



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 04:43 am BST

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

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

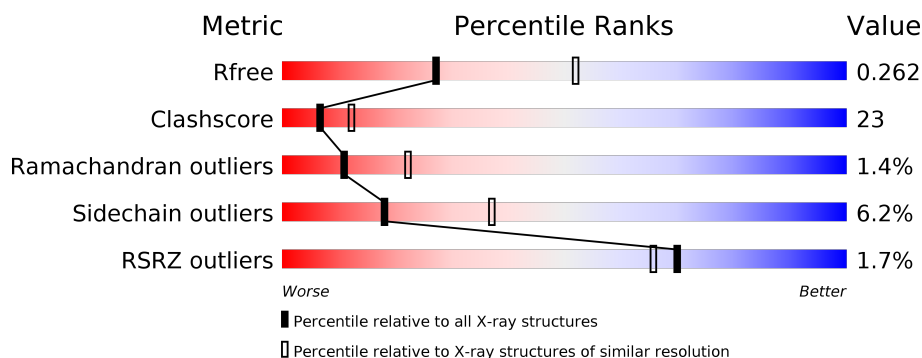
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.59 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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

Mol	Chain	Length	Quality of chain
1	A	266	<div> <div>61%</div> <div>30%</div> <div>5%</div> <div>.</div> </div>
1	B	266	<div> <div>60%</div> <div>33%</div> <div>.</div> <div>.</div> </div>
1	C	266	<div> <div>2%</div> <div>58%</div> <div>37%</div> <div>.</div> <div>.</div> </div>
1	D	266	<div> <div>%</div> <div>56%</div> <div>36%</div> <div>5%</div> <div>.</div> </div>
1	E	266	<div> <div>%</div> <div>54%</div> <div>39%</div> <div>.</div> <div>.</div> </div>
1	F	266	<div> <div>%</div> <div>54%</div> <div>40%</div> <div>.</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
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 4 unique types of molecules in this entry. The entry contains 33974 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Ureidoglycine aminohydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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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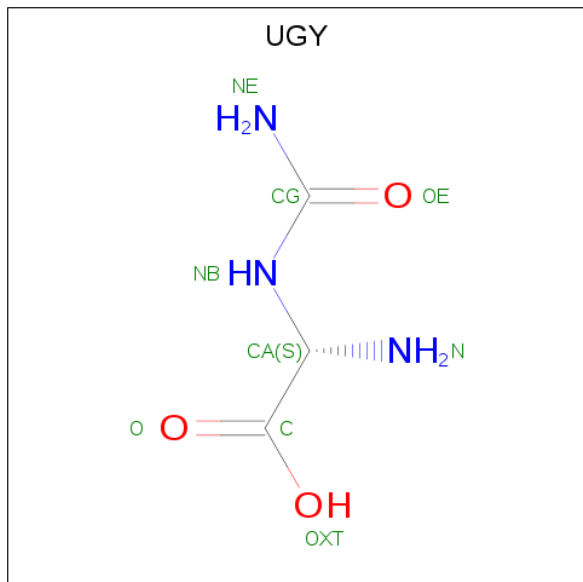
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Chain	Residue	Modelled	Actual	Comment	Reference
O	33	GLY	-	EXPRESSION TAG	UNP Q8GXV5
O	34	HIS	-	EXPRESSION TAG	UNP Q8GXV5
O	35	MET	-	EXPRESSION TAG	UNP Q8GXV5
P	33	GLY	-	EXPRESSION TAG	UNP Q8GXV5
P	34	HIS	-	EXPRESSION TAG	UNP Q8GXV5
P	35	MET	-	EXPRESSION 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 (2S)-amino(carbamoylamino)ethanoic acid (three-letter code: UGY) (formula: $C_3H_7N_3O_3$).



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

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

- Molecule 4 is water.

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

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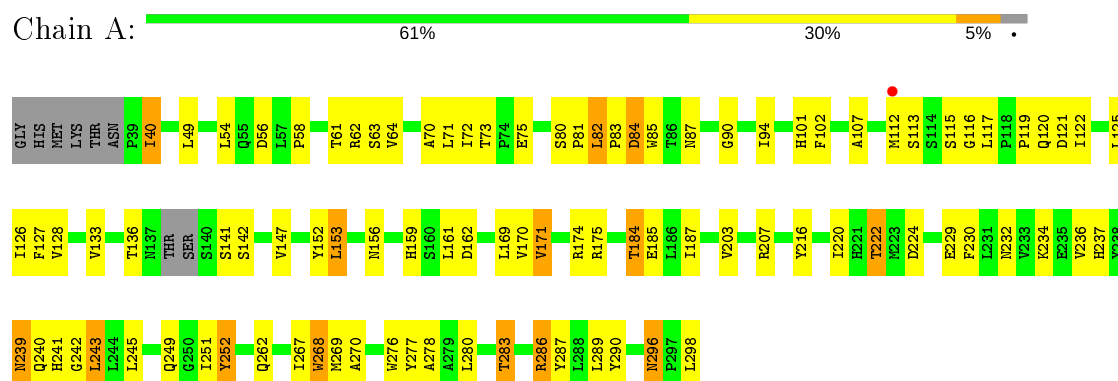
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	P	29	Total	O	0	0
			29	29		

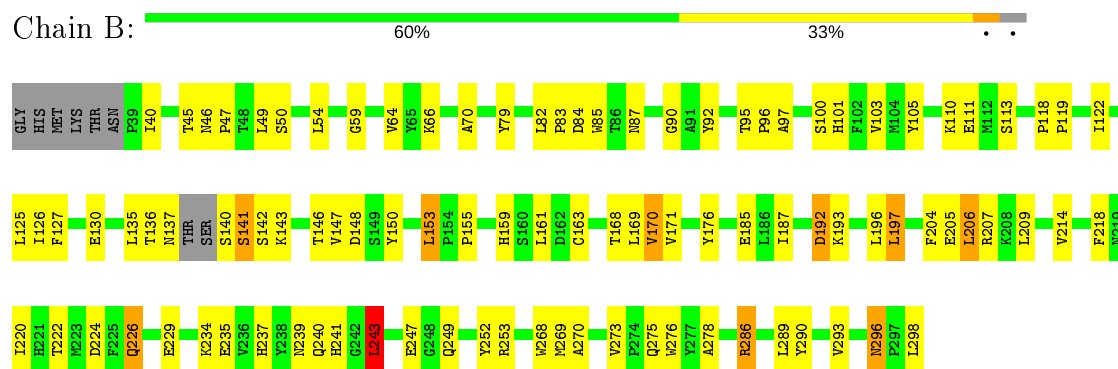
3 Residue-property plots

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

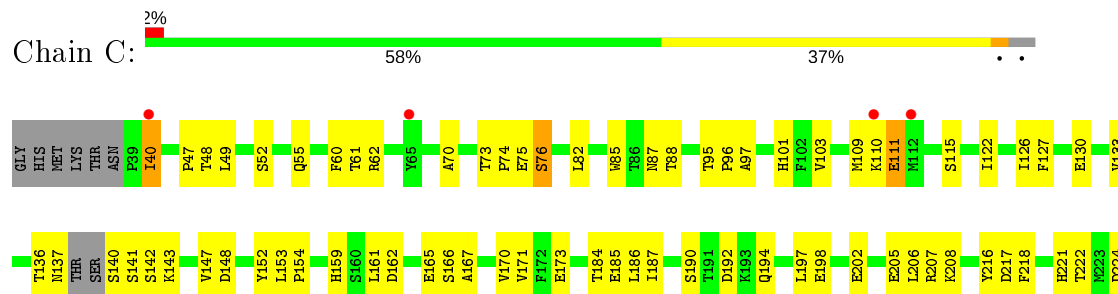
• Molecule 1: Ureidoglycine aminohydrolase



• Molecule 1: Ureidoglycine aminohydrolase

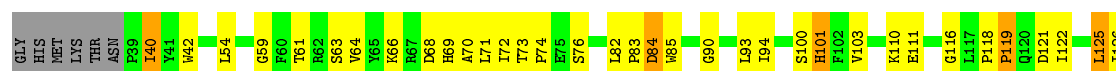


• Molecule 1: Ureidoglycine aminohydrolase





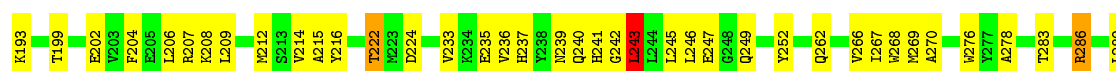
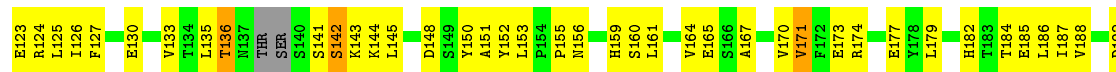
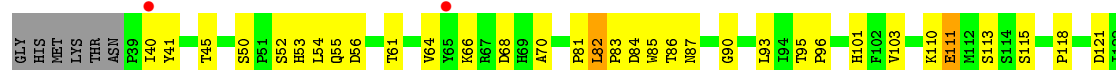
• Molecule 1: Ureidoglycine aminohydrolase



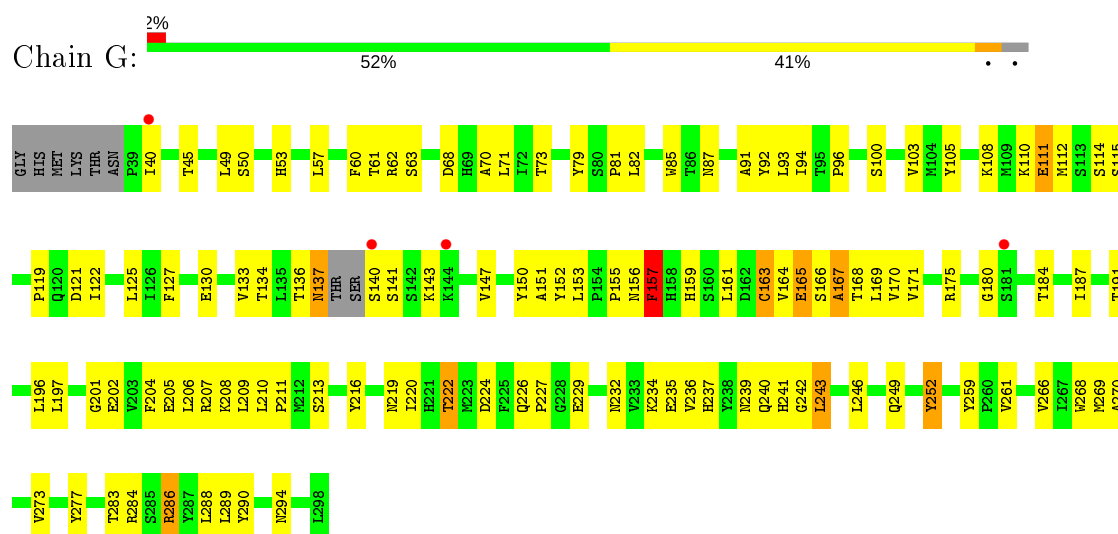
• Molecule 1: Ureidoglycine aminohydrolase



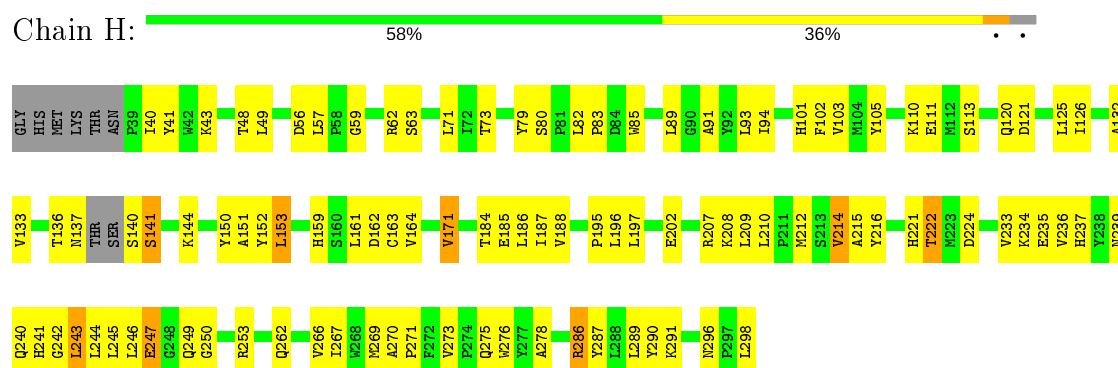
• Molecule 1: Ureidoglycine aminohydrolase



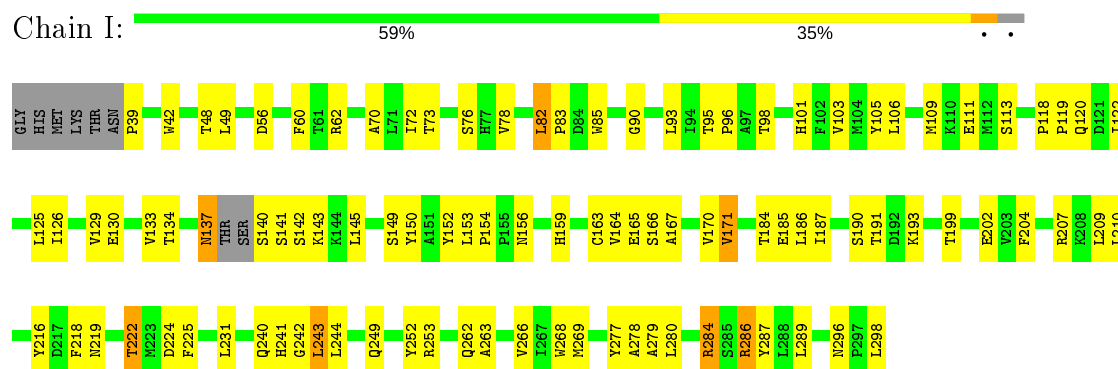
• Molecule 1: Ureidoglycine aminohydrolase



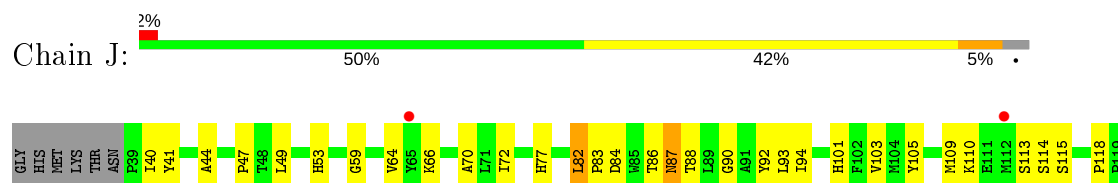
- Molecule 1: Ureidoglycine aminohydrolase

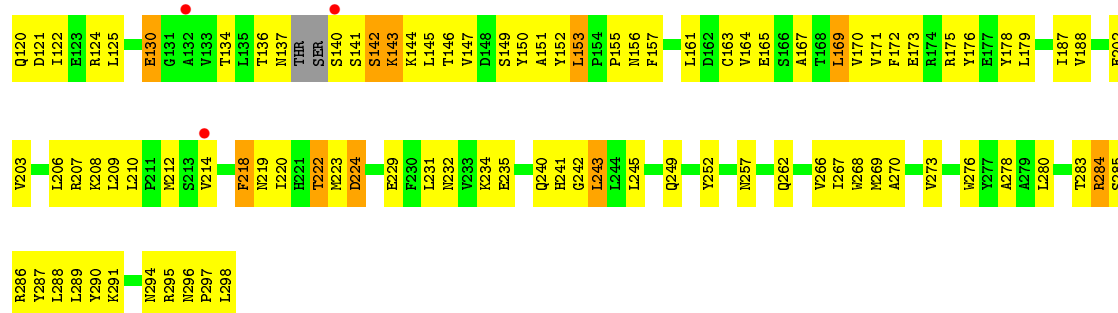


- Molecule 1: Ureidoglycine aminohydrolase

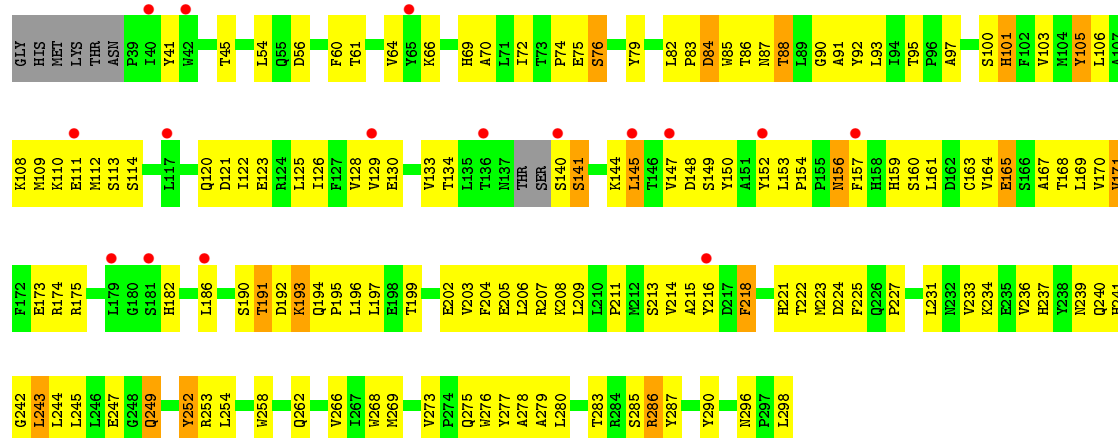
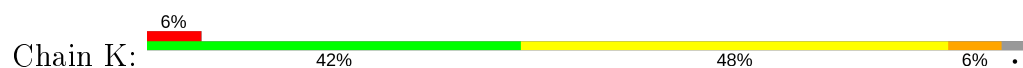


- Molecule 1: Ureidoglycine aminohydrolase

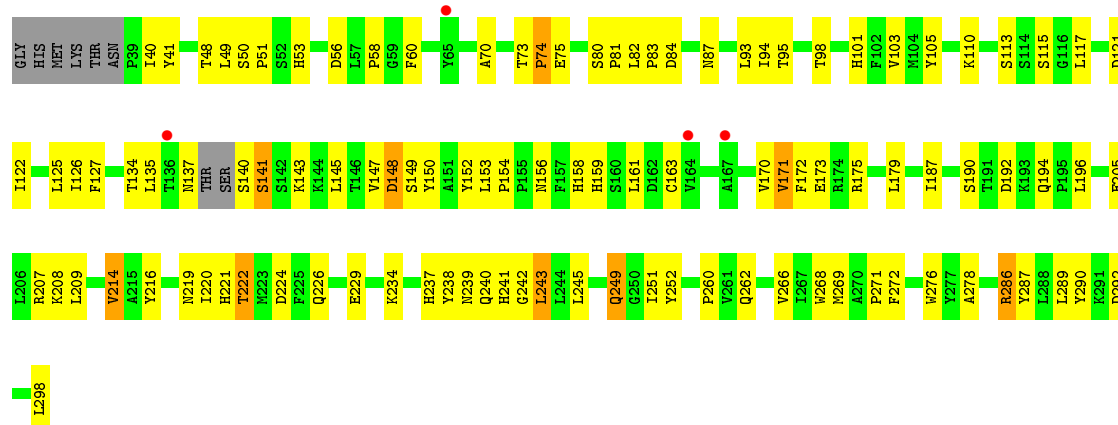




• Molecule 1: Ureidoglycine aminohydrolase

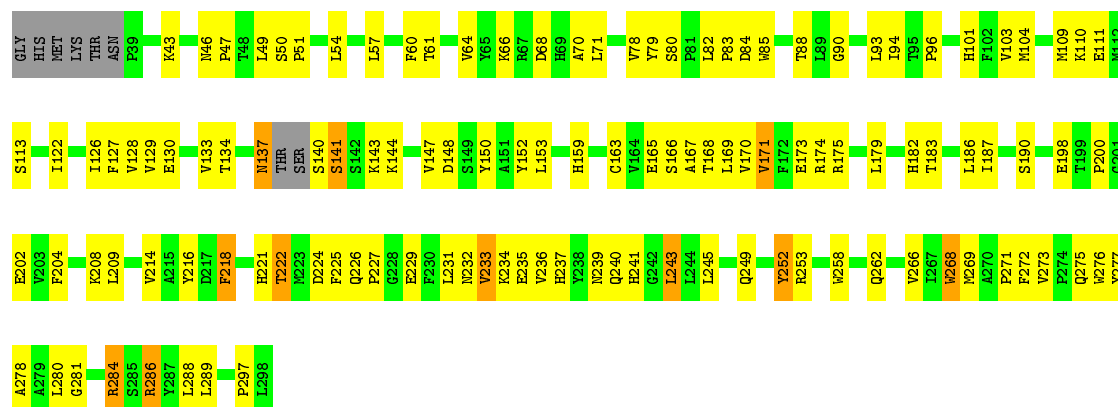


• Molecule 1: Ureidoglycine aminohydrolase

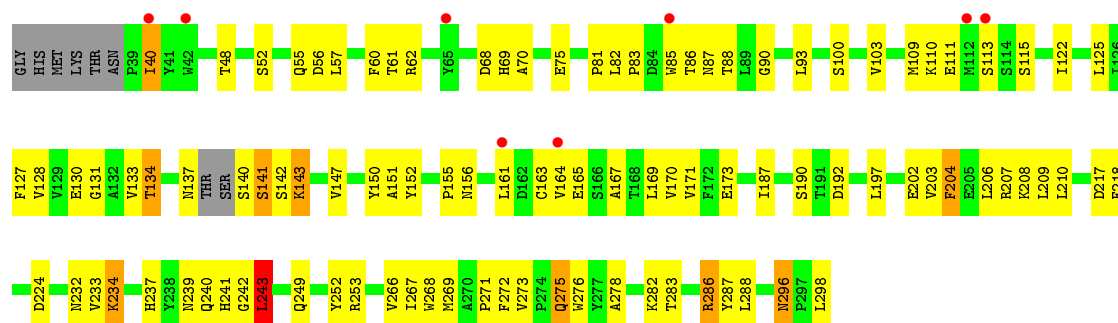


• Molecule 1: Ureidoglycine aminohydrolase

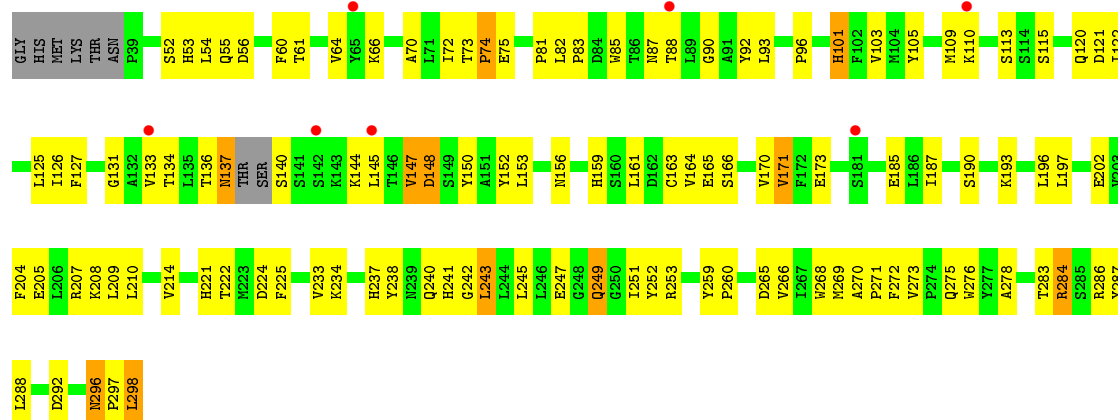




• Molecule 1: Ureidoglycine aminohydrolase



• 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, α , β , γ	93.10Å 174.89Å 154.30Å 90.00° 99.26° 90.00°	Depositor
Resolution (Å)	50.00 – 2.59 49.23 – 2.59	Depositor EDS
% Data completeness (in resolution range)	93.3 (50.00-2.59) 93.5 (49.23-2.59)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.27 (at 2.58Å)	Xtriage
Refinement program	CNS 1.21	Depositor
R, R_{free}	0.209 , 0.271 0.201 , 0.262	Depositor DCC
R_{free} test set	14964 reflections (9.99%)	wwPDB-VP
Wilson B-factor (Å ²)	43.1	Xtriage
Anisotropy	0.217	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 49.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	33974	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.63% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.43	0/2140	0.67	1/2920 (0.0%)
1	B	0.42	0/2140	0.68	1/2920 (0.0%)
1	C	0.43	0/2140	0.68	1/2920 (0.0%)
1	D	0.43	0/2140	0.67	1/2920 (0.0%)
1	E	0.42	0/2140	0.70	1/2920 (0.0%)
1	F	0.43	0/2140	0.68	2/2920 (0.1%)
1	G	0.44	0/2140	0.68	1/2920 (0.0%)
1	H	0.44	0/2140	0.69	1/2920 (0.0%)
1	I	0.43	0/2140	0.67	1/2920 (0.0%)
1	J	0.45	0/2140	0.67	1/2920 (0.0%)
1	K	0.47	0/2140	0.68	1/2920 (0.0%)
1	L	0.44	0/2140	0.69	1/2920 (0.0%)
1	M	0.43	0/2140	0.67	0/2920
1	N	0.45	0/2140	0.66	2/2920 (0.1%)
1	O	0.45	0/2140	0.67	1/2920 (0.0%)
1	P	0.45	0/2140	0.70	2/2920 (0.1%)
All	All	0.44	0/34240	0.68	18/46720 (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	M	0	1

