIS:O	2.01	0.61
1:C:345:LEU:HD11	1:C:465:LEU:HD22	1.82	0.61
1:C:315:GLY:C	1:C:316:ARG:HD2	2.21	0.61
1:E:602:THR:HG22	1:E:604:VAL:H	1.64	0.61
1:F:540:VAL:HG23	2:F:783:ADP:H1'	1.82	0.60
1:F:345:LEU:HD23	1:F:346:LYS:N	2.16	0.60
1:D:253:THR:HA	1:D:256:ILE:HD12	1.81	0.60
1:F:258:GLU:HG2	1:F:259:ALA:N	2.14	0.60
1:E:258:GLU:HG2	1:E:259:ALA:N	2.15	0.60
1:D:474:ALA:O	1:D:476:ILE:N	2.34	0.60
1:A:300:PRO:HG3	1:A:412:GLY:C	2.22	0.60
1:F:277:GLU:HB3	1:F:279:ILE:O	2.02	0.60
1:D:349:ILE:O	1:D:349:ILE:HD12	2.01	0.60
1:B:360:LYS:N	2:B:783:ADP:O1B	2.34	0.60
1:F:249:VAL:HG12	1:F:278:LYS:HG2	1.82	0.60
1:B:261:MET:H	1:B:262:PRO:HD3	1.66	0.60
1:D:560:ALA:O	1:D:562:GLU:HG3	2.01	0.60
1:A:560:ALA:O	1:A:562:GLU:HG3	2.01	0.60
1:C:477:PRO:HB2	1:C:480:LEU:HD23	1.82	0.60
1:C:738:ASN:O	1:C:741:ASP:HB2	2.00	0.60
1:D:361:THR:HB	2:D:783:ADP:O1A	2.01	0.60
1:E:315:GLY:C	1:E:316:ARG:HD2	2.22	0.60
1:C:579:LYS:HE2	1:C:579:LYS:O	2.01	0.60
1:F:586:GLN:N	1:F:586:GLN:OE1	2.34	0.60
1:D:444:PRO:HA	1:D:447:ASN:HD21	1.67	0.60
1:B:738:ASN:O	1:B:741:ASP:HB2	2.00	0.60
1:B:345:LEU:HD11	1:B:465:LEU:HD22	1.82	0.60
1:F:565:ARG:HG2	1:F:566:ILE:N	2.16	0.60
1:B:359:GLY:HA2	2:B:783:ADP:C5'	2.31	0.60
1:F:261:MET:H	1:F:262:PRO:HD3	1.67	0.60
1:D:335:TYR:HE2	1:D:465:LEU:HD21	1.65	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:260:GLY:O	1:D:261:MET:HB2	2.02	0.60
1:B:560:ALA:O	1:B:562:GLU:HG3	2.02	0.60
1:F:357:GLY:O	1:F:539:GLY:CA	2.49	0.60
1:B:260:GLY:O	1:B:261:MET:HB2	2.02	0.60
1:D:261:MET:N	1:D:262:PRO:HD3	2.17	0.60
1:A:345:LEU:HD23	1:A:346:LYS:N	2.16	0.60
1:C:444:PRO:HA	1:C:447:ASN:HD21	1.66	0.60
1:C:469:THR:HG22	1:C:470:ALA:N	2.17	0.60
1:F:380:LEU:HB2	1:F:422:GLU:O	2.02	0.60
1:A:642:TYR:CD2	1:A:761:LEU:HD12	2.37	0.60
1:D:357:GLY:O	1:D:540:VAL:N	2.33	0.59
1:A:565:ARG:HG2	1:A:566:ILE:N	2.16	0.59
1:F:315:GLY:C	1:F:316:ARG:HD2	2.23	0.59
1:A:420:LEU:H	1:A:420:LEU:HD22	1.66	0.59
1:C:441:VAL:HG13	1:C:442:LEU:HG	1.83	0.59
1:F:357:GLY:N	2:F:783:ADP:O2B	2.35	0.59
1:A:267:GLU:O	1:A:270:LEU:HB2	2.02	0.59
1:E:345:LEU:HD23	1:E:346:LYS:N	2.17	0.59
1:E:416:PRO:HD2	1:E:464:VAL:HG13	1.84	0.59
1:C:602:THR:HG21	1:C:604:VAL:HG22	1.83	0.59
1:A:277:GLU:HB3	1:A:279:ILE:O	2.01	0.59
1:C:496:GLU:O	1:C:500:ILE:HG13	2.03	0.59
1:C:380:LEU:HB2	1:C:422:GLU:O	2.02	0.59
1:B:267:GLU:HA	1:B:270:LEU:CG	2.32	0.59
1:A:261:MET:N	1:A:262:PRO:HD3	2.17	0.59
1:E:261:MET:H	1:E:262:PRO:HD3	1.67	0.59
1:F:261:MET:N	1:F:262:PRO:HD3	2.18	0.59
1:F:328:VAL:O	1:F:332:ILE:HG12	2.02	0.59
1:C:516:LYS:CE	1:C:516:LYS:HA	2.33	0.59
1:F:267:GLU:O	1:F:270:LEU:HB2	2.03	0.59
1:E:261:MET:N	1:E:262:PRO:HD3	2.17	0.59
1:B:380:LEU:HD12	1:B:423:ILE:HG23	1.83	0.59
1:B:249:VAL:HG12	1:B:278:LYS:HG2	1.82	0.59
1:A:341:LEU:HB3	1:C:514:GLY:O	2.03	0.59
1:B:267:GLU:HA	1:B:270:LEU:CD1	2.33	0.59
1:D:357:GLY:O	1:D:539:GLY:CA	2.51	0.59
1:F:260:GLY:O	1:F:261:MET:HB2	2.03	0.59
1:D:261:MET:H	1:D:262:PRO:HD3	1.66	0.59
1:D:357:GLY:N	2:D:783:ADP:O1B	2.34	0.59
1:C:260:GLY:O	1:C:261:MET:HB2	2.03	0.59
1:B:261:MET:N	1:B:262:PRO:HD3	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:335:TYR:HE2	1:A:465:LEU:HD21	1.67	0.59
1:E:420:LEU:HD21	1:E:466:PHE:HD2	1.68	0.59
1:C:569:THR:H	1:C:572:ASN:HB2	1.67	0.59
1:A:300:PRO:HB2	1:A:414:LEU:HB3	1.85	0.59
1:E:277:GLU:HB3	1:E:279:ILE:O	2.03	0.58
1:C:506:LEU:CD2	1:C:522:LEU:HD21	2.32	0.58
1:C:533:TYR:HB3	1:C:580:ARG:HD2	1.84	0.58
1:D:352:LEU:HD22	1:D:489:ILE:HD11	1.83	0.58
1:B:276:TYR:CZ	1:F:246:THR:HB	2.38	0.58
1:C:261:MET:N	1:C:262:PRO:HD3	2.18	0.58
1:E:380:LEU:HB2	1:E:422:GLU:O	2.03	0.58
1:B:349:ILE:O	1:B:349:ILE:HD12	2.03	0.58
1:C:565:ARG:HG2	1:C:566:ILE:N	2.16	0.58
1:E:589:THR:O	1:E:697:ARG:HD2	2.04	0.58
1:C:506:LEU:HD12	1:C:506:LEU:C	2.24	0.58
1:D:420:LEU:HD21	1:D:466:PHE:HD2	1.68	0.58
1:F:335:TYR:HE2	1:F:465:LEU:HD21	1.67	0.58
1:F:550:ILE:O	1:F:551:CYS:C	2.42	0.58
1:A:461:LEU:O	1:A:464:VAL:HG23	2.04	0.58
1:B:593:VAL:HB	1:E:708:ARG:NH2	2.18	0.58
1:A:261:MET:H	1:A:262:PRO:HD3	1.66	0.58
1:C:602:THR:CG2	1:C:604:VAL:HG22	2.33	0.58
1:C:336:LEU:O	1:C:339:GLN:N	2.37	0.58
1:E:317:LEU:O	1:E:317:LEU:HD23	2.04	0.58
1:F:506:LEU:CD2	1:F:522:LEU:HD21	2.33	0.58
1:E:590:GLU:HA	1:E:697:ARG:CD	2.33	0.58
1:A:671:VAL:CG2	1:A:672:PRO:HD2	2.33	0.58
1:E:613:VAL:HG23	1:E:685:ALA:HB1	1.86	0.58
1:D:477:PRO:HB2	1:D:480:LEU:HD23	1.85	0.58
1:A:267:GLU:HA	1:A:270:LEU:CG	2.34	0.58
1:C:584:TYR:CD1	1:C:584:TYR:C	2.76	0.58
1:C:267:GLU:HA	1:C:270:LEU:CG	2.33	0.58
1:A:260:GLY:O	1:A:261:MET:HB2	2.03	0.58
1:B:316:ARG:HD2	1:B:316:ARG:N	2.19	0.58
1:B:477:PRO:HB2	1:B:480:LEU:HD23	1.86	0.58
1:B:341:LEU:HD13	1:F:514:GLY:O	2.04	0.58
1:C:261:MET:H	1:C:262:PRO:HD3	1.68	0.58
1:E:260:GLY:O	1:E:261:MET:HB2	2.02	0.58
1:E:700:GLY:O	1:E:732:ILE:HA	2.04	0.58
1:C:705:ILE:HD11	1:C:761:LEU:HD21	1.86	0.57
1:F:294:ASP:HA	1:F:297:VAL:HG23	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:267:GLU:O	1:D:270:LEU:HB2	2.03	0.57
1:D:368:ALA:HB2	1:D:417:VAL:HG21	1.84	0.57
1:C:557:ALA:HB3	1:C:566:ILE:HD11	1.87	0.57
1:B:336:LEU:O	1:B:339:GLN:N	2.37	0.57
1:B:439:LEU:O	1:B:441:VAL:N	2.37	0.57
1:B:335:TYR:HE2	1:B:465:LEU:HD21	1.68	0.57
1:A:420:LEU:HD21	1:A:466:PHE:CD2	2.40	0.57
1:E:439:LEU:O	1:E:441:VAL:N	2.38	0.57
1:B:536:ARG:NH1	1:B:536:ARG:CG	2.65	0.57
1:F:420:LEU:HD21	1:F:466:PHE:HD2	1.70	0.57
1:F:461:LEU:O	1:F:464:VAL:HG23	2.05	0.57
1:E:613:VAL:HA	1:E:663:HIS:O	2.03	0.57
1:D:267:GLU:HA	1:D:270:LEU:CG	2.34	0.57
1:D:250:GLN:HA	1:D:253:THR:OG1	2.05	0.57
1:B:250:GLN:HA	1:B:253:THR:OG1	2.05	0.57
1:C:516:LYS:HZ1	1:C:516:LYS:HA	1.69	0.57
1:B:734:ALA:HB1	1:B:735:PRO:HD2	1.87	0.57
1:A:316:ARG:HD2	1:A:316:ARG:N	2.19	0.57
1:B:586:GLN:HE22	1:B:729:LEU:HA	1.70	0.57
1:E:497:LYS:HG2	1:E:540:VAL:HG12	1.86	0.57
1:A:506:LEU:HD12	1:A:506:LEU:C	2.24	0.57
1:C:267:GLU:HA	1:C:270:LEU:CD1	2.34	0.57
1:B:276:TYR:OH	1:F:247:GLY:N	2.37	0.57
1:E:262:PRO:HD2	1:E:301:TRP:CB	2.35	0.57
1:B:317:LEU:HD23	1:B:317:LEU:O	2.04	0.57
1:C:506:LEU:HD21	1:C:522:LEU:CD2	2.34	0.57
1:A:439:LEU:O	1:A:441:VAL:N	2.38	0.57
1:E:350:LEU:N	1:E:350:LEU:HD12	2.07	0.56
1:C:734:ALA:HB1	1:C:735:PRO:HD2	1.86	0.56
1:E:250:GLN:HA	1:E:253:THR:OG1	2.05	0.56
1:D:602:THR:HG21	1:D:604:VAL:HG22	1.87	0.56
1:F:332:ILE:HD12	1:F:367:ILE:HD11	1.86	0.56
1:E:565:ARG:HG2	1:E:566:ILE:N	2.20	0.56
1:B:350:LEU:HD23	1:B:487:ILE:HD11	1.87	0.56
1:C:250:GLN:HA	1:C:253:THR:OG1	2.05	0.56
1:B:290:ARG:O	1:B:293:ILE:HG22	2.05	0.56
1:B:294:ASP:HA	1:B:297:VAL:HG23	1.88	0.56
1:D:596:VAL:HG23	1:D:685:ALA:HB2	1.87	0.56
1:E:438:MET:O	1:E:439:LEU:C	2.44	0.56
1:C:294:ASP:HA	1:C:297:VAL:HG23	1.87	0.56
1:D:469:THR:O	1:D:470:ALA:HB2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:586:GLN:HG2	1:F:698:GLU:CG	2.27	0.56
1:D:362:SER:CB	2:D:783:ADP:H5'1	2.35	0.56
1:E:267:GLU:O	1:E:270:LEU:HB2	2.04	0.56
1:A:559:VAL:CG2	1:D:337:ALA:HB1	2.35	0.56
1:F:602:THR:HG21	1:F:604:VAL:HG22	1.86	0.56
1:A:294:ASP:HA	1:A:297:VAL:HG23	1.88	0.56
1:F:267:GLU:HA	1:F:270:LEU:CG	2.36	0.56
1:F:602:THR:CG2	1:F:604:VAL:HG22	2.36	0.56
1:A:557:ALA:HB3	1:A:566:ILE:HD11	1.88	0.56
1:E:294:ASP:HA	1:E:297:VAL:HG23	1.88	0.56
1:C:352:LEU:HD22	1:C:489:ILE:HD11	1.86	0.56
1:C:439:LEU:O	1:C:441:VAL:N	2.39	0.56
1:F:250:GLN:HA	1:F:253:THR:OG1	2.04	0.56
1:B:700:GLY:O	1:B:732:ILE:HA	2.06	0.56
1:D:636:ALA:C	1:D:638:ALA:H	2.08	0.56
1:A:350:LEU:N	1:A:350:LEU:HD12	2.11	0.56
1:E:316:ARG:N	1:E:316:ARG:HD2	2.21	0.56
1:F:560:ALA:O	1:F:562:GLU:HG3	2.05	0.56
1:D:380:LEU:HB2	1:D:422:GLU:O	2.05	0.56
1:E:579:LYS:O	1:E:579:LYS:HE2	2.06	0.56
1:A:250:GLN:HA	1:A:253:THR:OG1	2.05	0.56
1:B:756:ILE:HG13	1:B:767:HIS:CD2	2.41	0.55
1:C:290:ARG:O	1:C:293:ILE:HG22	2.06	0.55
1:A:328:VAL:O	1:A:332:ILE:HG12	2.05	0.55
1:A:336:LEU:O	1:A:339:GLN:N	2.39	0.55
1:E:267:GLU:HA	1:E:270:LEU:CG	2.37	0.55
1:F:267:GLU:HA	1:F:270:LEU:CD1	2.36	0.55
1:D:316:ARG:N	1:D:316:ARG:HD2	2.20	0.55
1:D:328:VAL:O	1:D:332:ILE:HG12	2.05	0.55
1:F:593:VAL:HG13	1:F:693:ARG:O	2.06	0.55
1:B:420:LEU:HD21	1:B:466:PHE:HD2	1.71	0.55
1:D:534:TYR:N	1:D:534:TYR:CD1	2.74	0.55
1:A:756:ILE:HG13	1:A:767:HIS:CD2	2.42	0.55
1:D:613:VAL:HA	1:D:663:HIS:O	2.05	0.55
2:B:783:ADP:O4'	2:B:783:ADP:O2A	2.24	0.55
1:B:579:LYS:O	1:B:579:LYS:HE2	2.05	0.55
1:D:579:LYS:HE2	1:D:579:LYS:O	2.05	0.55
1:D:350:LEU:N	1:D:350:LEU:HD12	2.14	0.55
1:D:439:LEU:O	1:D:441:VAL:N	2.39	0.55
1:A:469:THR:HG22	1:A:470:ALA:N	2.21	0.55
1:C:316:ARG:N	1:C:316:ARG:HD2	2.20	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:516:LYS:HA	1:B:516:LYS:CE	2.36	0.55
1:A:357:GLY:N	2:A:783:ADP:O2B	2.26	0.55
1:F:596:VAL:HG23	1:F:685:ALA:HB2	1.87	0.55
1:A:267:GLU:HA	1:A:270:LEU:CD1	2.36	0.55
1:E:290:ARG:O	1:E:293:ILE:HG22	2.06	0.55
1:D:290:ARG:O	1:D:293:ILE:HG22	2.06	0.55
1:E:548:ALA:O	1:E:549:ALA:C	2.45	0.55
1:F:317:LEU:HD23	1:F:317:LEU:O	2.07	0.55
1:C:613:VAL:HA	1:C:663:HIS:O	2.07	0.55
1:D:635:SER:O	1:D:638:ALA:HB3	2.07	0.55
1:A:380:LEU:HB2	1:A:422:GLU:O	2.06	0.55
1:B:355:PRO:O	1:B:358:VAL:HG22	2.07	0.55
1:D:336:LEU:O	1:D:339:GLN:N	2.39	0.55
1:E:624:LEU:H	1:E:624:LEU:HD12	1.72	0.55
1:C:378:ILE:HD13	1:C:420:LEU:CD1	2.37	0.55
1:F:734:ALA:HB1	1:F:735:PRO:HD2	1.88	0.55
2:A:783:ADP:O2A	2:A:783:ADP:O4'	2.24	0.55
1:F:316:ARG:N	1:F:316:ARG:HD2	2.21	0.55
1:F:349:ILE:HD12	1:F:349:ILE:O	2.06	0.55
1:D:461:LEU:O	1:D:464:VAL:HG23	2.07	0.54
1:E:756:ILE:HG13	1:E:767:HIS:CD2	2.42	0.54
1:B:599:LEU:H	1:B:599:LEU:HD22	1.71	0.54
1:D:573:LEU:HG	1:D:577:ILE:HD11	1.88	0.54
1:C:270:LEU:HD21	1:C:296:LEU:CD2	2.37	0.54
1:B:328:VAL:O	1:B:332:ILE:HG12	2.07	0.54
1:E:378:ILE:HD13	1:E:420:LEU:CD1	2.37	0.54
1:E:380:LEU:HD12	1:E:423:ILE:HG23	1.89	0.54
1:F:408:MET:HE2	1:F:408:MET:H	1.72	0.54
1:F:569:THR:CG2	1:F:572:ASN:H	2.20	0.54
1:D:602:THR:CG2	1:D:604:VAL:HG22	2.38	0.54
1:F:557:ALA:HB3	1:F:566:ILE:HD11	1.89	0.54
1:D:700:GLY:O	1:D:732:ILE:HA	2.08	0.54
1:D:362:SER:HB3	2:D:783:ADP:H5'1	1.89	0.54
1:D:516:LYS:O	1:D:519:ASN:HB2	2.07	0.54
1:E:360:LYS:HD2	1:E:469:THR:HG23	1.89	0.54
1:C:560:ALA:O	1:C:562:GLU:HG3	2.07	0.54
1:F:522:LEU:HB3	1:F:568:VAL:CG1	2.36	0.54
1:B:282:SER:HA	1:B:286:SER:HB3	1.89	0.54
1:B:708:ARG:HD3	1:F:613:VAL:O	2.07	0.54
1:A:273:LEU:HD13	1:A:289:ILE:HD12	1.90	0.54
1:F:290:ARG:O	1:F:293:ILE:HG22	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:267:GLU:HA	1:D:270:LEU:CD1	2.37	0.54
1:E:282:SER:HA	1:E:286:SER:HB3	1.90	0.54
1:D:579:LYS:NZ	1:D:579:LYS:H	2.05	0.54
1:C:536:ARG:CG	1:C:536:ARG:NH1	2.62	0.54
1:C:420:LEU:HD21	1:C:466:PHE:CD2	2.41	0.54
1:B:404:ILE:O	1:B:405:ILE:C	2.45	0.54
1:D:294:ASP:HA	1:D:297:VAL:HG23	1.90	0.54
1:A:700:GLY:O	1:A:732:ILE:HA	2.07	0.54
1:C:569:THR:CG2	1:C:572:ASN:H	2.21	0.54
1:D:516:LYS:HA	1:D:516:LYS:CE	2.37	0.54
1:B:350:LEU:N	1:B:350:LEU:HD12	2.10	0.54
1:E:267:GLU:HA	1:E:270:LEU:CD1	2.38	0.54
1:B:347:GLY:CA	1:B:444:PRO:HG3	2.38	0.54
1:A:613:VAL:HA	1:A:663:HIS:O	2.08	0.54
1:A:583:ARG:NH1	1:D:737:ASP:HB3	2.22	0.54
1:C:282:SER:HA	1:C:286:SER:HB3	1.90	0.54
1:B:469:THR:HG22	1:B:470:ALA:N	2.23	0.54
1:D:250:GLN:HA	1:D:253:THR:HG1	1.73	0.54
1:E:424:ASP:N	1:E:424:ASP:OD1	2.41	0.54
1:F:510:ILE:HG22	1:F:515:LEU:O	2.08	0.53
1:E:506:LEU:HD12	1:E:506:LEU:C	2.28	0.53
1:D:536:ARG:NH1	1:D:536:ARG:HG3	2.16	0.53
1:D:416:PRO:HD2	1:D:464:VAL:HG13	1.89	0.53
1:C:250:GLN:HA	1:C:253:THR:HG1	1.74	0.53
1:C:338:VAL:HG21	1:E:552:ARG:HG3	1.90	0.53
1:E:560:ALA:O	1:E:562:GLU:HG3	2.08	0.53
1:D:599:LEU:HD22	1:D:599:LEU:H	1.73	0.53
1:E:332:ILE:HD12	1:E:367:ILE:HD11	1.89	0.53
1:E:506:LEU:CD2	1:E:522:LEU:HD21	2.37	0.53
1:F:516:LYS:HE2	1:F:516:LYS:HA	1.90	0.53
1:A:540:VAL:CG2	2:A:783:ADP:C8	2.90	0.53
1:A:636:ALA:C	1:A:638:ALA:H	2.10	0.53
1:D:438:MET:O	1:D:439:LEU:C	2.47	0.53
1:A:282:SER:HA	1:A:286:SER:HB3	1.90	0.53
1:E:492:TYR:OH	2:E:783:ADP:N6	2.41	0.53
1:C:700:GLY:O	1:C:732:ILE:HA	2.07	0.53
1:B:438:MET:O	1:B:439:LEU:C	2.45	0.53
1:A:250:GLN:HA	1:A:253:THR:HG1	1.74	0.53
1:C:599:LEU:HD22	1:C:599:LEU:N	2.23	0.53
1:C:644:ARG:NE	1:C:657:HIS:CG	2.77	0.53
1:D:590:GLU:HA	1:D:697:ARG:CD	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:368:ALA:HB2	1:C:417:VAL:HG21	1.90	0.53
1:B:300:PRO:HB2	1:B:414:LEU:HB3	1.90	0.53
1:D:536:ARG:CG	1:D:536:ARG:NH1	2.64	0.53
1:E:461:LEU:O	1:E:464:VAL:HG23	2.09	0.53
1:F:362:SER:HB2	2:F:783:ADP:H5'1	1.89	0.53
1:A:705:ILE:HD11	1:A:761:LEU:HD21	1.91	0.53
1:E:534:TYR:N	1:E:534:TYR:CD1	2.77	0.53
1:A:747:GLU:H	1:A:747:GLU:CD	2.12	0.53
1:B:305:THR:HB	1:B:415:ASN:HD22	1.74	0.53
1:F:347:GLY:CA	1:F:444:PRO:HG3	2.37	0.53
1:A:347:GLY:CA	1:A:444:PRO:HG3	2.39	0.53
1:D:317:LEU:HD23	1:D:317:LEU:O	2.09	0.53
1:C:438:MET:O	1:C:439:LEU:C	2.46	0.53
1:F:644:ARG:NE	1:F:657:HIS:CG	2.77	0.53
1:B:557:ALA:HB3	1:B:566:ILE:HD11	1.90	0.53
1:E:611:ILE:HD12	1:E:681:THR:CG2	2.39	0.53
1:E:569:THR:CG2	1:E:572:ASN:H	2.22	0.53
1:B:380:LEU:HB2	1:B:422:GLU:O	2.08	0.53
1:A:380:LEU:HD12	1:A:423:ILE:HG23	1.91	0.53
1:E:307:ASP:HB3	1:E:309:LEU:HD21	1.91	0.53
1:D:533:TYR:HB3	1:D:580:ARG:HD2	1.91	0.53
1:A:408:MET:H	1:A:408:MET:HE2	1.74	0.53
1:F:439:LEU:O	1:F:441:VAL:N	2.41	0.53
1:B:277:GLU:C	1:B:279:ILE:N	2.62	0.53
1:E:599:LEU:HD22	1:E:599:LEU:H	1.74	0.53
1:A:438:MET:O	1:A:439:LEU:C	2.46	0.53
1:B:404:ILE:HG23	1:B:418:PHE:HE2	1.73	0.53
1:B:276:TYR:CE2	1:F:246:THR:HG21	2.43	0.53
1:E:328:VAL:O	1:E:332:ILE:HG12	2.09	0.53
1:A:635:SER:O	1:A:638:ALA:HB3	2.09	0.53
1:F:334:GLU:O	1:F:338:VAL:HB	2.09	0.53
1:F:506:LEU:HD21	1:F:522:LEU:CD2	2.37	0.52
1:E:506:LEU:HD21	1:E:522:LEU:CD2	2.38	0.52
1:B:671:VAL:CG2	1:B:672:PRO:HD2	2.37	0.52
1:B:644:ARG:NE	1:B:657:HIS:CG	2.77	0.52
1:B:636:ALA:C	1:B:638:ALA:H	2.12	0.52
1:E:593:VAL:HG13	1:E:693:ARG:O	2.08	0.52
1:D:497:LYS:HG2	1:D:540:VAL:HG12	1.91	0.52
1:F:282:SER:HA	1:F:286:SER:HB3	1.90	0.52
1:D:734:ALA:HB1	1:D:735:PRO:HD2	1.91	0.52
1:C:313:GLU:O	1:C:315:GLY:N	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:747:GLU:H	1:B:747:GLU:CD	2.10	0.52
1:E:536:ARG:NH1	1:E:536:ARG:CG	2.64	0.52
1:A:313:GLU:O	1:A:315:GLY:N	2.42	0.52
1:E:469:THR:HG22	1:E:470:ALA:N	2.25	0.52
1:A:644:ARG:HB3	1:C:616:SER:HB2	1.92	0.52
1:B:336:LEU:HA	1:B:339:GLN:HB3	1.92	0.52
1:F:493:THR:O	1:F:494:GLU:C	2.48	0.52
1:E:505:LEU:CD2	1:E:544:GLU:HG3	2.37	0.52
1:F:247:GLY:C	1:F:249:VAL:H	2.13	0.52
1:B:461:LEU:O	1:B:464:VAL:HG23	2.10	0.52
1:F:250:GLN:HA	1:F:253:THR:HG1	1.73	0.52
1:C:347:GLY:CA	1:C:444:PRO:HG3	2.40	0.52
1:A:644:ARG:NE	1:A:657:HIS:CG	2.77	0.52
1:B:635:SER:O	1:B:638:ALA:HB3	2.10	0.52
1:C:636:ALA:C	1:C:638:ALA:H	2.12	0.52
1:E:336:LEU:O	1:E:339:GLN:N	2.43	0.52
1:B:548:ALA:O	1:B:549:ALA:C	2.47	0.52
1:F:469:THR:HG22	1:F:470:ALA:N	2.24	0.52
1:F:378:ILE:HD13	1:F:420:LEU:CD1	2.39	0.52
1:C:406:GLN:O	1:C:407:GLY:C	2.48	0.52
1:A:404:ILE:O	1:A:405:ILE:C	2.47	0.52
1:F:448:SER:O	1:F:460:ASP:HA	2.08	0.52
1:B:448:SER:O	1:B:460:ASP:HA	2.10	0.52
1:D:378:ILE:HD13	1:D:420:LEU:CD1	2.40	0.52
1:A:406:GLN:O	1:A:407:GLY:C	2.48	0.52
1:A:290:ARG:O	1:A:293:ILE:HG22	2.10	0.52
1:A:469:THR:O	1:A:470:ALA:HB2	2.09	0.52
1:C:328:VAL:O	1:C:332:ILE:HG12	2.10	0.52
1:E:516:LYS:CE	1:E:516:LYS:HA	2.40	0.52
