



# Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 12:23 am BST

PDB ID : 4BTP  
Title : Structure of the capsid protein P1 of the bacteriophage phi8  
Authors : El Omari, K.; Sutton, G.; Ravantti, J.J.; Zhang, H.; Walter, T.S.; Grimes, J.M.; Bamford, D.H.; Stuart, D.I.; Mancini, E.J.  
Deposited on : 2013-06-18  
Resolution : 3.70 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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

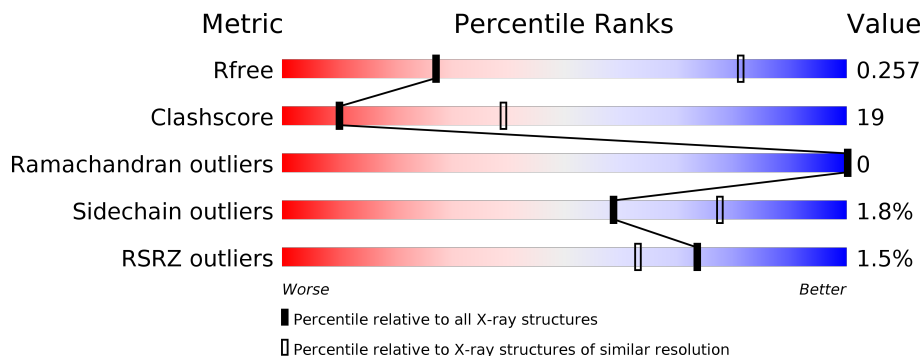
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

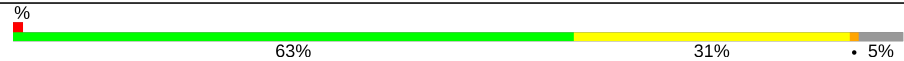
The reported resolution of this entry is 3.70 Å.

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



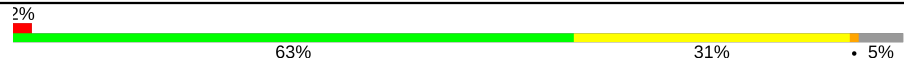

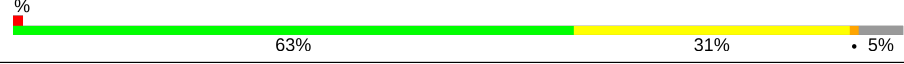

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1049 (3.88-3.52)
Clashscore	141614	1027 (3.86-3.54)
Ramachandran outliers	138981	1069 (3.88-3.52)
Sidechain outliers	138945	1065 (3.88-3.52)
RSRZ outliers	127900	1578 (3.90-3.50)

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

Mol	Chain	Length	Quality of chain
1	A	792	
1	B	792	
1	C	792	
1	D	792	
1	E	792	
1	F	792	

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Mol	Chain	Length	Quality of chain
1	G	792	
1	H	792	
1	I	792	
1	J	792	

## 2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 57630 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 p1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	749	5763	3634	998	1107	24	0	0	0
1	B	749	5763	3634	998	1107	24	0	0	0
1	C	749	5763	3634	998	1107	24	0	0	0
1	D	749	5763	3634	998	1107	24	0	0	0
1	E	749	5763	3634	998	1107	24	0	0	0
1	F	749	5763	3634	998	1107	24	0	0	0
1	G	749	5763	3634	998	1107	24	0	0	0
1	H	749	5763	3634	998	1107	24	0	0	0
1	I	749	5763	3634	998	1107	24	0	0	0
1	J	749	5763	3634	998	1107	24	0	0	0

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	419	ALA	GLY	engineered mutation	UNP Q9MC13
A	691	ASP	GLU	engineered mutation	UNP Q9MC13
A	716	ALA	GLY	conflict	UNP Q9MC13
B	419	ALA	GLY	engineered mutation	UNP Q9MC13
B	691	ASP	GLU	engineered mutation	UNP Q9MC13
B	716	ALA	GLY	conflict	UNP Q9MC13
C	419	ALA	GLY	engineered mutation	UNP Q9MC13
C	691	ASP	GLU	engineered mutation	UNP Q9MC13
C	716	ALA	GLY	conflict	UNP Q9MC13

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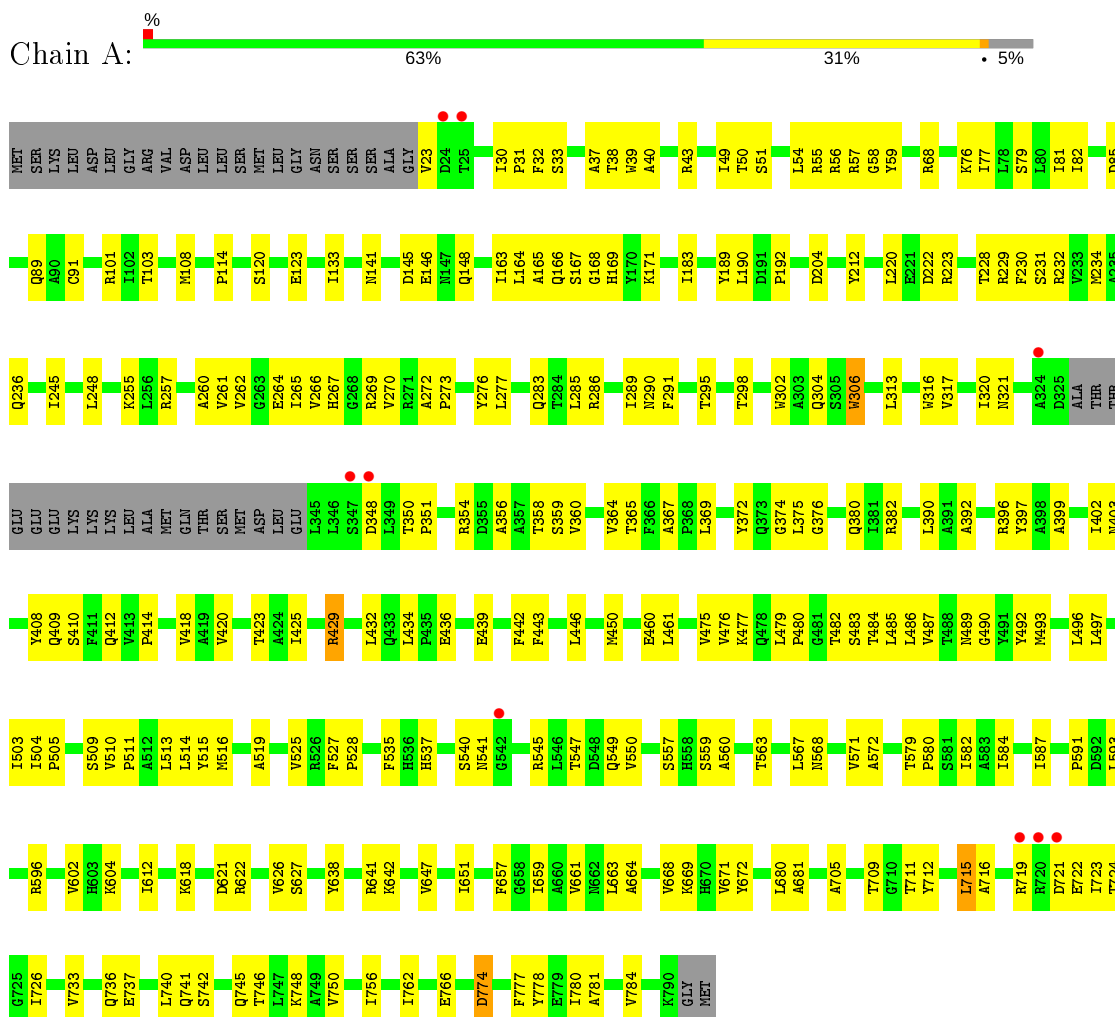
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Chain	Residue	Modelled	Actual	Comment	Reference
D	419	ALA	GLY	engineered mutation	UNP Q9MC13
D	691	ASP	GLU	engineered mutation	UNP Q9MC13
D	716	ALA	GLY	conflict	UNP Q9MC13
E	419	ALA	GLY	engineered mutation	UNP Q9MC13
E	691	ASP	GLU	engineered mutation	UNP Q9MC13
E	716	ALA	GLY	conflict	UNP Q9MC13
F	419	ALA	GLY	engineered mutation	UNP Q9MC13
F	691	ASP	GLU	engineered mutation	UNP Q9MC13
F	716	ALA	GLY	conflict	UNP Q9MC13
G	419	ALA	GLY	engineered mutation	UNP Q9MC13
G	691	ASP	GLU	engineered mutation	UNP Q9MC13
G	716	ALA	GLY	conflict	UNP Q9MC13
H	419	ALA	GLY	engineered mutation	UNP Q9MC13
H	691	ASP	GLU	engineered mutation	UNP Q9MC13
H	716	ALA	GLY	conflict	UNP Q9MC13
I	419	ALA	GLY	engineered mutation	UNP Q9MC13
I	691	ASP	GLU	engineered mutation	UNP Q9MC13
I	716	ALA	GLY	conflict	UNP Q9MC13
J	419	ALA	GLY	engineered mutation	UNP Q9MC13
J	691	ASP	GLU	engineered mutation	UNP Q9MC13
J	716	ALA	GLY	conflict	UNP Q9MC13

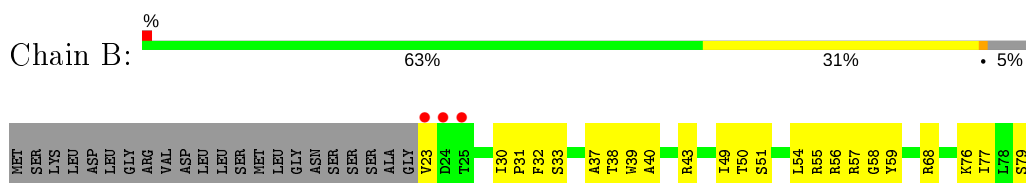
### 3 Residue-property plots

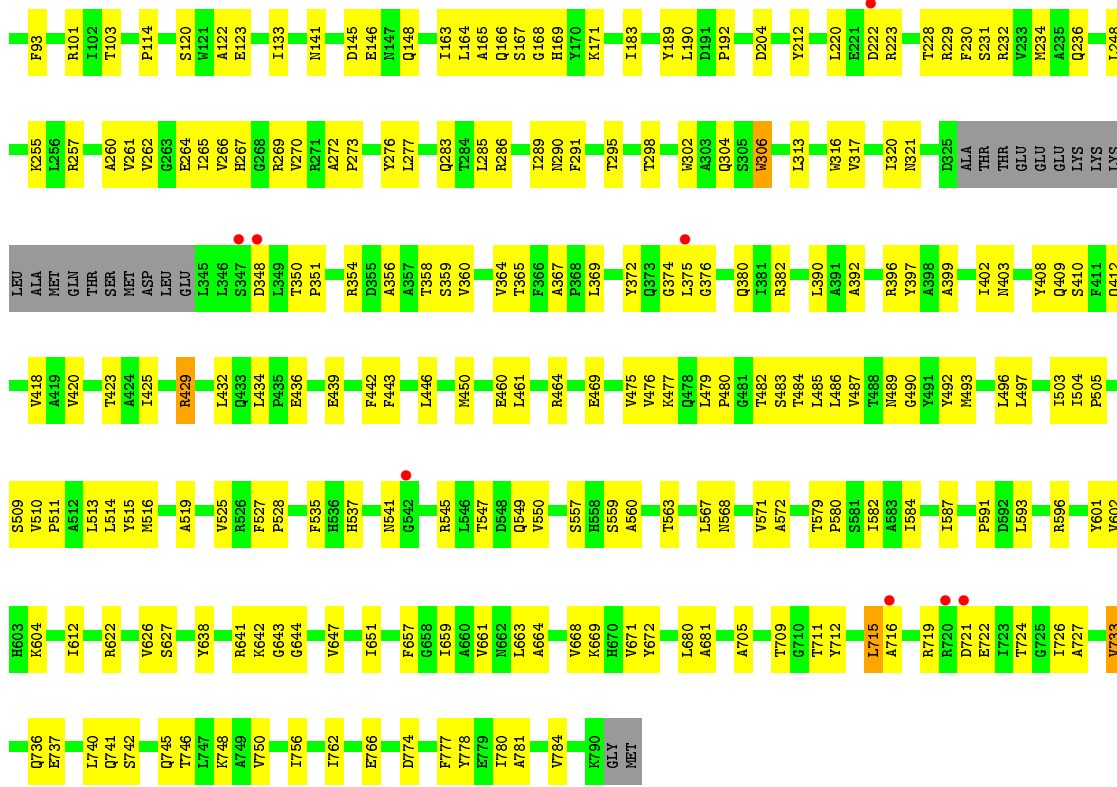
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

- Molecule 1: p1

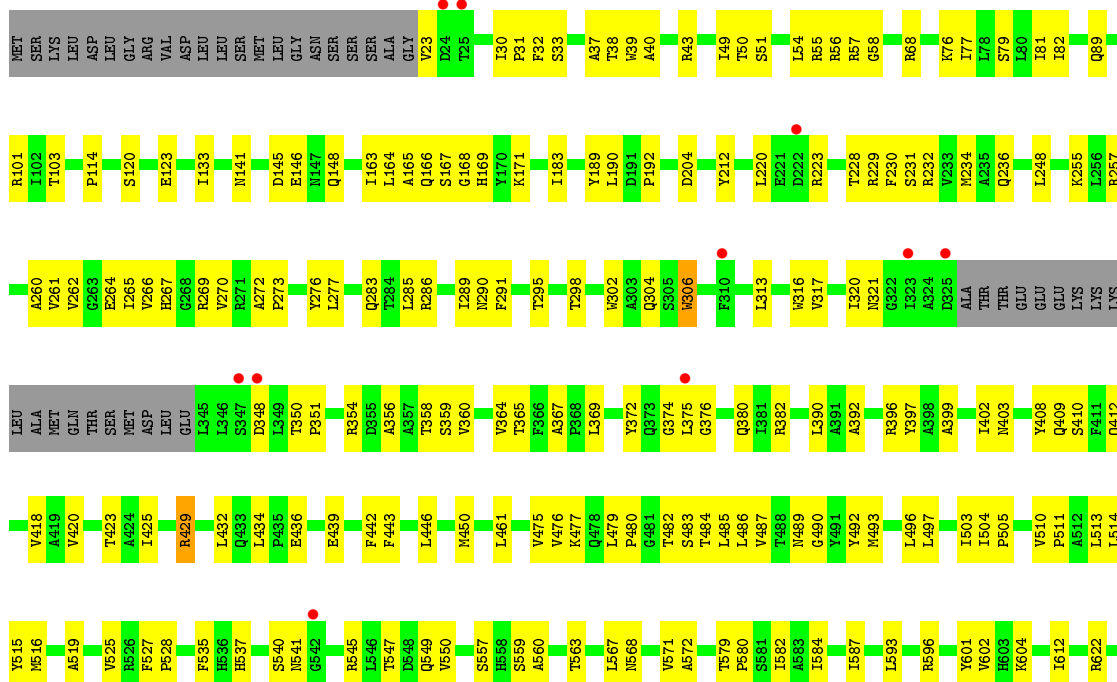


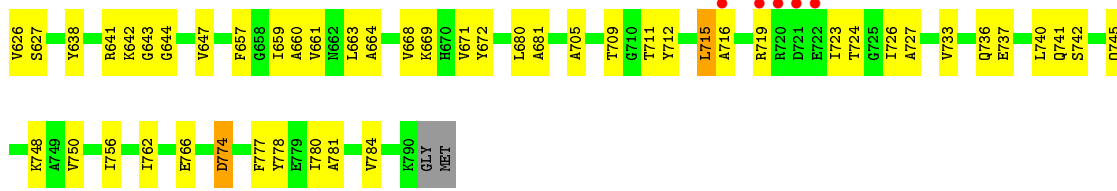
- Molecule 1: p1



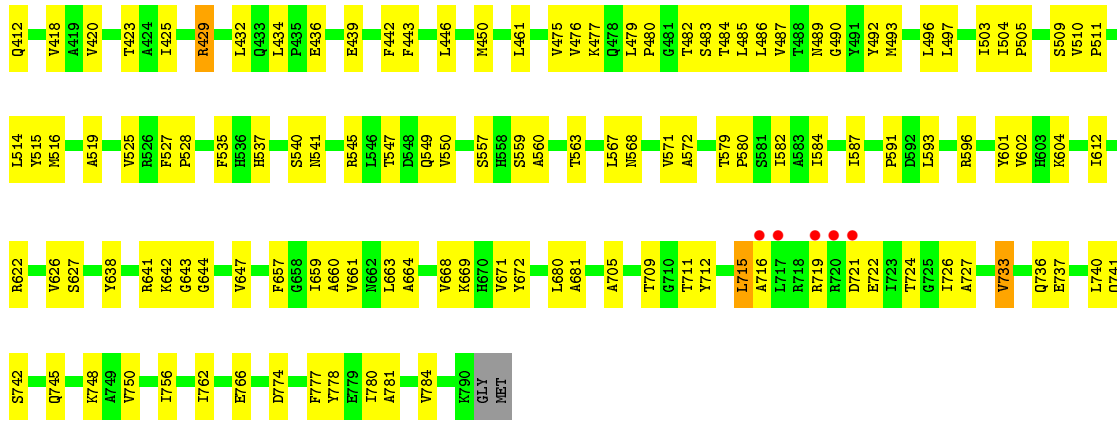
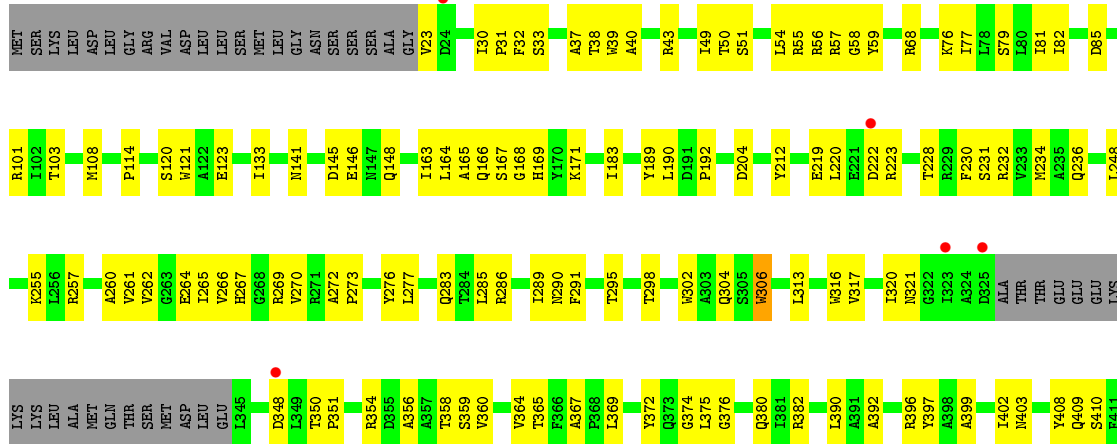