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	242	GLY	N-CA-C	-6.82	96.06	113.10
1	H	242	GLY	N-CA-C	-6.10	97.85	113.10
1	L	242	GLY	N-CA-C	-6.09	97.87	113.10
1	C	242	GLY	N-CA-C	-6.08	97.89	113.10
1	E	242	GLY	N-CA-C	-6.08	97.89	113.10
1	N	242	GLY	N-CA-C	-5.97	98.17	113.10
1	P	242	GLY	N-CA-C	-5.93	98.27	113.10
1	I	242	GLY	N-CA-C	-5.90	98.34	113.10
1	F	242	GLY	N-CA-C	-5.84	98.49	113.10
1	D	242	GLY	N-CA-C	-5.84	98.49	113.10
1	B	243	LEU	CA-CB-CG	5.59	128.16	115.30
1	J	242	GLY	N-CA-C	-5.52	99.29	113.10
1	A	242	GLY	N-CA-C	-5.50	99.34	113.10
1	P	243	LEU	CA-CB-CG	5.49	127.92	115.30
1	O	242	GLY	N-CA-C	-5.47	99.43	113.10
1	N	243	LEU	CA-CB-CG	5.38	127.67	115.30
1	K	242	GLY	N-CA-C	-5.31	99.83	113.10
1	F	243	LEU	CA-CB-CG	5.20	127.27	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	M	216	TYR	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2076	0	2034	76	0
1	B	2076	0	2034	84	0
1	C	2076	0	2034	83	0
1	D	2076	0	2034	107	0
1	E	2076	0	2034	98	0
1	F	2076	0	2034	96	0
1	G	2076	0	2034	106	0
1	H	2076	0	2034	97	0
1	I	2076	0	2034	81	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	J	2076	0	2034	118	0
1	K	2076	0	2034	162	0
1	L	2076	0	2034	98	0
1	M	2076	0	2034	95	0
1	N	2076	0	2034	89	0
1	O	2076	0	2034	102	0
1	P	2076	0	2034	138	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0
2	K	1	0	0	0	0
2	L	1	0	0	0	0
2	M	1	0	0	0	0
2	N	1	0	0	0	0
2	O	1	0	0	0	0
2	P	1	0	0	0	0
3	A	9	0	5	0	0
3	B	9	0	5	0	0
3	C	9	0	6	0	0
3	D	9	0	6	0	0
3	E	9	0	5	0	0
3	F	9	0	6	0	0
3	G	9	0	5	0	0
3	H	9	0	6	1	0
3	I	9	0	5	0	0
3	J	9	0	5	1	0
3	K	9	0	6	0	0
3	L	9	0	5	0	0
3	M	9	0	6	0	0
3	N	9	0	6	0	0
3	O	9	0	5	0	0
3	P	9	0	6	0	0
4	A	54	0	0	1	0
4	B	41	0	0	3	0
4	C	40	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	35	0	0	0	0
4	E	38	0	0	1	0
4	F	42	0	0	2	0
4	G	38	0	0	3	0
4	H	36	0	0	2	0
4	I	38	0	0	1	0
4	J	30	0	0	3	0
4	K	34	0	0	3	0
4	L	30	0	0	1	0
4	M	40	0	0	2	0
4	N	35	0	0	1	0
4	O	38	0	0	1	0
4	P	29	0	0	3	0
All	All	33974	0	32632	1541	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 23.

