



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:30 PM UTC

PDB ID : 4E2S / pdb\_00004e2s  
Title : Crystal structure of (S)-Ureidoglycine Aminohydrolase from Arabidopsis thaliana in complex with its substrate, (S)-Ureidoglycine  
Authors : Shin, I.; Rhee, S.  
Deposited on : 2012-03-09  
Resolution : 2.59 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

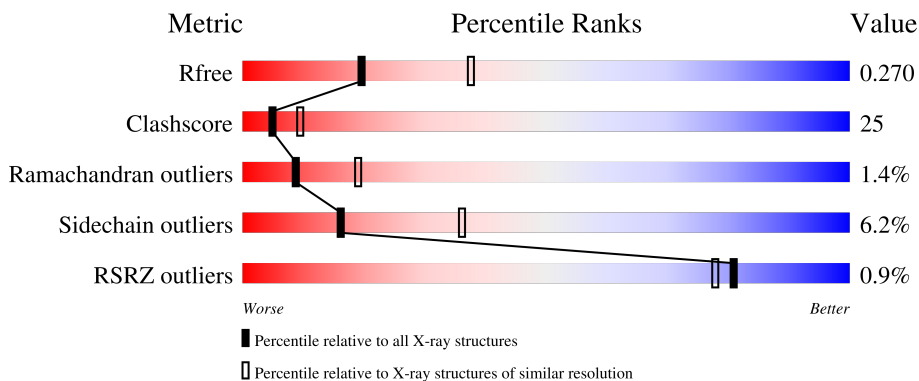
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.59 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))
$R_{free}$	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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 of 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	266	<div style="display: flex; align-items: center;"> <div style="width: 20px; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 100%; height: 20px; position: relative;"> <div style="width: 59%; height: 100%; background-color: green;"></div> <div style="width: 30%; height: 100%; background-color: yellow;"></div> <div style="width: 7%; height: 100%; background-color: orange;"></div> <div style="width: 4%; height: 100%; background-color: grey;"></div> </div> <div style="margin-left: 5px;">%</div> </div> <p style="text-align: center;">59% 30% 7% .</p>
1	B	266	<div style="width: 100%; height: 20px; position: relative;"> <div style="width: 57%; height: 100%; background-color: green;"></div> <div style="width: 35%; height: 100%; background-color: yellow;"></div> <div style="width: 8%; height: 100%; background-color: orange;"></div> <div style="width: 0%; height: 100%; background-color: red;"></div> <div style="width: 0%; height: 100%; background-color: grey;"></div> </div> <p style="text-align: center;">57% 35% . . .</p>
1	C	266	<div style="display: flex; align-items: center;"> <div style="width: 20px; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 100%; height: 20px; position: relative;"> <div style="width: 54%; height: 100%; background-color: green;"></div> <div style="width: 40%; height: 100%; background-color: yellow;"></div> <div style="width: 6%; height: 100%; background-color: orange;"></div> <div style="width: 0%; height: 100%; background-color: red;"></div> <div style="width: 0%; height: 100%; background-color: grey;"></div> </div> <div style="margin-left: 5px;">2%</div> </div> <p style="text-align: center;">54% 40% . .</p>
1	D	266	<div style="width: 100%; height: 20px; position: relative;"> <div style="width: 54%; height: 100%; background-color: green;"></div> <div style="width: 35%; height: 100%; background-color: yellow;"></div> <div style="width: 7%; height: 100%; background-color: orange;"></div> <div style="width: 4%; height: 100%; background-color: grey;"></div> </div> <p style="text-align: center;">54% 35% 7% .</p>
1	E	266	<div style="display: flex; align-items: center;"> <div style="width: 20px; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 100%; height: 20px; position: relative;"> <div style="width: 51%; height: 100%; background-color: green;"></div> <div style="width: 39%; height: 100%; background-color: yellow;"></div> <div style="width: 6%; height: 100%; background-color: orange;"></div> <div style="width: 4%; height: 100%; background-color: grey;"></div> </div> <div style="margin-left: 5px;">%</div> </div> <p style="text-align: center;">51% 39% 6% . .</p>

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Mol	Chain	Length	Quality of chain
1	F	266	 52% 41% . .
1	G	266	%  48% 43% 5% .
1	H	266	%  55% 37% 5% .
1	I	266	 56% 36% . .
1	J	266	 48% 44% 5% .
1	K	266	%  40% 51% 6% . .
1	L	266	%  53% 40% . .
1	M	266	 47% 46% . .
1	N	266	%  56% 36% 5% .
1	O	266	%  52% 41% . .
1	P	266	2%  45% 45% 6% .

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 33974 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 Ureidoglycine aminohydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	258	2076	1345	342	382	7	0	0	0
1	B	258	2076	1345	342	382	7	0	0	0
1	C	258	2076	1345	342	382	7	0	0	0
1	D	258	2076	1345	342	382	7	0	0	0
1	E	258	2076	1345	342	382	7	0	0	0
1	F	258	2076	1345	342	382	7	0	0	0
1	G	258	2076	1345	342	382	7	0	0	0
1	H	258	2076	1345	342	382	7	0	0	0
1	I	258	2076	1345	342	382	7	0	0	0
1	J	258	2076	1345	342	382	7	0	0	0
1	K	258	2076	1345	342	382	7	0	0	0
1	L	258	2076	1345	342	382	7	0	0	0
1	M	258	2076	1345	342	382	7	0	0	0
1	N	258	2076	1345	342	382	7	0	0	0
1	O	258	2076	1345	342	382	7	0	0	0
1	P	258	2076	1345	342	382	7	0	0	0

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	33	GLY	-	expression tag	UNP Q8GXXV5
A	34	HIS	-	expression tag	UNP Q8GXXV5
A	35	MET	-	expression tag	UNP Q8GXXV5
B	33	GLY	-	expression tag	UNP Q8GXXV5
B	34	HIS	-	expression tag	UNP Q8GXXV5
B	35	MET	-	expression tag	UNP Q8GXXV5
C	33	GLY	-	expression tag	UNP Q8GXXV5
C	34	HIS	-	expression tag	UNP Q8GXXV5
C	35	MET	-	expression tag	UNP Q8GXXV5
D	33	GLY	-	expression tag	UNP Q8GXXV5
D	34	HIS	-	expression tag	UNP Q8GXXV5
D	35	MET	-	expression tag	UNP Q8GXXV5
E	33	GLY	-	expression tag	UNP Q8GXXV5
E	34	HIS	-	expression tag	UNP Q8GXXV5
E	35	MET	-	expression tag	UNP Q8GXXV5
F	33	GLY	-	expression tag	UNP Q8GXXV5
F	34	HIS	-	expression tag	UNP Q8GXXV5
F	35	MET	-	expression tag	UNP Q8GXXV5
G	33	GLY	-	expression tag	UNP Q8GXXV5
G	34	HIS	-	expression tag	UNP Q8GXXV5
G	35	MET	-	expression tag	UNP Q8GXXV5
H	33	GLY	-	expression tag	UNP Q8GXXV5
H	34	HIS	-	expression tag	UNP Q8GXXV5
H	35	MET	-	expression tag	UNP Q8GXXV5
I	33	GLY	-	expression tag	UNP Q8GXXV5
I	34	HIS	-	expression tag	UNP Q8GXXV5
I	35	MET	-	expression tag	UNP Q8GXXV5
J	33	GLY	-	expression tag	UNP Q8GXXV5
J	34	HIS	-	expression tag	UNP Q8GXXV5
J	35	MET	-	expression tag	UNP Q8GXXV5
K	33	GLY	-	expression tag	UNP Q8GXXV5
K	34	HIS	-	expression tag	UNP Q8GXXV5
K	35	MET	-	expression tag	UNP Q8GXXV5
L	33	GLY	-	expression tag	UNP Q8GXXV5
L	34	HIS	-	expression tag	UNP Q8GXXV5
L	35	MET	-	expression tag	UNP Q8GXXV5
M	33	GLY	-	expression tag	UNP Q8GXXV5
M	34	HIS	-	expression tag	UNP Q8GXXV5
M	35	MET	-	expression tag	UNP Q8GXXV5
N	33	GLY	-	expression tag	UNP Q8GXXV5
N	34	HIS	-	expression tag	UNP Q8GXXV5
N	35	MET	-	expression tag	UNP Q8GXXV5

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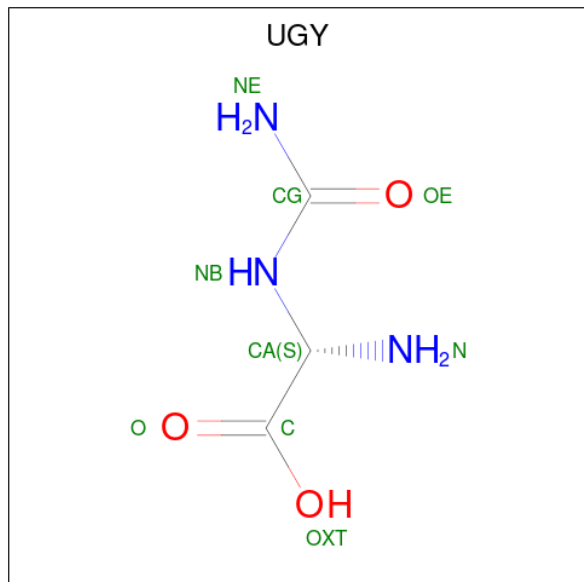
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Chain	Residue	Modelled	Actual	Comment	Reference
O	33	GLY	-	expression tag	UNP Q8GXXV5
O	34	HIS	-	expression tag	UNP Q8GXXV5
O	35	MET	-	expression tag	UNP Q8GXXV5
P	33	GLY	-	expression tag	UNP Q8GXXV5
P	34	HIS	-	expression tag	UNP Q8GXXV5
P	35	MET	-	expression tag	UNP Q8GXXV5

- Molecule 2 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Mn 1 1	0	0
2	B	1	Total Mn 1 1	0	0
2	C	1	Total Mn 1 1	0	0
2	D	1	Total Mn 1 1	0	0
2	E	1	Total Mn 1 1	0	0
2	F	1	Total Mn 1 1	0	0
2	G	1	Total Mn 1 1	0	0
2	H	1	Total Mn 1 1	0	0
2	I	1	Total Mn 1 1	0	0
2	J	1	Total Mn 1 1	0	0
2	K	1	Total Mn 1 1	0	0
2	L	1	Total Mn 1 1	0	0
2	M	1	Total Mn 1 1	0	0
2	N	1	Total Mn 1 1	0	0
2	O	1	Total Mn 1 1	0	0
2	P	1	Total Mn 1 1	0	0

- Molecule 3 is (2S)-amino(carbamoylamino)ethanoic acid (CCD ID: UGY) (formula:  $C_3H_7N_3O_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	Total 9	C 3	N 3	O 3	0	0
3	B	1	Total 9	C 3	N 3	O 3	0	0
3	C	1	Total 9	C 3	N 3	O 3	0	0
3	D	1	Total 9	C 3	N 3	O 3	0	0
3	E	1	Total 9	C 3	N 3	O 3	0	0
3	F	1	Total 9	C 3	N 3	O 3	0	0
3	G	1	Total 9	C 3	N 3	O 3	0	0
3	H	1	Total 9	C 3	N 3	O 3	0	0
3	I	1	Total 9	C 3	N 3	O 3	0	0
3	J	1	Total 9	C 3	N 3	O 3	0	0
3	K	1	Total 9	C 3	N 3	O 3	0	0
3	L	1	Total 9	C 3	N 3	O 3	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	M	1	Total	C	N	O	0	0
			9	3	3	3		
3	N	1	Total	C	N	O	0	0
			9	3	3	3		
3	O	1	Total	C	N	O	0	0
			9	3	3	3		
3	P	1	Total	C	N	O	0	0
			9	3	3	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	54	Total	O	0	0
			54	54		
4	B	41	Total	O	0	0
			41	41		
4	C	40	Total	O	0	0
			40	40		
4	D	35	Total	O	0	0
			35	35		
4	E	38	Total	O	0	0
			38	38		
4	F	42	Total	O	0	0
			42	42		
4	G	38	Total	O	0	0
			38	38		
4	H	36	Total	O	0	0
			36	36		
4	I	38	Total	O	0	0
			38	38		
4	J	30	Total	O	0	0
			30	30		
4	K	34	Total	O	0	0
			34	34		
4	L	30	Total	O	0	0
			30	30		
4	M	40	Total	O	0	0
			40	40		
4	N	35	Total	O	0	0
			35	35		
4	O	38	Total	O	0	0
			38	38		

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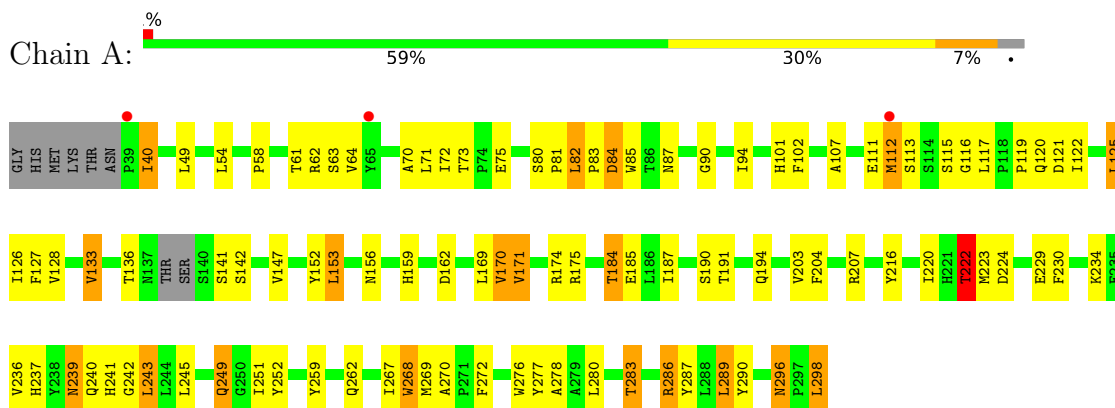
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
4	P	29	Total	O	0	0
			29	29		

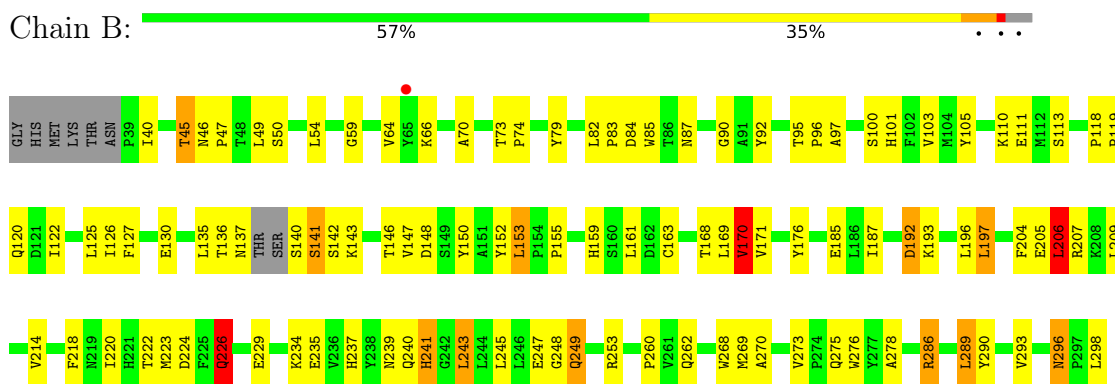
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

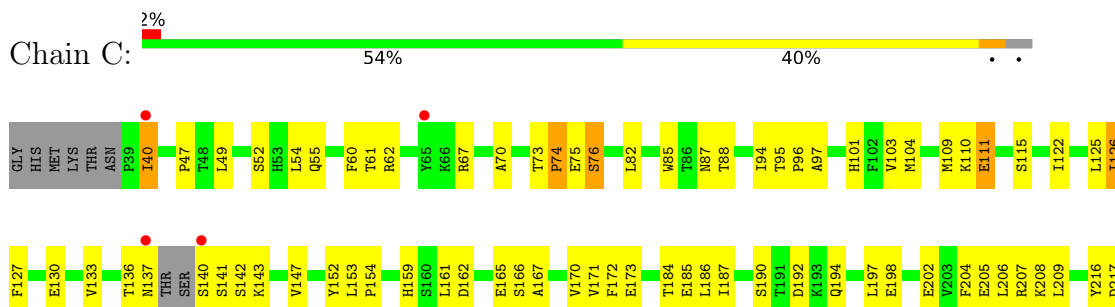
- Molecule 1: Ureidoglycine aminohydrolase

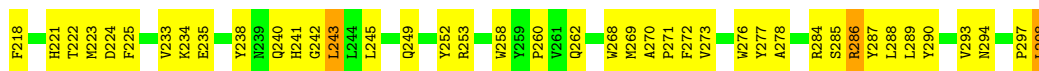


- Molecule 1: Ureidoglycine aminohydrolase

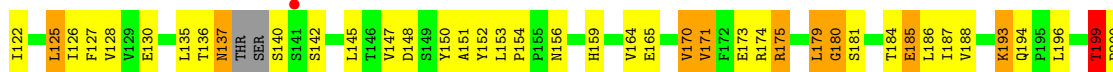


- Molecule 1: Ureidoglycine aminohydrolase

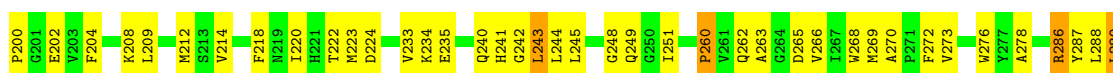
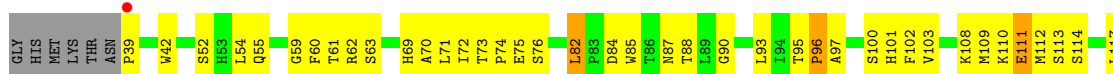




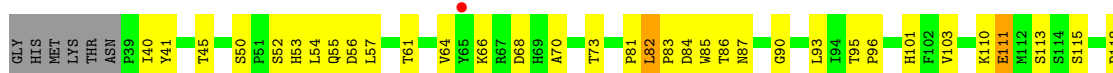
• Molecule 1: Ureidoglycine aminohydrolase



• Molecule 1: Ureidoglycine aminohydrolase



• Molecule 1: Ureidoglycine aminohydrolase



L289  
Y290  
N296  
P297  
L298

• Molecule 1: Ureidoglycine aminohydrolase

Chain G: 48% 43% 5%

GLY  
HIS  
MET  
LYS  
THR  
ASN  
P39  
L40  
T45  
N46  
L49  
S50  
H53  
L57  
F60  
T61  
R62  
S63  
V64  
V65  
K66  
R67  
D68  
R69  
A70  
L71  
I72  
I73  
P74  
Y79  
S80  
P81  
L82  
W85  
T86  
N87  
A91  
Y92  
L93  
I94  
T95  
P96  
S100  
H101  
F102  
L103  
M104  
Y105  
K108  
M109

K110  
E111  
M112  
S113  
S114  
S115  
G116  
L117  
P118  
P119  
Q120  
D121  
I122  
L125  
V126  
F127  
E130  
V133  
T134  
L135  
T136  
N137  
THR  
SER  
S140  
S141  
D142  
A143  
V147  
Y150  
A151  
Y152  
L153  
P154  
P155  
N156  
G157  
H158  
H159  
S160  
L161  
D162  
C163  
V164  
E165  
S166  
S100  
Q240  
H101  
T168  
L169  
F102  
V170  
M104  
V171  
R175  
Y176

G180  
T184  
I187  
T191  
L196  
L197  
E198  
P199  
D200  
G201  
E202  
V203  
F204  
E205  
L206  
R207  
K208  
L209  
L210  
P211  
N212  
S213  
V214  
D215  
Y216  
D217  
F218  
N219  
L220  
H221  
M223  
D224  
E225  
Q226  
Q227  
G228  
E229  
N232  
V233  
K234  
E235  
V236  
H237  
Y238  
M239  
Q240  
H241  
L243  
L246  
Q249

Y252  
Y259  
P260  
V261  
V266  
I267  
W268  
M269  
A270  
V273  
Y277  
T283  
R284  
S285  
R286  
L288  
L289  
Y290  
M294  
L298

• Molecule 1: Ureidoglycine aminohydrolase

Chain H: 55% 37% 5%

GLY  
HIS  
MET  
LYS  
THR  
ASN  
P39  
L40  
Y41  
W42  
K43  
T48  
L49  
D56  
L57  
P58  
G59  
R62  
S63  
V64  
Y65  
L71  
I72  
T73  
P74  
E75  
S76  
Y79  
S80  
L82  
P83  
D84  
W85  
T86  
N87  
L89  
G90  
A91  
Y92  
L93  
I94  
E105  
F102  
V103  
Y105  
K110  
E111  
M112  
S113  
Q120

D121  
L125  
I126  
V129  
A132  
V133  
T136  
N137  
THR  
SER  
S141  
K144  
Y150  
A151  
Y152  
L153  
H159  
S160  
L161  
D162  
C163  
V164  
V170  
V171  
T184  
E185  
L186  
I187  
V188  
P189  
L196  
L197  
E202  
V203  
F204  
E205  
L206  
R207  
K208  
L209  
L210  
P211  
N212  
S213  
V214  
A215  
Y216

H221  
T222  
M223  
D224  
V233  
K234  
E235  
H237  
V238  
N239  
Q240  
H241  
G242  
L243  
L244  
L245  
L246  
E247  
Q248  
Q249  
G250  
R253  
Q252  
V266  
I267  
W268  
M269  
P271  
F272  
D273  
V274  
Q275  
W276  
Y277  
A278  
R286  
Y287  
L288  
L289  
Y290  
K291  
D292  
V293  
N296  
P297  
L298

• Molecule 1: Ureidoglycine aminohydrolase

Chain I: 56% 36%

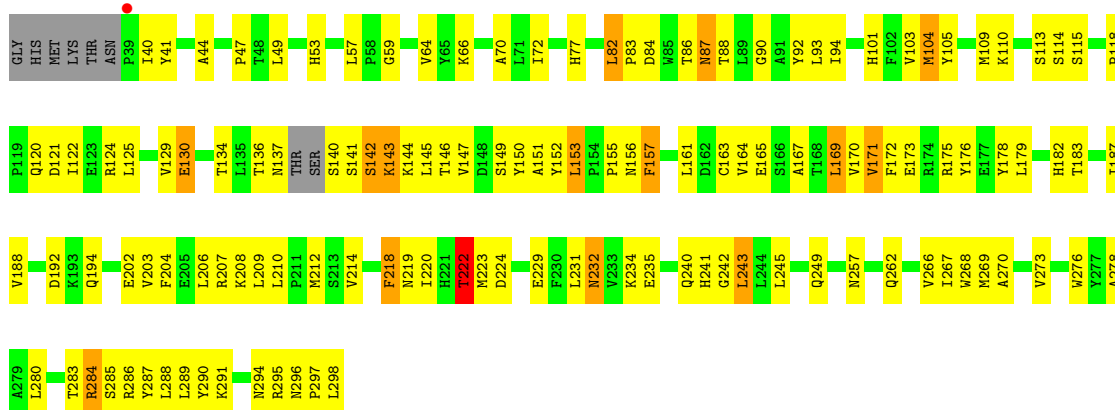
GLY  
HIS  
MET  
LYS  
THR  
ASN  
P39  
W42  
T45  
T48  
L49  
Q55  
D56  
L57  
F60  
T61  
R62  
A70  
L71  
I72  
I73  
S76  
H77  
V78  
L82  
P83  
W85  
G90  
L93  
T95  
P96  
A97  
T98  
H101  
F102  
V103  
M104  
Y105  
L106  
M109  
K110  
E111  
M112  
S113  
P118

P119  
Q120  
I122  
L125  
I126  
V129  
E130  
V133  
T134  
M137  
SER  
S140  
SER  
S140  
S141  
S142  
K143  
K144  
L145  
T146  
V147  
D148  
S149  
Y150  
A151  
Y152  
L153  
P154  
M156  
H159  
C163  
V164  
E165  
S166  
A167  
V170  
V171  
T184  
E185  
L186  
I187  
S190  
T191  
D192  
K193  
T199  
E202  
V203

F204  
K207  
K208  
L209  
L210  
Y216  
D217  
F218  
N219  
T222  
M223  
D224  
F225  
L231  
E235  
Q240  
H241  
G242  
L243  
L244  
Q249  
Y252  
R253  
Q262  
A263  
V266  
I267  
M268  
M269  
F272  
Y277  
A278  
A279  
L280  
R284  
S285  
R286  
Y287  
L288  
L289  
N296  
P297  
L298

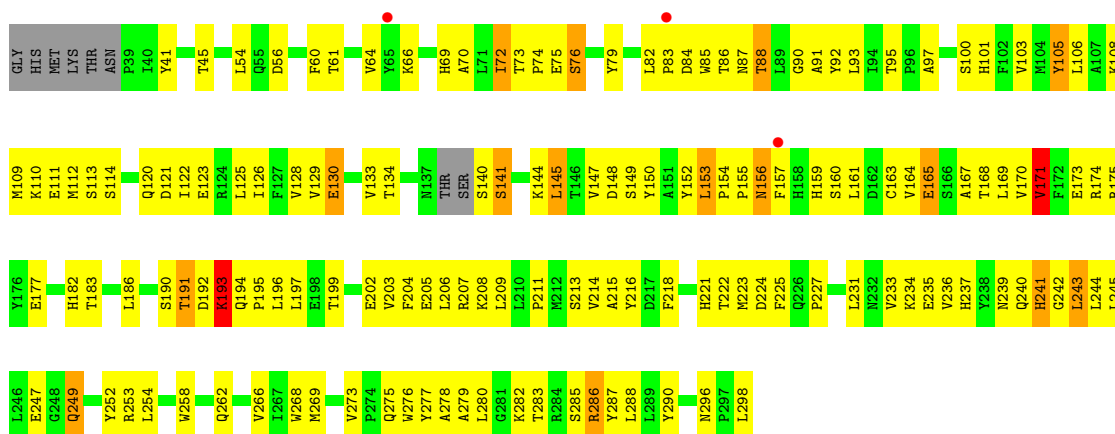
• Molecule 1: Ureidoglycine aminohydrolase

Chain J:  48% 44% 5% .