1:A:274:ASN:C	1:A:276:TYR:N	2.64	0.52
1:E:747:GLU:CD	1:E:747:GLU:H	2.13	0.52
1:B:414:LEU:C	1:B:416:PRO:HD3	2.30	0.52
1:D:569:THR:CG2	1:D:572:ASN:H	2.22	0.52
1:D:347:GLY:CA	1:D:444:PRO:HG3	2.38	0.52
1:F:714:ILE:HB	1:F:735:PRO:HG2	1.91	0.52
1:F:599:LEU:H	1:F:599:LEU:HD22	1.75	0.52
1:E:496:GLU:O	1:E:500:ILE:HG13	2.10	0.52
1:F:611:ILE:HD12	1:F:681:THR:CG2	2.39	0.52
1:F:686:LEU:HD22	1:F:686:LEU:O	2.10	0.52
1:C:506:LEU:HB3	1:C:507:PRO:CD	2.40	0.51
1:C:522:LEU:HB3	1:C:568:VAL:CG1	2.36	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:569:THR:HG22	1:B:572:ASN:OD1	2.10	0.51
1:D:613:VAL:HG23	1:D:685:ALA:HB1	1.92	0.51
1:D:274:ASN:C	1:D:276:TYR:N	2.63	0.51
1:D:557:ALA:HB3	1:D:566:ILE:HD11	1.92	0.51
1:B:706:THR:OG1	1:B:710:ARG:HB2	2.10	0.51
1:D:548:ALA:O	1:D:549:ALA:C	2.49	0.51
1:D:522:LEU:HB3	1:D:568:VAL:CG1	2.39	0.51
1:A:414:LEU:C	1:A:416:PRO:HD3	2.31	0.51
1:F:277:GLU:C	1:F:279:ILE:N	2.63	0.51
1:A:602:THR:HG21	1:A:604:VAL:HG22	1.90	0.51
1:C:656:PHE:C	1:C:658:GLU:H	2.13	0.51
1:B:408:MET:HE2	1:B:408:MET:H	1.75	0.51
1:A:624:LEU:HD12	1:A:624:LEU:H	1.74	0.51
1:B:506:LEU:HD12	1:B:506:LEU:O	2.10	0.51
1:E:273:LEU:HD13	1:E:289:ILE:HD12	1.92	0.51
1:E:404:ILE:O	1:E:405:ILE:C	2.49	0.51
1:F:362:SER:HB2	2:F:783:ADP:C5'	2.40	0.51
1:F:438:MET:O	1:F:439:LEU:C	2.48	0.51
1:A:516:LYS:HA	1:A:516:LYS:CE	2.41	0.51
1:A:714:ILE:HG23	1:A:715:GLY:N	2.24	0.51
1:A:308:LYS:O	1:A:309:LEU:HD23	2.11	0.51
1:A:569:THR:CG2	1:A:572:ASN:H	2.22	0.51
1:B:409:LYS:C	1:B:411:ALA:H	2.13	0.51
1:D:282:SER:HA	1:D:286:SER:HB3	1.91	0.51
1:B:624:LEU:H	1:B:624:LEU:HD12	1.75	0.51
1:F:506:LEU:C	1:F:506:LEU:HD12	2.30	0.51
1:F:569:THR:HG22	1:F:572:ASN:OD1	2.11	0.51
1:B:274:ASN:C	1:B:276:TYR:N	2.62	0.51
1:B:380:LEU:HD12	1:B:423:ILE:CG2	2.40	0.51
1:C:334:GLU:O	1:C:338:VAL:HB	2.11	0.51
1:F:533:TYR:HB3	1:F:580:ARG:HD2	1.92	0.51
1:C:624:LEU:H	1:C:624:LEU:HD12	1.76	0.51
1:D:273:LEU:HD13	1:D:289:ILE:HD12	1.92	0.51
1:E:274:ASN:C	1:E:276:TYR:N	2.64	0.51
1:D:420:LEU:HD21	1:D:466:PHE:CD2	2.46	0.51
1:E:262:PRO:CD	1:E:301:TRP:HB2	2.40	0.51
1:E:247:GLY:C	1:E:249:VAL:H	2.14	0.51
1:B:247:GLY:C	1:B:249:VAL:H	2.14	0.51
1:C:448:SER:O	1:C:460:ASP:HA	2.11	0.51
1:A:533:TYR:HB3	1:A:580:ARG:HD2	1.92	0.51
1:F:273:LEU:HD13	1:F:289:ILE:HD12	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:308:LYS:O	1:D:309:LEU:HD23	2.11	0.51
1:A:448:SER:O	1:A:460:ASP:HA	2.11	0.51
1:A:462:SER:HB2	1:A:463:LYS:HD2	1.93	0.51
1:D:404:ILE:O	1:D:405:ILE:C	2.49	0.51
1:E:569:THR:HG22	1:E:572:ASN:OD1	2.11	0.51
1:F:406:GLN:O	1:F:407:GLY:C	2.49	0.51
1:A:438:MET:O	1:A:440:GLU:N	2.44	0.51
1:C:747:GLU:H	1:C:747:GLU:CD	2.13	0.51
1:A:322:HIS:CE1	1:A:363:LEU:HD23	2.46	0.51
1:A:350:LEU:HD23	1:A:487:ILE:HD11	1.92	0.51
2:D:783:ADP:C4'	2:D:783:ADP:O2A	2.59	0.51
1:E:420:LEU:HD21	1:E:466:PHE:CD2	2.45	0.51
1:C:404:ILE:HG23	1:C:418:PHE:HE2	1.71	0.51
1:D:300:PRO:O	1:D:301:TRP:CD2	2.64	0.51
1:E:584:TYR:O	1:E:584:TYR:HD1	1.91	0.51
1:D:438:MET:O	1:D:440:GLU:N	2.44	0.51
1:A:286:SER:O	1:A:290:ARG:HB2	2.11	0.51
1:B:305:THR:HB	1:B:415:ASN:ND2	2.25	0.51
1:C:308:LYS:O	1:C:309:LEU:HD23	2.11	0.51
1:B:506:LEU:HD21	1:B:522:LEU:CD2	2.40	0.51
1:B:516:LYS:HA	1:B:516:LYS:HZ1	1.76	0.51
1:F:497:LYS:HG2	1:F:540:VAL:HG12	1.92	0.51
1:F:438:MET:O	1:F:440:GLU:N	2.44	0.51
1:E:347:GLY:CA	1:E:444:PRO:HG3	2.40	0.51
1:B:368:ALA:HB2	1:B:417:VAL:HG21	1.92	0.51
1:D:644:ARG:NE	1:D:657:HIS:CG	2.78	0.51
1:E:602:THR:HG22	1:E:603:THR:N	2.26	0.51
1:A:599:LEU:HD22	1:A:599:LEU:H	1.76	0.51
1:F:586:GLN:NE2	1:F:698:GLU:HA	2.16	0.51
1:B:250:GLN:HA	1:B:253:THR:HG1	1.74	0.51
1:B:286:SER:O	1:B:290:ARG:HB2	2.11	0.51
1:C:337:ALA:HB3	1:E:556:LYS:HA	1.92	0.51
1:A:334:GLU:O	1:A:338:VAL:HB	2.11	0.51
1:B:273:LEU:HD13	1:B:289:ILE:HD12	1.93	0.51
1:E:644:ARG:NE	1:E:657:HIS:CG	2.78	0.51
1:C:336:LEU:HA	1:C:339:GLN:HB3	1.93	0.51
1:F:700:GLY:O	1:F:732:ILE:HA	2.10	0.51
1:F:705:ILE:HD11	1:F:761:LEU:HD21	1.92	0.51
1:D:611:ILE:HD12	1:D:681:THR:CG2	2.41	0.51
1:F:624:LEU:HD12	1:F:624:LEU:H	1.75	0.51
1:B:506:LEU:CD2	1:B:522:LEU:HD21	2.38	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:274:ASN:O	1:B:276:TYR:N	2.43	0.50
1:E:557:ALA:HB3	1:E:566:ILE:HD11	1.93	0.50
1:D:550:ILE:O	1:D:551:CYS:C	2.47	0.50
1:D:536:ARG:HH11	1:D:536:ARG:CB	2.25	0.50
1:D:448:SER:O	1:D:460:ASP:HA	2.10	0.50
1:A:277:GLU:C	1:A:279:ILE:N	2.63	0.50
1:D:277:GLU:C	1:D:279:ILE:N	2.63	0.50
1:D:532:ARG:HG2	1:D:584:TYR:CD2	2.46	0.50
1:D:313:GLU:O	1:D:315:GLY:N	2.44	0.50
1:E:573:LEU:HG	1:E:577:ILE:HD11	1.93	0.50
1:B:322:HIS:CE1	1:B:363:LEU:HD23	2.46	0.50
1:B:621:LYS:O	1:B:661:ASP:OD1	2.29	0.50
1:D:714:ILE:HG23	1:D:715:GLY:N	2.25	0.50
1:F:549:ALA:HA	1:F:552:ARG:NH2	2.26	0.50
1:C:548:ALA:O	1:C:549:ALA:C	2.46	0.50
1:C:329:LYS:C	1:C:331:ARG:N	2.64	0.50
1:C:536:ARG:CB	1:C:536:ARG:HH11	2.24	0.50
1:C:414:LEU:C	1:C:416:PRO:HD3	2.31	0.50
1:F:286:SER:O	1:F:290:ARG:HB2	2.12	0.50
1:C:274:ASN:C	1:C:276:TYR:N	2.65	0.50
1:B:317:LEU:HD23	1:B:317:LEU:C	2.32	0.50
1:D:589:THR:O	1:D:697:ARG:HD2	2.12	0.50
1:D:624:LEU:HD12	1:D:624:LEU:H	1.76	0.50
1:B:299:LEU:O	1:B:299:LEU:HD12	2.11	0.50
1:D:406:GLN:O	1:D:407:GLY:C	2.50	0.50
1:C:300:PRO:HG3	1:C:412:GLY:HA2	1.94	0.50
1:F:546:GLN:OE1	1:F:577:ILE:HB	2.11	0.50
1:A:247:GLY:C	1:A:249:VAL:H	2.14	0.50
1:D:686:LEU:HD22	1:D:686:LEU:O	2.11	0.50
1:E:448:SER:O	1:E:460:ASP:HA	2.12	0.50
1:D:462:SER:HB2	1:D:463:LYS:HD2	1.94	0.50
1:A:329:LYS:O	1:A:331:ARG:N	2.44	0.50
1:C:439:LEU:H	1:C:439:LEU:CD2	2.20	0.50
1:B:438:MET:O	1:B:440:GLU:N	2.45	0.50
1:C:313:GLU:O	1:C:314:ALA:C	2.50	0.50
1:A:637:GLN:HG2	1:A:637:GLN:O	2.11	0.50
1:F:404:ILE:O	1:F:405:ILE:C	2.50	0.50
1:E:438:MET:O	1:E:440:GLU:N	2.43	0.50
1:D:313:GLU:O	1:D:314:ALA:C	2.50	0.50
1:D:593:VAL:HG13	1:D:693:ARG:O	2.12	0.50
1:A:534:TYR:CD1	1:A:534:TYR:N	2.80	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:350:LEU:HD23	1:C:487:ILE:HD11	1.93	0.50
1:E:733:ILE:HA	1:E:756:ILE:O	2.12	0.50
1:B:334:GLU:O	1:B:338:VAL:HB	2.11	0.50
1:C:317:LEU:HD23	1:C:317:LEU:C	2.31	0.50
1:A:424:ASP:HB2	1:A:475:THR:CG2	2.42	0.50
1:D:247:GLY:C	1:D:249:VAL:H	2.15	0.50
1:C:461:LEU:O	1:C:464:VAL:HG23	2.11	0.50
1:C:277:GLU:C	1:C:279:ILE:N	2.63	0.50
1:F:424:ASP:HB2	1:F:475:THR:CG2	2.42	0.50
1:E:469:THR:O	1:E:470:ALA:HB2	2.11	0.50
1:C:424:ASP:HB2	1:C:475:THR:CG2	2.42	0.50
1:A:602:THR:CG2	1:A:604:VAL:HG22	2.42	0.50
1:E:439:LEU:CD2	1:E:439:LEU:H	2.19	0.49
1:C:438:MET:O	1:C:440:GLU:N	2.45	0.49
1:C:362:SER:CB	2:C:783:ADP:H5'1	2.41	0.49
1:A:732:ILE:HG21	1:A:753:LEU:HD13	1.94	0.49
1:C:593:VAL:O	1:C:595:VAL:HG23	2.11	0.49
1:D:569:THR:HG23	1:D:572:ASN:H	1.78	0.49
1:B:596:VAL:HG23	1:B:685:ALA:HB2	1.93	0.49
1:C:702:THR:CG2	1:C:702:THR:O	2.60	0.49
1:A:424:ASP:N	1:A:424:ASP:OD1	2.45	0.49
1:A:313:GLU:O	1:A:314:ALA:C	2.49	0.49
1:B:687:VAL:O	1:B:691:THR:HG23	2.12	0.49
1:C:408:MET:HE2	1:C:408:MET:H	1.77	0.49
1:F:336:LEU:O	1:F:339:GLN:N	2.45	0.49
1:E:407:GLY:HA3	1:E:418:PHE:CZ	2.47	0.49
1:E:359:GLY:HA2	2:E:783:ADP:C5'	2.42	0.49
1:D:424:ASP:HB2	1:D:475:THR:CG2	2.41	0.49
1:E:313:GLU:O	1:E:315:GLY:N	2.44	0.49
1:B:462:SER:HB2	1:B:463:LYS:HD2	1.95	0.49
1:B:299:LEU:HD13	1:B:301:TRP:CZ2	2.47	0.49
1:F:404:ILE:HG23	1:F:418:PHE:HE2	1.70	0.49
1:A:520:LEU:HA	1:A:566:ILE:O	2.12	0.49
1:C:506:LEU:O	1:C:506:LEU:HD12	2.13	0.49
1:D:359:GLY:CA	2:D:783:ADP:O5'	2.58	0.49
1:E:406:GLN:O	1:E:407:GLY:C	2.51	0.49
1:F:455:ILE:O	1:F:456:GLU:C	2.51	0.49
1:E:255:LYS:NZ	1:E:255:LYS:HB3	2.28	0.49
1:B:550:ILE:O	1:B:551:CYS:C	2.49	0.49
1:A:686:LEU:O	1:A:686:LEU:HD22	2.12	0.49
1:A:464:VAL:O	1:A:466:PHE:CD1	2.63	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:739:GLU:C	1:D:741:ASP:H	2.15	0.49
1:E:637:GLN:HG2	1:E:637:GLN:O	2.12	0.49
1:D:637:GLN:O	1:D:637:GLN:HG2	2.11	0.49
1:D:742:ILE:O	1:D:742:ILE:HG22	2.13	0.49
1:A:506:LEU:HD21	1:A:522:LEU:CD2	2.42	0.49
1:F:548:ALA:O	1:F:549:ALA:C	2.51	0.49
1:B:313:GLU:O	1:B:315:GLY:N	2.46	0.49
1:F:308:LYS:O	1:F:309:LEU:HD23	2.12	0.49
1:A:596:VAL:HG23	1:A:685:ALA:HB2	1.94	0.49
1:B:378:ILE:HD13	1:B:420:LEU:CD1	2.43	0.49
1:A:404:ILE:HG23	1:A:418:PHE:HE2	1.72	0.49
1:A:734:ALA:HB1	1:A:735:PRO:CD	2.42	0.49
1:B:602:THR:HG21	1:B:604:VAL:HG22	1.94	0.49
1:E:734:ALA:HB1	1:E:735:PRO:CD	2.42	0.49
1:E:286:SER:O	1:E:290:ARG:HB2	2.13	0.49
1:D:286:SER:O	1:D:290:ARG:HB2	2.12	0.49
1:B:533:TYR:HB3	1:B:580:ARG:HD2	1.94	0.49
1:F:246:THR:HG23	1:F:250:GLN:NE2	2.28	0.49
1:F:255:LYS:NZ	1:F:255:LYS:HB3	2.28	0.49
1:A:407:GLY:HA3	1:A:418:PHE:CZ	2.48	0.49
1:C:584:TYR:O	1:C:584:TYR:HD1	1.95	0.49
1:A:708:ARG:NH2	1:C:593:VAL:HB	2.27	0.49
1:D:705:ILE:HD11	1:D:761:LEU:HD21	1.94	0.49
1:B:573:LEU:HG	1:B:577:ILE:HD11	1.95	0.48
1:E:313:GLU:O	1:E:314:ALA:C	2.51	0.48
1:D:317:LEU:C	1:D:317:LEU:HD23	2.33	0.48
1:C:506:LEU:O	1:C:507:PRO:C	2.49	0.48
1:C:756:ILE:HG13	1:C:767:HIS:CD2	2.48	0.48
1:D:255:LYS:HB3	1:D:255:LYS:NZ	2.28	0.48
1:F:551:CYS:O	1:F:554:ALA:HB3	2.13	0.48
1:A:336:LEU:HA	1:A:339:GLN:HB3	1.95	0.48
1:E:455:ILE:O	1:E:456:GLU:C	2.51	0.48
1:B:705:ILE:HD11	1:B:761:LEU:HD21	1.95	0.48
1:D:329:LYS:C	1:D:331:ARG:N	2.63	0.48
1:C:501:VAL:HG13	1:C:547:LEU:HD11	1.95	0.48
1:B:444:PRO:HA	1:B:447:ASN:ND2	2.28	0.48
1:B:714:ILE:HB	1:B:735:PRO:HG2	1.94	0.48
1:E:262:PRO:HG3	1:E:302:THR:OG1	2.13	0.48
1:D:656:PHE:CE2	1:D:690:LEU:HD11	2.48	0.48
1:C:247:GLY:C	1:C:249:VAL:H	2.15	0.48
1:E:602:THR:HG21	1:E:604:VAL:HG22	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:635:SER:O	1:C:638:ALA:HB3	2.13	0.48
1:C:536:ARG:HG3	1:C:536:ARG:NH1	2.16	0.48
1:E:602:THR:C	1:E:604:VAL:H	2.16	0.48
1:F:313:GLU:O	1:F:315:GLY:N	2.47	0.48
1:C:550:ILE:O	1:C:551:CYS:C	2.51	0.48
1:A:506:LEU:CD2	1:A:522:LEU:HD21	2.44	0.48
1:C:642:TYR:CD2	1:C:761:LEU:HD12	2.49	0.48
1:A:599:LEU:O	1:A:720:LYS:HE2	2.13	0.48
1:B:642:TYR:CE1	1:B:709:GLY:HA3	2.48	0.48
1:A:304:GLU:O	1:A:305:THR:C	2.50	0.48
1:E:686:LEU:O	1:E:686:LEU:HD22	2.14	0.48
1:B:350:LEU:H	1:B:350:LEU:CD1	2.10	0.48
1:C:404:ILE:O	1:C:405:ILE:C	2.51	0.48
1:F:331:ARG:HH22	1:F:485:GLU:CD	2.17	0.48
1:F:656:PHE:CG	1:F:657:HIS:N	2.80	0.48
1:E:424:ASP:HB2	1:E:475:THR:CG2	2.42	0.48
1:C:705:ILE:HD11	1:C:761:LEU:CD2	2.44	0.48
1:A:621:LYS:O	1:A:661:ASP:OD1	2.31	0.48
1:A:349:ILE:HD12	1:A:349:ILE:O	2.14	0.48
1:A:329:LYS:C	1:A:331:ARG:N	2.65	0.48
1:F:407:GLY:HA3	1:F:418:PHE:CZ	2.49	0.48
1:F:274:ASN:C	1:F:276:TYR:N	2.64	0.48
1:E:656:PHE:CG	1:E:657:HIS:N	2.82	0.48
1:E:262:PRO:HD2	1:E:301:TRP:HB3	1.94	0.48
1:C:462:SER:HB2	1:C:463:LYS:HD2	1.94	0.48
1:F:756:ILE:HG13	1:F:767:HIS:CD2	2.49	0.48
1:B:296:LEU:HD23	1:B:299:LEU:HD11	1.95	0.48
1:E:590:GLU:HA	1:E:697:ARG:HD3	1.96	0.48
1:B:536:ARG:HH11	1:B:536:ARG:CB	2.27	0.48
1:B:406:GLN:O	1:B:407:GLY:C	2.51	0.48
1:F:739:GLU:C	1:F:741:ASP:H	2.17	0.48
1:F:642:TYR:CE1	1:F:709:GLY:HA3	2.49	0.48
1:E:462:SER:HB2	1:E:463:LYS:HD2	1.95	0.48
1:C:273:LEU:HD13	1:C:289:ILE:HD12	1.95	0.48
1:C:712:LEU:HB3	1:C:713:PRO:CD	2.43	0.48
1:F:547:LEU:HA	1:F:547:LEU:HD23	1.75	0.48
1:E:408:MET:HE2	1:E:408:MET:H	1.79	0.48
1:D:656:PHE:C	1:D:658:GLU:H	2.16	0.48
1:E:579:LYS:H	1:E:579:LYS:NZ	2.12	0.48
1:F:336:LEU:HA	1:F:339:GLN:HB3	1.95	0.48
1:E:635:SER:O	1:E:638:ALA:HB3	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:334:GLU:O	1:E:338:VAL:HB	2.14	0.48
1:C:286:SER:O	1:C:290:ARG:HB2	2.14	0.48
1:E:270:LEU:HD21	1:E:296:LEU:CD2	2.43	0.48
1:E:357:GLY:H	2:E:783:ADP:PB	2.37	0.48
1:F:621:LYS:O	1:F:661:ASP:OD1	2.32	0.48
1:B:526:ALA:O	1:B:530:ILE:HG13	2.14	0.48
1:A:350:LEU:CD1	1:A:350:LEU:H	2.07	0.47
1:B:246:THR:HG23	1:B:250:GLN:NE2	2.29	0.47
1:F:536:ARG:HG3	1:F:536:ARG:NH1	2.21	0.47
1:C:656:PHE:CG	1:C:657:HIS:N	2.82	0.47
1:D:678:ALA:O	1:D:682:MET:HG2	2.14	0.47
1:C:329:LYS:O	1:C:331:ARG:N	2.47	0.47
1:E:277:GLU:C	1:E:279:ILE:N	2.64	0.47
1:E:416:PRO:HG2	1:E:464:VAL:HG13	1.96	0.47
1:F:420:LEU:HD21	1:F:466:PHE:CD2	2.47	0.47
1:F:362:SER:CB	2:F:783:ADP:H5'2	2.44	0.47
1:C:255:LYS:NZ	1:C:255:LYS:HB3	2.28	0.47
1:D:336:LEU:HA	1:D:339:GLN:HB3	1.96	0.47
1:F:642:TYR:CD2	1:F:761:LEU:HD12	2.49	0.47
1:E:276:TYR:CD1	1:E:277:GLU:N	2.83	0.47
1:C:613:VAL:HG23	1:C:685:ALA:HB1	1.95	0.47
1:B:536:ARG:NH1	1:B:536:ARG:HG3	2.18	0.47
1:C:733:ILE:HA	1:C:756:ILE:O	2.15	0.47
1:B:359:GLY:O	1:B:360:LYS:C	2.52	0.47
1:C:734:ALA:HB1	1:C:735:PRO:CD	2.45	0.47
1:D:360:LYS:HD2	1:D:469:THR:HG23	1.95	0.47
1:C:636:ALA:O	1:C:638:ALA:N	2.45	0.47
1:D:529:ASP:O	1:D:530:ILE:C	2.51	0.47
1:D:408:MET:H	1:D:408:MET:HE2	1.79	0.47
1:C:569:THR:HG23	1:C:571:LYS:N	2.16	0.47
1:E:414:LEU:C	1:E:416:PRO:HD3	2.33	0.47
1:B:424:ASP:HB2	1:B:475:THR:CG2	2.43	0.47
1:E:317:LEU:HD23	1:E:317:LEU:C	2.34	0.47
1:E:546:GLN:O	1:E:549:ALA:HB3	2.15	0.47
1:E:717:LEU:O	1:E:717:LEU:HD22	2.14	0.47
1:C:534:TYR:N	1:C:534:TYR:CD1	2.81	0.47
1:D:604:VAL:O	1:D:604:VAL:HG23	2.12	0.47
1:F:546:GLN:O	1:F:549:ALA:HB3	2.14	0.47
1:B:739:GLU:C	1:B:741:ASP:H	2.17	0.47
1:E:656:PHE:C	1:E:658:GLU:H	2.17	0.47
1:B:656:PHE:C	1:B:658:GLU:H	2.16	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:313:GLU:O	1:B:314:ALA:C	2.52	0.47
1:E:602:THR:C	1:E:604:VAL:N	2.67	0.47
1:E:336:LEU:HA	1:E:339:GLN:HB3	1.95	0.47
1:D:464:VAL:O	1:D:466:PHE:CD1	2.64	0.47
1:F:536:ARG:CG	1:F:536:ARG:NH1	2.67	0.47
1:C:407:GLY:HA3	1:C:418:PHE:CZ	2.49	0.47
1:C:733:ILE:CD1	1:C:768:ALA:HB2	2.45	0.47
1:F:313:GLU:O	1:F:314:ALA:C	2.53	0.47
1:F:599:LEU:HD22	1:F:599:LEU:N	2.29	0.47
1:C:546:GLN:O	1:C:549:ALA:HB3	2.15	0.47
1:E:364:ALA:O	1:E:365:LYS:C	2.53	0.47
1:A:478:GLY:N	1:A:479:PRO:HD2	2.30	0.47
1:F:493:THR:CG2	1:F:748:SER:HB2	2.20	0.47
1:F:613:VAL:HG23	1:F:685:ALA:HB1	1.97	0.47
1:A:452:ASP:O	1:A:455:ILE:HG22	2.15	0.47
1:A:246:THR:HG23	1:A:250:GLN:NE2	2.29	0.47
1:A:270:LEU:HD21	1:A:296:LEU:CD2	2.44	0.47
1:B:255:LYS:HB3	1:B:255:LYS:NZ	2.30	0.47
1:F:656:PHE:C	1:F:658:GLU:H	2.17	0.47
1:C:469:THR:O	1:C:470:ALA:HB2	2.15	0.47
1:E:308:LYS:O	1:E:309:LEU:HD23	2.14	0.47
1:C:611:ILE:HD12	1:C:681:THR:CG2	2.45	0.47
1:E:705:ILE:HD11	1:E:761:LEU:HD21	1.96	0.47
1:D:334:GLU:O	1:D:338:VAL:HB	2.15	0.47
1:E:705:ILE:HD12	1:E:705:ILE:HA	1.61	0.47
1:F:645:SER:O	1:F:647:THR:N	2.47	0.47
1:F:462:SER:HB2	1:F:463:LYS:HD2	1.95	0.47
1:A:647:THR:HG22	1:A:648:GLU:N	2.30	0.47
1:B:331:ARG:HH22	1:B:485:GLU:CD	2.17	0.47
1:D:506:LEU:HD21	1:D:522:LEU:CD2	2.42	0.47
1:D:414:LEU:C	1:D:416:PRO:HD3	2.35	0.47
1:E:739:GLU:C	1:E:741:ASP:H	2.17	0.47
1:F:534:TYR:CD2	1:F:577:ILE:HD12	2.50	0.47
1:B:656:PHE:CG	1:B:657:HIS:N	2.83	0.47
1:C:520:LEU:HA	1:C:566:ILE:O	2.15	0.47
1:B:584:TYR:CE2	1:B:728:GLY:HA3	2.49	0.47
1:B:452:ASP:O	1:B:455:ILE:HG22	2.15	0.47
1:D:455:ILE:O	1:D:456:GLU:C	2.54	0.47
1:A:506:LEU:O	1:A:506:LEU:HD12	2.15	0.47
1:B:282:SER:HB2	1:E:276:TYR:HH	1.80	0.47
1:E:274:ASN:O	1:E:276:TYR:N	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:572:ASN:O	1:A:573:LEU:C	2.53	0.47
1:B:569:THR:CG2	1:B:572:ASN:H	2.27	0.47
1:B:276:TYR:CD1	1:B:277:GLU:N	2.83	0.47
1:A:656:PHE:CG	1:A:657:HIS:N	2.82	0.47
1:B:255:LYS:O	1:B:258:GLU:HB3	2.15	0.47
1:B:260:GLY:O	1:B:261:MET:CB	2.63	0.47
1:F:656:PHE:CE2	1:F:690:LEU:HD11	2.50	0.47
1:A:680:ILE:HG22	1:A:705:ILE:HD13	1.97	0.47
