



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:25 AM UTC

PDB ID : 4E2Q / pdb_00004e2q
Title : Crystal Structure of (S)-Ureidoglycine Aminohydrolase from *Arabidopsis thaliana*
Authors : Shin, I.; Rhee, S.
Deposited on : 2012-03-09
Resolution : 2.50 Å (reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

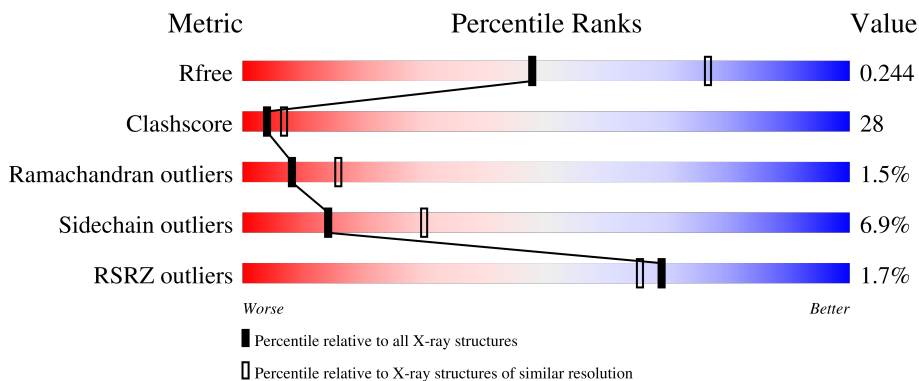
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of 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	 61% 31% . . .
1	B	266	 2% 59% 32% 6% . .
1	C	266	 2% 64% 29% 5% .
1	D	266	 57% 34% 5% .
1	E	266	 52% 41% . .

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Mol	Chain	Length	Quality of chain
1	F	266	53% 39% . . .
1	G	266	2% 48% 42% 7% .
1	H	266	2% 52% 41% 5% .
1	I	266	% 56% 35% 6% .
1	J	266	2% 50% 41% 5% .
1	K	266	6% 41% 46% 8% . .
1	L	266	% 47% 42% 7% .
1	M	266	3% 36% 53% 7% . .
1	N	266	2% 44% 47% 6% .
1	O	266	3% 36% 52% 9% .
1	P	266	2% 38% 51% 6% . .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 33964 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Ureidoglycine aminohydrolase.

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

There are 48 discrepancies between the modelled and reference sequences:

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

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

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

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

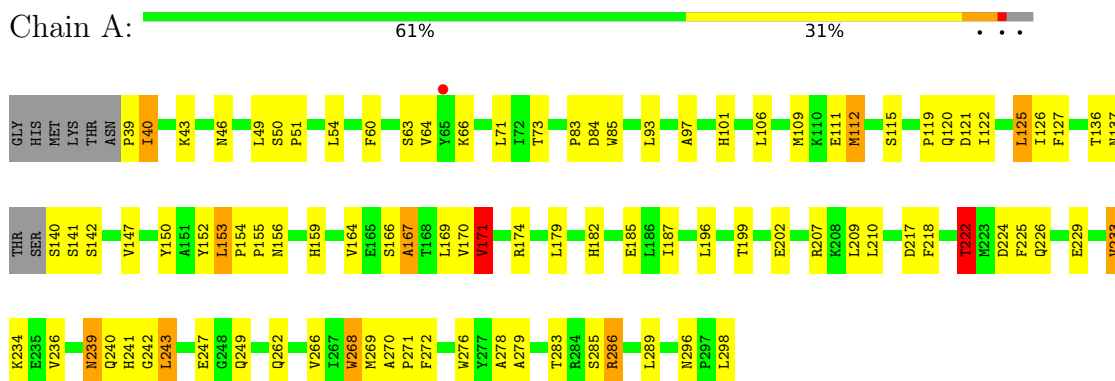
- Molecule 3 is water.

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

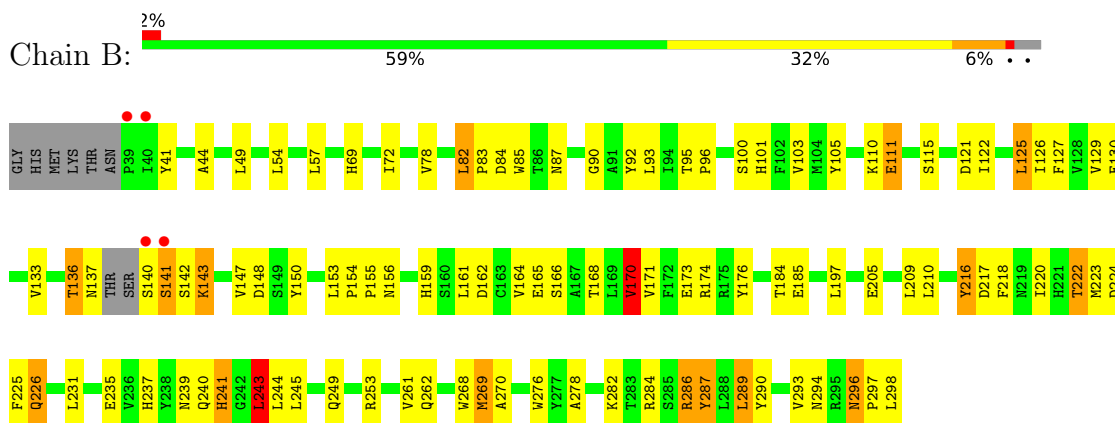
3 Residue-property plots

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

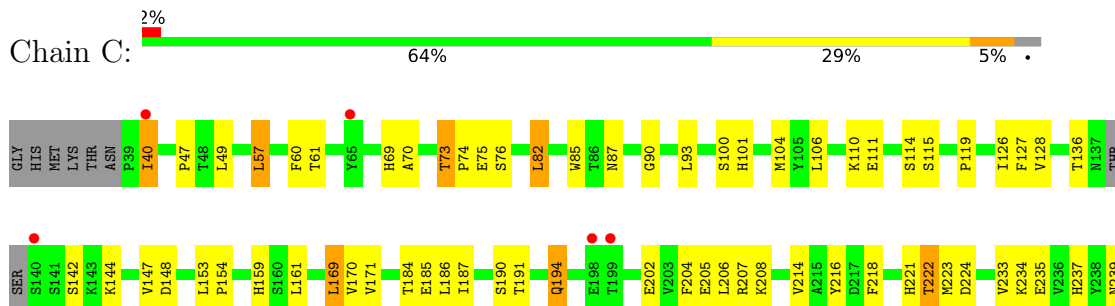
- Molecule 1: Ureidoglycine aminohydrolase



- Molecule 1: Ureidoglycine aminohydrolase



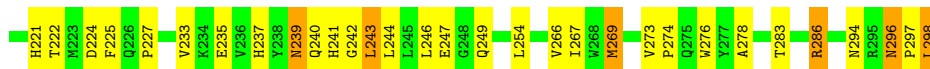
- Molecule 1: Ureidoglycine aminohydrolase





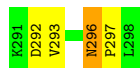
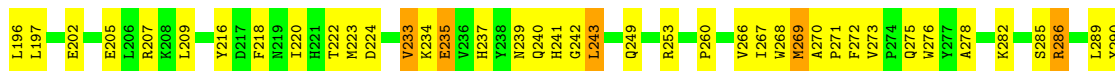
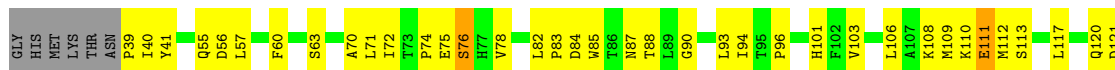
- Molecule 1: Ureidoglycine aminohydrolase

Chain D: 57% 34% 5%



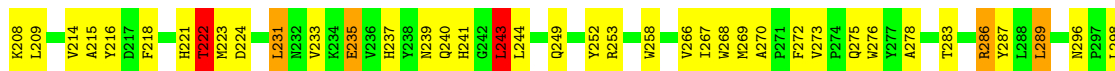
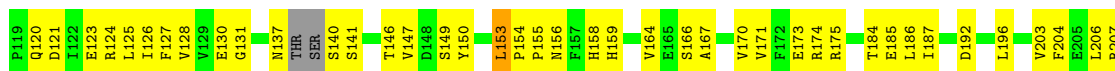
- Molecule 1: Ureidoglycine aminohydrolase