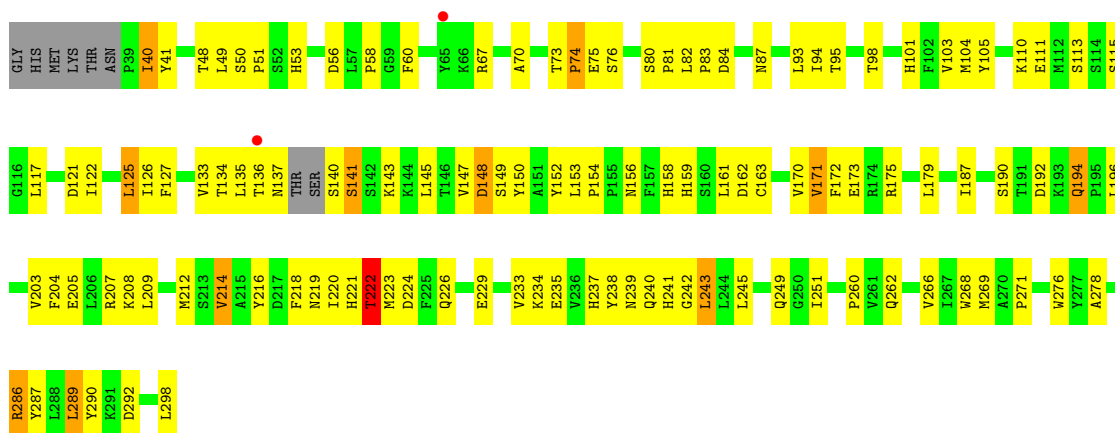
• Molecule 1: Ureidoglycine aminohydrolase

Chain K:  40% 51% 6% . .

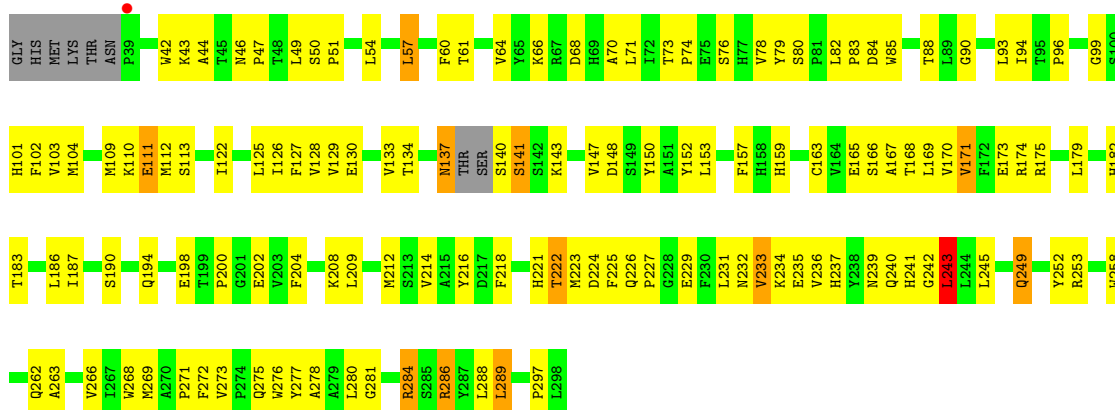


• Molecule 1: Ureidoglycine aminohydrolase

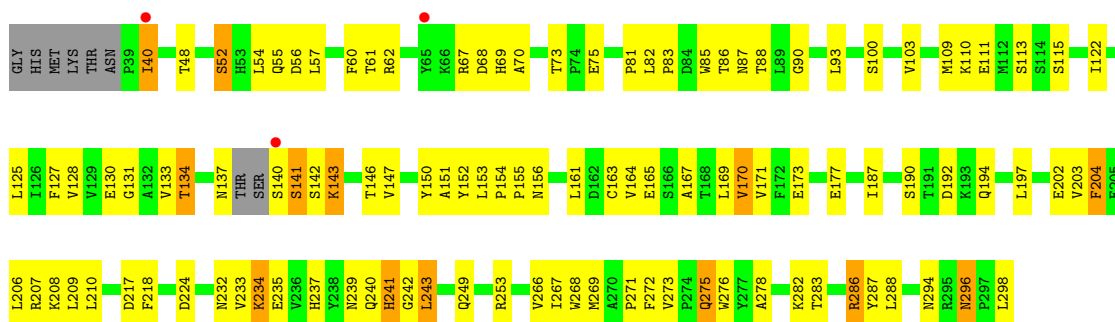
Chain L:  53% 40% . .



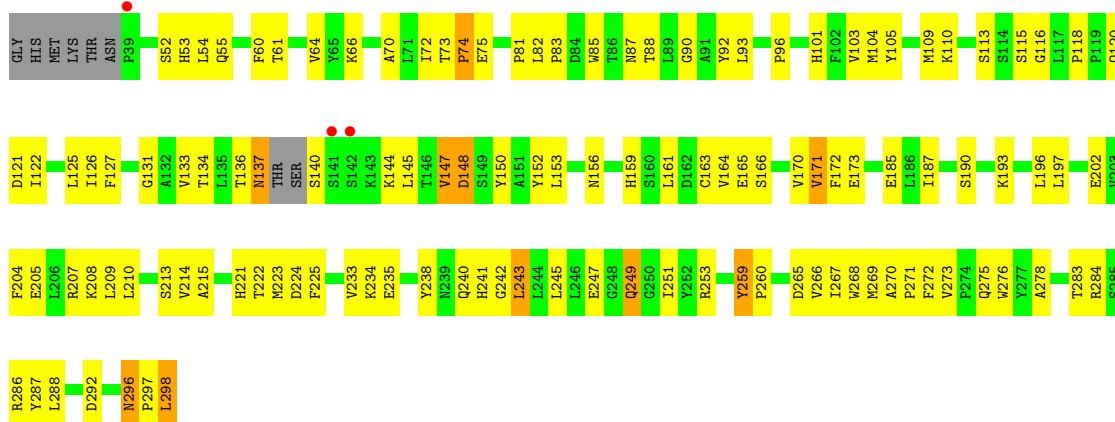
• Molecule 1: Ureidoglycine aminohydrolase

Chain M: 

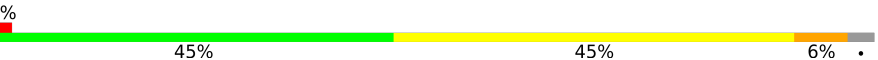
● Molecule 1: Ureidoglycine aminohydrolase

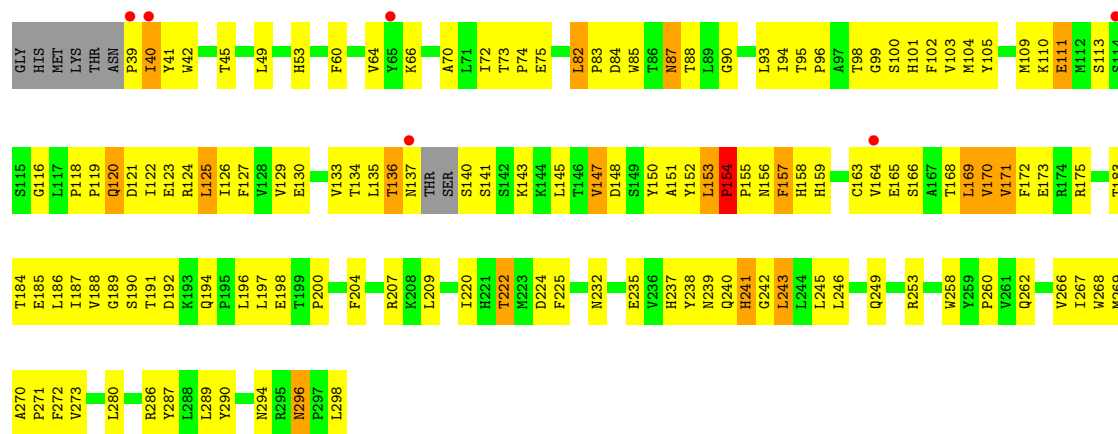
Chain N: 

● Molecule 1: Ureidoglycine aminohydrolase

Chain O: 

● Molecule 1: Ureidoglycine aminohydrolase

Chain P: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	93.10Å 174.89Å 154.30Å 90.00° 99.26° 90.00°	Depositor
Resolution (Å)	50.00 – 2.59 50.00 – 2.59	Depositor EDS
% Data completeness (in resolution range)	93.3 (50.00-2.59) 93.5 (50.00-2.59)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.27 (at 2.58Å)	Xtrriage
Refinement program	CNS 1.21	Depositor
R, $R_{free}$	0.209 , 0.271 0.208 , 0.270	Depositor DCC
$R_{free}$ test set	14964 reflections (9.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	43.1	Xtrriage
Anisotropy	0.217	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 47.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	33974	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.63% 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

### 5.1 Standard geometry

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

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	0.51	0/2140	0.93	8/2920 (0.3%)
1	B	0.48	0/2140	0.95	9/2920 (0.3%)
1	C	0.52	0/2140	0.96	6/2920 (0.2%)
1	D	0.51	0/2140	0.99	12/2920 (0.4%)
1	E	0.49	0/2140	0.99	9/2920 (0.3%)
1	F	0.50	0/2140	0.98	7/2920 (0.2%)
1	G	0.50	0/2140	1.00	15/2920 (0.5%)
1	H	0.51	0/2140	0.99	8/2920 (0.3%)
1	I	0.51	0/2140	0.96	11/2920 (0.4%)
1	J	0.52	0/2140	0.97	6/2920 (0.2%)
1	K	0.53	0/2140	1.01	11/2920 (0.4%)
1	L	0.49	0/2140	0.98	8/2920 (0.3%)
1	M	0.49	0/2140	0.99	10/2920 (0.3%)
1	N	0.49	0/2140	0.96	10/2920 (0.3%)
1	O	0.50	0/2140	0.94	4/2920 (0.1%)
1	P	0.51	0/2140	1.01	13/2920 (0.4%)
All	All	0.50	0/34240	0.98	147/46720 (0.3%)

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

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

There are no bond length outliers.

All (147) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	235	GLU	N-CA-C	8.55	122.91	110.42
1	P	294	ASN	N-CA-C	7.88	122.33	112.24
1	L	235	GLU	N-CA-C	7.79	121.52	110.23
1	P	235	GLU	N-CA-C	7.71	122.05	110.64
1	G	235	GLU	N-CA-C	7.59	120.94	110.24
1	D	235	GLU	N-CA-C	7.48	120.82	110.35
1	D	181	SER	N-CA-C	-7.42	104.27	112.72
1	H	235	GLU	N-CA-C	7.25	120.50	110.35
1	O	235	GLU	N-CA-C	7.24	120.88	110.24
1	G	242	GLY	N-CA-C	-7.22	96.06	113.18
1	I	235	GLU	N-CA-C	7.17	120.90	110.42
1	G	46	ASN	CA-C-N	7.05	127.02	119.76
1	G	46	ASN	C-N-CA	7.05	127.02	119.76
1	K	153	LEU	CA-C-N	7.03	127.62	120.38
1	K	153	LEU	C-N-CA	7.03	127.62	120.38
1	D	199	THR	CA-C-N	6.98	127.02	119.90
1	D	199	THR	C-N-CA	6.98	127.02	119.90
1	M	73	THR	CA-C-N	6.82	126.33	119.24
1	M	73	THR	C-N-CA	6.82	126.33	119.24
1	E	214	VAL	N-CA-C	6.68	118.23	110.62
1	K	171	VAL	N-CA-C	6.64	119.07	108.85
1	C	235	GLU	N-CA-C	6.53	119.84	110.24
1	D	209	LEU	N-CA-C	6.52	118.05	111.07
1	H	242	GLY	N-CA-C	-6.47	97.85	113.18
1	L	242	GLY	N-CA-C	-6.46	97.87	113.18
1	H	289	LEU	N-CA-C	6.46	119.23	108.13
1	C	242	GLY	N-CA-C	-6.45	97.89	113.18
1	E	242	GLY	N-CA-C	-6.45	97.89	113.18
1	N	242	GLY	N-CA-C	-6.33	98.17	113.18
1	K	73	THR	CA-C-N	6.33	127.75	119.84
1	K	73	THR	C-N-CA	6.33	127.75	119.84
1	P	242	GLY	N-CA-C	-6.29	98.27	113.18
1	I	242	GLY	N-CA-C	-6.26	98.34	113.18
1	A	222	THR	N-CA-C	-6.21	99.07	109.07
1	F	242	GLY	N-CA-C	-6.20	98.49	113.18
1	D	242	GLY	N-CA-C	-6.20	98.49	113.18
1	M	289	LEU	N-CA-C	6.19	118.54	108.26
1	M	57	LEU	CA-C-N	6.14	127.10	119.98
1	M	57	LEU	C-N-CA	6.14	127.10	119.98
1	K	288	LEU	N-CA-C	-6.09	100.57	110.20
1	D	175	ARG	N-CA-C	-6.05	100.69	109.59
1	P	170	VAL	N-CA-C	-6.04	101.75	109.30
1	H	170	VAL	N-CA-C	-5.99	99.80	108.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	241	HIS	N-CA-C	5.99	118.97	109.81
1	F	209	LEU	N-CA-C	5.99	119.05	111.69
1	N	170	VAL	N-CA-C	-5.98	99.01	107.75
1	A	272	PHE	N-CA-C	5.98	121.88	113.56
1	N	241	HIS	N-CA-C	5.97	118.49	109.23
1	N	294	ASN	N-CA-C	5.95	119.85	112.47
1	B	241	HIS	N-CA-C	5.94	118.44	109.41
1	G	170	VAL	N-CA-C	-5.94	99.32	107.99
1	M	243	LEU	N-CA-C	5.92	119.31	110.14
1	L	222	THR	N-CA-C	-5.90	100.09	109.59
1	O	118	PRO	N-CA-C	-5.90	103.50	110.70
1	I	57	LEU	CA-C-N	5.88	126.18	119.83
1	I	57	LEU	C-N-CA	5.88	126.18	119.83
1	J	242	GLY	N-CA-C	-5.86	99.29	113.18
1	I	272	PHE	N-CA-C	5.86	121.70	113.56
1	A	242	GLY	N-CA-C	-5.84	99.34	113.18
1	K	235	GLU	N-CA-C	5.84	118.95	110.42
1	M	194	GLN	CA-C-N	5.82	126.02	120.31
1	M	194	GLN	C-N-CA	5.82	126.02	120.31
1	C	209	LEU	N-CA-C	5.81	119.19	111.75
1	O	242	GLY	N-CA-C	-5.80	99.43	113.18
1	P	73	THR	CA-C-N	5.80	127.09	119.84
1	P	73	THR	C-N-CA	5.80	127.09	119.84
1	P	260	PRO	N-CA-C	-5.78	102.12	111.19
1	E	171	VAL	N-CA-C	5.77	116.99	108.45
1	D	57	LEU	CA-C-N	5.76	127.04	119.84
1	D	57	LEU	C-N-CA	5.76	127.04	119.84
1	P	153	LEU	CA-C-N	5.76	126.31	120.38
1	P	153	LEU	C-N-CA	5.76	126.31	120.38
1	K	193	LYS	N-CA-C	-5.74	106.50	112.93
1	E	289	LEU	N-CA-C	5.73	118.44	108.76
1	I	241	HIS	N-CA-C	5.73	118.40	109.52
1	H	57	LEU	CA-C-N	5.72	127.00	119.84
1	H	57	LEU	C-N-CA	5.72	127.00	119.84
1	H	293	VAL	N-CA-C	5.70	115.49	108.53
1	E	260	PRO	N-CA-C	-5.67	102.29	111.19
1	G	199	THR	CA-C-N	5.66	126.54	119.98
1	G	199	THR	C-N-CA	5.66	126.54	119.98
1	B	289	LEU	N-CA-C	5.65	117.84	108.13
1	N	67	ARG	N-CA-C	5.65	118.20	111.71
1	G	289	LEU	N-CA-C	5.63	117.61	108.26
1	K	242	GLY	N-CA-C	-5.63	99.83	113.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	289	LEU	N-CA-C	5.61	118.61	109.24
1	F	73	THR	CA-C-N	5.60	125.70	119.32
1	F	73	THR	C-N-CA	5.60	125.70	119.32
1	B	74	PRO	N-CA-C	5.60	121.31	113.53
1	L	194	GLN	CA-C-N	5.58	125.51	119.76
1	L	194	GLN	C-N-CA	5.58	125.51	119.76
1	C	260	PRO	N-CA-C	-5.55	102.48	111.19
1	B	170	VAL	N-CA-C	-5.54	100.41	108.17
1	G	171	VAL	N-CA-C	5.53	117.87	108.86
1	L	67	ARG	N-CA-C	5.49	116.94	111.07
1	D	170	VAL	N-CA-C	-5.48	99.99	107.99
1	E	248	GLY	N-CA-C	5.47	122.43	112.37
1	K	282	LYS	N-CA-C	-5.46	106.75	113.41
1	L	289	LEU	N-CA-C	5.45	118.34	108.69
1	L	136	THR	N-CA-C	5.44	119.06	107.70
1	J	57	LEU	CA-C-N	5.43	125.74	119.93
1	J	57	LEU	C-N-CA	5.43	125.74	119.93
1	H	206	LEU	N-CA-C	5.40	118.28	109.59
1	P	169	LEU	N-CA-C	5.39	118.96	107.70
1	B	260	PRO	N-CA-C	-5.37	102.76	111.19
1	J	171	VAL	N-CA-C	5.37	117.06	108.89
1	O	259	TYR	N-CA-C	5.34	117.94	109.40
1	A	194	GLN	CA-C-N	5.33	125.79	120.14
1	A	194	GLN	C-N-CA	5.33	125.79	120.14
1	C	272	PHE	N-CA-C	5.33	119.37	112.86
1	P	272	PHE	N-CA-C	5.32	121.81	113.72
1	M	99	GLY	N-CA-C	-5.32	107.45	114.95
1	B	206	LEU	N-CA-C	5.32	117.63	109.07
1	B	226	GLN	N-CA-C	-5.30	103.26	110.36
1	N	73	THR	CA-C-N	5.29	126.46	119.84
1	N	73	THR	C-N-CA	5.29	126.46	119.84
1	G	50	SER	CA-C-N	5.29	125.35	119.32
1	G	50	SER	C-N-CA	5.29	125.35	119.32
1	M	242	GLY	N-CA-C	-5.26	100.71	113.18
1	A	259	TYR	N-CA-C	5.24	118.56	108.45
1	I	62	ARG	N-CA-C	-5.23	106.90	113.28
1	I	171	VAL	N-CA-C	5.22	116.09	108.53
1	G	74	PRO	N-CA-C	5.17	121.31	113.81
1	E	128	VAL	N-CA-C	5.17	115.79	107.73
1	E	165	GLU	N-CA-C	5.17	120.05	113.18
1	P	241	HIS	N-CA-C	5.16	117.51	109.52
1	F	213	SER	N-CA-C	5.16	117.33	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	171	VAL	N-CA-C	5.15	117.26	108.86
1	I	73	THR	CA-C-N	5.15	126.28	119.84
1	I	73	THR	C-N-CA	5.15	126.28	119.84
1	D	260	PRO	N-CA-C	-5.14	102.53	111.32
1	J	222	THR	N-CA-C	-5.14	101.03	109.40
1	J	129	VAL	N-CA-C	-5.13	107.41	113.42
1	B	73	THR	CA-C-N	5.11	124.72	119.05
1	B	73	THR	C-N-CA	5.11	124.72	119.05
1	A	289	LEU	N-CA-C	5.11	116.91	108.13
1	G	117	LEU	CA-C-N	5.09	123.33	119.66
1	G	117	LEU	C-N-CA	5.09	123.33	119.66
1	F	57	LEU	CA-C-N	5.08	126.20	119.84
1	F	57	LEU	C-N-CA	5.08	126.20	119.84
1	P	99	GLY	N-CA-C	-5.07	107.80	114.95
1	E	166	SER	N-CA-C	5.06	116.10	108.46
1	N	194	GLN	CA-C-N	5.05	125.03	120.03
1	N	194	GLN	C-N-CA	5.05	125.03	120.03
1	G	67	ARG	N-CA-C	5.04	116.78	111.28
1	A	170	VAL	N-CA-C	-5.03	100.51	107.80
1	C	67	ARG	N-CA-C	5.02	116.44	111.07

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	M	216	TYR	Sidechain

## 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	2076	0	2034	80	0
1	B	2076	0	2034	93	0
1	C	2076	0	2034	95	0
1	D	2076	0	2034	114	0
1	E	2076	0	2034	102	0
1	F	2076	0	2034	99	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	2076	0	2034	115	0
1	H	2076	0	2034	105	0
1	I	2076	0	2034	87	0
1	J	2076	0	2034	125	0
1	K	2076	0	2034	172	0
1	L	2076	0	2034	105	0
1	M	2076	0	2034	110	0
1	N	2076	0	2034	96	0
1	O	2076	0	2034	108	0
1	P	2076	0	2034	144	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0
2	K	1	0	0	0	0
2	L	1	0	0	0	0
2	M	1	0	0	0	0
2	N	1	0	0	0	0
2	O	1	0	0	0	0
2	P	1	0	0	0	0
3	A	9	0	5	0	0
3	B	9	0	5	0	0
3	C	9	0	6	1	0
3	D	9	0	6	1	0
3	E	9	0	5	1	0
3	F	9	0	6	1	0
3	G	9	0	5	0	0
3	H	9	0	6	1	0
3	I	9	0	5	0	0
3	J	9	0	5	1	0
3	K	9	0	6	0	0
3	L	9	0	5	0	0
3	M	9	0	6	1	0
3	N	9	0	6	0	0
3	O	9	0	5	0	0
3	P	9	0	6	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	54	0	0	1	0
4	B	41	0	0	3	0
4	C	40	0	0	2	0
4	D	35	0	0	0	0
4	E	38	0	0	1	0
4	F	42	0	0	2	0
4	G	38	0	0	3	0
4	H	36	0	0	2	0
4	I	38	0	0	1	0
4	J	30	0	0	3	0
4	K	34	0	0	3	0
4	L	30	0	0	1	0
4	M	40	0	0	2	0
4	N	35	0	0	1	0
4	O	38	0	0	1	0
4	P	29	0	0	3	0
All	All	33974	0	32632	1663	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 25.