1:B:599:LEU:HD21	1:B:700:GLY:C	2.35	0.47
1:C:712:LEU:HB3	1:C:713:PRO:HD2	1.97	0.47
1:B:455:ILE:O	1:B:456:GLU:C	2.53	0.47
1:A:255:LYS:HB3	1:A:255:LYS:NZ	2.29	0.47
1:B:732:ILE:HD13	1:B:732:ILE:O	2.15	0.47
1:B:579:LYS:NZ	1:B:579:LYS:H	2.13	0.47
1:A:645:SER:O	1:A:647:THR:N	2.48	0.47
1:E:645:SER:O	1:E:647:THR:N	2.48	0.47
1:E:621:LYS:O	1:E:661:ASP:OD1	2.33	0.47
1:E:329:LYS:C	1:E:331:ARG:N	2.68	0.47
1:A:331:ARG:HH22	1:A:485:GLU:CD	2.18	0.46
1:F:540:VAL:CG2	2:F:783:ADP:H1'	2.45	0.46
1:D:702:THR:HG23	1:D:702:THR:O	2.16	0.46
1:D:444:PRO:HA	1:D:447:ASN:ND2	2.30	0.46
1:A:255:LYS:O	1:A:258:GLU:HB3	2.16	0.46
2:A:783:ADP:PA	2:A:783:ADP:O4'	2.71	0.46
1:A:317:LEU:C	1:A:317:LEU:HD23	2.34	0.46
1:F:593:VAL:O	1:F:595:VAL:HG23	2.15	0.46
1:C:732:ILE:HG21	1:C:753:LEU:HD13	1.97	0.46
1:B:636:ALA:O	1:B:638:ALA:N	2.46	0.46
1:E:331:ARG:HH22	1:E:485:GLU:CD	2.17	0.46
1:F:712:LEU:HB3	1:F:713:PRO:HD2	1.97	0.46
1:D:355:PRO:O	1:D:358:VAL:HG22	2.15	0.46
1:C:331:ARG:HH22	1:C:485:GLU:CD	2.18	0.46
1:F:360:LYS:CD	1:F:469:THR:HG23	2.41	0.46
1:E:404:ILE:HG23	1:E:418:PHE:HE2	1.72	0.46
1:F:496:GLU:O	1:F:500:ILE:HG13	2.14	0.46
1:D:246:THR:HG23	1:D:250:GLN:NE2	2.30	0.46
1:F:260:GLY:O	1:F:261:MET:CB	2.63	0.46
1:B:341:LEU:O	1:B:343:LYS:N	2.48	0.46
1:C:307:ASP:HB3	1:C:309:LEU:HD21	1.97	0.46
1:A:586:GLN:NE2	1:A:728:GLY:O	2.49	0.46
1:C:341:LEU:O	1:C:343:LYS:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:341:LEU:O	1:E:343:LYS:N	2.48	0.46
1:B:534:TYR:N	1:B:534:TYR:CD1	2.82	0.46
1:F:329:LYS:O	1:F:331:ARG:N	2.48	0.46
1:F:329:LYS:C	1:F:331:ARG:N	2.67	0.46
1:D:266:LYS:HG3	1:D:267:GLU:H	1.78	0.46
1:C:714:ILE:HG23	1:C:715:GLY:N	2.29	0.46
1:C:444:PRO:HA	1:C:447:ASN:ND2	2.30	0.46
1:E:246:THR:HG23	1:E:250:GLN:NE2	2.30	0.46
1:C:380:LEU:HD12	1:C:423:ILE:CG2	2.46	0.46
1:E:732:ILE:HG21	1:E:753:LEU:HD13	1.96	0.46
1:E:307:ASP:O	1:E:309:LEU:HG	2.16	0.46
1:B:678:ALA:O	1:B:682:MET:HG2	2.15	0.46
1:A:536:ARG:CB	1:A:536:ARG:HH11	2.28	0.46
1:D:569:THR:HG22	1:D:572:ASN:OD1	2.15	0.46
1:B:439:LEU:H	1:B:439:LEU:CD2	2.26	0.46
1:A:439:LEU:H	1:A:439:LEU:CD2	2.25	0.46
1:A:444:PRO:HA	1:A:447:ASN:ND2	2.28	0.46
1:C:579:LYS:NZ	1:C:579:LYS:H	2.14	0.46
1:D:636:ALA:O	1:D:638:ALA:N	2.40	0.46
1:E:636:ALA:C	1:E:638:ALA:H	2.17	0.46
1:F:352:LEU:HB3	1:F:360:LYS:HG2	1.96	0.46
1:A:409:LYS:C	1:A:411:ALA:H	2.17	0.46
1:F:734:ALA:HB1	1:F:735:PRO:CD	2.46	0.46
1:C:656:PHE:C	1:C:658:GLU:N	2.68	0.46
1:B:424:ASP:OD1	1:B:424:ASP:N	2.49	0.46
1:E:260:GLY:O	1:E:261:MET:CB	2.63	0.46
1:A:642:TYR:CE1	1:A:709:GLY:HA3	2.50	0.46
1:A:380:LEU:HD12	1:A:423:ILE:CG2	2.46	0.46
1:D:478:GLY:N	1:D:479:PRO:HD2	2.31	0.46
1:F:637:GLN:HG2	1:F:637:GLN:O	2.16	0.46
1:B:637:GLN:O	1:B:637:GLN:HG2	2.15	0.46
1:D:331:ARG:HH22	1:D:485:GLU:CD	2.18	0.46
1:C:536:ARG:CB	1:C:536:ARG:NH1	2.79	0.46
1:C:596:VAL:HG23	1:C:685:ALA:HB2	1.97	0.46
1:F:569:THR:HG23	1:F:572:ASN:H	1.79	0.46
1:F:444:PRO:HA	1:F:447:ASN:ND2	2.29	0.46
1:A:274:ASN:O	1:A:276:TYR:N	2.46	0.46
1:E:368:ALA:HB2	1:E:417:VAL:HG21	1.97	0.46
1:E:478:GLY:N	1:E:479:PRO:HD2	2.30	0.46
1:A:569:THR:HG22	1:A:572:ASN:OD1	2.16	0.46
1:E:409:LYS:C	1:E:411:ALA:H	2.19	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:409:LYS:C	1:F:411:ALA:H	2.18	0.46
1:C:246:THR:HG23	1:C:250:GLN:NE2	2.30	0.46
2:B:783:ADP:H2'	2:B:783:ADP:N3	2.30	0.46
1:B:734:ALA:HB1	1:B:735:PRO:CD	2.45	0.46
1:E:444:PRO:HA	1:E:447:ASN:ND2	2.30	0.46
1:B:710:ARG:HG2	1:B:710:ARG:HH21	1.81	0.46
1:F:322:HIS:CE1	1:F:363:LEU:HD23	2.50	0.46
1:E:322:HIS:CE1	1:E:363:LEU:HD23	2.51	0.46
1:A:311:LEU:O	1:A:312:LYS:C	2.54	0.46
1:C:645:SER:O	1:C:647:THR:N	2.49	0.46
1:A:505:LEU:CD2	1:A:544:GLU:HG3	2.44	0.46
1:B:329:LYS:C	1:B:331:ARG:N	2.66	0.46
1:E:506:LEU:HD12	1:E:506:LEU:O	2.15	0.46
1:D:407:GLY:HA3	1:D:418:PHE:CZ	2.50	0.46
1:C:266:LYS:HG3	1:C:267:GLU:H	1.80	0.46
1:A:260:GLY:O	1:A:261:MET:CB	2.64	0.46
1:A:604:VAL:HG23	1:A:604:VAL:O	2.16	0.46
1:D:656:PHE:CG	1:D:657:HIS:N	2.84	0.46
1:E:642:TYR:CE1	1:E:709:GLY:HA3	2.51	0.46
1:D:481:ARG:O	1:D:481:ARG:HG2	2.16	0.46
1:E:355:PRO:O	1:E:358:VAL:HG22	2.15	0.46
1:C:569:THR:HG22	1:C:572:ASN:OD1	2.16	0.46
1:B:290:ARG:HH12	1:E:273:LEU:HD21	1.80	0.46
1:D:329:LYS:O	1:D:331:ARG:N	2.48	0.46
1:D:350:LEU:HD23	1:D:487:ILE:HD11	1.97	0.46
1:C:510:ILE:HG22	1:C:515:LEU:O	2.15	0.46
1:A:456:GLU:OE2	1:C:291:ASN:ND2	2.49	0.46
1:F:534:TYR:N	1:F:534:TYR:CD1	2.84	0.46
1:E:714:ILE:HG23	1:E:715:GLY:N	2.30	0.46
1:C:260:GLY:O	1:C:261:MET:CB	2.64	0.46
1:D:367:ILE:HG22	1:D:368:ALA:N	2.28	0.46
1:A:636:ALA:O	1:A:638:ALA:N	2.43	0.46
1:F:622:LEU:HB2	1:F:662:ILE:HG12	1.98	0.46
1:D:733:ILE:HA	1:D:756:ILE:O	2.16	0.46
2:A:783:ADP:O1A	2:A:783:ADP:O1B	2.34	0.46
1:D:656:PHE:C	1:D:658:GLU:N	2.70	0.46
1:C:736:LYS:C	1:C:738:ASN:H	2.17	0.46
1:F:380:LEU:HD12	1:F:423:ILE:HG23	1.97	0.46
1:A:341:LEU:O	1:A:343:LYS:N	2.49	0.46
1:D:307:ASP:HB3	1:D:309:LEU:HD21	1.98	0.46
1:C:546:GLN:OE1	1:C:577:ILE:HB	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:645:SER:O	1:D:647:THR:N	2.48	0.46
1:A:378:ILE:HD13	1:A:420:LEU:CD1	2.45	0.45
1:D:496:GLU:O	1:D:497:LYS:C	2.55	0.45
1:B:276:TYR:CE2	1:F:246:THR:CG2	3.00	0.45
1:A:496:GLU:O	1:A:500:ILE:HG13	2.16	0.45
1:F:636:ALA:C	1:F:638:ALA:H	2.19	0.45
1:D:341:LEU:O	1:D:343:LYS:N	2.49	0.45
1:D:350:LEU:HA	1:D:485:GLU:O	2.16	0.45
1:A:656:PHE:C	1:A:658:GLU:H	2.17	0.45
1:F:255:LYS:O	1:F:258:GLU:HB3	2.16	0.45
1:C:469:THR:HG22	1:C:470:ALA:H	1.81	0.45
1:D:260:GLY:O	1:D:261:MET:CB	2.63	0.45
1:A:680:ILE:HG22	1:A:705:ILE:CD1	2.46	0.45
1:D:489:ILE:H	1:D:489:ILE:HG12	1.58	0.45
1:B:311:LEU:O	1:B:312:LYS:C	2.54	0.45
1:B:497:LYS:HG2	1:B:540:VAL:HG12	1.99	0.45
1:F:675:GLY:N	1:F:676:PRO:CD	2.79	0.45
1:C:455:ILE:O	1:C:456:GLU:C	2.54	0.45
1:B:604:VAL:HG23	1:B:604:VAL:O	2.15	0.45
1:B:656:PHE:C	1:B:658:GLU:N	2.70	0.45
1:D:452:ASP:O	1:D:455:ILE:HG22	2.17	0.45
1:B:711:VAL:N	1:B:759:SER:O	2.47	0.45
1:B:478:GLY:N	1:B:479:PRO:HD2	2.31	0.45
1:D:357:GLY:H	2:D:783:ADP:PB	2.39	0.45
1:A:455:ILE:O	1:A:456:GLU:C	2.53	0.45
1:B:276:TYR:OH	1:F:247:GLY:CA	2.64	0.45
1:C:380:LEU:HD12	1:C:423:ILE:HG23	1.98	0.45
1:B:645:SER:O	1:B:647:THR:N	2.49	0.45
1:B:505:LEU:CD2	1:B:544:GLU:HG3	2.45	0.45
1:D:506:LEU:O	1:D:507:PRO:C	2.55	0.45
1:C:714:ILE:HB	1:C:735:PRO:HG2	1.98	0.45
1:A:562:GLU:O	1:A:563:ARG:C	2.55	0.45
1:B:373:ARG:NE	1:B:415:ASN:OD1	2.50	0.45
1:F:597:THR:O	1:F:700:GLY:HA2	2.16	0.45
1:E:642:TYR:CD2	1:E:761:LEU:HD12	2.52	0.45
1:C:341:LEU:HB3	1:E:514:GLY:O	2.17	0.45
1:F:635:SER:O	1:F:638:ALA:HB3	2.16	0.45
1:E:706:THR:OG1	1:E:710:ARG:HB2	2.15	0.45
1:B:308:LYS:O	1:B:309:LEU:HD23	2.17	0.45
1:B:441:VAL:O	1:B:441:VAL:HG22	2.16	0.45
1:A:276:TYR:CD1	1:A:277:GLU:N	2.84	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:276:TYR:CD1	1:D:277:GLU:N	2.85	0.45
1:C:274:ASN:O	1:C:276:TYR:N	2.48	0.45
1:C:276:TYR:CD1	1:C:277:GLU:N	2.84	0.45
1:C:424:ASP:OD1	1:C:424:ASP:N	2.50	0.45
1:F:292:TYR:OH	1:F:455:ILE:HA	2.17	0.45
1:F:414:LEU:C	1:F:416:PRO:HD3	2.37	0.45
1:A:579:LYS:C	1:A:579:LYS:HE2	2.37	0.45
1:E:311:LEU:O	1:E:312:LYS:C	2.55	0.45
1:F:295:TRP:HZ3	1:F:405:ILE:HG21	1.81	0.45
1:C:714:ILE:HA	1:C:714:ILE:HD12	1.79	0.45
1:F:276:TYR:CD1	1:F:277:GLU:N	2.84	0.45
1:C:255:LYS:O	1:C:258:GLU:HB3	2.16	0.45
1:E:656:PHE:C	1:E:658:GLU:N	2.70	0.45
1:B:560:ALA:O	1:B:562:GLU:N	2.50	0.45
1:E:452:ASP:O	1:E:455:ILE:HG22	2.17	0.45
1:E:647:THR:HG22	1:E:648:GLU:N	2.32	0.45
1:D:621:LYS:O	1:D:661:ASP:OD1	2.35	0.45
1:B:464:VAL:O	1:B:466:PHE:CD1	2.63	0.45
1:C:439:LEU:O	1:C:440:GLU:C	2.55	0.45
1:B:439:LEU:O	1:B:440:GLU:C	2.55	0.45
1:D:424:ASP:OD1	1:D:424:ASP:N	2.50	0.45
1:A:493:THR:HG21	1:A:748:SER:CB	2.46	0.45
1:C:373:ARG:NE	1:C:415:ASN:OD1	2.50	0.45
1:B:364:ALA:O	1:B:365:LYS:C	2.55	0.45
1:D:598:GLY:HA2	1:D:701:MET:O	2.17	0.45
1:B:495:ILE:HA	1:B:495:ILE:HD13	1.78	0.45
1:D:747:GLU:CD	1:D:747:GLU:H	2.18	0.45
1:D:423:ILE:HD13	1:D:423:ILE:HG21	1.62	0.45
1:D:506:LEU:CD2	1:D:522:LEU:HD21	2.44	0.45
1:F:412:GLY:C	1:F:413:LYS:HG2	2.37	0.45
1:B:613:VAL:HG23	1:B:685:ALA:HB1	1.99	0.45
1:F:266:LYS:HG3	1:F:267:GLU:H	1.81	0.45
1:D:599:LEU:N	1:D:599:LEU:HD22	2.32	0.45
1:D:298:ALA:O	1:D:299:LEU:O	2.35	0.45
1:A:280:PRO:HB2	1:A:281:SER:H	1.67	0.45
1:B:505:LEU:HD23	1:B:505:LEU:HA	1.38	0.45
1:A:569:THR:HG23	1:A:571:LYS:N	2.19	0.45
1:A:536:ARG:CG	1:A:536:ARG:NH1	2.65	0.45
1:F:419:LEU:O	1:F:421:ASP:N	2.50	0.45
1:B:714:ILE:HG23	1:B:715:GLY:N	2.31	0.45
1:C:616:SER:O	1:C:661:ASP:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:599:LEU:HD22	1:B:599:LEU:N	2.31	0.45
1:F:732:ILE:HD13	1:F:732:ILE:O	2.17	0.45
1:C:647:THR:HG22	1:C:648:GLU:N	2.31	0.45
1:F:505:LEU:HD23	1:F:505:LEU:HA	1.38	0.44
1:B:266:LYS:HG3	1:B:267:GLU:H	1.82	0.44
1:B:414:LEU:HD12	1:B:414:LEU:C	2.37	0.44
1:D:439:LEU:O	1:D:440:GLU:C	2.55	0.44
1:F:478:GLY:N	1:F:479:PRO:HD2	2.31	0.44
1:E:712:LEU:HB3	1:E:713:PRO:HD2	1.99	0.44
1:B:296:LEU:O	1:B:299:LEU:HD11	2.16	0.44
1:E:536:ARG:HH11	1:E:536:ARG:CB	2.30	0.44
1:C:322:HIS:HA	2:C:783:ADP:N1	2.32	0.44
1:D:602:THR:C	1:D:604:VAL:N	2.71	0.44
1:D:274:ASN:O	1:D:276:TYR:N	2.45	0.44
1:A:493:THR:O	1:A:494:GLU:C	2.54	0.44
1:F:380:LEU:HD12	1:F:423:ILE:CG2	2.47	0.44
1:E:546:GLN:OE1	1:E:577:ILE:HB	2.17	0.44
1:D:732:ILE:HG21	1:D:753:LEU:HD13	1.99	0.44
1:F:732:ILE:HG21	1:F:753:LEU:HD13	1.99	0.44
1:B:496:GLU:O	1:B:497:LYS:C	2.54	0.44
1:D:616:SER:O	1:D:661:ASP:N	2.49	0.44
1:C:265:VAL:O	1:C:457:GLU:OE1	2.35	0.44
1:C:478:GLY:N	1:C:479:PRO:HD2	2.31	0.44
1:B:267:GLU:HA	1:B:270:LEU:HG	1.98	0.44
1:D:362:SER:HB3	2:D:783:ADP:C5'	2.47	0.44
1:B:569:THR:HG23	1:B:571:LYS:N	2.21	0.44
1:C:416:PRO:HD2	1:C:464:VAL:HG13	1.99	0.44
1:D:702:THR:CG2	1:D:702:THR:O	2.65	0.44
1:D:714:ILE:HB	1:D:735:PRO:HG2	2.00	0.44
1:A:736:LYS:C	1:A:738:ASN:H	2.20	0.44
1:F:452:ASP:O	1:F:455:ILE:HG22	2.17	0.44
1:C:346:LYS:HG3	1:C:348:PRO:HD2	1.99	0.44
1:F:520:LEU:HA	1:F:566:ILE:O	2.17	0.44
1:D:599:LEU:O	1:D:720:LYS:HE2	2.17	0.44
1:E:710:ARG:HH21	1:E:710:ARG:HG2	1.82	0.44
1:A:550:ILE:O	1:A:551:CYS:C	2.54	0.44
1:D:364:ALA:O	1:D:365:LYS:C	2.56	0.44
1:B:350:LEU:HA	1:B:485:GLU:O	2.18	0.44
1:B:420:LEU:HD21	1:B:466:PHE:CD2	2.50	0.44
1:B:407:GLY:HA3	1:B:418:PHE:CZ	2.52	0.44
1:C:621:LYS:O	1:C:661:ASP:OD1	2.35	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:520:LEU:HA	1:B:566:ILE:O	2.17	0.44
1:C:423:ILE:HG21	1:C:423:ILE:HD13	1.76	0.44
1:D:590:GLU:HA	1:D:697:ARG:HD3	1.99	0.44
1:B:280:PRO:HB2	1:B:281:SER:H	1.67	0.44
1:C:637:GLN:HA	1:C:640:PHE:HB3	1.99	0.44
1:C:569:THR:HG23	1:C:572:ASN:H	1.82	0.44
1:E:506:LEU:HB3	1:E:507:PRO:CD	2.45	0.44
1:B:299:LEU:O	1:B:301:TRP:CD1	2.70	0.44
1:E:569:THR:HG23	1:E:571:LYS:N	2.21	0.44
1:C:267:GLU:HG3	1:C:270:LEU:HD12	1.99	0.44
1:E:736:LYS:C	1:E:738:ASN:H	2.19	0.44
1:A:656:PHE:C	1:A:658:GLU:N	2.71	0.44
1:A:497:LYS:HG2	1:A:540:VAL:HG12	2.00	0.44
1:F:368:ALA:CB	1:F:417:VAL:HG21	2.47	0.44
1:B:642:TYR:CD2	1:B:761:LEU:HD12	2.53	0.44
1:A:546:GLN:O	1:A:549:ALA:HB3	2.17	0.44
1:A:495:ILE:HA	1:A:495:ILE:HD13	1.82	0.44
1:C:409:LYS:C	1:C:411:ALA:H	2.21	0.44
1:C:283:SER:N	1:C:286:SER:HB3	2.33	0.44
2:E:783:ADP:H5'2	2:E:783:ADP:C8	2.53	0.44
1:A:579:LYS:NZ	1:A:579:LYS:H	2.16	0.44
1:B:562:GLU:O	1:B:563:ARG:C	2.56	0.44
1:E:562:GLU:O	1:E:563:ARG:C	2.56	0.44
1:F:705:ILE:HD11	1:F:761:LEU:CD2	2.47	0.44
1:C:342:THR:HG22	1:C:344:SER:O	2.18	0.44
1:C:298:ALA:O	1:C:299:LEU:C	2.55	0.44
1:A:505:LEU:HA	1:A:505:LEU:HD23	1.45	0.44
1:B:522:LEU:HB3	1:B:568:VAL:CG1	2.43	0.44
1:B:262:PRO:HG2	1:B:302:THR:OG1	2.17	0.44
1:E:423:ILE:HG22	1:E:426:MET:HE1	1.99	0.44
1:E:604:VAL:HG23	1:E:604:VAL:O	2.17	0.44
1:E:597:THR:O	1:E:700:GLY:HA2	2.17	0.44
1:F:317:LEU:HD23	1:F:317:LEU:C	2.38	0.44
1:E:455:ILE:HG23	1:E:455:ILE:O	2.18	0.44
1:A:548:ALA:O	1:A:549:ALA:C	2.54	0.44
1:C:602:THR:C	1:C:604:VAL:N	2.70	0.44
1:D:586:GLN:HG3	1:D:698:GLU:HG2	2.00	0.44
1:E:255:LYS:O	1:E:258:GLU:HB3	2.18	0.44
1:E:295:TRP:O	1:E:299:LEU:HG	2.18	0.44
1:B:480:LEU:O	1:B:483:ARG:N	2.50	0.44
1:D:342:THR:HG22	1:D:344:SER:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:506:LEU:HD12	1:D:506:LEU:C	2.38	0.44
1:A:569:THR:HG23	1:A:572:ASN:H	1.82	0.44
1:E:300:PRO:HG3	1:E:413:LYS:N	2.32	0.44
1:D:441:VAL:HG22	1:D:441:VAL:O	2.17	0.44
1:B:736:LYS:C	1:B:738:ASN:H	2.20	0.44
1:F:579:LYS:H	1:F:579:LYS:NZ	2.15	0.44
1:D:255:LYS:O	1:D:258:GLU:HB3	2.17	0.44
1:C:532:ARG:HG2	1:C:584:TYR:CE2	2.53	0.44
1:C:675:GLY:N	1:C:676:PRO:CD	2.81	0.44
1:A:298:ALA:O	1:A:299:LEU:C	2.54	0.44
1:A:711:VAL:N	1:A:759:SER:O	2.47	0.44
1:A:675:GLY:N	1:A:676:PRO:CD	2.81	0.44
1:D:506:LEU:HD12	1:D:510:ILE:CG1	2.48	0.43
1:E:569:THR:HG23	1:E:572:ASN:H	1.82	0.43
1:B:546:GLN:O	1:B:549:ALA:HB3	2.18	0.43
1:D:756:ILE:HG13	1:D:767:HIS:CD2	2.54	0.43
1:A:439:LEU:O	1:A:440:GLU:C	2.55	0.43
1:A:267:GLU:HA	1:A:270:LEU:HG	1.99	0.43
1:A:271:LYS:CA	1:A:274:ASN:HB3	2.46	0.43
1:A:602:THR:C	1:A:604:VAL:H	2.21	0.43
1:F:346:LYS:HG3	1:F:348:PRO:HD2	2.00	0.43
1:A:493:THR:CG2	1:A:748:SER:HB2	2.47	0.43
1:C:333:LEU:HD23	1:C:336:LEU:HD12	2.00	0.43
1:B:335:TYR:O	1:B:335:TYR:CD2	2.71	0.43
1:A:357:GLY:H	2:A:783:ADP:PB	2.38	0.43
1:A:469:THR:HG22	1:A:470:ALA:H	1.83	0.43
1:C:557:ALA:CB	1:C:566:ILE:HD11	2.48	0.43
1:E:367:ILE:O	1:E:371:LEU:HD13	2.17	0.43
1:E:637:GLN:HA	1:E:640:PHE:HB3	2.00	0.43
1:D:712:LEU:HB3	1:D:713:PRO:CD	2.47	0.43
1:C:350:LEU:HA	1:C:485:GLU:O	2.18	0.43
1:E:350:LEU:CD1	1:E:350:LEU:H	2.09	0.43
1:A:496:GLU:O	1:A:497:LYS:C	2.56	0.43
1:C:642:TYR:CE1	1:C:709:GLY:HA3	2.52	0.43
1:B:514:GLY:O	1:E:341:LEU:HD13	2.17	0.43
1:A:536:ARG:CB	1:A:536:ARG:NH1	2.82	0.43
1:A:412:GLY:C	1:A:413:LYS:HG2	2.37	0.43
1:F:455:ILE:O	1:F:455:ILE:HG23	2.18	0.43
1:E:602:THR:CG2	1:E:604:VAL:HG22	2.49	0.43
1:C:562:GLU:O	1:C:563:ARG:C	2.56	0.43
1:E:616:SER:O	1:E:661:ASP:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:452:ASP:O	1:C:455:ILE:HG22	2.18	0.43
1:C:637:GLN:O	1:C:637:GLN:HG2	2.18	0.43
1:A:350:LEU:HA	1:A:485:GLU:O	2.19	0.43
1:E:439:LEU:O	1:E:440:GLU:C	2.57	0.43
1:D:439:LEU:H	1:D:439:LEU:CD2	2.24	0.43
1:F:439:LEU:CD2	1:F:439:LEU:H	2.26	0.43
1:C:493:THR:O	1:C:494:GLU:C	2.57	0.43
1:E:639:ALA:HB1	1:E:683:ALA:HB2	2.00	0.43
1:C:589:THR:O	1:C:697:ARG:NE	2.52	0.43
1:D:322:HIS:CE1	1:D:363:LEU:HD23	2.53	0.43
1:E:342:THR:HG22	1:E:344:SER:O	2.18	0.43
1:D:409:LYS:C	1:D:411:ALA:H	2.20	0.43
1:A:455:ILE:HG23	1:A:455:ILE:O	2.18	0.43
1:C:270:LEU:CD2	1:C:296:LEU:HD22	2.44	0.43
1:B:613:VAL:O	1:E:708:ARG:HD3	2.17	0.43
1:C:412:GLY:C	1:C:413:LYS:HG2	2.39	0.43
1:A:714:ILE:HB	1:A:735:PRO:HG2	2.00	0.43
1:A:739:GLU:C	1:A:741:ASP:H	2.21	0.43
1:B:602:THR:HG22	1:B:603:THR:N	2.33	0.43
1:B:735:PRO:O	1:B:738:ASN:HB2	2.18	0.43
2:E:783:ADP:C8	2:E:783:ADP:C5'	3.01	0.43
1:E:732:ILE:HD13	1:E:732:ILE:O	2.19	0.43
1:C:752:GLY:O	1:C:753:LEU:HD23	2.19	0.43
1:D:546:GLN:O	1:D:549:ALA:HB3	2.18	0.43
1:C:693:ARG:O	1:C:694:ALA:HB2	2.19	0.43
1:B:552:ARG:O	1:B:553:LYS:C	2.57	0.43
1:B:493:THR:O	1:B:494:GLU:C	2.57	0.43
1:B:267:GLU:HG3	1:B:270:LEU:HD12	2.01	0.43
1:B:299:LEU:CD1	1:B:301:TRP:NE1	2.82	0.43
1:E:300:PRO:HB2	1:E:414:LEU:CB	2.46	0.43