• Molecule 1: p1

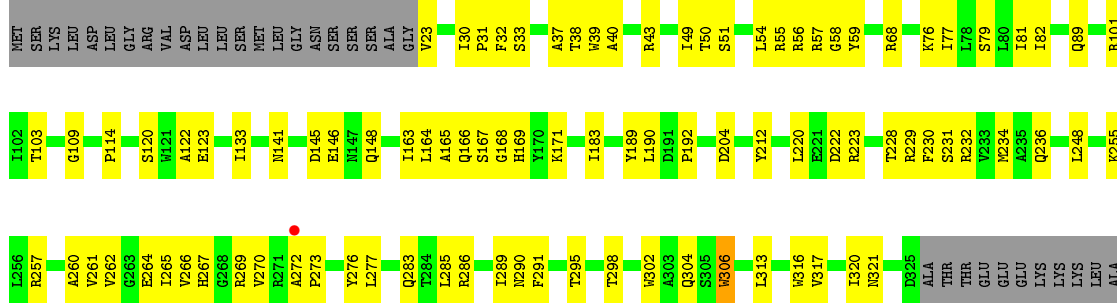




• Molecule 1: p1

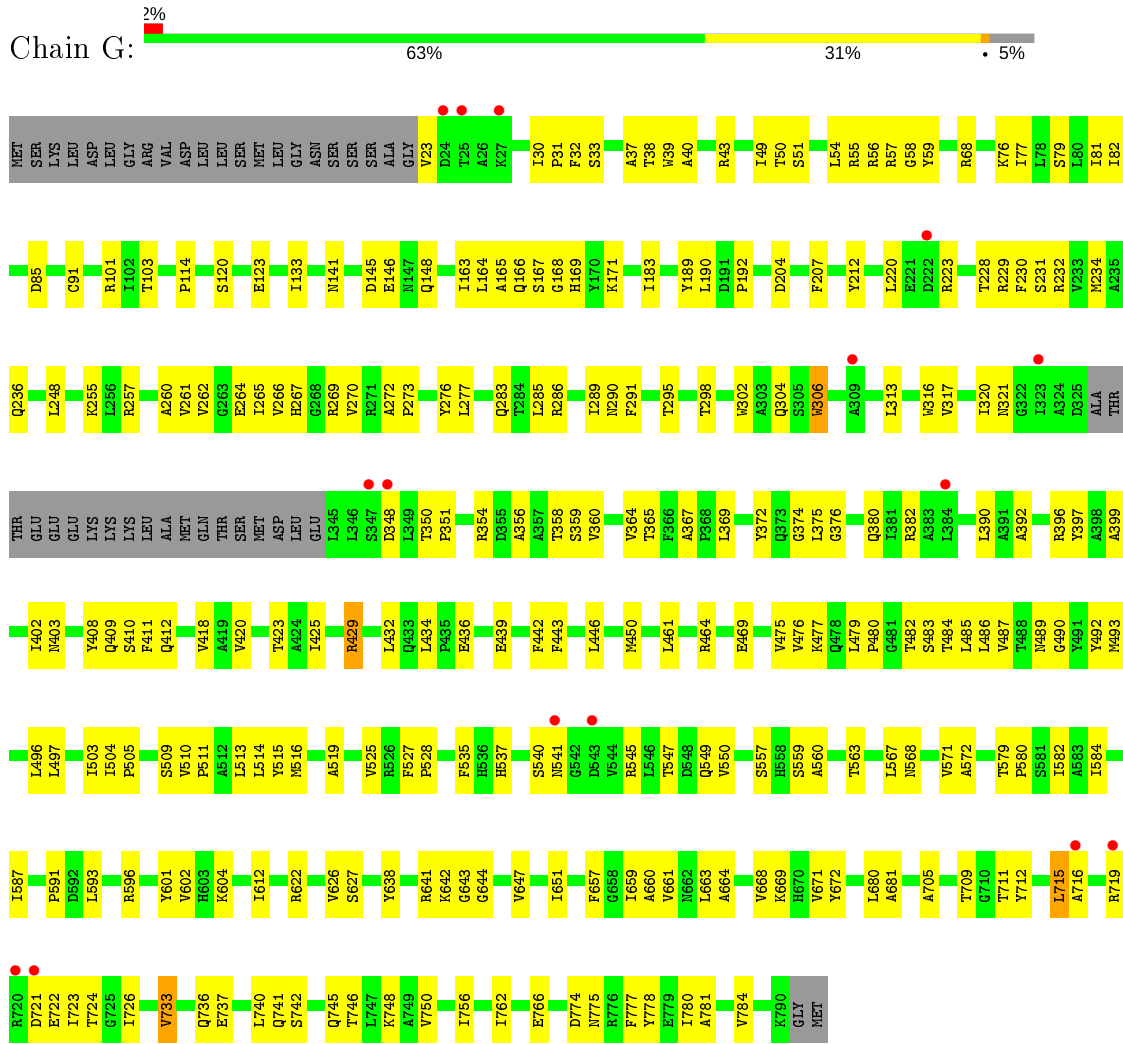


• Molecule 1: p1

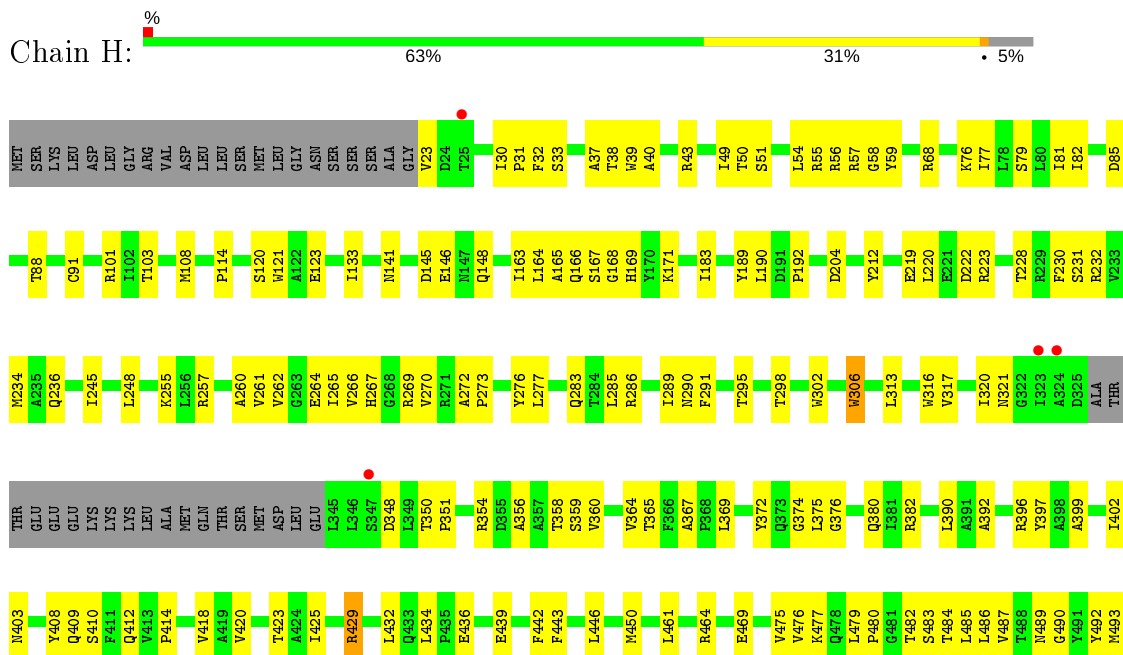


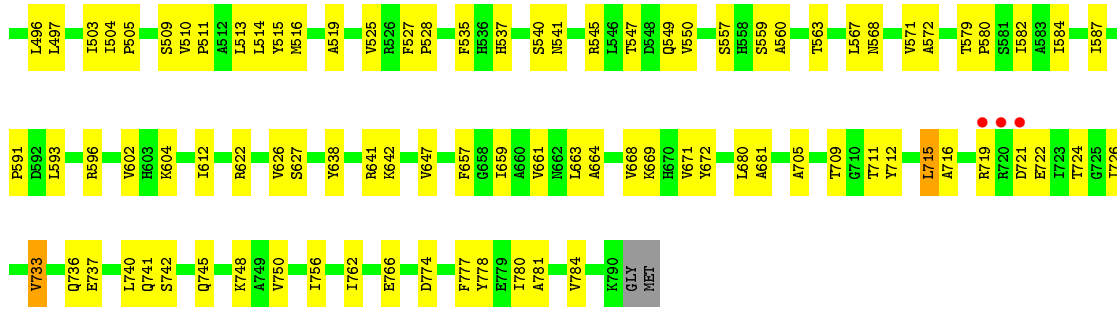




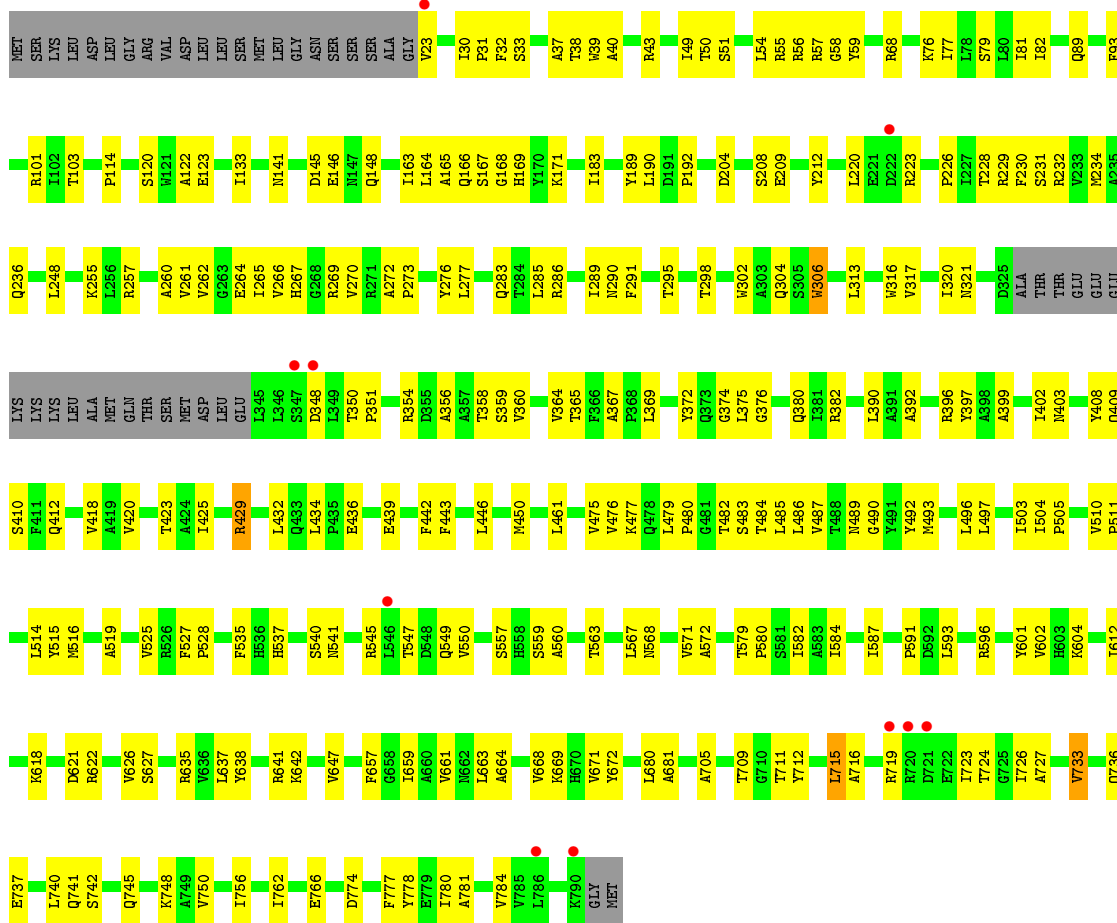


• Molecule 1: p1



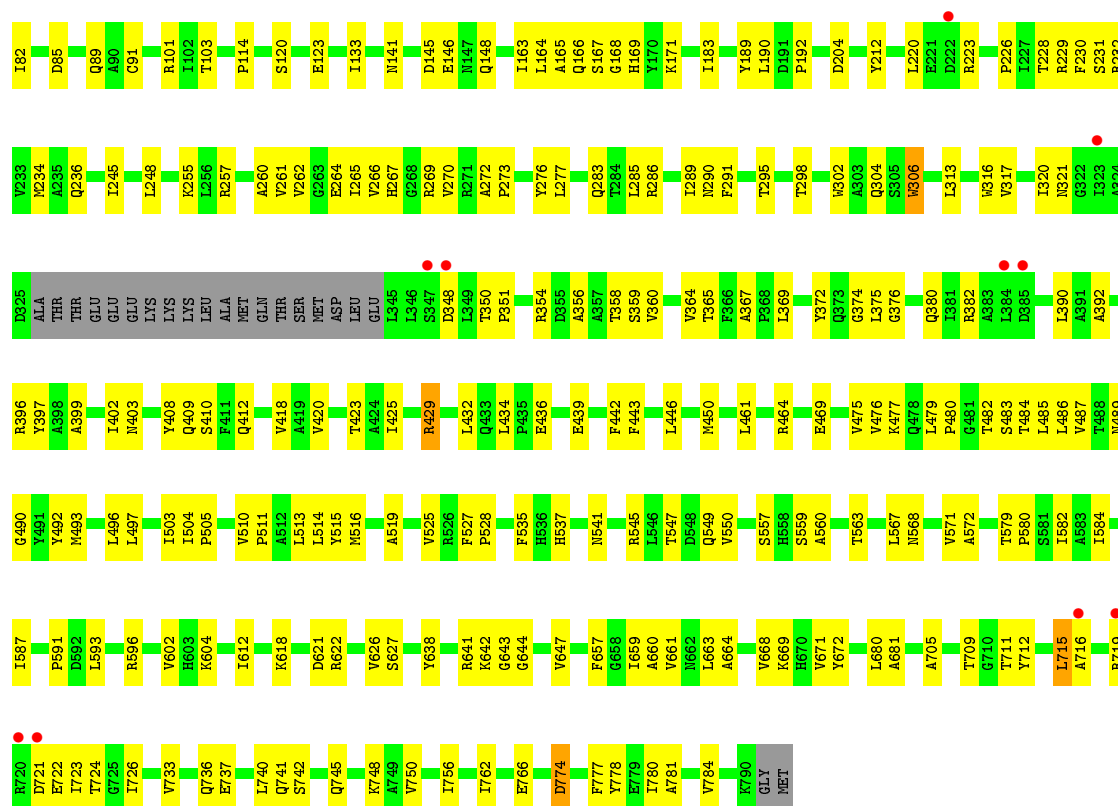


• Molecule 1: p1



• Molecule 1: p1





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	314.35Å 314.35Å 527.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.01 – 3.70 29.99 – 3.70	Depositor EDS
% Data completeness (in resolution range)	97.0 (30.01-3.70) 97.2 (29.99-3.70)	Depositor EDS
$R_{merge}$	0.17	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.19 (at 3.75Å)	Xtrriage
Refinement program	REFMAC 5.7.0032	Depositor
R, $R_{free}$	0.244 , 0.258 0.244 , 0.257	Depositor DCC
$R_{free}$ test set	13628 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	126.2	Xtrriage
Anisotropy	0.230	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 87.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	57630	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	142.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.41% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

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

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	0.36	0/5865	0.63	0/7957
1	B	0.36	0/5865	0.64	0/7957
1	C	0.36	0/5865	0.63	0/7957
1	D	0.36	0/5865	0.63	0/7957
1	E	0.36	0/5865	0.63	0/7957
1	F	0.36	0/5865	0.63	0/7957
1	G	0.36	0/5865	0.63	0/7957
1	H	0.36	0/5865	0.63	0/7957
1	I	0.36	0/5865	0.63	0/7957
1	J	0.36	0/5865	0.63	0/7957
All	All	0.36	0/58650	0.63	0/79570

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [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	5763	0	5773	228	0
1	B	5763	0	5773	232	0
1	C	5763	0	5773	220	0
1	D	5763	0	5773	225	6
1	E	5763	0	5773	228	0
1	F	5763	0	5773	227	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	5763	0	5773	227	0
1	H	5763	0	5773	232	6
1	I	5763	0	5773	228	0
1	J	5763	0	5773	230	0
All	All	57630	0	57730	2181	6

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 19.