Chain E: 52% 41%



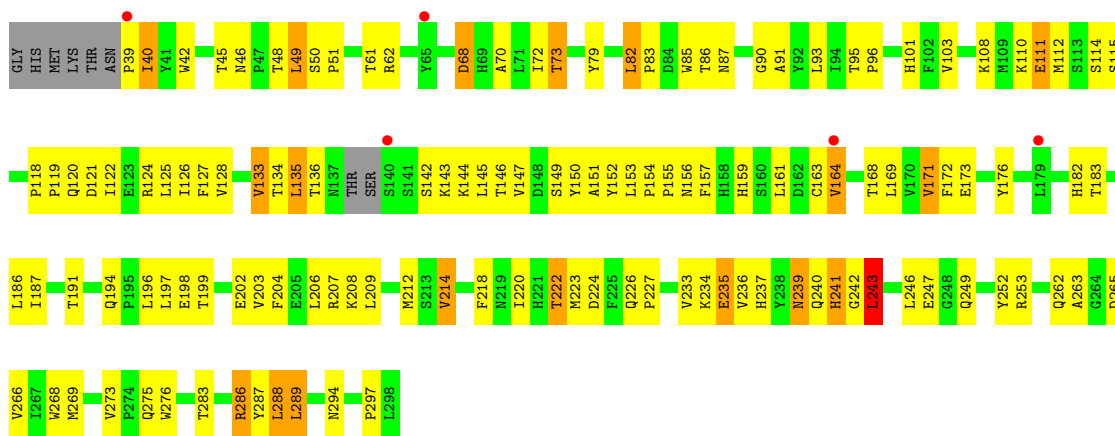
- Molecule 1: Ureidoglycine aminohydrolase