All (1663) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:122:ILE:HD13	1:K:298:LEU:HD13	1.30	1.09
1:D:82:LEU:HD13	1:D:90:GLY:HA3	1.34	1.07
1:P:87:ASN:HD21	1:P:110:LYS:HD2	1.19	1.02
1:G:164:VAL:HG23	1:G:165:GLU:H	1.27	0.99
1:D:40:ILE:H	1:D:40:ILE:HD12	1.24	0.99
1:B:82:LEU:HD13	1:B:90:GLY:HA3	1.45	0.99
1:C:115:SER:HB3	1:C:161:LEU:HB2	1.45	0.98
1:P:196:LEU:HD21	1:P:207:ARG:HH21	1.27	0.97
1:G:137:ASN:C	1:G:137:ASN:HD22	1.73	0.96
1:P:133:VAL:HG12	1:P:163:CYS:HB2	1.45	0.96
1:F:224:ASP:OD1	1:F:286:ARG:HD3	1.66	0.95
1:M:93:LEU:HD12	1:M:104:MET:HE2	1.45	0.95
1:K:224:ASP:OD2	1:K:286:ARG:HD3	1.66	0.95
1:N:40:ILE:HD12	1:N:40:ILE:H	1.31	0.94
1:G:87:ASN:OD1	1:G:110:LYS:HB2	1.67	0.93
1:P:40:ILE:H	1:P:40:ILE:HD12	1.35	0.92
1:J:143:LYS:H	1:J:143:LYS:HD2	1.33	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:101:HIS:H	1:B:240:GLN:HE22	1.19	0.91
1:E:82:LEU:HD13	1:E:90:GLY:HA3	1.50	0.91
1:D:296:ASN:ND2	1:D:298:LEU:H	1.69	0.91
1:L:70:ALA:HB3	1:L:268:TRP:HB3	1.55	0.89
1:K:87:ASN:ND2	1:K:110:LYS:HB2	1.89	0.88
1:H:82:LEU:HD12	1:H:83:PRO:HD2	1.55	0.87
1:P:87:ASN:HD21	1:P:110:LYS:CD	1.86	0.87
1:N:133:VAL:HG23	1:N:163:CYS:HB2	1.56	0.86
1:B:222:THR:HG23	1:B:286:ARG:HD2	1.56	0.85
1:J:82:LEU:HD13	1:J:90:GLY:HA3	1.58	0.85
1:N:202:GLU:OE1	1:N:233:VAL:HG12	1.75	0.85
1:P:130:GLU:HA	1:P:147:VAL:HG22	1.56	0.85
1:K:193:LYS:HA	1:K:193:LYS:HE3	1.56	0.85
1:K:190:SER:H	1:K:193:LYS:HB2	1.42	0.84
1:B:137:ASN:HA	4:B:402:HOH:O	1.77	0.84
1:D:296:ASN:HD22	1:D:298:LEU:H	1.19	0.84
1:P:296:ASN:HD22	1:P:298:LEU:H	1.20	0.84
1:H:208:LYS:NZ	1:H:212:MET:HE3	1.92	0.84
1:C:154:PRO:HG2	1:C:185:GLU:HA	1.60	0.83
1:D:196:LEU:HD11	1:D:207:ARG:NH2	1.92	0.83
1:M:224:ASP:OD2	1:M:286:ARG:HD3	1.79	0.83
1:A:239:ASN:H	1:A:239:ASN:HD22	1.24	0.82
1:C:207:ARG:HB2	1:C:222:THR:HG22	1.60	0.82
1:K:194:GLN:HE21	1:K:195:PRO:HD2	1.42	0.82
1:A:224:ASP:OD2	1:A:286:ARG:HD3	1.80	0.82
1:E:113:SER:OG	1:E:163:CYS:HB3	1.79	0.82
1:P:137:ASN:HA	1:P:159:HIS:HA	1.60	0.82
1:C:241:HIS:CD2	1:C:269:MET:HE3	2.14	0.82
1:E:208:LYS:HZ3	1:E:212:MET:HE3	1.45	0.81
1:J:169:LEU:N	1:J:169:LEU:HD23	1.96	0.81
1:B:126:ILE:HD13	1:B:161:LEU:HD11	1.62	0.81
1:O:247:GLU:HG2	1:O:286:ARG:HB3	1.63	0.81
1:P:296:ASN:ND2	1:P:298:LEU:H	1.77	0.81
1:D:224:ASP:OD2	1:D:286:ARG:HD3	1.81	0.80
1:D:165:GLU:HG3	1:E:165:GLU:OE1	1.80	0.80
1:M:208:LYS:HZ2	1:M:212:MET:HE3	1.44	0.80
1:A:40:ILE:H	1:A:40:ILE:HD12	1.46	0.80
1:H:137:ASN:HA	1:H:159:HIS:HA	1.63	0.80
1:G:40:ILE:H	1:G:40:ILE:HD12	1.47	0.80
1:I:243:LEU:HD12	1:I:244:LEU:N	1.96	0.80
1:N:296:ASN:HD22	1:N:298:LEU:H	1.29	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:234:LYS:HG2	1:G:61:THR:HB	1.63	0.80
1:N:87:ASN:ND2	1:N:110:LYS:HB2	1.96	0.79
1:P:196:LEU:CD2	1:P:207:ARG:HH21	1.94	0.79
1:P:64:VAL:HG11	1:P:66:LYS:HZ2	1.47	0.79
1:B:40:ILE:H	1:B:40:ILE:HD12	1.48	0.79
1:J:152:TYR:C	1:J:153:LEU:HD23	2.06	0.79
1:K:190:SER:O	1:K:193:LYS:N	2.14	0.79
1:O:110:LYS:HA	1:O:110:LYS:HE2	1.63	0.79
1:B:224:ASP:OD2	1:B:286:ARG:HD3	1.82	0.79
1:H:224:ASP:OD1	1:H:286:ARG:HD3	1.83	0.78
1:K:70:ALA:HB3	1:K:268:TRP:HB3	1.64	0.78
1:P:64:VAL:HG11	1:P:66:LYS:NZ	1.99	0.78
1:K:145:LEU:HD13	1:K:149:SER:HB3	1.64	0.78
1:F:111:GLU:HA	1:F:164:VAL:O	1.84	0.78
1:J:87:ASN:ND2	1:J:110:LYS:HB2	1.98	0.78
1:N:190:SER:HB3	1:N:192:ASP:OD1	1.83	0.78
1:E:101:HIS:H	1:E:240:GLN:HE22	1.30	0.78
1:L:40:ILE:H	1:L:40:ILE:HD12	1.48	0.78
1:B:119:PRO:HD2	1:B:122:ILE:HG13	1.66	0.78
1:N:93:LEU:HD13	1:N:266:VAL:HG21	1.64	0.77
1:G:70:ALA:HB3	1:G:268:TRP:HB3	1.66	0.77
1:K:64:VAL:HG11	1:K:66:LYS:HE3	1.66	0.77
1:K:211:PRO:HD2	1:K:216:TYR:CE2	2.20	0.77
1:I:224:ASP:OD2	1:I:286:ARG:HD3	1.83	0.77
1:O:296:ASN:HD22	1:O:298:LEU:H	1.33	0.77
1:J:146:THR:O	1:J:149:SER:HB3	1.85	0.77
1:A:40:ILE:HD12	1:A:40:ILE:N	1.99	0.76
1:L:87:ASN:ND2	1:L:110:LYS:HB2	2.00	0.76
1:K:126:ILE:HG22	1:K:171:VAL:HB	1.67	0.76
1:G:196:LEU:HD22	1:G:205:GLU:HB3	1.67	0.76
1:P:153:LEU:HD13	1:P:159:HIS:CD2	2.20	0.76
1:O:64:VAL:HG11	1:O:66:LYS:HE3	1.65	0.76
1:K:92:TYR:CE1	1:K:105:TYR:HD2	2.04	0.76
1:N:115:SER:HB3	1:N:161:LEU:HB2	1.66	0.76
1:P:224:ASP:OD1	1:P:286:ARG:HG3	1.84	0.76
1:G:115:SER:HB3	1:G:161:LEU:HB2	1.66	0.76
1:N:137:ASN:HB2	1:N:140:SER:HB3	1.68	0.76
1:N:61:THR:HB	1:O:234:LYS:HG2	1.66	0.76
1:P:133:VAL:HG12	1:P:163:CYS:CB	2.16	0.76
1:L:48:THR:HG21	1:N:55:GLN:HG2	1.66	0.75
1:I:93:LEU:HD12	1:I:105:TYR:HA	1.67	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:191:THR:HG21	1:P:286:ARG:NH2	2.00	0.75
1:J:175:ARG:HH11	1:J:175:ARG:HG3	1.50	0.75
1:N:82:LEU:HD13	1:N:90:GLY:HA3	1.69	0.75
1:M:208:LYS:NZ	1:M:212:MET:HE3	2.00	0.75
1:C:137:ASN:HD21	1:C:140:SER:HB2	1.52	0.74
1:E:93:LEU:HD13	1:E:266:VAL:HG21	1.67	0.74
1:L:121:ASP:H	1:L:156:ASN:HD21	1.32	0.74
1:K:241:HIS:HB2	1:K:269:MET:HB2	1.68	0.74
1:P:111:GLU:H	1:P:111:GLU:CD	1.96	0.74
1:P:154:PRO:HG2	1:P:185:GLU:HA	1.70	0.74
1:B:45:THR:HG22	1:B:46:ASN:OD1	1.88	0.74
1:D:127:PHE:HB3	1:D:170:VAL:CG1	2.18	0.74
1:P:135:LEU:HD23	1:P:136:THR:N	2.03	0.74
1:K:79:TYR:HA	1:K:91:ALA:HB2	1.69	0.73
1:D:119:PRO:HB2	1:D:122:ILE:HD12	1.68	0.73
1:L:190:SER:HB3	1:L:192:ASP:OD1	1.88	0.73
1:A:133:VAL:HG23	1:A:162:ASP:O	1.88	0.73
1:K:211:PRO:HB2	1:K:216:TYR:HE2	1.52	0.73
1:L:224:ASP:OD2	1:L:286:ARG:HD3	1.89	0.73
1:J:241:HIS:ND1	1:J:289:LEU:HD11	2.04	0.73
1:K:222:THR:HG23	1:K:286:ARG:HD2	1.69	0.73
1:L:93:LEU:HD13	1:L:266:VAL:HG21	1.71	0.73
1:C:197:LEU:HD12	1:C:208:LYS:HG3	1.71	0.73
1:P:85:TRP:CE3	1:P:88:THR:HG21	2.23	0.73
1:O:296:ASN:ND2	1:O:298:LEU:HB2	2.04	0.72
1:D:296:ASN:HD22	1:D:298:LEU:N	1.87	0.72
1:I:243:LEU:HD13	1:I:287:TYR:HB2	1.70	0.72
1:P:151:ALA:HA	1:P:187:ILE:O	1.89	0.72
1:J:93:LEU:HD13	1:J:266:VAL:HG21	1.71	0.72
1:O:190:SER:HB2	1:O:193:LYS:HG2	1.72	0.72
1:H:82:LEU:HG	1:H:85:TRP:CD1	2.25	0.72
1:L:153:LEU:HD22	1:L:159:HIS:CG	2.25	0.72
1:C:40:ILE:HD12	1:C:40:ILE:N	2.04	0.72
1:M:126:ILE:HG22	1:M:171:VAL:HB	1.71	0.72
1:I:109:MET:O	1:I:166:SER:HA	1.88	0.71
1:F:296:ASN:HD22	1:F:298:LEU:HB2	1.54	0.71
1:K:66:LYS:HD2	1:K:69:HIS:CE1	2.25	0.71
1:C:40:ILE:HD13	1:C:147:VAL:HG11	1.72	0.71
1:I:93:LEU:HD22	1:I:266:VAL:HG21	1.71	0.71
1:K:194:GLN:HA	1:K:194:GLN:NE2	2.05	0.71
1:G:121:ASP:H	1:G:156:ASN:HD21	1.37	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:87:ASN:ND2	1:P:110:LYS:HD2	2.00	0.71
1:E:61:THR:HG22	1:P:253:ARG:HH12	1.56	0.71
1:K:83:PRO:O	1:K:85:TRP:HD1	1.74	0.70
1:E:153:LEU:HD13	1:E:159:HIS:NE2	2.07	0.70
1:H:150:TYR:CE2	1:H:209:LEU:HB3	2.24	0.70
1:E:111:GLU:HA	1:E:165:GLU:HA	1.72	0.70
1:F:296:ASN:ND2	1:F:298:LEU:HB2	2.05	0.70
1:K:204:PHE:CE1	1:K:223:MET:HE3	2.26	0.70
1:L:147:VAL:O	1:L:148:ASP:HB2	1.92	0.70
1:A:296:ASN:HD22	1:A:298:LEU:H	1.39	0.70
1:K:193:LYS:HA	1:K:193:LYS:CE	2.20	0.70
1:P:101:HIS:H	1:P:240:GLN:HE22	1.39	0.70
1:H:247:GLU:HG3	1:H:286:ARG:HB3	1.74	0.70
1:P:85:TRP:CD1	1:P:116:GLY:H	2.10	0.70
1:H:202:GLU:OE2	1:H:233:VAL:HG12	1.91	0.70
1:H:208:LYS:HZ2	1:H:212:MET:HE3	1.57	0.70
1:K:227:PRO:HG3	1:K:283:THR:O	1.92	0.70
1:D:59:GLY:O	1:K:253:ARG:NH1	2.25	0.69
1:D:153:LEU:HD13	1:D:159:HIS:CD2	2.27	0.69
1:J:169:LEU:HD23	1:J:169:LEU:H	1.55	0.69
1:J:176:TYR:HE2	1:J:178:TYR:HA	1.57	0.69
1:K:86:THR:OG1	1:K:114:SER:N	2.26	0.69
1:K:170:VAL:O	1:K:170:VAL:HG13	1.91	0.69
1:M:110:LYS:HE2	1:M:110:LYS:HA	1.75	0.69
1:A:128:VAL:HG12	1:A:147:VAL:HA	1.74	0.69
1:H:184:THR:HB	1:H:216:TYR:CE1	2.27	0.69
1:B:101:HIS:N	1:B:240:GLN:HE22	1.91	0.69
1:G:164:VAL:HG23	1:G:165:GLU:N	2.05	0.69
1:J:113:SER:OG	1:J:163:CYS:HB3	1.93	0.69
1:K:72:ILE:N	1:K:72:ILE:HD12	2.07	0.69
1:K:109:MET:HB2	1:K:167:ALA:HB3	1.74	0.69
1:D:93:LEU:HD13	1:D:266:VAL:HG21	1.75	0.69
1:G:122:ILE:HD13	1:G:175:ARG:HA	1.74	0.69
1:J:124:ARG:O	1:J:153:LEU:HG	1.92	0.69
1:C:111:GLU:CD	1:C:111:GLU:H	2.00	0.69
1:E:39:PRO:HB2	1:E:42:TRP:HB2	1.74	0.69
1:F:101:HIS:H	1:F:240:GLN:HE22	1.41	0.69
1:G:175:ARG:HH11	1:G:175:ARG:HG3	1.57	0.69
1:H:136:THR:HG22	1:H:137:ASN:H	1.57	0.68
1:N:137:ASN:CB	1:N:140:SER:HB3	2.22	0.68
1:C:70:ALA:HB3	1:C:268:TRP:HB3	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:165:GLU:HG3	1:O:166:SER:H	1.57	0.68
1:K:243:LEU:HD13	1:K:287:TYR:HB2	1.74	0.68
1:J:224:ASP:OD1	1:J:286:ARG:HD3	1.93	0.68
1:K:145:LEU:HD13	1:K:149:SER:CB	2.23	0.68
1:D:154:PRO:HG2	1:D:185:GLU:HA	1.76	0.68
1:A:207:ARG:HB2	1:A:222:THR:HG22	1.76	0.68
1:D:121:ASP:H	1:D:156:ASN:HD21	1.41	0.68
1:J:87:ASN:HD21	1:J:110:LYS:HB2	1.59	0.67
1:O:70:ALA:HB3	1:O:268:TRP:HB3	1.76	0.67
1:D:64:VAL:HG11	1:D:66:LYS:HE3	1.75	0.67
1:K:190:SER:N	1:K:193:LYS:HB2	2.07	0.67
1:K:190:SER:O	1:K:192:ASP:N	2.28	0.67
1:K:103:VAL:CG2	1:K:173:GLU:HB2	2.25	0.67
1:I:93:LEU:HD11	1:I:106:LEU:HG	1.76	0.67
1:J:298:LEU:HD13	1:K:122:ILE:HD12	1.76	0.67
1:K:130:GLU:HA	1:K:147:VAL:HG22	1.77	0.67
1:B:127:PHE:HB3	1:B:170:VAL:HG13	1.76	0.67
1:H:132:ALA:HB1	1:H:144:LYS:HE3	1.75	0.67
1:D:101:HIS:H	1:D:240:GLN:HE22	1.41	0.67
1:K:194:GLN:NE2	1:K:195:PRO:HD2	2.10	0.67
1:K:114:SER:HA	1:K:161:LEU:O	1.96	0.66
1:L:140:SER:O	1:L:141:SER:HB3	1.94	0.66
1:M:237:HIS:CE1	1:M:239:ASN:HB2	2.30	0.66
1:A:82:LEU:HD13	1:A:90:GLY:HA3	1.76	0.66
1:F:93:LEU:HD13	1:F:266:VAL:HG21	1.76	0.66
1:J:130:GLU:HA	1:J:147:VAL:HG22	1.76	0.66
1:G:40:ILE:HD12	1:G:40:ILE:N	2.09	0.66
1:N:241:HIS:HB2	1:N:269:MET:HB2	1.78	0.66
1:C:207:ARG:HB2	1:C:222:THR:CG2	2.25	0.66
1:G:224:ASP:OD2	1:G:286:ARG:HB2	1.96	0.66
1:K:112:MET:N	1:K:164:VAL:O	2.25	0.66
1:L:196:LEU:HD11	1:L:207:ARG:HH21	1.60	0.66
1:F:241:HIS:HB2	1:F:269:MET:HB2	1.78	0.66
1:H:93:LEU:HD13	1:H:266:VAL:HG21	1.77	0.66
1:G:127:PHE:HB3	1:G:170:VAL:HG13	1.78	0.66
1:D:82:LEU:CD1	1:D:90:GLY:HA3	2.20	0.65
1:O:72:ILE:H	1:O:72:ILE:HD12	1.61	0.65
1:A:296:ASN:ND2	1:A:298:LEU:HB2	2.11	0.65
1:G:62:ARG:HB2	1:G:73:THR:HG21	1.78	0.65
1:N:70:ALA:HB3	1:N:268:TRP:HB3	1.78	0.65
1:M:133:VAL:HG22	1:M:134:THR:H	1.62	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:241:HIS:HB2	1:P:269:MET:HB2	1.78	0.65
1:M:137:ASN:C	1:M:137:ASN:HD22	2.04	0.65
1:F:243:LEU:C	1:F:243:LEU:HD12	2.22	0.65
1:H:133:VAL:HG23	1:H:162:ASP:C	2.21	0.65
1:L:127:PHE:HB3	1:L:170:VAL:HG13	1.79	0.65
1:L:220:ILE:HD13	1:L:290:TYR:HA	1.79	0.65
1:L:298:LEU:HD23	1:P:103:VAL:HG13	1.79	0.65
1:C:136:THR:HG22	1:C:142:SER:HB2	1.78	0.65
1:G:236:VAL:HG23	1:I:76:SER:HB3	1.79	0.65
1:K:164:VAL:HG23	1:K:165:GLU:N	2.12	0.65
1:C:202:GLU:OE2	1:C:233:VAL:HG12	1.96	0.64
1:D:70:ALA:HB3	1:D:268:TRP:HB3	1.79	0.64
1:G:243:LEU:C	1:G:243:LEU:HD12	2.22	0.64
1:B:241:HIS:HB2	1:B:269:MET:HB2	1.78	0.64
1:H:40:ILE:H	1:H:40:ILE:HD12	1.61	0.64
1:H:296:ASN:ND2	1:H:298:LEU:HB3	2.12	0.64
1:I:185:GLU:HG3	1:I:216:TYR:OH	1.97	0.64
1:J:208:LYS:HZ3	1:J:212:MET:HE3	1.62	0.64
1:B:101:HIS:H	1:B:240:GLN:NE2	1.91	0.64
1:G:40:ILE:HB	1:G:147:VAL:HG11	1.79	0.64
1:P:150:TYR:CE2	1:P:209:LEU:HB3	2.32	0.64
1:E:152:TYR:HB3	1:E:187:ILE:HB	1.78	0.64
1:I:72:ILE:N	1:I:72:ILE:HD12	2.13	0.64
1:L:234:LYS:HD2	1:L:234:LYS:N	2.11	0.64
1:A:94:ILE:CD1	1:A:268:TRP:HB2	2.27	0.64
1:H:82:LEU:HD12	1:H:83:PRO:CD	2.27	0.64
1:K:111:GLU:HA	1:K:164:VAL:O	1.97	0.64
1:O:64:VAL:CG1	1:O:66:LYS:HE3	2.28	0.64
1:B:153:LEU:HD13	1:B:159:HIS:NE2	2.13	0.64
1:C:224:ASP:OD2	1:C:286:ARG:HD3	1.98	0.64
1:J:64:VAL:HG11	1:J:66:LYS:NZ	2.13	0.64
1:C:109:MET:O	1:C:166:SER:HA	1.98	0.64
1:E:208:LYS:NZ	1:E:212:MET:HE3	2.13	0.64
1:I:120:GLN:HG3	1:I:156:ASN:HD21	1.62	0.64
1:K:222:THR:CG2	1:K:286:ARG:HD2	2.27	0.64
1:N:128:VAL:HA	1:N:169:LEU:HD23	1.80	0.64
1:E:243:LEU:HD12	1:E:244:LEU:N	2.13	0.64
1:H:243:LEU:C	1:H:243:LEU:HD12	2.23	0.64
1:P:121:ASP:H	1:P:156:ASN:HD21	1.44	0.64
1:F:127:PHE:HB3	1:F:170:VAL:CG1	2.26	0.64
1:O:137:ASN:ND2	1:O:140:SER:CB	2.61	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:164:VAL:HG23	1:P:165:GLU:H	1.63	0.63
1:D:196:LEU:HD11	1:D:207:ARG:CZ	2.28	0.63
1:K:252:TYR:CD1	1:K:277:TYR:HD1	2.16	0.63
1:P:168:THR:O	1:P:169:LEU:HD23	1.98	0.63
1:F:82:LEU:CD1	1:F:90:GLY:HA3	2.29	0.63
1:J:164:VAL:HG23	1:J:165:GLU:HG3	1.79	0.63
1:E:164:VAL:HG13	1:E:165:GLU:HG2	1.80	0.63
1:N:206:LEU:HD12	1:N:207:ARG:H	1.63	0.63
1:P:154:PRO:HG2	1:P:185:GLU:CA	2.29	0.63
1:P:243:LEU:C	1:P:243:LEU:HD12	2.24	0.63
1:B:87:ASN:ND2	1:B:110:LYS:HB2	2.13	0.63
1:E:296:ASN:HD22	1:E:298:LEU:HB2	1.63	0.63
1:H:245:LEU:HD12	1:H:287:TYR:HB3	1.80	0.63
1:A:207:ARG:HB2	1:A:222:THR:CG2	2.29	0.63
1:F:152:TYR:HB3	1:F:187:ILE:HB	1.81	0.63
1:H:103:VAL:HG13	1:N:298:LEU:HG	1.80	0.63
1:I:137:ASN:HB3	4:I:409:HOH:O	1.97	0.63
1:I:243:LEU:CD1	1:I:287:TYR:HB2	2.27	0.63
1:J:120:GLN:HG2	1:J:121:ASP:OD1	1.98	0.63
1:K:85:TRP:CE3	1:K:88:THR:HG21	2.33	0.63
1:O:207:ARG:HB2	1:O:222:THR:OG1	1.98	0.63
1:D:110:LYS:HB2	1:D:110:LYS:NZ	2.14	0.63
1:G:270:ALA:O	1:G:273:VAL:HG12	1.98	0.63
1:M:128:VAL:HG22	1:M:169:LEU:HD11	1.80	0.63
1:H:197:LEU:N	1:H:197:LEU:HD12	2.14	0.63
1:H:276:TRP:CH2	1:H:278:ALA:HB2	2.34	0.63
1:A:239:ASN:H	1:A:239:ASN:ND2	1.96	0.62
1:B:137:ASN:HB2	1:B:140:SER:HA	1.81	0.62
1:D:40:ILE:H	1:D:40:ILE:CD1	1.99	0.62
1:D:276:TRP:CH2	1:D:278:ALA:HB2	2.34	0.62
1:M:133:VAL:HG22	1:M:134:THR:N	2.13	0.62
1:B:296:ASN:HD22	1:B:298:LEU:H	1.45	0.62
1:I:137:ASN:HD22	1:I:137:ASN:N	1.96	0.62
1:P:196:LEU:HD21	1:P:207:ARG:NH2	2.07	0.62
1:D:207:ARG:HB2	1:D:222:THR:CG2	2.29	0.62
1:H:186:LEU:HD11	1:H:188:VAL:HG23	1.81	0.62
1:J:64:VAL:HG11	1:J:66:LYS:HZ3	1.63	0.62
1:A:127:PHE:HB3	1:A:170:VAL:HG13	1.80	0.62
1:D:207:ARG:HB2	1:D:222:THR:HG22	1.81	0.62
1:J:150:TYR:CZ	1:J:209:LEU:HB3	2.35	0.62
1:O:121:ASP:H	1:O:156:ASN:HD21	1.46	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:222:THR:HG23	1:F:286:ARG:HD2	1.80	0.62
1:K:231:LEU:HA	4:K:425:HOH:O	1.98	0.62
1:L:48:THR:HB	1:L:262:GLN:HE22	1.64	0.62
1:N:232:ASN:O	1:N:234:LYS:HE2	2.00	0.62
1:E:241:HIS:HB3	1:E:289:LEU:HD11	1.79	0.62
1:F:83:PRO:O	1:F:84:ASP:HB2	1.99	0.62
1:F:126:ILE:HG22	1:F:171:VAL:HB	1.82	0.62
1:H:208:LYS:HZ3	1:H:212:MET:HE3	1.61	0.62
1:A:40:ILE:H	1:A:40:ILE:CD1	2.06	0.62
1:B:140:SER:O	1:B:141:SER:HB2	2.00	0.62
1:G:115:SER:CB	1:G:161:LEU:HB2	2.30	0.62
1:H:243:LEU:HD13	1:H:287:TYR:HB2	1.80	0.62
1:H:298:LEU:HD23	1:H:298:LEU:C	2.25	0.62
1:J:82:LEU:CD1	1:J:90:GLY:HA3	2.28	0.62
1:L:226:GLN:HB2	1:L:229:GLU:OE1	2.00	0.62
1:N:206:LEU:HD12	1:N:207:ARG:N	2.14	0.62
1:G:40:ILE:H	1:G:40:ILE:CD1	2.13	0.62
1:J:206:LEU:HD12	1:J:207:ARG:N	2.14	0.62
1:F:85:TRP:CE3	1:F:115:SER:HA	2.35	0.62
1:O:131:GLY:HA3	1:O:166:SER:O	2.00	0.62
1:B:82:LEU:CD1	1:B:90:GLY:HA3	2.27	0.61
1:C:94:ILE:HD12	1:C:104:MET:HE3	1.80	0.61
1:L:150:TYR:CE2	1:L:209:LEU:HB3	2.34	0.61
1:M:128:VAL:HA	1:M:169:LEU:CD1	2.30	0.61
1:N:243:LEU:C	1:N:243:LEU:HD12	2.24	0.61
1:G:140:SER:HB2	4:G:421:HOH:O	1.99	0.61
1:J:243:LEU:C	1:J:243:LEU:HD12	2.25	0.61
1:L:121:ASP:H	1:L:156:ASN:ND2	1.98	0.61
1:O:137:ASN:ND2	1:O:140:SER:HB3	2.15	0.61
1:D:82:LEU:HD13	1:D:90:GLY:CA	2.22	0.61
1:K:122:ILE:HD13	1:K:175:ARG:HA	1.82	0.61
1:G:150:TYR:CZ	1:G:209:LEU:HB3	2.36	0.61
1:I:142:SER:O	1:I:143:LYS:HD2	2.01	0.61
1:M:150:TYR:CZ	1:M:209:LEU:HB3	2.36	0.61
1:P:130:GLU:CA	1:P:147:VAL:HG22	2.30	0.61
1:F:87:ASN:ND2	1:F:110:LYS:HB2	2.15	0.61
1:H:186:LEU:HD11	1:H:188:VAL:CG2	2.30	0.61
1:E:123:GLU:HG2	1:E:174:ARG:O	1.99	0.61
1:L:249:GLN:HE21	1:N:56:ASP:CG	2.08	0.61
1:C:87:ASN:ND2	1:C:110:LYS:HB2	2.14	0.61
1:P:169:LEU:O	1:P:171:VAL:HG12	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:296:ASN:HD22	1:P:298:LEU:N	1.97	0.61
1:G:121:ASP:H	1:G:156:ASN:ND2	1.99	0.61
1:L:243:LEU:C	1:L:243:LEU:HD12	2.25	0.61
1:J:273:VAL:HG13	1:J:273:VAL:O	2.00	0.61
1:O:147:VAL:O	1:O:148:ASP:HB2	1.99	0.61
1:C:101:HIS:H	1:C:240:GLN:HE22	1.47	0.61
1:D:111:GLU:HA	1:D:164:VAL:O	2.00	0.61
1:D:121:ASP:H	1:D:156:ASN:ND2	1.99	0.61
1:E:125:LEU:HD13	1:E:125:LEU:C	2.25	0.61
1:F:82:LEU:HD13	1:F:90:GLY:HA3	1.83	0.61
1:G:243:LEU:HD23	1:G:269:MET:CE	2.31	0.61
1:A:127:PHE:HB3	1:A:170:VAL:CG1	2.31	0.60
1:C:40:ILE:HD12	1:C:40:ILE:H	1.65	0.60
1:E:199:THR:HG23	1:E:200:PRO:HD2	1.81	0.60
1:M:150:TYR:CE2	1:M:209:LEU:HB3	2.36	0.60
1:G:157:PHE:C	1:G:157:PHE:CD2	2.79	0.60
1:A:153:LEU:HD13	1:A:159:HIS:NE2	2.15	0.60
1:K:105:TYR:CE1	1:K:171:VAL:HG22	2.37	0.60
1:K:249:GLN:HG2	1:K:280:LEU:O	2.01	0.60
1:M:64:VAL:HG12	1:M:71:LEU:HB3	1.82	0.60
1:E:296:ASN:HD21	1:E:298:LEU:HD12	1.67	0.60
1:O:205:GLU:HB2	1:O:224:ASP:HB2	1.84	0.60
1:F:144:LYS:O	1:F:145:LEU:HD23	2.01	0.60
1:B:137:ASN:OD1	1:B:140:SER:HA	2.02	0.60
1:B:150:TYR:CE2	1:B:209:LEU:HB3	2.37	0.60
1:G:127:PHE:HB3	1:G:170:VAL:CG1	2.31	0.60
1:G:137:ASN:C	1:G:137:ASN:ND2	2.46	0.60
1:J:101:HIS:H	1:J:240:GLN:HE22	1.49	0.60
1:B:268:TRP:CZ2	1:B:270:ALA:HB2	2.37	0.60
1:C:74:PRO:C	1:C:76:SER:H	2.10	0.60
1:F:184:THR:HB	1:F:216:TYR:CE1	2.37	0.60
1:C:104:MET:HE2	1:C:172:PHE:CE1	2.36	0.60
1:E:243:LEU:HD13	1:E:287:TYR:HB2	1.84	0.60
1:I:101:HIS:H	1:I:240:GLN:HE22	1.48	0.60
1:A:245:LEU:HA	1:A:287:TYR:HB3	1.84	0.59
1:D:84:ASP:O	1:D:116:GLY:HA3	2.01	0.59
1:H:62:ARG:HB2	1:H:73:THR:HG21	1.84	0.59
1:P:39:PRO:HB2	1:P:42:TRP:HB2	1.83	0.59
1:C:190:SER:HB3	1:C:192:ASP:OD1	2.01	0.59
1:F:208:LYS:NZ	1:F:212:MET:HE3	2.17	0.59
1:M:237:HIS:ND1	1:M:239:ASN:HB2	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:59:GLY:O	1:I:253:ARG:NH1	2.35	0.59
1:I:109:MET:HB3	1:I:113:SER:OG	2.02	0.59
1:J:136:THR:O	1:J:137:ASN:HB3	2.02	0.59
1:K:243:LEU:C	1:K:243:LEU:HD12	2.27	0.59
1:L:241:HIS:CG	1:L:289:LEU:HD11	2.38	0.59
1:M:153:LEU:HD13	1:M:159:HIS:CD2	2.37	0.59
1:M:64:VAL:CG2	1:M:66:LYS:HE3	2.32	0.59
1:O:153:LEU:HD13	1:O:159:HIS:CE1	2.38	0.59
1:N:155:PRO:O	1:N:156:ASN:HB2	2.02	0.59
1:E:128:VAL:HG22	1:E:169:LEU:CD2	2.31	0.59
1:G:130:GLU:HA	1:G:147:VAL:HG22	1.84	0.59
1:F:52:SER:O	1:F:55:GLN:HG2	2.02	0.59
1:G:197:LEU:HD22	1:G:208:LYS:HE3	1.84	0.59
1:K:153:LEU:HD22	1:K:159:HIS:CD2	2.38	0.59
1:B:47:PRO:HA	4:B:409:HOH:O	2.03	0.59
1:J:143:LYS:HD2	1:J:143:LYS:N	2.13	0.59
1:M:101:HIS:H	1:M:240:GLN:HE22	1.49	0.59
1:O:73:THR:HG22	1:O:265:ASP:OD1	2.02	0.59
1:P:87:ASN:ND2	1:P:87:ASN:C	2.61	0.59
1:P:113:SER:OG	1:P:163:CYS:HB3	2.03	0.59
1:D:233:VAL:HG13	1:D:235:GLU:HG3	1.83	0.59
1:E:82:LEU:CD1	1:E:90:GLY:HA3	2.30	0.59
1:M:49:LEU:HD11	1:M:54:LEU:HD21	1.84	0.59
1:G:184:THR:HB	1:G:216:TYR:CE1	2.37	0.58
1:M:222:THR:HG22	4:M:417:HOH:O	2.02	0.58
1:K:93:LEU:HD13	1:K:266:VAL:HG21	1.86	0.58
1:P:130:GLU:HA	1:P:147:VAL:CG2	2.32	0.58
1:O:202:GLU:HG3	1:O:204:PHE:HE2	1.67	0.58
1:F:125:LEU:C	1:F:125:LEU:HD13	2.28	0.58
1:H:120:GLN:O	1:H:121:ASP:HB2	2.04	0.58
