



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:06 PM GMT

PDB ID : 4E2Q  
Title : Crystal Structure of (S)-Ureidoglycine Aminohydrolase from Arabidopsis thaliana  
Authors : Shin, I.; Rhee, S.  
Deposited on : 2012-03-09  
Resolution : 2.50 Å(reported)

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

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

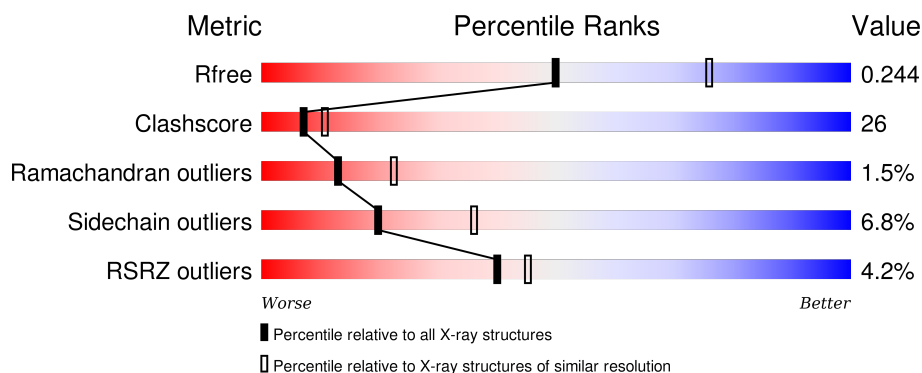
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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> <div>2%</div> <div>64% 30% . .</div> </div>
1	B	266	<div> <div>2%</div> <div>59% 33% 5% .</div> </div>
1	C	266	<div> <div>%</div> <div>65% 29% . .</div> </div>
1	D	266	<div> <div>%</div> <div>59% 32% 5% .</div> </div>
1	E	266	<div> <div>2%</div> <div>54% 40% . .</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	266	
1	G	266	
1	H	266	
1	I	266	
1	J	266	
1	K	266	
1	L	266	
1	M	266	
1	N	266	
1	O	266	
1	P	266	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 33964 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
1	A	258	Total	C	N	O	S	0	0	0
			2076	1345	342	382	7			
1	B	258	Total	C	N	O	S	0	0	0
			2076	1345	342	382	7			
1	C	258	Total	C	N	O	S	0	0	0
			2076	1345	342	382	7			
1	D	258	Total	C	N	O	S	0	0	0
			2076	1345	342	382	7			
1	E	258	Total	C	N	O	S	0	0	0
			2076	1345	342	382	7			
1	F	258	Total	C	N	O	S	0	0	0
			2076	1345	342	382	7			
1	G	258	Total	C	N	O	S	0	0	0
			2076	1345	342	382	7			
1	H	258	Total	C	N	O	S	0	0	0
			2076	1345	342	382	7			
1	I	258	Total	C	N	O	S	0	0	0
			2076	1345	342	382	7			
1	J	258	Total	C	N	O	S	0	0	0
			2076	1345	342	382	7			
1	K	258	Total	C	N	O	S	0	0	0
			2076	1345	342	382	7			
1	L	258	Total	C	N	O	S	0	0	0
			2076	1345	342	382	7			
1	M	258	Total	C	N	O	S	0	0	0
			2076	1345	342	382	7			
1	N	258	Total	C	N	O	S	0	0	0
			2076	1345	342	382	7			
1	O	258	Total	C	N	O	S	0	0	0
			2076	1345	342	382	7			
1	P	258	Total	C	N	O	S	0	0	0
			2076	1345	342	382	7			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	33	GLY	-	EXPRESSION TAG	UNP Q8GXV5
A	34	HIS	-	EXPRESSION TAG	UNP Q8GXV5
A	35	MET	-	EXPRESSION TAG	UNP Q8GXV5
B	33	GLY	-	EXPRESSION TAG	UNP Q8GXV5
B	34	HIS	-	EXPRESSION TAG	UNP Q8GXV5
B	35	MET	-	EXPRESSION TAG	UNP Q8GXV5
C	33	GLY	-	EXPRESSION TAG	UNP Q8GXV5
C	34	HIS	-	EXPRESSION TAG	UNP Q8GXV5
C	35	MET	-	EXPRESSION TAG	UNP Q8GXV5
D	33	GLY	-	EXPRESSION TAG	UNP Q8GXV5
D	34	HIS	-	EXPRESSION TAG	UNP Q8GXV5
D	35	MET	-	EXPRESSION TAG	UNP Q8GXV5
E	33	GLY	-	EXPRESSION TAG	UNP Q8GXV5
E	34	HIS	-	EXPRESSION TAG	UNP Q8GXV5
E	35	MET	-	EXPRESSION TAG	UNP Q8GXV5
F	33	GLY	-	EXPRESSION TAG	UNP Q8GXV5
F	34	HIS	-	EXPRESSION TAG	UNP Q8GXV5
F	35	MET	-	EXPRESSION TAG	UNP Q8GXV5
G	33	GLY	-	EXPRESSION TAG	UNP Q8GXV5
G	34	HIS	-	EXPRESSION TAG	UNP Q8GXV5
G	35	MET	-	EXPRESSION TAG	UNP Q8GXV5
H	33	GLY	-	EXPRESSION TAG	UNP Q8GXV5
H	34	HIS	-	EXPRESSION TAG	UNP Q8GXV5
H	35	MET	-	EXPRESSION TAG	UNP Q8GXV5
I	33	GLY	-	EXPRESSION TAG	UNP Q8GXV5
I	34	HIS	-	EXPRESSION TAG	UNP Q8GXV5
I	35	MET	-	EXPRESSION TAG	UNP Q8GXV5
J	33	GLY	-	EXPRESSION TAG	UNP Q8GXV5
J	34	HIS	-	EXPRESSION TAG	UNP Q8GXV5
J	35	MET	-	EXPRESSION TAG	UNP Q8GXV5
K	33	GLY	-	EXPRESSION TAG	UNP Q8GXV5
K	34	HIS	-	EXPRESSION TAG	UNP Q8GXV5
K	35	MET	-	EXPRESSION TAG	UNP Q8GXV5
L	33	GLY	-	EXPRESSION TAG	UNP Q8GXV5
L	34	HIS	-	EXPRESSION TAG	UNP Q8GXV5
L	35	MET	-	EXPRESSION TAG	UNP Q8GXV5
M	33	GLY	-	EXPRESSION TAG	UNP Q8GXV5
M	34	HIS	-	EXPRESSION TAG	UNP Q8GXV5
M	35	MET	-	EXPRESSION TAG	UNP Q8GXV5
N	33	GLY	-	EXPRESSION TAG	UNP Q8GXV5
N	34	HIS	-	EXPRESSION TAG	UNP Q8GXV5
N	35	MET	-	EXPRESSION TAG	UNP Q8GXV5

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Chain	Residue	Modelled	Actual	Comment	Reference
O	33	GLY	-	EXPRESSION TAG	UNP Q8GXV5
O	34	HIS	-	EXPRESSION TAG	UNP Q8GXV5
O	35	MET	-	EXPRESSION TAG	UNP Q8GXV5
P	33	GLY	-	EXPRESSION TAG	UNP Q8GXV5
P	34	HIS	-	EXPRESSION TAG	UNP Q8GXV5
P	35	MET	-	EXPRESSION TAG	UNP Q8GXV5

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

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

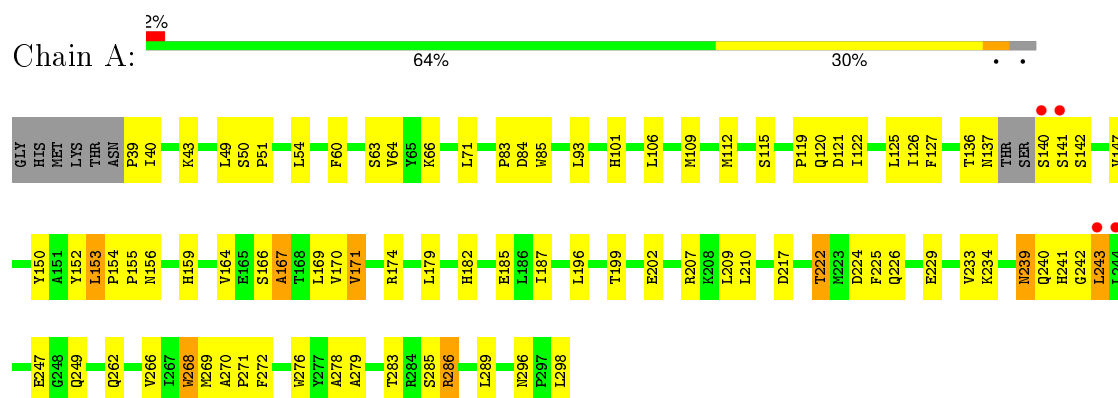
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	67	Total O 67 67	0	0
3	B	75	Total O 75 75	0	0
3	C	80	Total O 80 80	0	0
3	D	57	Total O 57 57	0	0
3	E	50	Total O 50 50	0	0
3	F	51	Total O 51 51	0	0
3	G	44	Total O 44 44	0	0
3	H	49	Total O 49 49	0	0
3	I	39	Total O 39 39	0	0
3	J	36	Total O 36 36	0	0
3	K	36	Total O 36 36	0	0
3	L	25	Total O 25 25	0	0
3	M	24	Total O 24 24	0	0
3	N	42	Total O 42 42	0	0
3	O	28	Total O 28 28	0	0
3	P	29	Total O 29 29	0	0

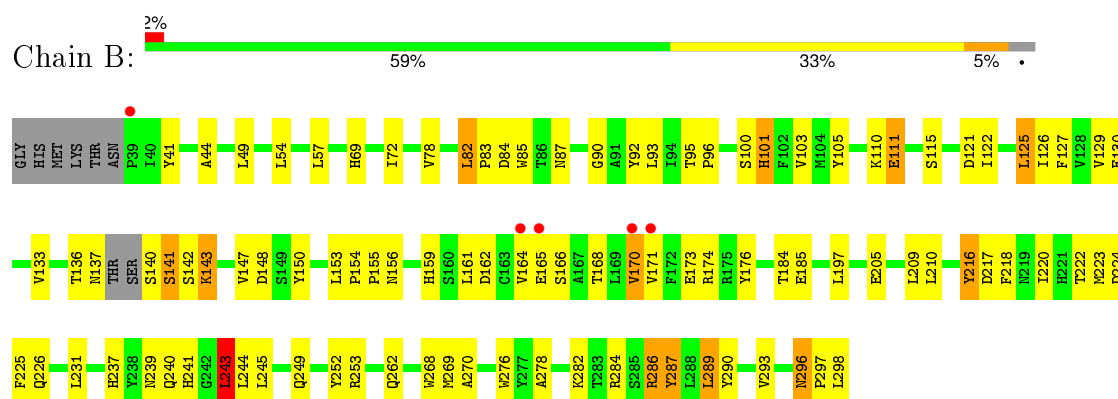
### 3 Residue-property plots [i](#)

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

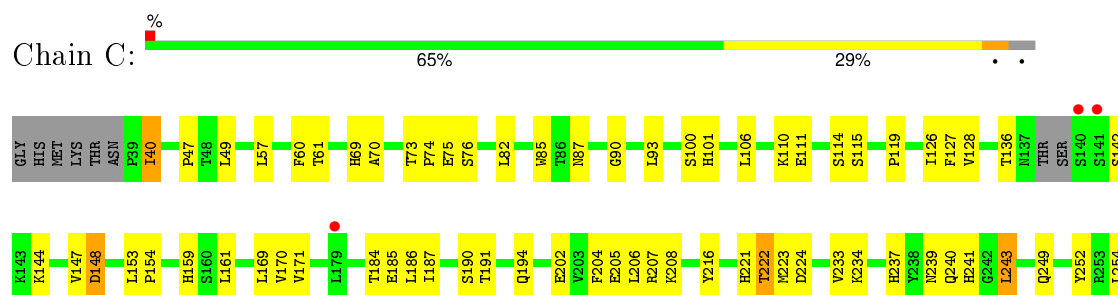
#### • Molecule 1: Ureidoglycine aminohydrolase



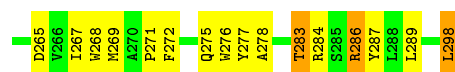
#### • Molecule 1: Ureidoglycine aminohydrolase



#### • Molecule 1: Ureidoglycine aminohydrolase



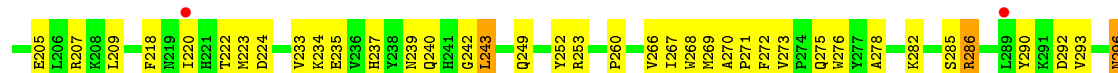
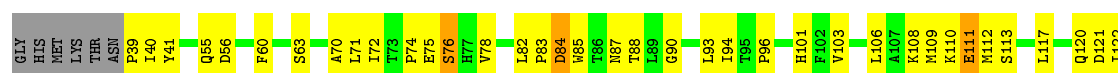




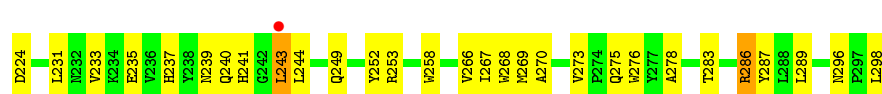
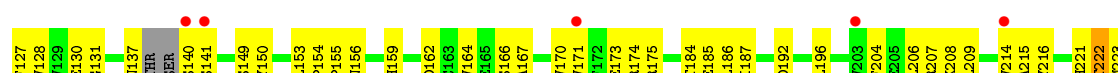
• Molecule 1: Ureidoglycine aminohydrolase



• Molecule 1: Ureidoglycine aminohydrolase

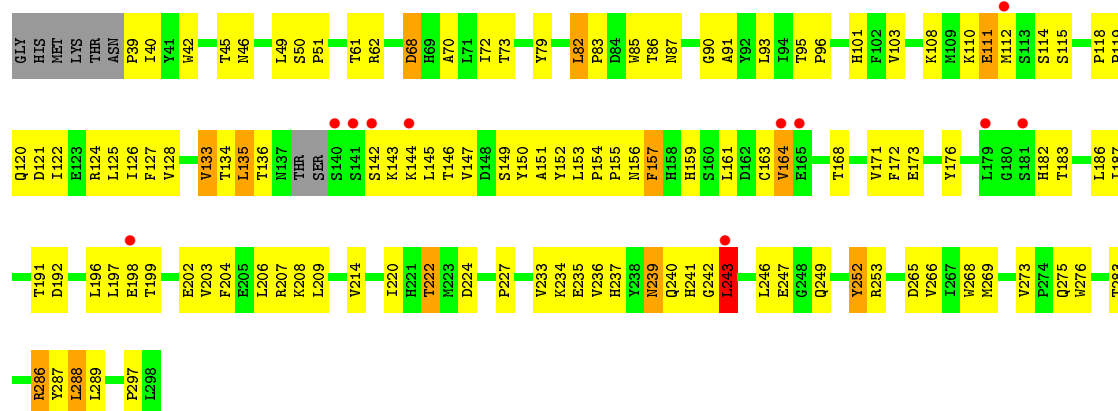


• Molecule 1: Ureidoglycine aminohydrolase

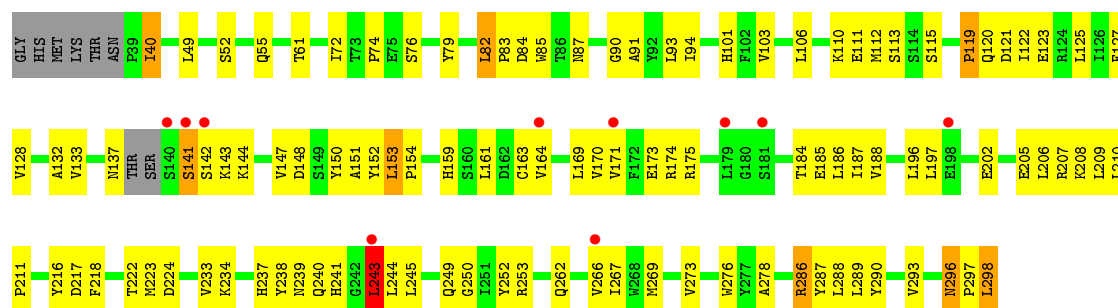


• Molecule 1: Ureidoglycine aminohydrolase

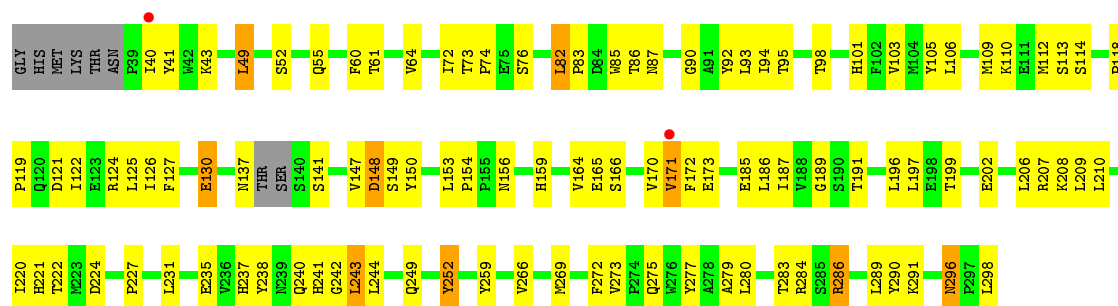




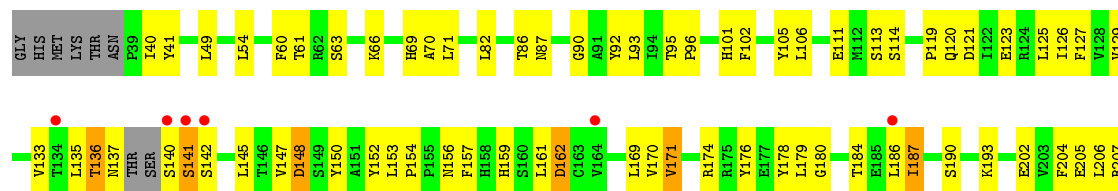
- Molecule 1: Ureidoglycine aminohydrolase

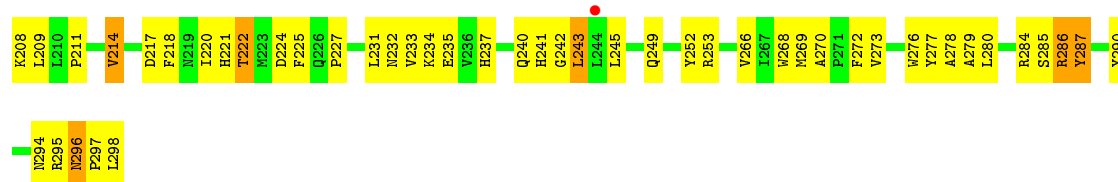


- Molecule 1: Ureidoglycine aminohydrolase

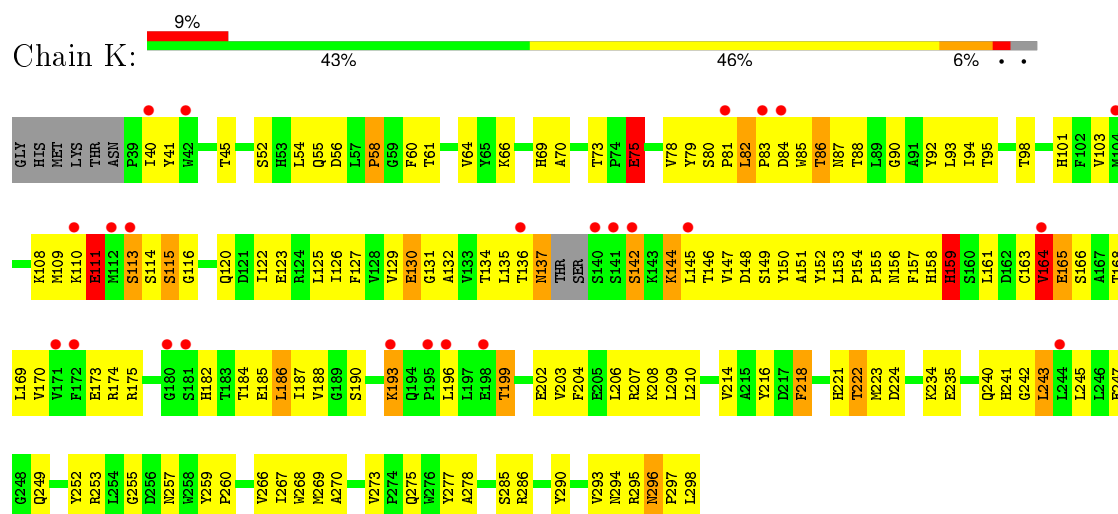


- Molecule 1: Ureidoglycine aminohydrolase

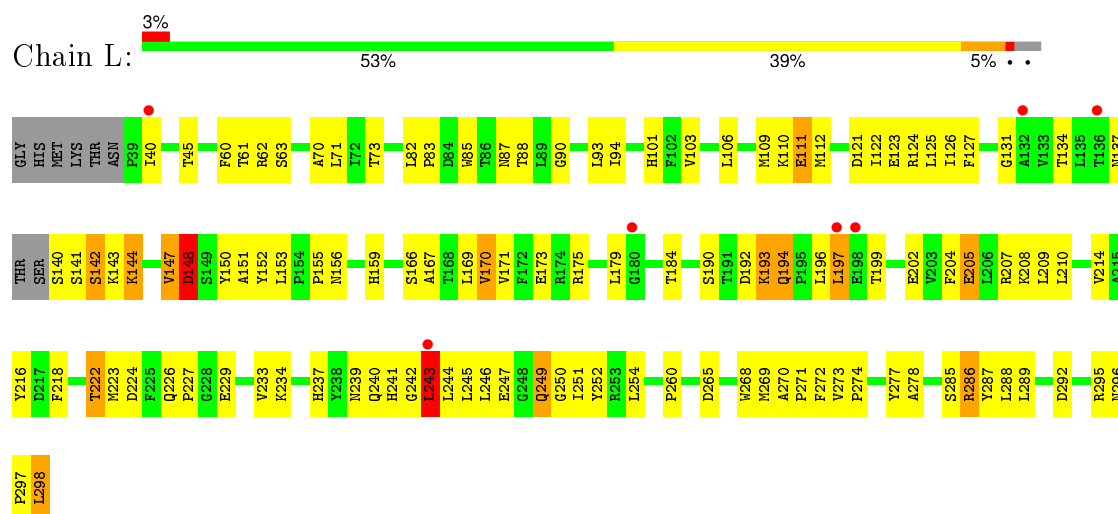




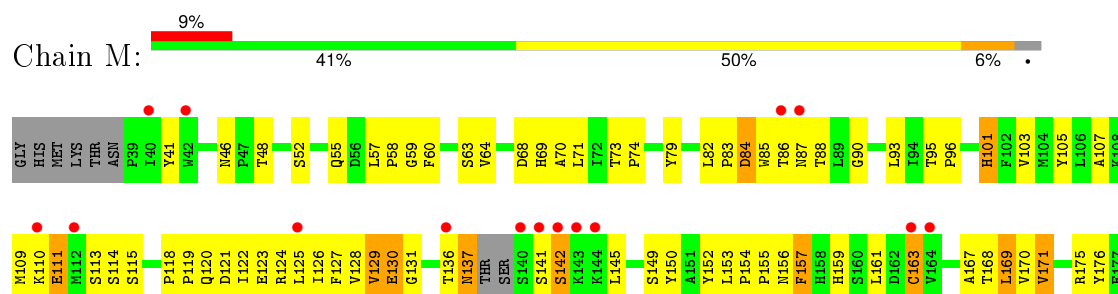
• Molecule 1: Ureidoglycine aminohydrolase