Chain F: 53% 39%

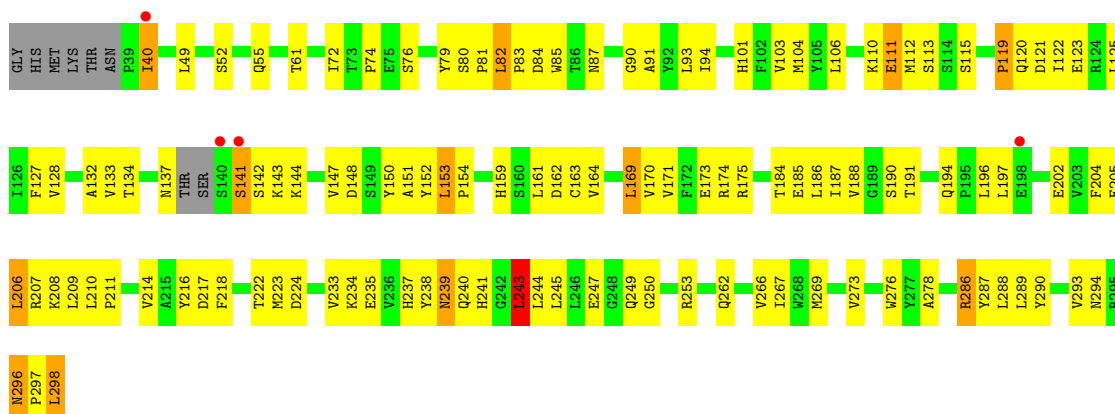


- Molecule 1: Ureidoglycine aminohydrolase

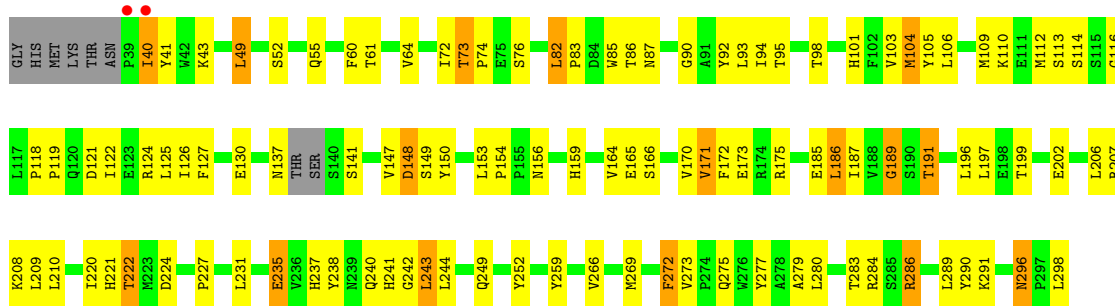
Chain G: 2% 48% 42% 7%



● Molecule 1: Ureidoglycine aminohydrolase



● Molecule 1: Ureidoglycine aminohydrolase

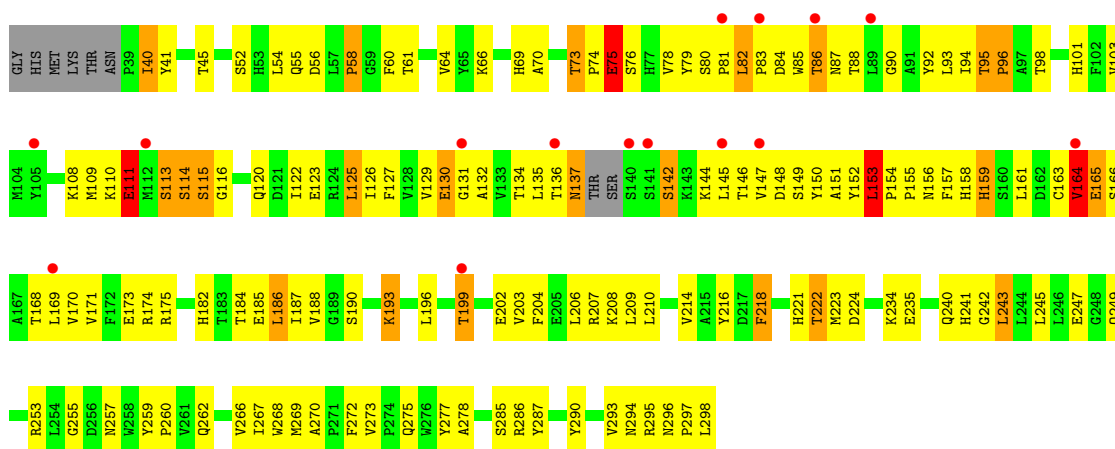


● Molecule 1: Ureidoglycine aminohydrolase

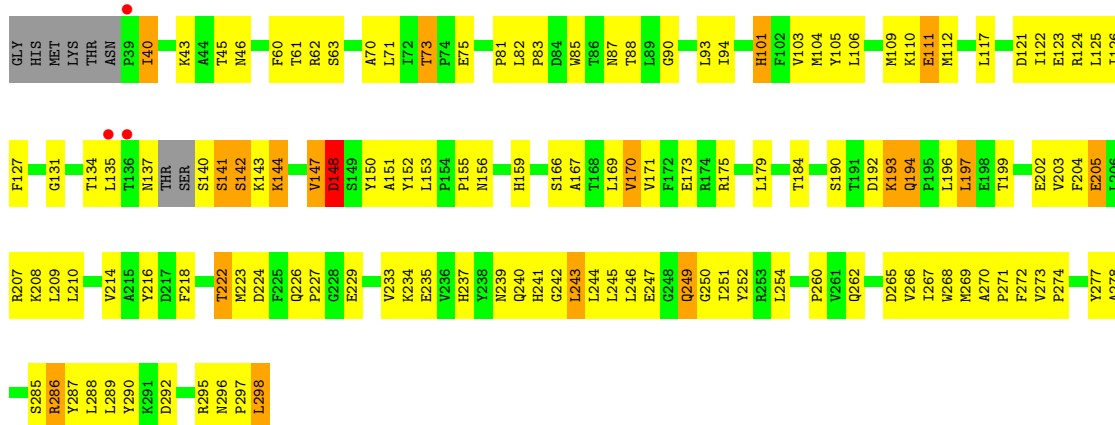




• Molecule 1: Ureidoglycine aminohydrolase

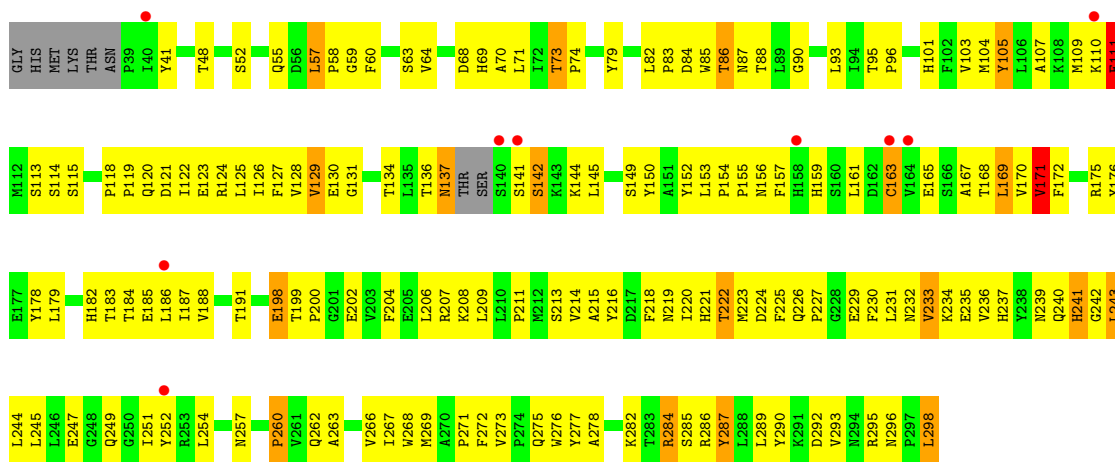


• Molecule 1: Ureidoglycine aminohydrolase

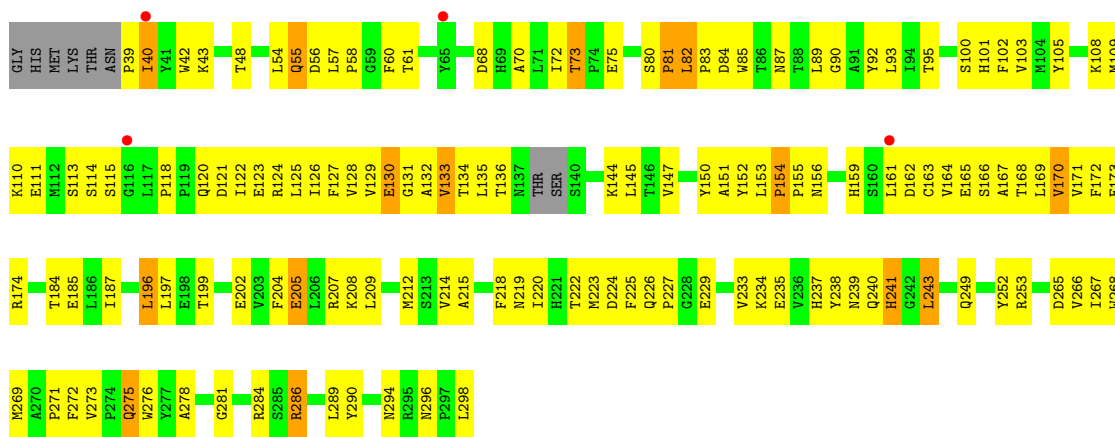


• Molecule 1: Ureidoglycine aminohydrolase

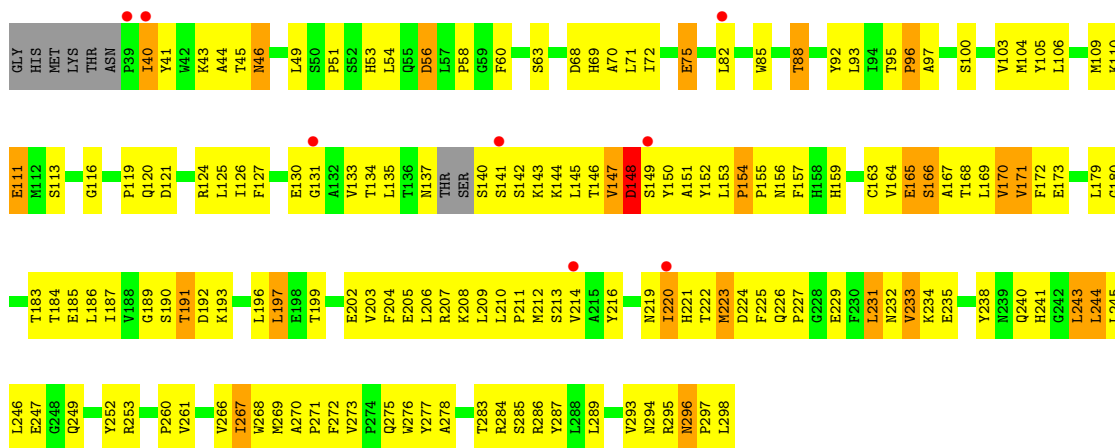




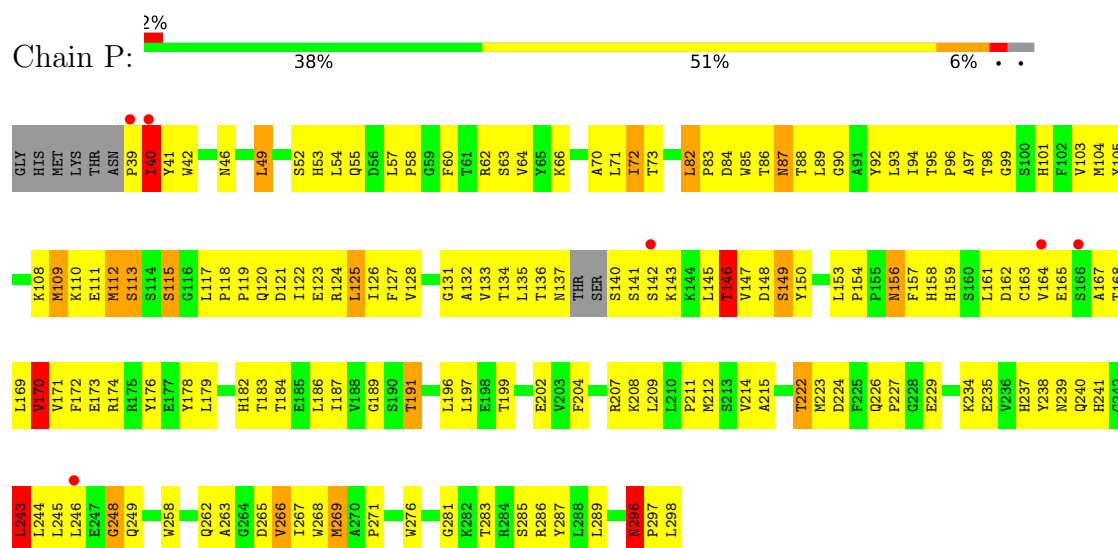
• Molecule 1: Ureidoglycine aminohydrolase



• 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	93.86Å 175.77Å 155.18Å 90.00° 99.39° 90.00°	Depositor
Resolution (Å)	50.00 – 2.50 50.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	89.1 (50.00-2.50) 97.7 (50.00-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.92 (at 2.51Å)	Xtrriage
Refinement program	CNS 1.21	Depositor
R, R_{free}	0.224 , 0.286 0.242 , 0.244	Depositor DCC
R_{free} test set	16554 reflections (9.69%)	wwPDB-VP
Wilson B-factor (Å ²)	44.5	Xtrriage
Anisotropy	0.248	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 42.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	33964	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

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

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 i

5.1 Standard geometry i

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.55	0/2140	1.00	9/2920 (0.3%)
1	B	0.53	1/2140 (0.0%)	0.98	8/2920 (0.3%)
1	C	0.56	1/2140 (0.0%)	0.98	13/2920 (0.4%)
1	D	0.54	1/2140 (0.0%)	0.98	8/2920 (0.3%)
1	E	0.55	1/2140 (0.0%)	1.01	8/2920 (0.3%)
1	F	0.51	0/2140	0.94	10/2920 (0.3%)
1	G	0.51	0/2140	1.00	13/2920 (0.4%)
1	H	0.54	1/2140 (0.0%)	1.00	7/2920 (0.2%)
1	I	0.54	1/2140 (0.0%)	1.01	8/2920 (0.3%)
1	J	0.51	0/2140	0.98	7/2920 (0.2%)
1	K	0.53	0/2140	0.99	9/2920 (0.3%)
1	L	0.51	0/2140	1.03	12/2920 (0.4%)
1	M	0.54	0/2140	1.00	13/2920 (0.4%)
1	N	0.54	0/2140	0.97	10/2920 (0.3%)
1	O	0.52	0/2140	1.02	8/2920 (0.3%)
1	P	0.53	1/2140 (0.0%)	1.00	16/2920 (0.5%)
All	All	0.53	7/34240 (0.0%)	0.99	159/46720 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	2
1	C	0	1
1	J	0	1
All	All	0	4