All (1541) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:122:ILE:HD13	1:K:298:LEU:HD13	1.30	1.09
1:D:82:LEU:HD13	1:D:90:GLY:HA3	1.34	1.07
1:P:87:ASN:HD21	1:P:110:LYS:HD2	1.19	1.02
1:G:164:VAL:HG23	1:G:165:GLU:H	1.27	0.99
1:D:40:ILE:H	1:D:40:ILE:HD12	1.24	0.99
1:B:82:LEU:HD13	1:B:90:GLY:HA3	1.45	0.99
1:C:115:SER:HB3	1:C:161:LEU:HB2	1.45	0.98
1:P:196:LEU:HD21	1:P:207:ARG:HH21	1.27	0.97
1:P:133:VAL:HG12	1:P:163:CYS:HB2	1.45	0.96
1:F:224:ASP:OD1	1:F:286:ARG:HD3	1.66	0.95
1:K:224:ASP:OD2	1:K:286:ARG:HD3	1.66	0.95
1:N:40:ILE:HD12	1:N:40:ILE:H	1.31	0.94
1:G:87:ASN:OD1	1:G:110:LYS:HB2	1.67	0.93
1:P:40:ILE:H	1:P:40:ILE:HD12	1.35	0.92
1:J:143:LYS:H	1:J:143:LYS:HD2	1.33	0.92
1:G:137:ASN:C	1:G:137:ASN:HD22	1.73	0.91
1:B:101:HIS:H	1:B:240:GLN:HE22	1.19	0.91
1:E:82:LEU:HD13	1:E:90:GLY:HA3	1.50	0.91
1:D:296:ASN:ND2	1:D:298:LEU:H	1.69	0.91
1:L:70:ALA:HB3	1:L:268:TRP:HB3	1.55	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:87:ASN:ND2	1:K:110:LYS:HB2	1.89	0.88
1:H:82:LEU:HD12	1:H:83:PRO:HD2	1.55	0.87
1:P:87:ASN:HD21	1:P:110:LYS:CD	1.86	0.87
1:N:133:VAL:HG23	1:N:163:CYS:HB2	1.56	0.86
1:B:222:THR:HG23	1:B:286:ARG:HD2	1.56	0.85
1:J:82:LEU:HD13	1:J:90:GLY:HA3	1.58	0.85
1:N:202:GLU:OE1	1:N:233:VAL:HG12	1.75	0.85
1:P:130:GLU:HA	1:P:147:VAL:HG22	1.56	0.85
1:K:193:LYS:HE3	1:K:193:LYS:HA	1.56	0.85
1:K:190:SER:H	1:K:193:LYS:HB2	1.42	0.84
1:B:137:ASN:HA	4:B:402:HOH:O	1.77	0.84
1:D:296:ASN:HD22	1:D:298:LEU:H	1.19	0.84
1:P:296:ASN:HD22	1:P:298:LEU:H	1.20	0.84
1:C:154:PRO:HG2	1:C:185:GLU:HA	1.60	0.83
1:D:196:LEU:HD11	1:D:207:ARG:NH2	1.92	0.83
1:M:224:ASP:OD2	1:M:286:ARG:HD3	1.79	0.83
1:A:239:ASN:HD22	1:A:239:ASN:H	1.24	0.82
1:C:207:ARG:HB2	1:C:222:THR:HG22	1.60	0.82
1:K:194:GLN:HE21	1:K:195:PRO:HD2	1.42	0.82
1:A:224:ASP:OD2	1:A:286:ARG:HD3	1.80	0.82
1:E:113:SER:OG	1:E:163:CYS:HB3	1.79	0.82
1:P:137:ASN:HA	1:P:159:HIS:HA	1.60	0.82
1:J:169:LEU:HD23	1:J:169:LEU:N	1.96	0.81
1:B:126:ILE:HD13	1:B:161:LEU:HD11	1.62	0.81
1:O:247:GLU:HG2	1:O:286:ARG:HB3	1.63	0.81
1:P:296:ASN:ND2	1:P:298:LEU:H	1.77	0.81
1:D:224:ASP:OD2	1:D:286:ARG:HD3	1.81	0.80
1:D:165:GLU:HG3	1:E:165:GLU:OE1	1.80	0.80
1:A:40:ILE:H	1:A:40:ILE:HD12	1.46	0.80
1:H:137:ASN:HA	1:H:159:HIS:HA	1.63	0.80
1:G:40:ILE:H	1:G:40:ILE:HD12	1.47	0.80
1:I:243:LEU:HD12	1:I:244:LEU:N	1.96	0.80
1:N:296:ASN:HD22	1:N:298:LEU:H	1.29	0.80
1:C:234:LYS:HG2	1:G:61:THR:HB	1.63	0.80
1:N:87:ASN:ND2	1:N:110:LYS:HB2	1.96	0.79
1:P:196:LEU:CD2	1:P:207:ARG:HH21	1.94	0.79
1:B:40:ILE:H	1:B:40:ILE:HD12	1.48	0.79
1:K:190:SER:O	1:K:193:LYS:N	2.14	0.79
1:O:110:LYS:HE2	1:O:110:LYS:HA	1.63	0.79
1:B:224:ASP:OD2	1:B:286:ARG:HD3	1.82	0.79
1:H:224:ASP:OD1	1:H:286:ARG:HD3	1.83	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:70:ALA:HB3	1:K:268:TRP:HB3	1.64	0.78
1:P:64:VAL:HG11	1:P:66:LYS:NZ	1.99	0.78
1:K:145:LEU:HD13	1:K:149:SER:HB3	1.64	0.78
1:F:111:GLU:HA	1:F:164:VAL:O	1.84	0.78
1:J:87:ASN:ND2	1:J:110:LYS:HB2	1.98	0.78
1:N:190:SER:HB3	1:N:192:ASP:OD1	1.83	0.78
1:E:101:HIS:H	1:E:240:GLN:HE22	1.30	0.78
1:L:40:ILE:HD12	1:L:40:ILE:H	1.48	0.78
1:B:119:PRO:HD2	1:B:122:ILE:HG13	1.66	0.78
1:N:93:LEU:HD13	1:N:266:VAL:HG21	1.64	0.77
1:G:70:ALA:HB3	1:G:268:TRP:HB3	1.66	0.77
1:K:64:VAL:HG11	1:K:66:LYS:HE3	1.66	0.77
1:K:211:PRO:HD2	1:K:216:TYR:CE2	2.20	0.77
1:I:224:ASP:OD2	1:I:286:ARG:HD3	1.83	0.77
1:O:296:ASN:HD22	1:O:298:LEU:H	1.33	0.77
1:J:146:THR:O	1:J:149:SER:HB3	1.85	0.77
1:A:40:ILE:N	1:A:40:ILE:HD12	1.99	0.76
1:L:87:ASN:ND2	1:L:110:LYS:HB2	2.00	0.76
1:K:126:ILE:HG22	1:K:171:VAL:HB	1.67	0.76
1:G:196:LEU:HD22	1:G:205:GLU:HB3	1.67	0.76
1:P:153:LEU:HD13	1:P:159:HIS:CD2	2.20	0.76
1:O:64:VAL:HG11	1:O:66:LYS:HE3	1.65	0.76
1:K:92:TYR:CE1	1:K:105:TYR:HD2	2.04	0.76
1:N:115:SER:HB3	1:N:161:LEU:HB2	1.66	0.76
1:P:224:ASP:OD1	1:P:286:ARG:HG3	1.84	0.76
1:G:115:SER:HB3	1:G:161:LEU:HB2	1.66	0.76
1:J:152:TYR:C	1:J:153:LEU:HD23	2.06	0.76
1:N:137:ASN:HB2	1:N:140:SER:HB3	1.68	0.76
1:N:61:THR:HB	1:O:234:LYS:HG2	1.66	0.76
1:P:133:VAL:HG12	1:P:163:CYS:CB	2.16	0.76
1:L:48:THR:HG21	1:N:55:GLN:HG2	1.66	0.75
1:I:93:LEU:HD12	1:I:105:TYR:HA	1.67	0.75
1:P:191:THR:HG21	1:P:286:ARG:NH2	2.00	0.75
1:J:175:ARG:HH11	1:J:175:ARG:HG3	1.50	0.75
1:N:82:LEU:HD13	1:N:90:GLY:HA3	1.69	0.75
1:C:137:ASN:HD21	1:C:140:SER:HB2	1.52	0.74
1:E:93:LEU:HD13	1:E:266:VAL:HG21	1.67	0.74
1:L:121:ASP:H	1:L:156:ASN:HD21	1.32	0.74
1:K:241:HIS:HB2	1:K:269:MET:HB2	1.68	0.74
1:P:154:PRO:HG2	1:P:185:GLU:HA	1.70	0.74
1:B:45:THR:HG22	1:B:46:ASN:OD1	1.88	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:127:PHE:HB3	1:D:170:VAL:CG1	2.18	0.74
1:P:135:LEU:HD23	1:P:136:THR:N	2.03	0.74
1:K:79:TYR:HA	1:K:91:ALA:HB2	1.69	0.73
1:D:119:PRO:HB2	1:D:122:ILE:HD12	1.68	0.73
1:L:190:SER:HB3	1:L:192:ASP:OD1	1.88	0.73
1:A:133:VAL:HG23	1:A:162:ASP:O	1.88	0.73
1:K:211:PRO:HB2	1:K:216:TYR:HE2	1.52	0.73
1:L:224:ASP:OD2	1:L:286:ARG:HD3	1.89	0.73
1:J:241:HIS:ND1	1:J:289:LEU:HD11	2.04	0.73
1:K:222:THR:HG23	1:K:286:ARG:HD2	1.69	0.73
1:L:93:LEU:HD13	1:L:266:VAL:HG21	1.71	0.73
1:C:197:LEU:HD12	1:C:208:LYS:HG3	1.71	0.73
1:P:85:TRP:CE3	1:P:88:THR:HG21	2.23	0.73
1:O:296:ASN:ND2	1:O:298:LEU:HB2	2.04	0.72
1:D:296:ASN:HD22	1:D:298:LEU:N	1.87	0.72
1:I:243:LEU:HD13	1:I:287:TYR:HB2	1.70	0.72
1:P:151:ALA:HA	1:P:187:ILE:O	1.89	0.72
1:J:93:LEU:HD13	1:J:266:VAL:HG21	1.71	0.72
1:O:190:SER:HB2	1:O:193:LYS:HG2	1.72	0.72
1:H:82:LEU:HG	1:H:85:TRP:CD1	2.25	0.72
1:L:153:LEU:HD22	1:L:159:HIS:CG	2.25	0.72
1:C:40:ILE:N	1:C:40:ILE:HD12	2.04	0.72
1:M:126:ILE:HG22	1:M:171:VAL:HB	1.71	0.72
1:I:109:MET:O	1:I:166:SER:HA	1.88	0.71
1:K:194:GLN:NE2	1:K:194:GLN:HA	2.05	0.71
1:F:296:ASN:HD22	1:F:298:LEU:HB2	1.54	0.71
1:K:66:LYS:HD2	1:K:69:HIS:CE1	2.25	0.71
1:C:40:ILE:HD13	1:C:147:VAL:HG11	1.72	0.71
1:I:93:LEU:HD22	1:I:266:VAL:HG21	1.71	0.71
1:G:121:ASP:H	1:G:156:ASN:HD21	1.37	0.71
1:P:87:ASN:ND2	1:P:110:LYS:HD2	2.00	0.71
1:E:61:THR:HG22	1:P:253:ARG:HH12	1.56	0.71
1:K:83:PRO:O	1:K:85:TRP:HD1	1.74	0.70
1:E:153:LEU:HD13	1:E:159:HIS:NE2	2.07	0.70
1:H:150:TYR:CE2	1:H:209:LEU:HB3	2.24	0.70
1:E:111:GLU:HA	1:E:165:GLU:HA	1.72	0.70
1:F:296:ASN:ND2	1:F:298:LEU:HB2	2.05	0.70
1:L:147:VAL:O	1:L:148:ASP:HB2	1.92	0.70
1:A:296:ASN:HD22	1:A:298:LEU:H	1.39	0.70
1:K:193:LYS:CE	1:K:193:LYS:HA	2.20	0.70
1:P:101:HIS:H	1:P:240:GLN:HE22	1.39	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:247:GLU:HG3	1:H:286:ARG:HB3	1.74	0.70
1:K:170:VAL:O	1:K:170:VAL:HG13	1.91	0.70
1:H:202:GLU:OE2	1:H:233:VAL:HG12	1.91	0.70
1:K:227:PRO:HG3	1:K:283:THR:O	1.92	0.70
1:D:59:GLY:O	1:K:253:ARG:NH1	2.25	0.69
1:D:153:LEU:HD13	1:D:159:HIS:CD2	2.27	0.69
1:P:111:GLU:H	1:P:111:GLU:CD	1.96	0.69
1:J:169:LEU:HD23	1:J:169:LEU:H	1.55	0.69
1:J:176:TYR:HE2	1:J:178:TYR:HA	1.57	0.69
1:K:86:THR:OG1	1:K:114:SER:N	2.26	0.69
1:M:110:LYS:HA	1:M:110:LYS:HE2	1.75	0.69
1:A:128:VAL:HG12	1:A:147:VAL:HA	1.74	0.69
1:H:184:THR:HB	1:H:216:TYR:CE1	2.27	0.69
1:J:113:SER:OG	1:J:163:CYS:HB3	1.93	0.69
1:K:109:MET:HB2	1:K:167:ALA:HB3	1.74	0.69
1:K:72:ILE:HD12	1:K:72:ILE:N	2.07	0.69
1:B:101:HIS:N	1:B:240:GLN:HE22	1.91	0.69
1:G:164:VAL:HG23	1:G:165:GLU:N	2.05	0.69
1:D:93:LEU:HD13	1:D:266:VAL:HG21	1.75	0.69
1:G:122:ILE:HD13	1:G:175:ARG:HA	1.74	0.69
1:J:124:ARG:O	1:J:153:LEU:HG	1.92	0.69
1:E:39:PRO:HB2	1:E:42:TRP:HB2	1.74	0.69
1:F:101:HIS:H	1:F:240:GLN:HE22	1.41	0.69
1:G:175:ARG:HG3	1:G:175:ARG:HH11	1.57	0.69
1:H:136:THR:HG22	1:H:137:ASN:H	1.57	0.68
1:N:137:ASN:CB	1:N:140:SER:HB3	2.22	0.68
1:C:70:ALA:HB3	1:C:268:TRP:HB3	1.75	0.68
1:O:165:GLU:HG3	1:O:166:SER:H	1.57	0.68
1:K:243:LEU:HD13	1:K:287:TYR:HB2	1.74	0.68
1:J:224:ASP:OD1	1:J:286:ARG:HD3	1.93	0.68
1:K:145:LEU:HD13	1:K:149:SER:CB	2.23	0.68
1:D:154:PRO:HG2	1:D:185:GLU:HA	1.76	0.68
1:A:207:ARG:HB2	1:A:222:THR:HG22	1.76	0.68
1:D:121:ASP:H	1:D:156:ASN:HD21	1.41	0.68
1:J:87:ASN:HD21	1:J:110:LYS:HB2	1.59	0.67
1:O:70:ALA:HB3	1:O:268:TRP:HB3	1.76	0.67
1:D:64:VAL:HG11	1:D:66:LYS:HE3	1.75	0.67
1:K:190:SER:N	1:K:193:LYS:HB2	2.07	0.67
1:K:190:SER:O	1:K:192:ASP:N	2.28	0.67
1:K:103:VAL:CG2	1:K:173:GLU:HB2	2.25	0.67
1:I:93:LEU:HD11	1:I:106:LEU:HG	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:298:LEU:HD13	1:K:122:ILE:HD12	1.76	0.67
1:K:130:GLU:HA	1:K:147:VAL:HG22	1.77	0.67
1:B:127:PHE:HB3	1:B:170:VAL:HG13	1.76	0.67
1:H:132:ALA:HB1	1:H:144:LYS:HE3	1.75	0.67
1:D:101:HIS:H	1:D:240:GLN:HE22	1.41	0.67
1:K:194:GLN:NE2	1:K:195:PRO:HD2	2.10	0.67
1:K:114:SER:HA	1:K:161:LEU:O	1.96	0.66
1:L:140:SER:O	1:L:141:SER:HB3	1.94	0.66
1:M:237:HIS:CE1	1:M:239:ASN:HB2	2.30	0.66
1:A:82:LEU:HD13	1:A:90:GLY:HA3	1.76	0.66
1:F:93:LEU:HD13	1:F:266:VAL:HG21	1.76	0.66
1:J:130:GLU:HA	1:J:147:VAL:HG22	1.76	0.66
1:G:40:ILE:N	1:G:40:ILE:HD12	2.09	0.66
1:N:241:HIS:HB2	1:N:269:MET:HB2	1.78	0.66
1:C:207:ARG:HB2	1:C:222:THR:CG2	2.25	0.66
1:G:224:ASP:OD2	1:G:286:ARG:HB2	1.96	0.66
1:K:112:MET:N	1:K:164:VAL:O	2.25	0.66
1:L:196:LEU:HD11	1:L:207:ARG:HH21	1.60	0.66
1:F:241:HIS:HB2	1:F:269:MET:HB2	1.78	0.66
1:H:93:LEU:HD13	1:H:266:VAL:HG21	1.77	0.66
1:G:127:PHE:HB3	1:G:170:VAL:HG13	1.78	0.66
1:D:82:LEU:CD1	1:D:90:GLY:HA3	2.20	0.65
1:O:72:ILE:H	1:O:72:ILE:HD12	1.61	0.65
1:A:296:ASN:ND2	1:A:298:LEU:HB2	2.11	0.65
1:G:62:ARG:HB2	1:G:73:THR:HG21	1.78	0.65
1:N:70:ALA:HB3	1:N:268:TRP:HB3	1.78	0.65
1:P:64:VAL:HG11	1:P:66:LYS:HZ2	1.58	0.65
1:G:137:ASN:C	1:G:137:ASN:ND2	2.46	0.65
1:M:133:VAL:HG22	1:M:134:THR:H	1.62	0.65
1:P:241:HIS:HB2	1:P:269:MET:HB2	1.78	0.65
1:L:127:PHE:HB3	1:L:170:VAL:HG13	1.79	0.65
1:L:220:ILE:HD13	1:L:290:TYR:HA	1.79	0.65
1:L:298:LEU:HD23	1:P:103:VAL:HG13	1.79	0.65
1:C:136:THR:HG22	1:C:142:SER:HB2	1.78	0.65
1:G:236:VAL:HG23	1:I:76:SER:HB3	1.79	0.65
1:K:164:VAL:HG23	1:K:165:GLU:N	2.12	0.65
1:C:202:GLU:OE2	1:C:233:VAL:HG12	1.96	0.64
1:D:70:ALA:HB3	1:D:268:TRP:HB3	1.79	0.64
1:B:241:HIS:HB2	1:B:269:MET:HB2	1.78	0.64
1:H:296:ASN:ND2	1:H:298:LEU:HB3	2.12	0.64
1:H:40:ILE:H	1:H:40:ILE:HD12	1.61	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:185:GLU:HG3	1:I:216:TYR:OH	1.97	0.64
1:B:101:HIS:H	1:B:240:GLN:NE2	1.91	0.64
1:G:40:ILE:HB	1:G:147:VAL:HG11	1.79	0.64
1:P:150:TYR:CE2	1:P:209:LEU:HB3	2.32	0.64
1:E:152:TYR:HB3	1:E:187:ILE:HB	1.78	0.64
1:I:72:ILE:N	1:I:72:ILE:HD12	2.13	0.64
1:L:234:LYS:N	1:L:234:LYS:HD2	2.11	0.64
1:C:111:GLU:CD	1:C:111:GLU:H	2.00	0.64
1:A:94:ILE:CD1	1:A:268:TRP:HB2	2.27	0.64
1:H:82:LEU:HD12	1:H:83:PRO:CD	2.27	0.64
1:K:111:GLU:HA	1:K:164:VAL:O	1.97	0.64
1:O:64:VAL:CG1	1:O:66:LYS:HE3	2.28	0.64
1:B:153:LEU:HD13	1:B:159:HIS:NE2	2.13	0.64
1:C:224:ASP:OD2	1:C:286:ARG:HD3	1.98	0.64
1:J:64:VAL:HG11	1:J:66:LYS:NZ	2.13	0.64
1:C:109:MET:O	1:C:166:SER:HA	1.98	0.64
1:I:120:GLN:HG3	1:I:156:ASN:HD21	1.62	0.64
1:K:222:THR:CG2	1:K:286:ARG:HD2	2.27	0.64
1:N:128:VAL:HA	1:N:169:LEU:HD23	1.80	0.64
1:E:243:LEU:HD12	1:E:244:LEU:N	2.13	0.64
1:P:121:ASP:H	1:P:156:ASN:HD21	1.44	0.64
1:F:127:PHE:HB3	1:F:170:VAL:CG1	2.26	0.64
1:O:137:ASN:ND2	1:O:140:SER:CB	2.61	0.63
1:P:164:VAL:HG23	1:P:165:GLU:H	1.63	0.63
1:D:196:LEU:HD11	1:D:207:ARG:CZ	2.28	0.63
1:K:252:TYR:CD1	1:K:277:TYR:HD1	2.16	0.63
1:P:168:THR:O	1:P:169:LEU:HD23	1.98	0.63
1:F:82:LEU:CD1	1:F:90:GLY:HA3	2.29	0.63
1:J:164:VAL:HG23	1:J:165:GLU:HG3	1.79	0.63
1:E:164:VAL:HG13	1:E:165:GLU:HG2	1.80	0.63
1:N:206:LEU:HD12	1:N:207:ARG:H	1.63	0.63
1:P:154:PRO:HG2	1:P:185:GLU:CA	2.29	0.63
1:B:87:ASN:ND2	1:B:110:LYS:HB2	2.13	0.63
1:E:296:ASN:HD22	1:E:298:LEU:HB2	1.63	0.63
1:H:245:LEU:HD12	1:H:287:TYR:HB3	1.80	0.63
1:A:207:ARG:HB2	1:A:222:THR:CG2	2.29	0.63
1:F:152:TYR:HB3	1:F:187:ILE:HB	1.81	0.63
1:H:103:VAL:HG13	1:N:298:LEU:HG	1.80	0.63
1:I:137:ASN:HB3	4:I:409:HOH:O	1.97	0.63
1:I:243:LEU:CD1	1:I:287:TYR:HB2	2.27	0.63
1:J:120:GLN:HG2	1:J:121:ASP:OD1	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:85:TRP:CE3	1:K:88:THR:HG21	2.33	0.63
1:O:207:ARG:HB2	1:O:222:THR:OG1	1.98	0.63
1:D:110:LYS:NZ	1:D:110:LYS:HB2	2.14	0.63
1:G:270:ALA:O	1:G:273:VAL:HG12	1.98	0.63
1:M:128:VAL:HG22	1:M:169:LEU:HD11	1.80	0.63
1:H:197:LEU:N	1:H:197:LEU:HD12	2.14	0.63
1:H:276:TRP:CH2	1:H:278:ALA:HB2	2.34	0.63
1:M:133:VAL:HG22	1:M:134:THR:N	2.13	0.63
1:A:239:ASN:H	1:A:239:ASN:ND2	1.96	0.62
1:B:137:ASN:HB2	1:B:140:SER:HA	1.81	0.62
1:D:276:TRP:CH2	1:D:278:ALA:HB2	2.34	0.62
1:D:40:ILE:H	1:D:40:ILE:CD1	1.99	0.62
1:B:296:ASN:HD22	1:B:298:LEU:H	1.45	0.62
1:I:137:ASN:N	1:I:137:ASN:HD22	1.96	0.62
1:P:196:LEU:HD21	1:P:207:ARG:NH2	2.07	0.62
1:D:207:ARG:HB2	1:D:222:THR:CG2	2.29	0.62
1:H:186:LEU:HD11	1:H:188:VAL:HG23	1.81	0.62
1:A:127:PHE:HB3	1:A:170:VAL:HG13	1.80	0.62
1:D:207:ARG:HB2	1:D:222:THR:HG22	1.81	0.62
1:J:150:TYR:CZ	1:J:209:LEU:HB3	2.35	0.62
1:O:121:ASP:H	1:O:156:ASN:HD21	1.46	0.62
1:F:222:THR:HG23	1:F:286:ARG:HD2	1.80	0.62
1:K:231:LEU:HA	4:K:425:HOH:O	1.98	0.62
1:L:48:THR:HB	1:L:262:GLN:HE22	1.64	0.62
1:N:232:ASN:O	1:N:234:LYS:HE2	2.00	0.62
1:E:241:HIS:HB3	1:E:289:LEU:HD11	1.79	0.62
1:F:126:ILE:HG22	1:F:171:VAL:HB	1.82	0.62
1:F:83:PRO:O	1:F:84:ASP:HB2	1.99	0.62
1:A:40:ILE:H	1:A:40:ILE:CD1	2.06	0.62
1:B:140:SER:O	1:B:141:SER:HB2	2.00	0.62
1:G:115:SER:CB	1:G:161:LEU:HB2	2.30	0.62
1:H:243:LEU:HD13	1:H:287:TYR:HB2	1.80	0.62
1:J:82:LEU:CD1	1:J:90:GLY:HA3	2.28	0.62
1:L:226:GLN:HB2	1:L:229:GLU:OE1	2.00	0.62
1:N:206:LEU:HD12	1:N:207:ARG:N	2.14	0.62
1:G:40:ILE:H	1:G:40:ILE:CD1	2.13	0.62
1:J:206:LEU:HD12	1:J:207:ARG:N	2.14	0.62
1:F:85:TRP:CE3	1:F:115:SER:HA	2.35	0.62
1:O:131:GLY:HA3	1:O:166:SER:O	2.00	0.62
1:B:82:LEU:CD1	1:B:90:GLY:HA3	2.27	0.61
1:L:150:TYR:CE2	1:L:209:LEU:HB3	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:128:VAL:HA	1:M:169:LEU:CD1	2.30	0.61