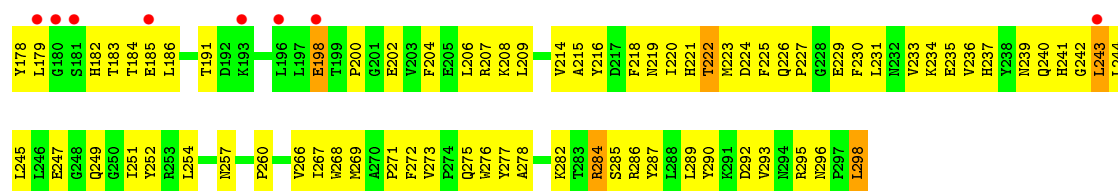


• Molecule 1: Ureidoglycine aminohydrolase

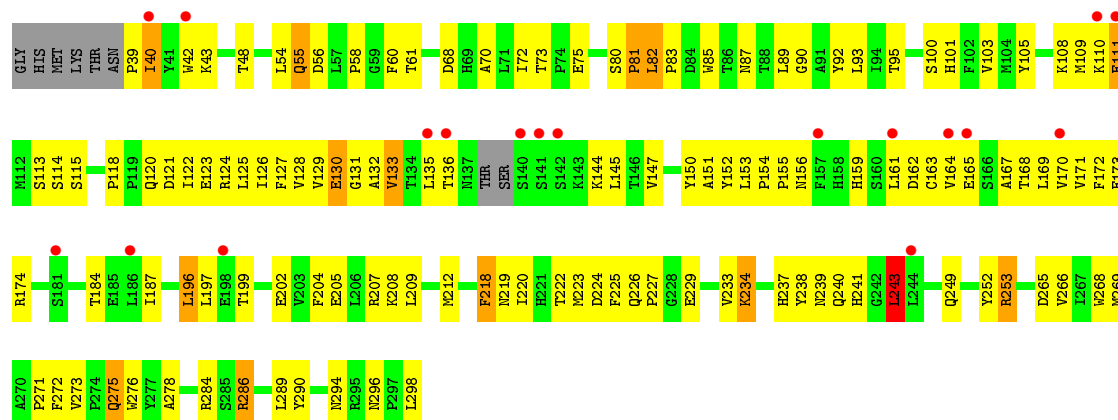


• Molecule 1: Ureidoglycine aminohydrolase

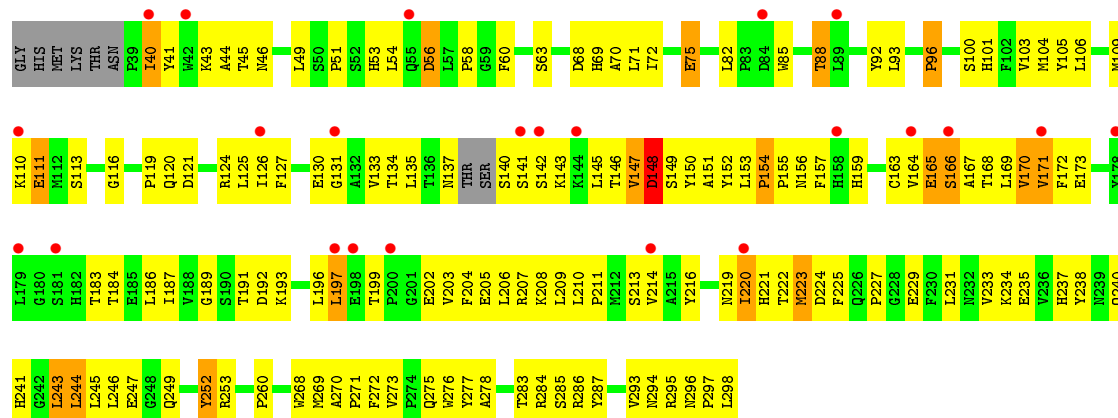
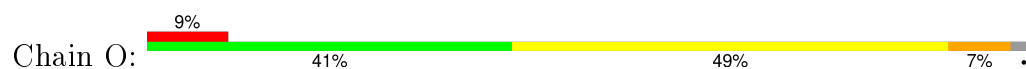




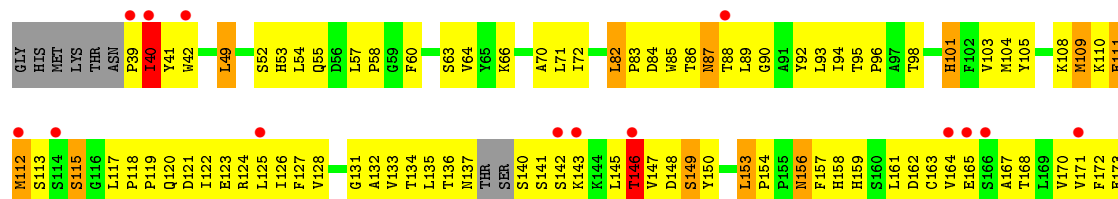
• Molecule 1: Ureidoglycine aminohydrolase

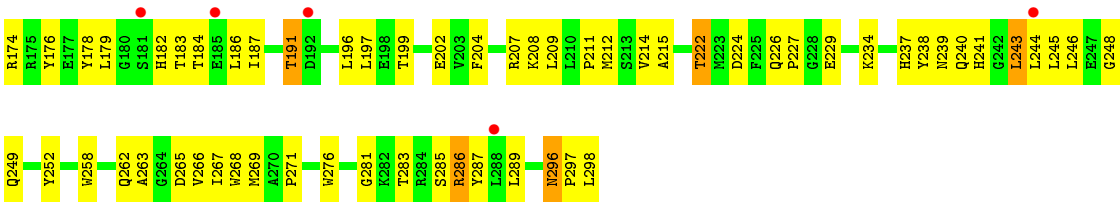


• Molecule 1: Ureidoglycine aminohydrolase



• Molecule 1: Ureidoglycine aminohydrolase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	93.86Å 175.77Å 155.18Å 90.00° 99.39° 90.00°	Depositor
Resolution (Å)	50.00 – 2.50 30.40 – 2.50	Depositor EDS
% Data completeness (in resolution range)	89.1 (50.00-2.50) 97.8 (30.40-2.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.92 (at 2.51Å)	Xtriage
Refinement program	CNS 1.21	Depositor
R, $R_{free}$	0.224 , 0.286 0.242 , 0.244	Depositor DCC
$R_{free}$ test set	16554 reflections (9.91%)	DCC
Wilson B-factor (Å <sup>2</sup> )	44.5	Xtriage
Anisotropy	0.248	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 47.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	0 of 167051 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	33964	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.56% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.44	0/2140	0.69	1/2920 (0.0%)
1	B	0.42	0/2140	0.69	1/2920 (0.0%)
1	C	0.45	0/2140	0.70	0/2920
1	D	0.43	0/2140	0.68	2/2920 (0.1%)
1	E	0.45	0/2140	0.70	1/2920 (0.0%)
1	F	0.43	0/2140	0.67	0/2920
1	G	0.45	0/2140	0.71	2/2920 (0.1%)
1	H	0.45	0/2140	0.71	1/2920 (0.0%)
1	I	0.44	0/2140	0.70	1/2920 (0.0%)
1	J	0.44	0/2140	0.68	1/2920 (0.0%)
1	K	0.47	0/2140	0.69	1/2920 (0.0%)
1	L	0.45	0/2140	0.69	2/2920 (0.1%)
1	M	0.47	0/2140	0.69	1/2920 (0.0%)
1	N	0.47	0/2140	0.68	1/2920 (0.0%)
1	O	0.47	0/2140	0.69	0/2920
1	P	0.46	0/2140	0.71	1/2920 (0.0%)
All	All	0.45	0/34240	0.69	16/46720 (0.0%)

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	B	0	2
1	C	0	1
1	J	0	1
All	All	0	4

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	242	GLY	N-CA-C	-6.13	97.78	113.10
1	A	242	GLY	N-CA-C	-6.02	98.06	113.10
1	M	242	GLY	N-CA-C	-5.72	98.80	113.10
1	J	242	GLY	N-CA-C	-5.66	98.94	113.10
1	N	243	LEU	CA-CB-CG	5.63	128.24	115.30
1	G	242	GLY	N-CA-C	-5.62	99.04	113.10
1	I	242	GLY	N-CA-C	-5.52	99.30	113.10
1	B	243	LEU	CA-CB-CG	5.46	127.85	115.30
1	D	242	GLY	N-CA-C	-5.42	99.55	113.10
1	G	243	LEU	CA-CB-CG	5.30	127.50	115.30
1	P	153	LEU	CA-CB-CG	-5.20	103.33	115.30
1	K	242	GLY	N-CA-C	-5.20	100.11	113.10
1	E	242	GLY	N-CA-C	-5.16	100.20	113.10
1	H	243	LEU	CA-CB-CG	5.16	127.16	115.30
1	D	153	LEU	CA-CB-CG	-5.03	103.73	115.30
1	L	243	LEU	CA-CB-CG	5.03	126.87	115.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	216	TYR	Sidechain
1	B	287	TYR	Sidechain
1	C	287	TYR	Sidechain
1	J	287	TYR	Sidechain

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2076	0	2034	73	0
1	B	2076	0	2034	78	0
1	C	2076	0	2034	71	0
1	D	2076	0	2034	89	0
1	E	2076	0	2034	100	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	116	0
1	H	2076	0	2034	100	0
1	I	2076	0	2034	100	0
1	J	2076	0	2034	110	0
1	K	2076	0	2034	153	0
1	L	2076	0	2034	131	0
1	M	2076	0	2034	148	0
1	N	2076	0	2034	130	0
1	O	2076	0	2034	158	0
1	P	2076	0	2034	164	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	67	0	0	4	0
3	B	75	0	0	3	0
3	C	80	0	0	2	0
3	D	57	0	0	2	0
3	E	50	0	0	5	0
3	F	51	0	0	6	0
3	G	44	0	0	2	0
3	H	49	0	0	2	0
3	I	39	0	0	1	0
3	J	36	0	0	2	0
3	K	36	0	0	4	0
3	L	25	0	0	0	0
3	M	24	0	0	3	0
3	N	42	0	0	1	0
3	O	28	0	0	5	0
3	P	29	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	33964	0	32544	1720	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 26.