1:N:234:LYS:HD3	1:N:234:LYS:N	2.18	0.58
1:O:202:GLU:HG3	1:O:204:PHE:CE2	2.39	0.58
1:P:119:PRO:HD2	1:P:122:ILE:HG13	1.85	0.58
1:B:137:ASN:HB2	1:B:141:SER:H	1.66	0.58
1:B:197:LEU:HB2	1:B:206:LEU:HD23	1.84	0.58
1:E:72:ILE:HD12	1:E:72:ILE:N	2.19	0.58
1:H:59:GLY:O	1:N:253:ARG:NH1	2.35	0.58
1:M:129:VAL:HG22	1:M:168:THR:O	2.04	0.58
1:N:40:ILE:H	1:N:40:ILE:CD1	2.06	0.58
1:C:40:ILE:H	1:C:40:ILE:CD1	2.17	0.58
1:C:204:PHE:CE1	1:C:223:MET:HE3	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:241:HIS:HB3	1:D:289:LEU:HD11	1.86	0.58
1:P:134:THR:HG23	1:P:143:LYS:O	2.03	0.58
1:P:109:MET:SD	1:P:169:LEU:HD11	2.43	0.58
1:B:153:LEU:HD13	1:B:159:HIS:CE1	2.38	0.58
1:H:298:LEU:HD23	1:H:298:LEU:OXT	2.04	0.58
1:B:204:PHE:CZ	1:B:223:MET:HE3	2.38	0.57
1:D:296:ASN:HD21	1:D:298:LEU:HB2	1.69	0.57
1:G:125:LEU:HD22	1:G:151:ALA:O	2.04	0.57
1:N:243:LEU:HG	1:N:267:ILE:HB	1.86	0.57
1:A:87:ASN:O	1:A:113:SER:HB2	2.04	0.57
1:D:122:ILE:HD13	1:K:298:LEU:CD1	2.20	0.57
1:M:137:ASN:C	1:M:137:ASN:ND2	2.59	0.57
1:A:121:ASP:H	1:A:156:ASN:HD21	1.51	0.57
1:A:243:LEU:HD23	1:A:269:MET:CE	2.33	0.57
1:D:151:ALA:HA	1:D:187:ILE:O	2.03	0.57
1:G:125:LEU:C	1:G:125:LEU:HD13	2.30	0.57
1:G:201:GLY:O	1:G:202:GLU:OE1	2.22	0.57
1:L:196:LEU:HD11	1:L:207:ARG:NH2	2.18	0.57
1:O:243:LEU:C	1:O:243:LEU:HD12	2.28	0.57
1:B:204:PHE:HE1	1:B:206:LEU:HB2	1.69	0.57
1:G:111:GLU:HA	1:G:164:VAL:O	2.04	0.57
1:K:190:SER:H	1:K:193:LYS:CB	2.17	0.57
1:M:47:PRO:HA	4:M:415:HOH:O	2.03	0.57
1:M:208:LYS:HE2	1:M:221:HIS:NE2	2.20	0.57
1:J:137:ASN:HD21	1:J:140:SER:N	2.03	0.57
1:K:150:TYR:CE1	1:K:209:LEU:HD22	2.39	0.57
1:P:84:ASP:HB3	4:P:424:HOH:O	2.05	0.57
1:A:268:TRP:CZ2	1:A:270:ALA:HB2	2.40	0.57
1:D:137:ASN:HD22	1:D:137:ASN:N	2.01	0.57
1:L:237:HIS:HB2	1:L:239:ASN:HD22	1.68	0.57
1:O:247:GLU:CG	1:O:286:ARG:HB3	2.33	0.57
1:P:136:THR:O	1:P:137:ASN:HB3	2.05	0.57
1:A:125:LEU:C	1:A:125:LEU:HD13	2.29	0.57
1:E:136:THR:HG23	1:E:160:SER:HB3	1.86	0.57
1:G:164:VAL:CG2	1:G:165:GLU:H	2.11	0.57
1:I:126:ILE:HG22	1:I:171:VAL:HB	1.87	0.57
1:M:79:TYR:HA	1:M:90:GLY:O	2.04	0.57
1:P:243:LEU:HG	1:P:267:ILE:HB	1.86	0.57
1:M:82:LEU:HG	1:M:85:TRP:CD1	2.40	0.57
1:N:152:TYR:HB3	1:N:187:ILE:HB	1.85	0.57
1:O:153:LEU:HD13	1:O:159:HIS:NE2	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:118:PRO:HD3	1:P:124:ARG:NH2	2.19	0.57
1:G:157:PHE:C	1:G:157:PHE:HD2	2.13	0.57
1:G:202:GLU:HB3	1:G:204:PHE:CE2	2.40	0.57
1:J:118:PRO:HB2	1:J:122:ILE:HB	1.86	0.57
1:J:218:PHE:CD1	1:J:218:PHE:C	2.82	0.57
1:J:234:LYS:HG2	1:K:61:THR:HB	1.87	0.57
1:O:72:ILE:HD12	1:O:72:ILE:N	2.19	0.57
1:K:204:PHE:CZ	1:K:223:MET:HE3	2.40	0.56
1:F:164:VAL:HG23	1:F:165:GLU:H	1.70	0.56
1:I:284:ARG:HD2	1:I:284:ARG:C	2.29	0.56
1:J:134:THR:HG23	1:J:144:LYS:HA	1.86	0.56
1:A:101:HIS:H	1:A:240:GLN:HE22	1.52	0.56
1:A:241:HIS:CG	1:A:289:LEU:HD11	2.40	0.56
1:D:136:THR:HG22	1:D:142:SER:HB2	1.86	0.56
1:D:196:LEU:CD1	1:D:207:ARG:NH2	2.67	0.56
1:F:153:LEU:HD13	1:F:159:HIS:NE2	2.20	0.56
1:F:164:VAL:HG23	1:F:165:GLU:N	2.20	0.56
1:J:241:HIS:CG	1:J:289:LEU:HD11	2.41	0.56
1:J:286:ARG:HG3	1:J:287:TYR:N	2.19	0.56
1:K:82:LEU:HD12	1:K:83:PRO:HD2	1.88	0.56
1:L:234:LYS:HD2	1:L:234:LYS:H	1.68	0.56
1:M:202:GLU:OE2	1:M:233:VAL:HG12	2.05	0.56
1:D:284:ARG:NH2	1:D:286:ARG:HH12	2.04	0.56
1:F:153:LEU:HD22	1:F:159:HIS:CG	2.40	0.56
1:J:94:ILE:O	1:J:103:VAL:HA	2.05	0.56
1:M:243:LEU:C	1:M:243:LEU:HD12	2.31	0.56
1:P:87:ASN:C	1:P:87:ASN:HD22	2.13	0.56
1:G:202:GLU:OE1	1:G:232:ASN:HB2	2.04	0.56
1:J:209:LEU:O	1:J:210:LEU:HD23	2.04	0.56
1:M:222:THR:HG23	1:M:286:ARG:HD2	1.88	0.56
1:O:164:VAL:HG23	1:O:165:GLU:N	2.19	0.56
1:I:280:LEU:HD21	1:J:280:LEU:HD21	1.88	0.56
1:B:113:SER:OG	1:B:163:CYS:HB3	2.06	0.56
1:J:208:LYS:NZ	1:J:212:MET:HE3	2.20	0.56
1:K:105:TYR:CE1	1:K:171:VAL:HG13	2.41	0.56
1:K:247:GLU:O	1:K:285:SER:HA	2.05	0.56
1:L:126:ILE:HG22	1:L:171:VAL:HB	1.87	0.56
1:E:251:ILE:HD13	1:E:260:PRO:HA	1.88	0.56
1:K:120:GLN:HG3	1:K:156:ASN:ND2	2.21	0.56
1:L:245:LEU:HD12	1:L:287:TYR:HB3	1.88	0.56
1:A:83:PRO:O	1:A:84:ASP:HB2	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:126:ILE:HG22	1:E:171:VAL:HB	1.88	0.56
1:F:208:LYS:HZ3	1:F:212:MET:HE3	1.70	0.56
1:L:82:LEU:HD21	1:L:105:TYR:CE1	2.41	0.56
1:O:93:LEU:HD13	1:O:266:VAL:HG21	1.87	0.56
1:P:243:LEU:HB3	1:P:289:LEU:HD12	1.88	0.56
1:B:276:TRP:CH2	1:B:278:ALA:HB2	2.41	0.56
1:E:69:HIS:HA	1:E:268:TRP:O	2.04	0.56
1:H:133:VAL:HG23	1:H:162:ASP:O	2.06	0.56
1:I:202:GLU:OE1	1:I:231:LEU:HD23	2.06	0.56
1:K:140:SER:O	1:K:141:SER:HB2	2.05	0.56
1:K:243:LEU:HD23	1:K:269:MET:HE1	1.88	0.56
1:A:87:ASN:O	1:A:87:ASN:CG	2.49	0.55
1:F:214:VAL:HG13	1:F:215:ALA:N	2.20	0.55
1:G:96:PRO:HD3	1:G:103:VAL:HG12	1.88	0.55
1:N:224:ASP:OD2	1:N:286:ARG:NE	2.39	0.55
1:A:296:ASN:HD22	1:A:298:LEU:N	2.04	0.55
1:F:170:VAL:O	1:F:170:VAL:HG13	2.06	0.55
1:I:49:LEU:HD22	1:K:54:LEU:CD2	2.37	0.55
1:M:83:PRO:O	1:M:84:ASP:HB2	2.05	0.55
1:H:136:THR:HG22	1:H:137:ASN:N	2.19	0.55
1:J:86:THR:O	1:J:87:ASN:C	2.49	0.55
1:K:153:LEU:HD22	1:K:159:HIS:CG	2.41	0.55
1:B:234:LYS:HE3	1:C:60:PHE:O	2.05	0.55
1:E:153:LEU:HD13	1:E:159:HIS:CD2	2.42	0.55
1:F:150:TYR:CD1	1:F:209:LEU:HD13	2.42	0.55
1:G:137:ASN:HB2	4:G:426:HOH:O	2.07	0.55
1:H:207:ARG:HG3	1:H:207:ARG:HH11	1.70	0.55
1:F:126:ILE:HG12	1:F:161:LEU:HD11	1.88	0.55
1:I:137:ASN:HD22	1:I:137:ASN:H	1.55	0.55
1:L:150:TYR:CZ	1:L:209:LEU:HB3	2.41	0.55
1:M:93:LEU:CD1	1:M:104:MET:HE2	2.27	0.55
1:D:296:ASN:ND2	1:D:298:LEU:HB2	2.21	0.55
1:E:243:LEU:HD12	1:E:243:LEU:C	2.30	0.55
1:G:150:TYR:CE2	1:G:209:LEU:HB3	2.42	0.55
1:H:153:LEU:HD22	1:H:159:HIS:CG	2.42	0.55
1:A:121:ASP:H	1:A:156:ASN:ND2	2.04	0.55
1:C:245:LEU:HD12	1:C:287:TYR:HB3	1.88	0.55
1:C:252:TYR:CD1	1:C:277:TYR:CD1	2.95	0.55
1:E:204:PHE:CZ	1:E:223:MET:HE3	2.41	0.55
1:K:164:VAL:HG23	1:K:165:GLU:H	1.71	0.55
1:P:121:ASP:H	1:P:156:ASN:ND2	2.02	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:191:THR:HG21	1:G:286:ARG:HH12	1.72	0.55
1:P:95:THR:O	1:P:98:THR:HG23	2.06	0.55
1:C:153:LEU:HD13	1:C:159:HIS:CG	2.42	0.55
1:H:243:LEU:HD12	1:H:244:LEU:N	2.22	0.55
1:J:296:ASN:HD21	1:J:298:LEU:HD12	1.72	0.55
1:A:153:LEU:HD13	1:A:159:HIS:CE1	2.42	0.55
1:G:286:ARG:HG3	1:G:286:ARG:O	2.06	0.55
1:L:245:LEU:HD23	1:L:262:GLN:C	2.32	0.55
1:P:70:ALA:HB3	1:P:268:TRP:HB3	1.88	0.55
1:P:133:VAL:CG1	1:P:163:CYS:HB2	2.27	0.55
1:L:101:HIS:H	1:L:240:GLN:HE22	1.53	0.54
1:D:243:LEU:C	1:D:243:LEU:HD12	2.32	0.54
1:J:235:GLU:OE1	3:J:302:UGY:N	2.40	0.54
1:O:150:TYR:CZ	1:O:209:LEU:HB3	2.41	0.54
1:A:224:ASP:OD2	1:A:286:ARG:HB2	2.07	0.54
1:C:185:GLU:O	1:C:187:ILE:HG12	2.08	0.54
1:F:86:THR:O	1:F:113:SER:HB2	2.07	0.54
1:K:150:TYR:CE2	1:K:209:LEU:HB3	2.42	0.54
1:L:103:VAL:CG2	1:L:173:GLU:HB2	2.37	0.54
1:K:100:SER:HA	1:K:240:GLN:HE22	1.72	0.54
1:K:144:LYS:HG2	1:K:144:LYS:O	2.05	0.54
1:N:130:GLU:HA	1:N:147:VAL:HG22	1.89	0.54
1:F:93:LEU:HD13	1:F:266:VAL:HG11	1.88	0.54
1:F:245:LEU:HD23	1:F:262:GLN:C	2.32	0.54
1:M:276:TRP:CH2	1:M:278:ALA:HB2	2.43	0.54
1:B:127:PHE:HB3	1:B:170:VAL:CG1	2.37	0.54
1:K:206:LEU:HD12	1:K:207:ARG:N	2.22	0.54
1:C:130:GLU:O	1:C:167:ALA:HA	2.07	0.54
1:D:125:LEU:C	1:D:125:LEU:HD13	2.32	0.54
1:B:150:TYR:CE1	1:B:209:LEU:HD22	2.42	0.54
1:G:137:ASN:HB3	1:G:140:SER:OG	2.07	0.54
1:H:126:ILE:HG22	1:H:171:VAL:HB	1.89	0.54
1:H:296:ASN:HD21	1:H:298:LEU:HB3	1.70	0.54
1:L:113:SER:OG	1:L:163:CYS:HB3	2.07	0.54
1:O:150:TYR:CE2	1:O:209:LEU:HB3	2.43	0.54
1:E:125:LEU:HD13	1:E:126:ILE:N	2.22	0.54
1:K:140:SER:O	1:K:141:SER:CB	2.55	0.54
1:N:164:VAL:HG23	1:N:165:GLU:H	1.72	0.54
1:N:271:PRO:O	1:N:272:PHE:HB2	2.07	0.54
1:E:74:PRO:O	1:E:76:SER:N	2.41	0.53
1:H:79:TYR:CD1	1:H:91:ALA:HB2	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:113:SER:OG	1:H:163:CYS:HB3	2.08	0.53
1:I:204:PHE:HB3	1:I:225:PHE:CE1	2.43	0.53
1:L:104:MET:HE1	1:L:266:VAL:HG13	1.91	0.53
1:N:243:LEU:HD13	1:N:287:TYR:HB2	1.90	0.53
1:P:245:LEU:HD23	1:P:262:GLN:C	2.34	0.53
1:B:95:THR:C	1:B:97:ALA:H	2.15	0.53
1:E:243:LEU:HD23	1:E:269:MET:HE2	1.90	0.53
1:F:70:ALA:HB3	1:F:268:TRP:HB3	1.90	0.53
1:F:136:THR:HG23	1:F:160:SER:O	2.09	0.53
1:G:226:GLN:O	1:G:229:GLU:HG3	2.08	0.53
1:A:61:THR:HB	1:D:234:LYS:HG2	1.90	0.53
1:C:276:TRP:CH2	1:C:278:ALA:HB2	2.43	0.53
1:C:241:HIS:CG	1:C:269:MET:HE3	2.43	0.53
1:D:54:LEU:HD23	1:G:49:LEU:HD22	1.89	0.53
1:K:213:SER:O	1:K:215:ALA:N	2.40	0.53
1:K:243:LEU:HD22	1:K:287:TYR:CD1	2.43	0.53
1:P:111:GLU:CD	1:P:111:GLU:N	2.65	0.53
1:C:234:LYS:HE3	1:G:60:PHE:O	2.08	0.53
1:J:145:LEU:HD22	1:J:149:SER:OG	2.08	0.53
1:K:190:SER:O	1:K:191:THR:C	2.51	0.53
1:L:125:LEU:C	1:L:125:LEU:HD13	2.33	0.53
1:O:185:GLU:O	1:O:187:ILE:HG12	2.09	0.53
1:P:296:ASN:ND2	1:P:298:LEU:HB2	2.24	0.53
1:E:82:LEU:O	1:E:85:TRP:HB2	2.08	0.53
1:E:202:GLU:OE2	1:E:233:VAL:HG12	2.09	0.53
1:E:208:LYS:NZ	1:E:212:MET:CE	2.72	0.53
1:I:241:HIS:HB2	1:I:269:MET:HB2	1.90	0.53
1:L:238:TYR:O	1:L:271:PRO:HB3	2.08	0.53
1:B:140:SER:O	1:B:141:SER:CB	2.57	0.53
1:E:63:SER:HA	1:E:71:LEU:O	2.09	0.53
1:C:243:LEU:HB2	1:C:288:LEU:O	2.09	0.53
1:D:68:ASP:OD2	1:D:273:VAL:HG23	2.09	0.53
1:D:127:PHE:HB3	1:D:170:VAL:HG13	1.90	0.53
1:E:74:PRO:C	1:E:76:SER:H	2.17	0.53
1:F:243:LEU:HG	1:F:267:ILE:HB	1.91	0.53
1:G:246:LEU:HD11	1:G:288:LEU:HD13	1.90	0.53
1:K:213:SER:C	1:K:215:ALA:H	2.16	0.53
1:N:152:TYR:HB2	1:N:210:LEU:HD21	1.91	0.53
1:P:116:GLY:HA2	4:P:424:HOH:O	2.09	0.53
1:P:191:THR:HG21	1:P:286:ARG:HH21	1.71	0.53
1:J:298:LEU:HD11	1:K:122:ILE:HG21	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:252:TYR:CD1	1:K:277:TYR:CD1	2.97	0.53
1:M:152:TYR:HB3	1:M:187:ILE:HB	1.91	0.53
1:P:127:PHE:HB3	1:P:170:VAL:CG1	2.39	0.53
1:A:82:LEU:CD1	1:A:90:GLY:HA3	2.38	0.53
1:E:52:SER:C	1:E:54:LEU:H	2.17	0.53
1:E:243:LEU:HD23	1:E:269:MET:CE	2.39	0.53
1:G:237:HIS:ND1	1:G:239:ASN:HB2	2.24	0.53
1:G:241:HIS:HB3	1:G:289:LEU:HD11	1.89	0.53
1:J:169:LEU:N	1:J:169:LEU:CD2	2.67	0.53
1:K:211:PRO:HB2	1:K:216:TYR:CE2	2.37	0.53
1:N:87:ASN:ND2	1:N:111:GLU:O	2.39	0.53
1:C:82:LEU:O	1:C:85:TRP:HB2	2.09	0.52
1:E:61:THR:HG22	1:P:253:ARG:NH1	2.22	0.52
1:G:156:ASN:HA	4:G:413:HOH:O	2.10	0.52
1:K:103:VAL:HG22	1:K:173:GLU:HB2	1.91	0.52
1:K:128:VAL:HG22	1:K:169:LEU:HD21	1.89	0.52
1:B:83:PRO:O	1:B:85:TRP:HD1	1.92	0.52
1:B:243:LEU:C	1:B:243:LEU:HD12	2.35	0.52
1:E:117:LEU:HD21	1:E:159:HIS:H	1.74	0.52
1:J:150:TYR:CE2	1:J:209:LEU:HB3	2.44	0.52
1:J:206:LEU:HD12	1:J:207:ARG:H	1.73	0.52
1:D:61:THR:HG22	1:K:253:ARG:NH1	2.24	0.52
1:E:114:SER:HA	1:E:161:LEU:O	2.09	0.52
1:H:207:ARG:HG3	1:H:207:ARG:NH1	2.24	0.52
1:K:113:SER:OG	1:K:163:CYS:HB3	2.09	0.52
1:K:224:ASP:OD2	1:K:286:ARG:CD	2.50	0.52
1:O:103:VAL:HG22	1:O:173:GLU:HB2	1.90	0.52
1:O:134:THR:OG1	1:O:144:LYS:HG2	2.09	0.52
1:O:267:ILE:HG21	1:O:269:MET:HE2	1.91	0.52
1:D:273:VAL:HG13	1:D:273:VAL:O	2.09	0.52
1:E:60:PHE:HZ	1:M:60:PHE:HZ	1.55	0.52
1:H:125:LEU:HD22	1:H:151:ALA:O	2.10	0.52
1:K:276:TRP:CH2	1:K:278:ALA:HB2	2.45	0.52
1:H:243:LEU:HD23	1:H:269:MET:HE1	1.91	0.52
1:I:126:ILE:C	1:I:126:ILE:HD12	2.34	0.52
1:J:268:TRP:CZ2	1:J:270:ALA:HB2	2.44	0.52
1:L:125:LEU:HD23	1:L:152:TYR:HB2	1.91	0.52
1:O:170:VAL:HG13	1:O:170:VAL:O	2.10	0.52
1:D:241:HIS:HB2	1:D:269:MET:HB2	1.92	0.52
1:K:290:TYR:C	1:K:290:TYR:CD2	2.87	0.52
1:O:121:ASP:H	1:O:156:ASN:ND2	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:127:PHE:HB3	1:C:170:VAL:CG1	2.40	0.52
1:H:241:HIS:HB3	1:H:289:LEU:HD11	1.91	0.52
1:N:131:GLY:HA3	1:N:167:ALA:HA	1.91	0.52
1:O:243:LEU:HB2	1:O:288:LEU:O	2.10	0.52
1:P:136:THR:O	1:P:137:ASN:CB	2.57	0.52
1:B:79:TYR:HA	1:B:90:GLY:O	2.10	0.52
1:K:74:PRO:C	1:K:76:SER:H	2.18	0.52
1:M:198:GLU:HG2	1:M:200:PRO:HD3	1.92	0.52
1:F:64:VAL:HG11	1:F:66:LYS:NZ	2.25	0.52
1:P:150:TYR:CZ	1:P:209:LEU:HB3	2.45	0.52
1:P:154:PRO:HB3	1:P:155:PRO:HD2	1.91	0.52
1:A:94:ILE:HD11	1:A:268:TRP:HB2	1.92	0.51
1:A:243:LEU:HG	1:A:267:ILE:HB	1.92	0.51
1:B:92:TYR:HA	1:B:105:TYR:HB3	1.92	0.51
1:C:152:TYR:HB3	1:C:187:ILE:HB	1.92	0.51
1:F:298:LEU:HD11	1:L:173:GLU:HB3	1.92	0.51
1:H:120:GLN:HG2	1:H:121:ASP:OD1	2.11	0.51
1:J:101:HIS:C	1:J:101:HIS:CD2	2.89	0.51
1:P:191:THR:HG22	1:P:207:ARG:HD2	1.91	0.51
1:A:243:LEU:HD12	1:A:243:LEU:C	2.36	0.51
1:A:243:LEU:HD21	1:A:252:TYR:CE1	2.45	0.51
1:E:241:HIS:HB2	1:E:269:MET:HB2	1.90	0.51
1:K:92:TYR:CE1	1:K:105:TYR:CD2	2.94	0.51
1:L:127:PHE:HB3	1:L:170:VAL:CG1	2.39	0.51
1:M:128:VAL:HA	1:M:169:LEU:HD12	1.92	0.51
1:N:142:SER:C	1:N:143:LYS:HD2	2.34	0.51
1:C:243:LEU:C	1:C:243:LEU:HD12	2.35	0.51
1:J:72:ILE:HD12	1:J:72:ILE:N	2.25	0.51
1:J:294:ASN:O	1:J:295:ARG:HG2	2.10	0.51
1:K:105:TYR:HE1	1:K:171:VAL:HG13	1.75	0.51
1:C:225:PHE:HB2	1:C:285:SER:HB2	1.92	0.51
1:K:273:VAL:O	1:K:273:VAL:HG13	2.10	0.51
1:P:94:ILE:HD12	1:P:104:MET:HE2	1.93	0.51
1:B:241:HIS:CE1	1:B:289:LEU:HD21	2.46	0.51
1:G:226:GLN:HB2	1:G:229:GLU:CD	2.36	0.51
1:H:245:LEU:HD23	1:H:262:GLN:C	2.35	0.51
1:I:125:LEU:C	1:I:125:LEU:HD13	2.35	0.51
1:J:141:SER:O	1:J:142:SER:HB2	2.11	0.51
1:L:134:THR:HG23	1:L:143:LYS:O	2.10	0.51
1:M:94:ILE:O	1:M:103:VAL:HA	2.11	0.51
1:P:82:LEU:CD1	1:P:90:GLY:HA3	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:130:GLU:HA	1:P:147:VAL:HG13	1.93	0.51
1:D:72:ILE:HD12	1:D:72:ILE:N	2.26	0.51
1:G:191:THR:HG21	1:G:286:ARG:NH1	2.26	0.51
1:L:207:ARG:HB2	1:L:222:THR:HG22	1.90	0.51
1:O:52:SER:O	1:O:55:GLN:HG2	2.10	0.51
1:O:109:MET:HB3	1:O:113:SER:OG	2.10	0.51
1:O:270:ALA:O	1:O:273:VAL:HG12	2.10	0.51
1:K:296:ASN:ND2	1:K:298:LEU:HD12	2.26	0.51
1:L:208:LYS:NZ	1:L:212:MET:HE3	2.25	0.51
1:P:135:LEU:HD23	1:P:135:LEU:C	2.35	0.51
1:A:152:TYR:HB3	1:A:187:ILE:HB	1.92	0.51
1:E:121:ASP:H	1:E:156:ASN:HD21	1.59	0.51
1:E:164:VAL:HG13	1:E:165:GLU:CG	2.41	0.51
1:E:270:ALA:O	1:E:273:VAL:HG12	2.10	0.51
1:I:82:LEU:CD2	1:I:90:GLY:HA3	2.40	0.51
1:K:202:GLU:OE1	1:K:202:GLU:HA	2.10	0.51
1:M:96:PRO:HD3	1:M:103:VAL:HG12	1.92	0.51
1:G:137:ASN:HB3	1:G:140:SER:CB	2.40	0.51
1:H:224:ASP:OD2	1:H:286:ARG:NH1	2.43	0.51
1:J:109:MET:HB2	1:J:167:ALA:HB3	1.92	0.51
1:K:218:PHE:C	1:K:218:PHE:CD1	2.88	0.51
1:M:140:SER:O	1:M:141:SER:CB	2.59	0.51
1:O:125:LEU:C	1:O:125:LEU:HD13	2.35	0.51
1:D:196:LEU:CD1	1:D:207:ARG:CZ	2.90	0.50
1:G:85:TRP:CE3	1:G:115:SER:HA	2.46	0.50
1:J:125:LEU:HD13	1:J:125:LEU:C	2.36	0.50
1:M:271:PRO:O	1:M:272:PHE:HB2	2.11	0.50
1:N:75:GLU:OE1	1:N:75:GLU:N	2.40	0.50
1:B:118:PRO:HB2	1:B:122:ILE:HB	1.92	0.50
1:D:126:ILE:C	1:D:126:ILE:HD12	2.37	0.50
1:F:186:LEU:O	1:F:187:ILE:HD13	2.11	0.50
1:G:236:VAL:CG2	1:I:76:SER:HB3	2.42	0.50
1:L:137:ASN:HD21	1:L:140:SER:N	2.10	0.50
1:O:153:LEU:HD13	1:O:159:HIS:CD2	2.46	0.50
1:B:111:GLU:H	1:B:111:GLU:CD	2.19	0.50
1:E:164:VAL:HG13	1:E:165:GLU:N	2.26	0.50
1:F:192:ASP:HA	4:F:417:HOH:O	2.10	0.50
1:I:140:SER:O	1:I:141:SER:HB3	2.11	0.50
1:I:170:VAL:HG13	1:I:170:VAL:O	2.11	0.50
1:K:111:GLU:HA	1:K:165:GLU:O	2.11	0.50
1:M:109:MET:HB3	1:M:113:SER:OG	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:118:PRO:HB2	1:P:122:ILE:HB	1.93	0.50
1:L:237:HIS:HB2	1:L:239:ASN:ND2	2.26	0.50
1:O:113:SER:OG	1:O:163:CYS:HB3	2.10	0.50
1:O:137:ASN:OD1	1:O:137:ASN:C	2.53	0.50
1:C:126:ILE:C	1:C:126:ILE:HD12	2.37	0.50
1:D:63:SER:HA	1:D:71:LEU:O	2.11	0.50
1:F:126:ILE:C	1:F:126:ILE:HD12	2.36	0.50
1:L:103:VAL:HG22	1:L:173:GLU:HB2	1.94	0.50
1:L:140:SER:O	1:L:141:SER:CB	2.59	0.50
1:B:146:THR:O	1:B:147:VAL:C	2.55	0.50
1:G:164:VAL:HG23	1:G:165:GLU:HG2	1.94	0.50
1:I:222:THR:HG23	1:I:286:ARG:HD2	1.94	0.50
1:M:137:ASN:HA	1:M:159:HIS:HA	1.93	0.50
1:M:253:ARG:NH1	1:O:61:THR:HG22	2.26	0.50
1:D:61:THR:HB	1:K:234:LYS:HG2	1.93	0.50
1:J:172:PHE:CE1	1:J:290:TYR:HB2	2.46	0.50
1:M:280:LEU:HD21	1:P:280:LEU:HD21	1.92	0.50
1:B:95:THR:O	1:B:97:ALA:N	2.45	0.50
1:D:127:PHE:HB3	1:D:170:VAL:HG12	1.92	0.50
1:F:155:PRO:O	1:F:156:ASN:HB2	2.12	0.50
1:I:72:ILE:HD12	1:I:72:ILE:H	1.74	0.50
1:I:152:TYR:HB3	1:I:187:ILE:HB	1.94	0.50
1:O:238:TYR:CE2	1:O:297:PRO:HB3	2.46	0.50
1:P:126:ILE:HD12	1:P:126:ILE:O	2.12	0.50
1:A:234:LYS:HD3	1:A:234:LYS:N	2.27	0.50
1:A:239:ASN:ND2	1:A:239:ASN:N	2.60	0.50
1:H:253:ARG:NH1	1:M:61:THR:HG22	2.26	0.50
1:J:179:LEU:HG	1:J:179:LEU:O	2.11	0.50
1:L:93:LEU:HD12	1:L:104:MET:HE2	1.93	0.50
1:L:298:LEU:HD13	1:P:122:ILE:HD12	1.94	0.50
1:P:175:ARG:HD3	4:P:426:HOH:O	2.11	0.50
1:E:70:ALA:HB3	1:E:268:TRP:HB3	1.93	0.49
1:F:56:ASP:HB2	1:H:48:THR:HG21	1.92	0.49
1:G:156:ASN:O	1:G:157:PHE:C	2.53	0.49
1:I:142:SER:C	1:I:143:LYS:HD2	2.37	0.49
1:M:218:PHE:CD1	1:M:218:PHE:C	2.90	0.49
1:N:68:ASP:OD2	1:N:273:VAL:HG23	2.11	0.49
1:O:247:GLU:OE2	1:O:284:ARG:NE	2.44	0.49
1:P:156:ASN:O	1:P:157:PHE:C	2.55	0.49
1:B:197:LEU:HB2	1:B:206:LEU:CD2	2.41	0.49
1:B:298:LEU:HD23	1:C:103:VAL:HG13	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:154:PRO:HG2	1:C:185:GLU:CA	2.38	0.49
1:G:134:THR:HG23	1:G:143:LYS:O	2.12	0.49
1:I:83:PRO:C	1:I:85:TRP:H	2.19	0.49
1:I:129:VAL:O	1:I:129:VAL:HG12	2.11	0.49
1:M:82:LEU:O	1:M:85:TRP:HB2	2.12	0.49
1:O:152:TYR:HB3	1:O:187:ILE:HB	1.95	0.49
1:C:74:PRO:C	1:C:76:SER:N	2.69	0.49
1:D:237:HIS:ND1	1:D:239:ASN:HB2	2.28	0.49
1:E:296:ASN:ND2	1:E:298:LEU:HB2	2.27	0.49
1:F:199:THR:HB	1:F:202:GLU:HB2	1.92	0.49
1:J:143:LYS:HG3	1:J:188:VAL:HG11	1.94	0.49
1:J:219:ASN:O	1:J:220:ILE:HD13	2.11	0.49
1:J:224:ASP:CG	1:J:286:ARG:HD3	2.37	0.49
1:O:152:TYR:HB2	1:O:210:LEU:HD21	1.95	0.49
1:O:204:PHE:CE2	1:O:223:MET:HE3	2.47	0.49
1:J:153:LEU:HD23	1:J:153:LEU:N	2.27	0.49
1:K:125:LEU:HD13	1:K:126:ILE:N	2.27	0.49
1:B:204:PHE:CE2	1:B:223:MET:HE3	2.48	0.49
1:F:93:LEU:CD1	1:F:266:VAL:HG21	2.42	0.49
1:M:245:LEU:HD23	1:M:262:GLN:C	2.37	0.49
1:N:87:ASN:HD21	1:N:110:LYS:HB2	1.75	0.49
1:P:133:VAL:O	1:P:145:LEU:HB2	2.12	0.49
1:I:152:TYR:O	1:I:186:LEU:HD12	2.12	0.49
1:L:115:SER:HB3	1:L:161:LEU:HB2	1.94	0.49
1:L:276:TRP:CH2	1:O:251:ILE:HD11	2.48	0.49
1:P:158:HIS:ND1	1:P:159:HIS:N	2.61	0.49
1:B:220:ILE:HD13	1:B:290:TYR:HA	1.95	0.49
1:E:87:ASN:ND2	1:E:110:LYS:HB2	2.28	0.49
1:G:63:SER:HA	1:G:71:LEU:O	2.12	0.49
1:O:81:PRO:O	1:O:83:PRO:HD3	2.13	0.49
1:B:298:LEU:HD11	1:C:122:ILE:HG21	1.95	0.49
1:D:237:HIS:CE1	1:D:239:ASN:HB2	2.48	0.49
1:E:82:LEU:HD23	1:E:85:TRP:CE2	2.48	0.49
1:E:234:LYS:HG2	1:F:61:THR:HB	1.94	0.49
1:G:114:SER:HA	1:G:161:LEU:O	2.13	0.49
1:O:87:ASN:ND2	1:O:110:LYS:HB2	2.26	0.49
1:O:164:VAL:CG2	1:O:165:GLU:N	2.75	0.49
1:B:150:TYR:CZ	1:B:209:LEU:HB3	2.48	0.49
1:C:74:PRO:O	1:C:76:SER:N	2.45	0.49
1:F:185:GLU:O	1:F:187:ILE:HG12	2.12	0.49