1:F:357:GLY:O	1:F:539:GLY:HA2	2.18	0.43
1:B:362:SER:HB3	2:B:783:ADP:H5'2	2.01	0.43
1:E:359:GLY:O	1:E:360:LYS:C	2.55	0.43
1:A:602:THR:C	1:A:604:VAL:N	2.72	0.43
1:F:656:PHE:C	1:F:658:GLU:N	2.71	0.43
1:D:311:LEU:O	1:D:312:LYS:C	2.57	0.43
1:B:416:PRO:HD2	1:B:464:VAL:HG13	2.01	0.43
1:F:579:LYS:C	1:F:579:LYS:HE2	2.38	0.43
1:D:293:ILE:O	1:D:297:VAL:HG23	2.19	0.43
1:E:602:THR:O	1:E:604:VAL:N	2.52	0.43
1:C:338:VAL:HG23	1:E:555:ALA:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:732:ILE:O	1:C:732:ILE:HD13	2.18	0.43
1:E:611:ILE:HG23	1:E:665:HIS:O	2.19	0.43
1:C:572:ASN:O	1:C:573:LEU:C	2.57	0.43
1:E:416:PRO:CD	1:E:464:VAL:HG13	2.49	0.43
1:C:378:ILE:HD13	1:C:420:LEU:HD12	1.99	0.43
1:F:350:LEU:HA	1:F:485:GLU:O	2.19	0.43
1:F:439:LEU:O	1:F:440:GLU:C	2.57	0.43
1:B:602:THR:CG2	1:B:604:VAL:HG22	2.48	0.43
1:F:274:ASN:O	1:F:276:TYR:N	2.46	0.43
1:D:332:ILE:CG2	1:D:367:ILE:HD11	2.49	0.43
1:A:599:LEU:HD22	1:A:599:LEU:N	2.32	0.43
1:D:647:THR:HG22	1:D:648:GLU:N	2.34	0.43
1:F:411:ALA:O	1:F:412:GLY:C	2.57	0.43
1:A:283:SER:N	1:A:286:SER:HB3	2.34	0.43
1:A:476:ILE:HG21	1:A:481:ARG:HB2	2.00	0.43
1:F:712:LEU:HB3	1:F:713:PRO:CD	2.48	0.43
1:F:747:GLU:CD	1:F:747:GLU:H	2.20	0.43
1:E:269:ALA:CB	1:E:457:GLU:OE1	2.67	0.43
1:B:301:TRP:O	1:B:414:LEU:HD21	2.19	0.42
1:D:329:LYS:C	1:D:331:ARG:H	2.22	0.42
1:F:569:THR:HG23	1:F:571:LYS:N	2.19	0.42
1:E:300:PRO:HG3	1:E:412:GLY:C	2.40	0.42
1:B:733:ILE:HA	1:B:756:ILE:O	2.19	0.42
1:D:411:ALA:O	1:D:412:GLY:C	2.57	0.42
1:B:593:VAL:HG13	1:B:693:ARG:O	2.19	0.42
1:B:273:LEU:O	1:B:276:TYR:HB2	2.19	0.42
1:D:267:GLU:HA	1:D:270:LEU:HG	2.00	0.42
1:E:489:ILE:H	1:E:489:ILE:HG12	1.65	0.42
1:A:656:PHE:CD2	1:A:657:HIS:N	2.87	0.42
1:A:333:LEU:HD23	1:A:336:LEU:HD12	2.01	0.42
1:D:642:TYR:CE1	1:D:709:GLY:HA3	2.54	0.42
1:B:637:GLN:HA	1:B:640:PHE:HB3	2.01	0.42
1:F:622:LEU:HB2	1:F:662:ILE:CG1	2.49	0.42
1:E:373:ARG:NE	1:E:415:ASN:OD1	2.52	0.42
1:B:622:LEU:HB2	1:B:662:ILE:HG12	2.01	0.42
1:E:682:MET:HE3	1:E:682:MET:HB3	1.68	0.42
1:F:678:ALA:O	1:F:682:MET:HG2	2.19	0.42
1:B:686:LEU:HD22	1:B:686:LEU:O	2.19	0.42
1:A:329:LYS:C	1:A:331:ARG:H	2.22	0.42
1:B:293:ILE:O	1:B:297:VAL:HG23	2.19	0.42
1:D:329:LYS:O	1:D:330:GLU:C	2.57	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:505:LEU:HD23	1:C:505:LEU:HA	1.43	0.42
1:C:505:LEU:CD2	1:C:544:GLU:HG3	2.47	0.42
1:B:546:GLN:OE1	1:B:577:ILE:HB	2.20	0.42
1:F:464:VAL:CG1	1:F:466:PHE:CE1	3.02	0.42
1:E:516:LYS:HZ1	1:E:516:LYS:HA	1.82	0.42
1:B:277:GLU:OE1	1:F:246:THR:N	2.52	0.42
1:E:656:PHE:CD2	1:E:657:HIS:N	2.87	0.42
1:B:579:LYS:C	1:B:579:LYS:HE2	2.40	0.42
1:B:647:THR:HG23	1:B:652:ILE:HG23	2.00	0.42
1:A:546:GLN:OE1	1:A:577:ILE:HB	2.19	0.42
1:E:550:ILE:O	1:E:551:CYS:C	2.58	0.42
1:D:403:ARG:O	1:D:403:ARG:CG	2.67	0.42
1:B:290:ARG:NH1	1:E:273:LEU:HD21	2.34	0.42
1:C:464:VAL:O	1:C:466:PHE:CD1	2.68	0.42
1:D:439:LEU:HD13	1:D:480:LEU:HD13	2.00	0.42
1:E:346:LYS:HG3	1:E:348:PRO:HD2	2.01	0.42
1:C:346:LYS:HZ1	1:E:513:HIS:CE1	2.36	0.42
1:D:256:ILE:CD1	1:D:293:ILE:HD11	2.48	0.42
1:F:562:GLU:O	1:F:563:ARG:C	2.58	0.42
1:C:597:THR:O	1:C:700:GLY:HA2	2.19	0.42
1:F:647:THR:HG22	1:F:648:GLU:N	2.34	0.42
1:B:455:ILE:HG23	1:B:455:ILE:O	2.19	0.42
1:D:712:LEU:HB3	1:D:713:PRO:HD2	2.01	0.42
1:A:342:THR:HG22	1:A:344:SER:O	2.20	0.42
1:B:712:LEU:HB3	1:B:713:PRO:HD2	2.01	0.42
1:B:569:THR:HG23	1:B:572:ASN:H	1.84	0.42
1:D:536:ARG:NH1	1:D:536:ARG:CB	2.82	0.42
1:A:456:GLU:O	1:A:457:GLU:HB2	2.20	0.42
1:B:359:GLY:HA2	2:B:783:ADP:H5'2	2.01	0.42
1:D:270:LEU:HD21	1:D:296:LEU:CD2	2.45	0.42
1:C:646:LYS:CD	1:C:646:LYS:H	2.32	0.42
1:E:298:ALA:O	1:E:299:LEU:C	2.57	0.42
1:C:455:ILE:O	1:C:455:ILE:HG23	2.18	0.42
1:A:373:ARG:NE	1:A:415:ASN:OD1	2.52	0.42
1:A:593:VAL:HG13	1:A:693:ARG:O	2.19	0.42
1:B:283:SER:N	1:B:286:SER:HB3	2.34	0.42
1:E:596:VAL:HG23	1:E:685:ALA:HB2	2.00	0.42
1:F:378:ILE:HD13	1:F:420:LEU:HD12	2.02	0.42
1:F:440:GLU:HG3	1:F:446:GLN:OE1	2.19	0.42
1:E:299:LEU:O	1:E:301:TRP:CE2	2.73	0.42
1:D:562:GLU:O	1:D:563:ARG:C	2.56	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:408:MET:N	1:B:408:MET:HE2	2.35	0.42
1:C:305:THR:O	1:C:307:ASP:N	2.52	0.42
1:A:506:LEU:O	1:A:507:PRO:C	2.58	0.42
1:A:522:LEU:HB3	1:A:568:VAL:CG1	2.45	0.42
1:E:505:LEU:HD23	1:E:505:LEU:HA	1.38	0.42
1:C:536:ARG:NH1	1:C:536:ARG:HB2	2.34	0.42
1:A:733:ILE:HA	1:A:756:ILE:O	2.19	0.42
1:F:283:SER:N	1:F:286:SER:HB3	2.35	0.42
1:D:602:THR:C	1:D:604:VAL:H	2.23	0.42
1:C:279:ILE:HA	1:C:280:PRO:HA	1.86	0.42
1:E:714:ILE:HB	1:E:735:PRO:HG2	2.00	0.42
1:B:656:PHE:CD2	1:B:657:HIS:N	2.88	0.42
1:A:561:GLU:O	1:A:562:GLU:HB2	2.19	0.42
1:E:561:GLU:O	1:E:562:GLU:HB2	2.19	0.42
1:E:599:LEU:N	1:E:599:LEU:HD22	2.34	0.42
1:F:599:LEU:O	1:F:720:LYS:HE2	2.20	0.42
1:E:365:LYS:HG3	1:E:375:PHE:CZ	2.55	0.42
1:C:311:LEU:O	1:C:312:LYS:C	2.56	0.42
1:C:627:LYS:O	1:C:627:LYS:HG3	2.20	0.42
1:F:342:THR:HG22	1:F:344:SER:O	2.20	0.42
1:B:460:ASP:O	1:B:461:LEU:HD23	2.18	0.42
1:F:496:GLU:O	1:F:497:LYS:C	2.58	0.42
1:A:266:LYS:HG3	1:A:267:GLU:H	1.82	0.42
1:F:256:ILE:CD1	1:F:293:ILE:HD11	2.49	0.42
1:D:279:ILE:HA	1:D:280:PRO:HA	1.86	0.42
1:C:271:LYS:CA	1:C:274:ASN:HB3	2.48	0.42
1:A:262:PRO:HD2	1:A:301:TRP:HB3	2.01	0.42
1:F:299:LEU:HA	1:F:300:PRO:HD3	1.69	0.42
1:D:283:SER:N	1:D:286:SER:HB3	2.34	0.42
1:F:705:ILE:HA	1:F:705:ILE:HD12	1.74	0.42
1:E:622:LEU:HB2	1:E:662:ILE:HG12	2.02	0.42
1:B:329:LYS:O	1:B:331:ARG:N	2.53	0.42
1:C:602:THR:C	1:C:604:VAL:H	2.22	0.42
1:B:271:LYS:CA	1:B:274:ASN:HB3	2.46	0.42
1:D:469:THR:HG22	1:D:470:ALA:N	2.34	0.42
1:A:480:LEU:O	1:A:483:ARG:N	2.53	0.42
1:A:747:GLU:N	1:A:747:GLU:CD	2.72	0.42
1:C:706:THR:OG1	1:C:710:ARG:HB2	2.19	0.42
1:A:573:LEU:HA	1:A:573:LEU:HD12	1.93	0.42
1:E:411:ALA:O	1:E:412:GLY:C	2.58	0.42
1:C:335:TYR:CD2	1:C:335:TYR:O	2.73	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:283:SER:N	1:E:286:SER:HB3	2.34	0.42
1:B:561:GLU:O	1:B:562:GLU:HB2	2.18	0.42
1:B:423:ILE:HG22	1:B:426:MET:HE1	2.00	0.42
1:D:579:LYS:HE2	1:D:579:LYS:C	2.39	0.42
1:C:593:VAL:HG13	1:C:693:ARG:O	2.19	0.42
1:D:705:ILE:HD11	1:D:761:LEU:CD2	2.50	0.42
1:B:486:ILE:CG2	1:B:487:ILE:N	2.82	0.42
1:D:505:LEU:HA	1:D:505:LEU:HD23	1.37	0.42
1:E:589:THR:O	1:E:697:ARG:CD	2.68	0.42
1:E:412:GLY:C	1:E:413:LYS:HG2	2.39	0.42
1:C:293:ILE:O	1:C:297:VAL:HG23	2.18	0.42
1:A:441:VAL:HG22	1:A:441:VAL:O	2.19	0.42
1:D:739:GLU:C	1:D:741:ASP:N	2.73	0.42
1:F:293:ILE:O	1:F:297:VAL:HG23	2.20	0.42
1:F:682:MET:HE3	1:F:682:MET:HB3	1.77	0.42
1:A:611:ILE:HD12	1:A:681:THR:CG2	2.50	0.42
1:B:342:THR:HG22	1:B:344:SER:O	2.20	0.42
1:C:329:LYS:O	1:C:332:ILE:N	2.41	0.41
1:E:506:LEU:O	1:E:507:PRO:C	2.58	0.41
1:F:536:ARG:CB	1:F:536:ARG:HH11	2.32	0.41
1:D:573:LEU:CG	1:D:577:ILE:HD11	2.50	0.41
1:F:519:ASN:HD22	1:F:519:ASN:HA	1.53	0.41
1:A:300:PRO:HG3	1:A:412:GLY:HA2	2.02	0.41
1:F:329:LYS:O	1:F:330:GLU:C	2.58	0.41
1:A:516:LYS:HZ1	1:A:516:LYS:HA	1.82	0.41
1:A:293:ILE:O	1:A:297:VAL:HG23	2.20	0.41
1:A:294:ASP:C	1:A:296:LEU:N	2.72	0.41
1:F:267:GLU:HA	1:F:270:LEU:HG	2.02	0.41
1:F:294:ASP:C	1:F:296:LEU:N	2.73	0.41
1:E:423:ILE:C	1:E:424:ASP:OD1	2.58	0.41
1:D:368:ALA:CB	1:D:417:VAL:HG21	2.48	0.41
1:C:680:ILE:HG22	1:C:705:ILE:HD13	2.02	0.41
1:B:732:ILE:HG21	1:B:753:LEU:HD13	2.02	0.41
1:B:747:GLU:N	1:B:747:GLU:CD	2.73	0.41
1:C:747:GLU:N	1:C:747:GLU:CD	2.73	0.41
1:C:355:PRO:O	1:C:358:VAL:HG22	2.20	0.41
1:D:495:ILE:HA	1:D:495:ILE:HD13	1.87	0.41
1:F:737:ASP:N	1:F:737:ASP:OD2	2.53	0.41
1:A:547:LEU:HA	1:A:547:LEU:HD23	1.78	0.41
1:F:341:LEU:O	1:F:343:LYS:N	2.53	0.41
1:D:496:GLU:O	1:D:500:ILE:HG13	2.18	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:734:ALA:HB1	1:D:735:PRO:CD	2.51	0.41
1:C:656:PHE:CD2	1:C:657:HIS:N	2.88	0.41
1:E:579:LYS:HE2	1:E:579:LYS:C	2.41	0.41
1:B:705:ILE:HA	1:B:705:ILE:HD12	1.75	0.41
1:E:350:LEU:HD23	1:E:487:ILE:HD11	2.02	0.41
1:B:693:ARG:O	1:B:694:ALA:HB2	2.19	0.41
1:E:736:LYS:HA	1:E:757:LEU:HB3	2.03	0.41
1:F:423:ILE:HG21	1:F:423:ILE:HD13	1.78	0.41
1:A:336:LEU:CD2	1:A:371:LEU:HD11	2.51	0.41
1:B:705:ILE:HD11	1:B:761:LEU:CD2	2.49	0.41
1:D:675:GLY:N	1:D:676:PRO:CD	2.83	0.41
1:C:529:ASP:O	1:C:530:ILE:C	2.58	0.41
1:A:622:LEU:HB2	1:A:662:ILE:HG12	2.03	0.41
1:D:547:LEU:HA	1:D:547:LEU:HD23	1.79	0.41
1:D:558:ILE:H	1:D:558:ILE:HG12	1.65	0.41
1:C:506:LEU:HD12	1:C:510:ILE:CG1	2.49	0.41
1:C:440:GLU:HG3	1:C:446:GLN:OE1	2.20	0.41
1:F:424:ASP:OD1	1:F:424:ASP:N	2.53	0.41
1:D:636:ALA:C	1:D:638:ALA:N	2.73	0.41
1:D:455:ILE:O	1:D:455:ILE:HG23	2.19	0.41
1:E:329:LYS:O	1:E:331:ARG:N	2.54	0.41
1:A:355:PRO:O	1:A:358:VAL:HG22	2.20	0.41
1:D:622:LEU:HB2	1:D:662:ILE:HG12	2.02	0.41
1:A:710:ARG:HG2	1:A:710:ARG:HH21	1.85	0.41
1:D:707:LEU:HD23	1:D:707:LEU:HA	1.92	0.41
1:B:412:GLY:C	1:B:413:LYS:HG2	2.39	0.41
1:C:267:GLU:HA	1:C:270:LEU:HB2	2.02	0.41
1:E:266:LYS:HG3	1:E:267:GLU:H	1.81	0.41
1:B:419:LEU:O	1:B:421:ASP:N	2.53	0.41
1:A:359:GLY:O	1:A:360:LYS:C	2.59	0.41
1:B:352:LEU:CD2	1:B:489:ILE:HD11	2.50	0.41
1:E:262:PRO:HD2	1:E:301:TRP:HB2	2.03	0.41
1:A:417:VAL:HG22	1:A:465:LEU:HB3	2.02	0.41
1:D:474:ALA:O	1:D:476:ILE:O	2.38	0.41
1:C:579:LYS:HE2	1:C:579:LYS:C	2.40	0.41
1:C:584:TYR:CD1	1:C:584:TYR:O	2.73	0.41
1:C:561:GLU:O	1:C:562:GLU:HB2	2.20	0.41
1:C:551:CYS:O	1:C:554:ALA:HB3	2.20	0.41
1:E:536:ARG:NH1	1:E:536:ARG:HG3	2.14	0.41
1:E:464:VAL:O	1:E:466:PHE:CD1	2.64	0.41
1:D:412:GLY:C	1:D:413:LYS:HG2	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:267:GLU:HA	1:C:270:LEU:HG	2.01	0.41
1:A:735:PRO:O	1:A:738:ASN:HB2	2.19	0.41
1:E:352:LEU:CD2	1:E:489:ILE:HD11	2.47	0.41
1:E:573:LEU:CG	1:E:577:ILE:HD11	2.51	0.41
1:E:717:LEU:HA	1:E:717:LEU:HD23	1.87	0.41
1:C:364:ALA:O	1:C:365:LYS:C	2.58	0.41
1:D:555:ALA:O	1:D:556:LYS:C	2.58	0.41
1:C:569:THR:HG22	1:C:572:ASN:H	1.86	0.41
1:E:273:LEU:O	1:E:276:TYR:HB2	2.20	0.41
1:D:460:ASP:O	1:D:461:LEU:HD23	2.20	0.41
1:A:414:LEU:HD12	1:A:414:LEU:C	2.41	0.41
1:B:276:TYR:HD1	1:B:277:GLU:N	2.17	0.41
1:A:736:LYS:HA	1:A:757:LEU:HB3	2.03	0.41
1:F:739:GLU:C	1:F:741:ASP:N	2.74	0.41
1:C:476:ILE:HG21	1:C:481:ARG:HB2	2.02	0.41
1:C:599:LEU:O	1:C:720:LYS:HE2	2.21	0.41
1:D:367:ILE:O	1:D:371:LEU:HD13	2.21	0.41
1:F:637:GLN:HA	1:F:640:PHE:HB3	2.02	0.41
1:E:678:ALA:O	1:E:682:MET:HG2	2.20	0.41
1:A:712:LEU:HB3	1:A:713:PRO:HD2	2.03	0.41
1:D:639:ALA:HB1	1:D:683:ALA:HA	2.03	0.41
1:B:506:LEU:CD1	1:B:506:LEU:C	2.88	0.41
1:D:506:LEU:HB3	1:D:507:PRO:CD	2.48	0.41
1:C:411:ALA:O	1:C:412:GLY:C	2.59	0.41
1:B:341:LEU:HB3	1:F:514:GLY:O	2.20	0.41
1:A:551:CYS:O	1:A:554:ALA:HB3	2.21	0.41
1:C:678:ALA:O	1:C:682:MET:HG2	2.21	0.41
1:F:567:THR:HG22	1:F:567:THR:O	2.21	0.41
1:E:271:LYS:CA	1:E:274:ASN:HB3	2.45	0.41
1:D:572:ASN:O	1:D:573:LEU:C	2.59	0.41
1:B:440:GLU:HG3	1:B:446:GLN:OE1	2.21	0.41
1:C:602:THR:HG22	1:C:603:THR:N	2.35	0.41
1:F:271:LYS:CA	1:F:274:ASN:HB3	2.46	0.41
1:E:359:GLY:HA2	2:E:783:ADP:H5'1	2.03	0.41
1:B:489:ILE:H	1:B:489:ILE:HG12	1.49	0.41
1:F:656:PHE:CD2	1:F:657:HIS:N	2.89	0.41
1:C:469:THR:CG2	1:C:470:ALA:N	2.82	0.41
1:B:332:ILE:CG2	1:B:367:ILE:HD11	2.51	0.41
1:A:761:LEU:HD23	1:A:761:LEU:HA	1.83	0.41
1:E:520:LEU:HA	1:E:566:ILE:O	2.21	0.41
1:F:561:GLU:O	1:F:562:GLU:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:305:THR:CG2	1:B:306:ASP:N	2.83	0.41
1:E:693:ARG:HB3	1:E:694:ALA:H	1.73	0.41
1:D:642:TYR:CD2	1:D:761:LEU:HD12	2.56	0.41
1:B:761:LEU:HA	1:B:761:LEU:HD23	1.95	0.41
1:A:304:GLU:O	1:A:304:GLU:HG2	2.20	0.41
1:A:616:SER:O	1:A:661:ASP:N	2.54	0.41
1:E:705:ILE:HD11	1:E:761:LEU:CD2	2.51	0.41
1:B:478:GLY:N	1:B:479:PRO:CD	2.84	0.41
1:D:298:ALA:O	1:D:299:LEU:C	2.59	0.41
1:A:364:ALA:O	1:A:365:LYS:C	2.56	0.41
1:F:707:LEU:HA	1:F:707:LEU:HD23	1.90	0.41
1:C:711:VAL:N	1:C:759:SER:O	2.51	0.41
1:B:598:GLY:HA2	1:B:701:MET:O	2.21	0.41
1:D:650:LEU:HD11	1:D:765:LEU:HD13	2.03	0.41
1:A:589:THR:O	1:A:590:GLU:CD	2.59	0.41
1:E:279:ILE:HA	1:E:280:PRO:HA	1.87	0.41
1:A:536:ARG:HB2	1:A:536:ARG:NH1	2.36	0.41
1:A:536:ARG:HG3	1:A:536:ARG:NH1	2.20	0.41
1:A:403:ARG:N	1:A:405:ILE:HG13	2.36	0.41
1:E:267:GLU:HA	1:E:270:LEU:HG	2.01	0.41
1:C:276:TYR:HD1	1:C:277:GLU:N	2.19	0.41
1:F:602:THR:C	1:F:604:VAL:N	2.75	0.41
1:D:752:GLY:O	1:D:753:LEU:HD23	2.21	0.41
1:D:551:CYS:O	1:D:554:ALA:HB3	2.21	0.41
1:B:622:LEU:HB2	1:B:662:ILE:CG1	2.51	0.41
1:D:403:ARG:HG2	1:D:403:ARG:O	2.21	0.41
1:C:710:ARG:HG2	1:C:710:ARG:HH21	1.86	0.41
1:B:294:ASP:C	1:B:296:LEU:N	2.72	0.40
1:E:536:ARG:NH2	1:E:583:ARG:O	2.47	0.40
1:C:256:ILE:CD1	1:C:293:ILE:HD11	2.46	0.40
1:B:602:THR:C	1:B:604:VAL:N	2.74	0.40
1:B:656:PHE:CE2	1:B:690:LEU:HD11	2.56	0.40
1:F:367:ILE:HG22	1:F:368:ALA:N	2.35	0.40
1:F:557:ALA:CB	1:F:566:ILE:HD11	2.50	0.40
1:A:557:ALA:CB	1:A:566:ILE:HD11	2.50	0.40
1:C:639:ALA:HB1	1:C:683:ALA:HA	2.04	0.40
1:C:329:LYS:C	1:C:331:ARG:H	2.22	0.40
1:A:329:LYS:O	1:A:330:GLU:C	2.59	0.40
1:D:331:ARG:NH1	1:D:485:GLU:OE1	2.46	0.40
1:B:536:ARG:NH1	1:B:536:ARG:CB	2.84	0.40
1:C:555:ALA:O	1:C:556:LYS:C	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:359:GLY:HA2	2:A:783:ADP:O5'	2.21	0.40
1:A:341:LEU:HD13	1:C:514:GLY:O	2.21	0.40
1:F:349:ILE:O	1:F:484:MET:HB2	2.21	0.40
1:C:708:ARG:NH2	1:E:593:VAL:HB	2.36	0.40
1:D:693:ARG:O	1:D:694:ALA:HB2	2.21	0.40
1:C:586:GLN:HB3	1:C:697:ARG:HE	1.86	0.40
1:D:373:ARG:NE	1:D:415:ASN:OD1	2.54	0.40
1:A:678:ALA:O	1:A:682:MET:HG2	2.21	0.40
1:B:572:ASN:O	1:B:573:LEU:C	2.60	0.40
1:D:534:TYR:CD2	1:D:577:ILE:HD12	2.56	0.40
1:D:440:GLU:HG3	1:D:446:GLN:OE1	2.21	0.40
1:A:270:LEU:CD2	1:A:296:LEU:HD22	2.48	0.40
1:D:267:GLU:HG3	1:D:270:LEU:HD12	2.04	0.40
1:A:714:ILE:HD12	1:A:714:ILE:HA	1.79	0.40
1:D:646:LYS:H	1:D:646:LYS:CD	2.31	0.40
1:E:656:PHE:CE2	1:E:690:LEU:HD11	2.56	0.40
1:B:367:ILE:HG22	1:B:368:ALA:N	2.36	0.40
1:C:533:TYR:CB	1:C:580:ARG:HD2	2.50	0.40
1:D:307:ASP:O	1:D:309:LEU:HG	2.21	0.40
1:B:645:SER:HA	1:F:616:SER:HA	2.03	0.40
1:F:355:PRO:O	1:F:358:VAL:HG22	2.21	0.40
1:C:687:VAL:O	1:C:691:THR:HG23	2.21	0.40
1:C:537:GLU:HG3	1:C:539:GLY:O	2.22	0.40
1:B:547:LEU:HD23	1:B:547:LEU:HA	1.76	0.40
1:B:464:VAL:CG1	1:B:466:PHE:CE1	3.04	0.40
1:E:267:GLU:HG3	1:E:270:LEU:HD12	2.03	0.40
1:A:262:PRO:HD2	1:A:301:TRP:CB	2.52	0.40
1:F:300:PRO:C	1:F:301:TRP:CG	2.94	0.40
1:B:560:ALA:O	1:B:561:GLU:C	2.59	0.40
1:D:526:ALA:O	1:D:530:ILE:HG13	2.21	0.40
1:A:478:GLY:N	1:A:479:PRO:CD	2.84	0.40
1:E:478:GLY:N	1:E:479:PRO:CD	2.85	0.40
1:D:483:ARG:HB3	1:D:483:ARG:NH2	2.37	0.40
1:A:510:ILE:HG22	1:A:515:LEU:O	2.21	0.40
1:E:613:VAL:HG13	1:E:664:ILE:HG12	2.02	0.40
1:A:408:MET:O	1:A:411:ALA:N	2.50	0.40
1:E:440:GLU:HG3	1:E:446:GLN:OE1	2.20	0.40
1:C:493:THR:CG2	1:C:748:SER:HB2	2.47	0.40
1:B:403:ARG:N	1:B:405:ILE:HG13	2.36	0.40
1:C:362:SER:HB2	2:C:783:ADP:C5'	2.49	0.40
1:F:276:TYR:HD1	1:F:277:GLU:N	2.19	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:561:GLU:O	1:D:562:GLU:HB2	2.21	0.40
1:B:305:THR:HG22	1:B:306:ASP:N	2.36	0.40
1:E:611:ILE:HD12	1:E:681:THR:HG22	2.02	0.40
1:E:622:LEU:HB2	1:E:662:ILE:CG1	2.51	0.40
1:A:302:THR:O	1:A:303:ASP:O	2.40	0.40
1:D:552:ARG:O	1:D:553:LYS:C	2.60	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:D:555:ALA:O	1:F:511:LYS:NZ[2_646]	2.14	0.06