All (1720) 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:K:130:GLU:HB3	1:K:168:THR:HB	1.36	1.06
1:P:121:ASP:H	1:P:156:ASN:ND2	1.53	1.05
1:L:137:ASN:HD21	1:L:140:SER:HB3	1.21	1.05
1:P:40:ILE:H	1:P:40:ILE:HD12	1.17	1.05
1:P:196:LEU:HD21	1:P:207:ARG:HH21	1.19	1.04
1:M:136:THR:HG22	1:M:142:SER:HB2	1.40	1.03
1:K:224:ASP:OD2	1:K:286:ARG:HD3	1.59	1.02
1:G:40:ILE:H	1:G:40:ILE:HD12	1.23	1.02
1:K:120:GLN:HG3	1:K:156:ASN:HD21	1.21	1.01
1:N:241:HIS:HB2	1:N:269:MET:HB2	1.42	1.01
1:C:136:THR:HG22	1:C:142:SER:HB2	1.42	1.00
1:F:224:ASP:OD1	1:F:286:ARG:HD3	1.62	0.99
1:J:296:ASN:HD22	1:J:297:PRO:HD2	1.27	0.98
1:P:133:VAL:HG23	1:P:163:CYS:HB3	1.43	0.97
1:P:72:ILE:HD13	1:P:266:VAL:HG12	1.47	0.97
1:H:224:ASP:OD2	1:H:286:ARG:HD3	1.64	0.97
1:O:205:GLU:HB2	1:O:224:ASP:HB2	1.46	0.96
1:A:40:ILE:H	1:A:40:ILE:HD12	1.27	0.96
1:N:284:ARG:HH22	1:N:286:ARG:HH21	0.99	0.96
1:G:115:SER:HB3	1:G:161:LEU:HB2	1.47	0.96
1:O:40:ILE:HD13	1:O:147:VAL:HG11	1.47	0.96
1:K:153:LEU:HD13	1:K:159:HIS:NE2	1.81	0.95
1:O:147:VAL:O	1:O:148:ASP:HB2	1.67	0.94
1:F:82:LEU:HD13	1:F:90:GLY:HA3	1.50	0.93
1:H:296:ASN:ND2	1:H:298:LEU:HB2	1.83	0.93
1:E:296:ASN:HD22	1:E:297:PRO:HD2	1.35	0.92
1:A:239:ASN:HD22	1:A:239:ASN:N	1.67	0.92
1:G:136:THR:HG22	1:G:142:SER:HB2	1.52	0.91
1:P:164:VAL:HG23	1:P:165:GLU:HG2	1.50	0.91
1:P:121:ASP:H	1:P:156:ASN:HD21	1.14	0.91
1:M:208:LYS:HB3	1:M:219:ASN:HD21	1.35	0.89
1:K:88:THR:HG22	1:K:109:MET:HA	1.53	0.89
1:O:241:HIS:HB2	1:O:269:MET:HB2	1.55	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:40:ILE:HD12	1:E:40:ILE:H	1.35	0.89
1:I:224:ASP:OD2	1:I:286:ARG:HD3	1.74	0.88
1:A:239:ASN:H	1:A:239:ASN:ND2	1.70	0.88
1:P:243:LEU:HB3	1:P:289:LEU:HD12	1.55	0.87
1:A:239:ASN:HD22	1:A:239:ASN:H	0.90	0.87
1:C:101:HIS:H	1:C:240:GLN:HE22	1.23	0.87
1:L:121:ASP:H	1:L:156:ASN:HD21	1.22	0.87
1:H:222:THR:HG23	1:H:286:ARG:HD2	1.55	0.87
1:N:284:ARG:NH2	1:N:286:ARG:HH21	1.71	0.86
1:B:224:ASP:OD2	1:B:286:ARG:HD3	1.74	0.86
1:L:144:LYS:HB2	1:L:144:LYS:NZ	1.90	0.85
1:D:296:ASN:HD22	1:D:298:LEU:H	1.24	0.84
1:K:222:THR:HG23	1:K:286:ARG:HD2	1.58	0.84
1:I:130:GLU:HA	1:I:147:VAL:HG22	1.60	0.84
1:M:68:ASP:OD2	1:M:273:VAL:HG23	1.78	0.83
1:G:224:ASP:OD2	1:G:286:ARG:HD3	1.79	0.83
1:E:82:LEU:HD13	1:E:90:GLY:HA3	1.60	0.82
1:A:222:THR:HG23	1:A:286:ARG:HD2	1.59	0.82
1:M:226:GLN:O	1:M:229:GLU:HG3	1.79	0.82
1:D:40:ILE:H	1:D:40:ILE:HD12	1.43	0.82
1:F:241:HIS:HB2	1:F:269:MET:HB2	1.62	0.82
1:G:246:LEU:HD11	1:G:288:LEU:HD13	1.58	0.82
1:M:185:GLU:HG2	1:M:216:TYR:OH	1.80	0.81
1:L:137:ASN:ND2	1:L:140:SER:HB3	1.93	0.81
1:N:133:VAL:HG23	1:N:163:CYS:HB2	1.62	0.81
1:O:166:SER:HB2	3:O:421:HOH:O	1.79	0.81
1:L:82:LEU:HD13	1:L:90:GLY:HA3	1.61	0.81
1:K:87:ASN:ND2	1:K:110:LYS:HB2	1.95	0.81
1:J:224:ASP:OD2	1:J:286:ARG:HD3	1.79	0.81
1:P:142:SER:O	1:P:143:LYS:HG2	1.80	0.81
1:B:87:ASN:ND2	1:B:110:LYS:HB2	1.96	0.81
1:J:205:GLU:HB2	1:J:224:ASP:HB2	1.62	0.81
1:H:87:ASN:ND2	1:H:110:LYS:HB2	1.95	0.81
1:E:101:HIS:H	1:E:240:GLN:HE22	1.30	0.80
1:A:122:ILE:HD12	1:D:298:LEU:HD22	1.62	0.80
1:P:121:ASP:N	1:P:156:ASN:HD21	1.80	0.80
1:M:154:PRO:HD2	1:M:157:PHE:HD1	1.46	0.80
1:M:96:PRO:HD3	1:M:103:VAL:HG12	1.64	0.80
1:M:145:LEU:HD22	1:M:149:SER:HB3	1.65	0.79
1:M:150:TYR:CE2	1:M:209:LEU:HB3	2.18	0.79
1:C:241:HIS:HB2	1:C:269:MET:HB2	1.61	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:241:HIS:HB2	1:K:269:MET:HB2	1.65	0.79
1:G:128:VAL:HG12	1:G:147:VAL:HA	1.65	0.79
1:N:82:LEU:HD13	1:N:90:GLY:HA3	1.63	0.78
1:P:40:ILE:CD1	1:P:40:ILE:H	1.95	0.78
1:H:40:ILE:H	1:H:40:ILE:HD12	1.48	0.78
1:O:152:TYR:HE2	1:O:184:THR:HB	1.47	0.78
1:O:49:LEU:HD22	1:P:54:LEU:HD23	1.66	0.78
1:F:93:LEU:HD13	1:F:266:VAL:HG21	1.63	0.78
1:H:137:ASN:HA	1:H:159:HIS:HA	1.65	0.78
1:M:87:ASN:ND2	1:M:110:LYS:HB2	2.00	0.77
1:K:88:THR:HG23	1:K:113:SER:OG	1.85	0.77
1:P:196:LEU:CD2	1:P:207:ARG:HH21	1.98	0.77
1:K:120:GLN:HG3	1:K:156:ASN:ND2	1.97	0.77
1:H:82:LEU:HD22	1:H:90:GLY:HA3	1.67	0.77
1:D:147:VAL:HG23	3:D:443:HOH:O	1.85	0.77
1:P:40:ILE:N	1:P:40:ILE:HD12	1.97	0.77
1:N:126:ILE:HD11	1:N:151:ALA:HB3	1.67	0.77
1:P:39:PRO:O	1:P:42:TRP:HB2	1.83	0.77
1:G:247:GLU:HB2	1:G:286:ARG:HB3	1.67	0.76
1:P:186:LEU:HD12	1:P:187:ILE:N	2.01	0.76
1:E:296:ASN:ND2	1:E:297:PRO:HD2	2.00	0.76
1:L:224:ASP:OD2	1:L:286:ARG:HD3	1.85	0.76
1:L:296:ASN:HD22	1:L:297:PRO:HD2	1.50	0.76
1:A:127:PHE:HB3	1:A:170:VAL:CG1	2.16	0.76
1:H:243:LEU:HD13	1:H:287:TYR:HB2	1.68	0.76
1:A:40:ILE:N	1:A:40:ILE:HD12	2.01	0.76
1:N:115:SER:HB3	1:N:161:LEU:HB2	1.67	0.76
1:L:40:ILE:H	1:L:40:ILE:HD12	1.51	0.75
1:K:86:THR:OG1	1:K:114:SER:HB3	1.87	0.75
1:B:82:LEU:HD13	1:B:90:GLY:HA3	1.68	0.75
1:N:197:LEU:HD13	1:N:208:LYS:HG3	1.69	0.75
1:G:125:LEU:HD13	1:G:126:ILE:N	2.03	0.74
1:D:64:VAL:HG11	1:D:66:LYS:HE3	1.69	0.74
1:I:252:TYR:CD1	1:I:277:TYR:HD1	2.04	0.74
1:P:72:ILE:H	1:P:72:ILE:HD12	1.52	0.74
1:O:49:LEU:HD23	1:P:57:LEU:HD12	1.70	0.74
1:K:150:TYR:CE2	1:K:209:LEU:HB3	2.23	0.74
1:O:296:ASN:ND2	1:O:298:LEU:HB2	2.02	0.74
1:G:101:HIS:H	1:G:240:GLN:HE22	1.36	0.74
1:O:207:ARG:HB2	1:O:222:THR:OG1	1.87	0.74
1:L:251:ILE:HD13	1:L:260:PRO:HA	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:101:HIS:H	1:D:240:GLN:HE22	1.35	0.74
1:D:276:TRP:CH2	1:D:278:ALA:HB2	2.23	0.74
1:N:284:ARG:HH22	1:N:286:ARG:NH2	1.80	0.74
1:D:82:LEU:HD13	1:D:90:GLY:HA3	1.70	0.74
1:L:101:HIS:H	1:L:240:GLN:HE22	1.35	0.73
1:N:196:LEU:HD22	1:N:196:LEU:N	2.03	0.73
1:P:128:VAL:HG23	1:P:148:ASP:N	2.02	0.73
1:J:135:LEU:HB2	1:J:145:LEU:HD11	1.70	0.73
1:K:40:ILE:HD12	1:K:40:ILE:N	2.04	0.73
1:B:153:LEU:HD13	1:B:159:HIS:CE1	2.24	0.73
1:H:111:GLU:H	1:H:111:GLU:CD	1.93	0.73
1:N:75:GLU:N	1:N:75:GLU:OE1	2.20	0.73
1:M:87:ASN:HD21	1:M:110:LYS:HB2	1.52	0.72
1:K:193:LYS:HE3	1:K:193:LYS:HA	1.70	0.72
1:P:241:HIS:HB2	1:P:269:MET:HB2	1.71	0.72
1:K:88:THR:HG22	1:K:109:MET:CA	2.19	0.72
1:A:262:GLN:HG2	1:C:57:LEU:HD21	1.70	0.72
1:M:137:ASN:HD22	1:M:137:ASN:H	1.36	0.72
1:L:87:ASN:ND2	1:L:110:LYS:HB2	2.04	0.72
1:A:127:PHE:HB3	1:A:170:VAL:HG13	1.70	0.72
1:I:280:LEU:HD21	1:J:280:LEU:HD21	1.72	0.72
1:D:239:ASN:H	1:D:239:ASN:HD22	1.36	0.72
1:O:127:PHE:HB3	1:O:170:VAL:HG13	1.72	0.72
1:I:164:VAL:HG23	1:I:165:GLU:N	2.05	0.71
1:K:145:LEU:HD11	1:K:188:VAL:HG13	1.71	0.71
1:A:40:ILE:H	1:A:40:ILE:CD1	2.01	0.71
1:C:224:ASP:OD2	1:C:286:ARG:HD3	1.89	0.71
1:M:202:GLU:OE2	1:M:233:VAL:HG12	1.89	0.71
1:G:40:ILE:N	1:G:40:ILE:HD12	2.04	0.71
1:O:153:LEU:HD13	1:O:159:HIS:CD2	2.25	0.71
1:G:70:ALA:HB3	1:G:268:TRP:HB3	1.72	0.71
1:P:82:LEU:CD1	1:P:90:GLY:HA3	2.20	0.71
1:M:234:LYS:HE3	1:O:60:PHE:O	1.89	0.71
1:I:121:ASP:H	1:I:156:ASN:HD21	1.39	0.71
1:P:224:ASP:OD2	1:P:286:ARG:HD3	1.90	0.71
1:J:150:TYR:CE2	1:J:209:LEU:HB3	2.25	0.71
1:P:128:VAL:HG23	1:P:148:ASP:H	1.53	0.70
1:P:186:LEU:HD12	1:P:187:ILE:H	1.56	0.70
1:M:128:VAL:HG22	1:M:169:LEU:HD21	1.73	0.70
1:N:95:THR:HG23	1:O:272:PHE:HZ	1.57	0.70
1:J:241:HIS:HB2	1:J:269:MET:HB2	1.70	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:153:LEU:HD13	1:H:159:HIS:CE1	2.27	0.70
1:K:218:PHE:HB2	1:K:290:TYR:CE1	2.26	0.70
1:O:235:GLU:HB2	1:O:275:GLN:HG3	1.74	0.70
1:L:127:PHE:HB3	1:L:170:VAL:HG13	1.73	0.70
1:E:93:LEU:HD13	1:E:266:VAL:HG21	1.74	0.70
1:D:137:ASN:HD21	1:D:140:SER:HB2	1.56	0.70
1:P:72:ILE:N	1:P:72:ILE:HD12	2.05	0.70
1:I:252:TYR:HD1	1:I:277:TYR:HD1	1.39	0.70
1:J:234:LYS:HG2	1:K:61:THR:HB	1.73	0.70
1:K:153:LEU:HD13	1:K:159:HIS:CD2	2.26	0.70
1:B:136:THR:HG22	1:B:142:SER:OG	1.92	0.70
1:B:243:LEU:HD12	1:B:244:LEU:N	2.07	0.70
1:O:49:LEU:HD23	1:P:57:LEU:CD1	2.22	0.69
1:G:133:VAL:HG23	1:G:163:CYS:HB2	1.74	0.69
1:D:59:GLY:O	1:K:253:ARG:NH1	2.25	0.69
1:O:260:PRO:O	1:P:57:LEU:HD22	1.92	0.69
1:D:241:HIS:HB2	1:D:269:MET:HB2	1.72	0.69
1:N:61:THR:HG22	1:O:253:ARG:NH1	2.08	0.69
1:P:133:VAL:CG2	1:P:163:CYS:HB3	2.18	0.69
1:P:128:VAL:HG21	1:P:146:THR:O	1.93	0.69
1:H:243:LEU:HD22	1:H:287:TYR:CD1	2.28	0.69
1:K:296:ASN:HD22	1:K:297:PRO:HD2	1.58	0.69
1:J:187:ILE:HD12	1:J:211:PRO:HD3	1.75	0.69
1:N:196:LEU:HD22	1:N:196:LEU:H	1.55	0.68
1:P:85:TRP:HA	1:P:115:SER:O	1.94	0.68
1:M:237:HIS:CE1	1:M:239:ASN:HB2	2.28	0.68
1:O:109:MET:HB2	1:O:167:ALA:HB3	1.74	0.68
1:L:147:VAL:HG12	1:L:148:ASP:N	2.08	0.68
1:L:150:TYR:CZ	1:L:209:LEU:HB3	2.28	0.68
1:J:126:ILE:HD13	1:J:161:LEU:HD11	1.74	0.68
1:E:122:ILE:HD12	1:P:298:LEU:HD13	1.74	0.68
1:H:241:HIS:HB2	1:H:269:MET:HB2	1.74	0.68
1:C:298:LEU:HG	1:G:103:VAL:HG13	1.74	0.68
1:I:121:ASP:H	1:I:156:ASN:ND2	1.91	0.68
1:B:87:ASN:HD21	1:B:110:LYS:HB2	1.59	0.68
1:L:122:ILE:HD13	1:L:175:ARG:HA	1.73	0.68
1:O:163:CYS:HA	3:O:412:HOH:O	1.94	0.68
1:B:241:HIS:HB2	1:B:269:MET:HB2	1.76	0.67
1:L:243:LEU:HD13	1:L:287:TYR:HB2	1.76	0.67
1:G:202:GLU:OE2	1:G:233:VAL:HG12	1.94	0.67
1:N:122:ILE:HD12	1:O:298:LEU:HD13	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:101:HIS:H	1:H:240:GLN:HE22	1.40	0.67
1:O:137:ASN:HD21	1:O:141:SER:H	1.41	0.67
1:C:154:PRO:HG2	1:C:185:GLU:HA	1.74	0.67
1:G:115:SER:CB	1:G:161:LEU:HB2	2.23	0.67
1:M:93:LEU:HD13	1:M:266:VAL:HG21	1.76	0.67
1:F:87:ASN:ND2	1:F:110:LYS:HB2	2.10	0.67
1:H:296:ASN:HD22	1:H:298:LEU:H	1.42	0.67
1:I:87:ASN:HD21	1:I:110:LYS:HB2	1.59	0.67
1:M:243:LEU:C	1:M:243:LEU:HD12	2.14	0.67
1:M:182:HIS:O	1:M:183:THR:HG23	1.95	0.67
1:K:110:LYS:O	1:K:113:SER:HB2	1.94	0.67
1:K:150:TYR:CD1	1:K:209:LEU:HD13	2.30	0.67
1:K:145:LEU:HB3	1:K:149:SER:HB2	1.76	0.67
1:A:241:HIS:HB2	1:A:269:MET:HB2	1.76	0.67
1:K:87:ASN:HD21	1:K:110:LYS:HB2	1.60	0.66
1:M:157:PHE:HE1	1:M:186:LEU:HB2	1.60	0.66
1:H:296:ASN:HD22	1:H:298:LEU:HB2	1.57	0.66
1:L:144:LYS:HB2	1:L:144:LYS:HZ3	1.59	0.66
1:F:40:ILE:HD12	1:F:40:ILE:H	1.60	0.66
1:K:66:LYS:HD2	1:K:69:HIS:CE1	2.30	0.66
1:I:153:LEU:HD13	1:I:159:HIS:CD2	2.30	0.66
1:E:40:ILE:HA	3:E:445:HOH:O	1.94	0.66
1:O:152:TYR:HB3	1:O:187:ILE:HB	1.77	0.66
1:L:103:VAL:CG2	1:L:173:GLU:HB2	2.26	0.66
1:N:296:ASN:ND2	1:N:298:LEU:HB2	2.10	0.66
1:L:137:ASN:HD21	1:L:140:SER:CB	2.05	0.66
1:E:154:PRO:HG2	1:E:185:GLU:HA	1.77	0.66
1:D:113:SER:OG	1:D:163:CYS:HB3	1.95	0.66
1:N:40:ILE:HD12	1:N:40:ILE:H	1.59	0.66
1:O:152:TYR:CE2	1:O:184:THR:HB	2.30	0.66
1:D:224:ASP:OD2	1:D:286:ARG:HD3	1.95	0.66
1:O:209:LEU:O	1:O:210:LEU:HD23	1.95	0.66
1:M:137:ASN:HB2	3:M:409:HOH:O	1.95	0.66
1:D:239:ASN:ND2	1:D:239:ASN:H	1.93	0.65
1:M:296:ASN:ND2	1:M:298:LEU:HB2	2.11	0.65
1:E:113:SER:OG	1:E:163:CYS:HB3	1.96	0.65
1:E:243:LEU:HG	1:E:267:ILE:HB	1.77	0.65
1:P:244:LEU:HD13	1:P:266:VAL:HG23	1.78	0.65
1:H:111:GLU:HA	1:H:164:VAL:O	1.95	0.65
1:K:247:GLU:O	1:K:285:SER:HA	1.97	0.65
1:B:147:VAL:O	1:B:148:ASP:HB2	1.95	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:145:LEU:HD22	1:K:149:SER:HB3	1.79	0.65
1:M:163:CYS:HA	3:M:401:HOH:O	1.96	0.65
1:D:87:ASN:ND2	1:D:110:LYS:HB2	2.10	0.65
1:C:147:VAL:O	1:C:148:ASP:HB2	1.95	0.65
1:J:153:LEU:HD13	1:J:159:HIS:CE1	2.31	0.65
1:H:184:THR:HB	1:H:216:TYR:CE1	2.32	0.65
1:B:140:SER:O	1:B:141:SER:HB2	1.96	0.65
1:C:234:LYS:HG2	1:G:61:THR:HB	1.77	0.65
1:A:136:THR:HG22	1:A:142:SER:HB2	1.78	0.65
1:N:95:THR:HG21	1:O:238:TYR:HB3	1.80	0.64
1:D:39:PRO:HG2	1:E:39:PRO:HG2	1.79	0.64
1:O:157:PHE:CE2	1:O:186:LEU:HD13	2.33	0.64
1:L:184:THR:HB	1:L:216:TYR:CE1	2.31	0.64
1:E:164:VAL:HG23	1:E:165:GLU:H	1.61	0.64
1:K:130:GLU:HB3	1:K:168:THR:CB	2.22	0.64
1:P:196:LEU:HD21	1:P:207:ARG:NH2	2.04	0.64
1:F:101:HIS:H	1:F:240:GLN:HE22	1.46	0.64
1:B:130:GLU:HB3	1:B:168:THR:HB	1.79	0.64
1:D:126:ILE:HG22	1:D:171:VAL:HB	1.80	0.64
1:F:243:LEU:HD12	1:F:243:LEU:C	2.17	0.64
1:F:150:TYR:CZ	1:F:209:LEU:HB3	2.33	0.64
1:F:150:TYR:CE2	1:F:209:LEU:HB3	2.33	0.64
1:K:199:THR:HB	1:K:202:GLU:HB2	1.79	0.64
1:L:202:GLU:OE2	1:L:233:VAL:HG12	1.97	0.64
1:O:244:LEU:HD12	1:O:245:LEU:N	2.13	0.64
1:N:243:LEU:HB3	1:N:289:LEU:HD12	1.79	0.64
1:N:204:PHE:HB3	1:N:225:PHE:CE1	2.32	0.64
1:K:103:VAL:CG2	1:K:173:GLU:HB2	2.28	0.64
1:J:101:HIS:H	1:J:240:GLN:HE22	1.45	0.64
1:G:134:THR:HG23	1:G:143:LYS:O	1.98	0.64
1:I:87:ASN:ND2	1:I:110:LYS:HB2	2.12	0.64
1:G:40:ILE:H	1:G:40:ILE:CD1	1.99	0.64
1:J:272:PHE:HZ	1:K:95:THR:HG23	1.61	0.64
1:I:252:TYR:CD1	1:I:277:TYR:CD1	2.86	0.64
1:L:87:ASN:HD21	1:L:110:LYS:HB2	1.62	0.64
1:O:163:CYS:SG	1:O:167:ALA:HB2	2.38	0.64
1:P:89:LEU:HG	1:P:110:LYS:NZ	2.13	0.63
1:L:207:ARG:HH11	1:L:207:ARG:HG3	1.63	0.63
1:P:153:LEU:HD13	1:P:159:HIS:CD2	2.32	0.63
1:L:243:LEU:HD12	1:L:244:LEU:N	2.13	0.63
1:I:127:PHE:HB3	1:I:170:VAL:CG1	2.28	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:153:LEU:HD13	1:I:159:HIS:NE2	2.13	0.63
1:K:144:LYS:HE2	1:K:146:THR:HG22	1.79	0.63
1:E:40:ILE:CD1	1:E:40:ILE:H	2.11	0.63
1:K:126:ILE:O	1:K:126:ILE:HD12	1.97	0.63
1:I:150:TYR:CE2	1:I:209:LEU:HB3	2.34	0.63
1:J:272:PHE:CZ	1:K:95:THR:HG23	2.34	0.63
1:H:61:THR:HB	1:N:234:LYS:HG2	1.79	0.63
1:L:153:LEU:HD13	1:L:159:HIS:NE2	2.14	0.63
1:H:120:GLN:O	1:H:121:ASP:HB2	1.99	0.63
1:F:86:THR:O	1:F:113:SER:HB2	1.98	0.63
1:K:235:GLU:HB2	1:K:275:GLN:HG3	1.80	0.63
1:J:170:VAL:O	1:J:170:VAL:HG13	1.98	0.63
1:P:153:LEU:HD13	1:P:159:HIS:CG	2.33	0.62
1:O:243:LEU:HD13	1:O:287:TYR:HB2	1.79	0.62
1:H:152:TYR:HE2	1:H:154:PRO:HG3	1.64	0.62
1:G:234:LYS:HG2	1:I:61:THR:HB	1.81	0.62
1:G:125:LEU:C	1:G:125:LEU:HD13	2.19	0.62
1:K:199:THR:HG21	1:K:204:PHE:CZ	2.34	0.62
1:E:207:ARG:HB2	1:E:222:THR:OG1	1.99	0.62
1:P:132:ALA:HB2	1:P:146:THR:HA	1.81	0.62
1:O:296:ASN:HD21	1:O:298:LEU:HB2	1.63	0.62
1:G:239:ASN:H	1:G:239:ASN:HD22	1.47	0.62
1:J:298:LEU:HD11	1:K:122:ILE:HG21	1.81	0.62
1:J:137:ASN:HD21	1:J:140:SER:N	1.98	0.62
1:K:144:LYS:HE2	1:K:146:THR:CG2	2.30	0.62
1:A:179:LEU:O	1:A:182:HIS:HB2	2.00	0.62
1:C:153:LEU:HD13	1:C:159:HIS:CD2	2.35	0.62
1:O:293:VAL:HG23	1:O:294:ASN:ND2	2.14	0.62
1:M:79:TYR:HA	1:M:90:GLY:O	1.99	0.62
1:G:239:ASN:H	1:G:239:ASN:ND2	1.96	0.62
1:B:121:ASP:H	1:B:156:ASN:HD21	1.47	0.62
1:F:124:ARG:HB2	1:F:173:GLU:HG2	1.80	0.62
1:M:157:PHE:CE1	1:M:186:LEU:HD22	2.35	0.62
1:L:126:ILE:HB	1:L:169:LEU:HD23	1.80	0.62
1:E:243:LEU:C	1:E:243:LEU:HD12	2.20	0.62
1:B:101:HIS:H	1:B:240:GLN:HE22	1.47	0.62
1:K:93:LEU:HD13	1:K:266:VAL:HG21	1.81	0.62
1:N:93:LEU:HD13	1:N:266:VAL:HG21	1.81	0.62
1:P:118:PRO:HD3	1:P:124:ARG:NH2	2.15	0.62
1:L:144:LYS:HB2	1:L:144:LYS:HZ2	1.65	0.61
1:K:296:ASN:HD22	1:K:297:PRO:CD	2.12	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:122:ILE:HD12	1:I:298:LEU:HD13	1.82	0.61
1:B:115:SER:HB3	1:B:161:LEU:HB2	1.82	0.61
1:G:243:LEU:HD12	1:G:243:LEU:C	2.20	0.61
1:L:270:ALA:O	1:L:273:VAL:HG12	2.00	0.61
1:A:241:HIS:CG	1:A:289:LEU:HD11	2.35	0.61
1:I:60:PHE:HZ	1:K:60:PHE:HZ	1.48	0.61
1:P:109:MET:HB2	1:P:167:ALA:HB3	1.82	0.61
1:L:152:TYR:O	1:L:153:LEU:HG	2.00	0.61
1:N:103:VAL:CG2	1:N:173:GLU:HB2	2.29	0.61
1:O:197:LEU:HD12	1:O:197:LEU:N	2.16	0.61
1:L:241:HIS:HB2	1:L:269:MET:HB2	1.83	0.61
1:D:49:LEU:HD11	1:G:49:LEU:HD11	1.82	0.61
1:H:202:GLU:OE2	1:H:233:VAL:HG12	1.99	0.61
1:N:92:TYR:CZ	1:O:297:PRO:HG3	2.35	0.61
1:K:152:TYR:HB2	1:K:210:LEU:HD21	1.80	0.61
1:D:82:LEU:CD1	1:D:90:GLY:HA3	2.30	0.61
1:A:241:HIS:ND1	1:A:289:LEU:HD11	2.15	0.61
1:J:273:VAL:HG13	1:J:273:VAL:O	2.00	0.61
1:B:220:ILE:HD13	1:B:290:TYR:HA	1.83	0.61
1:P:82:LEU:HD11	1:P:90:GLY:HA3	1.83	0.61
1:P:224:ASP:OD2	1:P:286:ARG:CD	2.49	0.61
1:D:126:ILE:O	1:D:126:ILE:HD12	2.01	0.61
1:K:134:THR:HA	1:K:144:LYS:HA	1.82	0.61
1:F:47:PRO:HA	3:F:413:HOH:O	2.01	0.61
1:F:96:PRO:HD3	1:F:103:VAL:HG12	1.82	0.61
1:A:296:ASN:HD22	1:A:298:LEU:H	1.48	0.61
1:E:202:GLU:OE2	1:E:233:VAL:HG12	2.00	0.61
1:P:245:LEU:O	1:P:263:ALA:HA	2.00	0.61
1:O:247:GLU:HG2	1:O:286:ARG:HB3	1.82	0.61
1:L:243:LEU:C	1:L:243:LEU:HD12	2.21	0.61
1:K:145:LEU:HD11	1:K:188:VAL:CG1	2.30	0.61
1:K:144:LYS:C	1:K:144:LYS:HD3	2.21	0.61
1:M:101:HIS:H	1:M:240:GLN:HE22	1.47	0.61
1:D:125:LEU:C	1:D:125:LEU:HD13	2.21	0.61
1:K:157:PHE:CZ	1:K:186:LEU:HD22	2.36	0.60
1:O:109:MET:HB3	1:O:113:SER:OG	2.00	0.60
1:B:121:ASP:H	1:B:156:ASN:ND2	1.99	0.60
1:A:296:ASN:ND2	1:A:298:LEU:H	2.00	0.60
1:G:241:HIS:HD2	1:G:275:GLN:HE22	1.48	0.60
1:O:204:PHE:HB3	1:O:225:PHE:CE1	2.36	0.60
1:P:296:ASN:HD22	1:P:298:LEU:H	1.47	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:223:MET:CE	1:B:289:LEU:HD22	2.31	0.60
1:H:150:TYR:CE2	1:H:209:LEU:HB3	2.36	0.60
1:M:225:PHE:O	1:M:284:ARG:HB2	2.02	0.60
1:F:54:LEU:HD23	1:H:49:LEU:HD22	1.82	0.60
1:F:224:ASP:OD1	1:F:286:ARG:HB2	2.01	0.60
1:E:122:ILE:HD13	1:E:175:ARG:HA	1.82	0.60
1:O:137:ASN:ND2	1:O:141:SER:N	2.49	0.60
1:J:40:ILE:HG22	1:J:41:TYR:CD2	2.36	0.60
1:K:137:ASN:HD22	1:K:137:ASN:N	1.98	0.60
1:B:237:HIS:CE1	1:B:239:ASN:HB2	2.36	0.60
1:I:82:LEU:HD13	1:I:90:GLY:HA3	1.83	0.60
1:C:276:TRP:CH2	1:C:278:ALA:HB2	2.36	0.60
1:N:234:LYS:N	1:N:234:LYS:HE2	2.17	0.60
1:P:199:THR:HG21	1:P:204:PHE:CE1	2.36	0.60
1:G:153:LEU:HD13	1:G:159:HIS:NE2	2.17	0.60
1:O:151:ALA:HA	1:O:187:ILE:O	2.02	0.60
1:F:125:LEU:C	1:F:125:LEU:HD13	2.22	0.60
1:I:72:ILE:N	1:I:72:ILE:HD12	2.17	0.60
1:I:252:TYR:HD1	1:I:277:TYR:CD1	2.19	0.60
1:I:241:HIS:HB2	1:I:269:MET:HB2	1.83	0.60
1:C:237:HIS:HB2	1:C:239:ASN:HD22	1.67	0.59
1:M:83:PRO:O	1:M:84:ASP:HB2	2.00	0.59
1:I:252:TYR:CE1	1:I:277:TYR:HB2	2.38	0.59
1:O:202:GLU:HG3	1:O:204:PHE:HE2	1.66	0.59
1:K:243:LEU:HD12	1:K:243:LEU:C	2.22	0.59
1:K:126:ILE:HG12	1:K:161:LEU:HD11	1.84	0.59
1:E:103:VAL:CG2	1:E:173:GLU:HB2	2.32	0.59
1:E:272:PHE:HE2	1:F:95:THR:HG1	1.50	0.59
1:E:117:LEU:HD21	1:E:159:HIS:H	1.66	0.59
1:K:122:ILE:HD13	1:K:175:ARG:HA	1.84	0.59
1:L:121:ASP:H	1:L:156:ASN:ND2	1.97	0.59
1:L:150:TYR:CE2	1:L:209:LEU:HB3	2.37	0.59
1:M:125:LEU:HD13	1:M:126:ILE:N	2.18	0.59
1:L:179:LEU:HD22	1:L:295:ARG:HD3	1.84	0.59
1:A:101:HIS:O	1:A:174:ARG:HG3	2.03	0.59
1:F:208:LYS:HD3	1:F:221:HIS:NE2	2.17	0.59
1:M:137:ASN:HD22	1:M:137:ASN:N	1.97	0.59
1:G:153:LEU:HD13	1:G:159:HIS:CE1	2.38	0.59
1:M:157:PHE:C	1:M:157:PHE:CD2	2.75	0.59
1:I:279:ALA:O	1:I:280:LEU:HD23	2.02	0.59
1:K:64:VAL:CG1	1:K:66:LYS:HE3	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:111:GLU:H	1:M:111:GLU:CD	2.05	0.59
1:H:87:ASN:HD21	1:H:110:LYS:HB2	1.65	0.59
1:I:164:VAL:HG23	1:I:165:GLU:H	1.67	0.59
1:L:126:ILE:HD13	1:L:169:LEU:HD23	1.85	0.59
1:K:64:VAL:HG11	1:K:66:LYS:HE3	1.83	0.59
1:D:103:VAL:HG23	1:D:173:GLU:HB2	1.84	0.59
1:C:101:HIS:N	1:C:240:GLN:HE22	1.97	0.59
1:M:296:ASN:ND2	1:O:119:PRO:HG2	2.18	0.59
1:P:127:PHE:HB3	1:P:170:VAL:HG13	1.85	0.59
1:C:70:ALA:HB3	1:C:268:TRP:HB3	1.84	0.59
1:P:243:LEU:HB3	1:P:289:LEU:CD1	2.32	0.59
1:P:52:SER:O	1:P:55:GLN:HG2	2.03	0.59
1:H:207:ARG:HB2	1:H:222:THR:HB	1.85	0.58
1:H:52:SER:O	1:H:55:GLN:HG2	2.03	0.58
1:N:133:VAL:HG23	1:N:163:CYS:CB	2.31	0.58
1:J:150:TYR:CZ	1:J:209:LEU:HB3	2.37	0.58
1:M:130:GLU:O	1:M:167:ALA:HA	2.03	0.58
1:F:184:THR:HB	1:F:216:TYR:CE1	2.38	0.58
1:E:55:GLN:HA	3:E:418:HOH:O	2.04	0.58
1:P:83:PRO:O	1:P:84:ASP:HB2	2.03	0.58
1:J:180:GLY:HA3	3:J:419:HOH:O	2.02	0.58
1:M:237:HIS:ND1	1:M:239:ASN:HB2	2.18	0.58
1:B:241:HIS:CE1	1:B:289:LEU:HD21	2.38	0.58
1:G:202:GLU:HB3	1:G:204:PHE:CE2	2.38	0.58
1:G:134:THR:OG1	1:G:144:LYS:HD3	2.02	0.58
1:M:125:LEU:C	1:M:125:LEU:HD13	2.23	0.58
1:D:243:LEU:HD12	1:D:244:LEU:N	2.17	0.58