1:H:111:GLU:HA	1:H:164:VAL:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:126:ILE:C	1:H:126:ILE:HD12	2.38	0.49
1:I:60:PHE:HZ	1:K:60:PHE:HZ	1.60	0.49
1:I:95:THR:O	1:I:98:THR:HG23	2.12	0.49
1:O:190:SER:HB2	1:O:193:LYS:CG	2.42	0.49
1:P:152:TYR:HB3	1:P:187:ILE:HB	1.95	0.49
1:C:186:LEU:O	1:C:187:ILE:HD13	2.12	0.49
1:D:126:ILE:HD12	1:D:126:ILE:O	2.13	0.49
1:E:62:ARG:NH2	1:E:265:ASP:OD2	2.46	0.49
1:F:54:LEU:CD2	1:H:49:LEU:HD22	2.43	0.49
1:F:121:ASP:H	1:F:156:ASN:ND2	2.11	0.49
1:H:185:GLU:O	1:H:187:ILE:HG12	2.13	0.49
1:I:130:GLU:O	1:I:167:ALA:HA	2.13	0.49
1:I:199:THR:HG21	1:I:204:PHE:O	2.13	0.49
1:J:124:ARG:HD2	1:J:153:LEU:HD12	1.95	0.49
1:O:284:ARG:HD2	1:O:284:ARG:C	2.38	0.49
1:B:270:ALA:O	1:B:273:VAL:HG12	2.13	0.48
1:D:110:LYS:HB2	1:D:110:LYS:HZ3	1.77	0.48
1:G:153:LEU:HD13	1:G:159:HIS:CD2	2.48	0.48
1:J:266:VAL:C	1:J:267:ILE:HD12	2.37	0.48
1:N:40:ILE:HB	1:N:147:VAL:HG11	1.95	0.48
1:N:203:VAL:O	1:N:204:PHE:C	2.56	0.48
1:P:152:TYR:HE2	1:P:184:THR:HB	1.79	0.48
1:F:290:TYR:C	1:F:290:TYR:CD2	2.91	0.48
1:G:111:GLU:O	1:G:112:MET:C	2.55	0.48
1:I:133:VAL:HG23	1:I:163:CYS:HB2	1.95	0.48
1:J:164:VAL:CG2	1:J:165:GLU:HG3	2.43	0.48
1:J:207:ARG:HB2	1:J:222:THR:CG2	2.43	0.48
1:J:207:ARG:HB2	1:J:222:THR:HG22	1.95	0.48
1:K:157:PHE:CZ	1:K:186:LEU:HD22	2.49	0.48
1:L:49:LEU:HD23	1:N:57:LEU:CD1	2.43	0.48
1:O:104:MET:HE3	1:O:172:PHE:CZ	2.49	0.48
1:P:127:PHE:HB3	1:P:170:VAL:HG13	1.95	0.48
1:B:54:LEU:HD23	1:J:49:LEU:HD22	1.94	0.48
1:C:142:SER:O	1:C:143:LYS:HD3	2.13	0.48
1:D:137:ASN:HD21	1:D:140:SER:C	2.22	0.48
1:F:133:VAL:HG21	1:F:161:LEU:HB3	1.95	0.48
1:K:269:MET:SD	1:K:275:GLN:OE1	2.71	0.48
1:L:192:ASP:OD1	1:L:192:ASP:N	2.47	0.48
1:M:232:ASN:O	1:M:234:LYS:HD3	2.14	0.48
1:N:128:VAL:HG22	1:N:169:LEU:HD21	1.95	0.48
1:O:127:PHE:HB3	1:O:170:VAL:CG1	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:SER:HA	1:A:71:LEU:O	2.13	0.48
1:B:130:GLU:HB3	1:B:168:THR:HB	1.95	0.48
1:C:85:TRP:CE3	1:C:88:THR:HG21	2.47	0.48
1:K:128:VAL:HG22	1:K:169:LEU:CD2	2.43	0.48
1:M:241:HIS:CG	1:M:289:LEU:HD11	2.48	0.48
1:M:252:TYR:OH	1:M:269:MET:HE1	2.13	0.48
1:A:58:PRO:HG3	1:D:230:PHE:CZ	2.48	0.48
1:B:153:LEU:HD13	1:B:159:HIS:CD2	2.48	0.48
1:B:222:THR:CG2	1:B:286:ARG:HD2	2.38	0.48
1:G:93:LEU:HD13	1:G:266:VAL:HG21	1.95	0.48
1:G:243:LEU:HD23	1:G:269:MET:HE1	1.95	0.48
1:H:214:VAL:HG13	1:H:215:ALA:N	2.28	0.48
1:I:186:LEU:O	1:I:187:ILE:HD13	2.12	0.48
1:J:151:ALA:HA	1:J:187:ILE:O	2.14	0.48
1:J:152:TYR:O	1:J:153:LEU:HD23	2.12	0.48
1:M:85:TRP:CE3	1:M:88:THR:HG21	2.48	0.48
1:D:226:GLN:HB2	1:D:229:GLU:OE1	2.14	0.48
1:F:111:GLU:H	1:F:111:GLU:HG2	1.36	0.48
1:I:243:LEU:HD12	1:I:243:LEU:C	2.37	0.48
1:J:297:PRO:HG3	1:K:92:TYR:CZ	2.48	0.48
1:K:87:ASN:CG	1:K:110:LYS:HB2	2.37	0.48
1:N:87:ASN:CG	1:N:110:LYS:HB2	2.37	0.48
1:N:137:ASN:OD1	1:N:140:SER:HB3	2.14	0.48
1:P:197:LEU:N	1:P:197:LEU:CD1	2.77	0.48
1:F:143:LYS:HD3	1:F:188:VAL:HG11	1.95	0.48
1:I:56:ASP:O	1:K:262:GLN:HB3	2.13	0.48
1:K:110:LYS:N	1:K:110:LYS:HD2	2.28	0.48
1:K:237:HIS:CE1	1:K:239:ASN:HB2	2.49	0.48
1:M:258:TRP:HB2	1:P:258:TRP:CD1	2.48	0.48
1:A:49:LEU:H	1:A:262:GLN:HE22	1.62	0.48
1:A:75:GLU:OE1	1:A:75:GLU:N	2.37	0.48
1:D:93:LEU:C	1:D:94:ILE:HG13	2.39	0.48
1:H:125:LEU:HD13	1:H:125:LEU:C	2.38	0.48
1:L:80:SER:O	1:L:81:PRO:C	2.56	0.48
1:M:130:GLU:O	1:M:167:ALA:HA	2.13	0.48
1:M:241:HIS:ND1	1:M:289:LEU:HD11	2.28	0.48
1:P:64:VAL:HG12	1:P:66:LYS:HG3	1.96	0.48
1:P:124:ARG:HG2	1:P:125:LEU:N	2.28	0.48
1:P:197:LEU:N	1:P:197:LEU:HD12	2.28	0.48
1:A:204:PHE:CE1	1:A:223:MET:HE3	2.48	0.48
1:A:277:TYR:CG	1:A:278:ALA:N	2.82	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:137:ASN:CG	1:B:140:SER:HA	2.38	0.48
1:C:104:MET:HE2	1:C:172:PHE:HE1	1.78	0.48
1:D:199:THR:HG21	1:D:204:PHE:CE1	2.49	0.48
1:D:206:LEU:HD12	1:D:207:ARG:N	2.28	0.48
1:D:296:ASN:ND2	1:D:298:LEU:N	2.49	0.48
1:F:121:ASP:H	1:F:156:ASN:HD21	1.62	0.48
1:H:41:TYR:CD2	1:H:246:LEU:HB3	2.49	0.48
1:H:41:TYR:CZ	1:H:246:LEU:HD13	2.49	0.48
1:J:245:LEU:HA	1:J:287:TYR:HB3	1.95	0.48
1:M:64:VAL:HG21	1:M:66:LYS:HE3	1.95	0.48
1:O:196:LEU:C	1:O:197:LEU:HD23	2.39	0.48
1:B:137:ASN:CB	1:B:140:SER:HA	2.43	0.48
1:J:270:ALA:O	1:J:273:VAL:HG12	2.13	0.48
1:L:207:ARG:HB2	1:L:222:THR:CG2	2.44	0.48
1:L:262:GLN:HB3	1:N:56:ASP:O	2.14	0.48
1:M:226:GLN:HB2	1:M:229:GLU:CD	2.38	0.48
1:P:83:PRO:O	1:P:84:ASP:HB2	2.14	0.48
1:C:153:LEU:HD13	1:C:159:HIS:CE1	2.49	0.47
1:D:125:LEU:HD13	1:D:126:ILE:N	2.30	0.47
1:E:59:GLY:O	1:P:253:ARG:NH1	2.47	0.47
1:G:209:LEU:O	1:G:210:LEU:HD23	2.13	0.47
1:I:164:VAL:HG23	1:I:165:GLU:N	2.29	0.47
1:J:245:LEU:HD23	1:J:262:GLN:C	2.39	0.47
1:N:140:SER:O	1:N:141:SER:HB3	2.13	0.47
1:H:270:ALA:O	1:H:273:VAL:HG12	2.14	0.47
1:J:92:TYR:HA	1:J:105:TYR:HB3	1.95	0.47
1:K:66:LYS:HD2	1:K:69:HIS:HE1	1.73	0.47
1:L:137:ASN:HB3	1:L:159:HIS:HA	1.96	0.47
1:N:217:ASP:O	1:N:218:PHE:HB3	2.13	0.47
1:O:238:TYR:CD2	1:O:297:PRO:HB3	2.49	0.47
1:A:101:HIS:O	1:A:174:ARG:HG3	2.14	0.47
1:D:137:ASN:N	1:D:137:ASN:ND2	2.63	0.47
1:G:222:THR:O	1:G:222:THR:HG22	2.13	0.47
1:N:125:LEU:C	1:N:125:LEU:HD13	2.39	0.47
1:D:243:LEU:HG	1:D:267:ILE:HB	1.96	0.47
1:E:52:SER:O	1:E:55:GLN:HG2	2.15	0.47
1:J:203:VAL:HG11	1:J:229:GLU:OE2	2.14	0.47
1:L:276:TRP:HH2	1:O:251:ILE:HD11	1.78	0.47
1:N:237:HIS:CE1	1:N:239:ASN:HB2	2.49	0.47
1:N:276:TRP:CH2	1:N:278:ALA:HB2	2.50	0.47
1:A:116:GLY:O	1:A:117:LEU:C	2.57	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:118:PRO:O	1:D:119:PRO:O	2.32	0.47
1:D:152:TYR:HB3	1:D:187:ILE:HB	1.96	0.47
1:F:64:VAL:HG11	1:F:66:LYS:HZ2	1.78	0.47
1:I:118:PRO:HB2	1:I:122:ILE:HB	1.95	0.47
1:J:276:TRP:CH2	1:J:278:ALA:HB2	2.49	0.47
1:O:147:VAL:O	1:O:148:ASP:CB	2.62	0.47
1:O:249:GLN:N	1:O:249:GLN:CD	2.72	0.47
1:P:41:TYR:CE1	1:P:246:LEU:HD13	2.50	0.47
1:E:88:THR:HA	1:E:108:LYS:O	2.13	0.47
1:E:88:THR:OG1	1:E:109:MET:HG2	2.15	0.47
1:E:109:MET:O	1:E:166:SER:HA	2.14	0.47
1:G:175:ARG:HG3	1:G:175:ARG:NH1	2.26	0.47
1:J:290:TYR:CD2	1:J:291:LYS:N	2.83	0.47
1:B:70:ALA:HB3	1:B:268:TRP:HB3	1.96	0.47
1:E:95:THR:O	1:E:97:ALA:N	2.48	0.47
1:F:182:HIS:CE1	1:F:214:VAL:HG11	2.49	0.47
1:G:68:ASP:HB2	1:G:273:VAL:HB	1.97	0.47
1:G:219:ASN:O	1:G:220:ILE:HD13	2.14	0.47
1:K:87:ASN:HD21	1:K:110:LYS:HB2	1.73	0.47
1:L:276:TRP:CH2	1:L:278:ALA:HB2	2.50	0.47
1:M:126:ILE:C	1:M:126:ILE:HD12	2.40	0.47
1:M:170:VAL:O	1:M:170:VAL:HG13	2.14	0.47
1:N:86:THR:O	1:N:113:SER:HA	2.14	0.47
1:N:197:LEU:HD22	1:N:208:LYS:HG3	1.97	0.47
1:O:145:LEU:N	1:O:145:LEU:HD12	2.30	0.47
1:O:245:LEU:HD12	1:O:287:TYR:HB3	1.97	0.47
1:B:125:LEU:HD13	1:B:126:ILE:N	2.30	0.47
1:D:224:ASP:OD1	1:D:286:ARG:NH1	2.48	0.47
1:I:262:GLN:O	1:I:263:ALA:C	2.57	0.47
1:J:283:THR:HB	4:J:417:HOH:O	2.13	0.47
1:P:96:PRO:HA	1:P:100:SER:O	2.15	0.47
1:A:251:ILE:HG12	1:A:280:LEU:CD1	2.45	0.47
1:D:194:GLN:NE2	1:D:194:GLN:HA	2.30	0.47
1:F:214:VAL:CG1	1:F:215:ALA:N	2.77	0.47
1:G:108:LYS:HD3	1:G:168:THR:HG23	1.97	0.47
1:H:243:LEU:HD23	1:H:269:MET:CE	2.44	0.47
1:K:125:LEU:HD13	1:K:125:LEU:C	2.40	0.47
1:L:73:THR:HB	1:L:74:PRO:HD2	1.96	0.47
1:M:153:LEU:HD13	1:M:159:HIS:NE2	2.30	0.47
1:P:238:TYR:C	1:P:238:TYR:CD2	2.93	0.47
1:B:161:LEU:HD13	1:B:169:LEU:HD21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:245:LEU:HD23	1:K:262:GLN:C	2.40	0.47
1:N:62:ARG:HD3	4:N:404:HOH:O	2.15	0.47
1:O:82:LEU:HD13	1:O:90:GLY:HA3	1.97	0.47
1:C:204:PHE:CD1	1:C:223:MET:HE3	2.51	0.46
1:F:40:ILE:HG22	1:F:41:TYR:CG	2.50	0.46
1:G:127:PHE:CE1	1:G:288:LEU:HD11	2.50	0.46
1:G:234:LYS:HE3	1:I:60:PHE:O	2.15	0.46
1:J:298:LEU:HD23	1:K:103:VAL:HG13	1.96	0.46
1:K:225:PHE:HB2	1:K:279:ALA:HB2	1.97	0.46
1:L:171:VAL:CG2	1:L:172:PHE:N	2.78	0.46
1:O:208:LYS:HE3	4:O:413:HOH:O	2.16	0.46
1:P:82:LEU:HD11	1:P:90:GLY:HA3	1.97	0.46
1:P:101:HIS:C	1:P:101:HIS:CD2	2.93	0.46
1:P:137:ASN:CA	1:P:159:HIS:HA	2.37	0.46
1:P:243:LEU:O	1:P:266:VAL:HG13	2.15	0.46
1:E:150:TYR:CE2	1:E:209:LEU:HB3	2.50	0.46
1:G:110:LYS:HA	1:G:110:LYS:HE2	1.96	0.46
1:H:63:SER:HA	1:H:71:LEU:O	2.15	0.46
1:H:82:LEU:CD1	1:H:83:PRO:HD2	2.36	0.46
1:I:150:TYR:CE2	1:I:209:LEU:HB3	2.51	0.46
1:N:170:VAL:O	1:N:170:VAL:HG13	2.15	0.46
1:O:137:ASN:ND2	1:O:140:SER:HB2	2.29	0.46
1:C:85:TRP:CE3	1:C:115:SER:HA	2.50	0.46
1:C:284:ARG:NH2	1:C:286:ARG:NH1	2.64	0.46
1:J:82:LEU:HD13	1:J:90:GLY:CA	2.39	0.46
1:A:136:THR:HG22	1:A:142:SER:CB	2.45	0.46
1:A:239:ASN:HD22	1:A:239:ASN:N	2.02	0.46
1:B:196:LEU:HD12	1:B:205:GLU:HB3	1.97	0.46
1:B:226:GLN:HB2	1:B:229:GLU:CD	2.40	0.46
1:D:61:THR:HG22	1:K:253:ARG:HH12	1.80	0.46
1:E:52:SER:C	1:E:54:LEU:N	2.71	0.46
1:E:154:PRO:HD3	1:E:186:LEU:HA	1.96	0.46
1:G:166:SER:O	1:G:167:ALA:HB2	2.14	0.46
1:I:119:PRO:HD2	1:I:122:ILE:HG13	1.97	0.46
1:K:93:LEU:CD1	1:K:266:VAL:HG21	2.45	0.46
1:L:117:LEU:HD21	1:L:158:HIS:CD2	2.51	0.46
1:C:243:LEU:HB3	1:C:289:LEU:HD12	1.98	0.46
1:I:70:ALA:HB3	1:I:268:TRP:HB3	1.98	0.46
1:B:204:PHE:CE1	1:B:206:LEU:HB2	2.48	0.46
1:C:252:TYR:CD1	1:C:277:TYR:HD1	2.34	0.46
1:D:284:ARG:NH2	1:D:286:ARG:NH1	2.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:233:VAL:O	1:E:233:VAL:HG13	2.15	0.46
1:I:109:MET:HB3	1:I:113:SER:HG	1.79	0.46
1:J:114:SER:HA	1:J:161:LEU:O	2.16	0.46
1:O:85:TRP:CD1	1:O:116:GLY:H	2.33	0.46
1:B:130:GLU:C	1:B:130:GLU:CD	2.84	0.46
1:E:62:ARG:HH22	1:E:265:ASP:CG	2.24	0.46
1:J:203:VAL:O	1:J:203:VAL:HG12	2.15	0.46
1:M:70:ALA:HB3	1:M:268:TRP:HB3	1.98	0.46
1:N:151:ALA:HA	1:N:187:ILE:O	2.16	0.46
1:O:202:GLU:OE2	1:O:233:VAL:HG12	2.15	0.46
1:A:184:THR:HG22	1:A:216:TYR:CE1	2.51	0.46
1:C:95:THR:O	1:C:97:ALA:N	2.49	0.46
1:F:141:SER:HB3	1:F:142:SER:H	1.55	0.46
1:F:204:PHE:HE1	1:F:206:LEU:HB2	1.81	0.46
1:H:224:ASP:OD1	1:H:286:ARG:CD	2.58	0.46
1:J:176:TYR:CE2	1:J:178:TYR:HA	2.43	0.46
1:K:123:GLU:HG2	1:K:174:ARG:O	2.14	0.46
1:M:273:VAL:HG13	1:M:273:VAL:O	2.14	0.46
1:D:103:VAL:CG2	1:D:173:GLU:HB2	2.46	0.46
1:D:153:LEU:HD13	1:D:159:HIS:CG	2.50	0.46
1:E:96:PRO:HA	1:E:100:SER:O	2.16	0.46
1:G:204:PHE:CD1	1:G:223:MET:HE3	2.51	0.46
1:G:206:LEU:HD21	1:G:208:LYS:HE2	1.98	0.46
1:J:170:VAL:HG13	1:J:170:VAL:O	2.15	0.46
1:K:164:VAL:CG2	1:K:165:GLU:N	2.78	0.46
1:K:194:GLN:HE21	1:K:194:GLN:HA	1.78	0.46
1:M:204:PHE:CZ	1:M:223:MET:HE3	2.51	0.46
1:O:96:PRO:HD3	1:O:103:VAL:HG12	1.97	0.46
1:P:204:PHE:HB3	1:P:225:PHE:CE1	2.51	0.46
1:A:54:LEU:CD2	1:C:49:LEU:HD22	2.46	0.46
1:A:82:LEU:HD12	1:A:82:LEU:HA	1.85	0.46
1:B:95:THR:C	1:B:97:ALA:N	2.73	0.46
1:L:241:HIS:HB2	1:L:269:MET:HB2	1.97	0.46
1:D:179:LEU:O	1:D:180:GLY:O	2.34	0.45
1:E:222:THR:HG22	1:E:288:LEU:HD12	1.98	0.45
1:F:151:ALA:HA	1:F:187:ILE:O	2.16	0.45
1:F:298:LEU:HG	1:L:103:VAL:HG11	1.97	0.45
1:H:125:LEU:HD23	1:H:152:TYR:HB2	1.98	0.45
1:K:100:SER:HA	1:K:240:GLN:NE2	2.31	0.45
1:K:211:PRO:CB	1:K:216:TYR:HE2	2.25	0.45
1:L:83:PRO:O	1:L:84:ASP:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:145:LEU:HD22	1:L:149:SER:HB3	1.99	0.45
1:L:204:PHE:CE1	1:L:223:MET:HE3	2.50	0.45
1:P:188:VAL:HG12	1:P:189:GLY:N	2.30	0.45
1:D:101:HIS:N	1:D:240:GLN:HE22	2.12	0.45
1:D:150:TYR:CE1	1:D:209:LEU:HD22	2.51	0.45
1:G:196:LEU:CD2	1:G:205:GLU:HB3	2.42	0.45
1:H:208:LYS:HG2	1:H:221:HIS:CD2	2.50	0.45
1:I:150:TYR:CE1	1:I:209:LEU:HD22	2.50	0.45
1:K:100:SER:CA	1:K:240:GLN:HE22	2.29	0.45
1:L:170:VAL:HG13	1:L:170:VAL:O	2.15	0.45
1:M:179:LEU:HD23	1:M:214:VAL:HG22	1.97	0.45
1:B:218:PHE:CD1	1:B:218:PHE:C	2.94	0.45
1:D:64:VAL:HG12	1:D:66:LYS:HG3	1.98	0.45
1:D:170:VAL:HG13	1:D:170:VAL:O	2.16	0.45
1:E:125:LEU:C	1:E:125:LEU:CD1	2.87	0.45
1:G:237:HIS:CE1	1:G:239:ASN:HB2	2.52	0.45
1:H:186:LEU:CD1	1:H:188:VAL:HG23	2.45	0.45
1:H:204:PHE:CZ	1:H:223:MET:HE3	2.51	0.45
1:J:47:PRO:HA	4:J:424:HOH:O	2.17	0.45
1:J:87:ASN:HD21	1:J:110:LYS:CB	2.29	0.45
1:K:163:CYS:SG	1:K:167:ALA:HB2	2.56	0.45
1:K:243:LEU:HD12	1:K:244:LEU:N	2.32	0.45
1:P:105:TYR:CE1	1:P:171:VAL:HG11	2.52	0.45
1:B:100:SER:HB3	1:B:268:TRP:CH2	2.51	0.45
1:C:198:GLU:HB2	1:H:197:LEU:O	2.16	0.45
1:E:117:LEU:HD11	1:E:158:HIS:CD2	2.52	0.45
1:I:243:LEU:HB2	1:I:289:LEU:HD12	1.99	0.45
1:J:77:HIS:NE2	4:J:401:HOH:O	2.35	0.45
1:L:147:VAL:O	1:L:148:ASP:CB	2.63	0.45
1:D:111:GLU:CD	1:D:111:GLU:H	2.24	0.45
1:D:128:VAL:HG12	1:D:147:VAL:HA	1.98	0.45
1:D:243:LEU:HD23	1:D:269:MET:CE	2.46	0.45
1:E:137:ASN:ND2	1:E:140:SER:HB3	2.31	0.45
1:F:237:HIS:HB2	1:F:239:ASN:HD22	1.82	0.45
1:F:262:GLN:HB3	1:H:56:ASP:O	2.16	0.45
1:H:243:LEU:HG	1:H:267:ILE:HB	1.98	0.45
1:J:179:LEU:HD23	1:J:214:VAL:HG22	1.98	0.45
1:L:95:THR:O	1:L:98:THR:HG23	2.16	0.45
1:L:205:GLU:HB2	1:L:224:ASP:HB2	1.98	0.45
1:N:133:VAL:HG23	1:N:163:CYS:CB	2.37	0.45
1:O:54:LEU:HD23	1:P:49:LEU:HD22	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:125:LEU:HD13	1:F:126:ILE:N	2.31	0.45
1:H:209:LEU:C	1:H:210:LEU:HD23	2.41	0.45
1:I:153:LEU:HD13	1:I:159:HIS:CD2	2.52	0.45
1:J:134:THR:HG23	1:J:144:LYS:CA	2.47	0.45
1:K:129:VAL:HB	1:K:168:THR:HB	1.98	0.45
1:K:133:VAL:HG22	1:K:134:THR:N	2.31	0.45
1:L:56:ASP:O	1:L:58:PRO:HD3	2.17	0.45
1:L:262:GLN:HE21	1:N:56:ASP:CB	2.30	0.45
1:L:262:GLN:NE2	1:N:56:ASP:HB2	2.32	0.45
1:M:64:VAL:HG22	1:M:66:LYS:HE3	1.97	0.45
1:P:237:HIS:CE1	1:P:239:ASN:HB2	2.52	0.45
1:D:72:ILE:HD12	1:D:72:ILE:H	1.81	0.45
1:F:179:LEU:HD23	1:F:214:VAL:HG22	1.99	0.45
1:G:227:PRO:HG3	1:G:283:THR:O	2.17	0.45
1:H:195:PRO:O	1:H:197:LEU:HD12	2.16	0.45
1:K:243:LEU:HD22	1:K:287:TYR:CE1	2.51	0.45
1:L:50:SER:OG	1:L:51:PRO:HD2	2.16	0.45
1:L:133:VAL:HG23	1:L:162:ASP:C	2.41	0.45
1:L:171:VAL:HG23	1:L:172:PHE:N	2.32	0.45
1:M:128:VAL:HG22	1:M:169:LEU:CD1	2.47	0.45
1:P:82:LEU:O	1:P:85:TRP:HB2	2.16	0.45
1:B:253:ARG:NH1	1:C:61:THR:HG22	2.32	0.45
1:F:237:HIS:CE1	1:F:239:ASN:HB2	2.51	0.45
1:H:290:TYR:CD2	1:H:291:LYS:N	2.85	0.45
1:K:95:THR:O	1:K:97:ALA:N	2.50	0.45
1:K:101:HIS:H	1:K:240:GLN:HE22	1.65	0.45
1:K:253:ARG:HD2	1:K:258:TRP:CZ2	2.52	0.45
1:L:40:ILE:HG22	1:L:41:TYR:CD2	2.51	0.45
1:N:150:TYR:CE2	1:N:209:LEU:HB3	2.52	0.45
1:P:72:ILE:HD12	1:P:72:ILE:H	1.81	0.45
1:P:123:GLU:O	1:P:173:GLU:HA	2.16	0.45
1:C:218:PHE:HA	1:C:293:VAL:HG22	1.98	0.45
1:D:184:THR:HB	1:D:216:TYR:CE1	2.51	0.45
1:E:103:VAL:CG2	1:E:173:GLU:HB2	2.47	0.45
1:G:82:LEU:O	1:G:85:TRP:HB2	2.17	0.45
1:J:175:ARG:HG3	1:J:175:ARG:NH1	2.22	0.45
1:J:223:MET:C	1:J:224:ASP:OD1	2.60	0.45
1:M:68:ASP:OD2	1:M:273:VAL:HG23	2.15	0.45
1:M:125:LEU:HD13	1:M:125:LEU:C	2.42	0.45
1:O:54:LEU:CD2	1:P:49:LEU:HD22	2.46	0.45
1:P:136:THR:O	1:P:137:ASN:ND2	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:TRP:CE3	1:A:115:SER:HA	2.52	0.45
1:A:126:ILE:HG22	1:A:171:VAL:HB	1.98	0.45
1:B:155:PRO:HG3	1:B:176:TYR:CD2	2.52	0.45
1:D:136:THR:HG22	1:D:142:SER:CB	2.46	0.45
1:H:43:LYS:HB2	4:H:413:HOH:O	2.17	0.45
1:I:209:LEU:O	1:I:210:LEU:HD23	2.17	0.45
1:J:241:HIS:HB2	1:J:269:MET:HB2	1.99	0.45
1:K:204:PHE:HB3	1:K:225:PHE:CE1	2.52	0.45
1:M:50:SER:HB2	1:M:51:PRO:HD2	1.98	0.45
1:M:269:MET:SD	1:M:275:GLN:OE1	2.76	0.45
1:O:120:GLN:O	1:O:122:ILE:HG12	2.17	0.45
1:C:194:GLN:NE2	4:C:431:HOH:O	2.50	0.44
1:E:73:THR:HG22	1:E:265:ASP:OD1	2.17	0.44
1:G:204:PHE:CE1	1:G:223:MET:HE3	2.52	0.44
1:G:211:PRO:C	1:G:213:SER:H	2.24	0.44
1:G:220:ILE:HD13	1:G:290:TYR:HA	1.99	0.44
1:H:94:ILE:O	1:H:103:VAL:HA	2.17	0.44
1:J:204:PHE:CE1	1:J:223:MET:HE3	2.53	0.44
1:L:219:ASN:OD1	1:L:220:ILE:N	2.50	0.44
1:P:85:TRP:HE3	1:P:88:THR:HG21	1.75	0.44
1:P:93:LEU:HD13	1:P:266:VAL:HG21	1.99	0.44
1:P:191:THR:CG2	1:P:286:ARG:NH2	2.75	0.44
1:B:207:ARG:HB2	1:B:222:THR:HB	1.99	0.44
1:D:64:VAL:CG1	1:D:66:LYS:HE3	2.45	0.44
1:F:207:ARG:NH2	4:F:436:HOH:O	2.50	0.44
1:L:117:LEU:HD12	1:L:117:LEU:N	2.32	0.44
1:L:292:ASP:OD1	1:L:292:ASP:N	2.51	0.44
1:M:152:TYR:O	1:M:186:LEU:HD12	2.16	0.44
1:N:111:GLU:HA	1:N:164:VAL:O	2.17	0.44
1:A:70:ALA:HB3	1:A:268:TRP:HB3	1.98	0.44
1:C:253:ARG:HD2	1:C:258:TRP:CZ2	2.52	0.44
1:H:140:SER:O	1:H:141:SER:HB2	2.17	0.44
1:H:290:TYR:CD2	1:H:290:TYR:C	2.96	0.44
1:J:232:ASN:HD22	1:J:232:ASN:HA	1.63	0.44
1:L:137:ASN:O	1:L:137:ASN:ND2	2.49	0.44
1:M:109:MET:O	1:M:166:SER:HA	2.18	0.44
1:M:182:HIS:NE2	1:M:214:VAL:HG11	2.33	0.44
1:N:88:THR:OG1	1:N:109:MET:HG2	2.17	0.44
1:P:45:THR:HG21	1:P:130:GLU:OE2	2.17	0.44
1:P:198:GLU:HG3	1:P:200:PRO:HD3	1.99	0.44
1:A:80:SER:O	1:A:81:PRO:C	2.60	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:247:GLU:CG	1:B:286:ARG:HB3	2.47	0.44
1:C:166:SER:O	1:C:167:ALA:HB2	2.16	0.44
1:D:223:MET:HE1	3:D:302:UGY:H2	1.81	0.44
1:E:218:PHE:CD1	1:E:218:PHE:C	2.96	0.44
1:H:56:ASP:C	1:H:58:PRO:HD3	2.43	0.44
1:I:102:PHE:CD1	1:I:102:PHE:C	2.95	0.44
1:J:103:VAL:HG22	1:J:173:GLU:O	2.18	0.44
1:N:61:THR:HB	1:O:234:LYS:CG	2.44	0.44
1:C:103:VAL:CG2	1:C:173:GLU:HB2	2.48	0.44
1:C:133:VAL:HG21	1:C:161:LEU:HB3	1.98	0.44
1:E:190:SER:HB2	1:E:192:ASP:OD1	2.17	0.44
1:F:118:PRO:HD3	1:F:124:ARG:NH2	2.33	0.44
1:G:226:GLN:O	1:G:227:PRO:C	2.59	0.44
1:H:237:HIS:ND1	1:H:239:ASN:HB2	2.33	0.44
1:I:153:LEU:HD13	1:I:159:HIS:NE2	2.32	0.44
1:O:133:VAL:HG22	1:O:134:THR:N	2.32	0.44
1:A:82:LEU:HD13	1:A:90:GLY:CA	2.47	0.44
1:A:122:ILE:HD13	1:A:175:ARG:HA	2.00	0.44
1:A:251:ILE:HG12	1:A:280:LEU:HD11	1.98	0.44
1:E:69:HIS:HE1	4:E:415:HOH:O	2.00	0.44
1:F:243:LEU:C	1:F:243:LEU:CD1	2.89	0.44
1:G:94:ILE:O	1:G:103:VAL:HA	2.18	0.44
1:H:250:GLY:HA3	1:H:278:ALA:O	2.18	0.44
1:J:164:VAL:HG23	1:J:165:GLU:CG	2.46	0.44
1:K:223:MET:O	1:K:286:ARG:HA	2.18	0.44
1:K:233:VAL:O	1:K:233:VAL:HG13	2.17	0.44
1:O:240:GLN:HG2	1:O:292:ASP:OD1	2.16	0.44
1:P:153:LEU:HD13	1:P:159:HIS:NE2	2.33	0.44
1:A:72:ILE:N	1:A:72:ILE:HD12	2.33	0.44
1:A:102:PHE:HE2	1:A:240:GLN:HE21	1.59	0.44
1:E:136:THR:CG2	1:E:160:SER:HB3	2.47	0.44
1:G:133:VAL:HG23	1:G:163:CYS:HB2	2.00	0.44
1:I:202:GLU:HB3	1:I:204:PHE:CE2	2.53	0.44
1:J:40:ILE:HG22	1:J:41:TYR:CD2	2.53	0.44
1:K:125:LEU:HD23	1:K:152:TYR:HB2	2.00	0.44
1:M:227:PRO:HB3	1:M:281:GLY:O	2.17	0.44
1:N:52:SER:C	1:N:54:LEU:H	2.24	0.44
1:N:60:PHE:O	1:O:234:LYS:HE3	2.17	0.44
1:O:147:VAL:O	1:O:147:VAL:HG22	2.17	0.44
1:O:276:TRP:CH2	1:O:278:ALA:HB2	2.52	0.44
1:A:83:PRO:O	1:A:84:ASP:CB	2.66	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:174:ARG:HG2	1:D:175:ARG:O	2.17	0.44
1:I:243:LEU:HD12	1:I:244:LEU:C	2.42	0.44
1:J:231:LEU:HD12	1:J:276:TRP:HA	2.00	0.44
1:K:211:PRO:O	1:K:216:TYR:HD2	2.00	0.44
1:L:153:LEU:HD22	1:L:159:HIS:CD2	2.53	0.44
1:M:133:VAL:CG2	1:M:134:THR:N	2.81	0.44
1:N:267:ILE:HG21	1:N:269:MET:HE2	1.98	0.44
1:B:248:GLY:C	1:B:249:GLN:NE2	2.76	0.44
1:C:297:PRO:HG3	1:G:92:TYR:CZ	2.53	0.44
1:D:110:LYS:O	1:D:111:GLU:C	2.60	0.44
1:E:223:MET:HE1	3:E:302:UGY:H2	1.82	0.44