All (2181) 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:J:270:VAL:HG21	1:J:317:VAL:HG12	1.19	1.17
1:B:270:VAL:HG21	1:B:317:VAL:HG12	1.19	1.17
1:B:270:VAL:CG2	1:B:317:VAL:HG12	1.76	1.15
1:C:270:VAL:CG2	1:C:317:VAL:HG12	1.76	1.15
1:D:270:VAL:CG2	1:D:317:VAL:HG12	1.77	1.15
1:A:270:VAL:HG21	1:A:317:VAL:HG12	1.19	1.15
1:G:270:VAL:CG2	1:G:317:VAL:HG12	1.76	1.14
1:H:270:VAL:HG21	1:H:317:VAL:HG12	1.19	1.14
1:H:270:VAL:CG2	1:H:317:VAL:HG12	1.76	1.14
1:I:270:VAL:CG2	1:I:317:VAL:HG12	1.77	1.14
1:A:270:VAL:CG2	1:A:317:VAL:HG12	1.76	1.14
1:E:270:VAL:CG2	1:E:317:VAL:HG12	1.76	1.14
1:C:270:VAL:HG21	1:C:317:VAL:HG12	1.19	1.13
1:F:270:VAL:CG2	1:F:317:VAL:HG12	1.77	1.13
1:J:270:VAL:CG2	1:J:317:VAL:HG12	1.76	1.13
1:E:270:VAL:HG21	1:E:317:VAL:HG12	1.19	1.12
1:G:270:VAL:HG21	1:G:317:VAL:HG12	1.19	1.11
1:F:270:VAL:HG21	1:F:317:VAL:HG12	1.19	1.10
1:I:270:VAL:HG21	1:I:317:VAL:HG12	1.19	1.09
1:D:270:VAL:HG21	1:D:317:VAL:HG12	1.19	1.09
1:J:255:LYS:NZ	1:J:359:SER:OG	2.02	0.93
1:G:255:LYS:NZ	1:G:359:SER:OG	2.02	0.93
1:F:255:LYS:NZ	1:F:359:SER:OG	2.02	0.93
1:A:255:LYS:NZ	1:A:359:SER:OG	2.02	0.93
1:E:255:LYS:NZ	1:E:359:SER:OG	2.02	0.93
1:A:23:VAL:HG21	1:A:32:PHE:HB3	1.51	0.92
1:E:23:VAL:HG21	1:E:32:PHE:HB3	1.52	0.92
1:C:255:LYS:NZ	1:C:359:SER:OG	2.02	0.92
1:D:255:LYS:NZ	1:D:359:SER:OG	2.01	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:23:VAL:HG21	1:C:32:PHE:HB3	1.52	0.91
1:D:23:VAL:HG21	1:D:32:PHE:HB3	1.52	0.91
1:H:255:LYS:NZ	1:H:359:SER:OG	2.02	0.91
1:B:255:LYS:NZ	1:B:359:SER:OG	2.02	0.91
1:F:23:VAL:HG21	1:F:32:PHE:HB3	1.52	0.91
1:J:23:VAL:HG21	1:J:32:PHE:HB3	1.52	0.91
1:H:23:VAL:HG21	1:H:32:PHE:HB3	1.52	0.91
1:I:255:LYS:NZ	1:I:359:SER:OG	2.02	0.91
1:I:23:VAL:HG21	1:I:32:PHE:HB3	1.51	0.90
1:B:23:VAL:HG21	1:B:32:PHE:HB3	1.51	0.90
1:I:270:VAL:HG21	1:I:317:VAL:CG1	2.03	0.89
1:G:23:VAL:HG21	1:G:32:PHE:HB3	1.52	0.89
1:G:270:VAL:HG21	1:G:317:VAL:CG1	2.03	0.89
1:B:270:VAL:HG21	1:B:317:VAL:CG1	2.03	0.89
1:D:270:VAL:HG21	1:D:317:VAL:CG1	2.03	0.88
1:F:270:VAL:HG21	1:F:317:VAL:CG1	2.03	0.88
1:E:270:VAL:HG21	1:E:317:VAL:CG1	2.03	0.88
1:H:270:VAL:HG21	1:H:317:VAL:CG1	2.03	0.88
1:E:306:TRP:HD1	1:E:313:LEU:HD13	1.39	0.88
1:B:306:TRP:HD1	1:B:313:LEU:HD13	1.40	0.87
1:A:270:VAL:HG21	1:A:317:VAL:CG1	2.03	0.87
1:C:270:VAL:HG21	1:C:317:VAL:CG1	2.03	0.87
1:J:306:TRP:HD1	1:J:313:LEU:HD13	1.39	0.87
1:H:306:TRP:HD1	1:H:313:LEU:HD13	1.39	0.87
1:F:306:TRP:HD1	1:F:313:LEU:HD13	1.39	0.86
1:D:306:TRP:HD1	1:D:313:LEU:HD13	1.39	0.86
1:I:306:TRP:HD1	1:I:313:LEU:HD13	1.39	0.86
1:A:306:TRP:HD1	1:A:313:LEU:HD13	1.39	0.86
1:C:306:TRP:HD1	1:C:313:LEU:HD13	1.39	0.85
1:D:403:ASN:OD1	1:D:436:GLU:HG2	1.77	0.85
1:J:403:ASN:OD1	1:J:436:GLU:HG2	1.77	0.85
1:J:270:VAL:HG21	1:J:317:VAL:CG1	2.03	0.85
1:G:306:TRP:HD1	1:G:313:LEU:HD13	1.39	0.85
1:G:403:ASN:OD1	1:G:436:GLU:HG2	1.77	0.85
1:E:403:ASN:OD1	1:E:436:GLU:HG2	1.77	0.84
1:B:403:ASN:OD1	1:B:436:GLU:HG2	1.77	0.84
1:A:403:ASN:OD1	1:A:436:GLU:HG2	1.77	0.84
1:C:270:VAL:CG2	1:C:317:VAL:CG1	2.56	0.84
1:D:270:VAL:CG2	1:D:317:VAL:CG1	2.56	0.84
1:B:23:VAL:CG2	1:B:32:PHE:HB3	2.08	0.83
1:A:270:VAL:CG2	1:A:317:VAL:CG1	2.56	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:316:TRP:CE2	1:C:320:ILE:HD11	2.14	0.83
1:F:403:ASN:OD1	1:F:436:GLU:HG2	1.77	0.83
1:C:403:ASN:OD1	1:C:436:GLU:HG2	1.77	0.83
1:E:270:VAL:CG2	1:E:317:VAL:CG1	2.56	0.83
1:E:316:TRP:CE2	1:E:320:ILE:HD11	2.14	0.83
1:I:23:VAL:CG2	1:I:32:PHE:HB3	2.08	0.83
1:J:23:VAL:CG2	1:J:32:PHE:HB3	2.09	0.83
1:C:23:VAL:CG2	1:C:32:PHE:HB3	2.09	0.83
1:D:316:TRP:CE2	1:D:320:ILE:HD11	2.13	0.83
1:G:316:TRP:CE2	1:G:320:ILE:HD11	2.13	0.83
1:H:403:ASN:OD1	1:H:436:GLU:HG2	1.77	0.83
1:J:316:TRP:CE2	1:J:320:ILE:HD11	2.13	0.83
1:E:306:TRP:CD1	1:E:313:LEU:HD13	2.13	0.83
1:G:306:TRP:CD1	1:G:313:LEU:HD13	2.13	0.83
1:I:403:ASN:OD1	1:I:436:GLU:HG2	1.77	0.83
1:A:306:TRP:CD1	1:A:313:LEU:HD13	2.13	0.83
1:F:316:TRP:CE2	1:F:320:ILE:HD11	2.13	0.83
1:A:23:VAL:CG2	1:A:32:PHE:HB3	2.08	0.83
1:A:316:TRP:CE2	1:A:320:ILE:HD11	2.13	0.83
1:B:270:VAL:CG2	1:B:317:VAL:CG1	2.56	0.83
1:F:270:VAL:CG2	1:F:317:VAL:CG1	2.56	0.83
1:I:306:TRP:CD1	1:I:313:LEU:HD13	2.13	0.83
1:H:270:VAL:CG2	1:H:317:VAL:CG1	2.56	0.83
1:B:306:TRP:CD1	1:B:313:LEU:HD13	2.14	0.82
1:D:306:TRP:CD1	1:D:313:LEU:HD13	2.13	0.82
1:I:316:TRP:CE2	1:I:320:ILE:HD11	2.13	0.82
1:E:23:VAL:CG2	1:E:32:PHE:HB3	2.08	0.82
1:I:270:VAL:CG2	1:I:317:VAL:CG1	2.56	0.82
1:J:270:VAL:CG2	1:J:317:VAL:CG1	2.56	0.82
1:H:316:TRP:CE2	1:H:320:ILE:HD11	2.13	0.82
1:J:306:TRP:CD1	1:J:313:LEU:HD13	2.13	0.82
1:H:23:VAL:CG2	1:H:32:PHE:HB3	2.09	0.82
1:B:316:TRP:CE2	1:B:320:ILE:HD11	2.14	0.82
1:F:306:TRP:CD1	1:F:313:LEU:HD13	2.13	0.82
1:D:23:VAL:CG2	1:D:32:PHE:HB3	2.09	0.82
1:H:306:TRP:CD1	1:H:313:LEU:HD13	2.13	0.81
1:C:306:TRP:CD1	1:C:313:LEU:HD13	2.13	0.81
1:F:23:VAL:CG2	1:F:32:PHE:HB3	2.09	0.81
1:G:270:VAL:CG2	1:G:317:VAL:CG1	2.56	0.81
1:H:171:LYS:O	1:I:232:ARG:NH2	2.13	0.81
1:C:39:TRP:CZ3	1:C:516:MET:HG2	2.17	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:23:VAL:CG2	1:G:32:PHE:HB3	2.09	0.81
1:B:228:THR:O	1:B:232:ARG:HG2	1.82	0.80
1:H:273:PRO:HB3	1:H:276:TYR:CD2	2.17	0.80
1:J:273:PRO:HB3	1:J:276:TYR:CD2	2.17	0.80
1:E:39:TRP:CZ3	1:E:516:MET:HG2	2.16	0.80
1:F:228:THR:O	1:F:232:ARG:HG2	1.82	0.80
1:F:504:ILE:HG13	1:F:510:VAL:HG21	1.64	0.80
1:G:273:PRO:HB3	1:G:276:TYR:CD2	2.17	0.80
1:G:39:TRP:CZ3	1:G:516:MET:HG2	2.17	0.80
1:I:228:THR:O	1:I:232:ARG:HG2	1.82	0.80
1:D:273:PRO:HB3	1:D:276:TYR:CD2	2.17	0.80
1:G:228:THR:O	1:G:232:ARG:HG2	1.82	0.80
1:I:504:ILE:HG13	1:I:510:VAL:HG21	1.64	0.79
1:C:228:THR:O	1:C:232:ARG:HG2	1.82	0.79
1:F:273:PRO:HB3	1:F:276:TYR:CD2	2.17	0.79
1:C:273:PRO:HB3	1:C:276:TYR:CD2	2.17	0.79
1:H:228:THR:O	1:H:232:ARG:HG2	1.82	0.79
1:A:228:THR:O	1:A:232:ARG:HG2	1.82	0.79
1:F:39:TRP:CZ3	1:F:516:MET:HG2	2.17	0.79
1:I:273:PRO:HB3	1:I:276:TYR:CD2	2.17	0.79
1:A:273:PRO:HB3	1:A:276:TYR:CD2	2.17	0.79
1:D:228:THR:O	1:D:232:ARG:HG2	1.81	0.79
1:H:39:TRP:CZ3	1:H:516:MET:HG2	2.18	0.79
1:J:39:TRP:CZ3	1:J:516:MET:HG2	2.18	0.79
1:D:504:ILE:HG13	1:D:510:VAL:HG21	1.64	0.78
1:H:123:GLU:CD	1:I:229:ARG:HH12	1.86	0.78
1:B:504:ILE:HG13	1:B:510:VAL:HG21	1.65	0.78
1:I:39:TRP:CZ3	1:I:516:MET:HG2	2.17	0.78
1:A:39:TRP:CZ3	1:A:516:MET:HG2	2.18	0.78
1:D:39:TRP:CZ3	1:D:516:MET:HG2	2.18	0.78
1:E:273:PRO:HB3	1:E:276:TYR:CD2	2.19	0.78
1:A:504:ILE:HG13	1:A:510:VAL:HG21	1.64	0.78
1:B:39:TRP:CZ3	1:B:516:MET:HG2	2.17	0.78
1:J:504:ILE:HG13	1:J:510:VAL:HG21	1.65	0.78
1:C:504:ILE:HG13	1:C:510:VAL:HG21	1.64	0.78
1:E:228:THR:O	1:E:232:ARG:HG2	1.82	0.77
1:E:504:ILE:HG13	1:E:510:VAL:HG21	1.65	0.77
1:B:273:PRO:HB3	1:B:276:TYR:CD2	2.19	0.77
1:J:228:THR:O	1:J:232:ARG:HG2	1.83	0.77
1:G:504:ILE:HG13	1:G:510:VAL:HG21	1.64	0.77
1:D:171:LYS:O	1:J:232:ARG:NH2	2.17	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:123:GLU:HG2	1:C:171:LYS:HD2	1.68	0.76
1:H:504:ILE:HG13	1:H:510:VAL:HG21	1.65	0.76
1:A:123:GLU:HG2	1:A:171:LYS:HD2	1.68	0.76
1:D:123:GLU:HG2	1:D:171:LYS:HD2	1.68	0.76
1:B:123:GLU:HG2	1:B:171:LYS:HD2	1.68	0.76
1:I:123:GLU:HG2	1:I:171:LYS:HD2	1.68	0.75
1:J:123:GLU:HG2	1:J:171:LYS:HD2	1.67	0.75
1:D:418:VAL:HG12	1:J:141:ASN:HD21	1.52	0.74
1:H:123:GLU:HG2	1:H:171:LYS:HD2	1.68	0.74
1:I:40:ALA:HB3	1:I:290:ASN:OD1	1.88	0.74
1:F:40:ALA:HB3	1:F:290:ASN:OD1	1.87	0.74
1:C:270:VAL:HG23	1:C:317:VAL:HG12	1.70	0.74
1:B:40:ALA:HB3	1:B:290:ASN:OD1	1.88	0.74
1:E:40:ALA:HB3	1:E:290:ASN:OD1	1.88	0.74
1:G:123:GLU:HG2	1:G:171:LYS:HD2	1.68	0.74
1:A:270:VAL:HG23	1:A:317:VAL:HG12	1.70	0.74
1:E:123:GLU:HG2	1:E:171:LYS:HD2	1.68	0.74
1:A:40:ALA:HB3	1:A:290:ASN:OD1	1.88	0.73
1:C:40:ALA:HB3	1:C:290:ASN:OD1	1.88	0.73
1:F:123:GLU:HG2	1:F:171:LYS:HD2	1.68	0.73
1:G:545:ARG:HD2	1:G:572:ALA:HB1	1.71	0.73
1:H:40:ALA:HB3	1:H:290:ASN:OD1	1.88	0.73
1:D:270:VAL:HG23	1:D:317:VAL:HG12	1.70	0.73
1:E:545:ARG:HD2	1:E:572:ALA:HB1	1.71	0.73
1:D:40:ALA:HB3	1:D:290:ASN:OD1	1.88	0.72
1:J:270:VAL:HG23	1:J:317:VAL:HG12	1.70	0.72
1:H:270:VAL:HG23	1:H:317:VAL:HG12	1.70	0.72
1:D:123:GLU:CD	1:J:229:ARG:HH12	1.93	0.72
1:G:40:ALA:HB3	1:G:290:ASN:OD1	1.88	0.72
1:F:545:ARG:HD2	1:F:572:ALA:HB1	1.71	0.72
1:H:545:ARG:HD2	1:H:572:ALA:HB1	1.71	0.72
1:G:270:VAL:HG23	1:G:317:VAL:HG12	1.70	0.72
1:I:545:ARG:HD2	1:I:572:ALA:HB1	1.71	0.72
1:C:306:TRP:CD1	1:C:313:LEU:CD1	2.73	0.71
1:G:306:TRP:CD1	1:G:313:LEU:CD1	2.73	0.71
1:H:39:TRP:CE3	1:H:289:ILE:HD11	2.25	0.71
1:J:40:ALA:HB3	1:J:290:ASN:OD1	1.88	0.71
1:E:270:VAL:HG23	1:E:317:VAL:HG12	1.70	0.71
1:B:545:ARG:HD2	1:B:572:ALA:HB1	1.71	0.71
1:A:306:TRP:CD1	1:A:313:LEU:CD1	2.74	0.71
1:C:545:ARG:HD2	1:C:572:ALA:HB1	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:306:TRP:CD1	1:D:313:LEU:CD1	2.73	0.71
1:G:39:TRP:CE3	1:G:289:ILE:HD11	2.25	0.71
1:H:306:TRP:CD1	1:H:313:LEU:CD1	2.74	0.71
1:C:39:TRP:CE3	1:C:289:ILE:HD11	2.26	0.71
1:E:306:TRP:CD1	1:E:313:LEU:CD1	2.74	0.71
1:F:306:TRP:CD1	1:F:313:LEU:CD1	2.73	0.71
1:I:39:TRP:CE3	1:I:289:ILE:HD11	2.26	0.71
1:E:145:ASP:HB3	1:E:148:GLN:HE21	1.56	0.71
1:F:39:TRP:CE3	1:F:289:ILE:HD11	2.26	0.71
1:H:418:VAL:HG12	1:I:141:ASN:HD21	1.55	0.71
1:D:39:TRP:CE3	1:D:289:ILE:HD11	2.25	0.70
1:J:39:TRP:CE3	1:J:289:ILE:HD11	2.25	0.70
1:B:306:TRP:CD1	1:B:313:LEU:CD1	2.74	0.70
1:D:316:TRP:CD2	1:D:320:ILE:HD11	2.26	0.70
1:I:270:VAL:HG23	1:I:317:VAL:HG12	1.70	0.70
1:J:316:TRP:CD2	1:J:320:ILE:HD11	2.26	0.70
1:I:306:TRP:CD1	1:I:313:LEU:CD1	2.74	0.70
1:I:316:TRP:CD2	1:I:320:ILE:HD11	2.27	0.70
1:A:145:ASP:HB3	1:A:148:GLN:HE21	1.56	0.70
1:C:412:GLN:HG2	1:C:423:THR:HG22	1.73	0.70
1:G:418:VAL:HG12	1:H:141:ASN:HD21	1.57	0.70
1:J:306:TRP:CD1	1:J:313:LEU:CD1	2.74	0.70
1:A:545:ARG:HD2	1:A:572:ALA:HB1	1.71	0.70
1:E:39:TRP:CE3	1:E:289:ILE:HD11	2.26	0.70
1:G:145:ASP:HB3	1:G:148:GLN:HE21	1.57	0.70
1:G:316:TRP:CD2	1:G:320:ILE:HD11	2.27	0.70
1:A:39:TRP:CE3	1:A:289:ILE:HD11	2.25	0.70
1:F:145:ASP:HB3	1:F:148:GLN:HE21	1.57	0.70
1:B:145:ASP:HB3	1:B:148:GLN:HE21	1.56	0.70
1:D:545:ARG:HD2	1:D:572:ALA:HB1	1.71	0.70
1:E:316:TRP:CD2	1:E:320:ILE:HD11	2.27	0.70
1:A:316:TRP:CD2	1:A:320:ILE:HD11	2.27	0.70
1:B:270:VAL:HG22	1:B:321:ASN:ND2	2.07	0.70
1:B:316:TRP:CD2	1:B:320:ILE:HD11	2.27	0.70
1:H:145:ASP:HB3	1:H:148:GLN:HE21	1.56	0.70
1:B:39:TRP:CE3	1:B:289:ILE:HD11	2.26	0.70
1:B:412:GLN:HG2	1:B:423:THR:HG22	1.73	0.70
1:J:545:ARG:HD2	1:J:572:ALA:HB1	1.71	0.70
1:A:412:GLN:HG2	1:A:423:THR:HG22	1.73	0.69
1:C:270:VAL:HG22	1:C:321:ASN:ND2	2.07	0.69
1:E:270:VAL:HG22	1:E:321:ASN:ND2	2.07	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:412:GLN:HG2	1:E:423:THR:HG22	1.73	0.69
1:A:418:VAL:HG12	1:B:141:ASN:HD21	1.58	0.69
1:D:270:VAL:HG22	1:D:321:ASN:ND2	2.07	0.69
1:C:316:TRP:CD2	1:C:320:ILE:HD11	2.27	0.69
1:D:412:GLN:HG2	1:D:423:THR:HG22	1.74	0.69
1:F:316:TRP:CD2	1:F:320:ILE:HD11	2.27	0.69
1:H:316:TRP:CD2	1:H:320:ILE:HD11	2.27	0.69
1:B:270:VAL:HG23	1:B:317:VAL:HG12	1.70	0.69
1:F:270:VAL:HG22	1:F:321:ASN:ND2	2.07	0.69
1:J:270:VAL:HG22	1:J:321:ASN:ND2	2.08	0.69
1:D:145:ASP:HB3	1:D:148:GLN:HE21	1.56	0.69
1:A:270:VAL:HG22	1:A:321:ASN:ND2	2.08	0.69
1:J:412:GLN:HG2	1:J:423:THR:HG22	1.73	0.69
1:H:412:GLN:HG2	1:H:423:THR:HG22	1.74	0.69
1:I:145:ASP:HB3	1:I:148:GLN:HE21	1.57	0.69
1:E:171:LYS:O	1:F:232:ARG:NH2	2.25	0.69
1:F:270:VAL:HG23	1:F:317:VAL:HG12	1.70	0.69
1:G:270:VAL:HG22	1:G:321:ASN:ND2	2.07	0.69
1:J:145:ASP:HB3	1:J:148:GLN:HE21	1.57	0.69
1:D:262:VAL:HG11	1:D:285:LEU:HD12	1.76	0.69
1:H:267:HIS:NE2	1:H:295:THR:HG23	2.09	0.68
1:I:267:HIS:NE2	1:I:295:THR:HG23	2.09	0.68
1:I:412:GLN:HG2	1:I:423:THR:HG22	1.73	0.68
1:A:262:VAL:HG11	1:A:285:LEU:HD12	1.76	0.68
1:D:267:HIS:NE2	1:D:295:THR:HG23	2.09	0.68
1:F:412:GLN:HG2	1:F:423:THR:HG22	1.74	0.68
1:I:270:VAL:HG22	1:I:321:ASN:ND2	2.07	0.68
1:J:267:HIS:NE2	1:J:295:THR:HG23	2.09	0.68
1:A:171:LYS:O	1:B:232:ARG:NH2	2.26	0.68
1:G:267:HIS:NE2	1:G:295:THR:HG23	2.09	0.68
1:G:412:GLN:HG2	1:G:423:THR:HG22	1.73	0.68
1:H:270:VAL:HG22	1:H:321:ASN:ND2	2.07	0.68
1:A:123:GLU:CD	1:B:229:ARG:HH12	1.96	0.68
1:B:262:VAL:HG11	1:B:285:LEU:HD12	1.76	0.68
1:E:267:HIS:NE2	1:E:295:THR:HG23	2.09	0.68
1:F:267:HIS:NE2	1:F:295:THR:HG23	2.09	0.68
1:C:145:ASP:HB3	1:C:148:GLN:HE21	1.56	0.68
1:F:545:ARG:HB2	1:F:572:ALA:HB3	1.76	0.67
1:H:262:VAL:HG11	1:H:285:LEU:HD12	1.76	0.67
1:H:545:ARG:HB2	1:H:572:ALA:HB3	1.77	0.67
1:A:545:ARG:HB2	1:A:572:ALA:HB3	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:267:HIS:NE2	1:B:295:THR:HG23	2.09	0.67
1:G:545:ARG:HB2	1:G:572:ALA:HB3	1.76	0.67
1:J:262:VAL:HG11	1:J:285:LEU:HD12	1.76	0.67
1:B:171:LYS:O	1:C:232:ARG:NH2	2.27	0.67
1:I:593:LEU:O	1:I:596:ARG:HB3	1.95	0.67
1:J:593:LEU:O	1:J:596:ARG:HB3	1.95	0.67
1:A:267:HIS:NE2	1:A:295:THR:HG23	2.09	0.67
1:C:262:VAL:HG11	1:C:285:LEU:HD12	1.76	0.67
1:G:262:VAL:HG11	1:G:285:LEU:HD12	1.76	0.67
1:I:545:ARG:HB2	1:I:572:ALA:HB3	1.76	0.67
1:A:593:LEU:O	1:A:596:ARG:HB3	1.95	0.67
1:D:545:ARG:HB2	1:D:572:ALA:HB3	1.76	0.67
1:E:123:GLU:CD	1:F:229:ARG:HH12	1.97	0.67
1:E:593:LEU:O	1:E:596:ARG:HB3	1.95	0.67
1:C:593:LEU:O	1:C:596:ARG:HB3	1.95	0.67
1:E:545:ARG:HB2	1:E:572:ALA:HB3	1.76	0.67
1:C:267:HIS:NE2	1:C:295:THR:HG23	2.09	0.67
1:J:545:ARG:HB2	1:J:572:ALA:HB3	1.77	0.66
1:E:262:VAL:HG11	1:E:285:LEU:HD12	1.76	0.66
1:B:545:ARG:HB2	1:B:572:ALA:HB3	1.77	0.66
1:H:593:LEU:O	1:H:596:ARG:HB3	1.95	0.66
1:I:262:VAL:HG11	1:I:285:LEU:HD12	1.76	0.66
1:B:593:LEU:O	1:B:596:ARG:HB3	1.95	0.66
1:B:266:VAL:HG13	1:B:286:ARG:HD2	1.78	0.65
1:F:262:VAL:HG11	1:F:285:LEU:HD12	1.76	0.65
1:G:266:VAL:HG13	1:G:286:ARG:HD2	1.78	0.65
1:F:593:LEU:O	1:F:596:ARG:HB3	1.95	0.65
1:A:266:VAL:HG13	1:A:286:ARG:HD2	1.78	0.65
1:D:593:LEU:O	1:D:596:ARG:HB3	1.95	0.65
1:G:593:LEU:O	1:G:596:ARG:HB3	1.95	0.65
1:C:266:VAL:HG13	1:C:286:ARG:HD2	1.79	0.65
1:C:545:ARG:HB2	1:C:572:ALA:HB3	1.77	0.65
1:J:266:VAL:HG13	1:J:286:ARG:HD2	1.79	0.65
1:B:272:ALA:N	1:B:273:PRO:CD	2.60	0.65
1:A:272:ALA:N	1:A:273:PRO:CD	2.60	0.64
1:D:272:ALA:N	1:D:273:PRO:CD	2.60	0.64
1:E:272:ALA:N	1:E:273:PRO:CD	2.60	0.64
1:F:418:VAL:HG12	1:G:141:ASN:HD21	1.61	0.64
1:H:266:VAL:HG13	1:H:286:ARG:HD2	1.79	0.64
1:I:272:ALA:N	1:I:273:PRO:CD	2.60	0.64
1:J:272:ALA:N	1:J:273:PRO:CD	2.60	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:230:PHE:O	1:F:234:MET:HG3	1.98	0.64
1:G:230:PHE:O	1:G:234:MET:HG3	1.98	0.64
1:G:272:ALA:N	1:G:273:PRO:CD	2.61	0.64
1:H:272:ALA:N	1:H:273:PRO:CD	2.61	0.64
1:E:230:PHE:O	1:E:234:MET:HG3	1.98	0.64
1:H:230:PHE:O	1:H:234:MET:HG3	1.97	0.64
1:C:230:PHE:O	1:C:234:MET:HG3	1.98	0.64
1:F:266:VAL:HG13	1:F:286:ARG:HD2	1.78	0.64
1:D:230:PHE:O	1:D:234:MET:HG3	1.98	0.64
1:J:39:TRP:CH2	1:J:516:MET:HA	2.33	0.64
1:C:39:TRP:CH2	1:C:516:MET:HA	2.33	0.64
1:D:266:VAL:HG13	1:D:286:ARG:HD2	1.78	0.64
1:F:547:THR:HG21	1:F:571:VAL:HG12	1.80	0.64
1:B:547:THR:HG21	1:B:571:VAL:HG12	1.80	0.63
1:C:272:ALA:N	1:C:273:PRO:CD	2.60	0.63
1:I:266:VAL:HG13	1:I:286:ARG:HD2	1.78	0.63
1:E:266:VAL:HG13	1:E:286:ARG:HD2	1.79	0.63
1:E:547:THR:HG21	1:E:571:VAL:HG12	1.80	0.63
1:G:39:TRP:CH2	1:G:516:MET:HA	2.33	0.63
1:A:232:ARG:NH2	1:J:171:LYS:O	2.30	0.63
1:A:547:THR:HG21	1:A:571:VAL:HG12	1.80	0.63
1:F:39:TRP:CH2	1:F:516:MET:HA	2.33	0.63
1:J:230:PHE:O	1:J:234:MET:HG3	1.98	0.63
1:B:716:ALA:HA	1:B:742:SER:OG	1.99	0.63
1:F:272:ALA:N	1:F:273:PRO:CD	2.61	0.63
1:D:39:TRP:CH2	1:D:516:MET:HA	2.34	0.63
1:I:230:PHE:O	1:I:234:MET:HG3	1.98	0.63
1:E:304:GLN:OE1	1:I:429:ARG:NE	2.28	0.63
1:J:547:THR:HG21	1:J:571:VAL:HG12	1.80	0.63
1:B:230:PHE:O	1:B:234:MET:HG3	1.98	0.63
1:H:716:ALA:HA	1:H:742:SER:OG	1.99	0.63
1:I:39:TRP:CH2	1:I:516:MET:HA	2.34	0.63
1:A:230:PHE:O	1:A:234:MET:HG3	1.98	0.63
1:A:39:TRP:CH2	1:A:516:MET:HA	2.34	0.63
1:B:39:TRP:CH2	1:B:516:MET:HA	2.33	0.63
1:E:716:ALA:HA	1:E:742:SER:OG	1.99	0.63
1:E:39:TRP:CH2	1:E:516:MET:HA	2.33	0.63
1:I:716:ALA:HA	1:I:742:SER:OG	1.99	0.63
1:H:547:THR:HG21	1:H:571:VAL:HG12	1.80	0.63
1:C:547:THR:HG21	1:C:571:VAL:HG12	1.80	0.62
1:A:39:TRP:CZ3	1:A:289:ILE:HD11	2.35	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:30:ILE:HG23	1:C:31:PRO:HD2	1.82	0.62
1:C:716:ALA:HA	1:C:742:SER:OG	2.00	0.62
1:G:716:ALA:HA	1:G:742:SER:OG	1.99	0.62
1:H:123:GLU:OE2	1:I:229:ARG:NH2	2.32	0.62
1:B:123:GLU:CD	1:C:229:ARG:HH12	2.03	0.62
1:E:232:ARG:NH2	1:I:171:LYS:O	2.32	0.62
1:I:547:THR:HG21	1:I:571:VAL:HG12	1.80	0.62
1:F:716:ALA:HA	1:F:742:SER:OG	1.99	0.62
1:G:547:THR:HG21	1:G:571:VAL:HG12	1.80	0.62
1:H:39:TRP:CZ3	1:H:289:ILE:HD11	2.35	0.62
1:E:30:ILE:HG23	1:E:31:PRO:HD2	1.82	0.62
1:G:39:TRP:CZ3	1:G:289:ILE:HD11	2.35	0.62
1:A:716:ALA:HA	1:A:742:SER:OG	1.99	0.62
1:A:429:ARG:NE	1:B:304:GLN:OE1	2.32	0.62
1:B:51:SER:HB2	1:B:56:ARG:HA	1.82	0.62
1:D:716:ALA:HA	1:D:742:SER:OG	1.99	0.62
1:D:39:TRP:CZ3	1:D:289:ILE:HD11	2.35	0.61
1:G:30:ILE:HG23	1:G:31:PRO:HD2	1.82	0.61
1:C:51:SER:HB2	1:C:56:ARG:HA	1.82	0.61
1:H:39:TRP:CH2	1:H:516:MET:HA	2.34	0.61
1:I:51:SER:HB2	1:I:56:ARG:HA	1.82	0.61
1:J:30:ILE:HG23	1:J:31:PRO:HD2	1.82	0.61
1:D:547:THR:HG21	1:D:571:VAL:HG12	1.80	0.61
1:J:716:ALA:HA	1:J:742:SER:OG	1.99	0.61
1:A:30:ILE:HG23	1:A:31:PRO:HD2	1.83	0.61
1:B:39:TRP:CZ3	1:B:289:ILE:HD11	2.35	0.61
1:D:30:ILE:HG23	1:D:31:PRO:HD2	1.82	0.61
1:B:30:ILE:HG23	1:B:31:PRO:HD2	1.83	0.61
1:C:39:TRP:CZ3	1:C:289:ILE:HD11	2.36	0.61
1:D:51:SER:HB2	1:D:56:ARG:HA	1.82	0.61
1:E:51:SER:HB2	1:E:56:ARG:HA	1.82	0.61
1:H:30:ILE:HG23	1:H:31:PRO:HD2	1.82	0.61
1:I:39:TRP:CZ3	1:I:289:ILE:HD11	2.35	0.61
1:B:76:LYS:O	1:B:79:SER:HB3	2.01	0.61
1:A:76:LYS:O	1:A:79:SER:HB3	2.01	0.61
1:E:76:LYS:O	1:E:79:SER:HB3	2.01	0.61
1:F:30:ILE:HG23	1:F:31:PRO:HD2	1.82	0.61
1:F:51:SER:HB2	1:F:56:ARG:HA	1.82	0.61
1:A:141:ASN:HD21	1:J:418:VAL:HG12	1.66	0.61
1:E:39:TRP:CZ3	1:E:289:ILE:HD11	2.36	0.61
1:F:39:TRP:CZ3	1:F:289:ILE:HD11	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:39:TRP:CZ3	1:J:289:ILE:HD11	2.35	0.61
1:I:76:LYS:O	1:I:79:SER:HB3	2.01	0.60
1:B:418:VAL:HG12	1:C:141:ASN:HD21	1.66	0.60
1:D:76:LYS:O	1:D:79:SER:HB3	2.01	0.60
1:A:51:SER:HB2	1:A:56:ARG:HA	1.82	0.60
1:G:51:SER:HB2	1:G:56:ARG:HA	1.82	0.60
1:H:76:LYS:O	1:H:79:SER:HB3	2.01	0.60
1:H:51:SER:HB2	1:H:56:ARG:HA	1.83	0.60
1:F:740:LEU:HD23	1:F:784:VAL:HG21	1.84	0.60
1:J:76:LYS:O	1:J:79:SER:HB3	2.01	0.60
1:F:76:LYS:O	1:F:79:SER:HB3	2.01	0.60
1:G:76:LYS:O	1:G:79:SER:HB3	2.01	0.60
1:H:480:PRO:HD2	1:H:567:LEU:CD2	2.32	0.60
1:C:480:PRO:HD2	1:C:567:LEU:CD2	2.32	0.60
1:E:740:LEU:HD23	1:E:784:VAL:HG21	1.84	0.60
1:J:51:SER:HB2	1:J:56:ARG:HA	1.82	0.60
1:E:141:ASN:HD21	1:I:418:VAL:HG12	1.66	0.60
1:I:30:ILE:HG23	1:I:31:PRO:HD2	1.82	0.60
1:C:740:LEU:HD23	1:C:784:VAL:HG21	1.84	0.59
1:I:480:PRO:HD2	1:I:567:LEU:CD2	2.32	0.59
1:I:740:LEU:HD23	1:I:784:VAL:HG21	1.84	0.59
1:A:740:LEU:HD23	1:A:784:VAL:HG21	1.84	0.59
1:B:480:PRO:HD2	1:B:567:LEU:CD2	2.32	0.59
1:F:480:PRO:HD2	1:F:567:LEU:CD2	2.32	0.59
1:A:50:THR:HG22	1:A:183:ILE:HB	1.85	0.59
1:B:740:LEU:HD23	1:B:784:VAL:HG21	1.84	0.59
1:C:418:VAL:HG12	1:D:141:ASN:HD21	1.66	0.59
1:E:480:PRO:HD2	1:E:567:LEU:CD2	2.32	0.59
1:I:50:THR:HG22	1:I:183:ILE:HB	1.85	0.59
1:C:76:LYS:O	1:C:79:SER:HB3	2.01	0.59
1:J:740:LEU:HD23	1:J:784:VAL:HG21	1.84	0.59
1:C:39:TRP:CD2	1:C:289:ILE:HD11	2.38	0.59
1:E:50:THR:HG22	1:E:183:ILE:HB	1.85	0.59
1:G:480:PRO:HD2	1:G:567:LEU:CD2	2.32	0.59
1:H:740:LEU:HD23	1:H:784:VAL:HG21	1.83	0.59
1:G:39:TRP:CD2	1:G:289:ILE:HD11	2.38	0.59
1:J:480:PRO:HD2	1:J:567:LEU:CD2	2.32	0.59
1:D:480:PRO:HD2	1:D:567:LEU:CD2	2.32	0.59
1:H:39:TRP:CD2	1:H:289:ILE:HD11	2.38	0.59
1:C:50:THR:HG22	1:C:183:ILE:HB	1.85	0.58
1:G:740:LEU:HD23	1:G:784:VAL:HG21	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:480:PRO:HD2	1:A:567:LEU:CD2	2.33	0.58
1:H:50:THR:HG22	1:H:183:ILE:HB	1.85	0.58
1:J:50:THR:HG22	1:J:183:ILE:HB	1.84	0.58
1:E:39:TRP:CD2	1:E:289:ILE:HD11	2.38	0.58
1:I:39:TRP:CD2	1:I:289:ILE:HD11	2.38	0.58
1:B:354:ARG:NH1	1:B:358:THR:HG22	2.19	0.58
1:C:30:ILE:HG23	1:C:31:PRO:CD	2.33	0.58
1:D:120:SER:OG	1:D:223:ARG:N	2.37	0.58
1:D:30:ILE:HG23	1:D:31:PRO:CD	2.34	0.58
1:D:740:LEU:HD23	1:D:784:VAL:HG21	1.84	0.58
1:A:39:TRP:CD2	1:A:289:ILE:HD11	2.38	0.58
1:E:30:ILE:HG23	1:E:31:PRO:CD	2.34	0.58
1:H:354:ARG:NH1	1:H:358:THR:HG22	2.19	0.58
1:C:723:ILE:HD11	1:D:509:SER:OG	2.03	0.58
1:F:30:ILE:HG23	1:F:31:PRO:CD	2.34	0.58
1:J:30:ILE:HG23	1:J:31:PRO:CD	2.34	0.58
1:F:354:ARG:NH1	1:F:358:THR:HG22	2.19	0.58
1:B:557:SER:OG	1:B:560:ALA:HB3	2.04	0.58
1:F:39:TRP:CD2	1:F:289:ILE:HD11	2.38	0.58
1:G:660:ALA:HB1	1:H:85:ASP:OD2	2.03	0.58
1:H:30:ILE:CG2	1:H:31:PRO:HD2	2.34	0.58
1:A:354:ARG:NH1	1:A:358:THR:HG22	2.19	0.57
1:B:103:THR:HG22	1:B:133:ILE:HA	1.86	0.57
1:B:30:ILE:HG23	1:B:31:PRO:CD	2.34	0.57
1:B:50:THR:HG22	1:B:183:ILE:HB	1.85	0.57
1:D:39:TRP:CD2	1:D:289:ILE:HD11	2.38	0.57
1:D:50:THR:HG22	1:D:183:ILE:HB	1.85	0.57
1:G:50:THR:HG22	1:G:183:ILE:HB	1.85	0.57
1:I:354:ARG:NH1	1:I:358:THR:HG22	2.19	0.57
1:A:229:ARG:HH12	1:J:123:GLU:CD	2.08	0.57
1:B:285:LEU:HD13	1:B:291:PHE:CE2	2.39	0.57
1:B:375:LEU:HB2	1:B:582:ILE:O	2.05	0.57
1:B:39:TRP:CD2	1:B:289:ILE:HD11	2.39	0.57
1:E:30:ILE:CG2	1:E:31:PRO:HD2	2.34	0.57
1:F:375:LEU:HB2	1:F:582:ILE:O	2.04	0.57
1:F:50:THR:HG22	1:F:183:ILE:HB	1.85	0.57
1:G:375:LEU:HB2	1:G:582:ILE:O	2.05	0.57
1:H:120:SER:OG	1:H:223:ARG:N	2.37	0.57
1:J:30:ILE:CG2	1:J:31:PRO:HD2	2.34	0.57
1:A:103:THR:HG22	1:A:133:ILE:HA	1.87	0.57
1:A:30:ILE:HG23	1:A:31:PRO:CD	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:ILE:CG2	1:A:31:PRO:HD2	2.34	0.57
1:A:712:TYR:HE2	1:A:750:VAL:HG21	1.70	0.57
1:D:30:ILE:CG2	1:D:31:PRO:HD2	2.34	0.57
1:F:120:SER:OG	1:F:223:ARG:N	2.37	0.57
1:G:30:ILE:CG2	1:G:31:PRO:HD2	2.34	0.57
1:G:557:SER:OG	1:G:560:ALA:HB3	2.05	0.57
1:H:375:LEU:HB2	1:H:582:ILE:O	2.05	0.57
1:H:557:SER:OG	1:H:560:ALA:HB3	2.05	0.57
1:J:557:SER:OG	1:J:560:ALA:HB3	2.04	0.57
1:B:120:SER:OG	1:B:223:ARG:N	2.37	0.57
1:I:557:SER:OG	1:I:560:ALA:HB3	2.05	0.57
1:J:270:VAL:HG11	1:J:320:ILE:HB	1.86	0.57
1:D:123:GLU:OE2	1:J:229:ARG:NH2	2.35	0.57
1:E:123:GLU:CG	1:E:171:LYS:HD2	2.35	0.57
1:I:120:SER:OG	1:I:223:ARG:N	2.38	0.57
1:I:375:LEU:HB2	1:I:582:ILE:O	2.05	0.57
1:J:39:TRP:CD2	1:J:289:ILE:HD11	2.38	0.57
1:A:55:ARG:NE	1:A:587:ILE:HD11	2.20	0.57
1:B:30:ILE:CG2	1:B:31:PRO:HD2	2.34	0.57
1:C:103:THR:HG22	1:C:133:ILE:HA	1.87	0.57
1:C:30:ILE:CG2	1:C:31:PRO:HD2	2.34	0.57
1:I:164:LEU:O	1:I:168:GLY:HA2	2.05	0.57
1:B:164:LEU:O	1:B:168:GLY:HA2	2.05	0.57
1:E:164:LEU:O	1:E:168:GLY:HA2	2.05	0.57
1:E:354:ARG:NH1	1:E:358:THR:HG22	2.19	0.57
1:E:55:ARG:NE	1:E:587:ILE:HD11	2.20	0.57
1:F:557:SER:OG	1:F:560:ALA:HB3	2.05	0.57
1:H:30:ILE:HG23	1:H:31:PRO:CD	2.34	0.57
1:I:123:GLU:CG	1:I:171:LYS:HD2	2.35	0.57
1:J:354:ARG:NH1	1:J:358:THR:HG22	2.19	0.57
1:G:164:LEU:O	1:G:168:GLY:HA2	2.05	0.57
1:G:354:ARG:NH1	1:G:358:THR:HG22	2.19	0.57
1:I:285:LEU:HD13	1:I:291:PHE:CE2	2.40	0.57
1:I:270:VAL:HG11	1:I:320:ILE:HB	1.87	0.57
1:A:285:LEU:HD13	1:A:291:PHE:CE2	2.40	0.57
1:C:712:TYR:HE2	1:C:750:VAL:HG21	1.70	0.57
1:D:164:LEU:O	1:D:168:GLY:HA2	2.05	0.57
1:E:375:LEU:HB2	1:E:582:ILE:O	2.05	0.57
1:F:171:LYS:O	1:G:232:ARG:NH2	2.38	0.57
1:G:712:TYR:HE2	1:G:750:VAL:HG21	1.70	0.57
1:D:123:GLU:CG	1:D:171:LYS:HD2	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:712:TYR:HE2	1:E:750:VAL:HG21	1.70	0.57
1:G:30:ILE:HG23	1:G:31:PRO:CD	2.34	0.57
1:H:285:LEU:HD13	1:H:291:PHE:CE2	2.39	0.57
1:B:123:GLU:CG	1:B:171:LYS:HD2	2.35	0.56
1:C:164:LEU:O	1:C:168:GLY:HA2	2.05	0.56
1:C:348:ASP:C	1:C:351:PRO:HD2	2.26	0.56
1:C:557:SER:OG	1:C:560:ALA:HB3	2.05	0.56
1:D:354:ARG:NH1	1:D:358:THR:HG22	2.19	0.56
1:D:55:ARG:NE	1:D:587:ILE:HD11	2.20	0.56
1:E:285:LEU:HD13	1:E:291:PHE:CE2	2.39	0.56
1:E:557:SER:OG	1:E:560:ALA:HB3	2.04	0.56
1:F:164:LEU:O	1:F:168:GLY:HA2	2.04	0.56
1:A:557:SER:OG	1:A:560:ALA:HB3	2.05	0.56
1:A:375:LEU:HB2	1:A:582:ILE:O	2.05	0.56
1:C:123:GLU:CG	1:C:171:LYS:HD2	2.35	0.56
1:C:270:VAL:HG11	1:C:320:ILE:HB	1.87	0.56
1:D:103:THR:HG22	1:D:133:ILE:HA	1.87	0.56
1:D:285:LEU:HD13	1:D:291:PHE:CE2	2.40	0.56
1:D:659:ILE:H	1:D:659:ILE:HD12	1.70	0.56
1:F:30:ILE:CG2	1:F:31:PRO:HD2	2.34	0.56
1:G:120:SER:OG	1:G:223:ARG:N	2.38	0.56
1:J:285:LEU:HD13	1:J:291:PHE:CE2	2.40	0.56
1:J:375:LEU:HB2	1:J:582:ILE:O	2.05	0.56
1:A:123:GLU:CG	1:A:171:LYS:HD2	2.35	0.56
1:D:375:LEU:HB2	1:D:582:ILE:O	2.04	0.56
1:E:120:SER:OG	1:E:223:ARG:N	2.38	0.56
1:E:659:ILE:H	1:E:659:ILE:HD12	1.70	0.56
1:F:659:ILE:H	1:F:659:ILE:HD12	1.70	0.56
1:G:103:THR:HG22	1:G:133:ILE:HA	1.86	0.56
1:H:164:LEU:O	1:H:168:GLY:HA2	2.04	0.56
1:I:30:ILE:CG2	1:I:31:PRO:HD2	2.34	0.56
1:I:30:ILE:HG23	1:I:31:PRO:CD	2.34	0.56
1:A:316:TRP:CZ2	1:A:320:ILE:HD11	2.41	0.56
1:C:120:SER:OG	1:C:223:ARG:N	2.39	0.56
1:D:557:SER:OG	1:D:560:ALA:HB3	2.05	0.56
1:E:103:THR:HG22	1:E:133:ILE:HA	1.87	0.56
1:E:229:ARG:HH12	1:I:123:GLU:CD	2.09	0.56
1:B:167:SER:OG	1:B:169:HIS:CD2	2.59	0.56
1:C:354:ARG:NH1	1:C:358:THR:HG22	2.19	0.56
1:D:348:ASP:C	1:D:351:PRO:HD2	2.26	0.56
1:E:270:VAL:HG11	1:E:320:ILE:HB	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:270:VAL:HG11	1:F:320:ILE:HB	1.87	0.56
1:F:49:ILE:HG23	1:F:50:THR:HG23	1.88	0.56
1:G:270:VAL:HG11	1:G:320:ILE:HB	1.87	0.56
1:G:348:ASP:C	1:G:351:PRO:HD2	2.25	0.56
1:G:55:ARG:NE	1:G:587:ILE:HD11	2.20	0.56
1:D:270:VAL:HG11	1:D:320:ILE:HB	1.87	0.56
1:F:285:LEU:HD13	1:F:291:PHE:CE2	2.40	0.56
1:G:503:ILE:HG22	1:G:515:TYR:CE1	2.40	0.56
1:H:55:ARG:NE	1:H:587:ILE:HD11	2.20	0.56
1:J:120:SER:OG	1:J:223:ARG:N	2.38	0.56
1:C:285:LEU:HD13	1:C:291:PHE:CE2	2.40	0.56
1:C:49:ILE:HG23	1:C:50:THR:HG23	1.87	0.56
1:D:49:ILE:HG23	1:D:50:THR:HG23	1.88	0.56
1:F:123:GLU:CG	1:F:171:LYS:HD2	2.35	0.56
1:F:712:TYR:HE2	1:F:750:VAL:HG21	1.70	0.56
1:I:103:THR:HG22	1:I:133:ILE:HA	1.88	0.56
1:I:167:SER:OG	1:I:169:HIS:CD2	2.59	0.56
1:I:659:ILE:HD12	1:I:659:ILE:H	1.70	0.56
1:B:55:ARG:NE	1:B:587:ILE:HD11	2.20	0.56
1:C:55:ARG:NE	1:C:587:ILE:HD11	2.20	0.56
1:H:712:TYR:HE2	1:H:750:VAL:HG21	1.70	0.56
1:J:659:ILE:HD12	1:J:659:ILE:H	1.71	0.56
1:C:375:LEU:HB2	1:C:582:ILE:O	2.04	0.56
1:D:316:TRP:CZ2	1:D:320:ILE:HD11	2.41	0.56
1:D:503:ILE:HG22	1:D:515:TYR:CE1	2.41	0.56
1:D:712:TYR:HE2	1:D:750:VAL:HG21	1.70	0.56
1:E:503:ILE:HG22	1:E:515:TYR:CE1	2.41	0.56
1:G:659:ILE:HD12	1:G:659:ILE:H	1.71	0.56
1:H:270:VAL:HG11	1:H:320:ILE:HB	1.87	0.56
1:H:348:ASP:C	1:H:351:PRO:HD2	2.26	0.56
1:I:348:ASP:C	1:I:351:PRO:HD2	2.26	0.56
1:I:712:TYR:HE2	1:I:750:VAL:HG21	1.70	0.56
1:A:167:SER:OG	1:A:169:HIS:CD2	2.59	0.56
1:A:120:SER:OG	1:A:223:ARG:N	2.38	0.56
1:A:270:VAL:HG11	1:A:320:ILE:HB	1.87	0.56
1:E:348:ASP:C	1:E:351:PRO:HD2	2.26	0.56
1:G:316:TRP:CZ2	1:G:320:ILE:HD11	2.41	0.56
1:H:49:ILE:HG23	1:H:50:THR:HG23	1.87	0.56
1:J:164:LEU:O	1:J:168:GLY:HA2	2.05	0.56
1:J:375:LEU:HD12	1:J:375:LEU:O	2.06	0.56
1:J:49:ILE:HG23	1:J:50:THR:HG23	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:503:ILE:HG22	1:A:515:TYR:CE1	2.41	0.56
1:I:55:ARG:NE	1:I:587:ILE:HD11	2.20	0.56
1:J:123:GLU:CG	1:J:171:LYS:HD2	2.35	0.56
1:B:270:VAL:HG11	1:B:320:ILE:HB	1.87	0.55
1:C:291:PHE:O	1:C:295:THR:HG22	2.07	0.55
1:F:348:ASP:C	1:F:351:PRO:HD2	2.26	0.55
1:H:503:ILE:HG22	1:H:515:TYR:CE1	2.41	0.55
1:H:659:ILE:HD12	1:H:659:ILE:H	1.71	0.55
1:I:316:TRP:CZ2	1:I:320:ILE:HD11	2.41	0.55
1:J:103:THR:HG22	1:J:133:ILE:HA	1.87	0.55
1:A:164:LEU:O	1:A:168:GLY:HA2	2.05	0.55
1:A:291:PHE:O	1:A:295:THR:HG22	2.07	0.55
1:B:375:LEU:O	1:B:375:LEU:HD12	2.06	0.55
1:B:712:TYR:HE2	1:B:750:VAL:HG21	1.70	0.55
1:D:375:LEU:O	1:D:375:LEU:HD12	2.06	0.55
1:F:103:THR:HG22	1:F:133:ILE:HA	1.87	0.55
1:G:167:SER:OG	1:G:169:HIS:CD2	2.60	0.55
1:G:285:LEU:HD13	1:G:291:PHE:CE2	2.40	0.55
1:H:123:GLU:CG	1:H:171:LYS:HD2	2.35	0.55
1:H:375:LEU:O	1:H:375:LEU:HD12	2.06	0.55
1:I:49:ILE:HG23	1:I:50:THR:HG23	1.87	0.55
1:J:291:PHE:O	1:J:295:THR:HG22	2.07	0.55
1:J:316:TRP:CZ2	1:J:320:ILE:HD11	2.41	0.55
1:C:503:ILE:HG22	1:C:515:TYR:CE1	2.42	0.55
1:D:204:ASP:O	1:D:248:LEU:HD11	2.06	0.55
1:D:291:PHE:O	1:D:295:THR:HG22	2.06	0.55
1:E:412:GLN:O	1:F:89:GLN:NE2	2.37	0.55
1:I:375:LEU:HD12	1:I:375:LEU:O	2.06	0.55
1:B:49:ILE:HG23	1:B:50:THR:HG23	1.88	0.55
1:H:103:THR:HG22	1:H:133:ILE:HA	1.86	0.55
1:J:348:ASP:C	1:J:351:PRO:HD2	2.26	0.55
1:J:503:ILE:HG22	1:J:515:TYR:CE1	2.41	0.55
1:J:712:TYR:HE2	1:J:750:VAL:HG21	1.70	0.55
1:A:49:ILE:HG23	1:A:50:THR:HG23	1.87	0.55
1:A:659:ILE:H	1:A:659:ILE:HD12	1.71	0.55
1:C:204:ASP:O	1:C:248:LEU:HD11	2.07	0.55
1:F:316:TRP:CZ2	1:F:320:ILE:HD11	2.41	0.55
1:I:291:PHE:O	1:I:295:THR:HG22	2.07	0.55
1:J:380:GLN:HB3	1:J:390:LEU:HD23	1.88	0.55
1:J:55:ARG:NE	1:J:587:ILE:HD11	2.21	0.55
1:C:375:LEU:HD12	1:C:375:LEU:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:659:ILE:HD12	1:C:659:ILE:H	1.70	0.55
1:E:316:TRP:CZ2	1:E:320:ILE:HD11	2.41	0.55
1:H:291:PHE:O	1:H:295:THR:HG22	2.07	0.55
1:A:348:ASP:C	1:A:351:PRO:HD2	2.26	0.55
1:D:380:GLN:HB3	1:D:390:LEU:HD23	1.89	0.55
1:E:204:ASP:O	1:E:248:LEU:HD11	2.07	0.55
1:E:375:LEU:HD12	1:E:375:LEU:O	2.07	0.55
1:G:49:ILE:HG23	1:G:50:THR:HG23	1.88	0.55
1:H:380:GLN:HB3	1:H:390:LEU:HD23	1.89	0.55
1:I:380:GLN:HB3	1:I:390:LEU:HD23	1.89	0.55
1:J:167:SER:OG	1:J:169:HIS:CD2	2.59	0.55
1:A:418:VAL:CG1	1:B:141:ASN:HD21	2.19	0.55
1:B:503:ILE:HG22	1:B:515:TYR:CE1	2.42	0.55
1:C:316:TRP:CZ2	1:C:320:ILE:HD11	2.41	0.55
1:F:167:SER:OG	1:F:169:HIS:CD2	2.60	0.55
1:G:375:LEU:O	1:G:375:LEU:HD12	2.07	0.55
1:H:167:SER:OG	1:H:169:HIS:CD2	2.60	0.55
1:H:204:ASP:O	1:H:248:LEU:HD11	2.07	0.55
1:J:204:ASP:O	1:J:248:LEU:HD11	2.07	0.55
1:A:204:ASP:O	1:A:248:LEU:HD11	2.07	0.55
1:A:375:LEU:O	1:A:375:LEU:HD12	2.06	0.55
1:B:291:PHE:O	1:B:295:THR:HG22	2.06	0.55
1:B:348:ASP:C	1:B:351:PRO:HD2	2.26	0.55
1:C:313:LEU:O	1:C:317:VAL:HG23	2.07	0.55
1:E:380:GLN:HB3	1:E:390:LEU:HD23	1.89	0.55
1:F:313:LEU:O	1:F:317:VAL:HG23	2.07	0.55
1:G:380:GLN:HB3	1:G:390:LEU:HD23	1.89	0.55
1:B:316:TRP:CZ2	1:B:320:ILE:HD11	2.41	0.54
1:B:659:ILE:HD12	1:B:659:ILE:H	1.70	0.54
1:D:476:VAL:HG13	1:D:485:LEU:HD13	1.89	0.54
1:F:204:ASP:O	1:F:248:LEU:HD11	2.07	0.54
1:F:375:LEU:HD12	1:F:375:LEU:O	2.06	0.54
1:F:476:VAL:HG13	1:F:485:LEU:HD13	1.89	0.54
1:F:55:ARG:NE	1:F:587:ILE:HD11	2.20	0.54
1:G:313:LEU:O	1:G:317:VAL:HG23	2.07	0.54
1:I:204:ASP:O	1:I:248:LEU:HD11	2.07	0.54
1:I:313:LEU:O	1:I:317:VAL:HG23	2.07	0.54
1:A:476:VAL:HG13	1:A:485:LEU:HD13	1.90	0.54
1:E:476:VAL:HG13	1:E:485:LEU:HD13	1.89	0.54
1:E:429:ARG:NE	1:F:304:GLN:OE1	2.40	0.54
1:A:313:LEU:O	1:A:317:VAL:HG23	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:412:GLN:O	1:B:89:GLN:NE2	2.39	0.54
1:C:167:SER:OG	1:C:169:HIS:CD2	2.60	0.54
1:E:167:SER:OG	1:E:169:HIS:CD2	2.60	0.54
1:F:291:PHE:O	1:F:295:THR:HG22	2.07	0.54
1:F:503:ILE:HG22	1:F:515:TYR:CE1	2.42	0.54
1:H:316:TRP:CZ2	1:H:320:ILE:HD11	2.41	0.54
1:H:418:VAL:CG1	1:I:141:ASN:HD21	2.19	0.54
1:A:123:GLU:OE2	1:B:229:ARG:NH2	2.40	0.54
1:A:380:GLN:HB3	1:A:390:LEU:HD23	1.89	0.54
1:D:313:LEU:O	1:D:317:VAL:HG23	2.07	0.54
1:E:291:PHE:O	1:E:295:THR:HG22	2.06	0.54
1:E:49:ILE:HG23	1:E:50:THR:HG23	1.88	0.54
1:B:204:ASP:O	1:B:248:LEU:HD11	2.07	0.54
1:B:476:VAL:HG13	1:B:485:LEU:HD13	1.89	0.54
1:G:204:ASP:O	1:G:248:LEU:HD11	2.07	0.54
1:G:476:VAL:HG13	1:G:485:LEU:HD13	1.89	0.54
1:D:167:SER:OG	1:D:169:HIS:CD2	2.60	0.54
1:J:313:LEU:O	1:J:317:VAL:HG23	2.07	0.54
1:C:146:GLU:OE2	1:C:604:LYS:NZ	2.38	0.54
1:C:476:VAL:HG13	1:C:485:LEU:HD13	1.89	0.54
1:E:313:LEU:O	1:E:317:VAL:HG23	2.07	0.54
1:B:313:LEU:O	1:B:317:VAL:HG23	2.07	0.54
1:G:291:PHE:O	1:G:295:THR:HG22	2.07	0.54
1:G:723:ILE:HD11	1:H:509:SER:OG	2.08	0.54
1:I:503:ILE:HG22	1:I:515:TYR:CE1	2.42	0.54
1:B:429:ARG:NE	1:C:304:GLN:OE1	2.40	0.54
1:E:270:VAL:HG23	1:E:317:VAL:CG1	2.34	0.54
1:F:380:GLN:HB3	1:F:390:LEU:HD23	1.89	0.54
1:I:56:ARG:HD2	1:I:671:VAL:HG22	1.90	0.54
1:D:418:VAL:CG1	1:J:141:ASN:HD21	2.19	0.54
1:B:380:GLN:HB3	1:B:390:LEU:HD23	1.89	0.54
1:I:146:GLU:OE2	1:I:604:LYS:NZ	2.38	0.54
1:J:476:VAL:HG13	1:J:485:LEU:HD13	1.89	0.54
1:A:497:LEU:HD12	1:A:511:PRO:HB2	1.91	0.53
1:C:40:ALA:HB1	1:C:192:PRO:HG3	1.91	0.53
1:E:418:VAL:HG12	1:F:141:ASN:HD21	1.73	0.53
1:F:56:ARG:HD2	1:F:671:VAL:HG22	1.90	0.53
1:H:313:LEU:O	1:H:317:VAL:HG23	2.07	0.53
1:H:476:VAL:HG13	1:H:485:LEU:HD13	1.89	0.53
1:B:270:VAL:HG23	1:B:317:VAL:CG1	2.34	0.53
1:G:568:ASN:O	1:G:571:VAL:O	2.26	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:145:ASP:OD1	1:I:146:GLU:N	2.41	0.53
1:J:40:ALA:HB1	1:J:192:PRO:HG3	1.90	0.53
1:D:497:LEU:HD12	1:D:511:PRO:HB2	1.90	0.53
1:F:58:GLY:O	1:F:669:LYS:HE2	2.09	0.53
1:G:270:VAL:HG23	1:G:317:VAL:CG1	2.34	0.53
1:A:736:GLN:O	1:A:781:ALA:HB1	2.09	0.53
1:B:146:GLU:OE2	1:B:604:LYS:NZ	2.39	0.53
1:B:40:ALA:HB1	1:B:192:PRO:HG3	1.91	0.53
1:B:568:ASN:O	1:B:571:VAL:O	2.26	0.53
1:C:380:GLN:HB3	1:C:390:LEU:HD23	1.89	0.53
1:D:568:ASN:O	1:D:571:VAL:O	2.26	0.53
1:I:58:GLY:O	1:I:669:LYS:HE2	2.08	0.53
1:A:40:ALA:HB1	1:A:192:PRO:HG3	1.91	0.53
1:A:568:ASN:O	1:A:571:VAL:O	2.26	0.53
1:G:40:ALA:HB1	1:G:192:PRO:HG3	1.90	0.53
1:G:56:ARG:HD2	1:G:671:VAL:HG22	1.91	0.53
1:H:568:ASN:O	1:H:571:VAL:O	2.26	0.53
1:I:568:ASN:O	1:I:571:VAL:O	2.27	0.53
1:J:56:ARG:HD2	1:J:671:VAL:HG22	1.91	0.53
1:A:56:ARG:HD2	1:A:671:VAL:HG22	1.90	0.53
1:D:40:ALA:HB1	1:D:192:PRO:HG3	1.90	0.53
1:H:146:GLU:OE2	1:H:604:LYS:NZ	2.39	0.53
1:H:736:GLN:O	1:H:781:ALA:HB1	2.09	0.53
1:B:490:GLY:HA2	1:B:493:MET:HG2	1.91	0.53
1:C:497:LEU:HD12	1:C:511:PRO:HB2	1.91	0.53
1:C:736:GLN:O	1:C:781:ALA:HB1	2.09	0.53
1:D:56:ARG:HD2	1:D:671:VAL:HG22	1.91	0.53
1:F:568:ASN:O	1:F:571:VAL:O	2.26	0.53
1:J:736:GLN:O	1:J:781:ALA:HB1	2.09	0.53
1:B:497:LEU:HD12	1:B:511:PRO:HB2	1.91	0.53
1:B:736:GLN:O	1:B:781:ALA:HB1	2.09	0.53
1:D:145:ASP:OD1	1:D:146:GLU:N	2.42	0.53
1:E:56:ARG:HD2	1:E:671:VAL:HG22	1.90	0.53
1:E:58:GLY:O	1:E:669:LYS:HE2	2.09	0.53
1:I:476:VAL:HG13	1:I:485:LEU:HD13	1.89	0.53
1:C:486:LEU:CD1	1:C:514:LEU:HD11	2.40	0.53
1:D:58:GLY:O	1:D:669:LYS:HE2	2.09	0.53
1:G:736:GLN:O	1:G:781:ALA:HB1	2.09	0.53
1:H:270:VAL:HG23	1:H:317:VAL:CG1	2.34	0.53
1:J:270:VAL:HG23	1:J:317:VAL:CG1	2.34	0.53
1:J:497:LEU:HD12	1:J:511:PRO:HB2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:490:GLY:HA2	1:A:493:MET:HG2	1.91	0.52
1:B:58:GLY:O	1:B:669:LYS:HE2	2.09	0.52
1:D:740:LEU:HD12	1:D:777:PHE:CE2	2.44	0.52
1:E:568:ASN:O	1:E:571:VAL:O	2.26	0.52
1:B:145:ASP:OD1	1:B:146:GLU:N	2.42	0.52
1:B:547:THR:OG1	1:B:549:GLN:OE1	2.28	0.52
1:B:56:ARG:HD2	1:B:671:VAL:HG22	1.90	0.52
1:B:715:LEU:HA	1:B:719:ARG:H	1.75	0.52
1:D:547:THR:OG1	1:D:549:GLN:OE1	2.28	0.52
1:E:490:GLY:HA2	1:E:493:MET:HG2	1.91	0.52
1:F:547:THR:OG1	1:F:549:GLN:OE1	2.28	0.52
1:G:123:GLU:CG	1:G:171:LYS:HD2	2.35	0.52
1:H:145:ASP:OD1	1:H:146:GLU:N	2.42	0.52
1:I:490:GLY:HA2	1:I:493:MET:HG2	1.91	0.52
1:A:740:LEU:HD12	1:A:777:PHE:CE2	2.44	0.52
1:C:56:ARG:HD2	1:C:671:VAL:HG22	1.90	0.52
1:C:58:GLY:O	1:C:669:LYS:HE2	2.09	0.52
1:C:740:LEU:HD12	1:C:777:PHE:CE2	2.44	0.52
1:F:264:GLU:OE2	1:F:298:THR:OG1	2.26	0.52
1:H:40:ALA:HB1	1:H:192:PRO:HG3	1.90	0.52
1:I:736:GLN:O	1:I:781:ALA:HB1	2.09	0.52
1:A:547:THR:OG1	1:A:549:GLN:OE1	2.28	0.52
1:C:490:GLY:HA2	1:C:493:MET:HG2	1.91	0.52
1:D:490:GLY:HA2	1:D:493:MET:HG2	1.91	0.52
1:D:736:GLN:O	1:D:781:ALA:HB1	2.09	0.52
1:E:736:GLN:O	1:E:781:ALA:HB1	2.09	0.52
1:F:146:GLU:OE2	1:F:604:LYS:NZ	2.38	0.52
1:G:740:LEU:HD12	1:G:777:PHE:CE2	2.44	0.52
1:J:380:GLN:HB3	1:J:390:LEU:CD2	2.40	0.52
1:A:58:GLY:O	1:A:669:LYS:HE2	2.09	0.52
1:D:380:GLN:HB3	1:D:390:LEU:CD2	2.40	0.52
1:E:497:LEU:HD12	1:E:511:PRO:HB2	1.90	0.52
1:F:145:ASP:OD1	1:F:146:GLU:N	2.43	0.52
1:F:736:GLN:O	1:F:781:ALA:HB1	2.09	0.52
1:F:723:ILE:HD11	1:G:509:SER:OG	2.09	0.52
1:H:285:LEU:HD13	1:H:291:PHE:CD2	2.45	0.52
1:H:58:GLY:O	1:H:669:LYS:HE2	2.09	0.52
1:D:409:GLN:HG3	1:D:661:VAL:HG13	1.92	0.52
1:E:145:ASP:OD1	1:E:146:GLU:N	2.42	0.52
1:E:285:LEU:HD13	1:E:291:PHE:CD2	2.45	0.52
1:E:30:ILE:CG2	1:E:31:PRO:CD	2.88	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:409:GLN:HG3	1:E:661:VAL:HG13	1.92	0.52
1:E:740:LEU:HD12	1:E:777:PHE:CE2	2.44	0.52
1:F:40:ALA:HB1	1:F:192:PRO:HG3	1.90	0.52
1:F:490:GLY:HA2	1:F:493:MET:HG2	1.91	0.52
1:H:39:TRP:CZ3	1:H:289:ILE:CD1	2.93	0.52
1:H:56:ARG:HD2	1:H:671:VAL:HG22	1.91	0.52
1:H:740:LEU:HD12	1:H:777:PHE:CE2	2.45	0.52
1:J:58:GLY:O	1:J:669:LYS:HE2	2.09	0.52
1:A:145:ASP:OD1	1:A:146:GLU:N	2.43	0.52
1:A:715:LEU:HA	1:A:719:ARG:H	1.75	0.52
1:B:285:LEU:HD13	1:B:291:PHE:CD2	2.45	0.52
1:B:486:LEU:CD1	1:B:514:LEU:HD11	2.40	0.52
1:C:568:ASN:O	1:C:571:VAL:O	2.27	0.52
1:D:659:ILE:N	1:D:659:ILE:HD12	2.25	0.52
1:E:486:LEU:CD1	1:E:514:LEU:HD11	2.40	0.52
1:E:547:THR:OG1	1:E:549:GLN:OE1	2.28	0.52
1:F:30:ILE:CG2	1:F:31:PRO:CD	2.88	0.52
1:F:380:GLN:HB3	1:F:390:LEU:CD2	2.40	0.52
1:G:39:TRP:CZ3	1:G:289:ILE:CD1	2.93	0.52
1:J:490:GLY:HA2	1:J:493:MET:HG2	1.91	0.52
1:A:659:ILE:N	1:A:659:ILE:HD12	2.25	0.52
1:E:380:GLN:HB3	1:E:390:LEU:CD2	2.40	0.52
1:G:145:ASP:OD1	1:G:146:GLU:N	2.43	0.52
1:G:486:LEU:CD1	1:G:514:LEU:HD11	2.40	0.52
1:G:715:LEU:HA	1:G:719:ARG:H	1.75	0.52
1:H:380:GLN:HB3	1:H:390:LEU:CD2	2.40	0.52
1:H:547:THR:OG1	1:H:549:GLN:OE1	2.28	0.52
1:I:380:GLN:HB3	1:I:390:LEU:CD2	2.40	0.52
1:J:409:GLN:HG3	1:J:661:VAL:HG13	1.92	0.52
1:J:568:ASN:O	1:J:571:VAL:O	2.26	0.52
1:J:715:LEU:HA	1:J:719:ARG:H	1.75	0.52
1:B:30:ILE:CG2	1:B:31:PRO:CD	2.88	0.52
1:B:409:GLN:HG3	1:B:661:VAL:HG13	1.92	0.52
1:D:30:ILE:CG2	1:D:31:PRO:CD	2.88	0.52
1:F:285:LEU:HD13	1:F:291:PHE:CD2	2.45	0.52
1:G:146:GLU:OE2	1:G:604:LYS:NZ	2.38	0.52
1:G:380:GLN:HB3	1:G:390:LEU:CD2	2.40	0.52
1:G:490:GLY:HA2	1:G:493:MET:HG2	1.91	0.52
1:H:497:LEU:HD12	1:H:511:PRO:HB2	1.91	0.52
1:I:486:LEU:CD1	1:I:514:LEU:HD11	2.40	0.52
1:I:740:LEU:HD12	1:I:777:PHE:CE2	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:145:ASP:OD1	1:J:146:GLU:N	2.42	0.52
1:J:740:LEU:HD12	1:J:777:PHE:CE2	2.45	0.52
1:E:40:ALA:HB1	1:E:192:PRO:HG3	1.91	0.52
1:F:486:LEU:CD1	1:F:514:LEU:HD11	2.39	0.52
1:H:264:GLU:OE2	1:H:298:THR:OG1	2.26	0.52
1:J:264:GLU:OE2	1:J:298:THR:OG1	2.26	0.52
1:J:30:ILE:CG2	1:J:31:PRO:CD	2.88	0.52
1:B:740:LEU:HD12	1:B:777:PHE:CE2	2.44	0.51
1:G:497:LEU:HD12	1:G:511:PRO:HB2	1.91	0.51
1:H:741:GLN:O	1:H:745:GLN:HG3	2.10	0.51
1:A:350:THR:OG1	1:A:351:PRO:HD3	2.11	0.51
1:B:380:GLN:HB3	1:B:390:LEU:CD2	2.40	0.51
1:D:715:LEU:HA	1:D:719:ARG:H	1.75	0.51
1:F:659:ILE:N	1:F:659:ILE:HD12	2.25	0.51
1:G:659:ILE:HD12	1:G:659:ILE:N	2.25	0.51
1:G:58:GLY:O	1:G:669:LYS:HE2	2.09	0.51
1:H:409:GLN:HG3	1:H:661:VAL:HG13	1.92	0.51
1:H:490:GLY:HA2	1:H:493:MET:HG2	1.90	0.51
1:I:40:ALA:HB1	1:I:192:PRO:HG3	1.90	0.51
1:J:547:THR:OG1	1:J:549:GLN:OE1	2.28	0.51
1:A:30:ILE:CG2	1:A:31:PRO:CD	2.89	0.51
1:A:39:TRP:CZ3	1:A:289:ILE:CD1	2.93	0.51
1:C:145:ASP:OD1	1:C:146:GLU:N	2.43	0.51
1:C:285:LEU:HD13	1:C:291:PHE:CD2	2.45	0.51
1:D:285:LEU:HD13	1:D:291:PHE:CD2	2.46	0.51
1:F:741:GLN:O	1:F:745:GLN:HG3	2.10	0.51
1:I:780:ILE:O	1:I:784:VAL:HG23	2.11	0.51
1:J:741:GLN:O	1:J:745:GLN:HG3	2.11	0.51
1:C:659:ILE:HD12	1:C:659:ILE:N	2.25	0.51
1:G:409:GLN:HG3	1:G:661:VAL:HG13	1.92	0.51
1:G:641:ARG:HG3	1:G:777:PHE:CE1	2.46	0.51
1:H:429:ARG:NE	1:I:304:GLN:OE1	2.40	0.51
1:I:659:ILE:HD12	1:I:659:ILE:N	2.25	0.51
1:J:350:THR:OG1	1:J:351:PRO:HD3	2.11	0.51
1:A:380:GLN:HB3	1:A:390:LEU:CD2	2.40	0.51
1:A:741:GLN:O	1:A:745:GLN:HG3	2.11	0.51
1:A:780:ILE:O	1:A:784:VAL:HG23	2.11	0.51
1:B:350:THR:OG1	1:B:351:PRO:HD3	2.10	0.51
1:B:780:ILE:O	1:B:784:VAL:HG23	2.11	0.51
1:C:741:GLN:O	1:C:745:GLN:HG3	2.11	0.51
1:E:659:ILE:N	1:E:659:ILE:HD12	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:741:GLN:O	1:E:745:GLN:HG3	2.10	0.51
1:F:409:GLN:HG3	1:F:661:VAL:HG13	1.92	0.51
1:F:497:LEU:HD12	1:F:511:PRO:HB2	1.91	0.51
1:F:740:LEU:HD12	1:F:777:PHE:CE2	2.45	0.51
1:I:39:TRP:CZ3	1:I:289:ILE:CD1	2.94	0.51
1:I:547:THR:OG1	1:I:549:GLN:OE1	2.28	0.51
1:J:442:PHE:CE2	1:J:681:ALA:HB1	2.46	0.51
1:J:486:LEU:CD1	1:J:514:LEU:HD11	2.40	0.51
1:C:442:PHE:CE2	1:C:681:ALA:HB1	2.46	0.51
1:E:429:ARG:HD2	1:E:661:VAL:HG11	1.93	0.51
1:E:641:ARG:HG3	1:E:777:PHE:CE1	2.46	0.51
1:F:350:THR:OG1	1:F:351:PRO:HD3	2.11	0.51
1:G:285:LEU:HD13	1:G:291:PHE:CD2	2.46	0.51
1:H:30:ILE:CG2	1:H:31:PRO:CD	2.88	0.51
1:H:350:THR:OG1	1:H:351:PRO:HD3	2.11	0.51
1:H:486:LEU:CD1	1:H:514:LEU:HD11	2.40	0.51
1:H:68:ARG:HH12	1:H:166:GLN:HG2	1.76	0.51
1:I:497:LEU:HD12	1:I:511:PRO:HB2	1.91	0.51
1:A:486:LEU:CD1	1:A:514:LEU:HD11	2.41	0.51
1:B:641:ARG:HG3	1:B:777:PHE:CE1	2.46	0.51
1:E:442:PHE:CE2	1:E:681:ALA:HB1	2.45	0.51
1:G:547:THR:OG1	1:G:549:GLN:OE1	2.28	0.51
1:C:715:LEU:HA	1:C:719:ARG:H	1.75	0.51
1:C:780:ILE:O	1:C:784:VAL:HG23	2.11	0.51
1:F:39:TRP:CZ3	1:F:289:ILE:CD1	2.94	0.51
1:H:641:ARG:HG3	1:H:777:PHE:CE1	2.46	0.51
1:J:780:ILE:O	1:J:784:VAL:HG23	2.11	0.51
1:A:146:GLU:OE2	1:A:604:LYS:NZ	2.38	0.51
1:A:285:LEU:HD13	1:A:291:PHE:CD2	2.46	0.51
1:A:31:PRO:HB3	1:A:528:PRO:HA	1.93	0.51
1:B:39:TRP:CZ3	1:B:289:ILE:CD1	2.94	0.51
1:C:145:ASP:CB	1:C:148:GLN:HE21	2.24	0.51
1:C:547:THR:OG1	1:C:549:GLN:OE1	2.28	0.51
1:D:146:GLU:OE2	1:D:604:LYS:NZ	2.39	0.51
1:C:429:ARG:NE	1:D:304:GLN:OE1	2.42	0.51
1:D:39:TRP:CZ3	1:D:289:ILE:CD1	2.93	0.51
1:C:660:ALA:HB1	1:D:85:ASP:OD2	2.10	0.51
1:I:270:VAL:HG23	1:I:317:VAL:CG1	2.34	0.51
1:I:409:GLN:HG3	1:I:661:VAL:HG13	1.91	0.51
1:I:741:GLN:O	1:I:745:GLN:HG3	2.10	0.51
1:I:641:ARG:HG3	1:I:777:PHE:CE1	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:409:GLN:HG3	1:A:661:VAL:HG13	1.92	0.51
1:I:442:PHE:CE2	1:I:681:ALA:HB1	2.46	0.51
1:B:31:PRO:HB3	1:B:528:PRO:HA	1.93	0.50
1:B:741:GLN:O	1:B:745:GLN:HG3	2.10	0.50
1:D:486:LEU:CD1	1:D:514:LEU:HD11	2.40	0.50
1:D:519:ALA:HB1	1:D:535:PHE:CE2	2.46	0.50
1:H:659:ILE:HD12	1:H:659:ILE:N	2.25	0.50
1:J:68:ARG:HH12	1:J:166:GLN:HG2	1.76	0.50
1:J:39:TRP:CZ3	1:J:289:ILE:CD1	2.93	0.50
1:B:519:ALA:HB1	1:B:535:PHE:CE2	2.46	0.50
1:B:659:ILE:N	1:B:659:ILE:HD12	2.25	0.50
1:C:380:GLN:HB3	1:C:390:LEU:CD2	2.40	0.50
1:F:68:ARG:HH12	1:F:166:GLN:HG2	1.77	0.50
1:F:519:ALA:HB1	1:F:535:PHE:CE2	2.47	0.50
1:F:641:ARG:HG3	1:F:777:PHE:CE1	2.47	0.50
1:G:31:PRO:HB3	1:G:528:PRO:HA	1.93	0.50
1:H:429:ARG:HD2	1:H:661:VAL:HG11	1.93	0.50
1:H:442:PHE:CE2	1:H:681:ALA:HB1	2.46	0.50
1:H:108:MET:HA	1:I:114:PRO:CG	2.42	0.50
1:I:68:ARG:HH12	1:I:166:GLN:HG2	1.76	0.50
1:I:30:ILE:CG2	1:I:31:PRO:CD	2.88	0.50
1:J:285:LEU:HD13	1:J:291:PHE:CD2	2.45	0.50
1:A:89:GLN:NE2	1:J:412:GLN:O	2.44	0.50
1:B:492:TYR:CE2	1:B:680:LEU:HA	2.46	0.50
1:C:350:THR:OG1	1:C:351:PRO:HD3	2.11	0.50
1:D:442:PHE:CE2	1:D:681:ALA:HB1	2.46	0.50
1:D:741:GLN:O	1:D:745:GLN:HG3	2.10	0.50
1:F:715:LEU:HA	1:F:719:ARG:H	1.75	0.50
1:F:745:GLN:HG2	1:F:766:GLU:OE2	2.12	0.50
1:G:30:ILE:CG2	1:G:31:PRO:CD	2.88	0.50
1:G:442:PHE:CE2	1:G:681:ALA:HB1	2.47	0.50
1:G:741:GLN:O	1:G:745:GLN:HG3	2.11	0.50
1:H:780:ILE:O	1:H:784:VAL:HG23	2.11	0.50
1:J:641:ARG:HG3	1:J:777:PHE:CE1	2.46	0.50
1:C:39:TRP:CZ3	1:C:289:ILE:CD1	2.94	0.50
1:C:429:ARG:HD2	1:C:661:VAL:HG11	1.93	0.50
1:D:492:TYR:CE2	1:D:680:LEU:HA	2.47	0.50
1:E:39:TRP:CZ3	1:E:289:ILE:CD1	2.94	0.50
1:E:780:ILE:O	1:E:784:VAL:HG23	2.11	0.50
1:G:420:VAL:CG1	1:G:602:VAL:HG13	2.42	0.50
1:I:519:ALA:HB1	1:I:535:PHE:CE2	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:418:VAL:CG1	1:C:141:ASN:HD21	2.25	0.50
1:B:429:ARG:HD2	1:B:661:VAL:HG11	1.93	0.50
1:C:31:PRO:HB3	1:C:528:PRO:HA	1.94	0.50
1:F:780:ILE:O	1:F:784:VAL:HG23	2.11	0.50
1:G:145:ASP:CB	1:G:148:GLN:HE21	2.24	0.50
1:G:68:ARG:HH12	1:G:166:GLN:HG2	1.77	0.50
1:G:492:TYR:CE2	1:G:680:LEU:HA	2.47	0.50
1:I:285:LEU:HD13	1:I:291:PHE:CD2	2.45	0.50
1:I:350:THR:OG1	1:I:351:PRO:HD3	2.11	0.50
1:J:382:ARG:HA	1:J:390:LEU:HA	1.94	0.50
1:A:492:TYR:CE2	1:A:680:LEU:HA	2.47	0.50
1:C:409:GLN:HG3	1:C:661:VAL:HG13	1.92	0.50
1:D:641:ARG:HG3	1:D:777:PHE:CE1	2.47	0.50
1:D:780:ILE:O	1:D:784:VAL:HG23	2.11	0.50
1:E:220:LEU:HD23	1:E:230:PHE:CD1	2.46	0.50
1:G:475:VAL:HG22	1:G:680:LEU:HD12	1.94	0.50
1:G:780:ILE:O	1:G:784:VAL:HG23	2.11	0.50
1:H:31:PRO:HB3	1:H:528:PRO:HA	1.93	0.50
1:J:659:ILE:HD12	1:J:659:ILE:N	2.25	0.50
1:C:270:VAL:HG23	1:C:317:VAL:CG1	2.34	0.50
1:C:492:TYR:CE2	1:C:680:LEU:HA	2.47	0.50
1:C:475:VAL:HG22	1:C:680:LEU:HD12	1.94	0.50
1:D:31:PRO:HB3	1:D:528:PRO:HA	1.94	0.50
1:D:429:ARG:HD2	1:D:661:VAL:HG11	1.93	0.50
1:E:350:THR:OG1	1:E:351:PRO:HD3	2.10	0.50
1:F:123:GLU:CD	1:G:229:ARG:HH12	2.15	0.50
1:F:270:VAL:HG23	1:F:317:VAL:CG1	2.34	0.50
1:F:429:ARG:HD2	1:F:661:VAL:HG11	1.94	0.50
1:G:220:LEU:HD23	1:G:230:PHE:CD1	2.47	0.50
1:G:264:GLU:OE2	1:G:298:THR:OG1	2.26	0.50
1:I:31:PRO:HB3	1:I:528:PRO:HA	1.93	0.50
1:A:519:ALA:HB1	1:A:535:PHE:CE2	2.46	0.50
1:A:475:VAL:HG22	1:A:680:LEU:HD12	1.94	0.50
1:B:412:GLN:O	1:C:89:GLN:NE2	2.42	0.50
1:C:30:ILE:CG2	1:C:31:PRO:CD	2.88	0.50
1:D:350:THR:OG1	1:D:351:PRO:HD3	2.11	0.50
1:D:642:LYS:HZ2	1:D:733:VAL:HG21	1.77	0.50
1:E:68:ARG:HH12	1:E:166:GLN:HG2	1.76	0.50
1:H:715:LEU:HA	1:H:719:ARG:H	1.75	0.50
1:I:145:ASP:CB	1:I:148:GLN:HE21	2.24	0.50
1:I:264:GLU:OE2	1:I:298:THR:OG1	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:715:LEU:HA	1:I:719:ARG:H	1.76	0.50
1:J:429:ARG:HD2	1:J:661:VAL:HG11	1.93	0.50
1:J:420:VAL:CG1	1:J:602:VAL:HG13	2.42	0.50
1:B:442:PHE:CE2	1:B:681:ALA:HB1	2.46	0.50
1:C:220:LEU:HD23	1:C:230:PHE:CD1	2.47	0.50
1:D:382:ARG:HA	1:D:390:LEU:HA	1.94	0.50
1:E:519:ALA:HB1	1:E:535:PHE:CE2	2.47	0.50
1:E:492:TYR:CE2	1:E:680:LEU:HA	2.46	0.50
1:E:715:LEU:HA	1:E:719:ARG:H	1.76	0.50
1:J:519:ALA:HB1	1:J:535:PHE:CE2	2.47	0.50
1:A:420:VAL:CG1	1:A:602:VAL:HG13	2.42	0.49
1:B:420:VAL:CG1	1:B:602:VAL:HG13	2.42	0.49
1:C:264:GLU:OE2	1:C:298:THR:OG1	2.26	0.49
1:D:420:VAL:CG1	1:D:602:VAL:HG13	2.42	0.49
1:H:220:LEU:HD23	1:H:230:PHE:CD1	2.47	0.49
1:H:492:TYR:CE2	1:H:680:LEU:HA	2.47	0.49
1:A:442:PHE:CE2	1:A:681:ALA:HB1	2.46	0.49
1:B:642:LYS:HZ2	1:B:733:VAL:HG21	1.77	0.49
1:C:541:ASN:HA	1:C:559:SER:HB3	1.95	0.49
1:C:68:ARG:HH12	1:C:166:GLN:HG2	1.76	0.49
1:D:745:GLN:HG2	1:D:766:GLU:OE2	2.12	0.49
1:I:492:TYR:CE2	1:I:680:LEU:HA	2.47	0.49
1:J:475:VAL:HG22	1:J:680:LEU:HD12	1.94	0.49
1:A:68:ARG:HH12	1:A:166:GLN:HG2	1.77	0.49
1:D:403:ASN:O	1:D:434:LEU:HB2	2.13	0.49
1:E:31:PRO:HB3	1:E:528:PRO:HA	1.93	0.49
1:G:350:THR:OG1	1:G:351:PRO:HD3	2.11	0.49
1:G:593:LEU:HD13	1:G:596:ARG:HD2	1.95	0.49
1:G:660:ALA:HB1	1:H:85:ASP:CG	2.32	0.49
1:I:420:VAL:CG1	1:I:602:VAL:HG13	2.42	0.49
1:I:429:ARG:HD2	1:I:661:VAL:HG11	1.93	0.49
1:I:745:GLN:HG2	1:I:766:GLU:OE2	2.12	0.49
1:J:745:GLN:HG2	1:J:766:GLU:OE2	2.12	0.49
1:A:429:ARG:HD2	1:A:661:VAL:HG11	1.93	0.49
1:C:641:ARG:HG3	1:C:777:PHE:CE1	2.47	0.49
1:D:145:ASP:CB	1:D:148:GLN:HE21	2.24	0.49
1:F:492:TYR:CE2	1:F:680:LEU:HA	2.47	0.49
1:F:442:PHE:CE2	1:F:681:ALA:HB1	2.46	0.49
1:G:429:ARG:HD2	1:G:661:VAL:HG11	1.93	0.49
1:G:745:GLN:HG2	1:G:766:GLU:OE2	2.12	0.49
1:J:390:LEU:O	1:J:484:THR:HG22	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:31:PRO:HB3	1:J:528:PRO:HA	1.93	0.49
1:C:403:ASN:O	1:C:434:LEU:HB2	2.13	0.49
1:D:475:VAL:HG22	1:D:680:LEU:HD12	1.94	0.49
1:C:519:ALA:HB1	1:C:535:PHE:CE2	2.47	0.49
1:D:68:ARG:HH12	1:D:166:GLN:HG2	1.77	0.49
1:D:537:HIS:O	1:D:560:ALA:HA	2.13	0.49
1:G:537:HIS:O	1:G:560:ALA:HA	2.13	0.49
1:H:745:GLN:HG2	1:H:766:GLU:OE2	2.12	0.49
1:A:403:ASN:O	1:A:434:LEU:HB2	2.13	0.49
1:A:541:ASN:HA	1:A:559:SER:HB3	1.95	0.49
1:A:745:GLN:HG2	1:A:766:GLU:OE2	2.12	0.49
1:A:641:ARG:HG3	1:A:777:PHE:CE1	2.47	0.49
1:B:382:ARG:HA	1:B:390:LEU:HA	1.94	0.49
1:B:745:GLN:HG2	1:B:766:GLU:OE2	2.12	0.49
1:D:541:ASN:HA	1:D:559:SER:HB3	1.94	0.49
1:F:475:VAL:HG22	1:F:680:LEU:HD12	1.94	0.49
1:H:412:GLN:O	1:I:89:GLN:NE2	2.42	0.49
1:H:519:ALA:HB1	1:H:535:PHE:CE2	2.47	0.49
1:H:420:VAL:CG1	1:H:602:VAL:HG13	2.42	0.49
1:J:541:ASN:HA	1:J:559:SER:HB3	1.95	0.49
1:A:593:LEU:HD13	1:A:596:ARG:HD2	1.95	0.49
1:C:390:LEU:O	1:C:484:THR:HG22	2.13	0.49
1:E:420:VAL:CG1	1:E:602:VAL:HG13	2.42	0.49
1:E:745:GLN:HG2	1:E:766:GLU:OE2	2.12	0.49
1:F:420:VAL:CG1	1:F:602:VAL:HG13	2.42	0.49
1:G:418:VAL:CG1	1:H:141:ASN:HD21	2.25	0.49
1:H:475:VAL:HG22	1:H:680:LEU:HD12	1.94	0.49
1:J:220:LEU:HD23	1:J:230:PHE:CD1	2.48	0.49
1:C:420:VAL:CG1	1:C:602:VAL:HG13	2.42	0.49
1:D:264:GLU:OE2	1:D:298:THR:OG1	2.26	0.49
1:E:264:GLU:OE2	1:E:298:THR:OG1	2.26	0.49
1:F:612:ILE:HD11	1:F:657:PHE:CD2	2.48	0.49
1:F:660:ALA:HB1	1:G:85:ASP:OD2	2.13	0.49
1:H:537:HIS:O	1:H:560:ALA:HA	2.13	0.49