1:C:111:GLU:CD	1:C:111:GLU:H	2.07	0.58
1:C:243:LEU:HD12	1:C:243:LEU:C	2.23	0.58
1:N:126:ILE:CD1	1:N:151:ALA:HB3	2.33	0.58
1:F:170:VAL:O	1:F:170:VAL:HG13	2.04	0.58
1:F:206:LEU:HD12	1:F:207:ARG:H	1.69	0.58
1:P:87:ASN:OD1	1:P:110:LYS:HE2	2.03	0.58
1:A:272:PHE:HE2	1:J:95:THR:HG1	1.51	0.58
1:F:296:ASN:HD22	1:F:298:LEU:H	1.50	0.58
1:K:218:PHE:HB2	1:K:290:TYR:HE1	1.69	0.58
1:P:92:TYR:CD1	1:P:105:TYR:HB3	2.39	0.58
1:N:95:THR:HG23	1:O:272:PHE:CZ	2.38	0.58
1:A:126:ILE:HG22	1:A:171:VAL:HB	1.84	0.58
1:P:145:LEU:HD22	1:P:149:SER:HB2	1.86	0.58
1:O:130:GLU:HA	3:O:419:HOH:O	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:40:ILE:N	1:F:40:ILE:HD12	2.18	0.58
1:N:202:GLU:OE2	1:N:233:VAL:HG12	2.04	0.58
1:P:84:ASP:HB3	3:P:415:HOH:O	2.02	0.58
1:K:158:HIS:O	1:K:159:HIS:HB3	2.02	0.57
1:M:126:ILE:HD12	1:M:126:ILE:O	2.03	0.57
1:N:222:THR:HG21	1:N:286:ARG:HH11	1.68	0.57
1:N:199:THR:HG21	1:N:204:PHE:CE1	2.38	0.57
1:L:152:TYR:HB2	1:L:210:LEU:HD21	1.85	0.57
1:N:109:MET:HB2	1:N:167:ALA:HB3	1.86	0.57
1:O:227:PRO:HG3	1:O:283:THR:O	2.03	0.57
1:E:296:ASN:ND2	3:E:411:HOH:O	2.37	0.57
1:P:82:LEU:HD13	1:P:90:GLY:HA3	1.86	0.57
1:O:154:PRO:HB2	1:O:157:PHE:HB2	1.86	0.57
1:A:122:ILE:HD12	1:D:298:LEU:CD2	2.32	0.57
1:N:135:LEU:HA	1:N:161:LEU:HD23	1.87	0.57
1:O:206:LEU:HD11	1:O:221:HIS:HB3	1.85	0.57
1:O:235:GLU:HB2	1:O:275:GLN:CG	2.34	0.57
1:L:109:MET:HB2	1:L:167:ALA:HB3	1.85	0.57
1:B:276:TRP:CH2	1:B:278:ALA:HB2	2.40	0.57
1:D:111:GLU:HA	1:D:164:VAL:O	2.05	0.57
1:P:243:LEU:HD23	1:P:289:LEU:HD13	1.85	0.57
1:N:234:LYS:H	1:N:234:LYS:HE2	1.69	0.57
1:J:82:LEU:HD13	1:J:90:GLY:HA3	1.86	0.57
1:I:49:LEU:HD22	1:K:54:LEU:HD23	1.87	0.57
1:E:137:ASN:CG	1:E:140:SER:HB2	2.23	0.57
1:O:82:LEU:O	1:O:85:TRP:HB2	2.03	0.57
1:O:49:LEU:CD2	1:P:54:LEU:HD23	2.33	0.57
1:L:101:HIS:H	1:L:240:GLN:NE2	2.02	0.57
1:J:141:SER:OG	1:J:142:SER:N	2.36	0.57
1:F:208:LYS:HD3	1:F:221:HIS:CD2	2.39	0.57
1:M:153:LEU:HD13	1:M:159:HIS:CD2	2.40	0.57
1:A:153:LEU:HD22	1:A:159:HIS:CG	2.40	0.57
1:K:101:HIS:H	1:K:240:GLN:HE22	1.53	0.57
1:C:186:LEU:O	1:C:187:ILE:HD13	2.05	0.57
1:B:85:TRP:CE3	1:B:115:SER:HA	2.40	0.56
1:D:243:LEU:C	1:D:243:LEU:HD12	2.25	0.56
1:N:130:GLU:HG2	1:N:131:GLY:N	2.19	0.56
1:A:152:TYR:HB3	1:A:187:ILE:HB	1.87	0.56
1:K:123:GLU:HG2	1:K:174:ARG:O	2.04	0.56
1:B:223:MET:HE1	1:B:289:LEU:HD22	1.87	0.56
1:G:243:LEU:HD13	1:G:287:TYR:HB2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:ASN:HD21	1:A:140:SER:N	2.03	0.56
1:K:52:SER:O	1:K:55:GLN:HG2	2.05	0.56
1:I:227:PRO:HG3	1:I:283:THR:O	2.04	0.56
1:O:192:ASP:OD1	1:O:193:LYS:HG2	2.05	0.56
1:K:82:LEU:O	1:K:85:TRP:HB2	2.05	0.56
1:L:83:PRO:O	1:L:85:TRP:HD1	1.88	0.56
1:I:186:LEU:HD12	1:I:187:ILE:N	2.20	0.56
1:B:150:TYR:CZ	1:B:209:LEU:HB3	2.40	0.56
1:N:125:LEU:O	1:N:171:VAL:HG23	2.05	0.56
1:D:100:SER:HB2	1:D:240:GLN:NE2	2.20	0.56
1:I:209:LEU:O	1:I:210:LEU:HD23	2.06	0.56
1:I:49:LEU:HD22	1:K:54:LEU:CD2	2.36	0.56
1:C:283:THR:HB	3:C:418:HOH:O	2.05	0.56
1:O:93:LEU:HD13	1:O:104:MET:HE2	1.87	0.56
1:B:296:ASN:HD22	1:B:298:LEU:H	1.53	0.56
1:K:125:LEU:O	1:K:125:LEU:HD13	2.06	0.56
1:D:237:HIS:HB2	1:D:239:ASN:HD22	1.71	0.56
1:N:40:ILE:HD13	1:N:147:VAL:HG11	1.88	0.56
1:L:199:THR:HG21	1:L:204:PHE:CE1	2.40	0.56
1:M:153:LEU:HD13	1:M:159:HIS:NE2	2.21	0.56
1:B:125:LEU:HD13	1:B:125:LEU:C	2.26	0.56
1:J:214:VAL:HG23	1:J:294:ASN:HB3	1.86	0.56
1:A:268:TRP:CZ2	1:A:270:ALA:HB2	2.41	0.56
1:F:243:LEU:HD12	1:F:244:LEU:N	2.20	0.56
1:M:127:PHE:HB3	1:M:170:VAL:CG1	2.36	0.56
1:H:186:LEU:O	1:H:187:ILE:HD13	2.05	0.56
1:H:245:LEU:HD23	1:H:262:GLN:C	2.26	0.56
1:A:63:SER:HA	1:A:71:LEU:O	2.06	0.56
1:N:72:ILE:HD12	1:N:72:ILE:H	1.70	0.56
1:J:102:PHE:HD2	1:J:240:GLN:HE21	1.54	0.56
1:G:253:ARG:HB3	1:G:276:TRP:HB3	1.88	0.56
1:L:249:GLN:HE21	1:N:56:ASP:CG	2.09	0.56
1:E:96:PRO:HD3	1:E:103:VAL:HG12	1.87	0.56
1:N:124:ARG:HA	1:N:172:PHE:O	2.06	0.56
1:K:127:PHE:HB3	1:K:170:VAL:HG13	1.87	0.56
1:K:223:MET:O	1:K:286:ARG:HA	2.06	0.55
1:P:153:LEU:CD2	1:P:186:LEU:HD13	2.36	0.55
1:A:101:HIS:H	1:A:240:GLN:HE22	1.54	0.55
1:F:196:LEU:HD21	1:F:207:ARG:NH1	2.21	0.55
1:I:126:ILE:O	1:I:126:ILE:HD12	2.06	0.55
1:K:190:SER:O	1:K:193:LYS:N	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:137:ASN:HD21	1:O:140:SER:HB3	1.70	0.55
1:M:243:LEU:HG	1:M:267:ILE:HB	1.88	0.55
1:O:197:LEU:HD12	1:O:197:LEU:H	1.70	0.55
1:G:234:LYS:HE3	1:I:60:PHE:O	2.06	0.55
1:D:50:SER:O	1:D:53:HIS:HB2	2.06	0.55
1:O:135:LEU:HB2	1:O:145:LEU:HD11	1.86	0.55
1:D:127:PHE:HB3	1:D:170:VAL:CG1	2.36	0.55
1:L:246:LEU:HD11	1:L:288:LEU:HB2	1.88	0.55
1:A:239:ASN:N	1:A:239:ASN:ND2	2.38	0.55
1:K:145:LEU:HB3	1:K:149:SER:CB	2.37	0.55
1:N:296:ASN:ND2	1:N:298:LEU:H	2.03	0.55
1:G:111:GLU:HA	1:G:164:VAL:O	2.07	0.55
1:A:83:PRO:O	1:A:84:ASP:HB2	2.06	0.55
1:P:128:VAL:CG2	1:P:149:SER:H	2.20	0.55
1:C:40:ILE:HD13	1:C:147:VAL:HG11	1.88	0.55
1:D:126:ILE:HG12	1:D:161:LEU:HD11	1.89	0.55
1:L:62:ARG:HH22	1:L:265:ASP:CG	2.09	0.55
1:K:132:ALA:HB1	1:K:144:LYS:HE3	1.87	0.55
1:O:183:THR:HG22	1:O:184:THR:N	2.22	0.55
1:H:125:LEU:HD22	1:H:151:ALA:O	2.06	0.55
1:C:202:GLU:OE2	1:C:233:VAL:HG12	2.07	0.55
1:D:296:ASN:ND2	1:D:298:LEU:H	2.02	0.55
1:L:175:ARG:HH11	1:L:175:ARG:HG3	1.72	0.55
1:O:204:PHE:CD1	1:O:223:MET:HG3	2.42	0.55
1:I:241:HIS:HB3	1:I:289:LEU:HD11	1.87	0.55
1:M:120:GLN:HG3	1:M:156:ASN:HD21	1.72	0.55
1:L:272:PHE:HZ	1:P:95:THR:HG23	1.71	0.55
1:L:205:GLU:HG3	1:L:224:ASP:HB2	1.87	0.55
1:O:271:PRO:O	1:O:272:PHE:HB2	2.07	0.55
1:D:137:ASN:OD1	1:D:140:SER:N	2.40	0.55
1:J:126:ILE:HD13	1:J:161:LEU:CD1	2.36	0.55
1:I:119:PRO:HD2	1:I:122:ILE:HG13	1.88	0.55
1:K:130:GLU:CB	1:K:168:THR:HB	2.26	0.54
1:K:185:GLU:O	1:K:185:GLU:HG3	2.05	0.54
1:N:196:LEU:H	1:N:196:LEU:CD2	2.20	0.54
1:O:70:ALA:HB3	1:O:268:TRP:HB3	1.89	0.54
1:D:202:GLU:OE2	1:D:233:VAL:HG12	2.07	0.54
1:J:176:TYR:HE2	1:J:178:TYR:HA	1.71	0.54
1:N:82:LEU:O	1:N:85:TRP:HB2	2.08	0.54
1:G:96:PRO:HD3	1:G:103:VAL:HG12	1.90	0.54
1:C:74:PRO:C	1:C:76:SER:H	2.10	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:53:HIS:CD2	1:O:53:HIS:H	2.24	0.54
1:K:70:ALA:HB3	1:K:268:TRP:HB3	1.90	0.54
1:O:220:ILE:HG22	1:O:220:ILE:O	2.06	0.54
1:M:121:ASP:H	1:M:156:ASN:ND2	2.05	0.54
1:A:93:LEU:HD13	1:A:266:VAL:HG21	1.88	0.54
1:P:226:GLN:HB2	1:P:229:GLU:CD	2.28	0.54
1:A:54:LEU:CD2	1:C:49:LEU:HD22	2.37	0.54
1:P:131:GLY:O	1:P:147:VAL:HG23	2.08	0.54
1:P:94:ILE:O	1:P:103:VAL:HA	2.07	0.54
1:A:54:LEU:HD23	1:C:49:LEU:HD22	1.89	0.54
1:C:93:LEU:HD11	1:C:106:LEU:HG	1.90	0.54
1:N:152:TYR:HB3	1:N:187:ILE:HB	1.89	0.54
1:H:90:GLY:HA2	1:H:106:LEU:O	2.07	0.54
1:H:119:PRO:HD2	1:H:122:ILE:HG13	1.89	0.54
1:L:153:LEU:HD13	1:L:159:HIS:CD2	2.42	0.54
1:O:92:TYR:HA	1:O:105:TYR:HB3	1.89	0.54
1:M:206:LEU:HD12	1:M:207:ARG:H	1.72	0.54
1:C:136:THR:HG22	1:C:142:SER:CB	2.26	0.54
1:K:218:PHE:CG	1:K:290:TYR:HE1	2.25	0.54
1:N:92:TYR:CE1	1:O:297:PRO:HG3	2.43	0.54
1:F:127:PHE:HB3	1:F:170:VAL:CG1	2.38	0.54
1:H:218:PHE:HA	1:H:293:VAL:HG22	1.88	0.54
1:G:118:PRO:HD3	1:G:124:ARG:CZ	2.38	0.54
1:C:126:ILE:O	1:C:126:ILE:HD12	2.07	0.54
1:F:150:TYR:CD1	1:F:209:LEU:HD13	2.43	0.54
1:J:82:LEU:CD1	1:J:90:GLY:HA3	2.37	0.54
1:N:118:PRO:HD3	1:N:124:ARG:NH1	2.22	0.54
1:G:121:ASP:H	1:G:156:ASN:ND2	2.06	0.54
1:L:125:LEU:HD13	1:L:125:LEU:C	2.27	0.54
1:D:154:PRO:HB3	1:D:184:THR:OG1	2.08	0.54
1:N:222:THR:CG2	1:N:286:ARG:HH11	2.21	0.54
1:N:224:ASP:OD2	1:N:286:ARG:HB2	2.08	0.54
1:E:40:ILE:O	1:E:41:TYR:HB2	2.08	0.54
1:C:101:HIS:H	1:C:240:GLN:NE2	2.01	0.54
1:H:110:LYS:HB3	1:H:111:GLU:OE2	2.08	0.54
1:H:154:PRO:HG2	1:H:185:GLU:HA	1.89	0.54
1:A:296:ASN:ND2	1:A:298:LEU:HB2	2.23	0.54
1:C:194:GLN:HB2	1:C:207:ARG:HD3	1.90	0.54
1:H:147:VAL:O	1:H:148:ASP:HB2	2.08	0.54
1:L:40:ILE:N	1:L:40:ILE:HD12	2.20	0.54
1:A:224:ASP:OD2	1:A:286:ARG:HD3	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:82:LEU:CD1	1:N:90:GLY:HA3	2.37	0.53
1:L:101:HIS:N	1:L:240:GLN:HE22	2.03	0.53
1:K:93:LEU:HD13	1:K:266:VAL:HG11	1.90	0.53
1:N:128:VAL:HA	1:N:169:LEU:HD23	1.89	0.53
1:G:136:THR:HG22	1:G:142:SER:CB	2.32	0.53
1:J:126:ILE:HD12	1:J:169:LEU:HD23	1.90	0.53
1:C:185:GLU:O	1:C:187:ILE:HG12	2.09	0.53
1:O:44:ALA:HB2	1:O:246:LEU:O	2.09	0.53
1:N:219:ASN:OD1	1:N:220:ILE:N	2.38	0.53
1:G:108:LYS:HG2	1:G:168:THR:HG23	1.89	0.53
1:F:128:VAL:HG23	1:F:149:SER:O	2.08	0.53
1:L:296:ASN:HD22	1:L:297:PRO:CD	2.21	0.53
1:D:154:PRO:HG2	1:D:185:GLU:HA	1.88	0.53
1:L:237:HIS:HB2	1:L:239:ASN:ND2	2.23	0.53
1:K:208:LYS:HG2	1:K:221:HIS:CD2	2.43	0.53
1:N:276:TRP:CH2	1:N:278:ALA:HB2	2.43	0.53
1:J:296:ASN:ND2	1:J:297:PRO:HD2	2.09	0.53
1:M:150:TYR:CZ	1:M:209:LEU:HB3	2.42	0.53
1:H:93:LEU:HD13	1:H:266:VAL:HG21	1.91	0.53
1:D:64:VAL:CG1	1:D:66:LYS:HE3	2.36	0.53
1:H:173:GLU:HB2	1:N:298:LEU:HD11	1.91	0.53
1:L:298:LEU:HD21	1:P:103:VAL:HG22	1.90	0.53
1:N:226:GLN:O	1:N:229:GLU:HG3	2.08	0.53
1:P:149:SER:HB3	3:P:427:HOH:O	2.09	0.53
1:B:72:ILE:HD12	1:B:72:ILE:N	2.24	0.53
1:F:185:GLU:O	1:F:187:ILE:HG12	2.09	0.53
1:D:204:PHE:HB3	1:D:225:PHE:CE1	2.44	0.53
1:I:127:PHE:HB3	1:I:170:VAL:HG12	1.90	0.53
1:P:246:LEU:O	1:P:263:ALA:HB1	2.09	0.53
1:N:120:GLN:HA	1:N:156:ASN:HD21	1.74	0.53
1:A:147:VAL:HG23	3:A:440:HOH:O	2.09	0.53
1:M:247:GLU:O	1:M:285:SER:HA	2.08	0.53
1:K:151:ALA:HA	1:K:187:ILE:O	2.08	0.53
1:B:129:VAL:O	1:B:129:VAL:HG12	2.07	0.53
1:L:147:VAL:CG1	1:L:148:ASP:N	2.72	0.53
1:J:125:LEU:C	1:J:125:LEU:HD13	2.29	0.53
1:B:226:GLN:NE2	1:B:284:ARG:HB3	2.24	0.53
1:D:196:LEU:HD21	1:D:207:ARG:NH2	2.24	0.53
1:J:93:LEU:HD13	1:J:266:VAL:HG21	1.90	0.53
1:O:270:ALA:O	1:O:273:VAL:HG12	2.08	0.53
1:B:222:THR:HG23	1:B:286:ARG:HD2	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:101:HIS:O	1:H:174:ARG:HG3	2.09	0.53
1:O:204:PHE:CE1	1:O:223:MET:HG3	2.43	0.53
1:F:153:LEU:HD13	1:F:159:HIS:NE2	2.24	0.53
1:J:218:PHE:C	1:J:218:PHE:CD1	2.81	0.53
1:P:179:LEU:O	1:P:182:HIS:HB2	2.09	0.53
1:P:113:SER:O	1:P:162:ASP:HA	2.09	0.53
1:G:222:THR:HG22	1:G:222:THR:O	2.08	0.53
1:O:88:THR:HG23	1:O:109:MET:HA	1.91	0.53
1:B:103:VAL:CG2	1:B:173:GLU:HB2	2.38	0.53
1:M:82:LEU:O	1:M:85:TRP:HB2	2.08	0.53
1:P:133:VAL:HA	1:P:163:CYS:CB	2.39	0.53
1:K:150:TYR:CZ	1:K:209:LEU:HB3	2.43	0.53
1:J:102:PHE:HD2	1:J:240:GLN:NE2	2.07	0.53
1:M:124:ARG:CG	1:M:125:LEU:H	2.22	0.53
1:N:152:TYR:HE2	1:N:184:THR:HB	1.74	0.53
1:N:120:GLN:O	1:N:121:ASP:HB2	2.07	0.53
1:D:45:THR:HG21	1:D:130:GLU:OE2	2.09	0.53
1:H:133:VAL:HG21	1:H:161:LEU:HB3	1.90	0.53
1:O:294:ASN:O	1:O:295:ARG:NH1	2.40	0.52
1:E:137:ASN:ND2	1:E:140:SER:HB2	2.24	0.52
1:L:152:TYR:C	1:L:153:LEU:HG	2.29	0.52
1:A:121:ASP:H	1:A:156:ASN:ND2	2.06	0.52
1:M:224:ASP:OD2	1:M:286:ARG:HD2	2.08	0.52
1:J:297:PRO:HG3	1:K:92:TYR:CZ	2.43	0.52
1:I:170:VAL:HG13	1:I:170:VAL:O	2.10	0.52
1:F:118:PRO:HD3	1:F:124:ARG:CZ	2.39	0.52
1:C:87:ASN:ND2	1:C:110:LYS:HB2	2.25	0.52
1:P:64:VAL:HG11	1:P:66:LYS:HE3	1.89	0.52
1:P:101:HIS:H	1:P:240:GLN:HE22	1.57	0.52
1:L:82:LEU:CD1	1:L:90:GLY:HA3	2.37	0.52
1:O:137:ASN:ND2	1:O:140:SER:HB3	2.24	0.52
1:G:62:ARG:HB2	1:G:73:THR:HG21	1.92	0.52
1:C:40:ILE:N	1:C:40:ILE:HD12	2.25	0.52
1:J:153:LEU:HD13	1:J:159:HIS:NE2	2.24	0.52
1:B:150:TYR:CE2	1:B:209:LEU:HB3	2.45	0.52
1:C:208:LYS:HG2	1:C:221:HIS:CD2	2.44	0.52
1:O:155:PRO:O	1:O:156:ASN:HB2	2.09	0.52
1:M:96:PRO:HD3	1:M:103:VAL:CG1	2.38	0.52
1:M:126:ILE:HG22	1:M:171:VAL:HB	1.92	0.52
1:B:127:PHE:HB3	1:B:170:VAL:HG13	1.92	0.52
1:F:253:ARG:NH1	1:L:61:THR:HG22	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:243:LEU:HD12	1:I:243:LEU:C	2.30	0.52
1:P:54:LEU:HD22	1:P:60:PHE:CD2	2.44	0.52
1:L:243:LEU:HB2	1:L:289:LEU:CD1	2.39	0.52
1:N:296:ASN:HD22	1:N:298:LEU:H	1.57	0.52
1:D:87:ASN:HD21	1:D:110:LYS:HB2	1.75	0.52
1:A:93:LEU:HD11	1:A:106:LEU:HG	1.91	0.52
1:O:125:LEU:HD13	1:O:126:ILE:N	2.25	0.52
1:B:92:TYR:HA	1:B:105:TYR:HB3	1.92	0.52
1:B:78:VAL:HG21	1:I:237:HIS:HD2	1.75	0.52
1:P:207:ARG:HB3	1:P:222:THR:OG1	2.10	0.52
1:P:70:ALA:HB3	1:P:268:TRP:HB3	1.91	0.52
1:I:93:LEU:HD13	1:I:266:VAL:HG21	1.92	0.52
1:H:234:LYS:HE3	1:M:60:PHE:O	2.09	0.52
1:N:100:SER:HA	1:N:240:GLN:HE22	1.74	0.52
1:G:127:PHE:CE1	1:G:209:LEU:HD11	2.45	0.52
1:J:135:LEU:HB2	1:J:145:LEU:CD1	2.38	0.52
1:K:126:ILE:C	1:K:126:ILE:HD12	2.29	0.52
1:N:68:ASP:OD2	1:N:273:VAL:HG23	2.10	0.52
1:M:122:ILE:HD13	1:M:175:ARG:HA	1.91	0.52
1:N:196:LEU:N	1:N:196:LEU:CD2	2.73	0.52
1:O:243:LEU:HD12	1:O:244:LEU:N	2.25	0.52
1:O:202:GLU:CD	1:O:231:LEU:HD23	2.30	0.52
1:K:196:LEU:HD21	1:K:207:ARG:NH2	2.25	0.52
1:O:150:TYR:CD1	1:O:209:LEU:HD13	2.45	0.51
1:L:137:ASN:O	1:L:137:ASN:OD1	2.28	0.51
1:E:90:GLY:HA2	1:E:106:LEU:O	2.11	0.51
1:B:140:SER:O	1:B:141:SER:CB	2.58	0.51
1:I:125:LEU:C	1:I:125:LEU:HD13	2.30	0.51
1:A:60:PHE:HZ	1:C:60:PHE:HZ	1.59	0.51
1:M:204:PHE:CE1	1:M:223:MET:HG2	2.46	0.51
1:H:243:LEU:C	1:H:243:LEU:HD12	2.30	0.51
1:A:296:ASN:HD22	1:A:298:LEU:HB2	1.74	0.51
1:C:100:SER:HB3	1:C:268:TRP:CH2	2.45	0.51
1:G:82:LEU:HD13	1:G:90:GLY:HA3	1.92	0.51
1:B:165:GLU:O	1:B:166:SER:HB3	2.10	0.51
1:C:184:THR:HB	1:C:216:TYR:CE1	2.45	0.51
1:P:111:GLU:O	1:P:112:MET:HB2	2.10	0.51
1:H:40:ILE:N	1:H:40:ILE:HD12	2.22	0.51
1:D:119:PRO:HG2	1:K:296:ASN:OD1	2.11	0.51
1:H:143:LYS:HD3	1:H:188:VAL:HG11	1.93	0.51
1:H:238:TYR:CE2	1:H:297:PRO:HB3	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:135:LEU:HA	1:P:161:LEU:HD23	1.92	0.51
1:G:150:TYR:CZ	1:G:209:LEU:HB3	2.46	0.51
1:O:197:LEU:CD1	1:O:207:ARG:HA	2.41	0.51
1:K:123:GLU:HB3	1:K:155:PRO:HD3	1.91	0.51
1:E:147:VAL:O	1:E:148:ASP:HB2	2.11	0.51
1:N:205:GLU:O	1:N:223:MET:HA	2.11	0.51
1:N:93:LEU:CD1	1:N:266:VAL:HG21	2.40	0.51
1:N:121:ASP:H	1:N:156:ASN:ND2	2.08	0.51
1:N:82:LEU:HD13	1:N:90:GLY:CA	2.38	0.51
1:G:101:HIS:N	1:G:240:GLN:HE22	2.07	0.51
1:B:243:LEU:C	1:B:243:LEU:HD12	2.31	0.51
1:L:202:GLU:HB3	1:L:204:PHE:CE2	2.46	0.51
1:L:207:ARG:HB2	1:L:222:THR:CG2	2.41	0.51
1:M:224:ASP:OD2	1:M:286:ARG:CD	2.59	0.51
1:I:101:HIS:H	1:I:240:GLN:HE22	1.58	0.51
1:J:147:VAL:O	1:J:148:ASP:HB2	2.10	0.51
1:M:157:PHE:CE1	1:M:186:LEU:HB2	2.44	0.51
1:O:93:LEU:HD11	1:O:106:LEU:HG	1.93	0.51
1:K:170:VAL:O	1:K:170:VAL:HG13	2.11	0.51
1:I:105:TYR:CE1	1:I:171:VAL:CG1	2.94	0.51
1:A:202:GLU:OE2	1:A:233:VAL:HG12	2.10	0.51
1:M:235:GLU:HB2	1:M:275:GLN:HG3	1.93	0.51
1:M:115:SER:HB3	1:M:161:LEU:HB2	1.93	0.51
1:J:63:SER:HA	1:J:71:LEU:O	2.11	0.51
1:J:66:LYS:HD2	1:J:69:HIS:CE1	2.46	0.51
1:F:214:VAL:HG13	1:F:215:ALA:N	2.26	0.51
1:H:298:LEU:O	1:M:96:PRO:HG2	2.09	0.51
1:O:130:GLU:HB3	1:O:168:THR:HB	1.93	0.51
1:M:145:LEU:CD2	1:M:149:SER:HB3	2.39	0.51
1:M:153:LEU:HD22	1:M:159:HIS:CG	2.46	0.51
1:M:41:TYR:HE2	1:M:247:GLU:OE1	1.93	0.51
1:H:239:ASN:H	1:H:239:ASN:HD22	1.59	0.51
1:M:179:LEU:CD2	1:M:214:VAL:HG22	2.40	0.51
1:L:197:LEU:HD22	1:L:208:LYS:HE3	1.93	0.51
1:M:157:PHE:HD2	1:M:157:PHE:C	2.14	0.50
1:K:40:ILE:O	1:K:41:TYR:HB2	2.11	0.50
1:O:240:GLN:HB3	1:O:271:PRO:HG3	1.93	0.50
1:G:153:LEU:HD23	1:G:186:LEU:CD1	2.40	0.50
1:C:114:SER:HA	1:C:161:LEU:O	2.11	0.50
1:L:155:PRO:O	1:L:156:ASN:HB2	2.11	0.50
1:L:251:ILE:CD1	1:L:260:PRO:HA	2.38	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:72:ILE:HD12	1:E:72:ILE:N	2.26	0.50
1:M:118:PRO:HD3	1:M:124:ARG:CZ	2.42	0.50
1:L:237:HIS:HB2	1:L:239:ASN:HD22	1.77	0.50
1:E:82:LEU:HD23	1:E:85:TRP:CD2	2.46	0.50
1:J:114:SER:HA	1:J:161:LEU:O	2.11	0.50
1:M:127:PHE:O	1:M:170:VAL:HG12	2.10	0.50
1:M:155:PRO:O	1:M:156:ASN:HB2	2.10	0.50
1:E:196:LEU:O	1:E:197:LEU:HD23	2.11	0.50
1:J:207:ARG:HG3	1:J:207:ARG:HH11	1.75	0.50
1:O:149:SER:HA	1:O:189:GLY:O	2.12	0.50
1:M:227:PRO:HG2	1:M:282:LYS:O	2.11	0.50
1:K:184:THR:HG22	1:K:216:TYR:CD1	2.46	0.50
1:L:205:GLU:CG	1:L:224:ASP:HB2	2.41	0.50
1:N:199:THR:OG1	1:N:202:GLU:HB2	2.12	0.50
1:E:40:ILE:HD12	1:E:40:ILE:N	2.16	0.50
1:O:207:ARG:HB2	1:O:222:THR:HG1	1.74	0.50
1:I:164:VAL:CG2	1:I:165:GLU:N	2.73	0.50
1:H:239:ASN:H	1:H:239:ASN:ND2	2.08	0.50
1:M:271:PRO:O	1:M:272:PHE:HB2	2.11	0.50
1:M:218:PHE:C	1:M:218:PHE:CD1	2.85	0.50
1:F:222:THR:HG23	1:F:286:ARG:HD2	1.92	0.50
1:C:205:GLU:HB2	1:C:224:ASP:HB2	1.94	0.50
1:B:155:PRO:HG3	1:B:176:TYR:CD2	2.47	0.50
1:G:157:PHE:CZ	1:G:186:LEU:HD22	2.46	0.50
1:P:126:ILE:HD12	1:P:126:ILE:C	2.32	0.50
1:N:133:VAL:O	1:N:145:LEU:N	2.41	0.50
1:N:133:VAL:CG2	1:N:163:CYS:HB2	2.38	0.50
1:N:40:ILE:HD12	1:N:40:ILE:N	2.27	0.50
1:N:199:THR:HG21	1:N:204:PHE:HE1	1.77	0.50
1:B:125:LEU:HD13	1:B:126:ILE:N	2.26	0.50
1:L:298:LEU:HD23	1:P:103:VAL:HG13	1.94	0.50
1:F:137:ASN:ND2	1:F:140:SER:N	2.59	0.50
1:P:128:VAL:HG23	1:P:128:VAL:O	2.11	0.50
1:K:88:THR:CG2	1:K:109:MET:HA	2.33	0.50
1:O:260:PRO:HB3	1:P:58:PRO:O	2.11	0.50
1:J:150:TYR:CD1	1:J:209:LEU:HD13	2.47	0.50
1:N:243:LEU:HB3	1:N:289:LEU:CD1	2.42	0.50
1:P:96:PRO:HD3	1:P:103:VAL:HG13	1.94	0.50
1:O:53:HIS:N	1:O:53:HIS:CD2	2.80	0.50
1:H:111:GLU:HB3	3:H:443:HOH:O	2.12	0.49
1:P:118:PRO:HB3	1:P:124:ARG:HH21	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:243:LEU:HG	1:K:267:ILE:HB	1.94	0.49
1:G:82:LEU:CD1	1:G:90:GLY:HA3	2.42	0.49
1:I:94:ILE:O	1:I:103:VAL:HA	2.11	0.49
1:K:87:ASN:CG	1:K:110:LYS:HB2	2.33	0.49
1:M:126:ILE:HD12	1:M:126:ILE:C	2.33	0.49
1:B:296:ASN:HD22	1:B:297:PRO:N	2.09	0.49
1:G:155:PRO:HG3	1:G:176:TYR:CD2	2.47	0.49
1:D:198:GLU:HG2	3:D:450:HOH:O	2.10	0.49
1:I:43:LYS:N	3:I:438:HOH:O	2.44	0.49
1:E:205:GLU:HB2	1:E:224:ASP:HB2	1.94	0.49
1:P:150:TYR:CZ	1:P:209:LEU:HB3	2.46	0.49
1:H:79:TYR:CD1	1:H:91:ALA:HB2	2.47	0.49
1:K:109:MET:SD	1:K:169:LEU:HD11	2.52	0.49
1:L:93:LEU:HD11	1:L:106:LEU:HG	1.95	0.49
1:G:241:HIS:CD2	1:G:275:GLN:HE22	2.28	0.49
1:K:208:LYS:HE2	1:K:221:HIS:NE2	2.27	0.49
1:N:70:ALA:HB3	1:N:268:TRP:HB3	1.94	0.49
1:N:87:ASN:ND2	1:N:110:LYS:HB2	2.27	0.49
1:L:63:SER:HA	1:L:71:LEU:O	2.13	0.49
1:M:230:PHE:CD1	1:M:230:PHE:O	2.65	0.49
1:B:205:GLU:HB2	1:B:224:ASP:HB2	1.93	0.49
1:J:133:VAL:O	1:J:145:LEU:HB2	2.11	0.49
1:N:243:LEU:O	1:N:266:VAL:HG13	2.12	0.49
1:L:196:LEU:HD11	1:L:207:ARG:NH2	2.27	0.49
1:D:49:LEU:CD1	1:G:49:LEU:HD11	2.42	0.49
1:I:90:GLY:HA2	1:I:106:LEU:O	2.12	0.49
1:D:41:TYR:CZ	1:D:246:LEU:HD13	2.47	0.49
1:K:131:GLY:HA3	1:K:166:SER:O	2.13	0.49
1:P:121:ASP:N	1:P:156:ASN:ND2	2.36	0.49
1:P:153:LEU:HD22	1:P:157:PHE:CD2	2.47	0.49
1:F:150:TYR:CG	1:F:209:LEU:HD13	2.48	0.49
1:I:150:TYR:CE1	1:I:209:LEU:HD22	2.47	0.49
1:B:296:ASN:ND2	1:B:298:LEU:H	2.11	0.49
1:P:95:THR:O	1:P:98:THR:HG23	2.13	0.49
1:G:120:GLN:HG3	1:G:156:ASN:HD21	1.77	0.49
1:D:154:PRO:HG2	1:D:185:GLU:CA	2.42	0.49
1:I:243:LEU:HD12	1:I:244:LEU:N	2.27	0.49
1:M:209:LEU:HG	1:M:220:ILE:O	2.12	0.49
1:C:241:HIS:CE1	1:C:289:LEU:HD21	2.47	0.49
1:H:94:ILE:O	1:H:103:VAL:HA	2.13	0.49
1:K:135:LEU:HA	1:K:161:LEU:HD23	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:83:PRO:O	1:B:84:ASP:HB2	2.12	0.49
1:F:196:LEU:HD21	1:F:207:ARG:CZ	2.42	0.49
1:D:170:VAL:HG13	1:D:170:VAL:O	2.12	0.49
1:P:64:VAL:CG1	1:P:66:LYS:HE3	2.43	0.49
1:D:153:LEU:HD13	1:D:159:HIS:NE2	2.27	0.49
1:C:73:THR:HG22	1:C:265:ASP:OD1	2.12	0.49
1:G:68:ASP:HB2	1:G:273:VAL:HB	1.94	0.49
1:P:111:GLU:HA	1:P:165:GLU:HA	1.95	0.49
1:B:243:LEU:HD13	1:B:287:TYR:HB2	1.94	0.49
1:J:101:HIS:O	1:J:174:ARG:HG3	2.12	0.49
1:C:153:LEU:HD13	1:C:159:HIS:NE2	2.27	0.49