1:G:140:SER:HB2	4:G:421:HOH:O	1.99	0.61
1:L:121:ASP:H	1:L:156:ASN:ND2	1.98	0.61
1:O:137:ASN:ND2	1:O:140:SER:HB3	2.15	0.61
1:D:82:LEU:HD13	1:D:90:GLY:CA	2.22	0.61
1:K:122:ILE:HD13	1:K:175:ARG:HA	1.82	0.61
1:G:150:TYR:CZ	1:G:209:LEU:HB3	2.36	0.61
1:I:142:SER:O	1:I:143:LYS:HD2	2.01	0.61
1:M:150:TYR:CZ	1:M:209:LEU:HB3	2.36	0.61
1:P:130:GLU:CA	1:P:147:VAL:HG22	2.30	0.61
1:F:87:ASN:ND2	1:F:110:LYS:HB2	2.15	0.61
1:H:186:LEU:HD11	1:H:188:VAL:CG2	2.30	0.61
1:E:123:GLU:HG2	1:E:174:ARG:O	1.99	0.61
1:C:87:ASN:ND2	1:C:110:LYS:HB2	2.14	0.61
1:P:169:LEU:O	1:P:171:VAL:HG12	2.00	0.61
1:P:296:ASN:HD22	1:P:298:LEU:N	1.97	0.61
1:G:121:ASP:H	1:G:156:ASN:ND2	1.99	0.61
1:H:133:VAL:HG23	1:H:162:ASP:C	2.21	0.61
1:J:273:VAL:O	1:J:273:VAL:HG13	2.00	0.61
1:O:147:VAL:O	1:O:148:ASP:HB2	1.99	0.61
1:C:101:HIS:H	1:C:240:GLN:HE22	1.47	0.61
1:D:111:GLU:HA	1:D:164:VAL:O	2.00	0.61
1:D:121:ASP:H	1:D:156:ASN:ND2	1.99	0.61
1:F:82:LEU:HD13	1:F:90:GLY:HA3	1.83	0.61
1:G:243:LEU:HD23	1:G:269:MET:CE	2.31	0.61
1:A:127:PHE:HB3	1:A:170:VAL:CG1	2.31	0.60
1:C:40:ILE:HD12	1:C:40:ILE:H	1.65	0.60
1:E:199:THR:HG23	1:E:200:PRO:HD2	1.81	0.60
1:M:150:TYR:CE2	1:M:209:LEU:HB3	2.36	0.60
1:A:153:LEU:HD13	1:A:159:HIS:NE2	2.15	0.60
1:F:243:LEU:HD12	1:F:243:LEU:C	2.22	0.60
1:K:105:TYR:CE1	1:K:171:VAL:HG22	2.37	0.60
1:K:249:GLN:HG2	1:K:280:LEU:O	2.01	0.60
1:M:64:VAL:HG12	1:M:71:LEU:HB3	1.82	0.60
1:E:296:ASN:HD21	1:E:298:LEU:HD12	1.67	0.60
1:O:205:GLU:HB2	1:O:224:ASP:HB2	1.84	0.60
1:F:144:LYS:O	1:F:145:LEU:HD23	2.01	0.60
1:B:137:ASN:OD1	1:B:140:SER:HA	2.02	0.60
1:B:150:TYR:CE2	1:B:209:LEU:HB3	2.37	0.60
1:G:127:PHE:HB3	1:G:170:VAL:CG1	2.31	0.60
1:J:101:HIS:H	1:J:240:GLN:HE22	1.49	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:268:TRP:CZ2	1:B:270:ALA:HB2	2.37	0.60
1:F:184:THR:HB	1:F:216:TYR:CE1	2.37	0.60
1:E:243:LEU:HD13	1:E:287:TYR:HB2	1.84	0.60
1:I:101:HIS:H	1:I:240:GLN:HE22	1.48	0.60
1:A:245:LEU:HA	1:A:287:TYR:HB3	1.84	0.59
1:D:84:ASP:O	1:D:116:GLY:HA3	2.01	0.59
1:H:62:ARG:HB2	1:H:73:THR:HG21	1.84	0.59
1:P:39:PRO:HB2	1:P:42:TRP:HB2	1.83	0.59
1:C:190:SER:HB3	1:C:192:ASP:OD1	2.01	0.59
1:M:237:HIS:ND1	1:M:239:ASN:HB2	2.17	0.59
1:B:59:GLY:O	1:I:253:ARG:NH1	2.35	0.59
1:E:208:LYS:HZ2	1:E:212:MET:HE1	1.67	0.59
1:I:109:MET:HB3	1:I:113:SER:OG	2.02	0.59
1:J:136:THR:O	1:J:137:ASN:HB3	2.02	0.59
1:L:241:HIS:CG	1:L:289:LEU:HD11	2.38	0.59
1:M:153:LEU:HD13	1:M:159:HIS:CD2	2.37	0.59
1:M:64:VAL:CG2	1:M:66:LYS:HE3	2.32	0.59
1:O:153:LEU:HD13	1:O:159:HIS:CE1	2.38	0.59
1:N:155:PRO:O	1:N:156:ASN:HB2	2.02	0.59
1:E:128:VAL:HG22	1:E:169:LEU:CD2	2.31	0.59
1:G:130:GLU:HA	1:G:147:VAL:HG22	1.84	0.59
1:G:243:LEU:HD12	1:G:243:LEU:C	2.22	0.59
1:F:52:SER:O	1:F:55:GLN:HG2	2.02	0.59
1:G:197:LEU:HD22	1:G:208:LYS:HE3	1.84	0.59
1:H:243:LEU:C	1:H:243:LEU:HD12	2.23	0.59
1:K:153:LEU:HD22	1:K:159:HIS:CD2	2.38	0.59
1:B:47:PRO:HA	4:B:409:HOH:O	2.03	0.59
1:J:143:LYS:N	1:J:143:LYS:HD2	2.13	0.59
1:M:101:HIS:H	1:M:240:GLN:HE22	1.49	0.59
1:O:73:THR:HG22	1:O:265:ASP:OD1	2.02	0.59
1:P:113:SER:OG	1:P:163:CYS:HB3	2.03	0.59
1:D:233:VAL:HG13	1:D:235:GLU:HG3	1.83	0.59
1:E:82:LEU:CD1	1:E:90:GLY:HA3	2.30	0.59
1:M:49:LEU:HD11	1:M:54:LEU:HD21	1.84	0.59
1:G:184:THR:HB	1:G:216:TYR:CE1	2.37	0.58
1:M:222:THR:HG22	4:M:417:HOH:O	2.02	0.58
1:K:93:LEU:HD13	1:K:266:VAL:HG21	1.86	0.58
1:P:130:GLU:HA	1:P:147:VAL:CG2	2.32	0.58
1:P:243:LEU:HD12	1:P:243:LEU:C	2.24	0.58
1:O:202:GLU:HG3	1:O:204:PHE:HE2	1.67	0.58
1:H:120:GLN:O	1:H:121:ASP:HB2	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:137:ASN:HD22	1:M:137:ASN:C	2.04	0.58
1:N:234:LYS:HD3	1:N:234:LYS:N	2.18	0.58
1:O:202:GLU:HG3	1:O:204:PHE:CE2	2.39	0.58
1:P:119:PRO:HD2	1:P:122:ILE:HG13	1.85	0.58
1:B:137:ASN:HB2	1:B:141:SER:H	1.66	0.58
1:B:197:LEU:HB2	1:B:206:LEU:HD23	1.84	0.58
1:E:72:ILE:HD12	1:E:72:ILE:N	2.19	0.58
1:H:59:GLY:O	1:N:253:ARG:NH1	2.35	0.58
1:M:129:VAL:HG22	1:M:168:THR:O	2.04	0.58
1:N:40:ILE:CD1	1:N:40:ILE:H	2.06	0.58
1:C:40:ILE:CD1	1:C:40:ILE:H	2.17	0.58
1:D:241:HIS:HB3	1:D:289:LEU:HD11	1.86	0.58
1:P:134:THR:HG23	1:P:143:LYS:O	2.03	0.58
1:P:109:MET:SD	1:P:169:LEU:HD11	2.43	0.58
1:B:153:LEU:HD13	1:B:159:HIS:CE1	2.38	0.58
1:H:298:LEU:OXT	1:H:298:LEU:HD23	2.04	0.58
1:D:296:ASN:HD21	1:D:298:LEU:HB2	1.69	0.57
1:G:125:LEU:HD22	1:G:151:ALA:O	2.04	0.57
1:N:243:LEU:HG	1:N:267:ILE:HB	1.86	0.57
1:A:87:ASN:O	1:A:113:SER:HB2	2.04	0.57
1:D:122:ILE:HD13	1:K:298:LEU:CD1	2.20	0.57
1:A:121:ASP:H	1:A:156:ASN:HD21	1.51	0.57
1:A:243:LEU:HD23	1:A:269:MET:CE	2.33	0.57
1:D:151:ALA:HA	1:D:187:ILE:O	2.03	0.57
1:G:201:GLY:O	1:G:202:GLU:OE1	2.22	0.57
1:L:196:LEU:HD11	1:L:207:ARG:NH2	2.18	0.57
1:B:204:PHE:HE1	1:B:206:LEU:HB2	1.69	0.57
1:G:111:GLU:HA	1:G:164:VAL:O	2.04	0.57
1:K:190:SER:H	1:K:193:LYS:CB	2.17	0.57
1:M:208:LYS:HE2	1:M:221:HIS:NE2	2.20	0.57
1:M:47:PRO:HA	4:M:415:HOH:O	2.03	0.57
1:H:298:LEU:HD23	1:H:298:LEU:C	2.25	0.57
1:J:137:ASN:HD21	1:J:140:SER:N	2.03	0.57
1:K:150:TYR:CE1	1:K:209:LEU:HD22	2.39	0.57
1:P:84:ASP:HB3	4:P:424:HOH:O	2.05	0.57
1:A:268:TRP:CZ2	1:A:270:ALA:HB2	2.40	0.57
1:D:137:ASN:HD22	1:D:137:ASN:N	2.01	0.57
1:L:237:HIS:HB2	1:L:239:ASN:HD22	1.68	0.57
1:O:247:GLU:CG	1:O:286:ARG:HB3	2.33	0.57
1:P:136:THR:O	1:P:137:ASN:HB3	2.05	0.57
1:E:136:THR:HG23	1:E:160:SER:HB3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:164:VAL:CG2	1:G:165:GLU:H	2.11	0.57
1:I:126:ILE:HG22	1:I:171:VAL:HB	1.87	0.57
1:M:79:TYR:HA	1:M:90:GLY:O	2.04	0.57
1:P:243:LEU:HG	1:P:267:ILE:HB	1.86	0.57
1:M:82:LEU:HG	1:M:85:TRP:CD1	2.40	0.57
1:N:152:TYR:HB3	1:N:187:ILE:HB	1.85	0.57
1:N:243:LEU:C	1:N:243:LEU:HD12	2.24	0.57
1:O:153:LEU:HD13	1:O:159:HIS:NE2	2.19	0.57
1:P:118:PRO:HD3	1:P:124:ARG:NH2	2.19	0.57
1:G:202:GLU:HB3	1:G:204:PHE:CE2	2.40	0.57
1:J:243:LEU:HD12	1:J:243:LEU:C	2.25	0.57
1:J:118:PRO:HB2	1:J:122:ILE:HB	1.86	0.57
1:J:234:LYS:HG2	1:K:61:THR:HB	1.87	0.57
1:O:72:ILE:N	1:O:72:ILE:HD12	2.19	0.57
1:E:125:LEU:C	1:E:125:LEU:HD13	2.25	0.56
1:L:243:LEU:C	1:L:243:LEU:HD12	2.25	0.56
1:M:137:ASN:ND2	1:M:137:ASN:C	2.59	0.56
1:F:164:VAL:HG23	1:F:165:GLU:H	1.70	0.56
1:J:134:THR:HG23	1:J:144:LYS:HA	1.86	0.56
1:F:153:LEU:HD13	1:F:159:HIS:NE2	2.20	0.56
1:F:164:VAL:HG23	1:F:165:GLU:N	2.20	0.56
1:J:241:HIS:CG	1:J:289:LEU:HD11	2.41	0.56
1:J:286:ARG:HG3	1:J:287:TYR:N	2.19	0.56
1:K:82:LEU:HD12	1:K:83:PRO:HD2	1.88	0.56
1:L:234:LYS:HD2	1:L:234:LYS:H	1.68	0.56
1:L:249:GLN:HE21	1:N:56:ASP:CG	2.08	0.56
1:M:202:GLU:OE2	1:M:233:VAL:HG12	2.05	0.56
1:A:101:HIS:H	1:A:240:GLN:HE22	1.52	0.56
1:A:241:HIS:CG	1:A:289:LEU:HD11	2.40	0.56
1:D:136:THR:HG22	1:D:142:SER:HB2	1.86	0.56
1:D:196:LEU:CD1	1:D:207:ARG:NH2	2.67	0.56
1:K:144:LYS:HG2	1:K:144:LYS:O	2.05	0.56
1:D:284:ARG:NH2	1:D:286:ARG:HH12	2.04	0.56
1:F:153:LEU:HD22	1:F:159:HIS:CG	2.40	0.56
1:J:94:ILE:O	1:J:103:VAL:HA	2.05	0.56
1:G:202:GLU:OE1	1:G:232:ASN:HB2	2.04	0.56
1:J:209:LEU:O	1:J:210:LEU:HD23	2.04	0.56
1:M:222:THR:HG23	1:M:286:ARG:HD2	1.88	0.56
1:M:83:PRO:O	1:M:84:ASP:HB2	2.05	0.56
1:O:164:VAL:HG23	1:O:165:GLU:N	2.19	0.56
1:I:280:LEU:HD21	1:J:280:LEU:HD21	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:113:SER:OG	1:B:163:CYS:HB3	2.06	0.56
1:K:105:TYR:CE1	1:K:171:VAL:HG13	2.41	0.56
1:K:247:GLU:O	1:K:285:SER:HA	2.05	0.56
1:L:126:ILE:HG22	1:L:171:VAL:HB	1.87	0.56
1:E:251:ILE:HD13	1:E:260:PRO:HA	1.88	0.56
1:G:157:PHE:CD2	1:G:157:PHE:C	2.79	0.56
1:K:120:GLN:HG3	1:K:156:ASN:ND2	2.21	0.56
1:L:245:LEU:HD12	1:L:287:TYR:HB3	1.88	0.56
1:A:83:PRO:O	1:A:84:ASP:HB2	2.06	0.56
1:E:126:ILE:HG22	1:E:171:VAL:HB	1.88	0.56
1:L:82:LEU:HD21	1:L:105:TYR:CE1	2.41	0.56
1:O:93:LEU:HD13	1:O:266:VAL:HG21	1.87	0.56
1:P:243:LEU:HB3	1:P:289:LEU:HD12	1.88	0.56
1:B:276:TRP:CH2	1:B:278:ALA:HB2	2.41	0.56
1:E:69:HIS:HA	1:E:268:TRP:O	2.04	0.56
1:H:133:VAL:HG23	1:H:162:ASP:O	2.06	0.56
1:I:202:GLU:OE1	1:I:231:LEU:HD23	2.06	0.56
1:K:140:SER:O	1:K:141:SER:HB2	2.05	0.56
1:F:214:VAL:HG13	1:F:215:ALA:N	2.20	0.55
1:G:96:PRO:HD3	1:G:103:VAL:HG12	1.88	0.55
1:N:224:ASP:OD2	1:N:286:ARG:NE	2.39	0.55
1:A:296:ASN:HD22	1:A:298:LEU:N	2.04	0.55
1:F:170:VAL:HG13	1:F:170:VAL:O	2.06	0.55
1:I:49:LEU:HD22	1:K:54:LEU:CD2	2.37	0.55
1:H:136:THR:HG22	1:H:137:ASN:N	2.19	0.55
1:K:153:LEU:HD22	1:K:159:HIS:CG	2.41	0.55
1:B:234:LYS:HE3	1:C:60:PHE:O	2.05	0.55
1:C:74:PRO:C	1:C:76:SER:H	2.10	0.55
1:E:153:LEU:HD13	1:E:159:HIS:CD2	2.42	0.55
1:F:150:TYR:CD1	1:F:209:LEU:HD13	2.42	0.55
1:G:137:ASN:HB2	4:G:426:HOH:O	2.07	0.55
1:H:207:ARG:HG3	1:H:207:ARG:HH11	1.70	0.55
1:F:126:ILE:HG12	1:F:161:LEU:HD11	1.88	0.55
1:I:137:ASN:H	1:I:137:ASN:HD22	1.55	0.55
1:L:150:TYR:CZ	1:L:209:LEU:HB3	2.41	0.55
1:D:296:ASN:ND2	1:D:298:LEU:HB2	2.21	0.55
1:G:150:TYR:CE2	1:G:209:LEU:HB3	2.42	0.55
1:H:153:LEU:HD22	1:H:159:HIS:CG	2.42	0.55
1:A:121:ASP:H	1:A:156:ASN:ND2	2.04	0.55
1:C:252:TYR:CD1	1:C:277:TYR:CD1	2.95	0.55
1:C:245:LEU:HD12	1:C:287:TYR:HB3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:164:VAL:HG23	1:K:165:GLU:H	1.71	0.55
1:P:121:ASP:H	1:P:156:ASN:ND2	2.02	0.55
1:G:191:THR:HG21	1:G:286:ARG:HH12	1.72	0.55
1:P:95:THR:O	1:P:98:THR:HG23	2.06	0.55
1:C:153:LEU:HD13	1:C:159:HIS:CG	2.42	0.55
1:H:243:LEU:HD12	1:H:244:LEU:N	2.22	0.55
1:J:296:ASN:HD21	1:J:298:LEU:HD12	1.72	0.55
1:K:243:LEU:HD12	1:K:243:LEU:C	2.27	0.55
1:A:153:LEU:HD13	1:A:159:HIS:CE1	2.42	0.55
1:G:286:ARG:HG3	1:G:286:ARG:O	2.06	0.55
1:J:64:VAL:HG11	1:J:66:LYS:HZ3	1.72	0.55
1:P:133:VAL:CG1	1:P:163:CYS:HB2	2.27	0.55
1:P:70:ALA:HB3	1:P:268:TRP:HB3	1.88	0.55
1:L:101:HIS:H	1:L:240:GLN:HE22	1.53	0.54
1:J:235:GLU:OE1	3:J:302:UGY:N	2.40	0.54
1:O:150:TYR:CZ	1:O:209:LEU:HB3	2.41	0.54
1:A:224:ASP:OD2	1:A:286:ARG:HB2	2.07	0.54
1:C:185:GLU:O	1:C:187:ILE:HG12	2.08	0.54
1:F:86:THR:O	1:F:113:SER:HB2	2.07	0.54
1:K:150:TYR:CE2	1:K:209:LEU:HB3	2.42	0.54
1:L:103:VAL:CG2	1:L:173:GLU:HB2	2.37	0.54
1:K:100:SER:HA	1:K:240:GLN:HE22	1.72	0.54
1:N:130:GLU:HA	1:N:147:VAL:HG22	1.89	0.54
1:F:125:LEU:C	1:F:125:LEU:HD13	2.28	0.54
1:F:93:LEU:HD13	1:F:266:VAL:HG11	1.88	0.54
1:M:276:TRP:CH2	1:M:278:ALA:HB2	2.43	0.54
1:P:87:ASN:C	1:P:87:ASN:ND2	2.61	0.54
1:B:127:PHE:HB3	1:B:170:VAL:CG1	2.37	0.54
1:K:206:LEU:HD12	1:K:207:ARG:N	2.22	0.54
1:C:130:GLU:O	1:C:167:ALA:HA	2.07	0.54
1:B:150:TYR:CE1	1:B:209:LEU:HD22	2.42	0.54
1:G:137:ASN:HB3	1:G:140:SER:OG	2.07	0.54
1:H:126:ILE:HG22	1:H:171:VAL:HB	1.89	0.54
1:H:296:ASN:HD21	1:H:298:LEU:HB3	1.70	0.54
1:L:113:SER:OG	1:L:163:CYS:HB3	2.07	0.54
1:O:150:TYR:CE2	1:O:209:LEU:HB3	2.43	0.54
1:E:125:LEU:HD13	1:E:126:ILE:N	2.22	0.54
1:K:140:SER:O	1:K:141:SER:CB	2.55	0.54
1:N:164:VAL:HG23	1:N:165:GLU:H	1.72	0.54
1:N:271:PRO:O	1:N:272:PHE:HB2	2.07	0.54
1:E:74:PRO:O	1:E:76:SER:N	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:113:SER:OG	1:H:163:CYS:HB3	2.08	0.53
1:H:79:TYR:CD1	1:H:91:ALA:HB2	2.43	0.53
1:I:204:PHE:HB3	1:I:225:PHE:CE1	2.43	0.53
1:N:243:LEU:HD13	1:N:287:TYR:HB2	1.90	0.53
1:F:136:THR:HG23	1:F:160:SER:O	2.09	0.53
1:F:70:ALA:HB3	1:F:268:TRP:HB3	1.90	0.53
1:G:226:GLN:O	1:G:229:GLU:HG3	2.08	0.53
1:A:61:THR:HB	1:D:234:LYS:HG2	1.90	0.53
1:C:276:TRP:CH2	1:C:278:ALA:HB2	2.43	0.53
1:D:54:LEU:HD23	1:G:49:LEU:HD22	1.89	0.53
1:K:213:SER:O	1:K:215:ALA:N	2.40	0.53
1:K:243:LEU:HD22	1:K:287:TYR:CD1	2.43	0.53
1:C:234:LYS:HE3	1:G:60:PHE:O	2.08	0.53
1:J:145:LEU:HD22	1:J:149:SER:OG	2.08	0.53
1:O:185:GLU:O	1:O:187:ILE:HG12	2.09	0.53
1:P:296:ASN:ND2	1:P:298:LEU:HB2	2.24	0.53
1:E:202:GLU:OE2	1:E:233:VAL:HG12	2.09	0.53
1:E:208:LYS:NZ	1:E:212:MET:CE	2.72	0.53
1:E:82:LEU:O	1:E:85:TRP:HB2	2.08	0.53
1:G:243:LEU:HD23	1:G:269:MET:HE2	1.90	0.53
1:I:241:HIS:HB2	1:I:269:MET:HB2	1.90	0.53
1:L:238:TYR:O	1:L:271:PRO:HB3	2.08	0.53
1:B:140:SER:O	1:B:141:SER:CB	2.57	0.53
1:E:63:SER:HA	1:E:71:LEU:O	2.09	0.53
1:C:243:LEU:HB2	1:C:288:LEU:O	2.09	0.53
1:D:127:PHE:HB3	1:D:170:VAL:HG13	1.90	0.53
1:D:68:ASP:OD2	1:D:273:VAL:HG23	2.09	0.53
1:F:243:LEU:HG	1:F:267:ILE:HB	1.91	0.53
1:G:246:LEU:HD11	1:G:288:LEU:HD13	1.90	0.53
1:N:152:TYR:HB2	1:N:210:LEU:HD21	1.91	0.53
1:P:116:GLY:HA2	4:P:424:HOH:O	2.09	0.53
1:P:191:THR:HG21	1:P:286:ARG:HH21	1.71	0.53
1:G:125:LEU:C	1:G:125:LEU:HD13	2.30	0.53
1:J:298:LEU:HD11	1:K:122:ILE:HG21	1.91	0.53
1:K:252:TYR:CD1	1:K:277:TYR:CD1	2.97	0.53
1:M:152:TYR:HB3	1:M:187:ILE:HB	1.91	0.53
1:O:243:LEU:C	1:O:243:LEU:HD12	2.28	0.53
1:P:127:PHE:HB3	1:P:170:VAL:CG1	2.39	0.53
1:A:82:LEU:CD1	1:A:90:GLY:HA3	2.38	0.53
1:E:243:LEU:HD23	1:E:269:MET:CE	2.39	0.53
1:G:237:HIS:ND1	1:G:239:ASN:HB2	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:241:HIS:HB3	1:G:289:LEU:HD11	1.89	0.53
1:J:169:LEU:CD2	1:J:169:LEU:N	2.67	0.53
1:K:211:PRO:HB2	1:K:216:TYR:CE2	2.37	0.53
1:N:87:ASN:ND2	1:N:111:GLU:O	2.39	0.53
1:C:82:LEU:O	1:C:85:TRP:HB2	2.09	0.52
1:E:61:THR:HG22	1:P:253:ARG:NH1	2.22	0.52
1:G:156:ASN:HA	4:G:413:HOH:O	2.10	0.52
1:K:103:VAL:HG22	1:K:173:GLU:HB2	1.91	0.52
1:K:128:VAL:HG22	1:K:169:LEU:HD21	1.89	0.52
1:P:64:VAL:HG11	1:P:66:LYS:HZ3	1.71	0.52
1:A:125:LEU:C	1:A:125:LEU:HD13	2.29	0.52
1:B:83:PRO:O	1:B:85:TRP:HD1	1.92	0.52
1:D:273:VAL:HG13	1:D:273:VAL:O	2.09	0.52
1:E:117:LEU:HD21	1:E:159:HIS:H	1.74	0.52
1:I:284:ARG:C	1:I:284:ARG:HD2	2.29	0.52
1:J:206:LEU:HD12	1:J:207:ARG:H	1.73	0.52
1:J:150:TYR:CE2	1:J:209:LEU:HB3	2.44	0.52
1:D:61:THR:HG22	1:K:253:ARG:NH1	2.24	0.52
1:E:114:SER:HA	1:E:161:LEU:O	2.09	0.52
1:E:208:LYS:HZ2	1:E:212:MET:CE	2.20	0.52
1:H:207:ARG:HG3	1:H:207:ARG:NH1	2.24	0.52
1:K:113:SER:OG	1:K:163:CYS:HB3	2.09	0.52
1:K:224:ASP:OD2	1:K:286:ARG:CD	2.50	0.52
1:O:103:VAL:HG22	1:O:173:GLU:HB2	1.90	0.52
1:O:134:THR:OG1	1:O:144:LYS:HG2	2.09	0.52
1:H:125:LEU:HD22	1:H:151:ALA:O	2.10	0.52