1:I:612:ILE:HD11	1:I:657:PHE:CD2	2.47	0.49
1:J:492:TYR:CE2	1:J:680:LEU:HA	2.47	0.49
1:A:220:LEU:HD23	1:A:230:PHE:CD1	2.47	0.49
1:B:475:VAL:HG22	1:B:680:LEU:HD12	1.94	0.49
1:B:432:LEU:HD13	1:B:756:ILE:HD11	1.95	0.49
1:E:141:ASN:HD21	1:I:418:VAL:CG1	2.26	0.49
1:E:593:LEU:HD13	1:E:596:ARG:HD2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:403:ASN:O	1:F:434:LEU:HB2	2.13	0.49
1:F:418:VAL:CG1	1:G:141:ASN:HD21	2.25	0.49
1:F:537:HIS:O	1:F:560:ALA:HA	2.13	0.49
1:G:519:ALA:HB1	1:G:535:PHE:CE2	2.47	0.49
1:I:475:VAL:HG22	1:I:680:LEU:HD12	1.94	0.49
1:J:612:ILE:HD11	1:J:657:PHE:CD2	2.48	0.49
1:A:382:ARG:HA	1:A:390:LEU:HA	1.95	0.48
1:B:68:ARG:HH12	1:B:166:GLN:HG2	1.76	0.48
1:B:408:TYR:HB3	1:B:425:ILE:HG23	1.95	0.48
1:C:432:LEU:HD13	1:C:756:ILE:HD11	1.95	0.48
1:C:593:LEU:HD13	1:C:596:ARG:HD2	1.95	0.48
1:D:660:ALA:HB1	1:J:85:ASP:OD2	2.13	0.48
1:F:31:PRO:HB3	1:F:528:PRO:HA	1.94	0.48
1:F:390:LEU:O	1:F:484:THR:HG22	2.13	0.48
1:G:390:LEU:O	1:G:484:THR:HG22	2.13	0.48
1:G:432:LEU:HD13	1:G:756:ILE:HD11	1.95	0.48
1:G:403:ASN:O	1:G:434:LEU:HB2	2.13	0.48
1:I:220:LEU:HD23	1:I:230:PHE:CD1	2.48	0.48
1:I:537:HIS:O	1:I:560:ALA:HA	2.13	0.48
1:J:432:LEU:HD13	1:J:756:ILE:HD11	1.95	0.48
1:A:432:LEU:HD13	1:A:756:ILE:HD11	1.95	0.48
1:B:403:ASN:O	1:B:434:LEU:HB2	2.13	0.48
1:B:541:ASN:HA	1:B:559:SER:HB3	1.95	0.48
1:C:382:ARG:HA	1:C:390:LEU:HA	1.94	0.48
1:D:390:LEU:O	1:D:484:THR:HG22	2.13	0.48
1:E:475:VAL:HG22	1:E:680:LEU:HD12	1.94	0.48
1:H:612:ILE:HD11	1:H:657:PHE:CD2	2.48	0.48
1:A:270:VAL:HG23	1:A:317:VAL:CG1	2.34	0.48
1:C:537:HIS:O	1:C:560:ALA:HA	2.13	0.48
1:E:390:LEU:O	1:E:484:THR:HG22	2.13	0.48
1:G:382:ARG:HA	1:G:390:LEU:HA	1.94	0.48
1:G:513:LEU:HD23	1:G:516:MET:HE3	1.95	0.48
1:I:382:ARG:HA	1:I:390:LEU:HA	1.95	0.48
1:I:403:ASN:O	1:I:434:LEU:HB2	2.13	0.48
1:B:390:LEU:O	1:B:484:THR:HG22	2.13	0.48
1:C:745:GLN:HG2	1:C:766:GLU:OE2	2.12	0.48
1:E:146:GLU:OE2	1:E:604:LYS:NZ	2.38	0.48
1:E:382:ARG:HA	1:E:390:LEU:HA	1.94	0.48
1:H:121:TRP:CE3	1:I:226:PRO:HG3	2.48	0.48
1:I:541:ASN:HA	1:I:559:SER:HB3	1.95	0.48
1:B:537:HIS:O	1:B:560:ALA:HA	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:122:ALA:HB1	1:F:114:PRO:HB2	1.95	0.48
1:F:541:ASN:HA	1:F:559:SER:HB3	1.95	0.48
1:G:721:ASP:HA	1:G:722:GLU:HA	1.57	0.48
1:H:541:ASN:HA	1:H:559:SER:HB3	1.94	0.48
1:I:432:LEU:HD13	1:I:756:ILE:HD11	1.95	0.48
1:J:403:ASN:O	1:J:434:LEU:HB2	2.13	0.48
1:B:220:LEU:HD23	1:B:230:PHE:CD1	2.47	0.48
1:E:612:ILE:HD11	1:E:657:PHE:CD2	2.48	0.48
1:F:220:LEU:HD23	1:F:230:PHE:CD1	2.48	0.48
1:F:593:LEU:HD13	1:F:596:ARG:HD2	1.96	0.48
1:H:382:ARG:HA	1:H:390:LEU:HA	1.95	0.48
1:H:390:LEU:O	1:H:484:THR:HG22	2.13	0.48
1:A:390:LEU:O	1:A:484:THR:HG22	2.13	0.48
1:A:513:LEU:HD23	1:A:516:MET:HE3	1.95	0.48
1:A:612:ILE:HD11	1:A:657:PHE:CD2	2.48	0.48
1:B:612:ILE:HD11	1:B:657:PHE:CD2	2.48	0.48
1:C:612:ILE:HD11	1:C:657:PHE:CD2	2.48	0.48
1:E:403:ASN:O	1:E:434:LEU:HB2	2.13	0.48
1:F:382:ARG:HA	1:F:390:LEU:HA	1.95	0.48
1:H:121:TRP:CZ3	1:I:226:PRO:HG3	2.49	0.48
1:H:408:TYR:HB3	1:H:425:ILE:HG23	1.96	0.48
1:A:509:SER:OG	1:J:723:ILE:HD11	2.13	0.48
1:A:537:HIS:O	1:A:560:ALA:HA	2.13	0.48
1:E:432:LEU:HD13	1:E:756:ILE:HD11	1.95	0.48
1:G:408:TYR:HB3	1:G:425:ILE:HG23	1.95	0.48
1:G:642:LYS:HZ2	1:G:733:VAL:HG21	1.77	0.48
1:I:612:ILE:HD11	1:I:657:PHE:HD2	1.79	0.48
1:J:146:GLU:OE2	1:J:604:LYS:NZ	2.38	0.48
1:B:593:LEU:HD13	1:B:596:ARG:HD2	1.96	0.48
1:E:541:ASN:HA	1:E:559:SER:HB3	1.95	0.48
1:H:432:LEU:HD13	1:H:756:ILE:HD11	1.95	0.48
1:J:537:HIS:O	1:J:560:ALA:HA	2.13	0.48
1:A:145:ASP:CB	1:A:148:GLN:HE21	2.23	0.48
1:D:220:LEU:HD23	1:D:230:PHE:CD1	2.48	0.48
1:E:145:ASP:CB	1:E:148:GLN:HE21	2.23	0.48
1:E:513:LEU:HD23	1:E:516:MET:HE3	1.96	0.48
1:G:612:ILE:HD11	1:G:657:PHE:CD2	2.49	0.48
1:H:403:ASN:O	1:H:434:LEU:HB2	2.13	0.48
1:J:612:ILE:HD11	1:J:657:PHE:HD2	1.79	0.48
1:A:612:ILE:HD11	1:A:657:PHE:HD2	1.79	0.47
1:B:145:ASP:CB	1:B:148:GLN:HE21	2.24	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:537:HIS:O	1:E:560:ALA:HA	2.13	0.47
1:F:432:LEU:HD13	1:F:756:ILE:HD11	1.95	0.47
1:H:108:MET:HA	1:I:114:PRO:HG2	1.96	0.47
1:B:260:ALA:HB2	1:B:302:TRP:HB3	1.96	0.47
1:B:264:GLU:OE2	1:B:298:THR:OG1	2.26	0.47
1:C:493:MET:HG3	1:C:496:LEU:HD12	1.96	0.47
1:D:260:ALA:HB2	1:D:302:TRP:HB3	1.96	0.47
1:E:408:TYR:HB3	1:E:425:ILE:HG23	1.96	0.47
1:F:396:ARG:HD3	1:F:443:PHE:CG	2.49	0.47
1:J:114:PRO:HA	1:J:228:THR:CG2	2.45	0.47
1:C:396:ARG:HD3	1:C:443:PHE:CG	2.49	0.47
1:D:593:LEU:HD13	1:D:596:ARG:HD2	1.95	0.47
1:D:705:ALA:O	1:D:709:THR:HG22	2.15	0.47
1:F:429:ARG:NE	1:G:304:GLN:OE1	2.42	0.47
1:I:477:LYS:O	1:I:486:LEU:HD23	2.15	0.47
1:I:390:LEU:O	1:I:484:THR:HG22	2.13	0.47
1:A:493:MET:HG3	1:A:496:LEU:HD12	1.96	0.47
1:C:114:PRO:HA	1:C:228:THR:CG2	2.45	0.47
1:C:705:ALA:O	1:C:709:THR:HG22	2.14	0.47
1:I:408:TYR:HB3	1:I:425:ILE:HG23	1.95	0.47
1:J:392:ALA:HB2	1:J:450:MET:HE2	1.96	0.47
1:B:477:LYS:O	1:B:486:LEU:HD23	2.15	0.47
1:B:493:MET:HG3	1:B:496:LEU:HD12	1.97	0.47
1:C:260:ALA:HB2	1:C:302:TRP:HB3	1.97	0.47
1:D:396:ARG:HD3	1:D:443:PHE:CG	2.49	0.47
1:D:612:ILE:HD11	1:D:657:PHE:CD2	2.49	0.47
1:F:705:ALA:O	1:F:709:THR:HG22	2.14	0.47
1:F:721:ASP:HA	1:F:722:GLU:HA	1.57	0.47
1:G:477:LYS:O	1:G:486:LEU:HD23	2.14	0.47
1:H:392:ALA:HB2	1:H:450:MET:HE2	1.97	0.47
1:H:612:ILE:HD11	1:H:657:PHE:HD2	1.79	0.47
1:H:642:LYS:HZ2	1:H:733:VAL:HG21	1.79	0.47
1:H:705:ALA:O	1:H:709:THR:HG22	2.15	0.47
1:I:114:PRO:HA	1:I:228:THR:CG2	2.44	0.47
1:B:33:SER:HA	1:B:525:VAL:O	2.15	0.47
1:C:33:SER:HA	1:C:525:VAL:O	2.15	0.47
1:C:477:LYS:O	1:C:486:LEU:HD23	2.14	0.47
1:D:477:LYS:O	1:D:486:LEU:HD23	2.14	0.47
1:E:493:MET:HG3	1:E:496:LEU:HD12	1.96	0.47
1:F:262:VAL:O	1:F:266:VAL:HG23	2.15	0.47
1:J:260:ALA:HB2	1:J:302:TRP:HB3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:374:GLY:HA3	1:J:375:LEU:HA	1.73	0.47
1:J:33:SER:HA	1:J:525:VAL:O	2.15	0.47
1:A:396:ARG:HD3	1:A:443:PHE:CG	2.49	0.47
1:A:705:ALA:O	1:A:709:THR:HG22	2.15	0.47
1:D:262:VAL:O	1:D:266:VAL:HG23	2.15	0.47
1:D:432:LEU:HD13	1:D:756:ILE:HD11	1.95	0.47
1:E:396:ARG:HD3	1:E:443:PHE:CG	2.49	0.47
1:F:408:TYR:HB3	1:F:425:ILE:HG23	1.96	0.47
1:F:642:LYS:HZ2	1:F:733:VAL:HG21	1.80	0.47
1:G:493:MET:HG3	1:G:496:LEU:HD12	1.96	0.47
1:G:705:ALA:O	1:G:709:THR:HG22	2.15	0.47
1:H:145:ASP:CB	1:H:148:GLN:HE21	2.23	0.47
1:I:396:ARG:HD3	1:I:443:PHE:CG	2.50	0.47
1:I:55:ARG:CZ	1:I:587:ILE:HD11	2.45	0.47
1:I:705:ALA:O	1:I:709:THR:HG22	2.15	0.47
1:J:262:VAL:O	1:J:266:VAL:HG23	2.15	0.47
1:J:721:ASP:HA	1:J:722:GLU:HA	1.57	0.47
1:A:264:GLU:OE2	1:A:298:THR:OG1	2.26	0.47
1:A:460:GLU:OE1	1:G:775:ASN:ND2	2.41	0.47
1:B:612:ILE:HD11	1:B:657:PHE:HD2	1.80	0.47
1:D:277:LEU:O	1:D:283:GLN:HG2	2.15	0.47
1:D:612:ILE:HD11	1:D:657:PHE:HD2	1.80	0.47
1:E:477:LYS:O	1:E:486:LEU:HD23	2.14	0.47
1:E:612:ILE:HD11	1:E:657:PHE:HD2	1.80	0.47
1:F:277:LEU:O	1:F:283:GLN:HG2	2.15	0.47
1:F:493:MET:HG3	1:F:496:LEU:HD12	1.96	0.47
1:I:390:LEU:O	1:I:549:GLN:NE2	2.48	0.47
1:J:114:PRO:HA	1:J:228:THR:HG21	1.97	0.47
1:J:396:ARG:HD3	1:J:443:PHE:CG	2.50	0.47
1:J:545:ARG:HB2	1:J:572:ALA:CB	2.45	0.47
1:J:593:LEU:HD13	1:J:596:ARG:HD2	1.96	0.47
1:A:477:LYS:O	1:A:486:LEU:HD23	2.15	0.47
1:C:277:LEU:O	1:C:283:GLN:HG2	2.15	0.47
1:E:545:ARG:HB2	1:E:572:ALA:CB	2.45	0.47
1:F:145:ASP:CB	1:F:148:GLN:HE21	2.24	0.47
1:F:477:LYS:O	1:F:486:LEU:HD23	2.15	0.47
1:G:277:LEU:O	1:G:283:GLN:HG2	2.15	0.47
1:G:33:SER:HA	1:G:525:VAL:O	2.15	0.47
1:G:541:ASN:HA	1:G:559:SER:HB3	1.95	0.47
1:C:354:ARG:HH12	1:C:358:THR:HG22	1.80	0.47
1:D:721:ASP:HA	1:D:722:GLU:HA	1.57	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:114:PRO:HA	1:F:228:THR:CG2	2.45	0.47
1:F:612:ILE:HD11	1:F:657:PHE:HD2	1.80	0.47
1:G:114:PRO:HA	1:G:228:THR:CG2	2.45	0.47
1:G:262:VAL:O	1:G:266:VAL:HG23	2.15	0.47
1:H:354:ARG:HH12	1:H:358:THR:HG22	1.80	0.47
1:J:257:ARG:O	1:J:261:VAL:HG23	2.15	0.47
1:J:477:LYS:O	1:J:486:LEU:HD23	2.15	0.47
1:J:493:MET:HG3	1:J:496:LEU:HD12	1.96	0.47
1:J:705:ALA:O	1:J:709:THR:HG22	2.15	0.47
1:B:396:ARG:HD3	1:B:443:PHE:CG	2.49	0.46
1:D:33:SER:HA	1:D:525:VAL:O	2.15	0.46
1:E:114:PRO:HA	1:E:228:THR:CG2	2.45	0.46
1:E:257:ARG:O	1:E:261:VAL:HG23	2.16	0.46
1:E:55:ARG:CZ	1:E:587:ILE:HD11	2.45	0.46
1:F:737:GLU:HG3	1:F:777:PHE:CZ	2.50	0.46
1:H:33:SER:HA	1:H:525:VAL:O	2.15	0.46
1:I:260:ALA:HB2	1:I:302:TRP:HB3	1.96	0.46
1:J:145:ASP:CB	1:J:148:GLN:HE21	2.24	0.46
1:C:612:ILE:HD11	1:C:657:PHE:HD2	1.80	0.46
1:H:277:LEU:O	1:H:283:GLN:HG2	2.15	0.46
1:H:396:ARG:HD3	1:H:443:PHE:CG	2.50	0.46
1:I:277:LEU:O	1:I:283:GLN:HG2	2.15	0.46
1:I:593:LEU:HD13	1:I:596:ARG:HD2	1.95	0.46
1:D:429:ARG:NE	1:J:304:GLN:OE1	2.45	0.46
1:A:257:ARG:O	1:A:261:VAL:HG23	2.16	0.46
1:A:262:VAL:O	1:A:266:VAL:HG23	2.15	0.46
1:A:33:SER:HA	1:A:525:VAL:O	2.15	0.46
1:B:262:VAL:O	1:B:266:VAL:HG23	2.15	0.46
1:B:390:LEU:O	1:B:549:GLN:NE2	2.49	0.46
1:B:705:ALA:O	1:B:709:THR:HG22	2.15	0.46
1:C:262:VAL:O	1:C:266:VAL:HG23	2.15	0.46
1:D:270:VAL:HG23	1:D:317:VAL:CG1	2.34	0.46
1:D:493:MET:HG3	1:D:496:LEU:HD12	1.96	0.46
1:E:317:VAL:HA	1:E:320:ILE:HD12	1.97	0.46
1:G:171:LYS:O	1:H:232:ARG:NH2	2.48	0.46
1:G:55:ARG:CZ	1:G:587:ILE:HD11	2.46	0.46
1:H:257:ARG:O	1:H:261:VAL:HG23	2.15	0.46
1:H:477:LYS:O	1:H:486:LEU:HD23	2.14	0.46
1:I:748:LYS:HA	1:I:762:ILE:HD13	1.97	0.46
1:J:408:TYR:HB3	1:J:425:ILE:HG23	1.96	0.46
1:A:260:ALA:HB2	1:A:302:TRP:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:354:ARG:HH12	1:A:358:THR:HG22	1.80	0.46
1:A:408:TYR:HB3	1:A:425:ILE:HG23	1.96	0.46
1:C:408:TYR:HB3	1:C:425:ILE:HG23	1.96	0.46
1:D:114:PRO:HA	1:D:228:THR:CG2	2.45	0.46
1:D:286:ARG:HH12	1:D:527:PHE:HB3	1.81	0.46
1:E:277:LEU:O	1:E:283:GLN:HG2	2.16	0.46
1:F:270:VAL:HG22	1:F:321:ASN:HD21	1.81	0.46
1:F:354:ARG:HH12	1:F:358:THR:HG22	1.80	0.46
1:H:260:ALA:HB2	1:H:302:TRP:HB3	1.96	0.46
1:H:493:MET:HG3	1:H:496:LEU:HD12	1.97	0.46
1:H:286:ARG:HH12	1:H:527:PHE:HB3	1.81	0.46
1:A:737:GLU:HG3	1:A:777:PHE:CZ	2.50	0.46
1:B:114:PRO:HA	1:B:228:THR:CG2	2.45	0.46
1:B:317:VAL:HA	1:B:320:ILE:HD12	1.97	0.46
1:C:114:PRO:HA	1:C:228:THR:HG21	1.97	0.46
1:D:257:ARG:O	1:D:261:VAL:HG23	2.16	0.46
1:D:408:TYR:HB3	1:D:425:ILE:HG23	1.95	0.46
1:D:392:ALA:HB2	1:D:450:MET:HE2	1.97	0.46
1:E:390:LEU:O	1:E:549:GLN:NE2	2.49	0.46
1:E:705:ALA:O	1:E:709:THR:HG22	2.15	0.46
1:F:55:ARG:CZ	1:F:587:ILE:HD11	2.46	0.46
1:F:748:LYS:HA	1:F:762:ILE:HD13	1.98	0.46
1:G:257:ARG:O	1:G:261:VAL:HG23	2.15	0.46
1:G:612:ILE:HD11	1:G:657:PHE:HD2	1.81	0.46
1:H:390:LEU:O	1:H:549:GLN:NE2	2.49	0.46
1:A:277:LEU:O	1:A:283:GLN:HG2	2.15	0.46
1:A:392:ALA:HB2	1:A:450:MET:HE2	1.98	0.46
1:D:390:LEU:O	1:D:549:GLN:NE2	2.49	0.46
1:D:402:ILE:O	1:D:434:LEU:HD12	2.16	0.46
1:E:354:ARG:HH12	1:E:358:THR:HG22	1.81	0.46
1:E:737:GLU:HG3	1:E:777:PHE:CZ	2.50	0.46
1:F:286:ARG:HH12	1:F:527:PHE:HB3	1.81	0.46
1:G:396:ARG:HD3	1:G:443:PHE:CG	2.50	0.46
1:G:408:TYR:HB3	1:G:425:ILE:CG2	2.46	0.46
1:H:540:SER:HA	1:H:541:ASN:HA	1.75	0.46
1:H:410:SER:HB3	1:H:664:ALA:HB2	1.98	0.46
1:I:273:PRO:CB	1:I:276:TYR:CD2	2.96	0.46
1:I:737:GLU:HG3	1:I:777:PHE:CZ	2.51	0.46
1:A:141:ASN:HD21	1:J:418:VAL:CG1	2.28	0.46
1:A:317:VAL:HA	1:A:320:ILE:HD12	1.98	0.46
1:A:55:ARG:CZ	1:A:587:ILE:HD11	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:114:PRO:HA	1:B:228:THR:HG21	1.98	0.46
1:B:277:LEU:O	1:B:283:GLN:HG2	2.15	0.46
1:C:55:ARG:CZ	1:C:587:ILE:HD11	2.46	0.46
1:D:410:SER:HB3	1:D:664:ALA:HB2	1.98	0.46
1:D:55:ARG:CZ	1:D:587:ILE:HD11	2.46	0.46
1:E:33:SER:HA	1:E:525:VAL:O	2.15	0.46
1:F:33:SER:HA	1:F:525:VAL:O	2.15	0.46
1:F:390:LEU:O	1:F:549:GLN:NE2	2.48	0.46
1:G:390:LEU:O	1:G:549:GLN:NE2	2.48	0.46
1:H:593:LEU:HD13	1:H:596:ARG:HD2	1.96	0.46
1:J:277:LEU:O	1:J:283:GLN:HG2	2.15	0.46
1:J:286:ARG:HH12	1:J:527:PHE:HB3	1.81	0.46
1:J:55:ARG:CZ	1:J:587:ILE:HD11	2.46	0.46
1:A:545:ARG:HB2	1:A:572:ALA:CB	2.45	0.46
1:B:264:GLU:OE1	1:B:269:ARG:HD2	2.16	0.46
1:B:374:GLY:HA3	1:B:375:LEU:HA	1.73	0.46
1:B:513:LEU:HD23	1:B:516:MET:HE3	1.97	0.46
1:C:286:ARG:HH12	1:C:527:PHE:HB3	1.81	0.46
1:E:264:GLU:OE1	1:E:269:ARG:HD2	2.16	0.46
1:G:410:SER:HB3	1:G:664:ALA:HB2	1.98	0.46
1:G:392:ALA:HB2	1:G:450:MET:HE2	1.98	0.46
1:H:37:ALA:O	1:H:369:LEU:HB2	2.16	0.46
1:H:737:GLU:HG3	1:H:777:PHE:CZ	2.51	0.46
1:I:262:VAL:O	1:I:266:VAL:HG23	2.15	0.46
1:J:399:ALA:HB2	1:J:584:ILE:HB	1.98	0.46
1:A:114:PRO:HA	1:A:228:THR:CG2	2.46	0.46
1:A:399:ALA:HB2	1:A:584:ILE:HB	1.98	0.46
1:A:479:LEU:HD11	1:A:567:LEU:HD23	1.98	0.46
1:B:257:ARG:O	1:B:261:VAL:HG23	2.16	0.46
1:B:402:ILE:O	1:B:434:LEU:HD12	2.16	0.46
1:B:737:GLU:HG3	1:B:777:PHE:CZ	2.50	0.46
1:C:317:VAL:HA	1:C:320:ILE:HD12	1.98	0.46
1:C:390:LEU:O	1:C:549:GLN:NE2	2.49	0.46
1:E:262:VAL:O	1:E:266:VAL:HG23	2.15	0.46
1:E:270:VAL:HG22	1:E:321:ASN:HD21	1.81	0.46
1:E:260:ALA:HB2	1:E:302:TRP:HB3	1.97	0.46
1:E:479:LEU:HD11	1:E:567:LEU:HD23	1.98	0.46
1:F:504:ILE:CG1	1:F:510:VAL:HG21	2.42	0.46
1:G:479:LEU:HD11	1:G:567:LEU:HD23	1.98	0.46
1:I:257:ARG:O	1:I:261:VAL:HG23	2.16	0.46
1:I:493:MET:HG3	1:I:496:LEU:HD12	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:410:SER:HB3	1:J:664:ALA:HB2	1.98	0.46
1:A:390:LEU:O	1:A:549:GLN:NE2	2.49	0.46
1:B:37:ALA:O	1:B:369:LEU:HB2	2.16	0.46
1:B:408:TYR:HB3	1:B:425:ILE:CG2	2.47	0.46
1:B:55:ARG:CZ	1:B:587:ILE:HD11	2.46	0.46
1:C:402:ILE:O	1:C:434:LEU:HD12	2.16	0.46
1:D:408:TYR:HB3	1:D:425:ILE:CG2	2.46	0.46
1:D:737:GLU:HG3	1:D:777:PHE:CZ	2.51	0.46
1:E:402:ILE:O	1:E:434:LEU:HD12	2.16	0.46
1:E:479:LEU:CD1	1:E:567:LEU:HD23	2.46	0.46
1:F:257:ARG:O	1:F:261:VAL:HG23	2.16	0.46
1:F:260:ALA:HB2	1:F:302:TRP:HB3	1.97	0.46
1:F:513:LEU:HD23	1:F:516:MET:HE1	1.98	0.46
1:H:408:TYR:HB3	1:H:425:ILE:CG2	2.47	0.46
1:H:399:ALA:HB2	1:H:584:ILE:HB	1.98	0.46
1:I:374:GLY:HA3	1:I:375:LEU:HA	1.74	0.46
1:I:402:ILE:O	1:I:434:LEU:HD12	2.16	0.46
1:I:504:ILE:CG1	1:I:510:VAL:HG21	2.43	0.46
1:B:54:LEU:CD2	1:B:375:LEU:HD23	2.46	0.45
1:B:399:ALA:HB2	1:B:584:ILE:HB	1.98	0.45
1:G:479:LEU:CD1	1:G:567:LEU:HD23	2.47	0.45
1:I:114:PRO:HA	1:I:228:THR:HG21	1.97	0.45
1:I:37:ALA:O	1:I:369:LEU:HB2	2.16	0.45
1:J:273:PRO:CB	1:J:276:TYR:CD2	2.96	0.45
1:J:479:LEU:HD11	1:J:567:LEU:HD23	1.98	0.45
1:J:740:LEU:HD21	1:J:780:ILE:HG22	1.98	0.45
1:A:410:SER:HB3	1:A:664:ALA:HB2	1.99	0.45
1:C:257:ARG:O	1:C:261:VAL:HG23	2.16	0.45
1:C:399:ALA:HB2	1:C:584:ILE:HB	1.99	0.45
1:C:740:LEU:HD21	1:C:780:ILE:HG22	1.98	0.45
1:D:354:ARG:HH12	1:D:358:THR:HG22	1.81	0.45
1:D:479:LEU:HD11	1:D:567:LEU:HD23	1.98	0.45
1:F:392:ALA:HB2	1:F:450:MET:HE2	1.98	0.45
1:F:402:ILE:O	1:F:434:LEU:HD12	2.16	0.45
1:F:545:ARG:HB2	1:F:572:ALA:CB	2.45	0.45
1:F:740:LEU:HD21	1:F:780:ILE:HG22	1.98	0.45
1:G:286:ARG:HH12	1:G:527:PHE:HB3	1.81	0.45
1:G:317:VAL:HA	1:G:320:ILE:HD12	1.98	0.45
1:G:740:LEU:HD21	1:G:780:ILE:HG22	1.99	0.45
1:H:317:VAL:HA	1:H:320:ILE:HD12	1.98	0.45
1:H:748:LYS:HA	1:H:762:ILE:HD13	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:740:LEU:HD21	1:H:780:ILE:HG22	1.98	0.45
1:I:33:SER:HA	1:I:525:VAL:O	2.15	0.45
1:A:479:LEU:CD1	1:A:567:LEU:HD23	2.47	0.45
1:A:85:ASP:OD2	1:J:660:ALA:HB1	2.16	0.45
1:B:563:THR:HG21	1:B:568:ASN:HB2	1.98	0.45
1:D:264:GLU:OE1	1:D:269:ARG:HD2	2.16	0.45
1:D:54:LEU:CD2	1:D:375:LEU:HD23	2.46	0.45
1:E:408:TYR:HB3	1:E:425:ILE:CG2	2.47	0.45
1:G:260:ALA:HB2	1:G:302:TRP:HB3	1.97	0.45
1:H:262:VAL:O	1:H:266:VAL:HG23	2.15	0.45
1:H:479:LEU:HB3	1:H:482:THR:OG1	2.17	0.45
1:J:23:VAL:HG21	1:J:32:PHE:CB	2.37	0.45
1:J:479:LEU:CD1	1:J:567:LEU:HD23	2.47	0.45
1:J:737:GLU:HG3	1:J:777:PHE:CZ	2.51	0.45
1:A:740:LEU:HD21	1:A:780:ILE:HG22	1.98	0.45
1:C:479:LEU:HB3	1:C:482:THR:OG1	2.17	0.45
1:C:54:LEU:CD2	1:C:375:LEU:HD23	2.46	0.45
1:C:737:GLU:HG3	1:C:777:PHE:CZ	2.50	0.45
1:E:748:LYS:HA	1:E:762:ILE:HD13	1.97	0.45
1:F:479:LEU:CD1	1:F:567:LEU:HD23	2.47	0.45
1:G:54:LEU:CD2	1:G:375:LEU:HD23	2.46	0.45
1:G:397:TYR:CE1	1:G:497:LEU:HD21	2.51	0.45
1:G:737:GLU:HG3	1:G:777:PHE:CZ	2.51	0.45
1:H:479:LEU:CD1	1:H:567:LEU:HD23	2.46	0.45
1:I:317:VAL:HA	1:I:320:ILE:HD12	1.98	0.45
1:D:412:GLN:O	1:J:89:GLN:NE2	2.48	0.45
1:A:37:ALA:O	1:A:369:LEU:HB2	2.16	0.45
1:A:402:ILE:O	1:A:434:LEU:HD12	2.16	0.45
1:A:479:LEU:HB3	1:A:482:THR:OG1	2.17	0.45
1:A:723:ILE:HD11	1:B:509:SER:OG	2.17	0.45
1:B:286:ARG:HH12	1:B:527:PHE:HB3	1.81	0.45
1:D:317:VAL:HA	1:D:320:ILE:HD12	1.98	0.45
1:E:54:LEU:CD2	1:E:375:LEU:HD23	2.46	0.45
1:E:37:ALA:O	1:E:369:LEU:HB2	2.17	0.45
1:G:273:PRO:CB	1:G:276:TYR:CD2	2.96	0.45
1:G:354:ARG:HH12	1:G:358:THR:HG22	1.81	0.45
1:G:402:ILE:O	1:G:434:LEU:HD12	2.16	0.45
1:I:354:ARG:HH12	1:I:358:THR:HG22	1.80	0.45
1:I:397:TYR:CE1	1:I:497:LEU:HD21	2.52	0.45
1:I:563:THR:HG21	1:I:568:ASN:HB2	1.98	0.45
1:J:390:LEU:O	1:J:549:GLN:NE2	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:286:ARG:HH12	1:A:527:PHE:HB3	1.81	0.45
1:A:54:LEU:CD2	1:A:375:LEU:HD23	2.46	0.45
1:B:479:LEU:HD11	1:B:567:LEU:HD23	1.98	0.45
1:B:740:LEU:HD21	1:B:780:ILE:HG22	1.99	0.45
1:C:410:SER:HB3	1:C:664:ALA:HB2	1.99	0.45
1:E:418:VAL:CG1	1:F:141:ASN:HD21	2.30	0.45
1:F:114:PRO:HA	1:F:228:THR:HG21	1.98	0.45
1:F:540:SER:HA	1:F:541:ASN:HA	1.75	0.45
1:G:748:LYS:HA	1:G:762:ILE:HD13	1.98	0.45
1:I:286:ARG:HH12	1:I:527:PHE:HB3	1.81	0.45
1:I:399:ALA:HB2	1:I:584:ILE:HB	1.98	0.45
1:I:479:LEU:CD1	1:I:567:LEU:HD23	2.46	0.45
1:J:37:ALA:O	1:J:369:LEU:HB2	2.16	0.45
1:A:145:ASP:HB3	1:A:148:GLN:HG3	1.99	0.45
1:A:748:LYS:HA	1:A:762:ILE:HD13	1.98	0.45
1:C:545:ARG:HB2	1:C:572:ALA:CB	2.45	0.45
1:D:748:LYS:HA	1:D:762:ILE:HD13	1.97	0.45
1:E:114:PRO:HA	1:E:228:THR:HG21	1.98	0.45
1:E:399:ALA:HB2	1:E:584:ILE:HB	1.99	0.45
1:F:317:VAL:HA	1:F:320:ILE:HD12	1.98	0.45
1:G:504:ILE:CG1	1:G:510:VAL:HG21	2.43	0.45
1:I:408:TYR:HB3	1:I:425:ILE:CG2	2.47	0.45
1:B:392:ALA:HB2	1:B:450:MET:HE2	1.99	0.45
1:C:563:THR:HG21	1:C:568:ASN:HB2	1.99	0.45
1:C:748:LYS:HA	1:C:762:ILE:HD13	1.98	0.45
1:D:114:PRO:HA	1:D:228:THR:HG21	1.98	0.45
1:D:37:ALA:O	1:D:369:LEU:HB2	2.17	0.45
1:D:479:LEU:CD1	1:D:567:LEU:HD23	2.47	0.45
1:D:563:THR:HG21	1:D:568:ASN:HB2	1.99	0.45
1:E:740:LEU:HD21	1:E:780:ILE:HG22	1.98	0.45
1:F:37:ALA:O	1:F:369:LEU:HB2	2.17	0.45
1:H:55:ARG:CZ	1:H:587:ILE:HD11	2.46	0.45
1:J:270:VAL:HG22	1:J:321:ASN:HD21	1.81	0.45
1:J:354:ARG:HH12	1:J:358:THR:HG22	1.80	0.45
1:C:260:ALA:O	1:C:264:GLU:HG2	2.17	0.45
1:C:479:LEU:CD1	1:C:567:LEU:HD23	2.47	0.45
1:D:399:ALA:HB2	1:D:584:ILE:HB	1.98	0.45
1:E:286:ARG:HH12	1:E:527:PHE:HB3	1.82	0.45
1:G:264:GLU:OE1	1:G:269:ARG:HD2	2.16	0.45
1:I:264:GLU:OE1	1:I:269:ARG:HD2	2.16	0.45
1:J:748:LYS:HA	1:J:762:ILE:HD13	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:408:TYR:HB3	1:A:425:ILE:CG2	2.47	0.45
1:D:260:ALA:O	1:D:264:GLU:HG2	2.17	0.45
1:D:740:LEU:HD21	1:D:780:ILE:HG22	1.99	0.45
1:E:414:PRO:HB3	1:F:142:LEU:HD22	1.98	0.45
1:G:37:ALA:O	1:G:369:LEU:HB2	2.16	0.45
1:G:545:ARG:HB2	1:G:572:ALA:CB	2.45	0.45
1:H:545:ARG:HB2	1:H:572:ALA:CB	2.45	0.45
1:I:40:ALA:CB	1:I:290:ASN:OD1	2.64	0.45
1:I:54:LEU:CD2	1:I:375:LEU:HD23	2.46	0.45
1:I:410:SER:HB3	1:I:664:ALA:HB2	1.98	0.45
1:I:545:ARG:HB2	1:I:572:ALA:CB	2.45	0.45
1:A:260:ALA:O	1:A:264:GLU:HG2	2.17	0.44
1:B:657:PHE:CD2	1:B:663:LEU:HD12	2.52	0.44
1:B:410:SER:HB3	1:B:664:ALA:HB2	1.99	0.44
1:C:145:ASP:HB3	1:C:148:GLN:HG3	1.99	0.44
1:D:545:ARG:HB2	1:D:572:ALA:CB	2.45	0.44
1:D:726:ILE:HA	1:D:727:ALA:HA	1.82	0.44
1:E:563:THR:HG21	1:E:568:ASN:HB2	1.99	0.44
1:F:399:ALA:HB2	1:F:584:ILE:HB	1.99	0.44
1:H:114:PRO:HA	1:H:228:THR:CG2	2.47	0.44
1:H:397:TYR:CE1	1:H:497:LEU:HD21	2.52	0.44
1:J:317:VAL:HA	1:J:320:ILE:HD12	1.98	0.44
1:J:54:LEU:CD2	1:J:375:LEU:HD23	2.46	0.44
1:J:408:TYR:HB3	1:J:425:ILE:CG2	2.47	0.44
1:A:232:ARG:O	1:A:236:GLN:HG3	2.18	0.44
1:B:260:ALA:O	1:B:264:GLU:HG2	2.17	0.44
1:B:40:ALA:CB	1:B:290:ASN:OD1	2.64	0.44
1:B:748:LYS:HA	1:B:762:ILE:HD13	1.98	0.44
1:C:273:PRO:CB	1:C:276:TYR:CD2	2.96	0.44
1:D:38:THR:HA	1:D:367:ALA:O	2.17	0.44
1:D:418:VAL:HG12	1:J:141:ASN:ND2	2.28	0.44
1:E:232:ARG:O	1:E:236:GLN:HG3	2.17	0.44
1:F:145:ASP:HB3	1:F:148:GLN:HG3	2.00	0.44
1:F:54:LEU:CD2	1:F:375:LEU:HD23	2.46	0.44
1:F:479:LEU:HB3	1:F:482:THR:OG1	2.17	0.44
1:G:255:LYS:NZ	1:G:359:SER:HG	2.13	0.44
1:H:503:ILE:HG21	1:H:515:TYR:CD2	2.53	0.44
1:E:89:GLN:NE2	1:I:412:GLN:O	2.44	0.44
1:I:479:LEU:HD11	1:I:567:LEU:HD23	1.98	0.44
1:D:108:MET:HA	1:J:114:PRO:CG	2.47	0.44
1:B:38:THR:HA	1:B:367:ALA:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:397:TYR:CE1	1:B:497:LEU:HD21	2.51	0.44
1:F:479:LEU:HD11	1:F:567:LEU:HD23	1.98	0.44
1:G:114:PRO:HA	1:G:228:THR:HG21	1.98	0.44
1:H:264:GLU:OE1	1:H:269:ARG:HD2	2.16	0.44
1:H:479:LEU:HD11	1:H:567:LEU:HD23	1.98	0.44
1:H:642:LYS:HG3	1:H:778:TYR:OH	2.17	0.44
1:I:740:LEU:HD21	1:I:780:ILE:HG22	1.99	0.44
1:A:264:GLU:OE1	1:A:269:ARG:HD2	2.16	0.44
1:C:37:ALA:O	1:C:369:LEU:HB2	2.17	0.44
1:C:418:VAL:CG1	1:D:141:ASN:HD21	2.31	0.44
1:D:715:LEU:N	1:D:716:ALA:HB3	2.33	0.44
1:E:410:SER:HB3	1:E:664:ALA:HB2	1.98	0.44
1:F:264:GLU:OE1	1:F:269:ARG:HD2	2.17	0.44
1:I:232:ARG:O	1:I:236:GLN:HG3	2.17	0.44
1:I:38:THR:HA	1:I:367:ALA:O	2.18	0.44
1:I:392:ALA:HB2	1:I:450:MET:HE2	1.99	0.44
1:I:642:LYS:HZ2	1:I:733:VAL:HG21	1.82	0.44
1:J:264:GLU:OE1	1:J:269:ARG:HD2	2.16	0.44
1:J:563:THR:HG21	1:J:568:ASN:HB2	1.99	0.44
1:A:563:THR:HG21	1:A:568:ASN:HB2	1.99	0.44
1:C:408:TYR:HB3	1:C:425:ILE:CG2	2.47	0.44
1:C:571:VAL:HA	1:C:572:ALA:HA	1.80	0.44
1:D:265:ILE:HD12	1:D:273:PRO:HG3	2.00	0.44
1:E:397:TYR:CE1	1:E:497:LEU:HD21	2.53	0.44
1:F:232:ARG:O	1:F:236:GLN:HG3	2.18	0.44
1:F:397:TYR:CE1	1:F:497:LEU:HD21	2.52	0.44
1:G:265:ILE:HD12	1:G:273:PRO:HG3	2.00	0.44
1:G:563:THR:HG21	1:G:568:ASN:HB2	1.98	0.44
1:H:232:ARG:O	1:H:236:GLN:HG3	2.18	0.44
1:H:402:ILE:O	1:H:434:LEU:HD12	2.16	0.44
1:H:715:LEU:N	1:H:716:ALA:HB3	2.33	0.44
1:J:265:ILE:HD12	1:J:273:PRO:HG3	2.00	0.44
1:J:397:TYR:CE1	1:J:497:LEU:HD21	2.52	0.44
1:J:642:LYS:HG3	1:J:778:TYR:OH	2.18	0.44
1:A:715:LEU:N	1:A:716:ALA:HB3	2.33	0.44
1:B:479:LEU:HB3	1:B:482:THR:OG1	2.17	0.44
1:C:264:GLU:OE1	1:C:269:ARG:HD2	2.16	0.44
1:D:374:GLY:HA3	1:D:375:LEU:HA	1.74	0.44
1:E:479:LEU:HB3	1:E:482:THR:OG1	2.17	0.44
1:E:503:ILE:HG21	1:E:515:TYR:CD2	2.53	0.44
1:E:504:ILE:HG22	1:E:505:PRO:HD2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:265:ILE:HD12	1:F:273:PRO:HG3	1.99	0.44
1:G:23:VAL:HG21	1:G:32:PHE:CB	2.36	0.44
1:G:399:ALA:HB2	1:G:584:ILE:HB	1.98	0.44
1:H:657:PHE:CD2	1:H:663:LEU:HD12	2.53	0.44
1:I:145:ASP:HB3	1:I:148:GLN:HG3	1.99	0.44
1:B:145:ASP:HB3	1:B:148:GLN:HG3	2.00	0.44
1:B:43:ARG:CG	1:B:365:THR:HG23	2.48	0.44
1:D:446:LEU:O	1:D:450:MET:HG2	2.18	0.44
1:E:657:PHE:CD2	1:E:663:LEU:HD12	2.53	0.44
1:F:260:ALA:O	1:F:264:GLU:HG2	2.17	0.44
1:F:408:TYR:HB3	1:F:425:ILE:CG2	2.47	0.44
1:F:657:PHE:CD2	1:F:663:LEU:HD12	2.53	0.44
1:G:479:LEU:HB3	1:G:482:THR:OG1	2.17	0.44
1:H:54:LEU:CD2	1:H:375:LEU:HD23	2.46	0.44
1:H:571:VAL:HA	1:H:572:ALA:HA	1.80	0.44
1:I:260:ALA:O	1:I:264:GLU:HG2	2.18	0.44
1:I:270:VAL:HG22	1:I:321:ASN:HD21	1.81	0.44
1:I:265:ILE:HD12	1:I:273:PRO:HG3	2.00	0.44
1:I:479:LEU:HB3	1:I:482:THR:OG1	2.17	0.44
1:J:402:ILE:O	1:J:434:LEU:HD12	2.17	0.44
1:J:479:LEU:HB3	1:J:482:THR:OG1	2.17	0.44
1:A:114:PRO:HA	1:A:228:THR:HG21	1.99	0.44
1:A:374:GLY:HA3	1:A:375:LEU:HA	1.73	0.44
1:B:446:LEU:O	1:B:450:MET:HG2	2.18	0.44
1:B:715:LEU:N	1:B:716:ALA:HB3	2.32	0.44
1:C:38:THR:HA	1:C:367:ALA:O	2.18	0.44
1:C:446:LEU:O	1:C:450:MET:HG2	2.18	0.44
1:E:642:LYS:HG3	1:E:778:TYR:OH	2.17	0.44
1:F:504:ILE:HG22	1:F:505:PRO:HD2	2.00	0.44
1:H:504:ILE:HG22	1:H:505:PRO:HD2	2.00	0.44
1:H:563:THR:HG21	1:H:568:ASN:HB2	1.99	0.44
1:J:190:LEU:HD13	1:J:190:LEU:O	2.18	0.44
1:J:260:ALA:O	1:J:264:GLU:HG2	2.17	0.44
1:A:38:THR:HA	1:A:367:ALA:O	2.18	0.44
1:A:642:LYS:HG3	1:A:778:TYR:OH	2.18	0.44
1:B:503:ILE:HG21	1:B:515:TYR:CD2	2.53	0.44
1:B:726:ILE:HA	1:B:727:ALA:HA	1.82	0.44
1:D:643:GLY:HA3	1:D:644:GLY:HA2	1.84	0.44
1:E:392:ALA:HB2	1:E:450:MET:HE2	2.00	0.44
1:F:410:SER:HB3	1:F:664:ALA:HB2	1.99	0.44
1:F:446:LEU:O	1:F:450:MET:HG2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:232:ARG:O	1:G:236:GLN:HG3	2.18	0.44
1:G:642:LYS:HG3	1:G:778:TYR:OH	2.17	0.44
1:H:260:ALA:O	1:H:264:GLU:HG2	2.17	0.44
1:H:40:ALA:CB	1:H:290:ASN:OD1	2.63	0.44
1:J:38:THR:HA	1:J:367:ALA:O	2.18	0.44
1:A:446:LEU:O	1:A:450:MET:HG2	2.18	0.43
1:C:392:ALA:HB2	1:C:450:MET:HE2	1.99	0.43
1:C:479:LEU:HD11	1:C:567:LEU:HD23	1.98	0.43
1:D:121:TRP:CZ3	1:J:226:PRO:HG3	2.53	0.43
1:D:163:ILE:HD13	1:D:212:TYR:CE2	2.53	0.43
1:D:439:GLU:OE2	1:D:489:ASN:ND2	2.51	0.43
1:E:145:ASP:HB3	1:E:148:GLN:HG3	1.99	0.43
1:F:38:THR:HA	1:F:367:ALA:O	2.18	0.43
1:G:260:ALA:O	1:G:264:GLU:HG2	2.17	0.43
1:G:504:ILE:HG22	1:G:505:PRO:HD2	2.00	0.43
1:H:145:ASP:HB3	1:H:148:GLN:HG3	1.99	0.43
1:H:446:LEU:O	1:H:450:MET:HG2	2.18	0.43
1:I:190:LEU:O	1:I:190:LEU:HD13	2.18	0.43
1:I:715:LEU:N	1:I:716:ALA:HB3	2.33	0.43
1:E:509:SER:OG	1:I:723:ILE:HD11	2.18	0.43
1:A:190:LEU:HD13	1:A:190:LEU:O	2.18	0.43
1:B:479:LEU:CD1	1:B:567:LEU:HD23	2.47	0.43
1:C:232:ARG:O	1:C:236:GLN:HG3	2.17	0.43
1:D:397:TYR:CE1	1:D:497:LEU:HD21	2.53	0.43
1:D:503:ILE:HG21	1:D:515:TYR:CD2	2.53	0.43
1:D:540:SER:HA	1:D:541:ASN:HA	1.75	0.43
1:D:642:LYS:HG3	1:D:778:TYR:OH	2.17	0.43
1:F:563:THR:HG21	1:F:568:ASN:HB2	1.99	0.43
1:G:446:LEU:O	1:G:450:MET:HG2	2.18	0.43
1:G:503:ILE:HG21	1:G:515:TYR:CD2	2.53	0.43
1:G:657:PHE:CD2	1:G:663:LEU:HD12	2.52	0.43
1:E:114:PRO:HB2	1:I:122:ALA:HB1	2.00	0.43
1:I:642:LYS:HG3	1:I:778:TYR:OH	2.18	0.43
1:J:145:ASP:HB3	1:J:148:GLN:HG3	2.00	0.43
1:J:446:LEU:O	1:J:450:MET:HG2	2.18	0.43
1:J:715:LEU:N	1:J:716:ALA:HB3	2.33	0.43
1:C:642:LYS:HG3	1:C:778:TYR:OH	2.18	0.43
1:D:232:ARG:O	1:D:236:GLN:HG3	2.18	0.43
1:D:270:VAL:HG22	1:D:321:ASN:HD21	1.81	0.43
1:D:479:LEU:HB3	1:D:482:THR:OG1	2.17	0.43
1:D:657:PHE:CD2	1:D:663:LEU:HD12	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:260:ALA:O	1:E:264:GLU:HG2	2.17	0.43
1:H:163:ILE:HD13	1:H:212:TYR:CE2	2.54	0.43
1:H:265:ILE:HD12	1:H:273:PRO:HG3	2.00	0.43
1:I:514:LEU:HD23	1:I:514:LEU:HA	1.91	0.43
1:A:270:VAL:HG22	1:A:321:ASN:HD21	1.81	0.43
1:A:304:GLN:OE1	1:J:429:ARG:NE	2.46	0.43
1:A:397:TYR:CE1	1:A:497:LEU:HD21	2.53	0.43
1:A:504:ILE:HG22	1:A:505:PRO:HD2	2.00	0.43
1:B:190:LEU:O	1:B:190:LEU:HD13	2.18	0.43
1:C:270:VAL:HG22	1:C:321:ASN:HD21	1.81	0.43
1:C:397:TYR:CE1	1:C:497:LEU:HD21	2.53	0.43
1:E:23:VAL:HG21	1:E:32:PHE:CB	2.36	0.43
1:E:715:LEU:N	1:E:716:ALA:HB3	2.33	0.43
1:H:190:LEU:O	1:H:190:LEU:HD13	2.18	0.43
1:I:163:ILE:HD13	1:I:212:TYR:CE2	2.54	0.43
1:I:446:LEU:O	1:I:450:MET:HG2	2.18	0.43
1:J:232:ARG:O	1:J:236:GLN:HG3	2.18	0.43
1:A:503:ILE:HG21	1:A:515:TYR:CD2	2.53	0.43
1:A:657:PHE:CD2	1:A:663:LEU:HD12	2.53	0.43
1:B:504:ILE:HG22	1:B:505:PRO:HD2	1.99	0.43
1:E:109:GLY:HA3	1:F:113:ARG:CD	2.48	0.43
1:E:374:GLY:HA3	1:E:375:LEU:HA	1.73	0.43
1:F:503:ILE:HG21	1:F:515:TYR:CD2	2.54	0.43
1:F:642:LYS:HG3	1:F:778:TYR:OH	2.18	0.43
1:F:715:LEU:N	1:F:716:ALA:HB3	2.33	0.43
1:G:38:THR:HA	1:G:367:ALA:O	2.18	0.43
1:I:356:ALA:O	1:I:360:VAL:HG23	2.19	0.43
1:I:504:ILE:HG22	1:I:505:PRO:HD2	2.00	0.43
1:J:356:ALA:O	1:J:360:VAL:HG23	2.19	0.43
1:B:265:ILE:HD12	1:B:273:PRO:HG3	2.00	0.43
1:B:642:LYS:HG3	1:B:778:TYR:OH	2.18	0.43
1:C:272:ALA:N	1:C:273:PRO:HD3	2.34	0.43
1:C:715:LEU:N	1:C:716:ALA:HB3	2.33	0.43
1:C:726:ILE:HA	1:C:727:ALA:HA	1.83	0.43
1:E:434:LEU:O	1:E:711:THR:HG21	2.18	0.43
1:E:571:VAL:HA	1:E:572:ALA:HA	1.80	0.43
1:F:23:VAL:HG21	1:F:32:PHE:CB	2.36	0.43
1:G:190:LEU:HD13	1:G:190:LEU:O	2.18	0.43
1:G:356:ALA:O	1:G:360:VAL:HG23	2.19	0.43
1:G:434:LEU:O	1:G:711:THR:HG21	2.19	0.43
1:I:657:PHE:CD2	1:I:663:LEU:HD12	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:503:ILE:HG21	1:J:515:TYR:CG	2.54	0.43
1:A:446:LEU:CD2	1:A:487:VAL:HG11	2.49	0.43
1:A:439:GLU:OE2	1:A:489:ASN:ND2	2.52	0.43
1:B:504:ILE:CG1	1:B:510:VAL:HG21	2.43	0.43
1:C:356:ALA:O	1:C:360:VAL:HG23	2.19	0.43
1:D:145:ASP:HB3	1:D:148:GLN:HG3	2.00	0.43
1:D:434:LEU:O	1:D:711:THR:HG21	2.19	0.43
1:E:190:LEU:O	1:E:190:LEU:HD13	2.18	0.43
1:F:434:LEU:O	1:F:711:THR:HG21	2.19	0.43
1:G:145:ASP:HB3	1:G:148:GLN:HG3	1.99	0.43
1:G:715:LEU:N	1:G:716:ALA:HB3	2.33	0.43
1:H:114:PRO:HA	1:H:228:THR:HG21	1.99	0.43
1:H:350:THR:N	1:H:351:PRO:CD	2.82	0.43
1:H:38:THR:HA	1:H:367:ALA:O	2.18	0.43
1:J:504:ILE:HG22	1:J:505:PRO:HD2	2.00	0.43
1:J:146:GLU:CD	1:J:604:LYS:HZ1	2.19	0.43
1:A:265:ILE:HD12	1:A:273:PRO:HG3	2.00	0.43
1:A:43:ARG:CG	1:A:365:THR:HG23	2.49	0.43
1:A:721:ASP:HA	1:A:722:GLU:HA	1.57	0.43
1:B:374:GLY:HA2	1:B:376:GLY:H	1.84	0.43
1:B:545:ARG:HB2	1:B:572:ALA:CB	2.45	0.43
1:E:356:ALA:O	1:E:360:VAL:HG23	2.19	0.43
1:E:425:ILE:HD12	1:E:593:LEU:HD22	2.01	0.43
1:E:439:GLU:OE2	1:E:489:ASN:ND2	2.52	0.43
1:E:446:LEU:O	1:E:450:MET:HG2	2.18	0.43
1:F:356:ALA:O	1:F:360:VAL:HG23	2.19	0.43
1:F:643:GLY:HA3	1:F:644:GLY:HA2	1.84	0.43
1:H:123:GLU:CD	1:I:229:ARG:NH1	2.65	0.43
1:I:446:LEU:CD2	1:I:487:VAL:HG11	2.49	0.43
1:J:439:GLU:OE2	1:J:489:ASN:ND2	2.52	0.43
1:A:272:ALA:N	1:A:273:PRO:HD3	2.34	0.43
1:A:402:ILE:HD12	1:A:668:VAL:CG1	2.49	0.43
1:B:122:ALA:HB1	1:C:114:PRO:HB2	2.00	0.43
1:B:272:ALA:N	1:B:273:PRO:HD3	2.33	0.43
1:B:354:ARG:HH12	1:B:358:THR:HG22	1.80	0.43
1:C:425:ILE:HD12	1:C:593:LEU:HD22	2.01	0.43
1:D:120:SER:HB3	1:D:222:ASP:HA	2.01	0.43
1:E:402:ILE:HD12	1:E:668:VAL:CG1	2.49	0.43
1:E:77:ILE:O	1:E:81:ILE:HG13	2.19	0.43
1:F:777:PHE:HA	1:F:780:ILE:HD12	2.01	0.43
1:H:721:ASP:HA	1:H:722:GLU:HA	1.57	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:425:ILE:HD12	1:I:593:LEU:HD22	2.01	0.43
1:J:43:ARG:CG	1:J:365:THR:HG23	2.49	0.43
1:J:503:ILE:HG21	1:J:515:TYR:CD2	2.53	0.43
1:A:356:ALA:O	1:A:360:VAL:HG23	2.19	0.43
1:B:356:ALA:O	1:B:360:VAL:HG23	2.19	0.43
1:C:657:PHE:CD2	1:C:663:LEU:HD12	2.53	0.43
1:E:43:ARG:CG	1:E:365:THR:HG23	2.48	0.43
1:E:51:SER:HB2	1:E:57:ARG:H	1.84	0.43
1:F:77:ILE:O	1:F:81:ILE:HG13	2.19	0.43
1:G:571:VAL:HA	1:G:572:ALA:HA	1.81	0.43
1:G:77:ILE:O	1:G:81:ILE:HG13	2.19	0.43
1:H:43:ARG:CG	1:H:365:THR:HG23	2.49	0.43
1:H:374:GLY:HA3	1:H:375:LEU:HA	1.73	0.43
1:H:434:LEU:O	1:H:711:THR:HG21	2.19	0.43
1:I:51:SER:HB2	1:I:57:ARG:H	1.84	0.43
1:J:163:ILE:HD13	1:J:212:TYR:CE2	2.54	0.43
1:A:350:THR:N	1:A:351:PRO:CD	2.82	0.42
1:A:77:ILE:O	1:A:81:ILE:HG13	2.19	0.42
1:B:503:ILE:HG21	1:B:515:TYR:CG	2.54	0.42
1:C:503:ILE:HG21	1:C:515:TYR:CD2	2.54	0.42
1:C:77:ILE:O	1:C:81:ILE:HG13	2.19	0.42
1:D:504:ILE:HG22	1:D:505:PRO:HD2	2.00	0.42
1:E:446:LEU:CD2	1:E:487:VAL:HG11	2.49	0.42
1:F:43:ARG:CG	1:F:365:THR:HG23	2.49	0.42
1:F:726:ILE:HA	1:F:727:ALA:HA	1.83	0.42
1:G:51:SER:HB2	1:G:57:ARG:H	1.84	0.42
1:H:261:VAL:HG13	1:H:316:TRP:HH2	1.85	0.42
1:A:434:LEU:O	1:A:711:THR:HG21	2.19	0.42
1:D:190:LEU:O	1:D:190:LEU:HD13	2.18	0.42
1:F:446:LEU:CD2	1:F:487:VAL:HG11	2.49	0.42
1:G:261:VAL:HG13	1:G:316:TRP:HH2	1.84	0.42
1:G:439:GLU:OE2	1:G:489:ASN:ND2	2.51	0.42
1:H:503:ILE:HG21	1:H:515:TYR:CG	2.54	0.42
1:I:434:LEU:O	1:I:711:THR:HG21	2.19	0.42
1:I:503:ILE:HG21	1:I:515:TYR:CD2	2.54	0.42
1:J:261:VAL:HG13	1:J:316:TRP:HH2	1.84	0.42
1:B:232:ARG:O	1:B:236:GLN:HG3	2.18	0.42
1:B:439:GLU:OE2	1:B:489:ASN:ND2	2.52	0.42
1:D:261:VAL:HG13	1:D:316:TRP:HH2	1.84	0.42
1:D:402:ILE:HD12	1:D:668:VAL:CG1	2.49	0.42
1:F:273:PRO:CB	1:F:276:TYR:CD2	2.96	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:163:ILE:HD13	1:G:212:TYR:CE2	2.53	0.42
1:H:402:ILE:HD12	1:H:668:VAL:CG1	2.49	0.42
1:H:68:ARG:HG3	1:H:165:ALA:CB	2.49	0.42
1:I:43:ARG:CG	1:I:365:THR:HG23	2.49	0.42
1:I:77:ILE:O	1:I:81:ILE:HG13	2.19	0.42
1:J:272:ALA:N	1:J:273:PRO:HD3	2.33	0.42
1:J:425:ILE:HD12	1:J:593:LEU:HD22	2.01	0.42
1:A:374:GLY:HA2	1:A:376:GLY:H	1.84	0.42
1:B:350:THR:N	1:B:351:PRO:CD	2.83	0.42
1:B:446:LEU:CD2	1:B:487:VAL:HG11	2.50	0.42
1:C:265:ILE:HD12	1:C:273:PRO:HG3	2.00	0.42
1:C:439:GLU:OE2	1:C:489:ASN:ND2	2.52	0.42
1:D:503:ILE:HG21	1:D:515:TYR:CG	2.54	0.42
1:E:38:THR:HA	1:E:367:ALA:O	2.18	0.42
1:G:350:THR:N	1:G:351:PRO:CD	2.82	0.42
1:G:418:VAL:HA	1:H:141:ASN:HD21	1.84	0.42
1:G:446:LEU:CD2	1:G:487:VAL:HG11	2.49	0.42
1:G:547:THR:HG23	1:G:550:VAL:HG23	2.02	0.42
1:G:643:GLY:HA3	1:G:644:GLY:HA2	1.84	0.42
1:J:657:PHE:CD2	1:J:663:LEU:HD12	2.54	0.42
1:A:261:VAL:HG13	1:A:316:TRP:HH2	1.84	0.42
1:A:40:ALA:CB	1:A:290:ASN:OD1	2.63	0.42
1:B:77:ILE:O	1:B:81:ILE:HG13	2.19	0.42
1:C:446:LEU:CD2	1:C:487:VAL:HG11	2.49	0.42
1:C:504:ILE:HG22	1:C:505:PRO:HD2	2.00	0.42
1:D:77:ILE:O	1:D:81:ILE:HG13	2.19	0.42
1:E:163:ILE:HD13	1:E:212:TYR:CE2	2.54	0.42
1:F:68:ARG:HG3	1:F:165:ALA:CB	2.50	0.42
1:F:190:LEU:O	1:F:190:LEU:HD13	2.18	0.42
1:H:101:ARG:HA	1:H:231:SER:HB3	2.02	0.42
1:H:273:PRO:CB	1:H:276:TYR:CD2	2.96	0.42
1:H:374:GLY:HA2	1:H:376:GLY:H	1.84	0.42
1:I:350:THR:N	1:I:351:PRO:CD	2.82	0.42
1:I:402:ILE:HD12	1:I:668:VAL:CG1	2.49	0.42
1:I:540:SER:HA	1:I:541:ASN:HA	1.74	0.42
1:A:141:ASN:HD21	1:J:418:VAL:HA	1.84	0.42
1:A:163:ILE:HD13	1:A:212:TYR:CE2	2.54	0.42
1:A:273:PRO:CB	1:A:276:TYR:CD2	2.96	0.42
1:A:547:THR:HG23	1:A:550:VAL:HG23	2.02	0.42
1:B:425:ILE:HD12	1:B:593:LEU:HD22	2.01	0.42
1:B:434:LEU:O	1:B:711:THR:HG21	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:51:SER:HB2	1:B:57:ARG:H	1.85	0.42
1:C:190:LEU:HD13	1:C:190:LEU:O	2.18	0.42
1:C:434:LEU:O	1:C:711:THR:HG21	2.19	0.42
1:C:82:ILE:N	1:C:82:ILE:HD12	2.34	0.42
1:D:374:GLY:HA2	1:D:376:GLY:H	1.85	0.42
1:D:446:LEU:CD2	1:D:487:VAL:HG11	2.49	0.42
1:D:68:ARG:HG3	1:D:165:ALA:CB	2.50	0.42
1:E:265:ILE:HD12	1:E:273:PRO:HG3	2.00	0.42
1:E:291:PHE:CE1	1:E:295:THR:HG21	2.54	0.42
1:E:374:GLY:HA2	1:E:376:GLY:H	1.84	0.42
1:E:503:ILE:HG21	1:E:515:TYR:CG	2.54	0.42
1:E:721:ASP:HA	1:E:722:GLU:HA	1.56	0.42
1:F:503:ILE:HG21	1:F:515:TYR:CG	2.55	0.42
1:G:503:ILE:HG21	1:G:515:TYR:CG	2.54	0.42
1:H:82:ILE:HD12	1:H:82:ILE:N	2.35	0.42
1:J:77:ILE:O	1:J:81:ILE:HG13	2.19	0.42
1:A:68:ARG:HG3	1:A:165:ALA:CB	2.50	0.42
1:B:163:ILE:HD13	1:B:212:TYR:CE2	2.54	0.42
1:B:261:VAL:HG13	1:B:316:TRP:HH2	1.85	0.42
1:B:402:ILE:HD12	1:B:668:VAL:CG1	2.49	0.42
1:B:777:PHE:HA	1:B:780:ILE:HD12	2.02	0.42
1:C:374:GLY:HA2	1:C:376:GLY:H	1.85	0.42
1:C:513:LEU:HA	1:C:516:MET:HE2	2.02	0.42
1:D:291:PHE:CE1	1:D:295:THR:HG21	2.55	0.42
1:D:356:ALA:O	1:D:360:VAL:HG23	2.19	0.42
1:D:777:PHE:HA	1:D:780:ILE:HD12	2.02	0.42
1:F:163:ILE:HD13	1:F:212:TYR:CE2	2.54	0.42
1:F:82:ILE:HD12	1:F:82:ILE:N	2.35	0.42
1:G:291:PHE:CE1	1:G:295:THR:HG21	2.55	0.42
1:H:446:LEU:CD2	1:H:487:VAL:HG11	2.50	0.42
1:H:513:LEU:HD23	1:H:516:MET:HE3	2.02	0.42
1:I:192:PRO:HB2	1:I:364:VAL:HG22	2.02	0.42
1:I:101:ARG:HA	1:I:231:SER:HB3	2.01	0.42
1:I:23:VAL:HG21	1:I:32:PHE:CB	2.36	0.42
1:J:374:GLY:HA2	1:J:376:GLY:H	1.85	0.42
1:J:643:GLY:HA3	1:J:644:GLY:HA2	1.84	0.42
1:A:51:SER:HB2	1:A:57:ARG:H	1.84	0.42
1:B:270:VAL:HG22	1:B:321:ASN:HD21	1.81	0.42
1:B:622:ARG:O	1:B:626:VAL:HG23	2.20	0.42
1:B:68:ARG:HG3	1:B:165:ALA:CB	2.50	0.42
1:C:402:ILE:HD12	1:C:668:VAL:CG1	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:68:ARG:HG3	1:C:165:ALA:CB	2.50	0.42
1:E:101:ARG:HA	1:E:231:SER:HB3	2.01	0.42
1:F:622:ARG:O	1:F:626:VAL:HG23	2.20	0.42
1:B:460:GLU:HG2	1:F:775:ASN:ND2	2.35	0.42
1:G:374:GLY:HA2	1:G:376:GLY:H	1.84	0.42
1:G:777:PHE:HA	1:G:780:ILE:HD12	2.02	0.42
1:H:480:PRO:HD2	1:H:567:LEU:HD22	2.02	0.42
1:H:622:ARG:O	1:H:626:VAL:HG23	2.20	0.42
1:I:439:GLU:OE2	1:I:489:ASN:ND2	2.52	0.42
1:J:493:MET:O	1:J:493:MET:HG3	2.20	0.42
1:J:434:LEU:O	1:J:711:THR:HG21	2.19	0.42
1:B:123:GLU:OE2	1:C:229:ARG:NH2	2.52	0.42
1:B:408:TYR:CB	1:B:425:ILE:CG2	2.98	0.42
1:B:408:TYR:CB	1:B:425:ILE:HG23	2.50	0.42
1:B:493:MET:O	1:B:493:MET:HG3	2.20	0.42
1:C:503:ILE:HG21	1:C:515:TYR:CG	2.54	0.42
1:E:540:SER:HA	1:E:541:ASN:HA	1.74	0.42
1:E:59:TYR:CE2	1:E:591:PRO:HD3	2.55	0.42
1:F:291:PHE:CE1	1:F:295:THR:HG21	2.54	0.42
1:F:439:GLU:OE2	1:F:489:ASN:ND2	2.53	0.42
1:F:493:MET:O	1:F:493:MET:HG3	2.20	0.42
1:G:540:SER:HA	1:G:541:ASN:HA	1.75	0.42
1:H:356:ALA:O	1:H:360:VAL:HG23	2.19	0.42
1:H:439:GLU:OE2	1:H:489:ASN:ND2	2.52	0.42
1:I:291:PHE:CE1	1:I:295:THR:HG21	2.55	0.42
1:A:503:ILE:HG21	1:A:515:TYR:CG	2.54	0.42
1:A:540:SER:HA	1:A:541:ASN:HA	1.75	0.42
1:C:43:ARG:CG	1:C:365:THR:HG23	2.49	0.42
1:C:504:ILE:CG1	1:C:510:VAL:HG21	2.43	0.42
1:D:408:TYR:CB	1:D:425:ILE:CG2	2.98	0.42
1:D:638:TYR:CE1	1:D:647:VAL:HG11	2.55	0.42
1:E:374:GLY:CA	1:E:376:GLY:H	2.33	0.42
1:F:101:ARG:HA	1:F:231:SER:HB3	2.02	0.42
1:F:261:VAL:HG13	1:F:316:TRP:HH2	1.84	0.42
1:F:350:THR:N	1:F:351:PRO:CD	2.82	0.42
1:G:622:ARG:O	1:G:626:VAL:HG23	2.20	0.42
1:I:503:ILE:HG21	1:I:515:TYR:CG	2.55	0.42
1:B:374:GLY:CA	1:B:376:GLY:H	2.33	0.41
1:C:163:ILE:HD13	1:C:212:TYR:CE2	2.55	0.41
1:C:374:GLY:HA3	1:C:375:LEU:HA	1.74	0.41
1:E:777:PHE:HA	1:E:780:ILE:HD12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:43:ARG:CG	1:G:365:THR:HG23	2.50	0.41
1:G:91:CYS:HG	1:G:207:PHE:HE2	1.65	0.41
1:G:411:PHE:CE2	1:H:88:THR:HG21	2.55	0.41
1:I:408:TYR:CB	1:I:425:ILE:HG23	2.50	0.41
1:J:101:ARG:HA	1:J:231:SER:HB3	2.01	0.41
1:D:108:MET:HA	1:J:114:PRO:HG2	2.02	0.41
1:J:192:PRO:HB2	1:J:364:VAL:HG22	2.02	0.41
1:J:68:ARG:HG3	1:J:165:ALA:CB	2.50	0.41
1:A:425:ILE:HD12	1:A:593:LEU:HD22	2.02	0.41
1:A:638:TYR:CE1	1:A:647:VAL:HG11	2.55	0.41
1:A:777:PHE:HA	1:A:780:ILE:HD12	2.02	0.41
1:C:192:PRO:HB2	1:C:364:VAL:HG22	2.02	0.41
1:C:40:ALA:CB	1:C:290:ASN:OD1	2.64	0.41
1:C:622:ARG:O	1:C:626:VAL:HG23	2.20	0.41
1:D:43:ARG:CG	1:D:365:THR:HG23	2.49	0.41
1:E:273:PRO:CB	1:E:276:TYR:CD2	2.98	0.41
1:E:350:THR:N	1:E:351:PRO:CD	2.82	0.41
1:E:171:LYS:HB3	1:F:232:ARG:NH2	2.35	0.41
1:G:402:ILE:HD12	1:G:668:VAL:CG1	2.50	0.41
1:G:418:VAL:HG12	1:H:141:ASN:ND2	2.30	0.41
1:H:192:PRO:HB2	1:H:364:VAL:HG22	2.01	0.41
1:H:291:PHE:CE1	1:H:295:THR:HG21	2.54	0.41
1:H:51:SER:HB2	1:H:57:ARG:H	1.85	0.41
1:H:77:ILE:O	1:H:81:ILE:HG13	2.19	0.41
1:I:82:ILE:N	1:I:82:ILE:HD12	2.35	0.41
1:C:291:PHE:CE1	1:C:295:THR:HG21	2.55	0.41
1:C:350:THR:N	1:C:351:PRO:CD	2.82	0.41
1:C:408:TYR:CB	1:C:425:ILE:CG2	2.98	0.41
1:D:192:PRO:HB2	1:D:364:VAL:HG22	2.02	0.41
1:D:82:ILE:N	1:D:82:ILE:HD12	2.36	0.41
1:E:408:TYR:CB	1:E:425:ILE:CG2	2.99	0.41
1:E:493:MET:HG3	1:E:493:MET:O	2.20	0.41
1:E:82:ILE:HD12	1:E:82:ILE:N	2.35	0.41
1:F:192:PRO:HB2	1:F:364:VAL:HG22	2.02	0.41
1:G:101:ARG:HA	1:G:231:SER:HB3	2.02	0.41
1:G:425:ILE:HD12	1:G:593:LEU:HD22	2.01	0.41
1:G:579:THR:HB	1:G:580:PRO:HD2	2.02	0.41
1:G:59:TYR:CE2	1:G:591:PRO:HD3	2.56	0.41
1:H:408:TYR:CB	1:H:425:ILE:CG2	2.98	0.41
1:I:261:VAL:HG13	1:I:316:TRP:HH2	1.85	0.41
1:I:374:GLY:HA2	1:I:376:GLY:H	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:PRO:HB2	1:A:364:VAL:HG22	2.02	0.41
1:A:493:MET:O	1:A:493:MET:HG3	2.20	0.41
1:B:190:LEU:CD2	1:B:290:ASN:ND2	2.83	0.41
1:C:171:LYS:O	1:D:232:ARG:NH2	2.51	0.41
1:C:643:GLY:HA3	1:C:644:GLY:HA2	1.84	0.41
1:D:350:THR:N	1:D:351:PRO:CD	2.83	0.41
1:D:425:ILE:O	1:D:596:ARG:HG3	2.21	0.41
1:E:403:ASN:O	1:E:403:ASN:OD1	2.38	0.41
1:E:425:ILE:O	1:E:596:ARG:HG3	2.21	0.41
1:E:420:VAL:HG12	1:E:602:VAL:HG13	2.03	0.41
1:E:622:ARG:O	1:E:626:VAL:HG23	2.20	0.41
1:F:402:ILE:HD12	1:F:668:VAL:CG1	2.49	0.41
1:F:403:ASN:OD1	1:F:403:ASN:O	2.38	0.41
1:F:408:TYR:CB	1:F:425:ILE:HG23	2.51	0.41
1:G:403:ASN:O	1:G:403:ASN:OD1	2.38	0.41
1:H:493:MET:HG3	1:H:493:MET:O	2.20	0.41
1:H:638:TYR:CE1	1:H:647:VAL:HG11	2.55	0.41
1:I:420:VAL:HG12	1:I:602:VAL:HG13	2.03	0.41
1:I:408:TYR:CB	1:I:425:ILE:CG2	2.98	0.41
1:I:726:ILE:HA	1:I:727:ALA:HA	1.83	0.41
1:A:101:ARG:HA	1:A:231:SER:HB3	2.02	0.41
1:A:291:PHE:CE1	1:A:295:THR:HG21	2.55	0.41
1:B:291:PHE:CE1	1:B:295:THR:HG21	2.55	0.41
1:B:403:ASN:O	1:B:403:ASN:OD1	2.38	0.41
1:B:579:THR:HB	1:B:580:PRO:HD2	2.02	0.41
1:B:59:TYR:CE2	1:B:591:PRO:HD3	2.55	0.41
1:B:420:VAL:HG12	1:B:602:VAL:HG13	2.03	0.41
1:C:408:TYR:CB	1:C:425:ILE:HG23	2.50	0.41
1:C:480:PRO:HD2	1:C:567:LEU:HD22	2.02	0.41
1:E:272:ALA:N	1:E:273:PRO:HD3	2.33	0.41
1:E:146:GLU:CD	1:E:604:LYS:HZ1	2.22	0.41
1:F:579:THR:HB	1:F:580:PRO:HD2	2.02	0.41
1:F:420:VAL:HG12	1:F:602:VAL:HG13	2.03	0.41
1:G:68:ARG:HG3	1:G:165:ALA:CB	2.50	0.41
1:H:306:TRP:CE3	1:H:306:TRP:HA	2.56	0.41
1:I:777:PHE:HA	1:I:780:ILE:HD12	2.02	0.41
1:J:51:SER:HB2	1:J:57:ARG:H	1.86	0.41
1:J:402:ILE:HD12	1:J:668:VAL:CG1	2.49	0.41
1:A:622:ARG:O	1:A:626:VAL:HG23	2.20	0.41
1:B:82:ILE:N	1:B:82:ILE:HD12	2.35	0.41
1:D:101:ARG:HA	1:D:231:SER:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:374:GLY:CA	1:D:376:GLY:H	2.34	0.41
1:D:403:ASN:OD1	1:D:403:ASN:O	2.38	0.41
1:D:59:TYR:CE2	1:D:591:PRO:HD3	2.56	0.41
1:E:261:VAL:HG13	1:E:316:TRP:HH2	1.84	0.41
1:E:627:SER:HB3	1:E:726:ILE:CD1	2.51	0.41
1:F:425:ILE:HD12	1:F:593:LEU:HD22	2.01	0.41
1:F:627:SER:HB3	1:F:726:ILE:CD1	2.51	0.41
1:G:374:GLY:CA	1:G:376:GLY:H	2.34	0.41
1:G:408:TYR:CB	1:G:425:ILE:CG2	2.98	0.41
1:H:120:SER:HB3	1:H:222:ASP:HA	2.02	0.41
1:H:425:ILE:O	1:H:596:ARG:HG3	2.21	0.41
1:I:493:MET:O	1:I:493:MET:HG3	2.20	0.41
1:I:59:TYR:CE2	1:I:591:PRO:HD3	2.56	0.41
1:I:622:ARG:O	1:I:626:VAL:HG23	2.20	0.41
1:J:350:THR:N	1:J:351:PRO:CD	2.83	0.41
1:J:82:ILE:HD12	1:J:82:ILE:N	2.35	0.41
1:A:579:THR:HB	1:A:580:PRO:HD2	2.02	0.41
1:B:101:ARG:HA	1:B:231:SER:HB3	2.01	0.41
1:B:638:TYR:CE1	1:B:647:VAL:HG11	2.56	0.41
1:C:374:GLY:CA	1:C:376:GLY:H	2.34	0.41
1:C:579:THR:HB	1:C:580:PRO:HD2	2.02	0.41
1:D:272:ALA:N	1:D:273:PRO:HD3	2.34	0.41
1:D:547:THR:HG23	1:D:550:VAL:HG23	2.02	0.41
1:D:627:SER:HB3	1:D:726:ILE:CD1	2.51	0.41
1:F:408:TYR:CB	1:F:425:ILE:CG2	2.98	0.41
1:F:547:THR:HG23	1:F:550:VAL:HG23	2.02	0.41
1:F:425:ILE:O	1:F:596:ARG:HG3	2.21	0.41
1:G:514:LEU:HD23	1:G:514:LEU:HA	1.91	0.41
1:H:40:ALA:CB	1:H:192:PRO:HG3	2.51	0.41
1:H:408:TYR:CB	1:H:425:ILE:HG23	2.50	0.41
1:H:547:THR:CG2	1:H:550:VAL:HG23	2.51	0.41
1:H:59:TYR:CE2	1:H:591:PRO:HD3	2.55	0.41
1:I:579:THR:HB	1:I:580:PRO:HD2	2.03	0.41
1:I:627:SER:HB3	1:I:726:ILE:CD1	2.51	0.41
1:J:291:PHE:CE1	1:J:295:THR:HG21	2.55	0.41
1:J:408:TYR:CB	1:J:425:ILE:CG2	2.99	0.41
1:J:513:LEU:HD23	1:J:516:MET:HE3	2.03	0.41
1:J:59:TYR:CE2	1:J:591:PRO:HD3	2.56	0.41
1:J:622:ARG:O	1:J:626:VAL:HG23	2.20	0.41
1:A:403:ASN:O	1:A:403:ASN:OD1	2.39	0.41
1:A:59:TYR:CE2	1:A:591:PRO:HD3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:ILE:HD12	1:A:82:ILE:N	2.36	0.41
1:B:547:THR:HG23	1:B:550:VAL:HG23	2.02	0.41
1:B:721:ASP:HA	1:B:722:GLU:HA	1.56	0.41
1:C:51:SER:HB2	1:C:57:ARG:H	1.85	0.41
1:C:627:SER:HB3	1:C:726:ILE:CD1	2.51	0.41
1:D:408:TYR:CB	1:D:425:ILE:HG23	2.50	0.41
1:D:504:ILE:CG1	1:D:510:VAL:HG21	2.43	0.41
1:E:418:VAL:HA	1:F:141:ASN:HD21	1.84	0.41
1:E:638:TYR:CE1	1:E:647:VAL:HG11	2.56	0.41
1:E:68:ARG:HG3	1:E:165:ALA:CB	2.50	0.41
1:F:547:THR:CG2	1:F:550:VAL:HG23	2.51	0.41
1:G:480:PRO:HB2	1:G:510:VAL:HG22	2.03	0.41
1:G:547:THR:CG2	1:G:550:VAL:HG23	2.51	0.41
1:H:403:ASN:OD1	1:H:403:ASN:O	2.39	0.41
1:H:425:ILE:HD12	1:H:593:LEU:HD22	2.01	0.41
1:H:514:LEU:HD23	1:H:514:LEU:HA	1.91	0.41
1:A:306:TRP:HA	1:A:306:TRP:CE3	2.56	0.41
1:A:374:GLY:CA	1:A:376:GLY:H	2.34	0.41
1:A:414:PRO:HG3	1:B:93:PHE:HD1	1.86	0.41
1:C:261:VAL:HG13	1:C:316:TRP:HH2	1.85	0.41
1:C:596:ARG:HB2	1:C:601:TYR:HE1	1.86	0.41
1:C:146:GLU:CD	1:C:604:LYS:HZ1	2.22	0.41
1:C:777:PHE:HA	1:C:780:ILE:HD12	2.02	0.41
1:D:493:MET:HG3	1:D:493:MET:O	2.20	0.41
1:D:51:SER:HB2	1:D:57:ARG:H	1.84	0.41
1:D:596:ARG:HB2	1:D:601:TYR:HE1	1.85	0.41
1:F:480:PRO:HD2	1:F:567:LEU:HD22	2.02	0.41
1:G:408:TYR:CB	1:G:425:ILE:HG23	2.50	0.41
1:G:464:ARG:HD3	1:G:469:GLU:OE2	2.21	0.41
1:G:82:ILE:N	1:G:82:ILE:HD12	2.35	0.41
1:H:270:VAL:HG22	1:H:321:ASN:HD21	1.81	0.41
1:H:777:PHE:HA	1:H:780:ILE:HD12	2.03	0.41
1:H:414:PRO:HG3	1:I:93:PHE:HD1	1.86	0.41
1:J:504:ILE:CG1	1:J:510:VAL:HG21	2.43	0.41
1:J:547:THR:HG23	1:J:550:VAL:HG23	2.02	0.41
1:J:627:SER:HB3	1:J:726:ILE:CD1	2.51	0.41
1:A:91:CYS:SG	1:A:245:ILE:HD11	2.61	0.41
1:B:40:ALA:CB	1:B:192:PRO:HG3	2.51	0.41
1:B:480:PRO:HD2	1:B:567:LEU:HD22	2.03	0.41
1:B:643:GLY:HA3	1:B:644:GLY:HA2	1.84	0.41
1:C:101:ARG:HA	1:C:231:SER:HB3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:273:PRO:CB	1:D:276:TYR:CD2	2.96	0.41
1:D:547:THR:CG2	1:D:550:VAL:HG23	2.51	0.41
1:D:622:ARG:O	1:D:626:VAL:HG23	2.20	0.41
1:F:91:CYS:SG	1:F:245:ILE:HD11	2.61	0.41
1:F:596:ARG:HB2	1:F:601:TYR:HE1	1.86	0.41
1:F:638:TYR:CE1	1:F:647:VAL:HG11	2.56	0.41
1:G:627:SER:HB3	1:G:726:ILE:CD1	2.51	0.41
1:H:464:ARG:HD3	1:H:469:GLU:OE2	2.21	0.41
1:I:208:SER:OG	1:I:209:GLU:N	2.54	0.41
1:I:638:TYR:CE1	1:I:647:VAL:HG11	2.56	0.41
1:J:403:ASN:O	1:J:403:ASN:OD1	2.38	0.41
1:J:446:LEU:CD2	1:J:487:VAL:HG11	2.50	0.41
1:J:480:PRO:HB2	1:J:510:VAL:HG22	2.03	0.41
1:J:514:LEU:HA	1:J:514:LEU:HD23	1.91	0.41
1:J:579:THR:HB	1:J:580:PRO:HD2	2.02	0.41
1:J:777:PHE:HA	1:J:780:ILE:HD12	2.02	0.41
1:A:408:TYR:CB	1:A:425:ILE:CG2	2.99	0.41
1:A:514:LEU:HD23	1:A:514:LEU:HA	1.91	0.41
1:B:120:SER:HB3	1:B:222:ASP:HA	2.03	0.41
1:B:627:SER:HB3	1:B:726:ILE:CD1	2.51	0.41
1:D:480:PRO:HB2	1:D:510:VAL:HG22	2.03	0.41
1:G:192:PRO:HB2	1:G:364:VAL:HG22	2.02	0.41
1:G:40:ALA:CB	1:G:192:PRO:HG3	2.51	0.41
1:H:91:CYS:SG	1:H:245:ILE:HD11	2.61	0.41
1:J:374:GLY:CA	1:J:376:GLY:H	2.34	0.41
1:J:547:THR:CG2	1:J:550:VAL:HG23	2.51	0.41
1:A:480:PRO:HD2	1:A:567:LEU:HD22	2.03	0.40
1:A:547:THR:CG2	1:A:550:VAL:HG23	2.51	0.40
1:B:464:ARG:HD3	1:B:469:GLU:OE2	2.22	0.40
1:B:596:ARG:HB2	1:B:601:TYR:HE1	1.86	0.40
1:C:403:ASN:OD1	1:C:403:ASN:O	2.38	0.40
1:C:540:SER:HA	1:C:541:ASN:HA	1.75	0.40
1:C:547:THR:HG23	1:C:550:VAL:HG23	2.02	0.40
1:E:408:TYR:CB	1:E:425:ILE:HG23	2.51	0.40
1:E:547:THR:HG23	1:E:550:VAL:HG23	2.02	0.40
1:E:579:THR:HB	1:E:580:PRO:HD2	2.03	0.40
1:F:374:GLY:HA2	1:F:376:GLY:H	1.85	0.40
1:F:51:SER:HB2	1:F:57:ARG:H	1.85	0.40
1:H:272:ALA:N	1:H:273:PRO:HD3	2.34	0.40
1:H:480:PRO:HB2	1:H:510:VAL:HG22	2.03	0.40
1:H:627:SER:HB3	1:H:726:ILE:CD1	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:68:ARG:HG3	1:I:165:ALA:CB	2.50	0.40
1:I:374:GLY:CA	1:I:376:GLY:H	2.34	0.40
1:I:425:ILE:O	1:I:596:ARG:HG3	2.21	0.40
1:A:108:MET:HA	1:B:114:PRO:CG	2.50	0.40
1:B:651:ILE:HG23	1:B:746:THR:HG22	2.04	0.40
1:D:514:LEU:HD23	1:D:514:LEU:HA	1.91	0.40
1:D:579:THR:HB	1:D:580:PRO:HD2	2.02	0.40
1:D:425:ILE:HD12	1:D:593:LEU:HD22	2.02	0.40
1:E:464:ARG:HD3	1:E:469:GLU:OE2	2.22	0.40
1:E:635:ARG:HE	1:E:637:LEU:HD21	1.86	0.40
1:G:493:MET:HG3	1:G:493:MET:O	2.20	0.40
1:G:651:ILE:HG23	1:G:746:THR:HG22	2.03	0.40
1:I:596:ARG:HB2	1:I:601:TYR:HE1	1.87	0.40
1:I:618:LYS:HB2	1:I:621:ASP:HB3	2.04	0.40
1:I:635:ARG:HE	1:I:637:LEU:HD21	1.86	0.40
1:J:306:TRP:CE3	1:J:306:TRP:HA	2.56	0.40
1:J:464:ARG:HD3	1:J:469:GLU:OE2	2.21	0.40
1:A:408:TYR:CB	1:A:425:ILE:HG23	2.51	0.40
1:A:618:LYS:HB2	1:A:621:ASP:HB3	2.03	0.40
1:B:273:PRO:CB	1:B:276:TYR:CD2	2.99	0.40
1:B:192:PRO:HB2	1:B:364:VAL:HG22	2.03	0.40
1:C:306:TRP:CE3	1:C:306:TRP:HA	2.56	0.40
1:E:120:SER:HB3	1:E:222:ASP:HA	2.04	0.40
1:E:480:PRO:HD2	1:E:567:LEU:HD22	2.03	0.40
1:E:618:LYS:HB2	1:E:621:ASP:HB3	2.03	0.40
1:F:59:TYR:CE2	1:F:591:PRO:HD3	2.56	0.40
1:F:618:LYS:HB2	1:F:621:ASP:HB3	2.04	0.40
1:F:651:ILE:HG23	1:F:746:THR:HG22	2.03	0.40
1:H:547:THR:HG23	1:H:550:VAL:HG23	2.02	0.40
1:I:403:ASN:O	1:I:403:ASN:OD1	2.38	0.40
1:A:120:SER:HB3	1:A:222:ASP:HA	2.04	0.40
1:B:425:ILE:O	1:B:596:ARG:HG3	2.21	0.40
1:C:425:ILE:O	1:C:596:ARG:HG3	2.21	0.40
1:C:638:TYR:CE1	1:C:647:VAL:HG11	2.56	0.40
1:E:547:THR:CG2	1:E:550:VAL:HG23	2.51	0.40
1:G:272:ALA:N	1:G:273:PRO:HD3	2.34	0.40
1:G:306:TRP:HA	1:G:306:TRP:CE3	2.56	0.40
1:G:596:ARG:HB2	1:G:601:TYR:HE1	1.86	0.40
1:H:374:GLY:CA	1:H:376:GLY:H	2.34	0.40
1:J:425:ILE:O	1:J:596:ARG:HG3	2.21	0.40
1:J:641:ARG:NH1	1:J:774:ASP:HA	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:638:TYR:CE1	1:J:647:VAL:HG11	2.55	0.40
1:A:425:ILE:O	1:A:596:ARG:HG3	2.21	0.40
1:A:627:SER:HB3	1:A:726:ILE:CD1	2.51	0.40
1:A:651:ILE:HG23	1:A:746:THR:HG22	2.03	0.40
1:A:641:ARG:NH1	1:A:774:ASP:HA	2.36	0.40
1:B:23:VAL:HG21	1:B:32:PHE:CB	2.36	0.40
1:B:306:TRP:CE3	1:B:306:TRP:HA	2.57	0.40
1:B:480:PRO:HB2	1:B:510:VAL:HG22	2.03	0.40
1:C:493:MET:HG3	1:C:493:MET:O	2.20	0.40
1:C:641:ARG:NH1	1:C:774:ASP:HA	2.37	0.40
1:E:190:LEU:CD2	1:E:290:ASN:ND2	2.85	0.40
1:E:461:LEU:HD23	1:E:485:LEU:CD2	2.52	0.40
1:F:272:ALA:N	1:F:273:PRO:HD3	2.34	0.40
1:G:638:TYR:CE1	1:G:647:VAL:HG11	2.56	0.40
1:H:579:THR:HB	1:H:580:PRO:HD2	2.03	0.40
1:I:190:LEU:CD2	1:I:290:ASN:ND2	2.84	0.40
1:I:547:THR:HG23	1:I:550:VAL:HG23	2.02	0.40
1:D:121:TRP:CE3	1:J:226:PRO:HG3	2.56	0.40
1:J:618:LYS:HB2	1:J:621:ASP:HB3	2.03	0.40
1:J:91:CYS:SG	1:J:245:ILE:HD11	2.61	0.40