1:G:157:PHE:CD2	1:G:157:PHE:C	2.85	0.49
1:P:127:PHE:HB3	1:P:170:VAL:CG1	2.43	0.49
1:M:176:TYR:OH	1:M:215:ALA:O	2.18	0.49
1:O:209:LEU:C	1:O:210:LEU:HD23	2.33	0.49
1:G:243:LEU:HD21	1:G:252:TYR:CE1	2.47	0.49
1:P:103:VAL:CG2	1:P:173:GLU:HB2	2.43	0.49
1:P:64:VAL:HG11	1:P:66:LYS:CE	2.42	0.49
1:N:227:PRO:HD3	1:N:284:ARG:HA	1.95	0.49
1:G:86:THR:HB	1:G:114:SER:OG	2.13	0.49
1:M:152:TYR:O	1:M:186:LEU:HD12	2.11	0.49
1:P:82:LEU:HB3	1:P:85:TRP:HB2	1.94	0.49
1:F:87:ASN:HD21	1:F:110:LYS:HB2	1.78	0.49
1:H:210:LEU:HB3	1:H:211:PRO:CD	2.42	0.49
1:G:236:VAL:HG23	1:I:76:SER:HB3	1.94	0.49
1:H:207:ARG:HG3	1:H:207:ARG:HH11	1.78	0.49
1:K:152:TYR:HE2	1:K:184:THR:HB	1.77	0.49
1:H:243:LEU:HD12	1:H:244:LEU:N	2.27	0.49
1:L:245:LEU:HD12	1:L:287:TYR:HB3	1.95	0.49
1:F:296:ASN:ND2	1:F:298:LEU:HB2	2.28	0.49
1:O:150:TYR:CE1	1:O:209:LEU:HD22	2.47	0.49
1:M:241:HIS:HB2	1:M:269:MET:HB2	1.95	0.49
1:N:153:LEU:HD13	1:N:159:HIS:CD2	2.48	0.49
1:F:63:SER:HA	1:F:71:LEU:O	2.13	0.49
1:M:198:GLU:HG3	1:M:200:PRO:HD3	1.94	0.49
1:K:154:PRO:HG2	1:K:185:GLU:HA	1.94	0.48
1:D:126:ILE:C	1:D:126:ILE:HD12	2.33	0.48
1:E:153:LEU:HD13	1:E:159:HIS:CE1	2.48	0.48
1:D:206:LEU:HD12	1:D:207:ARG:H	1.78	0.48
1:B:133:VAL:HG23	1:B:162:ASP:C	2.34	0.48
1:C:252:TYR:CE1	1:C:277:TYR:HB2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:40:ILE:CD1	1:K:40:ILE:N	2.73	0.48
1:K:296:ASN:HD22	1:K:297:PRO:N	2.09	0.48
1:O:137:ASN:HD21	1:O:141:SER:N	2.05	0.48
1:B:155:PRO:O	1:B:156:ASN:HB2	2.13	0.48
1:G:153:LEU:HD13	1:G:159:HIS:CD2	2.48	0.48
1:I:125:LEU:O	1:I:171:VAL:HG23	2.12	0.48
1:L:272:PHE:CZ	1:P:95:THR:HG23	2.48	0.48
1:C:208:LYS:HE2	1:C:221:HIS:NE2	2.28	0.48
1:E:133:VAL:HG13	1:E:145:LEU:HB2	1.94	0.48
1:L:82:LEU:HD13	1:L:90:GLY:CA	2.38	0.48
1:M:157:PHE:CZ	1:M:186:LEU:HD22	2.47	0.48
1:N:126:ILE:CG1	1:N:151:ALA:HB3	2.43	0.48
1:J:137:ASN:HB2	3:J:422:HOH:O	2.12	0.48
1:K:115:SER:OG	1:K:116:GLY:N	2.42	0.48
1:G:121:ASP:H	1:G:156:ASN:HD21	1.59	0.48
1:O:121:ASP:H	1:O:156:ASN:HD21	1.61	0.48
1:A:234:LYS:HG2	1:J:61:THR:HB	1.94	0.48
1:C:128:VAL:HG22	1:C:169:LEU:HD11	1.95	0.48
1:B:154:PRO:HG2	1:B:185:GLU:HA	1.96	0.48
1:P:244:LEU:HD12	1:P:265:ASP:O	2.12	0.48
1:H:296:ASN:HD21	1:H:298:LEU:HB2	1.74	0.48
1:O:241:HIS:HB2	1:O:269:MET:CB	2.35	0.48
1:L:207:ARG:HD2	1:L:222:THR:HG21	1.96	0.48
1:O:202:GLU:HG3	1:O:204:PHE:CE2	2.48	0.48
1:F:54:LEU:CD2	1:H:49:LEU:HD22	2.44	0.48
1:O:121:ASP:H	1:O:156:ASN:ND2	2.11	0.48
1:J:206:LEU:HD12	1:J:207:ARG:N	2.28	0.48
1:J:207:ARG:HB2	1:J:222:THR:HB	1.93	0.48
1:K:277:TYR:CG	1:K:278:ALA:N	2.81	0.48
1:C:127:PHE:HB3	1:C:170:VAL:HG13	1.95	0.48
1:A:164:VAL:HG22	3:A:427:HOH:O	2.12	0.48
1:F:70:ALA:HB3	1:F:268:TRP:HB3	1.94	0.48
1:E:150:TYR:CE1	1:E:209:LEU:HD22	2.49	0.48
1:M:184:THR:HB	1:M:216:TYR:CE1	2.49	0.48
1:P:153:LEU:CD1	1:P:159:HIS:CD2	2.96	0.48
1:B:101:HIS:H	1:B:240:GLN:NE2	2.10	0.48
1:I:125:LEU:HD13	1:I:126:ILE:N	2.29	0.48
1:L:254:LEU:HA	1:L:274:PRO:O	2.12	0.48
1:J:70:ALA:HB3	1:J:268:TRP:HB3	1.95	0.48
1:M:109:MET:HB3	1:M:113:SER:OG	2.13	0.48
1:P:156:ASN:N	1:P:156:ASN:ND2	2.60	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:240:GLN:HB3	1:E:271:PRO:HG3	1.96	0.48
1:M:157:PHE:HE1	1:M:186:LEU:HD22	1.79	0.48
1:L:234:LYS:N	1:L:234:LYS:HD2	2.29	0.48
1:G:297:PRO:HG3	1:I:92:TYR:CZ	2.48	0.48
1:G:62:ARG:NH2	1:G:265:ASP:OD1	2.46	0.48
1:M:204:PHE:CD1	1:M:223:MET:HG2	2.48	0.48
1:M:245:LEU:HA	1:M:287:TYR:HB3	1.95	0.48
1:L:247:GLU:O	1:L:285:SER:HA	2.13	0.48
1:K:81:PRO:O	1:K:83:PRO:HD3	2.13	0.48
1:F:112:MET:CE	1:F:164:VAL:HG12	2.43	0.48
1:A:64:VAL:CG1	1:A:66:LYS:HG3	2.44	0.48
1:O:103:VAL:HG22	1:O:173:GLU:HB2	1.96	0.48
1:A:240:GLN:HB3	1:A:271:PRO:HG3	1.95	0.48
1:H:85:TRP:CE3	1:H:115:SER:HA	2.48	0.48
1:D:74:PRO:C	1:D:76:SER:H	2.17	0.48
1:O:252:TYR:CE1	1:O:277:TYR:HB2	2.49	0.48
1:F:120:GLN:O	1:F:121:ASP:HB2	2.12	0.48
1:N:218:PHE:CD1	1:N:218:PHE:C	2.86	0.48
1:B:174:ARG:NH1	1:B:217:ASP:O	2.46	0.48
1:J:270:ALA:O	1:J:273:VAL:HG12	2.14	0.48
1:O:104:MET:HG3	1:O:172:PHE:CE1	2.49	0.48
1:M:121:ASP:H	1:M:156:ASN:HD21	1.62	0.48
1:F:137:ASN:HD21	1:F:140:SER:HB2	1.79	0.48
1:I:73:THR:HB	1:I:74:PRO:HD2	1.95	0.48
1:C:243:LEU:HG	1:C:267:ILE:HB	1.94	0.48
1:K:84:ASP:O	1:K:116:GLY:HA3	2.14	0.48
1:N:153:LEU:HD13	1:N:159:HIS:CE1	2.48	0.48
1:I:207:ARG:HH11	1:I:207:ARG:HG3	1.78	0.48
1:N:60:PHE:O	1:O:234:LYS:HE3	2.14	0.48
1:P:243:LEU:HG	1:P:267:ILE:HB	1.95	0.48
1:K:218:PHE:CB	1:K:290:TYR:HE1	2.27	0.48
1:O:164:VAL:HG23	1:O:165:GLU:HG2	1.96	0.48
1:O:54:LEU:HD23	1:P:49:LEU:HD22	1.96	0.48
1:K:152:TYR:CB	1:K:210:LEU:HD21	2.43	0.47
1:A:224:ASP:HA	1:A:285:SER:O	2.14	0.47
1:J:227:PRO:HD3	1:J:284:ARG:HA	1.96	0.47
1:E:101:HIS:N	1:E:240:GLN:HE22	2.06	0.47
1:D:64:VAL:HG12	1:D:66:LYS:HG3	1.96	0.47
1:D:82:LEU:HD13	1:D:90:GLY:CA	2.42	0.47
1:M:64:VAL:O	1:M:70:ALA:HA	2.14	0.47
1:E:164:VAL:HG23	1:E:165:GLU:N	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:103:VAL:HG22	1:K:173:GLU:HB2	1.95	0.47
1:L:207:ARG:HG3	1:L:207:ARG:NH1	2.29	0.47
1:L:62:ARG:NH2	1:L:265:ASP:OD2	2.44	0.47
1:A:166:SER:O	1:A:167:ALA:HB2	2.13	0.47
1:B:95:THR:HG23	1:I:272:PHE:HZ	1.79	0.47
1:J:152:TYR:C	1:J:153:LEU:HG	2.34	0.47
1:E:111:GLU:HA	1:E:164:VAL:O	2.14	0.47
1:L:196:LEU:HD12	1:L:196:LEU:N	2.28	0.47
1:F:253:ARG:HD2	1:F:258:TRP:CZ2	2.49	0.47
1:F:276:TRP:CH2	1:F:278:ALA:HB2	2.48	0.47
1:P:258:TRP:HZ3	1:P:276:TRP:CZ3	2.32	0.47
1:P:121:ASP:H	1:P:156:ASN:HD22	1.54	0.47
1:H:223:MET:O	1:H:286:ARG:HA	2.14	0.47
1:G:150:TYR:CE2	1:G:209:LEU:HB3	2.49	0.47
1:E:101:HIS:H	1:E:240:GLN:NE2	2.05	0.47
1:O:49:LEU:CD2	1:P:57:LEU:HD12	2.42	0.47
1:I:109:MET:O	1:I:166:SER:HA	2.15	0.47
1:O:140:SER:O	1:O:141:SER:CB	2.62	0.47
1:D:227:PRO:HG3	1:D:283:THR:O	2.14	0.47
1:F:66:LYS:HB3	3:F:423:HOH:O	2.14	0.47
1:J:253:ARG:HB3	1:J:276:TRP:HB3	1.96	0.47
1:B:54:LEU:HD23	1:J:49:LEU:HD22	1.95	0.47
1:J:186:LEU:HD12	1:J:187:ILE:H	1.78	0.47
1:M:70:ALA:HB3	1:M:268:TRP:HB3	1.96	0.47
1:N:204:PHE:C	1:N:204:PHE:CD1	2.88	0.47
1:O:82:LEU:HD23	1:O:85:TRP:CD2	2.49	0.47
1:G:155:PRO:O	1:G:156:ASN:HB2	2.14	0.47
1:K:206:LEU:HD11	1:K:221:HIS:HB3	1.95	0.47
1:D:150:TYR:CE2	1:D:209:LEU:HB3	2.50	0.47
1:M:222:THR:HG22	1:M:222:THR:O	2.13	0.47
1:E:87:ASN:ND2	1:E:110:LYS:HB2	2.29	0.47
1:M:130:GLU:CB	1:M:168:THR:HB	2.45	0.47
1:E:128:VAL:HB	1:E:146:THR:O	2.14	0.47
1:N:113:SER:O	1:N:162:ASP:HA	2.14	0.47
1:D:100:SER:HB2	1:D:240:GLN:HE22	1.80	0.47
1:L:126:ILE:HD13	1:L:169:LEU:CD2	2.44	0.47
1:E:272:PHE:HE2	1:F:95:THR:OG1	1.97	0.47
1:J:82:LEU:HD13	1:J:90:GLY:CA	2.44	0.47
1:I:206:LEU:HD12	1:I:207:ARG:H	1.79	0.47
1:F:55:GLN:HA	3:F:443:HOH:O	2.15	0.47
1:D:93:LEU:HD13	1:D:266:VAL:HG21	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:49:LEU:HD22	1:J:54:LEU:HD23	1.97	0.47
1:M:290:TYR:C	1:M:290:TYR:CD2	2.87	0.47
1:P:133:VAL:CB	1:P:163:CYS:HB3	2.43	0.47
1:H:298:LEU:HD13	1:M:122:ILE:HD12	1.97	0.47
1:E:96:PRO:HD3	1:E:103:VAL:CG1	2.45	0.47
1:F:206:LEU:HD12	1:F:207:ARG:N	2.29	0.47
1:C:126:ILE:C	1:C:126:ILE:HD12	2.35	0.47
1:D:152:TYR:HB3	1:D:187:ILE:HB	1.96	0.47
1:O:41:TYR:O	1:O:44:ALA:N	2.44	0.47
1:J:233:VAL:O	1:J:235:GLU:N	2.45	0.47
1:G:198:GLU:O	1:G:199:THR:HG23	2.15	0.47
1:P:108:LYS:NZ	1:P:168:THR:OG1	2.33	0.47
1:B:111:GLU:CD	1:B:111:GLU:H	2.18	0.47
1:B:164:VAL:HG23	3:B:433:HOH:O	2.14	0.47
1:N:238:TYR:O	1:N:271:PRO:HB3	2.15	0.47
1:K:152:TYR:C	1:K:153:LEU:HG	2.35	0.47
1:G:127:PHE:HE1	1:G:209:LEU:HD11	1.80	0.47
1:G:246:LEU:CD1	1:G:288:LEU:HD13	2.38	0.47
1:M:237:HIS:CG	1:M:239:ASN:HD22	2.33	0.47
1:N:296:ASN:HD22	1:N:298:LEU:HB2	1.79	0.47
1:G:153:LEU:HD23	1:G:186:LEU:HD11	1.97	0.47
1:G:186:LEU:O	1:G:187:ILE:HD13	2.15	0.47
1:I:105:TYR:CE1	1:I:171:VAL:HG11	2.50	0.47
1:O:120:GLN:HG2	1:O:121:ASP:OD2	2.14	0.47
1:L:60:PHE:HZ	1:N:60:PHE:HZ	1.62	0.47
1:F:39:PRO:HB2	1:F:42:TRP:HB2	1.97	0.47
1:F:93:LEU:CD1	1:F:266:VAL:HG21	2.40	0.47
1:I:86:THR:O	1:I:113:SER:HB2	2.14	0.47
1:E:276:TRP:CH2	1:E:278:ALA:HB2	2.50	0.47
1:E:83:PRO:O	1:E:84:ASP:HB2	2.15	0.47
1:P:176:TYR:CE2	1:P:178:TYR:HA	2.50	0.47
1:H:243:LEU:HG	1:H:267:ILE:HB	1.97	0.47
1:O:276:TRP:CH2	1:O:278:ALA:HB2	2.50	0.47
1:P:296:ASN:ND2	1:P:298:LEU:H	2.12	0.47
1:H:121:ASP:HB2	1:H:175:ARG:NH1	2.30	0.47
1:P:92:TYR:CE1	1:P:105:TYR:CD2	3.02	0.47
1:F:140:SER:O	1:F:141:SER:HB3	2.15	0.47
1:O:111:GLU:HA	1:O:165:GLU:HA	1.96	0.47
1:H:127:PHE:HB3	1:H:170:VAL:CG1	2.45	0.47
1:M:257:ASN:ND2	3:M:422:HOH:O	2.46	0.47
1:F:270:ALA:O	1:F:273:VAL:HG12	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:268:TRP:CZ2	1:B:270:ALA:HB2	2.50	0.47
1:N:39:PRO:O	1:N:42:TRP:HB2	2.15	0.47
1:P:133:VAL:HG22	1:P:134:THR:N	2.30	0.46
1:P:147:VAL:CG1	1:P:148:ASP:N	2.78	0.46
1:N:224:ASP:OD2	1:N:286:ARG:HD3	2.14	0.46
1:B:153:LEU:HD13	1:B:159:HIS:NE2	2.29	0.46
1:I:164:VAL:CG2	1:I:165:GLU:H	2.28	0.46
1:J:126:ILE:HD12	1:J:169:LEU:CD2	2.45	0.46
1:F:50:SER:HB2	1:F:51:PRO:HD2	1.95	0.46
1:E:126:ILE:HD12	1:E:126:ILE:C	2.35	0.46
1:J:154:PRO:HB3	1:J:184:THR:OG1	2.15	0.46
1:P:93:LEU:HD13	1:P:266:VAL:HG21	1.96	0.46
1:P:243:LEU:HD12	1:P:243:LEU:C	2.35	0.46
1:E:85:TRP:CE3	1:E:88:THR:HG21	2.51	0.46
1:F:125:LEU:HD13	1:F:126:ILE:N	2.30	0.46
1:M:124:ARG:CG	1:M:125:LEU:N	2.78	0.46
1:O:53:HIS:ND1	1:P:53:HIS:CG	2.83	0.46
1:O:41:TYR:CZ	1:O:246:LEU:HD13	2.50	0.46
1:G:50:SER:HB2	1:G:51:PRO:HD2	1.97	0.46
1:P:133:VAL:HG23	1:P:163:CYS:CB	2.30	0.46
1:P:82:LEU:O	1:P:85:TRP:HB2	2.15	0.46
1:E:72:ILE:HG21	1:E:93:LEU:HD22	1.97	0.46
1:B:137:ASN:ND2	1:B:140:SER:HA	2.30	0.46
1:F:243:LEU:HD13	1:F:287:TYR:HB2	1.98	0.46
1:F:153:LEU:HD22	1:F:159:HIS:CG	2.50	0.46
1:A:120:GLN:O	1:A:121:ASP:HB2	2.14	0.46
1:P:227:PRO:HB3	1:P:281:GLY:O	2.15	0.46
1:E:60:PHE:O	1:P:234:LYS:HE3	2.14	0.46
1:A:85:TRP:CE3	1:A:115:SER:HA	2.50	0.46
1:O:197:LEU:HD11	1:O:207:ARG:HA	1.96	0.46
1:L:147:VAL:HG12	1:L:148:ASP:H	1.80	0.46
1:H:241:HIS:CE1	1:H:289:LEU:HD21	2.51	0.46
1:B:101:HIS:O	1:B:174:ARG:HG3	2.15	0.46
1:P:101:HIS:O	1:P:174:ARG:HG3	2.15	0.46
1:J:123:GLU:OE2	1:J:217:ASP:OD1	2.32	0.46
1:K:111:GLU:HA	1:K:164:VAL:O	2.15	0.46
1:K:108:LYS:HG2	1:K:168:THR:OG1	2.15	0.46
1:E:296:ASN:HD22	1:E:297:PRO:CD	2.17	0.46
1:O:293:VAL:HG23	1:O:294:ASN:HD22	1.79	0.46
1:G:297:PRO:HB2	1:I:95:THR:HG21	1.96	0.46
1:D:127:PHE:HB3	1:D:170:VAL:HG13	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:298:LEU:HD23	1:P:103:VAL:CG1	2.46	0.46
1:E:275:GLN:NE2	3:E:444:HOH:O	2.48	0.46
1:J:176:TYR:CE2	1:J:178:TYR:HA	2.50	0.46
1:J:208:LYS:HE2	1:J:221:HIS:CE1	2.51	0.46
1:O:146:THR:O	1:O:147:VAL:C	2.53	0.46
1:N:196:LEU:HD11	1:N:207:ARG:NH2	2.30	0.46
1:K:175:ARG:HH11	1:K:175:ARG:HG3	1.80	0.46
1:I:126:ILE:HG22	1:I:171:VAL:HB	1.98	0.46
1:O:125:LEU:HD22	1:O:126:ILE:H	1.81	0.46
1:B:225:PHE:HZ	1:B:231:LEU:HD21	1.81	0.46
1:G:72:ILE:N	1:G:72:ILE:HD12	2.30	0.46
1:P:89:LEU:HG	1:P:110:LYS:HZ1	1.79	0.46
1:K:113:SER:HB2	1:K:163:CYS:SG	2.56	0.46
1:D:297:PRO:O	1:D:298:LEU:OXT	2.34	0.46
1:M:105:TYR:CE1	1:M:171:VAL:HG13	2.51	0.46
1:G:206:LEU:HA	1:G:222:THR:O	2.15	0.46
1:N:127:PHE:HB3	1:N:170:VAL:HG13	1.97	0.46
1:F:82:LEU:HD23	1:F:85:TRP:CD2	2.51	0.46
1:I:87:ASN:HD21	1:I:110:LYS:CB	2.26	0.46
1:O:150:TYR:CE2	1:O:209:LEU:HB3	2.51	0.46
1:L:268:TRP:CZ2	1:L:270:ALA:HB2	2.51	0.46
1:D:206:LEU:HD11	1:D:221:HIS:HB3	1.97	0.46
1:H:132:ALA:HB1	1:H:144:LYS:NZ	2.29	0.46
1:N:164:VAL:HG23	1:N:165:GLU:N	2.31	0.46
1:D:85:TRP:CE3	1:D:88:THR:HG21	2.51	0.46
1:P:121:ASP:CA	1:P:156:ASN:HD21	2.27	0.46
1:G:101:HIS:H	1:G:240:GLN:NE2	2.09	0.46
1:L:250:GLY:O	1:L:251:ILE:HD13	2.16	0.46
1:D:90:GLY:HA2	1:D:106:LEU:O	2.16	0.46
1:F:123:GLU:O	1:F:173:GLU:HA	2.16	0.46
1:C:115:SER:HB3	1:C:161:LEU:HB2	1.96	0.46
1:F:137:ASN:HD21	1:F:140:SER:CB	2.28	0.46
1:F:273:VAL:O	1:F:273:VAL:HG13	2.16	0.46
1:B:184:THR:HB	1:B:216:TYR:CE1	2.51	0.46
1:G:145:LEU:HB3	1:G:149:SER:CB	2.46	0.46
1:F:237:HIS:HB2	1:F:239:ASN:HD22	1.80	0.46
1:K:92:TYR:HB2	3:K:420:HOH:O	2.14	0.45
1:N:133:VAL:HG23	1:N:163:CYS:CA	2.46	0.45
1:H:82:LEU:HD22	1:H:90:GLY:CA	2.42	0.45
1:E:122:ILE:CD1	1:P:298:LEU:HD13	2.44	0.45
1:C:298:LEU:HD13	1:G:122:ILE:HD12	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:136:THR:HG22	1:K:142:SER:OG	2.16	0.45
1:L:131:GLY:HA3	1:L:167:ALA:HA	1.98	0.45
1:E:125:LEU:C	1:E:125:LEU:HD13	2.37	0.45
1:G:227:PRO:HG3	1:G:283:THR:O	2.16	0.45
1:D:273:VAL:HG13	1:D:273:VAL:O	2.16	0.45
1:F:249:GLN:N	1:F:249:GLN:OE1	2.50	0.45
1:D:218:PHE:CD1	1:D:218:PHE:C	2.90	0.45
1:O:56:ASP:HA	3:O:415:HOH:O	2.16	0.45
1:N:223:MET:O	1:N:286:ARG:HA	2.16	0.45
1:A:298:LEU:O	1:J:96:PRO:HG2	2.16	0.45
1:M:121:ASP:HA	1:M:155:PRO:HB2	1.98	0.45
1:G:62:ARG:HH11	1:G:62:ARG:HG3	1.82	0.45
1:H:237:HIS:CE1	1:H:239:ASN:HB2	2.51	0.45
1:M:252:TYR:OH	1:M:269:MET:CE	2.64	0.45
1:L:277:TYR:CG	1:L:278:ALA:N	2.84	0.45
1:J:187:ILE:HD12	1:J:211:PRO:CD	2.42	0.45
1:C:110:LYS:HB3	1:C:111:GLU:OE2	2.16	0.45
1:K:85:TRP:HA	1:K:115:SER:O	2.16	0.45
1:G:297:PRO:HG3	1:I:92:TYR:CE1	2.51	0.45
1:O:135:LEU:CB	1:O:145:LEU:HD11	2.47	0.45
1:O:133:VAL:O	1:O:145:LEU:HB2	2.16	0.45
1:K:208:LYS:HE2	1:K:221:HIS:CE1	2.51	0.45
1:G:203:VAL:HG22	3:G:410:HOH:O	2.16	0.45
1:F:155:PRO:O	1:F:156:ASN:HB2	2.17	0.45
1:D:109:MET:HB3	1:D:113:SER:OG	2.17	0.45
1:F:101:HIS:N	1:F:240:GLN:HE22	2.13	0.45
1:M:240:GLN:HG3	1:M:240:GLN:O	2.17	0.45
1:N:100:SER:CA	1:N:240:GLN:HE22	2.30	0.45
1:E:74:PRO:C	1:E:76:SER:H	2.19	0.45
1:P:238:TYR:O	1:P:271:PRO:HB3	2.17	0.45
1:O:40:ILE:HD13	1:O:147:VAL:CG1	2.32	0.45
1:I:130:GLU:CA	1:I:147:VAL:HG22	2.38	0.45
1:A:49:LEU:H	1:A:262:GLN:HE22	1.63	0.45
1:F:296:ASN:ND2	3:F:451:HOH:O	2.43	0.45
1:J:102:PHE:CD2	1:J:240:GLN:NE2	2.80	0.45
1:P:88:THR:OG1	1:P:109:MET:HA	2.16	0.45
1:O:202:GLU:OE1	1:O:231:LEU:HA	2.16	0.45
1:N:226:GLN:HB2	1:N:229:GLU:CD	2.37	0.45
1:O:63:SER:HA	1:O:71:LEU:O	2.16	0.45
1:F:131:GLY:HA3	1:F:166:SER:O	2.17	0.45
1:L:193:LYS:O	1:L:194:GLN:C	2.55	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:137:ASN:C	1:P:140:SER:HA	2.37	0.45
1:H:298:LEU:CD1	1:M:122:ILE:HG21	2.47	0.45
1:M:273:VAL:O	1:M:273:VAL:HG13	2.15	0.45
1:K:218:PHE:C	1:K:218:PHE:CD1	2.89	0.45
1:M:93:LEU:CD1	1:M:266:VAL:HG21	2.44	0.45
1:I:125:LEU:HD22	1:I:126:ILE:H	1.82	0.45
1:O:273:VAL:O	1:O:273:VAL:HG13	2.17	0.45
1:L:111:GLU:O	1:L:112:MET:C	2.54	0.45
1:O:147:VAL:O	1:O:148:ASP:CB	2.49	0.45
1:K:150:TYR:CE1	1:K:209:LEU:HD22	2.51	0.45
1:G:191:THR:O	1:G:207:ARG:HD3	2.16	0.45
1:E:56:ASP:OD2	1:M:48:THR:OG1	2.32	0.45
1:G:39:PRO:O	1:G:42:TRP:HB2	2.17	0.45
1:O:284:ARG:HG3	1:O:285:SER:N	2.31	0.45
1:O:72:ILE:N	1:O:72:ILE:HD12	2.32	0.45
1:A:226:GLN:HB2	1:A:229:GLU:HG3	1.99	0.45
1:D:237:HIS:HB2	1:D:239:ASN:ND2	2.32	0.45
1:E:117:LEU:HD11	1:E:158:HIS:CD2	2.52	0.45
1:J:233:VAL:O	1:J:233:VAL:HG13	2.17	0.45
1:E:63:SER:HA	1:E:71:LEU:O	2.17	0.45
1:J:86:THR:O	1:J:87:ASN:C	2.54	0.45
1:K:129:VAL:O	1:K:147:VAL:HG22	2.16	0.45
1:I:235:GLU:HB2	1:I:275:GLN:HG3	1.99	0.45
1:G:197:LEU:HD12	1:G:208:LYS:HE3	1.98	0.45
1:P:248:GLY:HA3	1:P:285:SER:HA	1.99	0.45
1:A:119:PRO:HB2	1:A:122:ILE:HG13	1.99	0.45
1:G:126:ILE:O	1:G:150:TYR:HB2	2.17	0.45
1:G:150:TYR:CD1	1:G:209:LEU:HD13	2.51	0.45
1:L:101:HIS:CE1	1:L:292:ASP:HB3	2.52	0.45
1:L:94:ILE:O	1:L:103:VAL:HA	2.17	0.45
1:H:103:VAL:CG1	1:N:298:LEU:HG	2.46	0.45
1:E:109:MET:HB3	1:E:113:SER:OG	2.17	0.45
1:H:152:TYR:CE2	1:H:154:PRO:HG3	2.49	0.45
1:M:129:VAL:HG23	1:M:168:THR:O	2.17	0.45
1:P:105:TYR:CE1	1:P:171:VAL:HG11	2.52	0.45
1:P:101:HIS:N	1:P:240:GLN:HE22	2.14	0.45
1:J:207:ARG:NH1	1:J:207:ARG:HG3	2.31	0.45
1:F:137:ASN:HD21	1:F:140:SER:N	2.13	0.45
1:O:203:VAL:HG23	1:O:229:GLU:OE2	2.16	0.45
1:N:89:LEU:HG	3:N:418:HOH:O	2.17	0.45
1:M:52:SER:O	1:M:55:GLN:HG2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:TYR:HB2	1:A:210:LEU:HD21	2.00	0.45
1:J:105:TYR:CE2	1:J:171:VAL:HG22	2.52	0.45
1:I:196:LEU:O	1:I:197:LEU:HD23	2.17	0.45
1:M:292:ASP:O	1:M:293:VAL:HG13	2.16	0.45
1:N:222:THR:HG23	1:N:286:ARG:HD3	1.97	0.44
1:L:40:ILE:CD1	1:L:40:ILE:H	2.26	0.44
1:L:243:LEU:HD23	1:L:269:MET:CE	2.47	0.44
1:L:204:PHE:CD1	1:L:223:MET:HE3	2.52	0.44
1:J:90:GLY:HA2	1:J:106:LEU:O	2.16	0.44
1:O:82:LEU:HD23	1:O:85:TRP:CE2	2.52	0.44
1:F:154:PRO:HG2	1:F:185:GLU:HA	1.99	0.44
1:A:121:ASP:H	1:A:156:ASN:HD21	1.65	0.44
1:H:83:PRO:O	1:H:84:ASP:HB2	2.16	0.44
1:E:223:MET:O	1:E:286:ARG:HA	2.16	0.44
1:A:150:TYR:CE2	1:A:209:LEU:HB3	2.52	0.44
1:I:52:SER:O	1:I:55:GLN:CG	2.65	0.44
1:I:147:VAL:O	1:I:148:ASP:HB2	2.16	0.44
1:H:40:ILE:H	1:H:40:ILE:CD1	2.06	0.44
1:E:152:TYR:HB3	1:E:187:ILE:HB	1.99	0.44
1:B:125:LEU:C	1:B:125:LEU:CD1	2.85	0.44
1:I:171:VAL:CG2	1:I:172:PHE:N	2.80	0.44
1:L:62:ARG:CB	1:L:73:THR:HG21	2.47	0.44
1:O:125:LEU:O	1:O:171:VAL:HG23	2.17	0.44
1:E:260:PRO:HB3	1:M:58:PRO:O	2.17	0.44
1:C:69:HIS:CD2	1:C:254:LEU:HD13	2.52	0.44
1:H:121:ASP:HB2	1:H:175:ARG:HH12	1.83	0.44
1:O:199:THR:HG21	1:O:204:PHE:O	2.17	0.44
1:M:124:ARG:HG2	1:M:125:LEU:N	2.32	0.44
1:M:287:TYR:HE1	1:M:289:LEU:HD22	1.82	0.44
1:J:154:PRO:HD2	1:J:157:PHE:CG	2.52	0.44
1:G:93:LEU:HD13	1:G:266:VAL:HG21	1.98	0.44
1:E:292:ASP:O	1:E:293:VAL:HG13	2.17	0.44
1:M:103:VAL:HG23	1:M:103:VAL:O	2.17	0.44
1:O:196:LEU:HD21	1:O:207:ARG:NH2	2.32	0.44
1:L:244:LEU:HD12	1:L:245:LEU:H	1.81	0.44
1:L:243:LEU:HB2	1:L:289:LEU:HD13	1.98	0.44
1:O:244:LEU:HD12	1:O:245:LEU:H	1.81	0.44
1:G:206:LEU:HD12	1:G:207:ARG:H	1.81	0.44
1:F:50:SER:HB2	1:F:51:PRO:CD	2.47	0.44
1:G:79:TYR:CD1	1:G:91:ALA:HB2	2.53	0.44
1:B:245:LEU:HD23	1:B:262:GLN:C	2.37	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:253:ARG:HB3	1:H:276:TRP:HB3	1.99	0.44
1:F:223:MET:O	1:F:286:ARG:HA	2.18	0.44
1:P:148:ASP:OD1	1:P:148:ASP:O	2.35	0.44
1:M:95:THR:HA	1:M:103:VAL:HG12	1.99	0.44
1:F:296:ASN:HB2	3:F:442:HOH:O	2.17	0.44
1:M:298:LEU:O	1:O:96:PRO:HG2	2.17	0.44
1:J:127:PHE:HB3	1:J:170:VAL:CG1	2.46	0.44
1:L:273:VAL:O	1:L:273:VAL:HG13	2.18	0.44
1:B:126:ILE:HD12	1:B:126:ILE:C	2.38	0.44
1:D:199:THR:HG21	1:D:204:PHE:CE1	2.52	0.44
1:G:207:ARG:HB2	1:G:222:THR:CG2	2.48	0.44
1:O:124:ARG:CG	1:O:125:LEU:N	2.80	0.44
1:C:85:TRP:CE3	1:C:115:SER:HA	2.52	0.44
1:J:231:LEU:HD12	1:J:276:TRP:HA	2.00	0.44
1:G:145:LEU:HB3	1:G:149:SER:HB3	1.99	0.44
1:E:94:ILE:CD1	1:E:268:TRP:HB2	2.48	0.44
1:J:204:PHE:HB3	1:J:225:PHE:CE1	2.53	0.44
1:A:276:TRP:CH2	1:A:278:ALA:HB2	2.52	0.44
1:L:123:GLU:OE1	1:L:218:PHE:HE2	2.01	0.44
1:P:132:ALA:CB	1:P:146:THR:HA	2.47	0.44
1:O:130:GLU:HB3	1:O:168:THR:CB	2.48	0.44
1:L:296:ASN:OD1	1:P:119:PRO:HG2	2.17	0.44
1:M:235:GLU:OE1	1:M:237:HIS:CD2	2.69	0.44
1:E:194:GLN:HB2	1:E:207:ARG:HD3	1.98	0.44
1:A:174:ARG:NH1	1:A:217:ASP:O	2.50	0.44
1:L:125:LEU:HD13	1:L:125:LEU:O	2.17	0.44
1:D:150:TYR:CD1	1:D:209:LEU:HD13	2.53	0.44
1:H:253:ARG:NH1	1:M:59:GLY:O	2.50	0.44
1:I:118:PRO:HD3	1:I:124:ARG:CZ	2.47	0.44
1:N:290:TYR:CD2	1:N:290:TYR:C	2.90	0.44
1:O:140:SER:O	1:O:141:SER:HB3	2.17	0.44
1:F:243:LEU:HG	1:F:267:ILE:HB	2.00	0.44
1:E:133:VAL:CG1	1:E:145:LEU:HB2	2.48	0.44
1:H:170:VAL:HG13	1:H:170:VAL:O	2.18	0.44
1:D:83:PRO:O	1:D:85:TRP:HD1	2.01	0.44
1:E:218:PHE:HA	1:E:293:VAL:HG22	1.99	0.44
1:P:134:THR:O	1:P:161:LEU:HA	2.18	0.44
1:O:224:ASP:OD2	1:O:286:ARG:HD3	2.17	0.44