1:K:276:TRP:CH2	1:K:278:ALA:HB2	2.45	0.52
1:E:60:PHE:HZ	1:M:60:PHE:HZ	1.55	0.52
1:G:157:PHE:HD2	1:G:157:PHE:C	2.13	0.52
1:J:268:TRP:CZ2	1:J:270:ALA:HB2	2.44	0.52
1:L:125:LEU:HD23	1:L:152:TYR:HB2	1.91	0.52
1:O:170:VAL:HG13	1:O:170:VAL:O	2.10	0.52
1:D:241:HIS:HB2	1:D:269:MET:HB2	1.92	0.52
1:J:218:PHE:C	1:J:218:PHE:CD1	2.82	0.52
1:O:121:ASP:H	1:O:156:ASN:ND2	2.08	0.52
1:C:127:PHE:HB3	1:C:170:VAL:CG1	2.40	0.52
1:H:241:HIS:HB3	1:H:289:LEU:HD11	1.91	0.52
1:N:131:GLY:HA3	1:N:167:ALA:HA	1.91	0.52
1:O:243:LEU:HB2	1:O:288:LEU:O	2.10	0.52
1:P:136:THR:O	1:P:137:ASN:CB	2.57	0.52
1:B:79:TYR:HA	1:B:90:GLY:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:198:GLU:HG2	1:M:200:PRO:HD3	1.92	0.52
1:P:87:ASN:C	1:P:87:ASN:HD22	2.13	0.52
1:F:64:VAL:HG11	1:F:66:LYS:NZ	2.25	0.52
1:P:150:TYR:CZ	1:P:209:LEU:HB3	2.45	0.52
1:P:154:PRO:HB3	1:P:155:PRO:HD2	1.91	0.52
1:A:243:LEU:HG	1:A:267:ILE:HB	1.92	0.51
1:A:94:ILE:HD11	1:A:268:TRP:HB2	1.92	0.51
1:B:92:TYR:HA	1:B:105:TYR:HB3	1.92	0.51
1:C:152:TYR:HB3	1:C:187:ILE:HB	1.92	0.51
1:H:120:GLN:HG2	1:H:121:ASP:OD1	2.11	0.51
1:F:298:LEU:HD11	1:L:173:GLU:HB3	1.92	0.51
1:P:191:THR:HG22	1:P:207:ARG:HD2	1.91	0.51
1:A:243:LEU:HD21	1:A:252:TYR:CE1	2.45	0.51
1:E:241:HIS:HB2	1:E:269:MET:HB2	1.90	0.51
1:K:92:TYR:CE1	1:K:105:TYR:CD2	2.94	0.51
1:L:127:PHE:HB3	1:L:170:VAL:CG1	2.39	0.51
1:M:128:VAL:HA	1:M:169:LEU:HD12	1.92	0.51
1:M:243:LEU:C	1:M:243:LEU:HD12	2.31	0.51
1:J:294:ASN:O	1:J:295:ARG:HG2	2.10	0.51
1:J:72:ILE:HD12	1:J:72:ILE:N	2.25	0.51
1:K:105:TYR:HE1	1:K:171:VAL:HG13	1.75	0.51
1:C:225:PHE:HB2	1:C:285:SER:HB2	1.92	0.51
1:K:273:VAL:O	1:K:273:VAL:HG13	2.10	0.51
1:B:241:HIS:CE1	1:B:289:LEU:HD21	2.46	0.51
1:J:141:SER:O	1:J:142:SER:HB2	2.11	0.51
1:L:134:THR:HG23	1:L:143:LYS:O	2.10	0.51
1:M:94:ILE:O	1:M:103:VAL:HA	2.11	0.51
1:P:130:GLU:HA	1:P:147:VAL:HG13	1.93	0.51
1:P:82:LEU:CD1	1:P:90:GLY:HA3	2.40	0.51
1:D:72:ILE:N	1:D:72:ILE:HD12	2.26	0.51
1:G:191:THR:HG21	1:G:286:ARG:NH1	2.26	0.51
1:L:207:ARG:HB2	1:L:222:THR:HG22	1.90	0.51
1:O:109:MET:HB3	1:O:113:SER:OG	2.10	0.51
1:O:270:ALA:O	1:O:273:VAL:HG12	2.10	0.51
1:O:52:SER:O	1:O:55:GLN:HG2	2.10	0.51
1:A:87:ASN:O	1:A:87:ASN:CG	2.49	0.51
1:K:296:ASN:ND2	1:K:298:LEU:HD12	2.26	0.51
1:A:152:TYR:HB3	1:A:187:ILE:HB	1.92	0.51
1:E:121:ASP:H	1:E:156:ASN:HD21	1.59	0.51
1:E:164:VAL:HG13	1:E:165:GLU:CG	2.41	0.51
1:E:270:ALA:O	1:E:273:VAL:HG12	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:82:LEU:CD2	1:I:90:GLY:HA3	2.40	0.51
1:K:202:GLU:HA	1:K:202:GLU:OE1	2.10	0.51
1:M:96:PRO:HD3	1:M:103:VAL:HG12	1.92	0.51
1:G:137:ASN:HB3	1:G:140:SER:CB	2.40	0.51
1:H:224:ASP:OD2	1:H:286:ARG:NH1	2.43	0.51
1:J:109:MET:HB2	1:J:167:ALA:HB3	1.92	0.51
1:J:86:THR:O	1:J:87:ASN:C	2.49	0.51
1:M:140:SER:O	1:M:141:SER:CB	2.59	0.51
1:D:196:LEU:CD1	1:D:207:ARG:CZ	2.90	0.50
1:G:85:TRP:CE3	1:G:115:SER:HA	2.46	0.50
1:M:271:PRO:O	1:M:272:PHE:HB2	2.11	0.50
1:N:75:GLU:N	1:N:75:GLU:OE1	2.40	0.50
1:B:118:PRO:HB2	1:B:122:ILE:HB	1.92	0.50
1:F:186:LEU:O	1:F:187:ILE:HD13	2.11	0.50
1:G:236:VAL:CG2	1:I:76:SER:HB3	2.42	0.50
1:L:137:ASN:HD21	1:L:140:SER:N	2.10	0.50
1:O:153:LEU:HD13	1:O:159:HIS:CD2	2.46	0.50
1:E:164:VAL:HG13	1:E:165:GLU:N	2.26	0.50
1:E:243:LEU:C	1:E:243:LEU:HD12	2.30	0.50
1:F:192:ASP:HA	4:F:417:HOH:O	2.10	0.50
1:I:140:SER:O	1:I:141:SER:HB3	2.11	0.50
1:I:170:VAL:HG13	1:I:170:VAL:O	2.11	0.50
1:K:111:GLU:HA	1:K:165:GLU:O	2.11	0.50
1:M:109:MET:HB3	1:M:113:SER:OG	2.12	0.50
1:P:118:PRO:HB2	1:P:122:ILE:HB	1.93	0.50
1:L:237:HIS:HB2	1:L:239:ASN:ND2	2.26	0.50
1:O:113:SER:OG	1:O:163:CYS:HB3	2.10	0.50
1:D:63:SER:HA	1:D:71:LEU:O	2.11	0.50
1:I:129:VAL:O	1:I:129:VAL:HG12	2.11	0.50
1:L:103:VAL:HG22	1:L:173:GLU:HB2	1.94	0.50
1:L:140:SER:O	1:L:141:SER:CB	2.59	0.50
1:G:164:VAL:HG23	1:G:165:GLU:HG2	1.94	0.50
1:I:222:THR:HG23	1:I:286:ARG:HD2	1.94	0.50
1:M:137:ASN:HA	1:M:159:HIS:HA	1.93	0.50
1:M:253:ARG:NH1	1:O:61:THR:HG22	2.26	0.50
1:J:172:PHE:CE1	1:J:290:TYR:HB2	2.46	0.50
1:D:61:THR:HB	1:K:234:LYS:HG2	1.93	0.50
1:L:245:LEU:HD23	1:L:262:GLN:C	2.32	0.50
1:M:280:LEU:HD21	1:P:280:LEU:HD21	1.92	0.50
1:B:95:THR:O	1:B:97:ALA:N	2.45	0.50
1:D:127:PHE:HB3	1:D:170:VAL:HG12	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:155:PRO:O	1:F:156:ASN:HB2	2.12	0.50
1:I:152:TYR:HB3	1:I:187:ILE:HB	1.94	0.50
1:I:72:ILE:H	1:I:72:ILE:HD12	1.74	0.50
1:O:238:TYR:CE2	1:O:297:PRO:HB3	2.46	0.50
1:P:126:ILE:HD12	1:P:126:ILE:O	2.12	0.50
1:A:234:LYS:N	1:A:234:LYS:HD3	2.27	0.50
1:A:239:ASN:N	1:A:239:ASN:ND2	2.60	0.50
1:H:253:ARG:NH1	1:M:61:THR:HG22	2.26	0.50
1:J:179:LEU:HG	1:J:179:LEU:O	2.11	0.50
1:L:298:LEU:HD13	1:P:122:ILE:HD12	1.94	0.50
1:P:175:ARG:HD3	4:P:426:HOH:O	2.11	0.50
1:D:243:LEU:C	1:D:243:LEU:HD12	2.32	0.49
1:E:70:ALA:HB3	1:E:268:TRP:HB3	1.93	0.49
1:F:56:ASP:HB2	1:H:48:THR:HG21	1.92	0.49
1:N:68:ASP:OD2	1:N:273:VAL:HG23	2.11	0.49
1:O:247:GLU:OE2	1:O:284:ARG:NE	2.44	0.49
1:B:197:LEU:HB2	1:B:206:LEU:CD2	2.41	0.49
1:B:298:LEU:HD23	1:C:103:VAL:HG13	1.94	0.49
1:C:154:PRO:HG2	1:C:185:GLU:CA	2.38	0.49
1:G:134:THR:HG23	1:G:143:LYS:O	2.12	0.49
1:M:82:LEU:O	1:M:85:TRP:HB2	2.12	0.49
1:O:152:TYR:HB3	1:O:187:ILE:HB	1.95	0.49
1:D:237:HIS:ND1	1:D:239:ASN:HB2	2.28	0.49
1:E:296:ASN:ND2	1:E:298:LEU:HB2	2.27	0.49
1:F:199:THR:HB	1:F:202:GLU:HB2	1.92	0.49
1:F:245:LEU:HD23	1:F:262:GLN:C	2.32	0.49
1:J:143:LYS:HG3	1:J:188:VAL:HG11	1.94	0.49
1:J:219:ASN:O	1:J:220:ILE:HD13	2.11	0.49
1:O:152:TYR:HB2	1:O:210:LEU:HD21	1.95	0.49
1:J:153:LEU:HD23	1:J:153:LEU:N	2.27	0.49
1:K:125:LEU:HD13	1:K:126:ILE:N	2.27	0.49
1:F:93:LEU:CD1	1:F:266:VAL:HG21	2.42	0.49
1:M:93:LEU:HD12	1:M:104:MET:HE1	1.93	0.49
1:N:87:ASN:HD21	1:N:110:LYS:HB2	1.75	0.49
1:P:133:VAL:O	1:P:145:LEU:HB2	2.12	0.49
1:I:152:TYR:O	1:I:186:LEU:HD12	2.12	0.49
1:L:115:SER:HB3	1:L:161:LEU:HB2	1.94	0.49
1:L:276:TRP:CH2	1:O:251:ILE:HD11	2.48	0.49
1:P:158:HIS:ND1	1:P:159:HIS:N	2.61	0.49
1:B:220:ILE:HD13	1:B:290:TYR:HA	1.95	0.49
1:D:125:LEU:C	1:D:125:LEU:HD13	2.32	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:87:ASN:ND2	1:E:110:LYS:HB2	2.28	0.49
1:G:63:SER:HA	1:G:71:LEU:O	2.12	0.49
1:O:81:PRO:O	1:O:83:PRO:HD3	2.13	0.49
1:B:298:LEU:HD11	1:C:122:ILE:HG21	1.95	0.49
1:D:237:HIS:CE1	1:D:239:ASN:HB2	2.48	0.49
1:E:82:LEU:HD23	1:E:85:TRP:CE2	2.48	0.49
1:E:234:LYS:HG2	1:F:61:THR:HB	1.94	0.49
1:G:114:SER:HA	1:G:161:LEU:O	2.13	0.49
1:O:164:VAL:CG2	1:O:165:GLU:N	2.75	0.49
1:O:87:ASN:ND2	1:O:110:LYS:HB2	2.26	0.49
1:B:150:TYR:CZ	1:B:209:LEU:HB3	2.48	0.49
1:C:74:PRO:O	1:C:76:SER:N	2.45	0.49
1:F:185:GLU:O	1:F:187:ILE:HG12	2.12	0.49
1:H:111:GLU:HA	1:H:164:VAL:O	2.13	0.49
1:I:60:PHE:HZ	1:K:60:PHE:HZ	1.60	0.49
1:I:95:THR:O	1:I:98:THR:HG23	2.12	0.49
1:O:190:SER:HB2	1:O:193:LYS:CG	2.42	0.49
1:P:152:TYR:HB3	1:P:187:ILE:HB	1.95	0.49
1:C:186:LEU:O	1:C:187:ILE:HD13	2.12	0.49
1:C:241:HIS:HB2	1:C:269:MET:HE2	1.94	0.49
1:D:126:ILE:O	1:D:126:ILE:HD12	2.13	0.49
1:E:62:ARG:NH2	1:E:265:ASP:OD2	2.46	0.49
1:F:121:ASP:H	1:F:156:ASN:ND2	2.11	0.49
1:F:54:LEU:CD2	1:H:49:LEU:HD22	2.43	0.49
1:H:185:GLU:O	1:H:187:ILE:HG12	2.13	0.49
1:I:130:GLU:O	1:I:167:ALA:HA	2.13	0.49
1:I:199:THR:HG21	1:I:204:PHE:O	2.13	0.49
1:J:124:ARG:HD2	1:J:153:LEU:HD12	1.95	0.49
1:P:245:LEU:HD23	1:P:262:GLN:C	2.34	0.49
1:B:270:ALA:O	1:B:273:VAL:HG12	2.13	0.48
1:B:95:THR:C	1:B:97:ALA:H	2.15	0.48
1:D:110:LYS:HZ3	1:D:110:LYS:HB2	1.77	0.48
1:G:153:LEU:HD13	1:G:159:HIS:CD2	2.48	0.48
1:M:93:LEU:HD12	1:M:104:MET:CE	2.42	0.48
1:N:40:ILE:HB	1:N:147:VAL:HG11	1.95	0.48
1:P:111:GLU:N	1:P:111:GLU:CD	2.65	0.48
1:P:152:TYR:HE2	1:P:184:THR:HB	1.79	0.48
1:E:208:LYS:HZ3	1:E:212:MET:HE3	1.78	0.48
1:I:133:VAL:HG23	1:I:163:CYS:HB2	1.95	0.48
1:J:164:VAL:CG2	1:J:165:GLU:HG3	2.43	0.48
1:J:207:ARG:HB2	1:J:222:THR:HG22	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:207:ARG:HB2	1:J:222:THR:CG2	2.43	0.48
1:K:157:PHE:CZ	1:K:186:LEU:HD22	2.49	0.48
1:L:49:LEU:HD23	1:N:57:LEU:CD1	2.43	0.48
1:P:127:PHE:HB3	1:P:170:VAL:HG13	1.95	0.48
1:C:142:SER:O	1:C:143:LYS:HD3	2.13	0.48
1:F:133:VAL:HG21	1:F:161:LEU:HB3	1.95	0.48
1:B:54:LEU:HD23	1:J:49:LEU:HD22	1.94	0.48
1:K:190:SER:O	1:K:191:THR:C	2.51	0.48
1:K:269:MET:SD	1:K:275:GLN:OE1	2.71	0.48
1:L:125:LEU:HD13	1:L:125:LEU:C	2.33	0.48
1:L:192:ASP:N	1:L:192:ASP:OD1	2.47	0.48
1:M:232:ASN:O	1:M:234:LYS:HD3	2.14	0.48
1:N:128:VAL:HG22	1:N:169:LEU:HD21	1.95	0.48
1:O:127:PHE:HB3	1:O:170:VAL:CG1	2.43	0.48
1:A:63:SER:HA	1:A:71:LEU:O	2.13	0.48
1:B:130:GLU:HB3	1:B:168:THR:HB	1.95	0.48
1:C:85:TRP:CE3	1:C:88:THR:HG21	2.47	0.48
1:K:128:VAL:HG22	1:K:169:LEU:CD2	2.43	0.48
1:M:241:HIS:CG	1:M:289:LEU:HD11	2.48	0.48
1:A:58:PRO:HG3	1:D:230:PHE:CZ	2.48	0.48
1:B:153:LEU:HD13	1:B:159:HIS:CD2	2.48	0.48
1:B:222:THR:CG2	1:B:286:ARG:HD2	2.38	0.48
1:E:272:PHE:HE2	1:F:95:THR:HG1	1.60	0.48
1:G:93:LEU:HD13	1:G:266:VAL:HG21	1.95	0.48
1:H:214:VAL:HG13	1:H:215:ALA:N	2.28	0.48
1:I:186:LEU:O	1:I:187:ILE:HD13	2.12	0.48
1:J:151:ALA:HA	1:J:187:ILE:O	2.14	0.48
1:J:152:TYR:O	1:J:153:LEU:HD23	2.12	0.48
1:M:85:TRP:CE3	1:M:88:THR:HG21	2.48	0.48
1:D:226:GLN:HB2	1:D:229:GLU:OE1	2.14	0.48
1:E:74:PRO:C	1:E:76:SER:H	2.17	0.48
1:F:111:GLU:H	1:F:111:GLU:HG2	1.36	0.48
1:J:297:PRO:HG3	1:K:92:TYR:CZ	2.48	0.48
1:N:137:ASN:OD1	1:N:140:SER:HB3	2.14	0.48
1:N:140:SER:O	1:N:141:SER:HB3	2.13	0.48
1:P:197:LEU:N	1:P:197:LEU:CD1	2.77	0.48
1:E:52:SER:C	1:E:54:LEU:H	2.17	0.48
1:F:143:LYS:HD3	1:F:188:VAL:HG11	1.95	0.48
1:I:56:ASP:O	1:K:262:GLN:HB3	2.13	0.48
1:K:110:LYS:N	1:K:110:LYS:HD2	2.28	0.48
1:K:237:HIS:CE1	1:K:239:ASN:HB2	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:258:TRP:HB2	1:P:258:TRP:CD1	2.48	0.48
1:A:49:LEU:H	1:A:262:GLN:HE22	1.62	0.48
1:A:75:GLU:OE1	1:A:75:GLU:N	2.37	0.48
1:C:241:HIS:CB	1:C:269:MET:HE2	2.43	0.48
1:K:213:SER:C	1:K:215:ALA:H	2.16	0.48
1:M:130:GLU:O	1:M:167:ALA:HA	2.13	0.48
1:M:241:HIS:ND1	1:M:289:LEU:HD11	2.28	0.48
1:P:124:ARG:HG2	1:P:125:LEU:N	2.28	0.48
1:P:197:LEU:HD12	1:P:197:LEU:N	2.28	0.48
1:P:64:VAL:HG12	1:P:66:LYS:HG3	1.96	0.48
1:A:277:TYR:CG	1:A:278:ALA:N	2.82	0.48
1:D:199:THR:HG21	1:D:204:PHE:CE1	2.49	0.48
1:D:206:LEU:HD12	1:D:207:ARG:N	2.28	0.48
1:D:296:ASN:ND2	1:D:298:LEU:N	2.49	0.48
1:F:121:ASP:H	1:F:156:ASN:HD21	1.62	0.48
1:H:41:TYR:CD2	1:H:246:LEU:HB3	2.49	0.48
1:H:41:TYR:CZ	1:H:246:LEU:HD13	2.49	0.48
1:J:245:LEU:HA	1:J:287:TYR:HB3	1.95	0.48
1:M:64:VAL:HG21	1:M:66:LYS:HE3	1.95	0.48
1:B:137:ASN:CB	1:B:140:SER:HA	2.43	0.48
1:B:243:LEU:HD12	1:B:243:LEU:C	2.35	0.48
1:J:270:ALA:O	1:J:273:VAL:HG12	2.13	0.48
1:L:207:ARG:HB2	1:L:222:THR:CG2	2.44	0.48
1:L:262:GLN:HB3	1:N:56:ASP:O	2.14	0.48
1:L:272:PHE:HE2	1:P:95:THR:HG1	1.62	0.48
1:P:83:PRO:O	1:P:84:ASP:HB2	2.14	0.48
1:C:153:LEU:HD13	1:C:159:HIS:CE1	2.49	0.47
1:D:125:LEU:HD13	1:D:126:ILE:N	2.30	0.47
1:G:209:LEU:O	1:G:210:LEU:HD23	2.13	0.47
1:I:164:VAL:HG23	1:I:165:GLU:N	2.29	0.47
1:E:59:GLY:O	1:P:253:ARG:NH1	2.47	0.47
1:H:270:ALA:O	1:H:273:VAL:HG12	2.14	0.47
1:J:92:TYR:HA	1:J:105:TYR:HB3	1.95	0.47
1:K:66:LYS:HD2	1:K:69:HIS:HE1	1.73	0.47
1:L:137:ASN:HB3	1:L:159:HIS:HA	1.96	0.47
1:N:217:ASP:O	1:N:218:PHE:HB3	2.13	0.47
1:O:238:TYR:CD2	1:O:297:PRO:HB3	2.49	0.47
1:A:101:HIS:O	1:A:174:ARG:HG3	2.14	0.47
1:D:137:ASN:ND2	1:D:137:ASN:N	2.63	0.47
1:G:222:THR:HG22	1:G:222:THR:O	2.13	0.47
1:I:126:ILE:C	1:I:126:ILE:HD12	2.34	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:243:LEU:HG	1:D:267:ILE:HB	1.96	0.47
1:E:52:SER:O	1:E:55:GLN:HG2	2.15	0.47
1:J:208:LYS:HZ2	1:J:212:MET:CE	2.26	0.47
1:J:203:VAL:HG11	1:J:229:GLU:OE2	2.14	0.47
1:K:290:TYR:CD2	1:K:290:TYR:C	2.87	0.47
1:L:276:TRP:HH2	1:O:251:ILE:HD11	1.78	0.47
1:N:237:HIS:CE1	1:N:239:ASN:HB2	2.49	0.47
1:N:276:TRP:CH2	1:N:278:ALA:HB2	2.50	0.47
1:D:118:PRO:O	1:D:119:PRO:O	2.32	0.47
1:D:152:TYR:HB3	1:D:187:ILE:HB	1.96	0.47
1:I:118:PRO:HB2	1:I:122:ILE:HB	1.95	0.47
1:J:276:TRP:CH2	1:J:278:ALA:HB2	2.49	0.47
1:N:142:SER:C	1:N:143:LYS:HD2	2.34	0.47
1:O:147:VAL:O	1:O:148:ASP:CB	2.62	0.47
1:P:41:TYR:CE1	1:P:246:LEU:HD13	2.50	0.47
1:E:88:THR:OG1	1:E:109:MET:HG2	2.15	0.47
1:E:109:MET:O	1:E:166:SER:HA	2.14	0.47
1:E:88:THR:HA	1:E:108:LYS:O	2.13	0.47
1:G:175:ARG:HG3	1:G:175:ARG:NH1	2.26	0.47
1:J:290:TYR:CD2	1:J:291:LYS:N	2.83	0.47
1:B:70:ALA:HB3	1:B:268:TRP:HB3	1.96	0.47
1:E:95:THR:O	1:E:97:ALA:N	2.48	0.47
1:F:182:HIS:CE1	1:F:214:VAL:HG11	2.49	0.47
1:G:68:ASP:HB2	1:G:273:VAL:HB	1.97	0.47
1:I:125:LEU:C	1:I:125:LEU:HD13	2.35	0.47
1:M:170:VAL:O	1:M:170:VAL:HG13	2.14	0.47
1:N:86:THR:O	1:N:113:SER:HA	2.14	0.47
1:N:197:LEU:HD22	1:N:208:LYS:HG3	1.97	0.47
1:G:219:ASN:O	1:G:220:ILE:HD13	2.14	0.47
1:K:87:ASN:HD21	1:K:110:LYS:HB2	1.73	0.47
1:K:74:PRO:C	1:K:76:SER:H	2.18	0.47
1:L:276:TRP:CH2	1:L:278:ALA:HB2	2.50	0.47
1:M:273:VAL:O	1:M:273:VAL:HG13	2.14	0.47
1:O:145:LEU:HD12	1:O:145:LEU:N	2.30	0.47
1:O:245:LEU:HD12	1:O:287:TYR:HB3	1.97	0.47
1:B:125:LEU:HD13	1:B:126:ILE:N	2.30	0.47
1:D:224:ASP:OD1	1:D:286:ARG:NH1	2.48	0.47
1:J:101:HIS:CD2	1:J:101:HIS:C	2.89	0.47
1:J:283:THR:HB	4:J:417:HOH:O	2.13	0.47
1:P:96:PRO:HA	1:P:100:SER:O	2.15	0.47
1:A:243:LEU:HD12	1:A:243:LEU:C	2.36	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:251:ILE:HG12	1:A:280:LEU:CD1	2.45	0.47
1:D:194:GLN:NE2	1:D:194:GLN:HA	2.30	0.47
1:F:214:VAL:CG1	1:F:215:ALA:N	2.77	0.47
1:G:108:LYS:HD3	1:G:168:THR:HG23	1.97	0.47
1:H:243:LEU:HD23	1:H:269:MET:CE	2.44	0.47
1:L:73:THR:HB	1:L:74:PRO:HD2	1.96	0.47
1:M:153:LEU:HD13	1:M:159:HIS:NE2	2.30	0.47
1:B:161:LEU:HD13	1:B:169:LEU:HD21	1.96	0.47
1:H:245:LEU:HD23	1:H:262:GLN:C	2.35	0.47
1:N:62:ARG:HD3	4:N:404:HOH:O	2.15	0.47
1:O:82:LEU:HD13	1:O:90:GLY:HA3	1.97	0.47
1:F:40:ILE:HG22	1:F:41:TYR:CG	2.50	0.46