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	269	MET	SD-CE	-7.74	1.60	1.79
1	B	269	MET	SD-CE	-6.11	1.64	1.79
1	C	104	MET	SD-CE	-5.79	1.65	1.79
1	E	269	MET	SD-CE	-5.67	1.65	1.79
1	H	104	MET	SD-CE	-5.64	1.65	1.79
1	P	269	MET	SD-CE	-5.23	1.66	1.79
1	I	104	MET	SD-CE	-5.13	1.66	1.79

All (159) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	235	GLU	N-CA-C	9.40	124.11	110.10
1	N	235	GLU	N-CA-C	8.94	123.47	110.42
1	G	235	GLU	N-CA-C	8.74	122.58	110.35
1	E	235	GLU	N-CA-C	8.47	122.18	110.24
1	L	117	LEU	CA-C-N	8.39	125.70	119.66
1	L	117	LEU	C-N-CA	8.39	125.70	119.66
1	I	235	GLU	N-CA-C	8.22	122.32	110.24
1	O	296	ASN	CA-C-N	8.17	127.89	119.56
1	O	296	ASN	C-N-CA	8.17	127.89	119.56
1	H	294	ASN	N-CA-C	7.51	121.75	111.54
1	D	235	GLU	N-CA-C	7.50	120.82	110.24
1	B	235	GLU	N-CA-C	7.47	120.77	110.24
1	P	235	GLU	N-CA-C	7.43	121.27	110.42
1	F	235	GLU	N-CA-C	7.37	121.18	110.42
1	O	289	LEU	N-CA-C	7.36	120.41	108.41
1	G	171	VAL	N-CA-C	7.20	119.18	108.46
1	I	73	THR	CA-C-N	7.10	128.72	119.84
1	I	73	THR	C-N-CA	7.10	128.72	119.84
1	C	235	GLU	N-CA-C	7.08	120.65	110.24
1	P	248	GLY	N-CA-C	7.01	123.91	112.84
1	D	57	LEU	CA-C-N	6.72	128.24	119.84
1	D	57	LEU	C-N-CA	6.72	128.24	119.84
1	J	294	ASN	N-CA-C	6.72	120.67	111.54
1	J	171	VAL	N-CA-C	6.68	118.22	108.53
1	L	135	LEU	N-CA-C	6.68	118.59	109.11
1	H	235	GLU	N-CA-C	6.61	119.61	110.35
1	N	170	VAL	N-CA-C	-6.56	98.29	107.80
1	N	241	HIS	N-CA-C	6.52	119.34	109.23
1	A	73	THR	CA-C-N	6.51	127.98	119.84
1	A	73	THR	C-N-CA	6.51	127.98	119.84
1	L	242	GLY	N-CA-C	-6.50	97.78	113.18
1	A	242	GLY	N-CA-C	-6.38	98.06	113.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	294	ASN	N-CA-C	6.29	120.21	111.90
1	E	241	HIS	N-CA-C	6.29	118.73	109.24
1	A	171	VAL	N-CA-C	6.28	117.52	108.48
1	G	241	HIS	N-CA-C	6.25	119.22	109.52
1	K	171	VAL	N-CA-C	6.25	117.48	108.48
1	J	206	LEU	N-CA-C	6.23	119.09	109.07
1	P	99	GLY	N-CA-C	-6.13	106.58	114.85
1	P	296	ASN	CA-C-N	6.10	127.47	119.84
1	P	296	ASN	C-N-CA	6.10	127.47	119.84
1	P	243	LEU	N-CA-C	6.10	118.44	109.24
1	M	199	THR	CA-C-N	6.08	126.40	119.83
1	M	199	THR	C-N-CA	6.08	126.40	119.83
1	C	73	THR	CA-C-N	6.08	127.43	119.84
1	C	73	THR	C-N-CA	6.08	127.43	119.84
1	M	242	GLY	N-CA-C	-6.07	98.80	113.18
1	N	57	LEU	CA-C-N	6.06	127.41	119.84
1	N	57	LEU	C-N-CA	6.06	127.41	119.84
1	C	194	GLN	CA-C-N	6.01	126.51	120.14
1	C	194	GLN	C-N-CA	6.01	126.51	120.14
1	J	242	GLY	N-CA-C	-6.01	98.94	113.18
1	M	241	HIS	N-CA-C	5.97	119.40	110.14
1	G	242	GLY	N-CA-C	-5.97	99.04	113.18
1	P	73	THR	CA-C-N	5.95	127.28	119.84
1	P	73	THR	C-N-CA	5.95	127.28	119.84
1	P	170	VAL	N-CA-C	-5.91	101.40	109.55
1	G	214	VAL	N-CA-C	5.89	119.29	111.17
1	L	73	THR	CA-C-N	5.87	127.17	119.84
1	L	73	THR	C-N-CA	5.87	127.17	119.84
1	I	242	GLY	N-CA-C	-5.86	99.30	113.18
1	B	170	VAL	N-CA-C	-5.85	99.32	107.80
1	M	111	GLU	N-CA-C	5.83	118.47	110.24
1	M	260	PRO	N-CA-C	-5.82	102.06	111.19
1	D	242	GLY	N-CA-C	-5.75	99.55	113.18
1	M	57	LEU	CA-C-N	5.69	126.02	119.93
1	M	57	LEU	C-N-CA	5.69	126.02	119.93
1	B	241	HIS	N-CA-C	5.67	118.46	109.50
1	E	57	LEU	CA-C-N	5.62	126.50	119.98
1	E	57	LEU	C-N-CA	5.62	126.50	119.98
1	M	287	TYR	N-CA-C	5.61	117.71	109.24
1	C	294	ASN	N-CA-C	5.60	119.29	111.90
1	G	294	ASN	N-CA-C	5.59	119.39	112.24
1	A	46	ASN	CA-C-N	5.58	125.86	119.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	46	ASN	C-N-CA	5.58	125.86	119.83
1	I	272	PHE	N-CA-C	5.56	121.29	113.56
1	P	46	ASN	CA-C-N	5.55	125.48	119.76
1	P	46	ASN	C-N-CA	5.55	125.48	119.76
1	F	82	LEU	CA-C-N	5.55	125.56	119.90
1	F	82	LEU	C-N-CA	5.55	125.56	119.90
1	G	73	THR	CA-C-N	5.55	126.78	119.84
1	G	73	THR	C-N-CA	5.55	126.78	119.84
1	K	153	LEU	CA-C-N	5.55	126.10	120.38
1	K	153	LEU	C-N-CA	5.55	126.10	120.38
1	N	281	GLY	N-CA-C	5.55	119.69	111.76
1	E	289	LEU	N-CA-C	5.53	118.48	108.69
1	K	242	GLY	N-CA-C	-5.52	100.11	113.18
1	F	243	LEU	N-CA-C	5.51	118.20	109.50
1	P	62	ARG	N-CA-C	-5.50	106.57	113.72
1	C	57	LEU	CA-C-N	5.50	126.71	119.84
1	C	57	LEU	C-N-CA	5.50	126.71	119.84
1	A	236	VAL	N-CA-C	-5.49	97.91	109.34
1	L	101	HIS	N-CA-C	-5.48	105.81	112.88
1	E	242	GLY	N-CA-C	-5.48	100.20	113.18
1	N	73	THR	CA-C-N	5.47	126.67	119.84
1	N	73	THR	C-N-CA	5.47	126.67	119.84
1	H	206	LEU	N-CA-C	5.46	118.71	109.76
1	H	194	GLN	CA-C-N	5.42	125.62	120.31
1	H	194	GLN	C-N-CA	5.42	125.62	120.31
1	G	289	LEU	N-CA-C	5.40	117.89	108.76
1	B	294	ASN	N-CA-C	5.39	122.29	110.80
1	L	267	ILE	N-CA-C	5.39	116.25	108.48
1	F	272	PHE	N-CA-C	5.38	121.04	113.56
1	G	243	LEU	N-CA-C	5.37	117.14	108.34
1	C	296	ASN	CA-C-N	5.37	125.18	119.28
1	C	296	ASN	C-N-CA	5.37	125.18	119.28
1	C	241	HIS	N-CA-C	5.36	117.83	109.52
1	I	191	THR	N-CA-C	5.35	117.55	111.02
1	F	289	LEU	N-CA-C	5.34	118.10	108.48
1	N	166	SER	N-CA-C	5.33	116.50	108.46
1	O	46	ASN	CA-C-N	5.32	126.14	120.13
1	O	46	ASN	C-N-CA	5.32	126.14	120.13
1	C	214	VAL	N-CA-C	5.32	120.40	109.34
1	D	111	GLU	N-CA-C	5.30	117.71	110.24
1	J	236	VAL	N-CA-C	-5.30	98.32	109.34
1	L	141	SER	CB-CA-C	-5.29	110.49	116.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	267	ILE	N-CA-C	5.28	115.88	108.17
1	P	97	ALA	N-CA-C	-5.28	106.81	113.20
1	B	226	GLN	N-CA-C	-5.28	103.01	110.29
1	M	73	THR	CA-C-N	5.27	126.43	119.84
1	M	73	THR	C-N-CA	5.27	126.43	119.84
1	D	209	LEU	N-CA-C	5.24	117.08	111.36
1	N	267	ILE	N-CA-C	5.24	115.44	108.11
1	C	260	PRO	N-CA-C	-5.22	102.39	111.32
1	I	189	GLY	N-CA-C	5.21	117.62	110.69
1	K	73	THR	CA-C-N	5.20	126.33	119.84
1	K	73	THR	C-N-CA	5.20	126.33	119.84
1	L	105	TYR	N-CA-C	5.18	116.86	109.14
1	G	194	GLN	CA-C-N	5.16	125.08	119.76
1	G	194	GLN	C-N-CA	5.16	125.08	119.76
1	M	105	TYR	N-CA-C	5.16	116.91	109.07
1	E	170	VAL	N-CA-C	-5.15	100.90	108.11
1	F	222	THR	N-CA-C	-5.15	100.85	109.24
1	A	222	THR	N-CA-C	-5.13	100.05	108.41
1	M	171	VAL	N-CA-C	5.12	115.75	108.42
1	K	114	SER	N-CA-C	5.12	117.41	108.76
1	B	243	LEU	N-CA-C	5.12	117.75	109.06
1	I	175	ARG	N-CA-C	-5.11	102.08	109.59
1	P	113	SER	N-CA-C	5.11	116.83	108.55
1	B	261	VAL	N-CA-C	5.11	116.72	108.85
1	O	212	MET	N-CA-C	-5.10	106.90	113.02
1	K	287	TYR	N-CA-C	5.09	117.54	109.50
1	O	261	VAL	N-CA-C	5.09	117.16	109.12
1	H	243	LEU	N-CA-C	5.08	117.11	109.23
1	D	171	VAL	N-CA-C	5.08	116.03	108.46
1	J	44	ALA	N-CA-C	-5.08	105.39	112.45
1	B	136	THR	CB-CA-C	-5.07	108.07	114.40
1	P	189	GLY	N-CA-C	5.07	119.84	111.59
1	P	169	LEU	N-CA-C	5.06	116.66	108.41
1	J	101	HIS	N-CA-C	-5.05	106.43	112.59
1	F	50	SER	CA-C-N	5.04	125.07	119.32
1	F	50	SER	C-N-CA	5.04	125.07	119.32
1	H	214	VAL	N-CA-C	5.03	119.81	109.34
1	E	216	TYR	N-CA-C	5.03	116.94	109.25
1	G	49	LEU	N-CA-C	-5.03	100.54	108.73
1	F	105	TYR	N-CA-C	5.02	116.68	108.55
1	K	272	PHE	N-CA-C	5.02	120.53	113.56
1	L	203	VAL	N-CA-C	5.01	116.93	112.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	97	ALA	N-CA-C	-5.01	105.95	111.71