1:M:145:LEU:HD22	1:M:149:SER:CB	2.44	0.44
1:L:240:GLN:HB3	1:L:271:PRO:HD3	1.98	0.44
1:J:133:VAL:HG23	1:J:162:ASP:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:110:LYS:H	1:E:113:SER:HB3	1.83	0.44
1:J:170:VAL:CG1	1:J:170:VAL:O	2.66	0.44
1:H:125:LEU:HD23	1:H:152:TYR:HB2	2.00	0.44
1:O:85:TRP:CD1	1:O:116:GLY:HA3	2.53	0.44
1:K:101:HIS:N	1:K:240:GLN:HE22	2.16	0.44
1:I:86:THR:HB	1:I:114:SER:OG	2.18	0.44
1:D:61:THR:HB	1:K:234:LYS:HG2	2.00	0.44
1:A:225:PHE:HB2	1:A:279:ALA:HB2	1.98	0.44
1:O:43:LYS:HA	1:O:46:ASN:O	2.18	0.44
1:P:40:ILE:O	1:P:41:TYR:C	2.57	0.44
1:M:154:PRO:HD2	1:M:157:PHE:CD1	2.37	0.44
1:P:119:PRO:HB2	1:P:122:ILE:CG1	2.48	0.44
1:N:208:LYS:HZ2	1:N:212:MET:HE3	1.82	0.44
1:M:243:LEU:C	1:M:243:LEU:CD1	2.85	0.44
1:O:96:PRO:HD3	1:O:103:VAL:HG12	2.00	0.44
1:N:243:LEU:HD12	1:N:243:LEU:C	2.37	0.44
1:B:296:ASN:C	1:B:296:ASN:HD22	2.21	0.44
1:C:74:PRO:C	1:C:76:SER:N	2.71	0.44
1:H:218:PHE:CA	1:H:293:VAL:HG22	2.48	0.44
1:O:126:ILE:HB	1:O:169:LEU:HD23	1.99	0.44
1:C:222:THR:O	1:C:222:THR:HG22	2.17	0.44
1:H:245:LEU:HD12	1:H:287:TYR:HB3	2.00	0.43
1:K:84:ASP:O	1:K:116:GLY:CA	2.66	0.43
1:E:220:ILE:HD13	1:E:290:TYR:HA	1.99	0.43
1:G:87:ASN:OD1	1:G:110:LYS:HB2	2.18	0.43
1:E:108:LYS:HD3	1:E:168:THR:HG23	1.99	0.43
1:A:243:LEU:HD12	1:A:243:LEU:C	2.39	0.43
1:N:253:ARG:HG3	1:N:253:ARG:HH11	1.82	0.43
1:A:122:ILE:CD1	1:D:298:LEU:HD22	2.42	0.43
1:M:128:VAL:HA	1:M:169:LEU:HD13	1.99	0.43
1:L:103:VAL:HG22	1:L:173:GLU:HB2	2.00	0.43
1:J:273:VAL:O	1:J:273:VAL:CG1	2.65	0.43
1:J:179:LEU:O	1:J:180:GLY:C	2.56	0.43
1:I:95:THR:O	1:I:98:THR:HG23	2.17	0.43
1:K:148:ASP:O	1:K:148:ASP:OD2	2.36	0.43
1:K:80:SER:O	1:K:90:GLY:N	2.44	0.43
1:K:153:LEU:HD23	1:K:186:LEU:CD1	2.48	0.43
1:O:208:LYS:HG2	1:O:221:HIS:CD2	2.54	0.43
1:L:251:ILE:HD11	1:N:58:PRO:HB2	2.01	0.43
1:M:267:ILE:HG22	1:M:268:TRP:N	2.33	0.43
1:K:202:GLU:HG3	1:K:204:PHE:HE2	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:118:PRO:CD	1:P:124:ARG:NH2	2.80	0.43
1:G:118:PRO:HD3	1:G:124:ARG:NH2	2.33	0.43
1:M:69:HIS:CD2	1:M:254:LEU:HD13	2.53	0.43
1:P:120:GLN:O	1:P:121:ASP:HB2	2.18	0.43
1:P:82:LEU:HA	1:P:82:LEU:HD12	1.68	0.43
1:J:125:LEU:HD13	1:J:126:ILE:N	2.34	0.43
1:K:127:PHE:HB3	1:K:170:VAL:CG1	2.48	0.43
1:D:197:LEU:HD12	1:D:208:LYS:HG3	1.99	0.43
1:N:150:TYR:CE2	1:N:209:LEU:HB3	2.53	0.43
1:E:234:LYS:N	1:E:234:LYS:HD3	2.32	0.43
1:P:40:ILE:CD1	1:P:40:ILE:N	2.69	0.43
1:G:146:THR:O	1:G:147:VAL:C	2.56	0.43
1:G:103:VAL:HG22	1:G:173:GLU:HB2	2.00	0.43
1:B:101:HIS:N	1:B:240:GLN:HE22	2.12	0.43
1:G:111:GLU:O	1:G:112:MET:C	2.56	0.43
1:F:235:GLU:HB2	1:F:275:GLN:HG3	2.01	0.43
1:I:202:GLU:OE1	1:I:231:LEU:HD23	2.18	0.43
1:J:277:TYR:CG	1:J:278:ALA:N	2.86	0.43
1:M:63:SER:HA	1:M:71:LEU:O	2.18	0.43
1:J:284:ARG:HH22	1:J:286:ARG:CZ	2.30	0.43
1:K:296:ASN:ND2	1:K:297:PRO:HD2	2.30	0.43
1:B:83:PRO:O	1:B:85:TRP:HD1	2.02	0.43
1:P:199:THR:HB	1:P:202:GLU:HB2	2.01	0.43
1:E:153:LEU:HD13	1:E:159:HIS:NE2	2.34	0.43
1:N:54:LEU:O	1:N:56:ASP:N	2.52	0.43
1:N:276:TRP:CZ2	1:N:278:ALA:HB2	2.54	0.43
1:F:186:LEU:O	1:F:187:ILE:HD13	2.19	0.43
1:I:207:ARG:HG3	1:I:207:ARG:NH1	2.34	0.43
1:N:271:PRO:O	1:N:272:PHE:HB2	2.18	0.43
1:B:253:ARG:NH1	1:C:61:THR:HG22	2.33	0.43
1:M:123:GLU:O	1:M:123:GLU:HG3	2.18	0.43
1:H:273:VAL:O	1:H:273:VAL:HG13	2.18	0.43
1:D:239:ASN:N	1:D:239:ASN:ND2	2.64	0.43
1:D:243:LEU:HG	1:D:267:ILE:HB	2.01	0.43
1:I:52:SER:O	1:I:55:GLN:HG2	2.19	0.43
1:E:282:LYS:HE3	3:H:427:HOH:O	2.18	0.43
1:A:39:PRO:N	3:A:454:HOH:O	2.51	0.43
1:L:45:THR:O	1:L:45:THR:HG22	2.18	0.43
1:P:86:THR:O	1:P:87:ASN:C	2.56	0.43
1:I:105:TYR:CZ	1:I:171:VAL:HG11	2.54	0.43
1:L:124:ARG:CG	1:L:125:LEU:N	2.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:207:ARG:HG3	1:G:207:ARG:HH11	1.83	0.43
1:E:144:LYS:O	1:E:145:LEU:HD23	2.19	0.43
1:A:234:LYS:HE3	1:J:60:PHE:O	2.18	0.43
1:L:190:SER:O	1:L:194:GLN:HG2	2.18	0.43
1:N:43:LYS:HE2	1:N:48:THR:OG1	2.18	0.43
1:F:111:GLU:HG2	1:F:111:GLU:H	1.56	0.43
1:P:133:VAL:HA	1:P:163:CYS:HB2	2.00	0.43
1:O:253:ARG:HB3	1:O:276:TRP:HB3	2.00	0.43
1:M:296:ASN:HD21	1:M:298:LEU:HB2	1.79	0.43
1:D:161:LEU:HD13	1:D:169:LEU:HD21	2.01	0.43
1:D:103:VAL:HG22	1:K:298:LEU:HD21	1.99	0.43
1:K:196:LEU:HD21	1:K:207:ARG:CZ	2.48	0.43
1:O:213:SER:HB3	1:O:216:TYR:CD2	2.54	0.43
1:A:262:GLN:HG2	1:C:57:LEU:CD2	2.44	0.43
1:K:95:THR:O	1:K:98:THR:HG23	2.19	0.43
1:K:134:THR:HG23	1:K:144:LYS:CA	2.48	0.43
1:M:130:GLU:HB3	1:M:168:THR:H	1.84	0.43
1:F:214:VAL:O	1:F:215:ALA:C	2.57	0.43
1:I:64:VAL:HG11	1:I:259:TYR:OH	2.18	0.43
1:N:237:HIS:CE1	1:N:239:ASN:HB2	2.54	0.43
1:B:282:LYS:HE3	3:B:462:HOH:O	2.19	0.43
1:F:130:GLU:O	1:F:167:ALA:HA	2.18	0.43
1:P:104:MET:CE	1:P:172:PHE:CZ	3.01	0.43
1:I:273:VAL:O	1:I:273:VAL:HG13	2.18	0.43
1:K:154:PRO:HB3	1:K:184:THR:OG1	2.19	0.42
1:L:82:LEU:HA	1:L:82:LEU:HD12	1.87	0.42
1:L:234:LYS:HE2	1:P:60:PHE:O	2.19	0.42
1:H:93:LEU:HD11	1:H:106:LEU:HG	2.01	0.42
1:D:113:SER:HG	1:D:163:CYS:HB3	1.83	0.42
1:E:135:LEU:HD11	1:E:159:HIS:HB2	2.00	0.42
1:C:110:LYS:HD3	1:C:110:LYS:HA	1.88	0.42
1:C:87:ASN:HD21	1:C:110:LYS:HB2	1.84	0.42
1:K:82:LEU:HB3	1:K:85:TRP:CG	2.54	0.42
1:N:155:PRO:O	1:N:156:ASN:HB2	2.18	0.42
1:I:86:THR:HB	1:I:114:SER:H	1.83	0.42
1:L:252:TYR:CE1	1:L:277:TYR:HB2	2.53	0.42
1:I:124:ARG:NE	1:I:173:GLU:OE2	2.52	0.42
1:C:82:LEU:HD13	1:C:90:GLY:HA3	2.00	0.42
1:M:73:THR:HB	1:M:74:PRO:HD2	2.01	0.42
1:D:254:LEU:HA	1:D:274:PRO:O	2.19	0.42
1:P:128:VAL:HG22	1:P:149:SER:H	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:207:ARG:HG3	1:H:207:ARG:NH1	2.34	0.42
1:H:122:ILE:CG2	1:N:298:LEU:HD13	2.48	0.42
1:L:152:TYR:CG	1:L:153:LEU:N	2.88	0.42
1:I:220:ILE:HD13	1:I:290:TYR:HA	1.99	0.42
1:C:237:HIS:ND1	1:C:239:ASN:HB2	2.33	0.42
1:M:130:GLU:CD	1:M:131:GLY:N	2.73	0.42
1:O:93:LEU:HD13	1:O:104:MET:CE	2.47	0.42
1:J:220:ILE:HD13	1:J:290:TYR:HA	2.00	0.42
1:E:268:TRP:CZ2	1:E:270:ALA:HB2	2.54	0.42
1:K:270:ALA:O	1:K:273:VAL:HG12	2.18	0.42
1:E:120:GLN:O	1:E:121:ASP:HB2	2.19	0.42
1:O:110:LYS:HE2	1:O:110:LYS:HA	2.01	0.42
1:P:87:ASN:C	1:P:87:ASN:OD1	2.58	0.42
1:L:207:ARG:HB2	1:L:222:THR:HG22	2.01	0.42
1:L:124:ARG:HG2	1:L:125:LEU:N	2.34	0.42
1:G:198:GLU:O	1:G:199:THR:CG2	2.67	0.42
1:J:208:LYS:HE2	1:J:221:HIS:NE2	2.34	0.42
1:P:238:TYR:CZ	1:P:239:ASN:OD1	2.72	0.42
1:I:208:LYS:HE2	1:I:221:HIS:CE1	2.54	0.42
1:G:93:LEU:HD13	1:G:266:VAL:HG11	2.01	0.42
1:L:106:LEU:HD23	1:L:170:VAL:HA	2.01	0.42
1:H:103:VAL:HG11	1:N:298:LEU:HG	2.01	0.42
1:K:54:LEU:HD12	1:K:75:GLU:HG3	2.01	0.42
1:D:185:GLU:O	1:D:187:ILE:HG12	2.19	0.42
1:O:125:LEU:C	1:O:125:LEU:HD13	2.40	0.42
1:N:129:VAL:HG23	1:N:170:VAL:HG12	2.01	0.42
1:P:104:MET:HE3	1:P:172:PHE:CZ	2.54	0.42
1:F:174:ARG:HG2	1:F:175:ARG:N	2.35	0.42
1:L:141:SER:OG	1:L:142:SER:N	2.52	0.42
1:P:153:LEU:HD23	1:P:186:LEU:HD13	2.01	0.42
1:O:208:LYS:HE3	1:O:221:HIS:NE2	2.34	0.42
1:E:93:LEU:HD13	1:E:266:VAL:HG11	2.00	0.42
1:D:137:ASN:HD21	1:D:140:SER:CB	2.26	0.42
1:J:169:LEU:N	1:J:169:LEU:HD12	2.34	0.42
1:J:101:HIS:CD2	1:J:101:HIS:C	2.93	0.42
1:O:100:SER:HB3	1:O:268:TRP:CH2	2.55	0.42
1:F:153:LEU:HD13	1:F:159:HIS:CE1	2.55	0.42
1:A:154:PRO:HG2	1:A:185:GLU:HA	2.00	0.42
1:P:191:THR:HG22	1:P:207:ARG:HH11	1.84	0.42
1:K:88:THR:HG22	1:K:109:MET:CB	2.50	0.42
1:G:125:LEU:CD1	1:G:125:LEU:C	2.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:126:ILE:HD13	1:N:161:LEU:HD11	2.01	0.42
1:P:153:LEU:HD22	1:P:157:PHE:CE2	2.55	0.42
1:P:82:LEU:CB	1:P:85:TRP:HB2	2.49	0.42
1:K:134:THR:HG23	1:K:144:LYS:HA	2.01	0.42
1:N:125:LEU:HD12	1:N:172:PHE:HD2	1.84	0.42
1:J:214:VAL:O	1:J:214:VAL:HG22	2.20	0.42
1:E:121:ASP:H	1:E:156:ASN:HD21	1.68	0.42
1:H:128:VAL:HG22	1:H:169:LEU:HD11	2.01	0.42
1:P:63:SER:HA	1:P:71:LEU:O	2.19	0.42
1:G:220:ILE:HA	1:G:289:LEU:O	2.20	0.42
1:I:165:GLU:HB3	1:I:166:SER:H	1.52	0.42
1:G:237:HIS:CE1	1:G:239:ASN:HB2	2.55	0.42
1:O:202:GLU:OE2	1:O:233:VAL:HG12	2.20	0.42
1:O:133:VAL:HG22	1:O:134:THR:N	2.34	0.42
1:C:206:LEU:HD12	1:C:207:ARG:H	1.83	0.42
1:E:125:LEU:HD13	1:E:126:ILE:N	2.34	0.42
1:K:164:VAL:HG23	1:K:165:GLU:H	1.85	0.42
1:D:83:PRO:O	1:D:84:ASP:HB2	2.19	0.42
1:B:218:PHE:HA	1:B:293:VAL:HG22	2.01	0.42
1:J:202:GLU:HA	1:J:232:ASN:HD22	1.85	0.42
1:N:111:GLU:H	1:N:111:GLU:CD	2.23	0.42
1:F:298:LEU:HD23	1:F:298:LEU:C	2.40	0.42
1:B:100:SER:HA	1:B:240:GLN:HE22	1.85	0.42
1:O:211:PRO:HB2	1:O:216:TYR:CE2	2.54	0.42
1:M:251:ILE:HD13	1:M:260:PRO:HA	2.01	0.42
1:N:73:THR:HG22	1:N:265:ASP:OD1	2.20	0.42
1:O:131:GLY:HA3	1:O:166:SER:O	2.19	0.42
1:J:153:LEU:HD22	1:J:159:HIS:CG	2.54	0.42
1:B:72:ILE:HG21	1:B:93:LEU:HD22	2.01	0.42
1:M:85:TRP:CE3	1:M:115:SER:HA	2.55	0.42
1:M:88:THR:CG2	1:M:109:MET:HG2	2.50	0.42
1:B:216:TYR:HA	3:B:443:HOH:O	2.20	0.42
1:F:175:ARG:NH1	1:F:175:ARG:HG3	2.35	0.42
1:J:190:SER:HB3	1:J:193:LYS:HG3	2.01	0.42
1:N:132:ALA:HB1	1:N:144:LYS:HE3	2.01	0.42
1:H:290:TYR:CD2	1:H:290:TYR:C	2.92	0.42
1:H:196:LEU:HD22	1:H:205:GLU:HB3	2.02	0.42
1:G:127:PHE:CZ	1:G:288:LEU:HD11	2.54	0.42
1:L:127:PHE:O	1:L:169:LEU:HA	2.19	0.42
1:F:298:LEU:HG	1:L:103:VAL:HG13	2.01	0.42
1:G:154:PRO:HD2	1:G:157:PHE:CD1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:62:ARG:HB2	1:L:73:THR:HG21	2.01	0.42
1:K:56:ASP:O	1:K:58:PRO:HD3	2.20	0.42
1:H:250:GLY:HA3	1:H:278:ALA:O	2.20	0.42
1:G:192:ASP:OD2	1:G:192:ASP:N	2.53	0.42
1:M:141:SER:O	1:M:142:SER:HB3	2.19	0.41
1:N:284:ARG:NH2	1:N:286:ARG:NH2	2.52	0.41
1:M:208:LYS:CB	1:M:219:ASN:HD21	2.17	0.41
1:H:72:ILE:HD13	1:H:93:LEU:O	2.20	0.41
1:G:172:PHE:O	1:G:173:GLU:HG3	2.20	0.41
1:K:73:THR:OG1	1:K:75:GLU:OE2	2.38	0.41
1:J:129:VAL:O	1:J:129:VAL:HG12	2.20	0.41
1:H:288:LEU:HA	1:H:288:LEU:HD12	1.89	0.41
1:G:114:SER:HA	1:G:161:LEU:O	2.19	0.41
1:C:271:PRO:O	1:C:272:PHE:HB2	2.20	0.41
1:F:296:ASN:ND2	1:F:298:LEU:CB	2.82	0.41
1:K:94:ILE:O	1:K:103:VAL:HA	2.20	0.41
1:G:135:LEU:HD23	1:G:143:LYS:HB2	2.01	0.41
1:I:127:PHE:HB3	1:I:170:VAL:HG13	2.01	0.41
1:H:125:LEU:HD13	1:H:125:LEU:C	2.40	0.41
1:G:151:ALA:HA	1:G:187:ILE:O	2.20	0.41
1:F:126:ILE:C	1:F:126:ILE:HD12	2.40	0.41
1:C:100:SER:HB3	1:C:268:TRP:CZ3	2.55	0.41
1:O:120:GLN:CG	1:O:121:ASP:OD2	2.68	0.41
1:H:123:GLU:OE2	1:H:217:ASP:OD1	2.38	0.41
1:M:276:TRP:CG	1:M:277:TYR:N	2.88	0.41
1:F:224:ASP:OD1	1:F:286:ARG:CD	2.50	0.41
1:N:82:LEU:HB3	1:N:85:TRP:CG	2.55	0.41
1:O:153:LEU:HD13	1:O:159:HIS:NE2	2.36	0.41
1:N:115:SER:CB	1:N:161:LEU:H	2.34	0.41
1:M:243:LEU:HD12	1:M:244:LEU:N	2.34	0.41
1:K:135:LEU:HD12	1:K:136:THR:H	1.86	0.41
1:J:40:ILE:O	1:J:41:TYR:HB2	2.20	0.41
1:E:253:ARG:HB3	1:E:276:TRP:HB3	2.02	0.41
1:B:69:HIS:HA	1:B:268:TRP:O	2.20	0.41
1:I:222:THR:HG23	1:I:286:ARG:HD2	2.02	0.41
1:O:296:ASN:HD21	1:O:298:LEU:HD12	1.85	0.41
1:M:267:ILE:CG2	1:M:268:TRP:N	2.83	0.41
1:F:296:ASN:ND2	1:F:298:LEU:H	2.18	0.41
1:L:196:LEU:N	1:L:196:LEU:CD1	2.83	0.41
1:G:152:TYR:O	1:G:186:LEU:HD12	2.21	0.41
1:E:135:LEU:HD13	1:E:161:LEU:HD23	2.00	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:125:LEU:CD1	1:M:125:LEU:C	2.89	0.41
1:F:127:PHE:HB3	1:F:170:VAL:HG13	2.02	0.41
1:J:294:ASN:O	1:J:295:ARG:HG2	2.21	0.41
1:A:155:PRO:O	1:A:156:ASN:HB2	2.21	0.41
1:E:70:ALA:HB3	1:E:268:TRP:HB3	2.01	0.41
1:P:197:LEU:HD12	1:P:208:LYS:HG3	2.01	0.41
1:I:149:SER:HA	1:I:189:GLY:O	2.20	0.41
1:B:41:TYR:O	1:B:44:ALA:HB3	2.20	0.41
1:F:94:ILE:O	1:F:103:VAL:HA	2.21	0.41
1:I:220:ILE:HA	1:I:289:LEU:O	2.21	0.41
1:B:209:LEU:O	1:B:210:LEU:HD23	2.19	0.41
1:E:273:VAL:O	1:E:273:VAL:HG13	2.19	0.41
1:B:57:LEU:HD23	1:B:57:LEU:HA	1.95	0.41
1:K:224:ASP:HA	1:K:285:SER:O	2.20	0.41
1:K:66:LYS:NZ	1:K:257:ASN:OD1	2.51	0.41
1:N:92:TYR:HA	1:N:105:TYR:HB3	2.03	0.41
1:L:85:TRP:CE3	1:L:88:THR:HG21	2.55	0.41
1:M:221:HIS:HB2	1:M:289:LEU:HB3	2.02	0.41
1:D:74:PRO:O	1:D:76:SER:N	2.54	0.41
1:K:294:ASN:O	1:K:295:ARG:HG2	2.21	0.41
1:J:120:GLN:HG3	1:J:156:ASN:HD21	1.85	0.41
1:H:197:LEU:HD12	1:H:208:LYS:HG3	2.02	0.41
1:M:137:ASN:ND2	1:M:137:ASN:H	2.11	0.41
1:O:163:CYS:C	3:O:416:HOH:O	2.58	0.41
1:L:244:LEU:HD12	1:L:245:LEU:N	2.36	0.41
1:E:243:LEU:HD12	1:E:243:LEU:O	2.19	0.41
1:J:137:ASN:ND2	1:J:140:SER:N	2.67	0.41
1:G:191:THR:HG22	1:G:207:ARG:HD2	2.01	0.41
1:M:85:TRP:CD2	1:M:115:SER:HA	2.55	0.41
1:N:100:SER:HB3	1:N:268:TRP:CH2	2.56	0.41
1:C:252:TYR:CD1	1:C:277:TYR:CD1	3.09	0.41
1:K:79:TYR:HA	1:K:90:GLY:O	2.20	0.41
1:P:117:LEU:HD11	1:P:158:HIS:CD2	2.55	0.41
1:I:83:PRO:O	1:I:85:TRP:HD1	2.02	0.41
1:F:204:PHE:CE2	1:F:231:LEU:HD11	2.55	0.41
1:A:196:LEU:HD21	1:A:207:ARG:CZ	2.50	0.41
1:A:125:LEU:HD13	1:A:125:LEU:C	2.41	0.41
1:K:185:GLU:O	1:K:186:LEU:C	2.58	0.41
1:K:113:SER:CB	1:K:163:CYS:SG	3.08	0.41
1:D:298:LEU:HD23	1:D:298:LEU:O	2.20	0.41
1:O:130:GLU:CD	1:O:131:GLY:N	2.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:205:GLU:HG2	1:L:205:GLU:H	1.61	0.41
1:E:243:LEU:HD23	1:E:269:MET:CE	2.50	0.41
1:G:241:HIS:HB2	1:G:269:MET:HB2	2.02	0.41
1:I:125:LEU:HD22	1:I:126:ILE:N	2.35	0.41
1:I:105:TYR:CZ	1:I:171:VAL:CG1	3.04	0.41
1:M:176:TYR:CE2	1:M:178:TYR:HA	2.56	0.41
1:K:147:VAL:O	1:K:148:ASP:HB3	2.21	0.41
1:E:237:HIS:HB2	1:E:239:ASN:HD22	1.86	0.41
1:P:243:LEU:HD23	1:P:289:LEU:CD1	2.51	0.41
1:C:240:GLN:HB3	1:C:271:PRO:HG3	2.02	0.41
1:H:111:GLU:O	1:H:112:MET:C	2.58	0.41
1:O:152:TYR:O	1:O:153:LEU:HD23	2.20	0.41
1:N:114:SER:HA	1:N:161:LEU:O	2.21	0.41
1:D:102:PHE:HD2	1:D:240:GLN:HE21	1.62	0.41
1:P:82:LEU:HB3	1:P:85:TRP:CG	2.56	0.41
1:M:107:ALA:N	1:M:169:LEU:O	2.46	0.41
1:J:243:LEU:HD23	1:J:269:MET:CE	2.51	0.41
1:B:142:SER:O	1:B:143:LYS:HD2	2.21	0.41
1:O:88:THR:CG2	1:O:109:MET:HG2	2.51	0.41
1:E:154:PRO:HG2	1:E:185:GLU:CA	2.49	0.41
1:E:111:GLU:O	1:E:112:MET:C	2.58	0.41
1:G:235:GLU:HB2	1:G:275:GLN:HG3	2.02	0.41
1:P:123:GLU:O	1:P:173:GLU:HA	2.21	0.41
1:G:108:LYS:HE2	1:G:168:THR:HG21	2.02	0.41
1:J:218:PHE:HE1	1:J:220:ILE:HG12	1.86	0.41
1:E:235:GLU:HB2	1:E:275:GLN:HG3	2.03	0.41
1:N:253:ARG:NH1	1:N:253:ARG:HG3	2.36	0.41
1:C:204:PHE:CE1	1:C:223:MET:HE3	2.56	0.41
1:H:141:SER:HB2	1:H:142:SER:H	1.60	0.41
1:D:155:PRO:O	1:D:156:ASN:HB2	2.21	0.41
1:L:226:GLN:HB2	1:L:229:GLU:OE1	2.21	0.41
1:P:125:LEU:C	1:P:125:LEU:HD13	2.41	0.41
1:N:108:LYS:NZ	1:N:168:THR:CG2	2.84	0.41
1:M:57:LEU:HD23	1:M:57:LEU:HA	1.81	0.41
1:H:74:PRO:C	1:H:76:SER:H	2.24	0.41
1:P:132:ALA:O	1:P:163:CYS:HB2	2.21	0.41
1:P:262:GLN:O	1:P:265:ASP:HB2	2.20	0.41
1:H:206:LEU:HD12	1:H:207:ARG:H	1.86	0.41
1:H:205:GLU:HB2	1:H:224:ASP:HB2	2.03	0.41
1:M:145:LEU:HB3	1:M:149:SER:HB2	2.02	0.41
1:O:207:ARG:O	1:O:221:HIS:HA	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:153:LEU:HA	1:I:154:PRO:HD3	1.96	0.41
1:F:243:LEU:CD1	1:F:243:LEU:C	2.86	0.41
1:M:130:GLU:HB3	1:M:168:THR:HB	2.02	0.41
1:H:113:SER:OG	1:H:163:CYS:HB3	2.20	0.41
1:J:207:ARG:HB2	1:J:222:THR:CG2	2.51	0.41
1:J:121:ASP:H	1:J:156:ASN:ND2	2.19	0.41
1:J:120:GLN:HA	1:J:156:ASN:ND2	2.36	0.41
1:H:197:LEU:HD12	1:H:208:LYS:HE3	2.03	0.41
1:I:40:ILE:O	1:I:41:TYR:HB2	2.20	0.41
1:L:134:THR:HG23	1:L:143:LYS:O	2.20	0.41
1:E:78:VAL:HG21	1:P:237:HIS:HD2	1.85	0.41
1:K:245:LEU:HD12	1:K:245:LEU:HA	1.90	0.41
1:M:86:THR:O	1:M:87:ASN:C	2.60	0.40
1:C:298:LEU:HD21	3:G:426:HOH:O	2.21	0.40
1:H:122:ILE:HG21	1:N:298:LEU:HD13	2.03	0.40
1:E:185:GLU:O	1:E:187:ILE:HG12	2.21	0.40
1:A:199:THR:HB	1:A:202:GLU:HB2	2.03	0.40
1:E:146:THR:O	1:E:149:SER:HB2	2.21	0.40
1:A:109:MET:HB2	1:A:167:ALA:HB3	2.04	0.40
1:D:85:TRP:CE3	1:D:115:SER:HA	2.56	0.40
1:J:92:TYR:HA	1:J:105:TYR:HB3	2.03	0.40
1:I:197:LEU:O	1:I:199:THR:HG23	2.21	0.40
1:L:218:PHE:C	1:L:218:PHE:CD1	2.94	0.40
1:O:68:ASP:O	1:O:69:HIS:HB3	2.21	0.40
1:E:285:SER:HB2	3:E:402:HOH:O	2.21	0.40
1:K:293:VAL:HG21	3:K:421:HOH:O	2.21	0.40
1:P:184:THR:HG22	1:P:215:ALA:O	2.21	0.40
1:E:123:GLU:HG2	1:E:174:ARG:O	2.20	0.40
1:A:50:SER:HB2	1:A:51:PRO:CD	2.51	0.40
1:K:259:TYR:HA	1:K:260:PRO:HD3	1.92	0.40
1:K:120:GLN:NE2	3:K:412:HOH:O	2.54	0.40
1:E:82:LEU:HB3	1:E:85:TRP:HB2	2.03	0.40
1:E:82:LEU:HB2	1:E:88:THR:O	2.21	0.40
1:A:247:GLU:O	1:A:285:SER:HA	2.21	0.40
1:J:135:LEU:O	1:J:136:THR:HG23	2.20	0.40
1:M:137:ASN:ND2	1:M:137:ASN:N	2.67	0.40
1:M:295:ARG:O	1:M:296:ASN:C	2.60	0.40
1:I:290:TYR:CD2	1:I:291:LYS:N	2.89	0.40
1:O:155:PRO:O	1:O:156:ASN:CB	2.68	0.40
1:L:123:GLU:OE1	1:L:218:PHE:CE2	2.73	0.40
1:F:62:ARG:HD3	3:F:404:HOH:O	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:83:PRO:C	1:G:85:TRP:H	2.24	0.40
1:C:272:PHE:HE2	1:G:95:THR:OG1	2.04	0.40
1:M:86:THR:HB	1:M:114:SER:OG	2.21	0.40
1:K:86:THR:N	1:K:114:SER:O	2.54	0.40
1:L:147:VAL:CG1	1:L:148:ASP:H	2.32	0.40
1:L:243:LEU:CD1	1:L:287:TYR:HB2	2.45	0.40
1:G:233:VAL:HG13	1:G:233:VAL:O	2.21	0.40
1:O:245:LEU:HD12	1:O:287:TYR:HB3	2.04	0.40
1:H:133:VAL:HG23	1:H:163:CYS:N	2.36	0.40
1:F:253:ARG:HH12	1:L:61:THR:HG22	1.86	0.40
1:P:150:TYR:CD1	1:P:209:LEU:HD13	2.56	0.40
1:G:273:VAL:O	1:G:273:VAL:HG13	2.20	0.40
1:E:145:LEU:HD22	1:E:149:SER:HB3	2.03	0.40
1:M:276:TRP:CH2	1:M:278:ALA:HB2	2.56	0.40
1:C:47:PRO:HA	3:C:407:HOH:O	2.20	0.40
1:J:237:HIS:HD2	1:K:78:VAL:HG21	1.86	0.40
1:J:245:LEU:HD12	1:J:287:TYR:HB3	2.04	0.40
1:K:109:MET:HB3	1:K:113:SER:HB3	2.03	0.40
1:O:49:LEU:HD23	1:P:57:LEU:HD11	1.99	0.40
1:J:279:ALA:O	1:J:280:LEU:HD23	2.22	0.40
1:P:296:ASN:HA	1:P:297:PRO:HD2	1.84	0.40
1:J:152:TYR:CG	1:J:153:LEU:N	2.89	0.40
1:P:245:LEU:HD12	1:P:287:TYR:HB3	2.03	0.40
1:I:92:TYR:CE1	1:I:105:TYR:CD2	3.09	0.40
1:M:191:THR:HG21	1:M:286:ARG:NH2	2.36	0.40
1:D:150:TYR:CG	1:D:209:LEU:HD13	2.56	0.40
1:J:86:THR:O	1:J:113:SER:HB2	2.21	0.40
1:N:81:PRO:O	1:N:83:PRO:HD3	2.21	0.40
1:F:233:VAL:O	1:F:233:VAL:HG13	2.21	0.40
1:I:238:TYR:CD2	1:I:238:TYR:C	2.95	0.40
1:N:275:GLN:HB3	1:N:275:GLN:HE21	1.63	0.40
1:P:110:LYS:HB3	1:P:111:GLU:OE1	2.21	0.40
1:N:115:SER:HB3	1:N:161:LEU:H	1.86	0.40
1:F:102:PHE:HE2	1:F:240:GLN:HE21	1.65	0.40
1:I:296:ASN:HD22	1:I:298:LEU:H	1.70	0.40
1:L:70:ALA:HB3	1:L:268:TRP:HB3	2.03	0.40
1:C:239:ASN:ND2	1:C:239:ASN:H	2.20	0.40
1:M:124:ARG:HG2	1:M:125:LEU:H	1.84	0.40
1:P:95:THR:HA	1:P:103:VAL:HG12	2.04	0.40
1:G:196:LEU:CD2	1:G:207:ARG:NH1	2.85	0.40
1:I:197:LEU:HD12	1:I:208:LYS:HG3	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:82:LEU:HA	1:C:82:LEU:HD12	1.92	0.40
1:O:51:PRO:HG3	1:O:75:GLU:CA	2.52	0.40
1:C:190:SER:O	1:C:191:THR:C	2.60	0.40
1:K:255:GLY:HA3	3:K:414:HOH:O	2.22	0.40
1:N:123:GLU:HG2	1:N:174:ARG:O	2.21	0.40
1:A:43:LYS:HG2	3:A:430:HOH:O	2.22	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%)	233 (92%)	18 (7%)	3 (1%)	16	29
1	B	254/266 (96%)	238 (94%)	14 (6%)	2 (1%)	24	41
1	C	254/266 (96%)	238 (94%)	14 (6%)	2 (1%)	24	41
1	D	254/266 (96%)	235 (92%)	17 (7%)	2 (1%)	24	41
1	E	254/266 (96%)	240 (94%)	13 (5%)	1 (0%)	39	61
1	F	254/266 (96%)	234 (92%)	20 (8%)	0	100	100
1	G	254/266 (96%)	228 (90%)	24 (9%)	2 (1%)	24	41
1	H	254/266 (96%)	227 (89%)	26 (10%)	1 (0%)	39	61
1	I	254/266 (96%)	241 (95%)	11 (4%)	2 (1%)	24	41
1	J	254/266 (96%)	231 (91%)	21 (8%)	2 (1%)	24	41
1	K	254/266 (96%)	222 (87%)	20 (8%)	12 (5%)	3	3
1	L	254/266 (96%)	220 (87%)	26 (10%)	8 (3%)	5	7
1	M	254/266 (96%)	220 (87%)	30 (12%)	4 (2%)	12	21
1	N	254/266 (96%)	227 (89%)	23 (9%)	4 (2%)	12	21
1	O	254/266 (96%)	216 (85%)	32 (13%)	6 (2%)	7	11