1:G:127:PHE:CE1	1:G:288:LEU:HD11	2.50	0.46
1:G:234:LYS:HE3	1:I:60:PHE:O	2.15	0.46
1:J:298:LEU:HD23	1:K:103:VAL:HG13	1.96	0.46
1:K:225:PHE:HB2	1:K:279:ALA:HB2	1.97	0.46
1:L:171:VAL:CG2	1:L:172:PHE:N	2.78	0.46
1:O:208:LYS:HE3	4:O:413:HOH:O	2.16	0.46
1:P:137:ASN:CA	1:P:159:HIS:HA	2.37	0.46
1:P:243:LEU:O	1:P:266:VAL:HG13	2.15	0.46
1:P:82:LEU:HD11	1:P:90:GLY:HA3	1.97	0.46
1:E:150:TYR:CE2	1:E:209:LEU:HB3	2.50	0.46
1:G:110:LYS:HE2	1:G:110:LYS:HA	1.96	0.46
1:G:226:GLN:HB2	1:G:229:GLU:CD	2.36	0.46
1:H:63:SER:HA	1:H:71:LEU:O	2.15	0.46
1:H:82:LEU:CD1	1:H:83:PRO:HD2	2.36	0.46
1:I:150:TYR:CE2	1:I:209:LEU:HB3	2.51	0.46
1:N:170:VAL:O	1:N:170:VAL:HG13	2.15	0.46
1:O:137:ASN:ND2	1:O:140:SER:HB2	2.29	0.46
1:C:284:ARG:NH2	1:C:286:ARG:NH1	2.64	0.46
1:C:85:TRP:CE3	1:C:115:SER:HA	2.50	0.46
1:J:82:LEU:HD13	1:J:90:GLY:CA	2.39	0.46
1:A:136:THR:HG22	1:A:142:SER:CB	2.45	0.46
1:A:239:ASN:HD22	1:A:239:ASN:N	2.02	0.46
1:B:196:LEU:HD12	1:B:205:GLU:HB3	1.97	0.46
1:C:243:LEU:HD12	1:C:243:LEU:C	2.35	0.46
1:E:154:PRO:HD3	1:E:186:LEU:HA	1.96	0.46
1:G:166:SER:O	1:G:167:ALA:HB2	2.14	0.46
1:I:119:PRO:HD2	1:I:122:ILE:HG13	1.97	0.46
1:D:61:THR:HG22	1:K:253:ARG:HH12	1.80	0.46
1:K:93:LEU:CD1	1:K:266:VAL:HG21	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:117:LEU:HD21	1:L:158:HIS:CD2	2.51	0.46
1:C:243:LEU:HB3	1:C:289:LEU:HD12	1.98	0.46
1:I:70:ALA:HB3	1:I:268:TRP:HB3	1.98	0.46
1:L:170:VAL:HG13	1:L:170:VAL:O	2.15	0.46
1:B:204:PHE:CE1	1:B:206:LEU:HB2	2.48	0.46
1:C:252:TYR:CD1	1:C:277:TYR:HD1	2.34	0.46
1:D:284:ARG:NH2	1:D:286:ARG:NH1	2.63	0.46
1:E:233:VAL:O	1:E:233:VAL:HG13	2.15	0.46
1:J:114:SER:HA	1:J:161:LEU:O	2.16	0.46
1:K:194:GLN:NE2	1:K:194:GLN:CA	2.74	0.46
1:P:135:LEU:C	1:P:135:LEU:HD23	2.35	0.46
1:J:203:VAL:O	1:J:203:VAL:HG12	2.15	0.46
1:K:218:PHE:C	1:K:218:PHE:CD1	2.88	0.46
1:M:70:ALA:HB3	1:M:268:TRP:HB3	1.98	0.46
1:N:151:ALA:HA	1:N:187:ILE:O	2.16	0.46
1:O:125:LEU:HD13	1:O:125:LEU:C	2.35	0.46
1:O:202:GLU:OE2	1:O:233:VAL:HG12	2.15	0.46
1:A:184:THR:HG22	1:A:216:TYR:CE1	2.51	0.46
1:C:95:THR:O	1:C:97:ALA:N	2.49	0.46
1:F:141:SER:HB3	1:F:142:SER:H	1.55	0.46
1:F:204:PHE:HE1	1:F:206:LEU:HB2	1.81	0.46
1:H:224:ASP:OD1	1:H:286:ARG:CD	2.58	0.46
1:J:125:LEU:C	1:J:125:LEU:HD13	2.36	0.46
1:J:176:TYR:CE2	1:J:178:TYR:HA	2.43	0.46
1:K:123:GLU:HG2	1:K:174:ARG:O	2.14	0.46
1:D:103:VAL:CG2	1:D:173:GLU:HB2	2.46	0.46
1:D:126:ILE:C	1:D:126:ILE:HD12	2.37	0.46
1:D:153:LEU:HD13	1:D:159:HIS:CG	2.50	0.46
1:E:96:PRO:HA	1:E:100:SER:O	2.16	0.46
1:G:206:LEU:HD21	1:G:208:LYS:HE2	1.98	0.46
1:J:170:VAL:HG13	1:J:170:VAL:O	2.15	0.46
1:K:164:VAL:CG2	1:K:165:GLU:N	2.78	0.46
1:K:194:GLN:HE21	1:K:194:GLN:HA	1.78	0.46
1:O:96:PRO:HD3	1:O:103:VAL:HG12	1.97	0.46
1:P:204:PHE:HB3	1:P:225:PHE:CE1	2.51	0.46
1:A:54:LEU:CD2	1:C:49:LEU:HD22	2.46	0.46
1:A:82:LEU:HD12	1:A:82:LEU:HA	1.85	0.46
1:B:111:GLU:H	1:B:111:GLU:CD	2.19	0.46
1:D:170:VAL:HG13	1:D:170:VAL:O	2.16	0.46
1:L:241:HIS:HB2	1:L:269:MET:HB2	1.97	0.46
1:C:166:SER:O	1:C:167:ALA:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:179:LEU:O	1:D:180:GLY:O	2.34	0.45
1:E:222:THR:HG22	1:E:288:LEU:HD12	1.98	0.45
1:F:151:ALA:HA	1:F:187:ILE:O	2.16	0.45
1:H:125:LEU:HD23	1:H:152:TYR:HB2	1.98	0.45
1:K:100:SER:HA	1:K:240:GLN:NE2	2.31	0.45
1:K:211:PRO:CB	1:K:216:TYR:HE2	2.25	0.45
1:F:298:LEU:HG	1:L:103:VAL:HG11	1.97	0.45
1:L:145:LEU:HD22	1:L:149:SER:HB3	1.99	0.45
1:L:83:PRO:O	1:L:84:ASP:HB2	2.16	0.45
1:O:137:ASN:OD1	1:O:137:ASN:C	2.53	0.45
1:P:188:VAL:HG12	1:P:189:GLY:N	2.30	0.45
1:D:150:TYR:CE1	1:D:209:LEU:HD22	2.51	0.45
1:D:101:HIS:N	1:D:240:GLN:HE22	2.12	0.45
1:F:126:ILE:C	1:F:126:ILE:HD12	2.36	0.45
1:G:196:LEU:CD2	1:G:205:GLU:HB3	2.42	0.45
1:H:208:LYS:HG2	1:H:221:HIS:CD2	2.50	0.45
1:I:150:TYR:CE1	1:I:209:LEU:HD22	2.50	0.45
1:K:100:SER:CA	1:K:240:GLN:HE22	2.29	0.45
1:M:179:LEU:HD23	1:M:214:VAL:HG22	1.97	0.45
1:C:126:ILE:HD12	1:C:126:ILE:C	2.37	0.45
1:D:64:VAL:HG12	1:D:66:LYS:HG3	1.98	0.45
1:G:237:HIS:CE1	1:G:239:ASN:HB2	2.52	0.45
1:H:186:LEU:CD1	1:H:188:VAL:HG23	2.45	0.45
1:J:47:PRO:HA	4:J:424:HOH:O	2.17	0.45
1:J:87:ASN:HD21	1:J:110:LYS:CB	2.29	0.45
1:K:163:CYS:SG	1:K:167:ALA:HB2	2.56	0.45
1:K:243:LEU:HD12	1:K:244:LEU:N	2.32	0.45
1:P:105:TYR:CE1	1:P:171:VAL:HG11	2.52	0.45
1:B:100:SER:HB3	1:B:268:TRP:CH2	2.51	0.45
1:B:146:THR:O	1:B:147:VAL:C	2.55	0.45
1:E:117:LEU:HD11	1:E:158:HIS:CD2	2.52	0.45
1:F:208:LYS:HZ2	1:F:212:MET:HE1	1.81	0.45
1:C:198:GLU:HB2	1:H:197:LEU:O	2.16	0.45
1:I:243:LEU:HB2	1:I:289:LEU:HD12	1.99	0.45
1:J:77:HIS:NE2	4:J:401:HOH:O	2.35	0.45
1:L:147:VAL:O	1:L:148:ASP:CB	2.63	0.45
1:D:128:VAL:HG12	1:D:147:VAL:HA	1.98	0.45
1:D:243:LEU:HD23	1:D:269:MET:CE	2.46	0.45
1:E:137:ASN:ND2	1:E:140:SER:HB3	2.31	0.45
1:F:237:HIS:HB2	1:F:239:ASN:HD22	1.82	0.45
1:F:262:GLN:HB3	1:H:56:ASP:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:243:LEU:HG	1:H:267:ILE:HB	1.98	0.45
1:J:179:LEU:HD23	1:J:214:VAL:HG22	1.98	0.45
1:L:205:GLU:HB2	1:L:224:ASP:HB2	1.98	0.45
1:L:95:THR:O	1:L:98:THR:HG23	2.16	0.45
1:N:133:VAL:HG23	1:N:163:CYS:CB	2.37	0.45
1:O:54:LEU:HD23	1:P:49:LEU:HD22	1.99	0.45
1:F:125:LEU:HD13	1:F:126:ILE:N	2.31	0.45
1:I:153:LEU:HD13	1:I:159:HIS:CD2	2.52	0.45
1:I:83:PRO:C	1:I:85:TRP:H	2.19	0.45
1:J:134:THR:HG23	1:J:144:LYS:CA	2.47	0.45
1:K:133:VAL:HG22	1:K:134:THR:N	2.31	0.45
1:K:129:VAL:HB	1:K:168:THR:HB	1.98	0.45
1:L:262:GLN:NE2	1:N:56:ASP:HB2	2.32	0.45
1:L:56:ASP:O	1:L:58:PRO:HD3	2.17	0.45
1:M:64:VAL:HG22	1:M:66:LYS:HE3	1.97	0.45
1:L:262:GLN:HE21	1:N:56:ASP:CB	2.30	0.45
1:P:237:HIS:CE1	1:P:239:ASN:HB2	2.52	0.45
1:D:72:ILE:H	1:D:72:ILE:HD12	1.81	0.45
1:F:179:LEU:HD23	1:F:214:VAL:HG22	1.99	0.45
1:G:156:ASN:O	1:G:157:PHE:C	2.53	0.45
1:G:227:PRO:HG3	1:G:283:THR:O	2.17	0.45
1:H:195:PRO:O	1:H:197:LEU:HD12	2.16	0.45
1:I:142:SER:C	1:I:143:LYS:HD2	2.37	0.45
1:K:243:LEU:HD22	1:K:287:TYR:CE1	2.51	0.45
1:L:171:VAL:HG23	1:L:172:PHE:N	2.32	0.45
1:L:50:SER:OG	1:L:51:PRO:HD2	2.16	0.45
1:M:128:VAL:HG22	1:M:169:LEU:CD1	2.47	0.45
1:M:218:PHE:C	1:M:218:PHE:CD1	2.90	0.45
1:P:156:ASN:O	1:P:157:PHE:C	2.55	0.45
1:P:82:LEU:O	1:P:85:TRP:HB2	2.16	0.45
1:A:56:ASP:OD2	1:C:48:THR:OG1	2.34	0.45
1:B:253:ARG:NH1	1:C:61:THR:HG22	2.32	0.45
1:F:237:HIS:CE1	1:F:239:ASN:HB2	2.51	0.45
1:H:290:TYR:CD2	1:H:291:LYS:N	2.85	0.45
1:K:101:HIS:H	1:K:240:GLN:HE22	1.65	0.45
1:K:253:ARG:HD2	1:K:258:TRP:CZ2	2.52	0.45
1:K:95:THR:O	1:K:97:ALA:N	2.50	0.45
1:L:40:ILE:HG22	1:L:41:TYR:CD2	2.51	0.45
1:N:150:TYR:CE2	1:N:209:LEU:HB3	2.52	0.45
1:P:123:GLU:O	1:P:173:GLU:HA	2.16	0.45
1:P:72:ILE:H	1:P:72:ILE:HD12	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:218:PHE:HA	1:C:293:VAL:HG22	1.98	0.45
1:D:184:THR:HB	1:D:216:TYR:CE1	2.51	0.45
1:E:103:VAL:CG2	1:E:173:GLU:HB2	2.47	0.45
1:G:82:LEU:O	1:G:85:TRP:HB2	2.17	0.45
1:J:175:ARG:HG3	1:J:175:ARG:NH1	2.22	0.45
1:J:224:ASP:CG	1:J:286:ARG:HD3	2.37	0.45
1:M:68:ASP:OD2	1:M:273:VAL:HG23	2.15	0.45
1:P:136:THR:O	1:P:137:ASN:ND2	2.49	0.45
1:O:54:LEU:CD2	1:P:49:LEU:HD22	2.46	0.45
1:A:126:ILE:HG22	1:A:171:VAL:HB	1.98	0.45
1:A:85:TRP:CE3	1:A:115:SER:HA	2.52	0.45
1:B:155:PRO:HG3	1:B:176:TYR:CD2	2.52	0.45
1:D:136:THR:HG22	1:D:142:SER:CB	2.46	0.45
1:H:43:LYS:HB2	4:H:413:HOH:O	2.17	0.45
1:I:209:LEU:O	1:I:210:LEU:HD23	2.17	0.45
1:J:241:HIS:HB2	1:J:269:MET:HB2	1.99	0.45
1:K:204:PHE:HB3	1:K:225:PHE:CE1	2.52	0.45
1:K:233:VAL:HG13	1:K:233:VAL:O	2.17	0.45
1:M:269:MET:SD	1:M:275:GLN:OE1	2.76	0.45
1:M:50:SER:HB2	1:M:51:PRO:HD2	1.98	0.45
1:O:120:GLN:O	1:O:122:ILE:HG12	2.17	0.45
1:C:194:GLN:NE2	4:C:431:HOH:O	2.50	0.44
1:E:73:THR:HG22	1:E:265:ASP:OD1	2.17	0.44
1:G:220:ILE:HD13	1:G:290:TYR:HA	1.99	0.44
1:H:94:ILE:O	1:H:103:VAL:HA	2.17	0.44
1:L:219:ASN:OD1	1:L:220:ILE:N	2.50	0.44
1:P:191:THR:CG2	1:P:286:ARG:NH2	2.75	0.44
1:P:85:TRP:HE3	1:P:88:THR:HG21	1.75	0.44
1:P:93:LEU:HD13	1:P:266:VAL:HG21	1.99	0.44
1:B:207:ARG:HB2	1:B:222:THR:HB	1.99	0.44
1:D:64:VAL:CG1	1:D:66:LYS:HE3	2.45	0.44
1:E:208:LYS:NZ	1:E:212:MET:HE3	2.32	0.44
1:F:207:ARG:NH2	4:F:436:HOH:O	2.50	0.44
1:L:117:LEU:HD12	1:L:117:LEU:N	2.32	0.44
1:L:292:ASP:OD1	1:L:292:ASP:N	2.51	0.44
1:M:152:TYR:O	1:M:186:LEU:HD12	2.16	0.44
1:M:245:LEU:HD23	1:M:262:GLN:C	2.37	0.44
1:N:111:GLU:HA	1:N:164:VAL:O	2.17	0.44
1:A:70:ALA:HB3	1:A:268:TRP:HB3	1.98	0.44
1:C:253:ARG:HD2	1:C:258:TRP:CZ2	2.52	0.44
1:H:140:SER:O	1:H:141:SER:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:232:ASN:HA	1:J:232:ASN:HD22	1.63	0.44
1:L:137:ASN:O	1:L:137:ASN:ND2	2.49	0.44
1:M:109:MET:O	1:M:166:SER:HA	2.18	0.44
1:M:182:HIS:NE2	1:M:214:VAL:HG11	2.33	0.44
1:N:88:THR:OG1	1:N:109:MET:HG2	2.17	0.44
1:P:198:GLU:HG3	1:P:200:PRO:HD3	1.99	0.44
1:P:45:THR:HG21	1:P:130:GLU:OE2	2.17	0.44
1:B:137:ASN:CG	1:B:140:SER:HA	2.38	0.44
1:B:247:GLU:CG	1:B:286:ARG:HB3	2.47	0.44
1:J:103:VAL:HG22	1:J:173:GLU:O	2.18	0.44
1:J:64:VAL:HG11	1:J:66:LYS:HZ2	1.83	0.44
1:N:61:THR:HB	1:O:234:LYS:CG	2.44	0.44
1:C:103:VAL:CG2	1:C:173:GLU:HB2	2.48	0.44
1:C:133:VAL:HG21	1:C:161:LEU:HB3	1.98	0.44
1:E:190:SER:HB2	1:E:192:ASP:OD1	2.17	0.44
1:E:243:LEU:HD23	1:E:269:MET:HE2	2.00	0.44
1:F:118:PRO:HD3	1:F:124:ARG:NH2	2.33	0.44
1:H:237:HIS:ND1	1:H:239:ASN:HB2	2.33	0.44
1:I:153:LEU:HD13	1:I:159:HIS:NE2	2.32	0.44
1:O:133:VAL:HG22	1:O:134:THR:N	2.32	0.44
1:A:122:ILE:HD13	1:A:175:ARG:HA	2.00	0.44
1:A:251:ILE:HG12	1:A:280:LEU:HD11	1.98	0.44
1:A:82:LEU:HD13	1:A:90:GLY:CA	2.47	0.44
1:E:69:HIS:HE1	4:E:415:HOH:O	2.00	0.44
1:G:94:ILE:O	1:G:103:VAL:HA	2.18	0.44
1:H:250:GLY:HA3	1:H:278:ALA:O	2.18	0.44
1:J:164:VAL:HG23	1:J:165:GLU:CG	2.46	0.44
1:K:223:MET:O	1:K:286:ARG:HA	2.18	0.44
1:O:240:GLN:HG2	1:O:292:ASP:OD1	2.16	0.44
1:P:153:LEU:HD13	1:P:159:HIS:NE2	2.33	0.44
1:A:102:PHE:HE2	1:A:240:GLN:HE21	1.59	0.44
1:A:72:ILE:HD12	1:A:72:ILE:N	2.33	0.44
1:E:136:THR:CG2	1:E:160:SER:HB3	2.47	0.44
1:G:133:VAL:HG23	1:G:163:CYS:HB2	2.00	0.44
1:H:126:ILE:C	1:H:126:ILE:HD12	2.38	0.44
1:I:202:GLU:HB3	1:I:204:PHE:CE2	2.53	0.44
1:J:266:VAL:C	1:J:267:ILE:HD12	2.37	0.44
1:J:40:ILE:HG22	1:J:41:TYR:CD2	2.53	0.44
1:K:125:LEU:HD23	1:K:152:TYR:HB2	2.00	0.44
1:M:227:PRO:HB3	1:M:281:GLY:O	2.17	0.44
1:N:203:VAL:O	1:N:204:PHE:C	2.56	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:147:VAL:HG22	1:O:147:VAL:O	2.17	0.44
1:N:60:PHE:O	1:O:234:LYS:HE3	2.17	0.44
1:O:276:TRP:CH2	1:O:278:ALA:HB2	2.52	0.44
1:A:83:PRO:O	1:A:84:ASP:CB	2.66	0.44
1:D:174:ARG:HG2	1:D:175:ARG:O	2.17	0.44
1:F:290:TYR:CD2	1:F:290:TYR:C	2.91	0.44
1:G:111:GLU:O	1:G:112:MET:C	2.55	0.44
1:J:231:LEU:HD12	1:J:276:TRP:HA	2.00	0.44
1:K:211:PRO:O	1:K:216:TYR:HD2	2.00	0.44
1:L:153:LEU:HD22	1:L:159:HIS:CD2	2.53	0.44
1:M:133:VAL:CG2	1:M:134:THR:N	2.81	0.44
1:C:297:PRO:HG3	1:G:92:TYR:CZ	2.53	0.44
1:D:137:ASN:HD21	1:D:140:SER:C	2.22	0.44
1:G:252:TYR:CD1	1:G:277:TYR:CD1	3.05	0.44
1:K:196:LEU:HD21	1:K:207:ARG:NH1	2.33	0.44
1:K:262:GLN:NE2	4:K:404:HOH:O	2.51	0.44
1:M:82:LEU:HD12	1:M:83:PRO:HD2	1.99	0.44
1:P:243:LEU:HB3	1:P:289:LEU:CD1	2.48	0.44
1:P:41:TYR:CZ	1:P:246:LEU:HD13	2.52	0.44
1:F:41:TYR:CD2	1:F:41:TYR:N	2.84	0.43
1:H:207:ARG:HB2	1:H:222:THR:CG2	2.48	0.43
1:I:126:ILE:O	1:I:126:ILE:HD12	2.18	0.43
1:I:279:ALA:O	1:I:280:LEU:HD23	2.18	0.43
1:K:90:GLY:HA2	1:K:106:LEU:O	2.18	0.43
1:M:140:SER:O	1:M:141:SER:HB3	2.17	0.43
1:M:252:TYR:CD1	1:M:277:TYR:CD1	3.06	0.43
1:P:245:LEU:HD12	1:P:287:TYR:HB3	2.00	0.43
1:D:135:LEU:O	1:D:142:SER:HA	2.18	0.43
1:E:133:VAL:HG22	1:E:134:THR:N	2.33	0.43
1:F:126:ILE:HD12	1:F:126:ILE:O	2.18	0.43
1:F:174:ARG:HH21	1:F:177:GLU:HG3	1.82	0.43
1:G:213:SER:O	1:G:294:ASN:ND2	2.51	0.43
1:H:222:THR:HG22	1:H:222:THR:O	2.18	0.43
1:K:164:VAL:HG23	1:K:165:GLU:HG2	2.00	0.43
1:O:241:HIS:HB2	1:O:269:MET:HB2	1.98	0.43
1:D:206:LEU:HD12	1:D:207:ARG:H	1.83	0.43
1:E:197:LEU:HD12	1:E:208:LYS:HG3	2.00	0.43
1:E:102:PHE:HD2	1:E:240:GLN:HE21	1.66	0.43
1:G:50:SER:O	1:G:53:HIS:HB2	2.18	0.43
1:H:208:LYS:HZ2	1:H:212:MET:HE2	1.83	0.43
1:K:87:ASN:CG	1:K:110:LYS:HB2	2.37	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:262:GLN:NE2	4:L:430:HOH:O	2.46	0.43
1:O:134:THR:O	1:O:161:LEU:HA	2.18	0.43
1:P:105:TYR:CE1	1:P:171:VAL:CG1	3.02	0.43
1:C:184:THR:HB	1:C:216:TYR:CE1	2.52	0.43
1:F:298:LEU:HG	1:L:103:VAL:CG1	2.48	0.43
1:H:237:HIS:CE1	1:H:239:ASN:HB2	2.53	0.43
1:H:237:HIS:HB3	1:M:78:VAL:HG21	2.00	0.43
1:I:134:THR:HG23	1:I:143:LYS:O	2.19	0.43
1:I:95:THR:HA	1:I:103:VAL:HG12	2.00	0.43
1:K:64:VAL:CG1	1:K:66:LYS:HE3	2.43	0.43
1:L:251:ILE:HD13	1:L:260:PRO:HA	1.99	0.43
1:N:87:ASN:CG	1:N:110:LYS:HB2	2.37	0.43
1:N:130:GLU:CG	1:N:131:GLY:N	2.81	0.43
1:N:93:LEU:CD1	1:N:266:VAL:HG21	2.40	0.43
1:O:253:ARG:HB3	1:O:276:TRP:HB3	2.00	0.43
1:O:284:ARG:C	1:O:284:ARG:HD2	2.38	0.43
1:P:207:ARG:HB3	1:P:222:THR:HB	1.99	0.43
1:B:235:GLU:HB2	1:B:275:GLN:HG3	2.00	0.43
1:C:115:SER:HB3	1:C:161:LEU:CB	2.33	0.43
1:C:217:ASP:O	1:C:218:PHE:HB3	2.18	0.43
1:F:64:VAL:HG12	1:F:66:LYS:HG3	2.00	0.43
1:G:82:LEU:HG	1:G:85:TRP:CD1	2.54	0.43
1:H:298:LEU:HD21	1:M:122:ILE:HD12	2.01	0.43
1:H:89:LEU:HD12	1:H:110:LYS:NZ	2.33	0.43
1:J:223:MET:O	1:J:286:ARG:HA	2.19	0.43
1:K:164:VAL:CG2	1:K:165:GLU:H	2.31	0.43
1:K:199:THR:HB	1:K:202:GLU:HB2	2.00	0.43
1:L:101:HIS:NE2	1:L:290:TYR:OH	2.44	0.43
1:L:220:ILE:HA	1:L:289:LEU:O	2.18	0.43
1:L:80:SER:O	1:L:81:PRO:C	2.56	0.43
1:P:120:GLN:OE1	1:P:121:ASP:N	2.52	0.43
1:A:230:PHE:HB2	1:A:277:TYR:O	2.19	0.43
1:C:270:ALA:O	1:C:273:VAL:HG12	2.18	0.43
1:D:93:LEU:C	1:D:94:ILE:HG13	2.39	0.43
1:E:276:TRP:CH2	1:E:278:ALA:HB2	2.54	0.43
1:E:52:SER:C	1:E:54:LEU:N	2.71	0.43
1:F:135:LEU:HB2	1:F:145:LEU:HD11	2.01	0.43
1:H:125:LEU:HD13	1:H:125:LEU:C	2.38	0.43
1:K:101:HIS:N	1:K:240:GLN:HE22	2.17	0.43