There are no chirality outliers.

All (4) planarity outliers are listed below:

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

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2076	0	2034	78	0
1	B	2076	0	2034	79	0
1	C	2076	0	2034	74	0
1	D	2076	0	2034	93	0
1	E	2076	0	2034	103	0
1	F	2076	0	2034	108	0
1	G	2076	0	2034	126	0
1	H	2076	0	2034	109	0
1	I	2076	0	2034	105	0
1	J	2076	0	2034	121	0
1	K	2076	0	2034	168	0
1	L	2076	0	2034	141	0
1	M	2076	0	2034	156	0
1	N	2076	0	2034	136	0
1	O	2076	0	2034	171	0
1	P	2076	0	2034	168	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0
2	K	1	0	0	0	0
2	L	1	0	0	0	0
2	M	1	0	0	0	0
2	N	1	0	0	0	0
2	O	1	0	0	0	0
2	P	1	0	0	0	0
3	A	67	0	0	4	0
3	B	75	0	0	3	0
3	C	80	0	0	2	0
3	D	57	0	0	2	0
3	E	50	0	0	5	0
3	F	51	0	0	6	0
3	G	44	0	0	2	0
3	H	49	0	0	3	0
3	I	39	0	0	1	0
3	J	36	0	0	2	0
3	K	36	0	0	4	0
3	L	25	0	0	0	0
3	M	24	0	0	3	0
3	N	42	0	0	1	0
3	O	28	0	0	5	0
3	P	29	0	0	2	0
All	All	33964	0	32544	1835	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 28.