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	P	254/266 (96%)	211 (83%)	32 (13%)	11 (4%)	3	4
All	All	4064/4256 (96%)	3661 (90%)	341 (8%)	62 (2%)	13	22

All (62) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	141	SER
1	I	141	SER
1	K	115	SER
1	L	148	ASP
1	O	147	VAL
1	O	148	ASP
1	P	115	SER
1	P	146	THR
1	A	167	ALA
1	D	142	SER
1	K	159	HIS
1	K	186	LEU
1	K	214	VAL
1	M	142	SER
1	N	294	ASN
1	P	87	ASN
1	P	191	THR
1	C	75	GLU
1	D	75	GLU
1	K	58	PRO
1	K	142	SER
1	K	165	GLU
1	L	142	SER
1	L	151	ALA
1	L	194	GLN
1	N	55	GLN
1	P	40	ILE
1	A	141	SER
1	C	119	PRO
1	E	75	GLU
1	H	119	PRO
1	I	112	MET
1	J	119	PRO
1	K	182	HIS
1	L	193	LYS
1	M	119	PRO

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Mol	Chain	Res	Type
1	M	231	LEU
1	O	165	GLU
1	P	154	PRO
1	P	214	VAL
1	A	112	MET
1	G	182	HIS
1	K	111	GLU
1	K	164	VAL
1	P	109	MET
1	P	112	MET
1	P	211	PRO
1	G	119	PRO
1	J	214	VAL
1	K	75	GLU
1	K	203	VAL
1	N	81	PRO
1	N	154	PRO
1	O	154	PRO
1	P	141	SER
1	L	147	VAL
1	O	58	PRO
1	B	96	PRO
1	L	227	PRO
1	M	236	VAL
1	L	214	VAL
1	O	220	ILE