1:L:190:SER:O	1:L:194:GLN:HG2	2.18	0.43
1:M:226:GLN:HB2	1:M:229:GLU:CD	2.38	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:150:TYR:CD1	1:O:209:LEU:HD13	2.53	0.43
1:O:196:LEU:C	1:O:197:LEU:HD23	2.39	0.43
1:B:185:GLU:O	1:B:187:ILE:HG12	2.19	0.43
1:I:243:LEU:HD12	1:I:243:LEU:C	2.37	0.43
1:I:96:PRO:HD3	1:I:103:VAL:HG12	2.00	0.43
1:J:234:LYS:N	1:J:234:LYS:HD3	2.33	0.43
1:N:243:LEU:HD23	1:N:269:MET:HE1	1.99	0.43
1:P:103:VAL:CG2	1:P:173:GLU:HB2	2.48	0.43
1:A:283:THR:HG21	4:A:430:HOH:O	2.19	0.43
1:F:127:PHE:HB3	1:F:170:VAL:HG12	1.97	0.43
1:F:41:TYR:CZ	1:F:246:LEU:HD13	2.54	0.43
1:H:298:LEU:CD2	1:M:122:ILE:HD12	2.49	0.43
1:J:245:LEU:HD23	1:J:262:GLN:C	2.39	0.43
1:J:66:LYS:HE2	1:J:257:ASN:HD21	1.83	0.43
1:N:81:PRO:O	1:N:83:PRO:HD3	2.19	0.43
1:O:253:ARG:O	1:O:275:GLN:HA	2.19	0.43
1:P:124:ARG:HA	1:P:172:PHE:O	2.18	0.43
1:P:190:SER:HB3	1:P:192:ASP:OD1	2.19	0.43
1:B:64:VAL:HG12	1:B:66:LYS:HG2	2.00	0.43
1:E:133:VAL:HG23	1:E:162:ASP:O	2.19	0.43
1:E:224:ASP:OD2	1:E:286:ARG:HD3	2.18	0.43
1:F:192:ASP:OD2	1:F:193:LYS:N	2.52	0.43
1:G:79:TYR:CD1	1:G:91:ALA:HB2	2.54	0.43
1:H:105:TYR:CE2	1:H:171:VAL:HG22	2.53	0.43
1:K:208:LYS:HE2	1:K:221:HIS:CE1	2.54	0.43
1:K:258:TRP:CD1	1:K:258:TRP:N	2.87	0.43
1:H:234:LYS:HG2	1:M:61:THR:HB	2.01	0.43
1:N:125:LEU:C	1:N:125:LEU:HD13	2.39	0.43
1:P:100:SER:HB3	1:P:268:TRP:CH2	2.54	0.43
1:P:273:VAL:HG13	1:P:273:VAL:O	2.18	0.43
1:D:100:SER:HB2	1:D:240:GLN:NE2	2.34	0.43
1:D:204:PHE:HB3	1:D:225:PHE:CE1	2.54	0.43
1:M:93:LEU:HD13	1:M:266:VAL:HG21	2.01	0.43
1:N:275:GLN:HE21	1:N:275:GLN:HB3	1.66	0.43
1:O:165:GLU:CG	1:O:166:SER:H	2.22	0.43
1:B:126:ILE:HD13	1:B:161:LEU:CD1	2.41	0.42
1:C:224:ASP:OD1	1:C:286:ARG:NH1	2.52	0.42
1:G:57:LEU:HD23	1:G:57:LEU:HA	1.84	0.42
1:I:48:THR:OG1	1:K:56:ASP:OD2	2.29	0.42
1:L:53:HIS:O	1:N:48:THR:HG22	2.19	0.42
1:M:127:PHE:HB3	1:M:170:VAL:CG1	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:69:HIS:HA	1:N:268:TRP:O	2.19	0.42
1:O:137:ASN:HD22	1:O:140:SER:CB	2.30	0.42
1:A:116:GLY:O	1:A:117:LEU:C	2.57	0.42
1:A:120:GLN:HG3	1:A:156:ASN:ND2	2.33	0.42
1:A:220:ILE:HD13	1:A:290:TYR:HA	2.01	0.42
1:D:83:PRO:O	1:D:84:ASP:HB2	2.18	0.42
1:E:296:ASN:ND2	1:E:298:LEU:HD12	2.31	0.42
1:H:186:LEU:HD12	1:H:187:ILE:N	2.34	0.42
1:I:120:GLN:CG	1:I:156:ASN:HD21	2.31	0.42
1:O:249:GLN:CD	1:O:249:GLN:N	2.72	0.42
1:O:224:ASP:OD2	1:O:286:ARG:HD3	2.20	0.42
1:E:220:ILE:HA	1:E:289:LEU:O	2.20	0.42
1:E:82:LEU:HD23	1:E:85:TRP:CD2	2.55	0.42
1:G:68:ASP:N	1:G:68:ASP:OD1	2.51	0.42
1:I:252:TYR:CE1	1:I:277:TYR:HB2	2.55	0.42
1:J:137:ASN:ND2	1:J:140:SER:N	2.67	0.42
1:J:202:GLU:OE2	1:J:202:GLU:HA	2.20	0.42
1:L:187:ILE:HD11	1:L:216:TYR:OH	2.18	0.42
1:M:57:LEU:HA	1:M:57:LEU:HD23	1.87	0.42
1:A:203:VAL:HG21	1:A:229:GLU:HG2	2.01	0.42
1:B:126:ILE:HG13	1:B:126:ILE:O	2.19	0.42
1:C:170:VAL:O	1:C:170:VAL:HG13	2.19	0.42
1:C:52:SER:O	1:C:55:GLN:HG2	2.20	0.42
1:I:190:SER:HB3	1:I:193:LYS:HG2	2.01	0.42
1:J:88:THR:HG23	1:J:109:MET:HA	2.01	0.42
1:L:153:LEU:HA	1:L:154:PRO:HD3	1.87	0.42
1:N:130:GLU:HG2	1:N:131:GLY:H	1.83	0.42
1:E:233:VAL:HG13	1:E:235:GLU:HG3	2.01	0.42
1:F:41:TYR:CE1	1:F:246:LEU:HD13	2.54	0.42
1:H:140:SER:O	1:H:141:SER:CB	2.67	0.42
1:H:102:PHE:HE2	1:H:240:GLN:HE21	1.64	0.42
1:H:275:GLN:OE1	3:H:302:UGY:NE	2.52	0.42
1:H:57:LEU:HD23	1:H:57:LEU:HA	1.94	0.42
1:I:149:SER:O	1:I:150:TYR:HB3	2.20	0.42
1:K:41:TYR:OH	1:K:286:ARG:NH2	2.53	0.42
1:L:179:LEU:HD23	1:L:214:VAL:CG2	2.49	0.42
1:M:174:ARG:HG2	1:M:175:ARG:N	2.34	0.42
1:P:158:HIS:O	1:P:159:HIS:HB3	2.19	0.42
1:O:53:HIS:CD2	1:P:53:HIS:CE1	3.07	0.42
1:A:237:HIS:CE1	1:A:239:ASN:HB2	2.55	0.42
1:G:100:SER:HA	1:G:240:GLN:HE22	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:208:LYS:NZ	1:H:212:MET:HE3	2.35	0.42
1:I:262:GLN:O	1:I:263:ALA:C	2.57	0.42
1:K:88:THR:OG1	1:K:109:MET:HA	2.19	0.42
1:M:126:ILE:HD12	1:M:126:ILE:C	2.40	0.42
1:O:60:PHE:HZ	1:P:60:PHE:HZ	1.67	0.42
1:M:253:ARG:HH12	1:O:61:THR:HG22	1.84	0.42
1:P:110:LYS:HB3	1:P:111:GLU:OE2	2.19	0.42
1:A:62:ARG:HB2	1:A:73:THR:HG21	2.02	0.42
1:B:135:LEU:O	1:B:142:SER:HA	2.20	0.42
1:B:237:HIS:CE1	1:B:239:ASN:HB2	2.53	0.42
1:I:218:PHE:HD1	1:I:219:ASN:N	2.17	0.42
1:I:222:THR:HG22	1:I:222:THR:O	2.20	0.42
1:K:125:LEU:HD13	1:K:125:LEU:C	2.40	0.42
1:L:134:THR:HG22	1:L:135:LEU:N	2.35	0.42
1:N:282:LYS:HE2	1:N:282:LYS:N	2.34	0.42
1:O:259:TYR:HA	1:O:260:PRO:HD3	1.89	0.42
1:P:75:GLU:OE1	1:P:75:GLU:N	2.47	0.42
1:C:62:ARG:NH1	1:C:73:THR:HG21	2.35	0.42
1:D:147:VAL:O	1:D:148:ASP:CB	2.67	0.42
1:D:245:LEU:HD12	1:D:287:TYR:HB3	2.02	0.42
1:H:235:GLU:HB2	1:H:275:GLN:HG3	2.02	0.42
1:J:115:SER:HB3	1:J:161:LEU:HB2	2.00	0.42
1:M:133:VAL:CG2	1:M:134:THR:H	2.30	0.42
1:M:101:HIS:N	1:M:240:GLN:HE22	2.16	0.42
1:M:94:ILE:CD1	1:M:268:TRP:HB2	2.49	0.42
1:N:127:PHE:HB3	1:N:170:VAL:CG1	2.49	0.42
1:P:238:TYR:CD2	1:P:238:TYR:C	2.93	0.42
1:D:137:ASN:ND2	1:D:140:SER:N	2.67	0.42
1:F:144:LYS:HG3	1:F:145:LEU:N	2.34	0.42
1:F:82:LEU:HD11	1:F:90:GLY:HA3	2.02	0.42
1:J:288:LEU:HA	1:J:288:LEU:HD12	1.81	0.42
1:K:245:LEU:HD23	1:K:262:GLN:C	2.40	0.42
1:O:101:HIS:H	1:O:240:GLN:HE22	1.68	0.42
1:P:101:HIS:CD2	1:P:101:HIS:C	2.93	0.42
1:P:152:TYR:O	1:P:154:PRO:HD3	2.19	0.42
1:P:232:ASN:HA	1:P:232:ASN:HD22	1.71	0.42
1:B:49:LEU:HD13	1:J:53:HIS:HB3	2.02	0.42
1:C:238:TYR:O	1:C:271:PRO:HB3	2.20	0.42
1:C:47:PRO:HA	4:C:405:HOH:O	2.19	0.42
1:C:49:LEU:H	1:C:262:GLN:HE22	1.67	0.42
1:F:130:GLU:O	1:F:167:ALA:HA	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:41:TYR:CE2	1:H:246:LEU:HD13	2.55	0.42
1:J:134:THR:HA	1:J:144:LYS:HA	2.02	0.42
1:K:206:LEU:HD12	1:K:207:ARG:H	1.81	0.42
1:K:83:PRO:O	1:K:84:ASP:HB2	2.19	0.42
1:N:140:SER:O	1:N:141:SER:CB	2.68	0.42
1:O:196:LEU:HD21	1:O:207:ARG:NH2	2.35	0.42
1:P:165:GLU:O	1:P:166:SER:OG	2.30	0.42
1:A:185:GLU:O	1:A:187:ILE:HG12	2.20	0.41
1:B:226:GLN:HB2	1:B:229:GLU:CD	2.40	0.41
1:D:111:GLU:H	1:D:111:GLU:CD	2.24	0.41
1:E:122:ILE:HD13	1:E:175:ARG:HA	2.01	0.41
1:E:298:LEU:HD23	1:F:103:VAL:HG13	2.02	0.41
1:J:83:PRO:O	1:J:84:ASP:HB2	2.20	0.41
1:L:94:ILE:O	1:L:103:VAL:HA	2.19	0.41
1:M:243:LEU:HB2	1:M:288:LEU:O	2.20	0.41
1:N:240:GLN:HB3	1:N:271:PRO:HG3	2.01	0.41
1:P:87:ASN:OD1	1:P:110:LYS:HB2	2.20	0.41
1:C:74:PRO:C	1:C:76:SER:N	2.69	0.41
1:E:74:PRO:C	1:E:76:SER:N	2.74	0.41
1:H:196:LEU:CD2	1:H:207:ARG:NH1	2.83	0.41
1:K:170:VAL:O	1:K:170:VAL:CG1	2.62	0.41
1:K:121:ASP:HB2	1:K:175:ARG:NH1	2.35	0.41
1:K:88:THR:OG1	1:K:109:MET:HG2	2.20	0.41
1:L:208:LYS:HG2	1:L:221:HIS:CD2	2.54	0.41
1:N:134:THR:HG22	1:N:134:THR:O	2.19	0.41
1:N:204:PHE:HE1	1:N:206:LEU:HB2	1.84	0.41
1:N:267:ILE:HG22	1:N:269:MET:HG3	2.00	0.41
1:A:276:TRP:CG	1:J:59:GLY:HA2	2.55	0.41
1:C:190:SER:O	1:C:194:GLN:HG2	2.21	0.41
1:E:130:GLU:O	1:E:167:ALA:HA	2.19	0.41
1:F:123:GLU:O	1:F:173:GLU:HA	2.20	0.41
1:F:233:VAL:O	1:F:233:VAL:HG13	2.20	0.41
1:F:68:ASP:O	1:F:270:ALA:HB3	2.19	0.41
1:K:150:TYR:CZ	1:K:209:LEU:HB3	2.56	0.41
1:K:202:GLU:HB3	1:K:204:PHE:CE2	2.55	0.41
1:M:133:VAL:HG23	1:M:163:CYS:HB2	2.03	0.41
1:O:85:TRP:CE3	1:O:88:THR:HG21	2.56	0.41
1:P:190:SER:O	1:P:194:GLN:HG2	2.20	0.41
1:P:220:ILE:HD13	1:P:290:TYR:HA	2.02	0.41
1:B:296:ASN:ND2	1:B:298:LEU:H	2.16	0.41
1:D:101:HIS:H	1:D:240:GLN:NE2	2.15	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:40:ILE:HD12	1:F:40:ILE:N	2.35	0.41
1:F:40:ILE:HG22	1:F:41:TYR:CD2	2.55	0.41
1:J:245:LEU:HD12	1:J:287:TYR:HB3	2.02	0.41
1:K:194:GLN:HG3	1:K:209:LEU:HA	2.02	0.41
1:K:69:HIS:HB2	1:K:254:LEU:HD13	2.02	0.41
1:A:107:ALA:HB3	1:A:169:LEU:HB2	2.03	0.41
1:C:153:LEU:HD13	1:C:159:HIS:CD2	2.56	0.41
1:F:241:HIS:CG	1:F:289:LEU:HD11	2.56	0.41
1:F:64:VAL:HG11	1:F:66:LYS:HZ3	1.85	0.41
1:G:92:TYR:HA	1:G:105:TYR:HB3	2.02	0.41
1:J:273:VAL:O	1:J:273:VAL:CG1	2.67	0.41
1:K:121:ASP:H	1:K:156:ASN:ND2	2.19	0.41
1:K:197:LEU:HD12	1:K:208:LYS:HG3	2.01	0.41
1:K:204:PHE:CD1	1:K:223:MET:HE2	2.55	0.41
1:M:225:PHE:O	1:M:284:ARG:HB2	2.20	0.41
1:B:163:CYS:HA	4:B:422:HOH:O	2.19	0.41
1:B:218:PHE:HA	1:B:293:VAL:HG22	2.03	0.41
1:B:95:THR:C	1:B:97:ALA:N	2.73	0.41
1:D:199:THR:HA	1:D:200:PRO:HD2	1.84	0.41
1:E:245:LEU:HD12	1:E:287:TYR:HB3	2.03	0.41
1:E:268:TRP:CZ2	1:E:270:ALA:HB2	2.56	0.41
1:H:241:HIS:CG	1:H:289:LEU:HD11	2.56	0.41
1:H:82:LEU:HA	1:H:83:PRO:HD3	1.95	0.41
1:J:220:ILE:HA	1:J:289:LEU:O	2.20	0.41
1:K:148:ASP:OD1	1:K:191:THR:HB	2.21	0.41
1:L:179:LEU:HD23	1:L:214:VAL:HG22	2.03	0.41
1:M:297:PRO:HG3	1:O:92:TYR:CZ	2.55	0.41
1:O:126:ILE:HG22	1:O:171:VAL:HB	2.02	0.41
1:A:40:ILE:N	1:A:40:ILE:CD1	2.66	0.41
1:D:76:SER:HB3	1:K:236:VAL:HB	2.03	0.41
1:D:42:TRP:CE2	1:E:39:PRO:HG3	2.55	0.41
1:F:81:PRO:O	1:F:83:PRO:HD3	2.20	0.41
1:I:154:PRO:HB3	1:I:184:THR:OG1	2.20	0.41
1:I:82:LEU:HD21	1:I:90:GLY:HA3	2.02	0.41
1:N:122:ILE:HG23	1:O:298:LEU:HD11	2.03	0.41
1:O:113:SER:N	1:O:163:CYS:O	2.50	0.41
1:O:204:PHE:HB3	1:O:225:PHE:CE1	2.55	0.41
1:O:245:LEU:HA	1:O:245:LEU:HD12	1.90	0.41
1:F:50:SER:H	1:F:53:HIS:CE1	2.39	0.41
1:G:130:GLU:HA	1:G:147:VAL:CG2	2.51	0.41
1:H:83:PRO:O	1:H:85:TRP:HD1	2.04	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:191:THR:O	1:I:207:ARG:HD3	2.21	0.41
1:I:277:TYR:CG	1:I:278:ALA:N	2.88	0.41
1:I:39:PRO:HB2	1:I:42:TRP:HB2	2.01	0.41
1:J:41:TYR:O	1:J:44:ALA:HB3	2.20	0.41
1:K:205:GLU:HB2	1:K:224:ASP:HB2	2.03	0.41
1:K:86:THR:HG22	4:K:424:HOH:O	2.21	0.41
1:L:122:ILE:HD13	1:L:175:ARG:HA	2.01	0.41
1:L:262:GLN:HE21	1:N:56:ASP:HB2	1.85	0.41
1:M:166:SER:O	1:M:167:ALA:HB2	2.21	0.41
1:N:83:PRO:O	1:N:85:TRP:HD1	2.04	0.41
1:P:129:VAL:O	1:P:147:VAL:HG13	2.21	0.41
1:C:133:VAL:HG23	1:C:162:ASP:O	2.20	0.41
1:E:125:LEU:CD1	1:E:125:LEU:C	2.87	0.41
1:E:39:PRO:O	1:E:42:TRP:HB2	2.21	0.41
1:G:211:PRO:C	1:G:213:SER:H	2.24	0.41
1:H:240:GLN:HB3	1:H:271:PRO:HG3	2.02	0.41
1:L:298:LEU:HA	1:L:298:LEU:HD23	1.87	0.41
1:M:237:HIS:CG	1:M:239:ASN:HD22	2.39	0.41
1:N:100:SER:HB2	1:N:240:GLN:NE2	2.35	0.41
1:O:82:LEU:HD21	1:O:105:TYR:CE1	2.56	0.41
1:P:137:ASN:OD1	1:P:140:SER:HB2	2.21	0.41
1:P:243:LEU:CD1	1:P:243:LEU:C	2.88	0.41
1:B:82:LEU:HD23	1:B:85:TRP:CD2	2.56	0.41
1:C:298:LEU:HG	1:G:103:VAL:HG13	2.02	0.41
1:G:155:PRO:O	1:G:156:ASN:CB	2.69	0.41
1:G:259:TYR:O	1:G:261:VAL:HG13	2.21	0.41
1:H:62:ARG:HD3	4:H:410:HOH:O	2.21	0.41
1:J:284:ARG:HH22	1:J:286:ARG:NH2	2.19	0.41
1:K:243:LEU:HD13	1:K:287:TYR:CB	2.46	0.41
1:M:103:VAL:HG22	1:M:173:GLU:HB2	2.03	0.41
1:N:103:VAL:HG22	1:N:173:GLU:HB2	2.02	0.41
1:N:197:LEU:HD23	1:N:208:LYS:HE3	2.02	0.41
1:P:152:TYR:O	1:P:186:LEU:HA	2.21	0.41
1:B:218:PHE:CD1	1:B:218:PHE:C	2.94	0.41
1:C:153:LEU:HD13	1:C:159:HIS:ND1	2.36	0.41
1:C:216:TYR:O	1:C:294:ASN:ND2	2.47	0.41
1:E:82:LEU:HB3	1:E:85:TRP:HB2	2.03	0.41
1:F:276:TRP:CH2	1:F:278:ALA:HB2	2.55	0.41
1:G:153:LEU:HD13	1:G:159:HIS:NE2	2.35	0.41
1:G:235:GLU:HG2	1:I:78:VAL:CG2	2.50	0.41
1:J:155:PRO:O	1:J:156:ASN:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:296:ASN:HD21	1:K:298:LEU:HD12	1.86	0.41
1:G:196:LEU:HD21	1:G:207:ARG:NH1	2.35	0.40
1:G:62:ARG:CB	1:G:73:THR:HG21	2.49	0.40
1:G:235:GLU:HG2	1:I:78:VAL:HG22	2.03	0.40
1:K:108:LYS:HD3	1:K:168:THR:HG23	2.03	0.40
1:K:85:TRP:HB3	1:K:88:THR:CG2	2.51	0.40
1:M:202:GLU:HG3	1:M:204:PHE:CE2	2.55	0.40
1:P:267:ILE:HG22	1:P:269:MET:HG3	2.03	0.40
1:B:226:GLN:O	1:B:229:GLU:HG3	2.21	0.40
1:B:40:ILE:CD1	1:B:40:ILE:H	2.24	0.40
1:C:206:LEU:CD1	1:C:221:HIS:HB3	2.50	0.40
1:H:209:LEU:C	1:H:210:LEU:HD23	2.41	0.40
1:I:243:LEU:HD12	1:I:244:LEU:C	2.42	0.40
1:I:62:ARG:HB2	1:I:73:THR:HG21	2.03	0.40
1:J:296:ASN:ND2	1:J:298:LEU:HB2	2.37	0.40
1:P:153:LEU:HD13	1:P:159:HIS:CG	2.56	0.40
1:A:232:ASN:O	1:A:234:LYS:NZ	2.39	0.40
1:C:110:LYS:HE2	1:C:110:LYS:HA	2.04	0.40
1:C:205:GLU:HB2	1:C:224:ASP:HB2	2.02	0.40
1:D:68:ASP:O	1:D:69:HIS:HB3	2.21	0.40
1:J:208:LYS:NZ	1:J:212:MET:CE	2.85	0.40
1:J:70:ALA:HB3	1:J:268:TRP:HB3	2.03	0.40
1:L:126:ILE:HG21	1:L:161:LEU:HD11	2.03	0.40
1:M:122:ILE:HD13	1:M:175:ARG:HA	2.04	0.40
1:O:208:LYS:HG2	1:O:221:HIS:CD2	2.56	0.40
1:O:85:TRP:CD2	1:O:115:SER:HA	2.55	0.40
1:A:80:SER:O	1:A:81:PRO:C	2.60	0.40
1:B:192:ASP:OD2	1:B:193:LYS:HE3	2.21	0.40
1:D:145:LEU:HD21	1:D:188:VAL:HG13	2.03	0.40
1:E:62:ARG:HH22	1:E:265:ASP:CG	2.24	0.40
1:F:85:TRP:CD2	1:F:115:SER:HA	2.56	0.40
1:F:115:SER:HB3	1:F:161:LEU:HB2	2.03	0.40
1:F:170:VAL:CG1	1:F:170:VAL:O	2.68	0.40
1:L:60:PHE:HZ	1:N:60:PHE:HZ	1.68	0.40
1:N:103:VAL:CG2	1:N:173:GLU:HB2	2.51	0.40
1:O:271:PRO:O	1:O:272:PHE:HB2	2.21	0.40
1:D:186:LEU:HD11	1:D:188:VAL:CG2	2.51	0.40
1:D:73:THR:HB	1:D:74:PRO:HD2	2.04	0.40
1:D:82:LEU:O	1:D:85:TRP:HB2	2.22	0.40
1:G:152:TYR:HB3	1:G:187:ILE:HB	2.03	0.40
1:H:208:LYS:HZ2	1:H:212:MET:CE	2.33	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:105:TYR:HE1	1:K:171:VAL:CG1	2.34	0.40
1:K:153:LEU:HA	1:K:154:PRO:HD3	1.86	0.40
1:N:243:LEU:HD23	1:N:269:MET:CE	2.52	0.40
1:O:103:VAL:CG2	1:O:173:GLU:HB2	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	254/266 (96%)	231 (91%)	18 (7%)	5 (2%)	7	14
1	B	254/266 (96%)	235 (92%)	15 (6%)	4 (2%)	9	19
1	C	254/266 (96%)	236 (93%)	15 (6%)	3 (1%)	13	27
1	D	254/266 (96%)	235 (92%)	16 (6%)	3 (1%)	13	27
1	E	254/266 (96%)	234 (92%)	18 (7%)	2 (1%)	19	39
1	F	254/266 (96%)	238 (94%)	14 (6%)	2 (1%)	19	39
1	G	254/266 (96%)	224 (88%)	24 (9%)	6 (2%)	6	10
1	H	254/266 (96%)	236 (93%)	15 (6%)	3 (1%)	13	27
1	I	254/266 (96%)	236 (93%)	18 (7%)	0	100	100
1	J	254/266 (96%)	225 (89%)	25 (10%)	4 (2%)	9	19
1	K	254/266 (96%)	220 (87%)	27 (11%)	7 (3%)	5	7
1	L	254/266 (96%)	238 (94%)	13 (5%)	3 (1%)	13	27
1	M	254/266 (96%)	229 (90%)	20 (8%)	5 (2%)	7	14
1	N	254/266 (96%)	228 (90%)	24 (9%)	2 (1%)	19	39
1	O	254/266 (96%)	229 (90%)	22 (9%)	3 (1%)	13	27
1	P	254/266 (96%)	224 (88%)	24 (9%)	6 (2%)	6	10