## 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	490/543 (90%)	350 (71%)	97 (20%)	43 (9%)	1	10
1	B	490/543 (90%)	354 (72%)	94 (19%)	42 (9%)	1	10
1	C	490/543 (90%)	347 (71%)	104 (21%)	39 (8%)	1	12
1	D	490/543 (90%)	350 (71%)	102 (21%)	38 (8%)	1	12
1	E	490/543 (90%)	350 (71%)	102 (21%)	38 (8%)	1	12
1	F	490/543 (90%)	352 (72%)	99 (20%)	39 (8%)	1	12
All	All	2940/3258 (90%)	2103 (72%)	598 (20%)	239 (8%)	1	11

All (239) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	276	TYR
1	A	288	VAL

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Mol	Chain	Res	Type
1	A	303	ASP
1	A	304	GLU
1	A	314	ALA
1	A	407	GLY
1	A	412	GLY
1	A	424	ASP
1	A	439	LEU
1	A	440	GLU
1	A	455	ILE
1	A	475	THR
1	A	560	ALA
1	A	646	LYS
1	A	693	ARG
1	B	276	TYR
1	B	288	VAL
1	B	314	ALA
1	B	405	ILE
1	B	407	GLY
1	B	412	GLY
1	B	424	ASP
1	B	439	LEU
1	B	440	GLU
1	B	455	ILE
1	B	475	THR
1	B	560	ALA
1	B	646	LYS
1	B	693	ARG
1	C	276	TYR
1	C	288	VAL
1	C	306	ASP
1	C	314	ALA
1	C	407	GLY
1	C	412	GLY
1	C	424	ASP
1	C	439	LEU
1	C	440	GLU
1	C	455	ILE
1	C	475	THR
1	C	646	LYS
1	C	693	ARG
1	D	276	TYR
1	D	288	VAL