All (6) 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:219:GLU:OE1	1:H:219:GLU:OE2[6_476]	1.30	0.90
1:D:219:GLU:OE1	1:H:219:GLU:CD[6_476]	1.35	0.85
1:D:219:GLU:OE1	1:H:219:GLU:OE1[6_476]	1.40	0.80
1:D:219:GLU:OE2	1:H:219:GLU:OE1[6_476]	1.40	0.80
1:D:219:GLU:CD	1:H:219:GLU:OE1[6_476]	1.43	0.77
1:D:219:GLU:CD	1:H:219:GLU:CD[6_476]	1.93	0.27

## 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	745/792 (94%)	712 (96%)	33 (4%)	0	100	100
1	B	745/792 (94%)	711 (95%)	34 (5%)	0	100	100
1	C	745/792 (94%)	712 (96%)	33 (4%)	0	100	100
1	D	745/792 (94%)	712 (96%)	33 (4%)	0	100	100
1	E	745/792 (94%)	712 (96%)	33 (4%)	0	100	100
1	F	745/792 (94%)	712 (96%)	33 (4%)	0	100	100
1	G	745/792 (94%)	712 (96%)	33 (4%)	0	100	100
1	H	745/792 (94%)	712 (96%)	33 (4%)	0	100	100
1	I	745/792 (94%)	712 (96%)	33 (4%)	0	100	100
1	J	745/792 (94%)	712 (96%)	33 (4%)	0	100	100
All	All	7450/7920 (94%)	7119 (96%)	331 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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	622/663 (94%)	611 (98%)	11 (2%)	59	77
1	B	622/663 (94%)	611 (98%)	11 (2%)	59	77
1	C	622/663 (94%)	611 (98%)	11 (2%)	59	77
1	D	622/663 (94%)	611 (98%)	11 (2%)	59	77
1	E	622/663 (94%)	611 (98%)	11 (2%)	59	77
1	F	622/663 (94%)	611 (98%)	11 (2%)	59	77
1	G	622/663 (94%)	611 (98%)	11 (2%)	59	77
1	H	622/663 (94%)	611 (98%)	11 (2%)	59	77
1	I	622/663 (94%)	611 (98%)	11 (2%)	59	77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	J	622/663 (94%)	611 (98%)	11 (2%)	59	77
All	All	6220/6630 (94%)	6110 (98%)	110 (2%)	59	77