All (1835) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:130:GLU:HB3	1:K:168:THR:HB	1.36	1.06
1:L:137:ASN:HD21	1:L:140:SER:HB3	1.21	1.05
1:P:121:ASP:H	1:P:156:ASN:ND2	1.53	1.05
1:P:40:ILE:H	1:P:40:ILE:HD12	1.17	1.05
1:P:196:LEU:HD21	1:P:207:ARG:HH21	1.19	1.04
1:M:136:THR:HG22	1:M:142:SER:HB2	1.40	1.03
1:G:40:ILE:H	1:G:40:ILE:HD12	1.23	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:224:ASP:OD2	1:K:286:ARG:HD3	1.59	1.02
1:K:120:GLN:HG3	1:K:156:ASN:HD21	1.21	1.01
1:N:241:HIS:HB2	1:N:269:MET:HB2	1.42	1.01
1:C:136:THR:HG22	1:C:142:SER:HB2	1.42	1.00
1:F:224:ASP:OD1	1:F:286:ARG:HD3	1.62	0.99
1:J:296:ASN:HD22	1:J:297:PRO:HD2	1.27	0.98
1:P:133:VAL:HG23	1:P:163:CYS:HB3	1.43	0.97
1:P:72:ILE:HD13	1:P:266:VAL:HG12	1.47	0.97
1:H:224:ASP:OD2	1:H:286:ARG:HD3	1.64	0.97
1:O:205:GLU:HB2	1:O:224:ASP:HB2	1.46	0.96
1:A:40:ILE:H	1:A:40:ILE:HD12	1.27	0.96
1:N:284:ARG:HH22	1:N:286:ARG:HH21	0.99	0.96
1:G:115:SER:HB3	1:G:161:LEU:HB2	1.47	0.96
1:O:40:ILE:HD13	1:O:147:VAL:HG11	1.47	0.96
1:K:153:LEU:HD13	1:K:159:HIS:NE2	1.81	0.95
1:O:147:VAL:O	1:O:148:ASP:HB2	1.67	0.94
1:F:82:LEU:HD13	1:F:90:GLY:HA3	1.50	0.93
1:H:296:ASN:ND2	1:H:298:LEU:HB2	1.83	0.93
1:A:239:ASN:HD22	1:A:239:ASN:N	1.67	0.92
1:E:296:ASN:HD22	1:E:297:PRO:HD2	1.35	0.92
1:G:136:THR:HG22	1:G:142:SER:HB2	1.52	0.91
1:P:164:VAL:HG23	1:P:165:GLU:HG2	1.50	0.91
1:P:121:ASP:H	1:P:156:ASN:HD21	1.14	0.91
1:M:208:LYS:HB3	1:M:219:ASN:HD21	1.35	0.89
1:K:88:THR:HG22	1:K:109:MET:HA	1.53	0.89
1:O:241:HIS:HB2	1:O:269:MET:HB2	1.55	0.89
1:E:40:ILE:H	1:E:40:ILE:HD12	1.35	0.89
1:I:224:ASP:OD2	1:I:286:ARG:HD3	1.74	0.88
1:A:239:ASN:H	1:A:239:ASN:ND2	1.70	0.88
1:P:243:LEU:HB3	1:P:289:LEU:HD12	1.55	0.87
1:A:239:ASN:HD22	1:A:239:ASN:H	0.90	0.87
1:C:101:HIS:H	1:C:240:GLN:HE22	1.23	0.87
1:L:121:ASP:H	1:L:156:ASN:HD21	1.22	0.87
1:H:222:THR:HG23	1:H:286:ARG:HD2	1.55	0.87
1:B:224:ASP:OD2	1:B:286:ARG:HD3	1.74	0.86
1:N:284:ARG:NH2	1:N:286:ARG:HH21	1.71	0.86
1:F:112:MET:HE1	1:F:164:VAL:HG12	1.58	0.86
1:L:144:LYS:HB2	1:L:144:LYS:NZ	1.90	0.85
1:P:104:MET:HE3	1:P:172:PHE:CZ	2.10	0.85
1:D:296:ASN:HD22	1:D:298:LEU:H	1.24	0.84
1:K:222:THR:HG23	1:K:286:ARG:HD2	1.58	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:130:GLU:HA	1:I:147:VAL:HG22	1.60	0.84
1:M:68:ASP:OD2	1:M:273:VAL:HG23	1.78	0.83
1:G:224:ASP:OD2	1:G:286:ARG:HD3	1.79	0.83
1:E:82:LEU:HD13	1:E:90:GLY:HA3	1.60	0.82
1:A:222:THR:HG23	1:A:286:ARG:HD2	1.59	0.82
1:D:40:ILE:H	1:D:40:ILE:HD12	1.43	0.82
1:M:226:GLN:O	1:M:229:GLU:HG3	1.79	0.82
1:F:241:HIS:HB2	1:F:269:MET:HB2	1.62	0.82
1:G:246:LEU:HD11	1:G:288:LEU:HD13	1.58	0.82
1:M:185:GLU:HG2	1:M:216:TYR:OH	1.80	0.81
1:L:137:ASN:ND2	1:L:140:SER:HB3	1.93	0.81
1:N:133:VAL:HG23	1:N:163:CYS:HB2	1.62	0.81
1:L:82:LEU:HD13	1:L:90:GLY:HA3	1.61	0.81
1:O:166:SER:HB2	3:O:421:HOH:O	1.79	0.81
1:K:87:ASN:ND2	1:K:110:LYS:HB2	1.95	0.81
1:J:224:ASP:OD2	1:J:286:ARG:HD3	1.79	0.81
1:P:142:SER:O	1:P:143:LYS:HG2	1.80	0.81
1:B:87:ASN:ND2	1:B:110:LYS:HB2	1.96	0.81
1:H:87:ASN:ND2	1:H:110:LYS:HB2	1.95	0.81
1:J:205:GLU:HB2	1:J:224:ASP:HB2	1.62	0.81
1:E:101:HIS:H	1:E:240:GLN:HE22	1.30	0.80
1:A:122:ILE:HD12	1:D:298:LEU:HD22	1.62	0.80
1:P:121:ASP:N	1:P:156:ASN:HD21	1.80	0.80
1:M:154:PRO:HD2	1:M:157:PHE:HD1	1.46	0.80
1:M:96:PRO:HD3	1:M:103:VAL:HG12	1.64	0.80
1:M:145:LEU:HD22	1:M:149:SER:HB3	1.65	0.79
1:C:241:HIS:HB2	1:C:269:MET:HB2	1.61	0.79
1:M:150:TYR:CE2	1:M:209:LEU:HB3	2.18	0.79
1:K:241:HIS:HB2	1:K:269:MET:HB2	1.65	0.79
1:G:128:VAL:HG12	1:G:147:VAL:HA	1.65	0.79
1:N:82:LEU:HD13	1:N:90:GLY:HA3	1.63	0.78
1:P:40:ILE:H	1:P:40:ILE:CD1	1.95	0.78
1:H:40:ILE:H	1:H:40:ILE:HD12	1.48	0.78
1:O:49:LEU:HD22	1:P:54:LEU:HD23	1.66	0.78
1:O:152:TYR:HE2	1:O:184:THR:HB	1.47	0.78
1:B:223:MET:HE1	1:B:289:LEU:HD22	1.65	0.78
1:F:93:LEU:HD13	1:F:266:VAL:HG21	1.63	0.78
1:H:137:ASN:HA	1:H:159:HIS:HA	1.65	0.78
1:H:111:GLU:H	1:H:111:GLU:CD	1.93	0.77
1:M:87:ASN:ND2	1:M:110:LYS:HB2	2.00	0.77
1:K:88:THR:HG23	1:K:113:SER:OG	1.85	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:196:LEU:CD2	1:P:207:ARG:HH21	1.98	0.77
1:K:120:GLN:HG3	1:K:156:ASN:ND2	1.97	0.77
1:H:82:LEU:HD22	1:H:90:GLY:HA3	1.67	0.77
1:D:147:VAL:HG23	3:D:443:HOH:O	1.85	0.77
1:N:126:ILE:HD11	1:N:151:ALA:HB3	1.67	0.77
1:P:39:PRO:O	1:P:42:TRP:HB2	1.83	0.77
1:P:40:ILE:HD12	1:P:40:ILE:N	1.97	0.77
1:G:247:GLU:HB2	1:G:286:ARG:HB3	1.67	0.76
1:P:186:LEU:HD12	1:P:187:ILE:N	2.01	0.76
1:E:296:ASN:ND2	1:E:297:PRO:HD2	2.00	0.76
1:L:224:ASP:OD2	1:L:286:ARG:HD3	1.85	0.76
1:L:296:ASN:HD22	1:L:297:PRO:HD2	1.50	0.76
1:A:127:PHE:HB3	1:A:170:VAL:CG1	2.16	0.76
1:H:243:LEU:HD13	1:H:287:TYR:HB2	1.68	0.76
1:A:40:ILE:HD12	1:A:40:ILE:N	2.01	0.76
1:N:115:SER:HB3	1:N:161:LEU:HB2	1.67	0.76
1:L:40:ILE:H	1:L:40:ILE:HD12	1.51	0.75
1:K:86:THR:OG1	1:K:114:SER:HB3	1.87	0.75
1:B:82:LEU:HD13	1:B:90:GLY:HA3	1.68	0.75