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Mol	Chain	Res	Type
1	D	314	ALA
1	D	407	GLY
1	D	412	GLY
1	D	424	ASP
1	D	439	LEU
1	D	440	GLU
1	D	455	ILE
1	D	475	THR
1	D	560	ALA
1	D	646	LYS
1	D	693	ARG
1	E	276	TYR
1	E	288	VAL
1	E	314	ALA
1	E	407	GLY
1	E	412	GLY
1	E	424	ASP
1	E	439	LEU
1	E	440	GLU
1	E	455	ILE
1	E	475	THR
1	E	560	ALA
1	E	646	LYS
1	E	693	ARG
1	F	276	TYR
1	F	288	VAL
1	F	314	ALA
1	F	407	GLY
1	F	412	GLY
1	F	424	ASP
1	F	439	LEU
1	F	440	GLU
1	F	455	ILE
1	F	475	THR
1	F	560	ALA
1	F	646	LYS
1	F	693	ARG
1	A	275	ARG
1	A	281	SER
1	A	313	GLU
1	A	405	ILE
1	A	474	ALA

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Mol	Chain	Res	Type
1	A	514	GLY
1	A	603	THR
1	A	629	GLY
1	A	645	SER
1	B	275	ARG
1	B	281	SER
1	B	304	GLU
1	B	313	GLU
1	B	420	LEU
1	B	474	ALA
1	B	514	GLY
1	B	629	GLY
1	B	645	SER
1	C	275	ARG
1	C	281	SER
1	C	313	GLU
1	C	405	ILE
1	C	474	ALA
1	C	514	GLY
1	C	560	ALA
1	C	629	GLY
1	C	645	SER
1	D	275	ARG
1	D	281	SER
1	D	313	GLU
1	D	405	ILE
1	D	474	ALA
1	D	514	GLY
1	D	587	ALA
1	D	629	GLY
1	D	645	SER
1	E	275	ARG
1	E	281	SER
1	E	313	GLU
1	E	405	ILE
1	E	474	ALA
1	E	514	GLY
1	E	629	GLY
1	F	275	ARG
1	F	281	SER
1	F	303	ASP
1	F	313	GLU