All (110) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	189	TYR
1	A	306	TRP
1	A	372	TYR
1	A	429	ARG
1	A	461	LEU
1	A	483	SER
1	A	672	TYR
1	A	715	LEU
1	A	724	THR
1	A	733	VAL
1	A	774	ASP
1	B	189	TYR
1	B	306	TRP
1	B	372	TYR
1	B	429	ARG
1	B	461	LEU
1	B	483	SER
1	B	672	TYR
1	B	715	LEU
1	B	724	THR
1	B	733	VAL
1	B	774	ASP
1	C	189	TYR
1	C	306	TRP
1	C	372	TYR
1	C	429	ARG
1	C	461	LEU
1	C	483	SER
1	C	672	TYR
1	C	715	LEU
1	C	724	THR
1	C	733	VAL
1	C	774	ASP
1	D	189	TYR
1	D	306	TRP
1	D	372	TYR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	D	429	ARG
1	D	461	LEU
1	D	483	SER
1	D	672	TYR
1	D	715	LEU
1	D	724	THR
1	D	733	VAL
1	D	774	ASP
1	E	189	TYR
1	E	306	TRP
1	E	372	TYR
1	E	429	ARG
1	E	461	LEU
1	E	483	SER
1	E	672	TYR
1	E	715	LEU
1	E	724	THR
1	E	733	VAL
1	E	774	ASP
1	F	189	TYR
1	F	306	TRP
1	F	372	TYR
1	F	429	ARG
1	F	461	LEU
1	F	483	SER
1	F	672	TYR
1	F	715	LEU
1	F	724	THR
1	F	733	VAL
1	F	774	ASP
1	G	189	TYR
1	G	306	TRP
1	G	372	TYR
1	G	429	ARG
1	G	461	LEU
1	G	483	SER
1	G	672	TYR
1	G	715	LEU
1	G	724	THR
1	G	733	VAL
1	G	774	ASP
1	H	189	TYR