1:G:252:TYR:CD1	1:G:277:TYR:CD1	3.05	0.44
1:I:218:PHE:CD1	1:I:218:PHE:C	2.95	0.44
1:I:296:ASN:HD22	1:I:296:ASN:C	2.25	0.44
1:K:196:LEU:HD21	1:K:207:ARG:NH1	2.33	0.44
1:K:262:GLN:NE2	4:K:404:HOH:O	2.51	0.44
1:L:290:TYR:CD2	1:L:290:TYR:C	2.96	0.44
1:M:82:LEU:HD12	1:M:83:PRO:HD2	1.99	0.44
1:P:41:TYR:CZ	1:P:246:LEU:HD13	2.52	0.44
1:P:243:LEU:HB3	1:P:289:LEU:CD1	2.48	0.44
1:F:41:TYR:N	1:F:41:TYR:CD2	2.84	0.43
1:H:207:ARG:HB2	1:H:222:THR:CG2	2.48	0.43
1:I:126:ILE:HD12	1:I:126:ILE:O	2.18	0.43
1:I:279:ALA:O	1:I:280:LEU:HD23	2.18	0.43
1:K:90:GLY:HA2	1:K:106:LEU:O	2.18	0.43
1:M:140:SER:O	1:M:141:SER:HB3	2.17	0.43
1:M:252:TYR:CD1	1:M:277:TYR:CD1	3.06	0.43
1:P:245:LEU:HD12	1:P:287:TYR:HB3	2.00	0.43
1:D:101:HIS:C	1:D:101:HIS:CD2	2.95	0.43
1:D:135:LEU:O	1:D:142:SER:HA	2.18	0.43
1:E:133:VAL:HG22	1:E:134:THR:N	2.33	0.43
1:F:126:ILE:HD12	1:F:126:ILE:O	2.18	0.43
1:F:174:ARG:HH21	1:F:177:GLU:HG3	1.82	0.43
1:G:213:SER:O	1:G:294:ASN:ND2	2.51	0.43
1:H:222:THR:O	1:H:222:THR:HG22	2.18	0.43
1:K:164:VAL:HG23	1:K:165:GLU:HG2	2.00	0.43
1:O:241:HIS:HB2	1:O:269:MET:HB2	1.98	0.43
1:A:204:PHE:CD1	1:A:223:MET:HE3	2.53	0.43
1:D:125:LEU:C	1:D:125:LEU:CD1	2.91	0.43
1:D:206:LEU:HD12	1:D:207:ARG:H	1.83	0.43
1:D:218:PHE:CD1	1:D:218:PHE:C	2.95	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:102:PHE:HD2	1:E:240:GLN:HE21	1.66	0.43
1:E:197:LEU:HD12	1:E:208:LYS:HG3	2.00	0.43
1:G:50:SER:O	1:G:53:HIS:HB2	2.18	0.43
1:K:213:SER:C	1:K:215:ALA:N	2.76	0.43
1:L:262:GLN:NE2	4:L:430:HOH:O	2.46	0.43
1:M:262:GLN:O	1:M:263:ALA:C	2.61	0.43
1:O:134:THR:O	1:O:161:LEU:HA	2.18	0.43
1:P:105:TYR:CE1	1:P:171:VAL:CG1	3.02	0.43
1:A:190:SER:O	1:A:191:THR:C	2.60	0.43
1:C:184:THR:HB	1:C:216:TYR:CE1	2.52	0.43
1:E:74:PRO:C	1:E:76:SER:N	2.74	0.43
1:E:262:GLN:O	1:E:263:ALA:C	2.58	0.43
1:F:298:LEU:HG	1:L:103:VAL:CG1	2.48	0.43
1:H:237:HIS:HB3	1:M:78:VAL:HG21	2.00	0.43
1:H:237:HIS:CE1	1:H:239:ASN:HB2	2.53	0.43
1:I:95:THR:HA	1:I:103:VAL:HG12	2.00	0.43
1:I:134:THR:HG23	1:I:143:LYS:O	2.19	0.43
1:K:64:VAL:CG1	1:K:66:LYS:HE3	2.43	0.43
1:L:251:ILE:HD13	1:L:260:PRO:HA	1.99	0.43
1:N:93:LEU:CD1	1:N:266:VAL:HG21	2.40	0.43
1:N:130:GLU:CG	1:N:131:GLY:N	2.81	0.43
1:O:204:PHE:CZ	1:O:223:MET:HE3	2.54	0.43
1:O:253:ARG:HB3	1:O:276:TRP:HB3	2.00	0.43
1:P:207:ARG:HB3	1:P:222:THR:HB	1.99	0.43
1:P:296:ASN:HD22	1:P:296:ASN:C	2.27	0.43
1:B:235:GLU:HB2	1:B:275:GLN:HG3	2.00	0.43
1:C:111:GLU:CD	1:C:111:GLU:N	2.74	0.43
1:C:115:SER:HB3	1:C:161:LEU:CB	2.33	0.43
1:C:217:ASP:O	1:C:218:PHE:HB3	2.18	0.43
1:C:270:ALA:O	1:C:271:PRO:C	2.61	0.43
1:F:64:VAL:HG12	1:F:66:LYS:HG3	2.00	0.43
1:G:82:LEU:HG	1:G:85:TRP:CD1	2.54	0.43
1:H:89:LEU:HD12	1:H:110:LYS:NZ	2.33	0.43
1:H:298:LEU:HD21	1:M:122:ILE:HD12	2.01	0.43
1:J:223:MET:O	1:J:286:ARG:HA	2.19	0.43
1:K:164:VAL:CG2	1:K:165:GLU:H	2.31	0.43
1:K:199:THR:HB	1:K:202:GLU:HB2	2.00	0.43
1:L:101:HIS:NE2	1:L:290:TYR:OH	2.44	0.43
1:L:220:ILE:HA	1:L:289:LEU:O	2.18	0.43
1:M:223:MET:HE1	3:M:302:UGY:H2	1.84	0.43
1:P:64:VAL:HG11	1:P:66:LYS:HZ1	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:120:GLN:OE1	1:P:121:ASP:N	2.52	0.43
1:A:230:PHE:HB2	1:A:277:TYR:O	2.19	0.43
1:C:270:ALA:O	1:C:273:VAL:HG12	2.18	0.43
1:E:276:TRP:CH2	1:E:278:ALA:HB2	2.54	0.43
1:F:135:LEU:HB2	1:F:145:LEU:HD11	2.01	0.43
1:G:290:TYR:CD2	1:G:290:TYR:C	2.96	0.43
1:K:101:HIS:N	1:K:240:GLN:HE22	2.17	0.43
1:L:190:SER:O	1:L:194:GLN:HG2	2.18	0.43
1:O:150:TYR:CD1	1:O:209:LEU:HD13	2.53	0.43
1:B:185:GLU:O	1:B:187:ILE:HG12	2.19	0.43
1:I:96:PRO:HD3	1:I:103:VAL:HG12	2.00	0.43
1:J:234:LYS:HD3	1:J:234:LYS:N	2.33	0.43
1:M:157:PHE:C	1:M:157:PHE:CD2	2.97	0.43
1:P:103:VAL:CG2	1:P:173:GLU:HB2	2.48	0.43
1:P:130:GLU:C	1:P:147:VAL:HG22	2.42	0.43
1:A:283:THR:HG21	4:A:430:HOH:O	2.19	0.43
1:F:41:TYR:CZ	1:F:246:LEU:HD13	2.54	0.43
1:F:127:PHE:HB3	1:F:170:VAL:HG12	1.97	0.43
1:G:101:HIS:CD2	1:G:101:HIS:C	2.97	0.43
1:H:298:LEU:CD2	1:M:122:ILE:HD12	2.49	0.43
1:J:66:LYS:HE2	1:J:257:ASN:HD21	1.83	0.43
1:N:81:PRO:O	1:N:83:PRO:HD3	2.19	0.43
1:O:253:ARG:O	1:O:275:GLN:HA	2.19	0.43
1:P:124:ARG:HA	1:P:172:PHE:O	2.18	0.43
1:P:190:SER:HB3	1:P:192:ASP:OD1	2.19	0.43
1:B:64:VAL:HG12	1:B:66:LYS:HG2	2.00	0.43
1:E:133:VAL:HG23	1:E:162:ASP:O	2.19	0.43
1:E:224:ASP:OD2	1:E:286:ARG:HD3	2.18	0.43
1:F:192:ASP:OD2	1:F:193:LYS:N	2.52	0.43
1:G:79:TYR:CD1	1:G:91:ALA:HB2	2.54	0.43
1:H:74:PRO:C	1:H:76:SER:H	2.27	0.43
1:H:105:TYR:CE2	1:H:171:VAL:HG22	2.53	0.43
1:H:234:LYS:HG2	1:M:61:THR:HB	2.01	0.43
1:K:208:LYS:HE2	1:K:221:HIS:CE1	2.54	0.43
1:K:258:TRP:CD1	1:K:258:TRP:N	2.87	0.43
1:P:100:SER:HB3	1:P:268:TRP:CH2	2.54	0.43
1:P:273:VAL:HG13	1:P:273:VAL:O	2.18	0.43
1:C:101:HIS:CD2	1:C:101:HIS:C	2.97	0.43
1:D:100:SER:HB2	1:D:240:GLN:NE2	2.34	0.43
1:D:204:PHE:HB3	1:D:225:PHE:CE1	2.54	0.43
1:G:158:HIS:ND1	1:G:158:HIS:C	2.77	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:93:LEU:HD13	1:M:266:VAL:HG21	2.01	0.43
1:N:275:GLN:HE21	1:N:275:GLN:HB3	1.66	0.43
1:O:165:GLU:CG	1:O:166:SER:H	2.22	0.43
1:P:243:LEU:C	1:P:243:LEU:CD1	2.88	0.43
1:B:126:ILE:HD13	1:B:161:LEU:CD1	2.41	0.42
1:C:224:ASP:OD1	1:C:286:ARG:NH1	2.52	0.42
1:G:57:LEU:HD23	1:G:57:LEU:HA	1.84	0.42
1:L:53:HIS:O	1:N:48:THR:HG22	2.19	0.42
1:M:127:PHE:HB3	1:M:170:VAL:CG1	2.49	0.42
1:N:69:HIS:HA	1:N:268:TRP:O	2.19	0.42
1:N:218:PHE:CD1	1:N:218:PHE:C	2.96	0.42
1:O:137:ASN:HD22	1:O:140:SER:CB	2.30	0.42
1:A:120:GLN:HG3	1:A:156:ASN:ND2	2.33	0.42
1:A:125:LEU:C	1:A:125:LEU:CD1	2.92	0.42
1:A:220:ILE:HD13	1:A:290:TYR:HA	2.01	0.42
1:D:83:PRO:O	1:D:84:ASP:HB2	2.18	0.42
1:E:272:PHE:HE2	1:F:95:THR:HG1	1.66	0.42
1:E:296:ASN:ND2	1:E:298:LEU:HD12	2.31	0.42
1:H:186:LEU:HD12	1:H:187:ILE:N	2.34	0.42
1:I:120:GLN:CG	1:I:156:ASN:HD21	2.31	0.42
1:J:157:PHE:CD2	1:J:157:PHE:C	2.97	0.42
1:O:224:ASP:OD2	1:O:286:ARG:HD3	2.20	0.42
1:B:245:LEU:HD23	1:B:262:GLN:C	2.44	0.42
1:C:95:THR:C	1:C:97:ALA:H	2.28	0.42
1:E:82:LEU:HD23	1:E:85:TRP:CD2	2.55	0.42
1:E:220:ILE:HA	1:E:289:LEU:O	2.20	0.42
1:G:68:ASP:OD1	1:G:68:ASP:N	2.51	0.42
1:I:252:TYR:CE1	1:I:277:TYR:HB2	2.55	0.42
1:J:104:MET:HE2	1:J:172:PHE:CZ	2.53	0.42
1:J:137:ASN:ND2	1:J:140:SER:N	2.67	0.42
1:J:202:GLU:HA	1:J:202:GLU:OE2	2.20	0.42
1:L:187:ILE:HD11	1:L:216:TYR:OH	2.18	0.42
1:M:57:LEU:HD23	1:M:57:LEU:HA	1.87	0.42
1:M:74:PRO:C	1:M:76:SER:N	2.77	0.42
1:A:203:VAL:HG21	1:A:229:GLU:HG2	2.01	0.42
1:B:126:ILE:O	1:B:126:ILE:HG13	2.19	0.42
1:C:52:SER:O	1:C:55:GLN:HG2	2.20	0.42
1:C:170:VAL:O	1:C:170:VAL:HG13	2.19	0.42
1:I:190:SER:HB3	1:I:193:LYS:HG2	2.01	0.42
1:J:88:THR:HG23	1:J:109:MET:HA	2.01	0.42
1:L:153:LEU:HA	1:L:154:PRO:HD3	1.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:74:PRO:C	1:M:76:SER:H	2.26	0.42
1:N:130:GLU:HG2	1:N:131:GLY:H	1.83	0.42
1:P:125:LEU:HD13	1:P:125:LEU:C	2.44	0.42
1:A:111:GLU:O	1:A:112:MET:C	2.63	0.42
1:B:296:ASN:HD22	1:B:296:ASN:C	2.28	0.42
1:E:233:VAL:HG13	1:E:235:GLU:HG3	2.01	0.42
1:F:41:TYR:CE1	1:F:246:LEU:HD13	2.54	0.42
1:H:57:LEU:HD23	1:H:57:LEU:HA	1.94	0.42
1:H:102:PHE:HE2	1:H:240:GLN:HE21	1.64	0.42
1:H:111:GLU:H	1:H:111:GLU:CD	2.28	0.42
1:H:140:SER:O	1:H:141:SER:CB	2.67	0.42
1:H:275:GLN:OE1	3:H:302:UGY:NE	2.52	0.42
1:I:48:THR:OG1	1:K:56:ASP:OD2	2.29	0.42
1:K:41:TYR:OH	1:K:286:ARG:NH2	2.53	0.42
1:L:179:LEU:HD23	1:L:214:VAL:CG2	2.49	0.42
1:M:174:ARG:HG2	1:M:175:ARG:N	2.34	0.42
1:N:52:SER:C	1:N:54:LEU:N	2.76	0.42
1:O:53:HIS:CD2	1:P:53:HIS:CE1	3.07	0.42
1:P:158:HIS:O	1:P:159:HIS:HB3	2.19	0.42
1:A:237:HIS:CE1	1:A:239:ASN:HB2	2.55	0.42
1:B:152:TYR:C	1:B:152:TYR:CD2	2.96	0.42
1:G:100:SER:HA	1:G:240:GLN:HE22	1.84	0.42
1:K:88:THR:OG1	1:K:109:MET:HA	2.19	0.42
1:M:253:ARG:HH12	1:O:61:THR:HG22	1.84	0.42
1:O:60:PHE:HZ	1:P:60:PHE:HZ	1.67	0.42
1:P:110:LYS:HB3	1:P:111:GLU:OE2	2.19	0.42
1:A:62:ARG:HB2	1:A:73:THR:HG21	2.02	0.42
1:B:135:LEU:O	1:B:142:SER:HA	2.20	0.42
1:B:237:HIS:CE1	1:B:239:ASN:HB2	2.53	0.42
1:I:218:PHE:HD1	1:I:219:ASN:N	2.17	0.42
1:I:222:THR:O	1:I:222:THR:HG22	2.20	0.42
1:L:134:THR:HG22	1:L:135:LEU:N	2.35	0.42
1:N:282:LYS:HE2	1:N:282:LYS:N	2.34	0.42
1:O:259:TYR:HA	1:O:260:PRO:HD3	1.89	0.42
1:P:75:GLU:OE1	1:P:75:GLU:N	2.47	0.42
1:C:62:ARG:NH1	1:C:73:THR:HG21	2.35	0.42
1:D:147:VAL:O	1:D:148:ASP:CB	2.67	0.42
1:D:245:LEU:HD12	1:D:287:TYR:HB3	2.02	0.42
1:H:235:GLU:HB2	1:H:275:GLN:HG3	2.02	0.42
1:I:209:LEU:C	1:I:210:LEU:HD23	2.45	0.42
1:J:115:SER:HB3	1:J:161:LEU:HB2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:191:THR:C	1:K:193:LYS:H	2.27	0.42
1:M:94:ILE:CD1	1:M:268:TRP:HB2	2.49	0.42
1:M:101:HIS:N	1:M:240:GLN:HE22	2.16	0.42
1:M:133:VAL:CG2	1:M:134:THR:H	2.30	0.42
1:N:127:PHE:HB3	1:N:170:VAL:CG1	2.49	0.42
1:P:270:ALA:O	1:P:271:PRO:C	2.63	0.42
1:D:137:ASN:ND2	1:D:140:SER:N	2.67	0.42
1:F:82:LEU:HD11	1:F:90:GLY:HA3	2.02	0.42
1:F:144:LYS:HG3	1:F:145:LEU:N	2.34	0.42
1:J:288:LEU:HD12	1:J:288:LEU:HA	1.81	0.42
1:M:111:GLU:O	1:M:112:MET:C	2.63	0.42
1:M:249:GLN:CD	1:M:249:GLN:N	2.77	0.42
1:O:101:HIS:H	1:O:240:GLN:HE22	1.68	0.42
1:P:152:TYR:O	1:P:154:PRO:HD3	2.19	0.42
1:P:232:ASN:HD22	1:P:232:ASN:HA	1.71	0.42
1:B:49:LEU:HD13	1:J:53:HIS:HB3	2.02	0.42
1:C:47:PRO:HA	4:C:405:HOH:O	2.19	0.42
1:C:49:LEU:H	1:C:262:GLN:HE22	1.67	0.42
1:C:238:TYR:O	1:C:271:PRO:HB3	2.20	0.42
1:D:243:LEU:HD23	1:D:269:MET:HE1	2.02	0.42
1:F:130:GLU:O	1:F:167:ALA:HA	2.20	0.42
1:H:41:TYR:CE2	1:H:246:LEU:HD13	2.55	0.42
1:J:134:THR:HA	1:J:144:LYS:HA	2.02	0.42
1:K:193:LYS:O	1:K:194:GLN:CD	2.63	0.42
1:K:206:LEU:HD12	1:K:207:ARG:H	1.81	0.42
1:N:140:SER:O	1:N:141:SER:CB	2.68	0.42
1:O:196:LEU:HD21	1:O:207:ARG:NH2	2.35	0.42
1:P:165:GLU:O	1:P:166:SER:OG	2.30	0.42
1:A:185:GLU:O	1:A:187:ILE:HG12	2.20	0.41
1:E:101:HIS:C	1:E:101:HIS:CD2	2.98	0.41
1:E:122:ILE:HD13	1:E:175:ARG:HA	2.01	0.41
1:E:298:LEU:HD23	1:F:103:VAL:HG13	2.02	0.41
1:H:204:PHE:CE1	1:H:223:MET:HE3	2.56	0.41
1:J:83:PRO:O	1:J:84:ASP:HB2	2.20	0.41
1:K:83:PRO:O	1:K:84:ASP:HB2	2.19	0.41
1:L:94:ILE:O	1:L:103:VAL:HA	2.19	0.41
1:M:243:LEU:HB2	1:M:288:LEU:O	2.20	0.41
1:N:146:THR:O	1:N:147:VAL:C	2.61	0.41
1:N:240:GLN:HB3	1:N:271:PRO:HG3	2.01	0.41
1:P:87:ASN:OD1	1:P:110:LYS:HB2	2.20	0.41
1:H:196:LEU:CD2	1:H:207:ARG:NH1	2.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:88:THR:OG1	1:K:109:MET:HG2	2.20	0.41
1:K:101:HIS:CD2	1:K:101:HIS:C	2.98	0.41
1:K:121:ASP:HB2	1:K:175:ARG:NH1	2.35	0.41
1:K:170:VAL:O	1:K:170:VAL:CG1	2.62	0.41
1:L:208:LYS:HG2	1:L:221:HIS:CD2	2.54	0.41
1:N:134:THR:O	1:N:134:THR:HG22	2.19	0.41
1:N:204:PHE:HE1	1:N:206:LEU:HB2	1.84	0.41
1:N:267:ILE:HG22	1:N:269:MET:HG3	2.00	0.41
1:A:276:TRP:CG	1:J:59:GLY:HA2	2.55	0.41
1:C:190:SER:O	1:C:194:GLN:HG2	2.21	0.41
1:E:130:GLU:O	1:E:167:ALA:HA	2.19	0.41
1:F:68:ASP:O	1:F:270:ALA:HB3	2.19	0.41
1:F:123:GLU:O	1:F:173:GLU:HA	2.20	0.41
1:F:233:VAL:HG13	1:F:233:VAL:O	2.20	0.41
1:K:150:TYR:CZ	1:K:209:LEU:HB3	2.56	0.41
1:K:202:GLU:HB3	1:K:204:PHE:CE2	2.55	0.41
1:M:133:VAL:HG23	1:M:163:CYS:HB2	2.03	0.41
1:N:130:GLU:CD	1:N:131:GLY:N	2.78	0.41
1:O:85:TRP:CE3	1:O:88:THR:HG21	2.56	0.41
1:P:102:PHE:CD1	1:P:102:PHE:C	2.98	0.41
1:P:190:SER:O	1:P:194:GLN:HG2	2.20	0.41
1:P:220:ILE:HD13	1:P:290:TYR:HA	2.02	0.41
1:B:296:ASN:ND2	1:B:298:LEU:H	2.16	0.41
1:C:290:TYR:CD2	1:C:290:TYR:C	2.98	0.41
1:D:101:HIS:H	1:D:240:GLN:NE2	2.15	0.41
1:F:40:ILE:HG22	1:F:41:TYR:CD2	2.55	0.41
1:F:40:ILE:HD12	1:F:40:ILE:N	2.35	0.41
1:G:218:PHE:CD1	1:G:218:PHE:C	2.99	0.41
1:I:146:THR:O	1:I:147:VAL:C	2.63	0.41
1:J:245:LEU:HD12	1:J:287:TYR:HB3	2.02	0.41
1:K:69:HIS:HB2	1:K:254:LEU:HD13	2.02	0.41
1:K:194:GLN:HG3	1:K:209:LEU:HA	2.02	0.41
1:A:107:ALA:HB3	1:A:169:LEU:HB2	2.03	0.41
1:C:153:LEU:HD13	1:C:159:HIS:CD2	2.56	0.41
1:F:241:HIS:CG	1:F:289:LEU:HD11	2.56	0.41
1:G:92:TYR:HA	1:G:105:TYR:HB3	2.02	0.41
1:J:273:VAL:O	1:J:273:VAL:CG1	2.67	0.41
1:K:121:ASP:H	1:K:156:ASN:ND2	2.19	0.41
1:K:197:LEU:HD12	1:K:208:LYS:HG3	2.01	0.41
1:L:74:PRO:C	1:L:76:SER:H	2.28	0.41
1:M:102:PHE:CD1	1:M:102:PHE:C	2.97	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:225:PHE:O	1:M:284:ARG:HB2	2.20	0.41
1:B:83:PRO:C	1:B:85:TRP:H	2.29	0.41
1:B:163:CYS:HA	4:B:422:HOH:O	2.19	0.41
1:B:218:PHE:HA	1:B:293:VAL:HG22	2.03	0.41
1:D:199:THR:HA	1:D:200:PRO:HD2	1.84	0.41
1:E:245:LEU:HD12	1:E:287:TYR:HB3	2.03	0.41
1:E:268:TRP:CZ2	1:E:270:ALA:HB2	2.56	0.41
1:H:82:LEU:HA	1:H:83:PRO:HD3	1.95	0.41
1:H:241:HIS:CG	1:H:289:LEU:HD11	2.56	0.41
1:H:243:LEU:C	1:H:243:LEU:CD1	2.93	0.41
1:I:149:SER:O	1:I:150:TYR:HB3	2.20	0.41
1:J:220:ILE:HA	1:J:289:LEU:O	2.20	0.41
1:K:148:ASP:OD1	1:K:191:THR:HB	2.21	0.41
1:L:179:LEU:HD23	1:L:214:VAL:HG22	2.03	0.41
1:M:297:PRO:HG3	1:O:92:TYR:CZ	2.55	0.41
1:O:126:ILE:HG22	1:O:171:VAL:HB	2.02	0.41
1:A:40:ILE:N	1:A:40:ILE:CD1	2.66	0.41
1:D:42:TRP:CE2	1:E:39:PRO:HG3	2.55	0.41
1:D:76:SER:HB3	1:K:236:VAL:HB	2.03	0.41
1:D:193:LYS:C	1:D:194:GLN:HE21	2.28	0.41
1:F:81:PRO:O	1:F:83:PRO:HD3	2.20	0.41
1:I:82:LEU:HD21	1:I:90:GLY:HA3	2.02	0.41
1:I:154:PRO:HB3	1:I:184:THR:OG1	2.20	0.41
1:J:182:HIS:C	1:J:183:THR:HG23	2.45	0.41
1:N:122:ILE:HG23	1:O:298:LEU:HD11	2.03	0.41
1:O:113:SER:N	1:O:163:CYS:O	2.50	0.41
1:O:204:PHE:HB3	1:O:225:PHE:CE1	2.55	0.41
1:O:213:SER:C	1:O:215:ALA:N	2.78	0.41
1:O:245:LEU:HD12	1:O:245:LEU:HA	1.90	0.41
1:F:50:SER:H	1:F:53:HIS:CE1	2.39	0.41
1:G:130:GLU:HA	1:G:147:VAL:CG2	2.51	0.41
1:H:83:PRO:O	1:H:85:TRP:HD1	2.04	0.41
1:I:39:PRO:HB2	1:I:42:TRP:HB2	2.01	0.41
1:I:191:THR:O	1:I:207:ARG:HD3	2.21	0.41
1:I:277:TYR:CG	1:I:278:ALA:N	2.88	0.41
1:J:41:TYR:O	1:J:44:ALA:HB3	2.20	0.41
1:K:86:THR:HG22	4:K:424:HOH:O	2.21	0.41
1:K:95:THR:C	1:K:97:ALA:N	2.78	0.41
1:K:155:PRO:C	1:K:156:ASN:OD1	2.63	0.41
1:K:205:GLU:HB2	1:K:224:ASP:HB2	2.03	0.41
1:L:122:ILE:HD13	1:L:175:ARG:HA	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:262:GLN:HE21	1:N:56:ASP:HB2	1.85	0.41
1:M:42:TRP:C	1:M:44:ALA:N	2.78	0.41
1:N:83:PRO:O	1:N:85:TRP:HD1	2.04	0.41
1:N:153:LEU:O	1:N:154:PRO:C	2.64	0.41
1:N:243:LEU:C	1:N:243:LEU:CD1	2.94	0.41
1:P:129:VAL:O	1:P:147:VAL:HG13	2.21	0.41
1:A:249:GLN:CD	1:A:249:GLN:N	2.79	0.41
1:B:82:LEU:HD23	1:B:85:TRP:CD2	2.56	0.41
1:C:52:SER:C	1:C:54:LEU:N	2.79	0.41
1:C:133:VAL:HG23	1:C:162:ASP:O	2.20	0.41
1:C:223:MET:HE1	3:C:302:UGY:H2	1.85	0.41
1:C:298:LEU:HG	1:G:103:VAL:HG13	2.02	0.41
1:E:39:PRO:O	1:E:42:TRP:HB2	2.21	0.41
1:G:155:PRO:O	1:G:156:ASN:CB	2.69	0.41
1:G:259:TYR:O	1:G:261:VAL:HG13	2.21	0.41
1:H:62:ARG:HD3	4:H:410:HOH:O	2.21	0.41
1:H:240:GLN:HB3	1:H:271:PRO:HG3	2.02	0.41
1:J:284:ARG:HH22	1:J:286:ARG:NH2	2.19	0.41
1:K:243:LEU:HD13	1:K:287:TYR:CB	2.46	0.41
1:L:298:LEU:HD23	1:L:298:LEU:HA	1.87	0.41
1:M:101:HIS:C	1:M:101:HIS:CD2	2.98	0.41
1:M:103:VAL:HG22	1:M:173:GLU:HB2	2.03	0.41
1:M:237:HIS:CG	1:M:239:ASN:HD22	2.39	0.41
1:N:100:SER:HB2	1:N:240:GLN:NE2	2.35	0.41
1:N:103:VAL:HG22	1:N:173:GLU:HB2	2.02	0.41
1:N:197:LEU:HD23	1:N:208:LYS:HE3	2.02	0.41
1:O:82:LEU:HD21	1:O:105:TYR:CE1	2.56	0.41
1:P:137:ASN:OD1	1:P:140:SER:HB2	2.21	0.41
1:P:152:TYR:O	1:P:186:LEU:HA	2.21	0.41
1:C:153:LEU:HD13	1:C:159:HIS:ND1	2.36	0.41
1:C:216:TYR:O	1:C:294:ASN:ND2	2.47	0.41
1:E:82:LEU:HB3	1:E:85:TRP:HB2	2.03	0.41
1:F:276:TRP:CH2	1:F:278:ALA:HB2	2.55	0.41
1:G:153:LEU:HD13	1:G:159:HIS:NE2	2.35	0.41
1:G:235:GLU:HG2	1:I:78:VAL:CG2	2.50	0.41
1:J:155:PRO:O	1:J:156:ASN:HB2	2.21	0.41
1:J:243:LEU:C	1:J:243:LEU:CD1	2.93	0.41
1:K:191:THR:C	1:K:193:LYS:N	2.78	0.41
1:K:296:ASN:HD21	1:K:298:LEU:HD12	1.86	0.41
1:C:125:LEU:C	1:C:125:LEU:HD13	2.46	0.40
1:G:62:ARG:CB	1:G:73:THR:HG21	2.49	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:176:TYR:OH	1:G:215:ALA:O	2.32	0.40
1:G:196:LEU:HD21	1:G:207:ARG:NH1	2.35	0.40
1:G:235:GLU:HG2	1:I:78:VAL:HG22	2.03	0.40
1:J:192:ASP:C	1:J:194:GLN:H	2.29	0.40
1:K:85:TRP:HB3	1:K:88:THR:CG2	2.51	0.40
1:K:105:TYR:C	1:K:105:TYR:CD1	2.99	0.40
1:K:108:LYS:HD3	1:K:168:THR:HG23	2.03	0.40
1:M:202:GLU:HG3	1:M:204:PHE:CE2	2.55	0.40
1:P:267:ILE:HG22	1:P:269:MET:HG3	2.03	0.40
1:B:40:ILE:H	1:B:40:ILE:CD1	2.24	0.40
1:B:196:LEU:C	1:B:197:LEU:HD13	2.46	0.40
1:B:226:GLN:O	1:B:229:GLU:HG3	2.21	0.40
1:C:206:LEU:CD1	1:C:221:HIS:HB3	2.50	0.40
1:D:86:THR:O	1:D:87:ASN:C	2.65	0.40
1:F:223:MET:HE1	3:F:302:UGY:H2	1.86	0.40
1:I:62:ARG:HB2	1:I:73:THR:HG21	2.03	0.40
1:J:296:ASN:ND2	1:J:298:LEU:HB2	2.37	0.40
1:P:153:LEU:HD13	1:P:159:HIS:CG	2.56	0.40
1:C:110:LYS:HA	1:C:110:LYS:HE2	2.04	0.40
1:C:205:GLU:HB2	1:C:224:ASP:HB2	2.02	0.40
1:E:112:MET:HE3	1:E:112:MET:HB3	1.99	0.40
1:J:70:ALA:HB3	1:J:268:TRP:HB3	2.03	0.40
1:J:208:LYS:NZ	1:J:212:MET:CE	2.85	0.40
1:L:126:ILE:HG21	1:L:161:LEU:HD11	2.03	0.40
1:M:122:ILE:HD13	1:M:175:ARG:HA	2.04	0.40
1:O:85:TRP:CD2	1:O:115:SER:HA	2.55	0.40
1:O:208:LYS:HG2	1:O:221:HIS:CD2	2.56	0.40
1:B:192:ASP:OD2	1:B:193:LYS:HE3	2.21	0.40
1:D:145:LEU:HD21	1:D:188:VAL:HG13	2.03	0.40
1:F:85:TRP:CD2	1:F:115:SER:HA	2.56	0.40
1:F:115:SER:HB3	1:F:161:LEU:HB2	2.03	0.40
1:F:170:VAL:CG1	1:F:170:VAL:O	2.68	0.40
1:G:284:ARG:HD2	1:G:284:ARG:C	2.47	0.40
1:L:60:PHE:HZ	1:N:60:PHE:HZ	1.68	0.40
1:L:218:PHE:CD1	1:L:218:PHE:C	3.00	0.40
1:N:103:VAL:CG2	1:N:173:GLU:HB2	2.51	0.40
1:O:271:PRO:O	1:O:272:PHE:HB2	2.21	0.40
1:D:73:THR:HB	1:D:74:PRO:HD2	2.04	0.40
1:D:82:LEU:O	1:D:85:TRP:HB2	2.22	0.40
1:D:186:LEU:HD11	1:D:188:VAL:CG2	2.51	0.40
1:G:152:TYR:HB3	1:G:187:ILE:HB	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:85:TRP:CE3	1:K:109:MET:HE3	2.56	0.40
1:K:105:TYR:HE1	1:K:171:VAL:CG1	2.34	0.40
1:K:153:LEU:HA	1:K:154:PRO:HD3	1.86	0.40
1:M:166:SER:O	1:M:167:ALA:HB2	2.21	0.40
1:N:243:LEU:HD23	1:N:269:MET:CE	2.52	0.40
1:O:103:VAL:CG2	1:O:173:GLU:HB2	2.51	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	254/266 (96%)	231 (91%)	18 (7%)	5 (2%)	6	12
1	B	254/266 (96%)	235 (92%)	15 (6%)	4 (2%)	7	16
1	C	254/266 (96%)	236 (93%)	15 (6%)	3 (1%)	10	23
1	D	254/266 (96%)	235 (92%)	16 (6%)	3 (1%)	10	23
1	E	254/266 (96%)	234 (92%)	18 (7%)	2 (1%)	16	34
1	F	254/266 (96%)	238 (94%)	14 (6%)	2 (1%)	16	34
1	G	254/266 (96%)	224 (88%)	24 (9%)	6 (2%)	4	9
1	H	254/266 (96%)	236 (93%)	15 (6%)	3 (1%)	10	23
1	I	254/266 (96%)	236 (93%)	18 (7%)	0	100	100
1	J	254/266 (96%)	225 (89%)	25 (10%)	4 (2%)	7	16
1	K	254/266 (96%)	220 (87%)	27 (11%)	7 (3%)	4	6
1	L	254/266 (96%)	238 (94%)	13 (5%)	3 (1%)	10	23
1	M	254/266 (96%)	229 (90%)	20 (8%)	5 (2%)	6	12
1	N	254/266 (96%)	228 (90%)	24 (9%)	2 (1%)	16	34
1	O	254/266 (96%)	229 (90%)	22 (9%)	3 (1%)	10	23