1:N:197:LEU:HD13	1:N:208:LYS:HG3	1.69	0.75
1:G:125:LEU:HD13	1:G:126:ILE:N	2.03	0.74
1:D:64:VAL:HG11	1:D:66:LYS:HE3	1.69	0.74
1:I:252:TYR:CD1	1:I:277:TYR:HD1	2.04	0.74
1:O:49:LEU:HD23	1:P:57:LEU:HD12	1.70	0.74
1:P:72:ILE:HD12	1:P:72:ILE:H	1.52	0.74
1:K:150:TYR:CE2	1:K:209:LEU:HB3	2.23	0.74
1:O:296:ASN:ND2	1:O:298:LEU:HB2	2.02	0.74
1:G:101:HIS:H	1:G:240:GLN:HE22	1.36	0.74
1:O:207:ARG:HB2	1:O:222:THR:OG1	1.87	0.74
1:D:101:HIS:H	1:D:240:GLN:HE22	1.35	0.74
1:D:276:TRP:CH2	1:D:278:ALA:HB2	2.23	0.74
1:L:251:ILE:HD13	1:L:260:PRO:HA	1.68	0.74
1:D:82:LEU:HD13	1:D:90:GLY:HA3	1.70	0.74
1:N:284:ARG:HH22	1:N:286:ARG:NH2	1.80	0.74
1:L:101:HIS:H	1:L:240:GLN:HE22	1.35	0.73
1:N:196:LEU:HD22	1:N:196:LEU:N	2.03	0.73
1:J:135:LEU:HB2	1:J:145:LEU:HD11	1.70	0.73
1:P:128:VAL:HG23	1:P:148:ASP:N	2.02	0.73
1:K:40:ILE:HD12	1:K:40:ILE:N	2.04	0.73
1:B:153:LEU:HD13	1:B:159:HIS:CE1	2.24	0.73
1:N:75:GLU:OE1	1:N:75:GLU:N	2.20	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:87:ASN:HD21	1:M:110:LYS:HB2	1.52	0.72
1:N:208:LYS:NZ	1:N:212:MET:HE3	2.03	0.72
1:K:193:LYS:HA	1:K:193:LYS:HE3	1.70	0.72
1:P:241:HIS:HB2	1:P:269:MET:HB2	1.71	0.72
1:K:88:THR:HG22	1:K:109:MET:CA	2.19	0.72
1:A:262:GLN:HG2	1:C:57:LEU:HD21	1.70	0.72
1:M:137:ASN:HD22	1:M:137:ASN:H	1.36	0.72
1:L:87:ASN:ND2	1:L:110:LYS:HB2	2.04	0.72
1:N:208:LYS:HZ2	1:N:212:MET:HE3	1.55	0.72
1:A:127:PHE:HB3	1:A:170:VAL:HG13	1.70	0.72
1:I:280:LEU:HD21	1:J:280:LEU:HD21	1.72	0.72
1:D:239:ASN:H	1:D:239:ASN:HD22	1.36	0.72
1:O:127:PHE:HB3	1:O:170:VAL:HG13	1.72	0.72
1:I:164:VAL:HG23	1:I:165:GLU:N	2.05	0.71
1:K:145:LEU:HD11	1:K:188:VAL:HG13	1.71	0.71
1:A:40:ILE:H	1:A:40:ILE:CD1	2.01	0.71
1:C:224:ASP:OD2	1:C:286:ARG:HD3	1.89	0.71
1:M:202:GLU:OE2	1:M:233:VAL:HG12	1.89	0.71
1:M:243:LEU:C	1:M:243:LEU:HD12	2.14	0.71
1:G:40:ILE:HD12	1:G:40:ILE:N	2.04	0.71
1:G:70:ALA:HB3	1:G:268:TRP:HB3	1.72	0.71
1:O:153:LEU:HD13	1:O:159:HIS:CD2	2.25	0.71
1:P:82:LEU:CD1	1:P:90:GLY:HA3	2.20	0.71
1:I:121:ASP:H	1:I:156:ASN:HD21	1.39	0.71
1:M:234:LYS:HE3	1:O:60:PHE:O	1.89	0.71
1:P:224:ASP:OD2	1:P:286:ARG:HD3	1.90	0.71
1:J:150:TYR:CE2	1:J:209:LEU:HB3	2.25	0.71
1:M:128:VAL:HG22	1:M:169:LEU:HD21	1.73	0.70
1:O:93:LEU:HD13	1:O:104:MET:HE2	1.73	0.70
1:P:128:VAL:HG23	1:P:148:ASP:H	1.53	0.70
1:P:186:LEU:HD12	1:P:187:ILE:H	1.56	0.70
1:J:241:HIS:HB2	1:J:269:MET:HB2	1.70	0.70
1:N:95:THR:HG23	1:O:272:PHE:HZ	1.57	0.70
1:H:153:LEU:HD13	1:H:159:HIS:CE1	2.27	0.70
1:K:218:PHE:HB2	1:K:290:TYR:CE1	2.26	0.70
1:L:127:PHE:HB3	1:L:170:VAL:HG13	1.73	0.70
1:O:235:GLU:HB2	1:O:275:GLN:HG3	1.74	0.70
1:D:137:ASN:HD21	1:D:140:SER:HB2	1.56	0.70
1:E:93:LEU:HD13	1:E:266:VAL:HG21	1.74	0.70
1:P:72:ILE:HD12	1:P:72:ILE:N	2.05	0.70
1:I:252:TYR:HD1	1:I:277:TYR:HD1	1.39	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:234:LYS:HG2	1:K:61:THR:HB	1.73	0.70
1:B:136:THR:HG22	1:B:142:SER:OG	1.92	0.70
1:B:243:LEU:HD12	1:B:244:LEU:N	2.07	0.70
1:K:153:LEU:HD13	1:K:159:HIS:CD2	2.26	0.70
1:D:59:GLY:O	1:K:253:ARG:NH1	2.25	0.69
1:G:133:VAL:HG23	1:G:163:CYS:HB2	1.74	0.69
1:O:49:LEU:HD23	1:P:57:LEU:CD1	2.22	0.69
1:O:260:PRO:O	1:P:57:LEU:HD22	1.92	0.69
1:D:241:HIS:HB2	1:D:269:MET:HB2	1.72	0.69
1:N:61:THR:HG22	1:O:253:ARG:NH1	2.08	0.69
1:P:133:VAL:CG2	1:P:163:CYS:HB3	2.18	0.69
1:F:243:LEU:C	1:F:243:LEU:HD12	2.17	0.69
1:H:243:LEU:HD22	1:H:287:TYR:CD1	2.28	0.69
1:K:296:ASN:HD22	1:K:297:PRO:HD2	1.58	0.69
1:P:128:VAL:HG21	1:P:146:THR:O	1.93	0.69
1:J:187:ILE:HD12	1:J:211:PRO:HD3	1.75	0.69
1:N:196:LEU:HD22	1:N:196:LEU:H	1.55	0.68
1:M:237:HIS:CE1	1:M:239:ASN:HB2	2.28	0.68
1:O:109:MET:HB2	1:O:167:ALA:HB3	1.74	0.68
1:P:85:TRP:HA	1:P:115:SER:O	1.94	0.68
1:K:243:LEU:HD23	1:K:269:MET:HE1	1.75	0.68
1:L:147:VAL:HG12	1:L:148:ASP:N	2.08	0.68
1:L:150:TYR:CZ	1:L:209:LEU:HB3	2.28	0.68
1:J:126:ILE:HD13	1:J:161:LEU:HD11	1.74	0.68
1:C:298:LEU:HG	1:G:103:VAL:HG13	1.74	0.68
1:E:122:ILE:HD12	1:P:298:LEU:HD13	1.74	0.68
1:H:241:HIS:HB2	1:H:269:MET:HB2	1.74	0.68
1:I:121:ASP:H	1:I:156:ASN:ND2	1.91	0.68
1:B:87:ASN:HD21	1:B:110:LYS:HB2	1.59	0.68
1:L:122:ILE:HD13	1:L:175:ARG:HA	1.73	0.68
1:O:163:CYS:HA	3:O:412:HOH:O	1.94	0.68
1:B:241:HIS:HB2	1:B:269:MET:HB2	1.76	0.67
1:G:202:GLU:OE2	1:G:233:VAL:HG12	1.94	0.67
1:L:243:LEU:HD13	1:L:287:TYR:HB2	1.76	0.67
1:C:154:PRO:HG2	1:C:185:GLU:HA	1.74	0.67
1:H:101:HIS:H	1:H:240:GLN:HE22	1.40	0.67
1:N:122:ILE:HD12	1:O:298:LEU:HD13	1.76	0.67
1:O:137:ASN:HD21	1:O:141:SER:H	1.41	0.67
1:G:115:SER:CB	1:G:161:LEU:HB2	2.23	0.67
1:F:87:ASN:ND2	1:F:110:LYS:HB2	2.10	0.67
1:M:93:LEU:HD13	1:M:266:VAL:HG21	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:243:LEU:C	1:G:243:LEU:HD12	2.20	0.67
1:H:296:ASN:HD22	1:H:298:LEU:H	1.42	0.67
1:I:87:ASN:HD21	1:I:110:LYS:HB2	1.59	0.67
1:M:182:HIS:O	1:M:183:THR:HG23	1.95	0.67
1:K:110:LYS:O	1:K:113:SER:HB2	1.94	0.67
1:K:145:LEU:HB3	1:K:149:SER:HB2	1.76	0.67