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Mol	Chain	Res	Type
1	H	306	TRP
1	H	372	TYR
1	H	429	ARG
1	H	461	LEU
1	H	483	SER
1	H	672	TYR
1	H	715	LEU
1	H	724	THR
1	H	733	VAL
1	H	774	ASP
1	I	189	TYR
1	I	306	TRP
1	I	372	TYR
1	I	429	ARG
1	I	461	LEU
1	I	483	SER
1	I	672	TYR
1	I	715	LEU
1	I	724	THR
1	I	733	VAL
1	I	774	ASP
1	J	189	TYR
1	J	306	TRP
1	J	372	TYR
1	J	429	ARG
1	J	461	LEU
1	J	483	SER
1	J	672	TYR
1	J	715	LEU
1	J	724	THR
1	J	733	VAL
1	J	774	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (73) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	130	ASN
1	A	141	ASN
1	A	148	GLN
1	A	169	HIS
1	A	288	ASN
1	A	549	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	741	GLN
1	B	130	ASN
1	B	141	ASN
1	B	148	GLN
1	B	169	HIS
1	B	249	ASN
1	B	288	ASN
1	B	549	GLN
1	B	741	GLN
1	C	130	ASN
1	C	141	ASN
1	C	148	GLN
1	C	169	HIS
1	C	288	ASN
1	C	549	GLN
1	C	741	GLN
1	D	130	ASN
1	D	141	ASN
1	D	148	GLN
1	D	169	HIS
1	D	288	ASN
1	D	741	GLN
1	E	130	ASN
1	E	141	ASN
1	E	148	GLN
1	E	169	HIS
1	E	249	ASN
1	E	288	ASN
1	E	549	GLN
1	E	741	GLN
1	F	130	ASN
1	F	141	ASN
1	F	148	GLN
1	F	169	HIS
1	F	288	ASN
1	F	549	GLN
1	F	729	GLN
1	F	741	GLN
1	F	775	ASN
1	G	130	ASN
1	G	141	ASN
1	G	148	GLN