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	P	254/266 (96%)	224 (88%)	24 (9%)	6 (2%)	4	9
All	All	4064/4256 (96%)	3698 (91%)	308 (8%)	58 (1%)	9	19

All (58) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	141	SER
1	B	141	SER
1	C	141	SER
1	D	119	PRO
1	G	165	GLU
1	J	142	SER
1	K	141	SER
1	K	191	THR
1	K	214	VAL
1	M	141	SER
1	N	141	SER
1	C	75	GLU
1	D	180	GLY
1	D	294	ASN
1	E	75	GLU
1	G	180	GLY
1	J	157	PHE
1	K	182	HIS
1	L	75	GLU
1	L	141	SER
1	M	235	GLU
1	O	148	ASP
1	P	154	PRO
1	C	96	PRO
1	F	235	GLU
1	F	236	VAL
1	G	141	SER
1	G	167	ALA
1	K	75	GLU
1	K	165	GLU
1	P	87	ASN
1	P	148	ASP
1	P	157	PHE
1	A	112	MET
1	E	96	PRO
1	J	284	ARG

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Mol	Chain	Res	Type
1	M	43	LYS
1	P	141	SER
1	B	84	ASP
1	B	96	PRO
1	G	157	PHE
1	H	141	SER
1	O	74	PRO
1	A	84	ASP
1	J	87	ASN
1	L	214	VAL
1	M	165	GLU
1	N	204	PHE
1	A	236	VAL
1	G	119	PRO
1	H	214	VAL
1	O	214	VAL
1	A	119	PRO
1	B	214	VAL
1	K	203	VAL
1	M	236	VAL
1	P	147	VAL
1	H	236	VAL