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Mol	Chain	Res	Type
1	F	405	ILE
1	F	420	LEU
1	F	514	GLY
1	F	629	GLY
1	F	645	SER
1	A	262	PRO
1	A	342	THR
1	A	416	PRO
1	A	420	LEU
1	A	456	GLU
1	A	637	GLN
1	B	262	PRO
1	B	303	ASP
1	B	342	THR
1	B	456	GLU
1	B	561	GLU
1	B	637	GLN
1	B	672	PRO
1	C	262	PRO
1	C	342	THR
1	C	416	PRO
1	C	456	GLU
1	C	672	PRO
1	D	262	PRO
1	D	299	LEU
1	D	342	THR
1	D	416	PRO
1	D	456	GLU
1	D	561	GLU
1	D	603	THR
1	D	637	GLN
1	D	672	PRO
1	E	262	PRO
1	E	306	ASP
1	E	342	THR
1	E	416	PRO
1	E	456	GLU
1	E	637	GLN
1	E	645	SER
1	E	672	PRO
1	F	262	PRO
1	F	342	THR

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Mol	Chain	Res	Type
1	F	416	PRO
1	F	456	GLU
1	F	474	ALA
1	F	603	THR
1	F	672	PRO
1	A	280	PRO
1	A	305	THR
1	A	330	GLU
1	A	561	GLU
1	A	672	PRO
1	B	280	PRO
1	B	416	PRO
1	B	694	ALA
1	C	280	PRO
1	C	420	LEU
1	C	561	GLU
1	C	637	GLN
1	D	280	PRO
1	E	280	PRO
1	E	420	LEU
1	E	603	THR
1	F	280	PRO
1	F	421	ASP
1	F	637	GLN
1	A	248	GLU
1	A	272	GLU
1	A	591	ASP
1	B	248	GLU
1	B	270	LEU
1	B	272	GLU
1	B	323	HIS
1	B	603	THR
1	C	248	GLU
1	C	270	LEU
1	C	272	GLU
1	C	421	ASP
1	D	248	GLU
1	D	270	LEU
1	D	272	GLU
1	D	304	GLU
1	D	420	LEU
1	E	248	GLU

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Mol	Chain	Res	Type
1	E	270	LEU
1	E	561	GLU
1	F	248	GLU
1	F	270	LEU
1	F	272	GLU
1	F	561	GLU
1	A	261	MET
1	A	270	LEU
1	A	421	ASP
1	B	261	MET
1	B	421	ASP
1	C	261	MET
1	C	330	GLU
1	D	261	MET
1	E	261	MET
1	E	272	GLU
1	F	261	MET
1	C	324	GLY
1	E	324	GLY
1	F	652	ILE
1	B	324	GLY
1	B	652	ILE
1	F	324	GLY
1	C	652	ILE
1	A	324	GLY
1	A	652	ILE
1	E	652	ILE

### 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	415/454 (91%)	361 (87%)	54 (13%)	5	25
1	B	415/454 (91%)	358 (86%)	57 (14%)	4	23
1	C	415/454 (91%)	357 (86%)	58 (14%)	4	23

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	415/454 (91%)	358 (86%)	57 (14%)	4	23
1	E	415/454 (91%)	357 (86%)	58 (14%)	4	23
1	F	415/454 (91%)	360 (87%)	55 (13%)	5	24
All	All	2490/2724 (91%)	2151 (86%)	339 (14%)	5	24

All (339) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	263	ASP
1	A	294	ASP
1	A	296	LEU
1	A	312	LYS
1	A	313	GLU
1	A	316	ARG
1	A	331	ARG
1	A	350	LEU
1	A	367	ILE
1	A	378	ILE
1	A	408	MET
1	A	442	LEU
1	A	455	ILE
1	A	463	LYS
1	A	465	LEU
1	A	471	ASN
1	A	475	THR
1	A	489	ILE
1	A	493	THR
1	A	504	HIS
1	A	506	LEU
1	A	516	LYS
1	A	519	ASN
1	A	522	LEU
1	A	532	ARG
1	A	534	TYR
1	A	536	ARG
1	A	543	LEU
1	A	565	ARG
1	A	568	VAL
1	A	579	LYS
1	A	590	GLU
1	A	592	GLN

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Mol	Chain	Res	Type
1	A	608	THR
1	A	624	LEU
1	A	635	SER
1	A	646	LYS
1	A	656	PHE
1	A	660	TYR
1	A	661	ASP
1	A	666	VAL
1	A	671	VAL
1	A	682	MET
1	A	686	LEU
1	A	705	ILE
1	A	714	ILE
1	A	717	LEU
1	A	731	THR
1	A	732	ILE
1	A	738	ASN
1	A	747	GLU
1	A	748	SER
1	A	759	SER
1	A	762	ASP
1	B	263	ASP
1	B	294	ASP
1	B	296	LEU
1	B	299	LEU
1	B	312	LYS
1	B	313	GLU
1	B	316	ARG
1	B	331	ARG
1	B	350	LEU
1	B	367	ILE
1	B	378	ILE
1	B	408	MET
1	B	423	ILE
1	B	442	LEU
1	B	455	ILE
1	B	463	LYS
1	B	465	LEU
1	B	475	THR
1	B	489	ILE
1	B	493	THR
1	B	504	HIS

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Mol	Chain	Res	Type
1	B	506	LEU
1	B	516	LYS
1	B	519	ASN
1	B	522	LEU
1	B	536	ARG
1	B	543	LEU
1	B	565	ARG
1	B	568	VAL
1	B	579	LYS
1	B	589	THR
1	B	590	GLU
1	B	592	GLN
1	B	599	LEU
1	B	608	THR
1	B	624	LEU
1	B	635	SER
1	B	646	LYS
1	B	656	PHE
1	B	660	TYR
1	B	661	ASP
1	B	666	VAL
1	B	671	VAL
1	B	682	MET
1	B	686	LEU
1	B	705	ILE
1	B	714	ILE
1	B	717	LEU
1	B	731	THR
1	B	732	ILE
1	B	738	ASN
1	B	747	GLU
1	B	748	SER
1	B	759	SER
1	B	762	ASP
1	B	767	HIS
1	B	770	VAL
1	C	263	ASP
1	C	294	ASP
1	C	296	LEU
1	C	300	PRO
1	C	303	ASP
1	C	305	THR

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Mol	Chain	Res	Type
1	C	312	LYS
1	C	313	GLU
1	C	316	ARG
1	C	331	ARG
1	C	350	LEU
1	C	367	ILE
1	C	378	ILE
1	C	408	MET
1	C	442	LEU
1	C	455	ILE
1	C	463	LYS
1	C	465	LEU
1	C	475	THR
1	C	489	ILE
1	C	493	THR
1	C	504	HIS
1	C	506	LEU
1	C	516	LYS
1	C	519	ASN
1	C	522	LEU
1	C	532	ARG
1	C	536	ARG
1	C	543	LEU
1	C	565	ARG
1	C	568	VAL
1	C	579	LYS
1	C	583	ARG
1	C	592	GLN
1	C	599	LEU
1	C	608	THR
1	C	624	LEU
1	C	635	SER
1	C	646	LYS
1	C	656	PHE
1	C	660	TYR
1	C	661	ASP
1	C	666	VAL
1	C	671	VAL
1	C	682	MET
1	C	686	LEU
1	C	705	ILE
1	C	714	ILE

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Mol	Chain	Res	Type
1	C	717	LEU
1	C	731	THR
1	C	732	ILE
1	C	738	ASN
1	C	741	ASP
1	C	747	GLU
1	C	748	SER
1	C	759	SER
1	C	762	ASP
1	C	767	HIS
1	D	263	ASP
1	D	294	ASP
1	D	296	LEU
1	D	303	ASP
1	D	305	THR
1	D	312	LYS
1	D	313	GLU
1	D	316	ARG
1	D	331	ARG
1	D	350	LEU
1	D	367	ILE
1	D	378	ILE
1	D	423	ILE
1	D	442	LEU
1	D	455	ILE
1	D	463	LYS
1	D	465	LEU
1	D	475	THR
1	D	489	ILE
1	D	493	THR
1	D	506	LEU
1	D	516	LYS
1	D	519	ASN
1	D	522	LEU
1	D	532	ARG
1	D	536	ARG
1	D	543	LEU
1	D	565	ARG
1	D	568	VAL
1	D	579	LYS
1	D	583	ARG
1	D	589	THR

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Mol	Chain	Res	Type
1	D	592	GLN
1	D	599	LEU
1	D	608	THR
1	D	624	LEU
1	D	635	SER
1	D	646	LYS
1	D	656	PHE
1	D	660	TYR
1	D	661	ASP
1	D	666	VAL
1	D	671	VAL
1	D	682	MET
1	D	686	LEU
1	D	705	ILE
1	D	714	ILE
1	D	717	LEU
1	D	731	THR
1	D	732	ILE
1	D	738	ASN
1	D	747	GLU
1	D	748	SER
1	D	749	VAL
1	D	759	SER
1	D	762	ASP
1	D	770	VAL
1	E	263	ASP
1	E	294	ASP
1	E	296	LEU
1	E	312	LYS
1	E	313	GLU
1	E	316	ARG
1	E	331	ARG
1	E	350	LEU
1	E	367	ILE
1	E	378	ILE
1	E	408	MET
1	E	442	LEU
1	E	455	ILE
1	E	463	LYS
1	E	465	LEU
1	E	471	ASN
1	E	475	THR

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Mol	Chain	Res	Type
1	E	489	ILE
1	E	493	THR
1	E	506	LEU
1	E	515	LEU
1	E	516	LYS
1	E	519	ASN
1	E	522	LEU
1	E	532	ARG
1	E	536	ARG
1	E	543	LEU
1	E	565	ARG
1	E	568	VAL
1	E	579	LYS
1	E	588	GLU
1	E	590	GLU
1	E	592	GLN
1	E	593	VAL
1	E	599	LEU
1	E	608	THR
1	E	624	LEU
1	E	635	SER
1	E	646	LYS
1	E	656	PHE
1	E	660	TYR
1	E	661	ASP
1	E	666	VAL
1	E	671	VAL
1	E	682	MET
1	E	686	LEU
1	E	705	ILE
1	E	714	ILE
1	E	717	LEU
1	E	731	THR
1	E	732	ILE
1	E	738	ASN
1	E	741	ASP
1	E	747	GLU
1	E	748	SER
1	E	759	SER
1	E	762	ASP
1	E	767	HIS
1	F	263	ASP