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Mol	Chain	Res	Type
1	G	169	HIS
1	G	288	ASN
1	G	549	GLN
1	G	741	GLN
1	H	130	ASN
1	H	141	ASN
1	H	148	GLN
1	H	169	HIS
1	H	288	ASN
1	H	549	GLN
1	H	741	GLN
1	I	130	ASN
1	I	141	ASN
1	I	148	GLN
1	I	169	HIS
1	I	288	ASN
1	I	549	GLN
1	I	741	GLN
1	J	130	ASN
1	J	141	ASN
1	J	148	GLN
1	J	169	HIS
1	J	288	ASN
1	J	549	GLN
1	J	741	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	749/792 (94%)	-0.35	9 (1%) 79 69	85, 134, 194, 235	0
1	B	749/792 (94%)	-0.32	11 (1%) 73 63	79, 127, 189, 230	0
1	C	749/792 (94%)	-0.28	15 (2%) 65 53	86, 144, 202, 250	0
1	D	749/792 (94%)	-0.30	10 (1%) 77 67	88, 138, 198, 241	0
1	E	749/792 (94%)	-0.31	10 (1%) 77 67	86, 131, 189, 231	0
1	F	749/792 (94%)	-0.26	14 (1%) 66 55	88, 146, 206, 239	0
1	G	749/792 (94%)	-0.29	15 (2%) 65 53	85, 140, 199, 240	0
1	H	749/792 (94%)	-0.31	7 (0%) 84 76	83, 136, 199, 238	0
1	I	749/792 (94%)	-0.28	10 (1%) 77 67	86, 134, 199, 246	0
1	J	749/792 (94%)	-0.29	14 (1%) 66 55	87, 138, 199, 235	0
All	All	7490/7920 (94%)	-0.30	115 (1%) 73 63	79, 137, 198, 250	0

All (115) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	720	ARG	7.7
1	D	720	ARG	7.4
1	H	720	ARG	6.3
1	F	720	ARG	5.9
1	G	720	ARG	5.9
1	A	720	ARG	5.4
1	B	720	ARG	5.3
1	F	222	ASP	5.2
1	E	720	ARG	5.2
1	I	720	ARG	4.9
1	G	721	ASP	4.8
1	J	720	ARG	4.7
1	D	719	ARG	4.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	J	222	ASP	4.1
1	C	721	ASP	4.0
1	G	347	SER	3.9
1	I	222	ASP	3.8
1	G	719	ARG	3.8
1	F	716	ALA	3.7
1	C	716	ALA	3.7
1	E	348	ASP	3.7
1	A	719	ARG	3.6
1	F	721	ASP	3.6
1	H	721	ASP	3.6
1	D	721	ASP	3.6
1	C	719	ARG	3.5
1	E	542	GLY	3.5
1	G	716	ALA	3.4
1	C	222	ASP	3.4
1	E	716	ALA	3.4
1	C	347	SER	3.3
1	F	348	ASP	3.2
1	B	348	ASP	3.2
1	D	716	ALA	3.2
1	A	721	ASP	3.2
1	A	542	GLY	3.1
1	C	348	ASP	3.1
1	B	23	VAL	3.1
1	I	23	VAL	3.1
1	F	25	THR	3.1
1	F	309	ALA	3.1
1	A	25	THR	3.0
1	D	222	ASP	3.0
1	J	25	THR	3.0
1	A	347	SER	2.9
1	I	348	ASP	2.9
1	B	721	ASP	2.9
1	J	719	ARG	2.9
1	J	348	ASP	2.9
1	I	546	LEU	2.9
1	B	347	SER	2.8
1	G	323	ILE	2.8
1	F	719	ARG	2.8
1	A	24	ASP	2.8
1	B	222	ASP	2.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	G	348	ASP	2.8
1	I	719	ARG	2.8
1	F	23	VAL	2.8
1	J	721	ASP	2.7
1	E	721	ASP	2.7
1	C	323	ILE	2.7
1	F	28	GLY	2.6
1	F	24	ASP	2.6
1	B	542	GLY	2.6
1	J	347	SER	2.6
1	G	25	THR	2.6
1	I	790	LYS	2.5
1	G	543	ASP	2.5
1	F	347	SER	2.5
1	D	348	ASP	2.5
1	F	27	LYS	2.5
1	H	25	THR	2.5
1	B	716	ALA	2.5
1	E	272	ALA	2.5
1	D	325	ASP	2.5
1	E	541	ASN	2.5
1	J	384	LEU	2.5
1	J	24	ASP	2.5
1	G	309	ALA	2.5
1	E	543	ASP	2.4
1	I	347	SER	2.4
1	I	721	ASP	2.4
1	J	716	ALA	2.4
1	B	24	ASP	2.4
1	D	717	LEU	2.4
1	E	719	ARG	2.4
1	A	348	ASP	2.3
1	D	323	ILE	2.3
1	G	384	LEU	2.3
1	F	310	PHE	2.3
1	D	24	ASP	2.3
1	B	375	LEU	2.3
1	G	27	LYS	2.3
1	G	541	ASN	2.3
1	C	542	GLY	2.3
1	G	24	ASP	2.3
1	E	347	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	25	THR	2.3
1	A	324	ALA	2.3
1	J	27	LYS	2.2
1	G	222	ASP	2.2
1	B	25	THR	2.2
1	C	375	LEU	2.1
1	C	310	PHE	2.1
1	C	722	GLU	2.1
1	H	324	ALA	2.1
1	H	323	ILE	2.1
1	J	385	ASP	2.1
1	H	347	SER	2.1
1	J	323	ILE	2.1
1	J	28	GLY	2.1
1	I	786	LEU	2.0
1	H	719	ARG	2.0
1	C	24	ASP	2.0
1	C	325	ASP	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.