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	4064/4256 (96%)	3698 (91%)	308 (8%)	58 (1%)	11	22

All (58) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	141	SER
1	B	141	SER
1	C	141	SER
1	D	119	PRO
1	G	165	GLU
1	J	142	SER
1	K	141	SER
1	K	191	THR
1	K	214	VAL
1	M	141	SER
1	N	141	SER
1	C	75	GLU
1	D	180	GLY
1	D	294	ASN
1	E	75	GLU
1	G	180	GLY
1	J	157	PHE
1	K	182	HIS
1	L	75	GLU
1	L	141	SER
1	M	235	GLU
1	O	148	ASP
1	P	154	PRO
1	C	96	PRO
1	F	235	GLU
1	F	236	VAL
1	G	141	SER
1	G	167	ALA
1	K	75	GLU
1	K	165	GLU
1	P	87	ASN
1	P	148	ASP
1	P	157	PHE
1	A	112	MET
1	E	96	PRO
1	J	284	ARG
1	M	43	LYS

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

5.3.2 Protein sidechains ⓘ

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%)	214 (93%)	16 (7%)	15	30
1	B	230/237 (97%)	213 (93%)	17 (7%)	13	28
1	C	230/237 (97%)	220 (96%)	10 (4%)	29	54
1	D	230/237 (97%)	215 (94%)	15 (6%)	17	34
1	E	230/237 (97%)	218 (95%)	12 (5%)	23	46
1	F	230/237 (97%)	215 (94%)	15 (6%)	17	34
1	G	230/237 (97%)	215 (94%)	15 (6%)	17	34
1	H	230/237 (97%)	220 (96%)	10 (4%)	29	54

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	230/237 (97%)	218 (95%)	12 (5%)	23	46
1	J	230/237 (97%)	217 (94%)	13 (6%)	20	41
1	K	230/237 (97%)	214 (93%)	16 (7%)	15	30
1	L	230/237 (97%)	222 (96%)	8 (4%)	36	62
1	M	230/237 (97%)	209 (91%)	21 (9%)	9	18
1	N	230/237 (97%)	216 (94%)	14 (6%)	18	38
1	O	230/237 (97%)	214 (93%)	16 (7%)	15	30
1	P	230/237 (97%)	213 (93%)	17 (7%)	13	28
All	All	3680/3792 (97%)	3453 (94%)	227 (6%)	18	37

All (227) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	ILE
1	A	64	VAL
1	A	82	LEU
1	A	153	LEU
1	A	161	LEU
1	A	171	VAL
1	A	184	THR
1	A	222	THR
1	A	239	ASN
1	A	243	LEU
1	A	249	GLN
1	A	252	TYR
1	A	268	TRP
1	A	283	THR
1	A	286	ARG
1	A	296	ASN
1	B	50	SER
1	B	103	VAL
1	B	136	THR
1	B	143	LYS
1	B	148	ASP
1	B	153	LEU
1	B	170	VAL
1	B	171	VAL
1	B	192	ASP
1	B	197	LEU

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Mol	Chain	Res	Type
1	B	206	LEU
1	B	226	GLN
1	B	243	LEU
1	B	249	GLN
1	B	252	TYR
1	B	286	ARG
1	B	296	ASN
1	C	40	ILE
1	C	76	SER
1	C	111	GLU
1	C	148	ASP
1	C	165	GLU
1	C	171	VAL
1	C	243	LEU
1	C	249	GLN
1	C	286	ARG
1	C	298	LEU
1	D	40	ILE
1	D	84	ASP
1	D	101	HIS
1	D	125	LEU
1	D	137	ASN
1	D	171	VAL
1	D	179	LEU
1	D	199	THR
1	D	213	SER
1	D	222	THR
1	D	243	LEU
1	D	249	GLN
1	D	275	GLN
1	D	284	ARG
1	D	286	ARG
1	E	130	GLU
1	E	136	THR
1	E	147	VAL
1	E	165	GLU
1	E	166	SER
1	E	171	VAL
1	E	191	THR
1	E	192	ASP
1	E	243	LEU
1	E	249	GLN

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Mol	Chain	Res	Type
1	E	252	TYR
1	E	286	ARG
1	F	45	THR
1	F	82	LEU
1	F	96	PRO
1	F	111	GLU
1	F	136	THR
1	F	142	SER
1	F	148	ASP
1	F	171	VAL
1	F	222	THR
1	F	243	LEU
1	F	247	GLU
1	F	249	GLN
1	F	252	TYR
1	F	283	THR
1	F	286	ARG
1	G	45	THR
1	G	81	PRO
1	G	111	GLU
1	G	136	THR
1	G	137	ASN
1	G	157	PHE
1	G	163	CYS
1	G	169	LEU
1	G	171	VAL
1	G	222	THR
1	G	243	LEU
1	G	249	GLN
1	G	252	TYR
1	G	284	ARG
1	G	286	ARG
1	H	80	SER
1	H	101	HIS
1	H	153	LEU
1	H	161	LEU
1	H	171	VAL
1	H	222	THR
1	H	243	LEU
1	H	247	GLU
1	H	249	GLN
1	H	286	ARG

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Mol	Chain	Res	Type
1	I	82	LEU
1	I	111	GLU
1	I	137	ASN
1	I	145	LEU
1	I	171	VAL
1	I	222	THR
1	I	243	LEU
1	I	249	GLN
1	I	284	ARG
1	I	286	ARG
1	I	296	ASN
1	I	298	LEU
1	J	82	LEU
1	J	130	GLU
1	J	143	LYS
1	J	153	LEU
1	J	169	LEU
1	J	171	VAL
1	J	218	PHE
1	J	222	THR
1	J	224	ASP
1	J	243	LEU
1	J	249	GLN
1	J	252	TYR
1	J	285	SER
1	K	45	THR
1	K	76	SER
1	K	84	ASP
1	K	88	THR
1	K	101	HIS
1	K	105	TYR
1	K	145	LEU
1	K	156	ASN
1	K	160	SER
1	K	171	VAL
1	K	193	LYS
1	K	218	PHE
1	K	243	LEU
1	K	249	GLN
1	K	252	TYR
1	K	286	ARG
1	L	74	PRO

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Mol	Chain	Res	Type
1	L	148	ASP
1	L	171	VAL
1	L	222	THR
1	L	243	LEU
1	L	249	GLN
1	L	252	TYR
1	L	286	ARG
1	M	46	ASN
1	M	80	SER
1	M	111	GLU
1	M	137	ASN
1	M	143	LYS
1	M	144	LYS
1	M	147	VAL
1	M	148	ASP
1	M	171	VAL
1	M	183	THR
1	M	190	SER
1	M	218	PHE
1	M	222	THR
1	M	231	LEU
1	M	233	VAL
1	M	243	LEU
1	M	249	GLN
1	M	252	TYR
1	M	268	TRP
1	M	284	ARG
1	M	286	ARG
1	N	40	ILE
1	N	52	SER
1	N	134	THR
1	N	143	LYS
1	N	171	VAL
1	N	234	LYS
1	N	243	LEU
1	N	249	GLN
1	N	252	TYR
1	N	275	GLN
1	N	283	THR
1	N	286	ARG
1	N	288	LEU
1	N	296	ASN

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Mol	Chain	Res	Type
1	O	56	ASP
1	O	74	PRO
1	O	75	GLU
1	O	101	HIS
1	O	136	THR
1	O	137	ASN
1	O	147	VAL
1	O	171	VAL
1	O	237	HIS
1	O	243	LEU
1	O	249	GLN
1	O	252	TYR
1	O	283	THR
1	O	284	ARG
1	O	296	ASN
1	O	298	LEU
1	P	40	ILE
1	P	74	PRO
1	P	82	LEU
1	P	84	ASP
1	P	87	ASN
1	P	101	HIS
1	P	111	GLU
1	P	120	GLN
1	P	130	GLU
1	P	136	THR
1	P	171	VAL
1	P	183	THR
1	P	222	THR
1	P	243	LEU
1	P	249	GLN
1	P	252	TYR
1	P	296	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (107) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	87	ASN
1	A	156	ASN
1	A	182	HIS
1	A	239	ASN
1	A	240	GLN

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Mol	Chain	Res	Type
1	A	257	ASN
1	A	262	GLN
1	A	296	ASN
1	B	87	ASN
1	B	120	GLN
1	B	156	ASN
1	B	239	ASN
1	B	240	GLN
1	B	249	GLN
1	B	262	GLN
1	B	296	ASN
1	C	137	ASN
1	C	156	ASN
1	C	194	GLN
1	C	239	ASN
1	C	240	GLN
1	C	249	GLN
1	C	262	GLN
1	D	137	ASN
1	D	156	ASN
1	D	194	GLN
1	D	221	HIS
1	D	239	ASN
1	D	240	GLN
1	D	249	GLN
1	D	262	GLN
1	D	296	ASN
1	E	77	HIS
1	E	156	ASN
1	E	158	HIS
1	E	194	GLN
1	E	240	GLN
1	E	249	GLN
1	E	296	ASN
1	F	87	ASN
1	F	156	ASN
1	F	239	ASN
1	F	240	GLN
1	F	249	GLN
1	F	296	ASN
1	G	137	ASN
1	G	156	ASN

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

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Mol	Chain	Res	Type
1	N	221	HIS
1	N	240	GLN
1	N	249	GLN
1	N	262	GLN
1	N	296	ASN
1	O	53	HIS
1	O	87	ASN
1	O	137	ASN
1	O	156	ASN
1	O	239	ASN
1	O	240	GLN
1	O	296	ASN
1	P	87	ASN
1	P	156	ASN
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 32 ligands modelled in this entry, 16 are monoatomic - leaving 16 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	UGY	N	302	2	4,8,8	1.31	1 (25%)	3,10,10	1.29	1 (33%)
3	UGY	K	302	2	4,8,8	0.87	0	3,10,10	1.11	0
3	UGY	H	302	2	4,8,8	0.45	0	3,10,10	1.00	0
3	UGY	M	302	2	4,8,8	1.17	1 (25%)	3,10,10	1.07	0
3	UGY	J	302	2	4,8,8	0.82	0	3,10,10	1.12	0
3	UGY	G	302	2	4,8,8	0.67	0	3,10,10	1.19	0
3	UGY	D	302	2	4,8,8	0.71	0	3,10,10	1.12	0
3	UGY	I	302	2	4,8,8	1.07	0	3,10,10	1.36	1 (33%)
3	UGY	F	302	2	4,8,8	1.03	0	3,10,10	1.37	1 (33%)
3	UGY	C	302	2	4,8,8	0.80	0	3,10,10	1.17	0
3	UGY	E	302	2	4,8,8	1.38	1 (25%)	3,10,10	1.23	1 (33%)
3	UGY	B	302	2	4,8,8	0.97	0	3,10,10	1.14	0
3	UGY	A	302	2	4,8,8	0.84	0	3,10,10	1.23	1 (33%)
3	UGY	P	302	2	4,8,8	0.82	0	3,10,10	1.13	0
3	UGY	O	302	2	4,8,8	0.97	0	3,10,10	0.95	0
3	UGY	L	302	2	4,8,8	1.46	1 (25%)	3,10,10	1.16	0

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

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	UGY	L	302	2	-	0/3/8/8	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	302	UGY	CA-NB	2.67	1.49	1.45
3	N	302	UGY	CA-NB	2.38	1.48	1.45
3	E	302	UGY	CA-NB	2.37	1.48	1.45
3	M	302	UGY	CA-NB	2.07	1.48	1.45

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	302	UGY	OE-CG-NE	-2.29	119.28	123.22
3	I	302	UGY	OE-CG-NE	-2.19	119.46	123.22
3	N	302	UGY	OE-CG-NE	-2.15	119.53	123.22
3	A	302	UGY	OE-CG-NE	-2.02	119.76	123.22
3	E	302	UGY	OE-CG-NE	-2.00	119.78	123.22

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	302	UGY	1	0
3	J	302	UGY	1	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th 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 ²)	Q<0.9
1	A	258/266 (96%)	-0.11	1 (0%) 92 91	26, 36, 51, 57	0
1	B	258/266 (96%)	-0.03	0 100 100	25, 37, 47, 53	0
1	C	258/266 (96%)	-0.01	4 (1%) 72 68	21, 36, 51, 64	0
1	D	258/266 (96%)	-0.07	2 (0%) 86 84	24, 36, 50, 64	0
1	E	258/266 (96%)	-0.13	2 (0%) 86 84	25, 38, 53, 62	0
1	F	258/266 (96%)	-0.13	2 (0%) 86 84	26, 37, 49, 60	0
1	G	258/266 (96%)	0.13	4 (1%) 72 68	26, 43, 59, 70	0
1	H	258/266 (96%)	-0.17	0 100 100	24, 36, 50, 62	0
1	I	258/266 (96%)	0.01	0 100 100	25, 39, 51, 64	0
1	J	258/266 (96%)	0.26	5 (1%) 66 62	28, 44, 57, 67	0
1	K	258/266 (96%)	0.52	16 (6%) 20 15	30, 48, 63, 70	0
1	L	258/266 (96%)	0.16	4 (1%) 72 68	26, 42, 51, 63	0
1	M	258/266 (96%)	-0.02	0 100 100	27, 41, 55, 67	0
1	N	258/266 (96%)	0.09	8 (3%) 49 42	28, 41, 55, 66	0
1	O	258/266 (96%)	0.34	7 (2%) 54 48	30, 43, 56, 63	0
1	P	258/266 (96%)	0.41	16 (6%) 20 15	28, 45, 61, 65	0
All	All	4128/4256 (96%)	0.08	71 (1%) 70 66	21, 40, 56, 70	0

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	140	SER	4.2
1	D	141	SER	3.9
1	K	157	PHE	3.6
1	K	145	LEU	3.2
1	P	65	TYR	3.1

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Mol	Chain	Res	Type	RSRZ
1	G	181	SER	3.1
1	K	40	ILE	3.0
1	K	42	TRP	3.0
1	P	135	LEU	3.0
1	K	147	VAL	2.9
1	K	181	SER	2.9
1	O	133	VAL	2.8
1	N	112	MET	2.8
1	C	110	LYS	2.8
1	O	145	LEU	2.8
1	F	40	ILE	2.8
1	F	65	TYR	2.7
1	N	42	TRP	2.7
1	L	167	ALA	2.7
1	P	136	THR	2.7
1	P	132	ALA	2.6
1	O	88	THR	2.6
1	P	161	LEU	2.6
1	G	40	ILE	2.6
1	C	40	ILE	2.6
1	J	214	VAL	2.6
1	P	188	VAL	2.6
1	K	179	LEU	2.6
1	E	117	LEU	2.6
1	O	142	SER	2.6
1	P	112	MET	2.5
1	P	186	LEU	2.5
1	N	65	TYR	2.5
1	P	165	GLU	2.5
1	K	152	TYR	2.5
1	N	113	SER	2.5
1	N	164	VAL	2.4
1	K	111	GLU	2.4
1	P	114	SER	2.4
1	N	161	LEU	2.4
1	J	65	TYR	2.4
1	P	130	GLU	2.4
1	K	65	TYR	2.4
1	J	140	SER	2.3
1	K	216	TYR	2.3
1	P	164	VAL	2.3
1	K	186	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	J	132	ALA	2.3
1	P	137	ASN	2.3
1	L	136	THR	2.3
1	O	65	TYR	2.3
1	N	85	TRP	2.3
1	L	65	TYR	2.3
1	O	110	LYS	2.2
1	K	117	LEU	2.2
1	K	140	SER	2.2
1	P	129	VAL	2.2
1	A	112	MET	2.2
1	K	129	VAL	2.2
1	J	112	MET	2.1
1	N	40	ILE	2.1
1	P	133	VAL	2.1
1	P	39	PRO	2.1
1	O	181	SER	2.1
1	C	65	TYR	2.1
1	D	164	VAL	2.0
1	K	136	THR	2.0
1	E	140	SER	2.0
1	L	164	VAL	2.0
1	G	144	LYS	2.0
1	C	112	MET	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. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	UGY	K	302	9/9	0.88	0.17	51,52,55,55	0
3	UGY	I	302	9/9	0.90	0.17	45,50,53,54	0
3	UGY	L	302	9/9	0.91	0.16	55,55,58,59	0
3	UGY	G	302	9/9	0.94	0.14	53,54,59,61	0
3	UGY	N	302	9/9	0.95	0.18	38,40,43,44	0
3	UGY	F	302	9/9	0.95	0.17	43,46,47,47	0
3	UGY	J	302	9/9	0.95	0.14	56,56,58,58	0
3	UGY	D	302	9/9	0.95	0.16	41,43,47,49	0
3	UGY	H	302	9/9	0.95	0.18	43,45,49,51	0
3	UGY	B	302	9/9	0.96	0.14	46,47,49,50	0
3	UGY	A	302	9/9	0.96	0.16	45,46,50,52	0
3	UGY	M	302	9/9	0.96	0.13	50,51,53,53	0
3	UGY	C	302	9/9	0.96	0.14	40,43,47,49	0
3	UGY	P	302	9/9	0.96	0.13	32,36,44,46	0
3	UGY	O	302	9/9	0.97	0.12	44,46,48,49	0
2	MN	C	301	1/1	0.98	0.11	29,29,29,29	0
2	MN	H	301	1/1	0.98	0.12	33,33,33,33	0
2	MN	J	301	1/1	0.98	0.15	47,47,47,47	0
3	UGY	E	302	9/9	0.98	0.10	38,41,42,43	0
2	MN	M	301	1/1	0.99	0.11	41,41,41,41	0
2	MN	D	301	1/1	0.99	0.12	31,31,31,31	0
2	MN	A	301	1/1	0.99	0.12	36,36,36,36	0
2	MN	F	301	1/1	0.99	0.13	36,36,36,36	0
2	MN	N	301	1/1	0.99	0.14	32,32,32,32	0
2	MN	E	301	1/1	0.99	0.10	31,31,31,31	0
2	MN	P	301	1/1	0.99	0.11	33,33,33,33	0
2	MN	O	301	1/1	0.99	0.12	39,39,39,39	0
2	MN	K	301	1/1	0.99	0.11	36,36,36,36	0
2	MN	I	301	1/1	0.99	0.12	35,35,35,35	0
2	MN	B	301	1/1	0.99	0.13	32,32,32,32	0
2	MN	G	301	1/1	0.99	0.09	31,31,31,31	0
2	MN	L	301	1/1	1.00	0.13	38,38,38,38	0

6.5 Other polymers

There are no such residues in this entry.