### 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	230/237 (97%)	213 (93%)	17 (7%)	13	29
1	B	230/237 (97%)	212 (92%)	18 (8%)	11	26
1	C	230/237 (97%)	219 (95%)	11 (5%)	23	47
1	D	230/237 (97%)	214 (93%)	16 (7%)	14	31
1	E	230/237 (97%)	214 (93%)	16 (7%)	14	31
1	F	230/237 (97%)	215 (94%)	15 (6%)	15	35
1	G	230/237 (97%)	216 (94%)	14 (6%)	17	37

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	230/237 (97%)	217 (94%)	13 (6%)	18	40
1	I	230/237 (97%)	216 (94%)	14 (6%)	17	37
1	J	230/237 (97%)	217 (94%)	13 (6%)	18	40
1	K	230/237 (97%)	214 (93%)	16 (7%)	14	31
1	L	230/237 (97%)	219 (95%)	11 (5%)	23	47
1	M	230/237 (97%)	213 (93%)	17 (7%)	13	29
1	N	230/237 (97%)	216 (94%)	14 (6%)	17	37
1	O	230/237 (97%)	219 (95%)	11 (5%)	23	47
1	P	230/237 (97%)	216 (94%)	14 (6%)	17	37
All	All	3680/3792 (97%)	3450 (94%)	230 (6%)	16	36

All (230) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	ILE
1	A	64	VAL
1	A	82	LEU
1	A	125	LEU
1	A	133	VAL
1	A	153	LEU
1	A	171	VAL
1	A	184	THR
1	A	222	THR
1	A	239	ASN
1	A	243	LEU
1	A	249	GLN
1	A	268	TRP
1	A	283	THR
1	A	286	ARG
1	A	296	ASN
1	A	298	LEU
1	B	45	THR
1	B	50	SER
1	B	103	VAL
1	B	120	GLN
1	B	136	THR
1	B	143	LYS
1	B	148	ASP
1	B	153	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	170	VAL
1	B	171	VAL
1	B	192	ASP
1	B	197	LEU
1	B	206	LEU
1	B	226	GLN
1	B	243	LEU
1	B	249	GLN
1	B	286	ARG
1	B	296	ASN
1	C	40	ILE
1	C	74	PRO
1	C	76	SER
1	C	111	GLU
1	C	126	ILE
1	C	165	GLU
1	C	171	VAL
1	C	243	LEU
1	C	249	GLN
1	C	286	ARG
1	C	298	LEU
1	D	40	ILE
1	D	82	LEU
1	D	110	LYS
1	D	111	GLU
1	D	125	LEU
1	D	130	GLU
1	D	137	ASN
1	D	171	VAL
1	D	179	LEU
1	D	185	GLU
1	D	193	LYS
1	D	199	THR
1	D	222	THR
1	D	243	LEU
1	D	249	GLN
1	D	286	ARG
1	E	82	LEU
1	E	84	ASP
1	E	111	GLU
1	E	125	LEU
1	E	130	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	E	136	THR
1	E	137	ASN
1	E	147	VAL
1	E	153	LEU
1	E	165	GLU
1	E	171	VAL
1	E	191	THR
1	E	192	ASP
1	E	243	LEU
1	E	249	GLN
1	E	286	ARG
1	F	45	THR
1	F	82	LEU
1	F	96	PRO
1	F	111	GLU
1	F	136	THR
1	F	142	SER
1	F	148	ASP
1	F	171	VAL
1	F	203	VAL
1	F	222	THR
1	F	243	LEU
1	F	247	GLU
1	F	249	GLN
1	F	283	THR
1	F	286	ARG
1	G	40	ILE
1	G	45	THR
1	G	81	PRO
1	G	111	GLU
1	G	136	THR
1	G	137	ASN
1	G	157	PHE
1	G	169	LEU
1	G	171	VAL
1	G	222	THR
1	G	243	LEU
1	G	249	GLN
1	G	252	TYR
1	G	286	ARG
1	H	80	SER
1	H	82	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	H	87	ASN
1	H	111	GLU
1	H	129	VAL
1	H	153	LEU
1	H	161	LEU
1	H	171	VAL
1	H	222	THR
1	H	243	LEU
1	H	247	GLU
1	H	249	GLN
1	H	286	ARG
1	I	45	THR
1	I	55	GLN
1	I	72	ILE
1	I	82	LEU
1	I	111	GLU
1	I	137	ASN
1	I	145	LEU
1	I	171	VAL
1	I	222	THR
1	I	243	LEU
1	I	249	GLN
1	I	286	ARG
1	I	296	ASN
1	I	298	LEU
1	J	82	LEU
1	J	104	MET
1	J	130	GLU
1	J	143	LYS
1	J	153	LEU
1	J	169	LEU
1	J	171	VAL
1	J	218	PHE
1	J	222	THR
1	J	232	ASN
1	J	243	LEU
1	J	249	GLN
1	J	285	SER
1	K	45	THR
1	K	72	ILE
1	K	76	SER
1	K	88	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	K	105	TYR
1	K	130	GLU
1	K	145	LEU
1	K	156	ASN
1	K	160	SER
1	K	171	VAL
1	K	177	GLU
1	K	183	THR
1	K	193	LYS
1	K	243	LEU
1	K	249	GLN
1	K	286	ARG
1	L	40	ILE
1	L	74	PRO
1	L	111	GLU
1	L	125	LEU
1	L	148	ASP
1	L	171	VAL
1	L	203	VAL
1	L	222	THR
1	L	233	VAL
1	L	243	LEU
1	L	286	ARG
1	M	46	ASN
1	M	80	SER
1	M	111	GLU
1	M	137	ASN
1	M	143	LYS
1	M	147	VAL
1	M	148	ASP
1	M	171	VAL
1	M	183	THR
1	M	190	SER
1	M	222	THR
1	M	231	LEU
1	M	233	VAL
1	M	243	LEU
1	M	249	GLN
1	M	284	ARG
1	M	286	ARG
1	N	40	ILE
1	N	52	SER

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Mol	Chain	Res	Type
1	N	134	THR
1	N	143	LYS
1	N	171	VAL
1	N	177	GLU
1	N	234	LYS
1	N	243	LEU
1	N	249	GLN
1	N	275	GLN
1	N	283	THR
1	N	286	ARG
1	N	288	LEU
1	N	296	ASN
1	O	74	PRO
1	O	75	GLU
1	O	136	THR
1	O	137	ASN
1	O	147	VAL
1	O	171	VAL
1	O	243	LEU
1	O	249	GLN
1	O	283	THR
1	O	296	ASN
1	O	298	LEU
1	P	40	ILE
1	P	74	PRO
1	P	82	LEU
1	P	111	GLU
1	P	120	GLN
1	P	125	LEU
1	P	136	THR
1	P	154	PRO
1	P	171	VAL
1	P	183	THR
1	P	222	THR
1	P	243	LEU
1	P	249	GLN
1	P	296	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (117) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	156	ASN
1	A	182	HIS
1	A	194	GLN
1	A	239	ASN
1	A	240	GLN
1	A	249	GLN
1	A	257	ASN
1	A	262	GLN
1	A	296	ASN
1	B	87	ASN
1	B	120	GLN
1	B	156	ASN
1	B	240	GLN
1	B	249	GLN
1	B	262	GLN
1	B	296	ASN
1	C	46	ASN
1	C	137	ASN
1	C	156	ASN
1	C	194	GLN
1	C	239	ASN
1	C	240	GLN
1	C	249	GLN
1	C	262	GLN
1	D	55	GLN
1	D	137	ASN
1	D	156	ASN
1	D	158	HIS
1	D	194	GLN
1	D	239	ASN
1	D	240	GLN
1	D	249	GLN
1	D	296	ASN
1	E	46	ASN
1	E	156	ASN
1	E	158	HIS
1	E	194	GLN
1	E	240	GLN
1	E	249	GLN
1	E	296	ASN
1	F	46	ASN
1	F	156	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	F	194	GLN
1	F	239	ASN
1	F	240	GLN
1	F	249	GLN
1	F	296	ASN
1	G	55	GLN
1	G	137	ASN
1	G	156	ASN
1	G	226	GLN
1	G	240	GLN
1	G	249	GLN
1	G	294	ASN
1	H	156	ASN
1	H	221	HIS
1	H	240	GLN
1	H	249	GLN
1	H	262	GLN
1	H	296	ASN
1	I	55	GLN
1	I	120	GLN
1	I	137	ASN
1	I	156	ASN
1	I	182	HIS
1	I	240	GLN
1	I	296	ASN
1	J	87	ASN
1	J	156	ASN
1	J	158	HIS
1	J	194	GLN
1	J	232	ASN
1	J	240	GLN
1	J	249	GLN
1	J	257	ASN
1	J	296	ASN
1	K	156	ASN
1	K	194	GLN
1	K	221	HIS
1	K	240	GLN
1	K	249	GLN
1	K	296	ASN
1	L	156	ASN
1	L	158	HIS

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Mol	Chain	Res	Type
1	L	239	ASN
1	L	240	GLN
1	L	249	GLN
1	L	257	ASN
1	L	262	GLN
1	M	46	ASN
1	M	69	HIS
1	M	156	ASN
1	M	239	ASN
1	M	240	GLN
1	M	249	GLN
1	M	262	GLN
1	N	194	GLN
1	N	226	GLN
1	N	240	GLN
1	N	262	GLN
1	N	296	ASN
1	O	46	ASN
1	O	53	HIS
1	O	87	ASN
1	O	137	ASN
1	O	156	ASN
1	O	239	ASN
1	O	240	GLN
1	O	296	ASN
1	P	46	ASN
1	P	87	ASN
1	P	156	ASN
1	P	232	ASN
1	P	240	GLN
1	P	249	GLN
1	P	296	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 32 ligands modelled in this entry, 16 are monoatomic - leaving 16 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
3	UGY	A	302	2	7,8,8	2.42	3 (42%)	4,10,10	1.49	1 (25%)
3	UGY	H	302	2	7,8,8	2.00	1 (14%)	4,10,10	1.26	1 (25%)
3	UGY	D	302	2	7,8,8	2.18	3 (42%)	4,10,10	1.53	1 (25%)
3	UGY	G	302	2	7,8,8	1.21	1 (14%)	4,10,10	1.54	1 (25%)
3	UGY	I	302	2	7,8,8	1.19	1 (14%)	4,10,10	1.69	1 (25%)
3	UGY	J	302	2	7,8,8	1.28	1 (14%)	4,10,10	1.47	1 (25%)
3	UGY	E	302	2	7,8,8	1.67	2 (28%)	4,10,10	1.48	1 (25%)
3	UGY	B	302	2	7,8,8	2.29	3 (42%)	4,10,10	1.53	1 (25%)
3	UGY	L	302	2	7,8,8	2.45	4 (57%)	4,10,10	1.41	1 (25%)
3	UGY	C	302	2	7,8,8	2.32	3 (42%)	4,10,10	1.54	1 (25%)
3	UGY	P	302	2	7,8,8	1.20	1 (14%)	4,10,10	1.51	1 (25%)
3	UGY	K	302	2	7,8,8	1.43	1 (14%)	4,10,10	1.39	1 (25%)
3	UGY	O	302	2	7,8,8	2.23	3 (42%)	4,10,10	1.44	1 (25%)
3	UGY	F	302	2	7,8,8	2.34	3 (42%)	4,10,10	1.58	1 (25%)
3	UGY	N	302	2	7,8,8	1.55	2 (28%)	4,10,10	1.54	1 (25%)
3	UGY	M	302	2	7,8,8	2.20	4 (57%)	4,10,10	1.52	1 (25%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	UGY	A	302	2	-	1/7/8/8	-
3	UGY	H	302	2	-	0/7/8/8	-
3	UGY	D	302	2	-	1/7/8/8	-
3	UGY	G	302	2	-	0/7/8/8	-
3	UGY	I	302	2	-	1/7/8/8	-
3	UGY	J	302	2	-	1/7/8/8	-
3	UGY	E	302	2	-	1/7/8/8	-
3	UGY	B	302	2	-	2/7/8/8	-
3	UGY	L	302	2	-	2/7/8/8	-
3	UGY	C	302	2	-	1/7/8/8	-
3	UGY	P	302	2	-	1/7/8/8	-
3	UGY	K	302	2	-	1/7/8/8	-
3	UGY	O	302	2	-	2/7/8/8	-
3	UGY	F	302	2	-	1/7/8/8	-
3	UGY	N	302	2	-	1/7/8/8	-
3	UGY	M	302	2	-	1/7/8/8	-

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	302	UGY	CA-C	-5.11	1.49	1.56
3	B	302	UGY	O-C	4.26	1.34	1.22
3	O	302	UGY	O-C	4.22	1.34	1.22
3	A	302	UGY	CA-C	-4.12	1.50	1.56
3	D	302	UGY	O-C	4.12	1.34	1.22
3	L	302	UGY	O-C	4.00	1.33	1.22
3	M	302	UGY	O-C	4.00	1.33	1.22
3	F	302	UGY	O-C	3.86	1.33	1.22
3	C	302	UGY	O-C	3.75	1.33	1.22
3	C	302	UGY	CA-C	-3.66	1.51	1.56
3	A	302	UGY	O-C	3.62	1.32	1.22
3	L	302	UGY	CA-C	-3.52	1.51	1.56
3	F	302	UGY	CA-C	-3.48	1.51	1.56
3	E	302	UGY	CA-C	-3.33	1.51	1.56
3	K	302	UGY	CA-C	-3.07	1.52	1.56
3	N	302	UGY	CA-C	-2.91	1.52	1.56
3	A	302	UGY	OXT-C	-2.86	1.21	1.30
3	B	302	UGY	CA-C	-2.85	1.52	1.56
3	D	302	UGY	CA-C	-2.82	1.52	1.56
3	C	302	UGY	OXT-C	-2.77	1.21	1.30
3	J	302	UGY	CA-C	-2.73	1.52	1.56
3	F	302	UGY	OXT-C	-2.68	1.22	1.30
3	G	302	UGY	CA-C	-2.67	1.52	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	O	302	UGY	CA-C	-2.66	1.52	1.56
3	L	302	UGY	CA-NB	2.66	1.49	1.45
3	B	302	UGY	OXT-C	-2.60	1.22	1.30
3	M	302	UGY	CA-C	-2.59	1.52	1.56
3	D	302	UGY	OXT-C	-2.56	1.22	1.30
3	O	302	UGY	OXT-C	-2.52	1.22	1.30
3	M	302	UGY	OXT-C	-2.43	1.22	1.30
3	P	302	UGY	CA-C	-2.39	1.53	1.56
3	N	302	UGY	CA-NB	2.36	1.48	1.45
3	E	302	UGY	CA-NB	2.36	1.48	1.45
3	L	302	UGY	OXT-C	-2.29	1.23	1.30
3	I	302	UGY	CA-C	-2.09	1.53	1.56
3	M	302	UGY	CA-NB	2.06	1.48	1.45

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	302	UGY	OXT-C-O	-2.68	117.99	124.08
3	M	302	UGY	OXT-C-O	-2.60	118.19	124.08
3	D	302	UGY	OXT-C-O	-2.56	118.27	124.08
3	B	302	UGY	OXT-C-O	-2.55	118.30	124.08
3	C	302	UGY	OXT-C-O	-2.53	118.35	124.08
3	G	302	UGY	OXT-C-O	-2.52	118.36	124.08
3	P	302	UGY	OXT-C-O	-2.51	118.38	124.08
3	O	302	UGY	OXT-C-O	-2.51	118.39	124.08
3	J	302	UGY	OXT-C-O	-2.42	118.58	124.08
3	N	302	UGY	OXT-C-O	-2.41	118.61	124.08
3	F	302	UGY	OXT-C-O	-2.41	118.62	124.08
3	A	302	UGY	OXT-C-O	-2.36	118.72	124.08
3	E	302	UGY	OXT-C-O	-2.32	118.81	124.08
3	K	302	UGY	OXT-C-O	-2.25	118.97	124.08
3	L	302	UGY	OXT-C-O	-2.24	118.99	124.08
3	H	302	UGY	OXT-C-O	-2.03	119.48	124.08

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	K	302	UGY	OXT-C-CA-N
3	L	302	UGY	OXT-C-CA-N
3	N	302	UGY	OXT-C-CA-N
3	J	302	UGY	C-CA-NB-CG

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Mol	Chain	Res	Type	Atoms
3	P	302	UGY	C-CA-NB-CG
3	A	302	UGY	OXT-C-CA-N
3	B	302	UGY	OXT-C-CA-N
3	C	302	UGY	OXT-C-CA-N
3	D	302	UGY	OXT-C-CA-N
3	E	302	UGY	OXT-C-CA-N
3	F	302	UGY	OXT-C-CA-N
3	M	302	UGY	OXT-C-CA-N
3	O	302	UGY	OXT-C-CA-N
3	B	302	UGY	C-CA-NB-CG
3	I	302	UGY	C-CA-NB-CG
3	L	302	UGY	O-C-CA-N
3	O	302	UGY	C-CA-NB-CG

There are no ring outliers.

7 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	302	UGY	1	0
3	D	302	UGY	1	0
3	J	302	UGY	1	0
3	E	302	UGY	1	0
3	C	302	UGY	1	0
3	F	302	UGY	1	0
3	M	302	UGY	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	258/266 (96%)	-0.06	3 (1%) 76 73	26, 36, 51, 57	0
1	B	258/266 (96%)	-0.10	1 (0%) 88 86	25, 37, 47, 53	0
1	C	258/266 (96%)	-0.05	4 (1%) 70 66	21, 36, 51, 64	0
1	D	258/266 (96%)	-0.07	2 (0%) 82 80	24, 36, 50, 64	0
1	E	258/266 (96%)	-0.00	2 (0%) 82 80	25, 38, 53, 62	0
1	F	258/266 (96%)	-0.07	1 (0%) 88 86	26, 37, 49, 60	0
1	G	258/266 (96%)	0.18	2 (0%) 82 80	26, 43, 59, 70	0
1	H	258/266 (96%)	-0.12	3 (1%) 76 73	24, 36, 50, 62	0
1	I	258/266 (96%)	-0.02	1 (0%) 88 86	25, 39, 51, 64	0
1	J	258/266 (96%)	0.26	1 (0%) 88 86	28, 44, 57, 67	0
1	K	258/266 (96%)	0.54	3 (1%) 76 73	30, 48, 63, 70	0
1	L	258/266 (96%)	0.05	2 (0%) 82 80	26, 42, 51, 63	0
1	M	258/266 (96%)	0.04	1 (0%) 88 86	27, 41, 55, 67	0
1	N	258/266 (96%)	0.06	3 (1%) 76 73	28, 41, 55, 66	0
1	O	258/266 (96%)	0.09	3 (1%) 76 73	30, 43, 56, 63	0
1	P	258/266 (96%)	0.27	6 (2%) 61 55	28, 45, 61, 65	0
All	All	4128/4256 (96%)	0.06	38 (0%) 81 78	21, 40, 56, 70	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	P	65	TYR	3.6
1	D	141	SER	3.3
1	A	112	MET	3.3
1	N	65	TYR	3.2
1	F	65	TYR	3.1

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Mol	Chain	Res	Type	RSRZ
1	O	39	PRO	3.0
1	A	39	PRO	3.0
1	D	65	TYR	2.7
1	N	40	ILE	2.7
1	P	114	SER	2.7
1	A	65	TYR	2.6
1	L	65	TYR	2.6
1	N	140	SER	2.5
1	J	39	PRO	2.5
1	M	39	PRO	2.5
1	B	65	TYR	2.5
1	K	157	PHE	2.5
1	P	137	ASN	2.4
1	E	140	SER	2.4
1	G	39	PRO	2.4
1	C	137	ASN	2.2
1	C	140	SER	2.2
1	H	140	SER	2.2
1	P	164	VAL	2.2
1	C	65	TYR	2.2
1	P	40	ILE	2.2
1	L	136	THR	2.2
1	E	39	PRO	2.2
1	K	83	PRO	2.2
1	H	65	TYR	2.2
1	I	39	PRO	2.2
1	G	65	TYR	2.1
1	C	40	ILE	2.1
1	K	65	TYR	2.1
1	O	142	SER	2.0
1	P	39	PRO	2.0
1	H	39	PRO	2.0
1	O	141	SER	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 oligosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	UGY	K	302	9/9	0.88	0.12	51,52,55,55	0
3	UGY	G	302	9/9	0.89	0.13	53,54,59,61	0
3	UGY	L	302	9/9	0.89	0.13	55,55,58,59	0
3	UGY	I	302	9/9	0.90	0.10	45,50,53,54	0
3	UGY	B	302	9/9	0.90	0.11	46,47,49,50	0
3	UGY	H	302	9/9	0.90	0.12	43,45,49,51	0
3	UGY	F	302	9/9	0.91	0.11	43,46,47,47	0
3	UGY	D	302	9/9	0.91	0.11	41,43,47,49	0
3	UGY	M	302	9/9	0.91	0.09	50,51,53,53	0
3	UGY	N	302	9/9	0.91	0.10	38,40,43,44	0
3	UGY	A	302	9/9	0.92	0.11	45,46,50,52	0
3	UGY	C	302	9/9	0.93	0.09	40,43,47,49	0
3	UGY	J	302	9/9	0.94	0.09	56,56,58,58	0
3	UGY	O	302	9/9	0.94	0.09	44,46,48,49	0
3	UGY	P	302	9/9	0.94	0.08	32,36,44,46	0
3	UGY	E	302	9/9	0.96	0.07	38,41,42,43	0
2	MN	A	301	1/1	0.98	0.03	36,36,36,36	0
2	MN	B	301	1/1	0.99	0.03	32,32,32,32	0
2	MN	C	301	1/1	0.99	0.03	29,29,29,29	0
2	MN	E	301	1/1	0.99	0.02	31,31,31,31	0
2	MN	H	301	1/1	0.99	0.02	33,33,33,33	0
2	MN	I	301	1/1	0.99	0.03	35,35,35,35	0
2	MN	J	301	1/1	0.99	0.04	47,47,47,47	0
2	MN	L	301	1/1	0.99	0.03	38,38,38,38	0
2	MN	N	301	1/1	0.99	0.04	32,32,32,32	0
2	MN	D	301	1/1	1.00	0.03	31,31,31,31	0
2	MN	M	301	1/1	1.00	0.02	41,41,41,41	0
2	MN	F	301	1/1	1.00	0.03	36,36,36,36	0
2	MN	O	301	1/1	1.00	0.02	39,39,39,39	0
2	MN	P	301	1/1	1.00	0.02	33,33,33,33	0
2	MN	G	301	1/1	1.00	0.02	31,31,31,31	0
2	MN	K	301	1/1	1.00	0.03	36,36,36,36	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.