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	230/237 (97%)	220 (96%)	10 (4%)	35	61
1	B	230/237 (97%)	216 (94%)	14 (6%)	23	42
1	C	230/237 (97%)	218 (95%)	12 (5%)	29	51
1	D	230/237 (97%)	211 (92%)	19 (8%)	14	26

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	230/237 (97%)	216 (94%)	14 (6%)	23	42
1	F	230/237 (97%)	218 (95%)	12 (5%)	29	51
1	G	230/237 (97%)	211 (92%)	19 (8%)	14	26
1	H	230/237 (97%)	219 (95%)	11 (5%)	31	55
1	I	230/237 (97%)	216 (94%)	14 (6%)	23	42
1	J	230/237 (97%)	216 (94%)	14 (6%)	23	42
1	K	230/237 (97%)	211 (92%)	19 (8%)	14	26
1	L	230/237 (97%)	216 (94%)	14 (6%)	23	42
1	M	230/237 (97%)	213 (93%)	17 (7%)	17	31
1	N	230/237 (97%)	212 (92%)	18 (8%)	16	29
1	O	230/237 (97%)	206 (90%)	24 (10%)	9	16
1	P	230/237 (97%)	212 (92%)	18 (8%)	16	29
All	All	3680/3792 (97%)	3431 (93%)	249 (7%)	20	36

All (249) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	153	LEU
1	A	169	LEU
1	A	171	VAL
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	B	82	LEU
1	B	101	HIS
1	B	111	GLU
1	B	125	LEU
1	B	143	LYS
1	B	170	VAL
1	B	171	VAL
1	B	197	LEU
1	B	243	LEU
1	B	249	GLN
1	B	252	TYR

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Mol	Chain	Res	Type
1	B	286	ARG
1	B	289	LEU
1	B	296	ASN
1	C	40	ILE
1	C	144	LYS
1	C	148	ASP
1	C	171	VAL
1	C	222	THR
1	C	243	LEU
1	C	249	GLN
1	C	275	GLN
1	C	283	THR
1	C	284	ARG
1	C	286	ARG
1	C	298	LEU
1	D	40	ILE
1	D	82	LEU
1	D	101	HIS
1	D	103	VAL
1	D	111	GLU
1	D	112	MET
1	D	125	LEU
1	D	134	THR
1	D	148	ASP
1	D	153	LEU
1	D	171	VAL
1	D	199	THR
1	D	239	ASN
1	D	243	LEU
1	D	247	GLU
1	D	249	GLN
1	D	286	ARG
1	D	296	ASN
1	D	298	LEU
1	E	76	SER
1	E	84	ASP
1	E	111	GLU
1	E	136	THR
1	E	148	ASP
1	E	165	GLU
1	E	166	SER
1	E	171	VAL

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Mol	Chain	Res	Type
1	E	198	GLU
1	E	243	LEU
1	E	249	GLN
1	E	252	TYR
1	E	286	ARG
1	E	296	ASN
1	F	56	ASP
1	F	111	GLU
1	F	112	MET
1	F	162	ASP
1	F	171	VAL
1	F	192	ASP
1	F	222	THR
1	F	243	LEU
1	F	252	TYR
1	F	283	THR
1	F	286	ARG
1	F	289	LEU
1	G	45	THR
1	G	46	ASN
1	G	68	ASP
1	G	82	LEU
1	G	111	GLU
1	G	133	VAL
1	G	135	LEU
1	G	157	PHE
1	G	164	VAL
1	G	171	VAL
1	G	183	THR
1	G	214	VAL
1	G	222	THR
1	G	239	ASN
1	G	243	LEU
1	G	249	GLN
1	G	252	TYR
1	G	286	ARG
1	G	288	LEU
1	H	40	ILE
1	H	82	LEU
1	H	141	SER
1	H	153	LEU
1	H	171	VAL

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Mol	Chain	Res	Type
1	H	243	LEU
1	H	249	GLN
1	H	252	TYR
1	H	286	ARG
1	H	296	ASN
1	H	298	LEU
1	I	49	LEU
1	I	82	LEU
1	I	130	GLU
1	I	137	ASN
1	I	148	ASP
1	I	171	VAL
1	I	185	GLU
1	I	191	THR
1	I	243	LEU
1	I	249	GLN
1	I	252	TYR
1	I	284	ARG
1	I	286	ARG
1	I	296	ASN
1	J	111	GLU
1	J	136	THR
1	J	141	SER
1	J	148	ASP
1	J	162	ASP
1	J	171	VAL
1	J	187	ILE
1	J	222	THR
1	J	243	LEU
1	J	249	GLN
1	J	252	TYR
1	J	285	SER
1	J	286	ARG
1	J	296	ASN
1	K	45	THR
1	K	75	GLU
1	K	82	LEU
1	K	86	THR
1	K	111	GLU
1	K	113	SER
1	K	130	GLU
1	K	137	ASN

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Mol	Chain	Res	Type
1	K	144	LYS
1	K	159	HIS
1	K	164	VAL
1	K	193	LYS
1	K	199	THR
1	K	218	PHE
1	K	222	THR
1	K	243	LEU
1	K	249	GLN
1	K	252	TYR
1	K	296	ASN
1	L	111	GLU
1	L	144	LYS
1	L	148	ASP
1	L	166	SER
1	L	170	VAL
1	L	171	VAL
1	L	192	ASP
1	L	197	LEU
1	L	205	GLU
1	L	222	THR
1	L	243	LEU
1	L	249	GLN
1	L	286	ARG
1	L	298	LEU
1	M	46	ASN
1	M	84	ASP
1	M	101	HIS
1	M	111	GLU
1	M	129	VAL
1	M	130	GLU
1	M	137	ASN
1	M	157	PHE
1	M	163	CYS
1	M	169	LEU
1	M	171	VAL
1	M	198	GLU
1	M	222	THR
1	M	243	LEU
1	M	249	GLN
1	M	284	ARG
1	M	298	LEU

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Mol	Chain	Res	Type
1	N	40	ILE
1	N	55	GLN
1	N	80	SER
1	N	82	LEU
1	N	101	HIS
1	N	111	GLU
1	N	130	GLU
1	N	133	VAL
1	N	136	THR
1	N	196	LEU
1	N	218	PHE
1	N	234	LYS
1	N	243	LEU
1	N	249	GLN
1	N	252	TYR
1	N	253	ARG
1	N	275	GLN
1	N	286	ARG
1	O	40	ILE
1	O	45	THR
1	O	56	ASP
1	O	75	GLU
1	O	88	THR
1	O	96	PRO
1	O	101	HIS
1	O	111	GLU
1	O	142	SER
1	O	143	LYS
1	O	148	ASP
1	O	166	SER
1	O	170	VAL
1	O	171	VAL
1	O	191	THR
1	O	197	LEU
1	O	214	VAL
1	O	219	ASN
1	O	223	MET
1	O	237	HIS
1	O	243	LEU
1	O	244	LEU
1	O	249	GLN
1	O	252	TYR

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Mol	Chain	Res	Type
1	P	40	ILE
1	P	49	LEU
1	P	82	LEU
1	P	101	HIS
1	P	111	GLU
1	P	136	THR
1	P	146	THR
1	P	149	SER
1	P	156	ASN
1	P	183	THR
1	P	212	MET
1	P	222	THR
1	P	243	LEU
1	P	249	GLN
1	P	252	TYR
1	P	283	THR
1	P	286	ARG
1	P	296	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (125) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	77	HIS
1	A	156	ASN
1	A	221	HIS
1	A	239	ASN
1	A	240	GLN
1	A	249	GLN
1	A	262	GLN
1	A	296	ASN
1	B	55	GLN
1	B	87	ASN
1	B	120	GLN
1	B	156	ASN
1	B	226	GLN
1	B	239	ASN
1	B	240	GLN
1	B	249	GLN
1	B	262	GLN
1	B	296	ASN
1	C	87	ASN
1	C	239	ASN

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Mol	Chain	Res	Type
1	C	240	GLN
1	C	249	GLN
1	C	262	GLN
1	C	296	ASN
1	D	46	ASN
1	D	137	ASN
1	D	156	ASN
1	D	239	ASN
1	D	240	GLN
1	D	249	GLN
1	D	296	ASN
1	E	87	ASN
1	E	156	ASN
1	E	239	ASN
1	E	240	GLN
1	E	249	GLN
1	E	296	ASN
1	F	87	ASN
1	F	137	ASN
1	F	239	ASN
1	F	240	GLN
1	F	262	GLN
1	F	296	ASN
1	G	156	ASN
1	G	182	HIS
1	G	226	GLN
1	G	239	ASN
1	G	240	GLN
1	G	249	GLN
1	G	262	GLN
1	G	275	GLN
1	H	87	ASN
1	H	156	ASN
1	H	221	HIS
1	H	239	ASN
1	H	240	GLN
1	H	249	GLN
1	H	262	GLN
1	H	296	ASN
1	I	55	GLN
1	I	87	ASN
1	I	120	GLN

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Mol	Chain	Res	Type
1	I	137	ASN
1	I	156	ASN
1	I	194	GLN
1	I	237	HIS
1	I	239	ASN
1	I	249	GLN
1	I	296	ASN
1	J	55	GLN
1	J	156	ASN
1	J	232	ASN
1	J	240	GLN
1	J	249	GLN
1	J	257	ASN
1	J	262	GLN
1	J	296	ASN
1	K	87	ASN
1	K	120	GLN
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	120	GLN
1	L	137	ASN
1	L	156	ASN
1	L	239	ASN
1	L	240	GLN
1	L	296	ASN
1	M	87	ASN
1	M	137	ASN
1	M	156	ASN
1	M	219	ASN
1	M	221	HIS
1	M	226	GLN
1	M	239	ASN
1	M	240	GLN
1	M	249	GLN
1	M	257	ASN
1	M	262	GLN
1	M	296	ASN
1	N	137	ASN

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Mol	Chain	Res	Type
1	N	156	ASN
1	N	239	ASN
1	N	240	GLN
1	N	249	GLN
1	N	262	GLN
1	N	296	ASN
1	O	101	HIS
1	O	137	ASN
1	O	156	ASN
1	O	221	HIS
1	O	240	GLN
1	O	249	GLN
1	O	262	GLN
1	O	294	ASN
1	O	296	ASN
1	P	156	ASN
1	P	194	GLN
1	P	221	HIS
1	P	232	ASN
1	P	240	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 carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 16 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.



There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	258/266 (96%)	-0.04	4 (1%) 74 78	20, 32, 47, 64	0
1	B	258/266 (96%)	-0.02	5 (1%) 70 73	18, 33, 47, 55	0
1	C	258/266 (96%)	0.04	3 (1%) 81 83	18, 32, 50, 63	0
1	D	258/266 (96%)	-0.03	3 (1%) 81 83	19, 34, 47, 62	0
1	E	258/266 (96%)	0.11	6 (2%) 64 67	19, 37, 53, 65	0
1	F	258/266 (96%)	0.14	9 (3%) 48 53	24, 38, 50, 66	0
1	G	258/266 (96%)	0.29	11 (4%) 39 44	22, 41, 58, 70	0
1	H	258/266 (96%)	0.15	10 (3%) 43 48	24, 38, 54, 66	0
1	I	258/266 (96%)	0.20	2 (0%) 87 89	24, 41, 53, 66	0
1	J	258/266 (96%)	0.30	7 (2%) 58 62	27, 44, 57, 73	0
1	K	258/266 (96%)	0.61	24 (9%) 11 11	26, 46, 63, 70	0
1	L	258/266 (96%)	0.32	7 (2%) 58 62	33, 47, 58, 65	0
1	M	258/266 (96%)	0.53	23 (8%) 12 13	27, 48, 61, 67	0
1	N	258/266 (96%)	0.38	18 (6%) 19 22	26, 46, 59, 66	0
1	O	258/266 (96%)	0.57	23 (8%) 12 13	31, 50, 59, 71	0
1	P	258/266 (96%)	0.59	19 (7%) 17 19	28, 52, 64, 67	0
All	All	4128/4256 (96%)	0.26	174 (4%) 40 45	18, 41, 58, 73	0

All (174) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	140	SER	6.1
1	G	140	SER	5.6
1	K	141	SER	5.3
1	M	164	VAL	5.3
1	P	164	VAL	5.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	M	140	SER	5.1
1	G	164	VAL	4.8
1	G	141	SER	4.6
1	F	140	SER	4.4
1	N	141	SER	4.3
1	K	140	SER	4.2
1	O	214	VAL	4.2
1	H	140	SER	4.0
1	O	164	VAL	4.0
1	N	40	ILE	4.0
1	K	196	LEU	4.0
1	G	144	LYS	3.9
1	K	42	TRP	3.8
1	M	198	GLU	3.8
1	N	164	VAL	3.7
1	M	142	SER	3.7
1	D	141	SER	3.7
1	O	131	GLY	3.6
1	M	141	SER	3.6
1	J	141	SER	3.6
1	M	42	TRP	3.5
1	O	198	GLU	3.5
1	H	181	SER	3.5
1	K	145	LEU	3.5
1	O	178	TYR	3.4
1	P	39	PRO	3.4
1	L	136	THR	3.3
1	O	144	LYS	3.3
1	H	243	LEU	3.3
1	E	171	VAL	3.3
1	G	165	GLU	3.3
1	K	142	SER	3.3
1	O	141	SER	3.3
1	G	179	LEU	3.2
1	A	140	SER	3.2
1	O	142	SER	3.2
1	M	163	CYS	3.2
1	P	146	THR	3.2
1	P	112	MET	3.2
1	P	166	SER	3.2
1	M	243	LEU	3.1
1	O	179	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	H	141	SER	3.1
1	L	198	GLU	3.1
1	F	112	MET	3.1
1	A	141	SER	3.1
1	J	164	VAL	3.1
1	N	198	GLU	3.1
1	P	244	LEU	3.0
1	M	112	MET	3.0
1	E	125	LEU	3.0
1	N	165	GLU	3.0
1	G	198	GLU	2.9
1	P	171	VAL	2.9
1	O	197	LEU	2.9
1	M	143	LYS	2.9
1	M	40	ILE	2.9
1	O	200	PRO	2.9
1	P	142	SER	2.9
1	C	179	LEU	2.9
1	M	144	LYS	2.9
1	J	142	SER	2.8
1	P	125	LEU	2.8
1	N	140	SER	2.8
1	K	112	MET	2.8
1	P	88	THR	2.8
1	D	140	SER	2.8
1	F	141	SER	2.8
1	G	142	SER	2.8
1	N	42	TRP	2.7
1	N	136	THR	2.7
1	P	114	SER	2.7
1	K	136	THR	2.7
1	E	170	VAL	2.7
1	L	132	ALA	2.7
1	I	171	VAL	2.6
1	K	181	SER	2.6
1	M	87	ASN	2.6
1	H	179	LEU	2.6
1	K	83	PRO	2.6
1	H	171	VAL	2.6
1	P	181	SER	2.6
1	J	134	THR	2.6
1	P	165	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	M	86	THR	2.6
1	N	170	VAL	2.5
1	L	180	GLY	2.5
1	N	111	GLU	2.5
1	L	40	ILE	2.5
1	O	220	ILE	2.5
1	P	192	ASP	2.5
1	C	140	SER	2.5
1	K	171	VAL	2.5
1	G	112	MET	2.5
1	K	198	GLU	2.5
1	N	181	SER	2.5
1	F	171	VAL	2.5
1	A	243	LEU	2.5
1	J	186	LEU	2.5
1	L	243	LEU	2.5
1	K	104	MET	2.5
1	M	193	LYS	2.4
1	O	110	LYS	2.4
1	K	180	GLY	2.4
1	I	40	ILE	2.4
1	O	89	LEU	2.4
1	N	142	SER	2.4
1	M	185	GLU	2.4
1	F	214	VAL	2.4
1	G	243	LEU	2.4
1	K	84	ASP	2.4
1	M	136	THR	2.4
1	G	181	SER	2.4
1	F	243	LEU	2.4
1	O	40	ILE	2.4
1	P	185	GLU	2.4
1	K	110	LYS	2.3
1	H	198	GLU	2.3
1	K	40	ILE	2.3
1	N	161	LEU	2.3
1	O	166	SER	2.3
1	O	171	VAL	2.3
1	F	104	MET	2.3
1	K	195	PRO	2.3
1	M	110	LYS	2.3
1	N	244	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	O	42	TRP	2.3
1	B	164	VAL	2.3
1	P	288	LEU	2.3
1	N	110	LYS	2.2
1	O	181	SER	2.2
1	N	157	PHE	2.2
1	B	165	GLU	2.2
1	M	181	SER	2.2
1	M	179	LEU	2.2
1	P	143	LYS	2.2
1	B	39	PRO	2.2
1	O	55	GLN	2.2
1	O	84	ASP	2.2
1	K	193	LYS	2.2
1	N	186	LEU	2.2
1	K	164	VAL	2.2
1	K	172	PHE	2.2
1	L	197	LEU	2.2
1	B	171	VAL	2.1
1	F	40	ILE	2.1
1	A	244	LEU	2.1
1	E	289	LEU	2.1
1	M	180	GLY	2.1
1	C	141	SER	2.1
1	K	81	PRO	2.1
1	O	158	HIS	2.1
1	O	126	ILE	2.1
1	B	170	VAL	2.1
1	H	266	VAL	2.1
1	H	164	VAL	2.1
1	P	42	TRP	2.1
1	P	40	ILE	2.1
1	J	244	LEU	2.1
1	K	244	LEU	2.1
1	M	125	LEU	2.1
1	N	135	LEU	2.1
1	K	113	SER	2.1
1	H	142	SER	2.0
1	D	170	VAL	2.0
1	F	203	VAL	2.0
1	E	220	ILE	2.0
1	M	196	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	E	140	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	MN	O	301	1/1	0.94	0.10	-	47,47,47,47	0
2	MN	P	301	1/1	0.99	0.18	-	44,44,44,44	0
2	MN	I	301	1/1	0.99	0.13	-	34,34,34,34	0
2	MN	K	301	1/1	0.99	0.17	-	40,40,40,40	0
2	MN	E	301	1/1	0.98	0.16	-	29,29,29,29	0
2	MN	G	301	1/1	0.99	0.14	-	34,34,34,34	0
2	MN	H	301	1/1	0.98	0.15	-	36,36,36,36	0
2	MN	A	301	1/1	0.98	0.17	-	33,33,33,33	0
2	MN	C	301	1/1	0.97	0.14	-	30,30,30,30	0
2	MN	N	301	1/1	0.99	0.12	-	41,41,41,41	0
2	MN	J	301	1/1	0.97	0.19	-	51,51,51,51	0
2	MN	L	301	1/1	0.97	0.13	-	46,46,46,46	0
2	MN	F	301	1/1	0.98	0.10	-	36,36,36,36	0
2	MN	B	301	1/1	0.98	0.17	-	32,32,32,32	0
2	MN	D	301	1/1	0.98	0.16	-	30,30,30,30	0
2	MN	M	301	1/1	0.99	0.10	-	48,48,48,48	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.