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Mol	Chain	Res	Type
1	F	294	ASP
1	F	296	LEU
1	F	305	THR
1	F	312	LYS
1	F	313	GLU
1	F	316	ARG
1	F	331	ARG
1	F	350	LEU
1	F	367	ILE
1	F	378	ILE
1	F	423	ILE
1	F	442	LEU
1	F	455	ILE
1	F	463	LYS
1	F	465	LEU
1	F	475	THR
1	F	489	ILE
1	F	493	THR
1	F	506	LEU
1	F	516	LYS
1	F	519	ASN
1	F	522	LEU
1	F	532	ARG
1	F	536	ARG
1	F	543	LEU
1	F	565	ARG
1	F	568	VAL
1	F	579	LYS
1	F	588	GLU
1	F	589	THR
1	F	592	GLN
1	F	608	THR
1	F	624	LEU
1	F	635	SER
1	F	646	LYS
1	F	656	PHE
1	F	660	TYR
1	F	661	ASP
1	F	666	VAL
1	F	671	VAL
1	F	682	MET
1	F	686	LEU

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Mol	Chain	Res	Type
1	F	705	ILE
1	F	706	THR
1	F	714	ILE
1	F	717	LEU
1	F	731	THR
1	F	732	ILE
1	F	738	ASN
1	F	747	GLU
1	F	748	SER
1	F	759	SER
1	F	762	ASP
1	F	767	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	250	GLN
1	A	767	HIS
1	B	250	GLN
1	B	446	GLN
1	B	586	GLN
1	B	767	HIS
1	C	250	GLN
1	C	291	ASN
1	C	446	GLN
1	C	586	GLN
1	C	767	HIS
1	D	250	GLN
1	D	767	HIS
1	E	250	GLN
1	E	767	HIS
1	F	250	GLN
1	F	446	GLN
1	F	767	HIS

### 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 ⓘ

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
2	ADP	A	783	-	22,29,29	1.28	2 (9%)	27,45,45	2.53	6 (22%)
2	ADP	B	783	-	22,29,29	1.00	1 (4%)	27,45,45	2.27	7 (25%)
2	ADP	C	783	-	22,29,29	1.17	1 (4%)	27,45,45	2.40	10 (37%)
2	ADP	D	783	-	22,29,29	1.33	3 (13%)	27,45,45	2.52	11 (40%)
2	ADP	E	783	-	22,29,29	1.12	2 (9%)	27,45,45	2.46	11 (40%)
2	ADP	F	783	-	22,29,29	1.02	1 (4%)	27,45,45	2.17	8 (29%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ADP	A	783	-	-	0/12/32/32	0/3/3/3
2	ADP	B	783	-	-	0/12/32/32	0/3/3/3
2	ADP	C	783	-	-	0/12/32/32	0/3/3/3
2	ADP	D	783	-	-	0/12/32/32	0/3/3/3
2	ADP	E	783	-	-	0/12/32/32	0/3/3/3
2	ADP	F	783	-	-	0/12/32/32	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	783	ADP	PB-O3B	-2.23	1.46	1.54
2	D	783	ADP	C5-N7	-2.07	1.32	1.39
2	A	783	ADP	C2-N3	2.04	1.35	1.32
2	E	783	ADP	C2-N3	2.30	1.36	1.32
2	B	783	ADP	C5-C4	2.75	1.46	1.40
2	F	783	ADP	C5-C4	3.07	1.47	1.40
2	E	783	ADP	C5-C4	3.40	1.48	1.40
2	D	783	ADP	C5-C4	3.56	1.48	1.40
2	C	783	ADP	C5-C4	3.93	1.49	1.40
2	A	783	ADP	C5-C4	4.29	1.50	1.40

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	783	ADP	PA-O3A-PB	-8.87	102.94	132.67
2	B	783	ADP	N3-C2-N1	-7.15	123.42	128.89
2	F	783	ADP	N3-C2-N1	-6.44	123.96	128.89
2	E	783	ADP	C4-C5-N7	-6.12	103.85	109.48
2	D	783	ADP	N3-C2-N1	-5.64	124.57	128.89
2	B	783	ADP	PA-O3A-PB	-5.59	113.92	132.67
2	C	783	ADP	PA-O3A-PB	-5.54	114.10	132.67
2	D	783	ADP	C2'-C1'-N9	-5.38	106.07	114.29
2	A	783	ADP	C4-C5-N7	-5.38	104.53	109.48
2	C	783	ADP	N3-C2-N1	-5.34	124.80	128.89
2	E	783	ADP	PA-O3A-PB	-4.86	116.38	132.67
2	F	783	ADP	PA-O3A-PB	-4.76	116.69	132.67
2	E	783	ADP	N3-C2-N1	-4.61	125.37	128.89
2	D	783	ADP	PA-O3A-PB	-4.28	118.32	132.67
2	C	783	ADP	C4-C5-N7	-3.96	105.83	109.48
2	D	783	ADP	C4-C5-N7	-3.96	105.83	109.48
2	B	783	ADP	C2'-C1'-N9	-3.88	108.36	114.29
2	E	783	ADP	C2'-C1'-N9	-3.75	108.56	114.29
2	E	783	ADP	C4'-O4'-C1'	-3.40	105.99	109.72
2	F	783	ADP	C2'-C3'-C4'	-3.39	95.65	102.61
2	F	783	ADP	C4-C5-N7	-3.11	106.62	109.48
2	C	783	ADP	C2'-C3'-C4'	-3.07	96.31	102.61
2	B	783	ADP	C4-C5-N7	-2.98	106.74	109.48
2	A	783	ADP	C2'-C1'-N9	-2.72	110.14	114.29
2	C	783	ADP	O5'-C5'-C4'	-2.65	99.34	109.12
2	B	783	ADP	O2'-C2'-C3'	-2.60	103.37	111.83
2	E	783	ADP	O5'-C5'-C4'	-2.59	99.57	109.12
2	A	783	ADP	N3-C2-N1	-2.53	126.96	128.89
2	F	783	ADP	O2'-C2'-C3'	-2.43	103.93	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	783	ADP	O4'-C4'-C5'	-2.38	100.80	109.32
2	E	783	ADP	O5'-PA-O1A	-2.37	100.40	109.62
2	D	783	ADP	O3B-PB-O3A	-2.37	94.35	105.09
2	F	783	ADP	O5'-C5'-C4'	-2.24	100.86	109.12
2	C	783	ADP	O2'-C2'-C3'	-2.15	104.82	111.83
2	C	783	ADP	O5'-PA-O1A	-2.07	101.57	109.62
2	B	783	ADP	O3A-PA-O5'	2.01	108.27	102.94
2	D	783	ADP	O2B-PB-O1B	2.02	117.09	110.58
2	D	783	ADP	O5'-C5'-C4'	2.05	116.67	109.12
2	D	783	ADP	O3B-PB-O2B	2.12	115.44	107.38
2	F	783	ADP	C1'-N9-C4	2.15	130.18	126.94
2	E	783	ADP	O2A-PA-O1A	2.18	124.36	112.53
2	B	783	ADP	O3B-PB-O1B	2.26	117.87	110.58
2	E	783	ADP	O3B-PB-O1B	2.35	118.13	110.58
2	D	783	ADP	C2-N1-C6	2.39	123.03	118.77
2	E	783	ADP	O3B-PB-O2B	2.58	117.19	107.38
2	F	783	ADP	O3B-PB-O2B	2.58	117.20	107.38
2	C	783	ADP	O2A-PA-O1A	2.64	126.84	112.53
2	A	783	ADP	O3B-PB-O1B	2.68	119.21	110.58
2	C	783	ADP	O3B-PB-O2B	3.34	120.09	107.38
2	D	783	ADP	C1'-N9-C4	3.75	132.59	126.94
2	A	783	ADP	C1'-N9-C4	4.43	133.62	126.94
2	C	783	ADP	C1'-N9-C4	4.63	133.93	126.94
2	D	783	ADP	O3A-PA-O5'	5.01	116.23	102.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 44 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	783	ADP	7	0
2	B	783	ADP	7	0
2	C	783	ADP	6	0
2	D	783	ADP	11	0
2	E	783	ADP	6	0
2	F	783	ADP	7	0

## 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

### 6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å <sup>2</sup> )	Q<0.9
1	A	496/543 (91%)	0.21	26 (5%)	31 28	69, 145, 461, 643	0
1	B	496/543 (91%)	0.25	30 (6%)	25 23	75, 143, 456, 637	0
1	C	496/543 (91%)	0.40	42 (8%)	13 13	71, 145, 458, 683	0
1	D	496/543 (91%)	0.48	56 (11%)	7 7	65, 145, 463, 696	0
1	E	496/543 (91%)	0.50	58 (11%)	6 6	75, 146, 466, 682	0
1	F	496/543 (91%)	0.32	42 (8%)	13 13	78, 148, 457, 672	0
All	All	2976/3258 (91%)	0.36	254 (8%)	13 13	65, 145, 464, 696	0

All (254) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	287	SER	15.5
1	E	246	THR	13.8
1	B	246	THR	10.8
1	F	278	LYS	10.5
1	B	282	SER	10.3
1	C	288	VAL	9.0
1	A	246	THR	8.9
1	C	257	GLU	8.8
1	B	251	THR	8.5
1	B	248	GLU	8.4
1	E	251	THR	7.4
1	C	249	VAL	7.2
1	E	282	SER	6.7
1	D	278	LYS	6.5
1	D	246	THR	6.5
1	E	247	GLY	6.2
1	C	246	THR	6.1
1	A	259	ALA	5.8
1	C	247	GLY	5.7

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Mol	Chain	Res	Type	RSRZ
1	E	250	GLN	5.6
1	C	289	ILE	5.6
1	C	286	SER	5.6
1	F	307	ASP	5.6
1	B	254	GLU	5.6
1	D	252	LEU	5.3
1	D	615	LEU	5.3
1	E	281	SER	4.9
1	C	301	TRP	4.9
1	A	463	LYS	4.8
1	B	278	LYS	4.8
1	C	300	PRO	4.8
1	E	290	ARG	4.8
1	C	250	GLN	4.8
1	E	276	TYR	4.7
1	C	337	ALA	4.7
1	D	302	THR	4.6
1	B	289	ILE	4.5
1	E	459	PHE	4.5
1	D	342	THR	4.5
1	C	427	SER	4.5
1	E	293	ILE	4.4
1	C	256	ILE	4.4
1	F	277	GLU	4.4
1	E	277	GLU	4.4
1	B	279	ILE	4.4
1	C	282	SER	4.4
1	B	307	ASP	4.3
1	D	620	GLY	4.3
1	D	279	ILE	4.3
1	E	285	GLU	4.2
1	F	644	ARG	4.2
1	F	288	VAL	4.1
1	E	347	GLY	4.1
1	F	627	LYS	4.1
1	D	757	LEU	4.1
1	F	472	ASN	4.0
1	B	252	LEU	4.0
1	D	289	ILE	4.0
1	D	286	SER	4.0
1	D	689	ALA	3.9
1	F	279	ILE	3.9

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Mol	Chain	Res	Type	RSRZ
1	C	290	ARG	3.9
1	D	662	ILE	3.9
1	F	345	LEU	3.9
1	F	289	ILE	3.9
1	E	615	LEU	3.8
1	A	456	GLU	3.8
1	E	295	TRP	3.8
1	D	614	SER	3.8
1	B	247	GLY	3.8
1	A	251	THR	3.8
1	A	337	ALA	3.7
1	D	456	GLU	3.7
1	F	676	PRO	3.7
1	F	459	PHE	3.6
1	F	272	GLU	3.6
1	B	337	ALA	3.6
1	B	257	GLU	3.6
1	F	246	THR	3.6
1	A	338	VAL	3.6
1	C	248	GLU	3.5
1	C	283	SER	3.5
1	E	344	SER	3.5
1	B	286	SER	3.4
1	C	414	LEU	3.4
1	D	344	SER	3.4
1	E	471	ASN	3.4
1	D	624	LEU	3.3
1	A	663	HIS	3.3
1	C	455	ILE	3.3
1	E	289	ILE	3.3
1	D	641	SER	3.3
1	B	342	THR	3.3
1	F	344	SER	3.3
1	C	662	ILE	3.3
1	F	664	ILE	3.3
1	B	281	SER	3.3
1	D	657	HIS	3.2
1	A	285	GLU	3.2
1	B	276	TYR	3.2
1	E	338	VAL	3.2
1	E	278	LYS	3.1
1	E	564	LYS	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	444	PRO	3.1
1	D	644	ARG	3.1
1	C	338	VAL	3.0
1	E	288	VAL	3.0
1	D	594	GLY	3.0
1	F	725	HIS	3.0
1	D	472	ASN	3.0
1	D	756	ILE	3.0
1	F	290	ARG	3.0
1	E	279	ILE	3.0
1	B	341	LEU	2.9
1	E	532	ARG	2.9
1	D	301	TRP	2.9
1	F	663	HIS	2.9
1	C	284	ALA	2.9
1	E	296	LEU	2.9
1	D	699	VAL	2.9
1	F	373	ARG	2.9
1	E	343	LYS	2.9
1	B	255	LYS	2.9
1	B	444	PRO	2.8
1	D	596	VAL	2.8
1	B	295	TRP	2.8
1	A	341	LEU	2.8
1	A	343	LYS	2.8
1	E	342	THR	2.8
1	E	591	ASP	2.8
1	F	731	THR	2.8
1	A	734	ALA	2.7
1	F	732	ILE	2.7
1	E	755	PHE	2.7
1	D	288	VAL	2.7
1	E	413	LYS	2.7
1	C	663	HIS	2.7
1	F	540	VAL	2.7
1	D	639	ALA	2.7
1	A	462	SER	2.7
1	D	755	PHE	2.7
1	D	613	VAL	2.7
1	D	251	THR	2.7
1	E	257	GLU	2.6
1	C	558	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	F	261	MET	2.6
1	D	444	PRO	2.6
1	B	284	ALA	2.6
1	C	565	ARG	2.6
1	F	617	PRO	2.6
1	E	584	TYR	2.6
1	E	249	VAL	2.6
1	B	259	ALA	2.6
1	F	577	ILE	2.6
1	D	337	ALA	2.6
1	C	278	LYS	2.6
1	C	465	LEU	2.6
1	C	566	ILE	2.6
1	C	341	LEU	2.6
1	D	648	GLU	2.6
1	F	248	GLU	2.6
1	E	360	LYS	2.6
1	D	277	GLU	2.6
1	F	301	TRP	2.5
1	D	345	LEU	2.5
1	F	620	GLY	2.5
1	C	456	GLU	2.5
1	A	262	PRO	2.5
1	F	276	TYR	2.5
1	C	307	ASP	2.5
1	D	622	LEU	2.5
1	A	427	SER	2.5
1	E	286	SER	2.5
1	B	288	VAL	2.5
1	E	337	ALA	2.5
1	E	558	ILE	2.5
1	F	259	ALA	2.5
1	D	654	PRO	2.4
1	E	301	TRP	2.4
1	B	301	TRP	2.4
1	F	662	ILE	2.4
1	D	768	ALA	2.4
1	A	445	GLU	2.4
1	D	690	LEU	2.4
1	D	412	GLY	2.4
1	C	342	THR	2.4
1	E	335	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	283	SER	2.3
1	A	258	GLU	2.3
1	E	267	GLU	2.3
1	A	458	THR	2.3
1	F	616	SER	2.3
1	D	445	GLU	2.3
1	E	294	ASP	2.3
1	A	437	ALA	2.3
1	E	440	GLU	2.3
1	E	252	LEU	2.3
1	E	721	ALA	2.3
1	D	275	ARG	2.3
1	C	251	THR	2.3
1	C	445	GLU	2.3
1	E	341	LEU	2.3
1	C	344	SER	2.3
1	B	440	GLU	2.2
1	C	615	LEU	2.2
1	D	769	LEU	2.2
1	F	444	PRO	2.2
1	D	666	VAL	2.2
1	D	462	SER	2.2
1	E	268	THR	2.2
1	B	454	TYR	2.2
1	C	454	TYR	2.2
1	F	426	MET	2.2
1	C	345	LEU	2.2
1	A	255	LYS	2.2
1	E	323	HIS	2.2
1	B	280	PRO	2.2
1	E	421	ASP	2.2
1	B	273	LEU	2.2
1	D	437	ALA	2.2
1	E	280	PRO	2.2
1	F	729	LEU	2.2
1	E	705	ILE	2.2
1	A	615	LEU	2.2
1	D	632	MET	2.1
1	A	614	SER	2.1
1	D	307	ASP	2.1
1	E	562	GLU	2.1
1	C	291	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	564	LYS	2.1
1	F	296	LEU	2.1
1	D	273	LEU	2.1
1	E	463	LYS	2.1
1	A	644	ARG	2.1
1	D	680	ILE	2.1
1	F	710	ARG	2.1
1	D	599	LEU	2.1
1	B	462	SER	2.1
1	E	594	GLY	2.1
1	D	640	PHE	2.1
1	E	656	PHE	2.1
1	F	286	SER	2.1
1	E	458	THR	2.1
1	E	345	LEU	2.1
1	F	497	LYS	2.0
1	A	702	THR	2.0
1	D	695	VAL	2.0
1	E	450	PHE	2.0
1	F	321	GLU	2.0
1	C	639	ALA	2.0
1	A	459	PHE	2.0
1	F	543	LEU	2.0
1	D	287	SER	2.0
1	E	271	LYS	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors

of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	ADP	D	783	27/27	0.73	0.31	0.96	30,142,369,458	0
2	ADP	C	783	27/27	0.89	0.30	0.65	57,125,341,462	0
2	ADP	B	783	27/27	0.91	0.25	0.11	73,123,341,499	0
2	ADP	A	783	27/27	0.91	0.22	-0.04	55,104,341,499	0
2	ADP	F	783	27/27	0.92	0.22	-0.20	57,123,341,482	0
2	ADP	E	783	27/27	0.93	0.19	-0.79	53,114,341,491	0

## 6.5 Other polymers

There are no such residues in this entry.