1:K:150:TYR:CD1	1:K:209:LEU:HD13	2.30	0.67
1:A:241:HIS:HB2	1:A:269:MET:HB2	1.76	0.67
1:E:243:LEU:C	1:E:243:LEU:HD12	2.20	0.66
1:K:87:ASN:HD21	1:K:110:LYS:HB2	1.60	0.66
1:M:157:PHE:HE1	1:M:186:LEU:HB2	1.60	0.66
1:F:40:ILE:HD12	1:F:40:ILE:H	1.60	0.66
1:H:296:ASN:HD22	1:H:298:LEU:HB2	1.57	0.66
1:L:144:LYS:HB2	1:L:144:LYS:HZ3	1.59	0.66
1:I:153:LEU:HD13	1:I:159:HIS:CD2	2.30	0.66
1:K:66:LYS:HD2	1:K:69:HIS:CE1	2.30	0.66
1:E:40:ILE:HA	3:E:445:HOH:O	1.94	0.66
1:L:103:VAL:CG2	1:L:173:GLU:HB2	2.26	0.66
1:N:296:ASN:ND2	1:N:298:LEU:HB2	2.10	0.66
1:O:152:TYR:HB3	1:O:187:ILE:HB	1.77	0.66
1:D:113:SER:OG	1:D:163:CYS:HB3	1.95	0.66
1:E:154:PRO:HG2	1:E:185:GLU:HA	1.77	0.66
1:L:137:ASN:HD21	1:L:140:SER:CB	2.05	0.66
1:N:40:ILE:HD12	1:N:40:ILE:H	1.59	0.66
1:G:125:LEU:HD13	1:G:125:LEU:C	2.19	0.66
1:O:152:TYR:CE2	1:O:184:THR:HB	2.30	0.66
1:D:224:ASP:OD2	1:D:286:ARG:HD3	1.95	0.66
1:O:209:LEU:O	1:O:210:LEU:HD23	1.95	0.66
1:M:137:ASN:HB2	3:M:409:HOH:O	1.95	0.66
1:D:239:ASN:H	1:D:239:ASN:ND2	1.93	0.65
1:L:243:LEU:C	1:L:243:LEU:HD12	2.21	0.65
1:M:296:ASN:ND2	1:M:298:LEU:HB2	2.11	0.65
1:D:125:LEU:C	1:D:125:LEU:HD13	2.21	0.65
1:E:113:SER:OG	1:E:163:CYS:HB3	1.96	0.65
1:E:243:LEU:HG	1:E:267:ILE:HB	1.77	0.65
1:H:111:GLU:HA	1:H:164:VAL:O	1.95	0.65
1:P:244:LEU:HD13	1:P:266:VAL:HG23	1.78	0.65
1:B:147:VAL:O	1:B:148:ASP:HB2	1.95	0.65
1:K:247:GLU:O	1:K:285:SER:HA	1.97	0.65
1:K:145:LEU:HD22	1:K:149:SER:HB3	1.79	0.65
1:M:163:CYS:HA	3:M:401:HOH:O	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:144:LYS:HD3	1:K:144:LYS:C	2.21	0.65
1:C:147:VAL:O	1:C:148:ASP:HB2	1.95	0.65
1:D:87:ASN:ND2	1:D:110:LYS:HB2	2.10	0.65
1:J:153:LEU:HD13	1:J:159:HIS:CE1	2.31	0.65
1:H:184:THR:HB	1:H:216:TYR:CE1	2.32	0.65
1:B:140:SER:O	1:B:141:SER:HB2	1.96	0.65
1:A:136:THR:HG22	1:A:142:SER:HB2	1.78	0.65
1:C:234:LYS:HG2	1:G:61:THR:HB	1.77	0.65
1:F:125:LEU:C	1:F:125:LEU:HD13	2.22	0.65
1:D:39:PRO:HG2	1:E:39:PRO:HG2	1.79	0.64
1:N:95:THR:HG21	1:O:238:TYR:HB3	1.80	0.64
1:O:157:PHE:CE2	1:O:186:LEU:HD13	2.33	0.64
1:E:164:VAL:HG23	1:E:165:GLU:H	1.61	0.64
1:K:204:PHE:CZ	1:K:223:MET:HE3	2.31	0.64
1:L:184:THR:HB	1:L:216:TYR:CE1	2.31	0.64
1:F:101:HIS:H	1:F:240:GLN:HE22	1.46	0.64
1:J:208:LYS:NZ	1:J:212:MET:HE3	2.11	0.64
1:K:130:GLU:HB3	1:K:168:THR:CB	2.22	0.64
1:P:196:LEU:HD21	1:P:207:ARG:NH2	2.04	0.64
1:B:130:GLU:HB3	1:B:168:THR:HB	1.79	0.64
1:D:126:ILE:HG22	1:D:171:VAL:HB	1.80	0.64
1:F:150:TYR:CZ	1:F:209:LEU:HB3	2.33	0.64
1:K:243:LEU:C	1:K:243:LEU:HD12	2.22	0.64
1:F:150:TYR:CE2	1:F:209:LEU:HB3	2.33	0.64
1:J:208:LYS:HZ3	1:J:212:MET:HE3	1.62	0.64
1:K:199:THR:HB	1:K:202:GLU:HB2	1.79	0.64
1:L:202:GLU:OE2	1:L:233:VAL:HG12	1.97	0.64
1:N:204:PHE:HB3	1:N:225:PHE:CE1	2.32	0.64
1:N:243:LEU:HB3	1:N:289:LEU:HD12	1.79	0.64
1:O:244:LEU:HD12	1:O:245:LEU:N	2.13	0.64
1:G:134:THR:HG23	1:G:143:LYS:O	1.98	0.64
1:J:101:HIS:H	1:J:240:GLN:HE22	1.45	0.64
1:K:103:VAL:CG2	1:K:173:GLU:HB2	2.28	0.64
1:I:87:ASN:ND2	1:I:110:LYS:HB2	2.12	0.64
1:G:40:ILE:H	1:G:40:ILE:CD1	1.99	0.64
1:G:208:LYS:NZ	1:G:212:MET:HE3	2.13	0.64
1:J:272:PHE:HZ	1:K:95:THR:HG23	1.61	0.64
1:M:111:GLU:H	1:M:111:GLU:CD	2.05	0.64
1:I:252:TYR:CD1	1:I:277:TYR:CD1	2.86	0.64
1:L:87:ASN:HD21	1:L:110:LYS:HB2	1.62	0.64
1:M:157:PHE:C	1:M:157:PHE:CD2	2.75	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:163:CYS:SG	1:O:167:ALA:HB2	2.38	0.64
1:L:207:ARG:HH11	1:L:207:ARG:HG3	1.63	0.63
1:P:89:LEU:HG	1:P:110:LYS:NZ	2.13	0.63
1:I:127:PHE:HB3	1:I:170:VAL:CG1	2.28	0.63
1:L:243:LEU:HD12	1:L:244:LEU:N	2.13	0.63
1:P:153:LEU:HD13	1:P:159:HIS:CD2	2.32	0.63
1:I:153:LEU:HD13	1:I:159:HIS:NE2	2.13	0.63
1:K:144:LYS:HE2	1:K:146:THR:HG22	1.79	0.63
1:E:40:ILE:H	1:E:40:ILE:CD1	2.11	0.63
1:K:126:ILE:HD12	1:K:126:ILE:O	1.97	0.63
1:C:111:GLU:CD	1:C:111:GLU:H	2.07	0.63
1:I:150:TYR:CE2	1:I:209:LEU:HB3	2.34	0.63
1:M:125:LEU:HD13	1:M:125:LEU:C	2.23	0.63
1:H:61:THR:HB	1:N:234:LYS:HG2	1.79	0.63
1:J:272:PHE:CZ	1:K:95:THR:HG23	2.34	0.63
1:L:153:LEU:HD13	1:L:159:HIS:NE2	2.14	0.63
1:F:86:THR:O	1:F:113:SER:HB2	1.98	0.63
1:H:120:GLN:O	1:H:121:ASP:HB2	1.99	0.63
1:K:235:GLU:HB2	1:K:275:GLN:HG3	1.80	0.63
1:J:170:VAL:HG13	1:J:170:VAL:O	1.98	0.63
1:G:234:LYS:HG2	1:I:61:THR:HB	1.81	0.62
1:H:152:TYR:HE2	1:H:154:PRO:HG3	1.64	0.62
1:O:243:LEU:HD13	1:O:287:TYR:HB2	1.79	0.62
1:P:153:LEU:HD13	1:P:159:HIS:CG	2.33	0.62
1:E:207:ARG:HB2	1:E:222:THR:OG1	1.99	0.62
1:K:199:THR:HG21	1:K:204:PHE:CZ	2.34	0.62
1:G:239:ASN:H	1:G:239:ASN:HD22	1.47	0.62
1:J:204:PHE:CZ	1:J:223:MET:HE3	2.34	0.62
1:J:298:LEU:HD11	1:K:122:ILE:HG21	1.81	0.62
1:O:296:ASN:HD21	1:O:298:LEU:HB2	1.63	0.62
1:P:132:ALA:HB2	1:P:146:THR:HA	1.81	0.62
1:C:243:LEU:C	1:C:243:LEU:HD12	2.23	0.62
1:J:137:ASN:HD21	1:J:140:SER:N	1.98	0.62
1:K:144:LYS:HE2	1:K:146:THR:CG2	2.30	0.62
1:A:179:LEU:O	1:A:182:HIS:HB2	2.00	0.62
1:C:153:LEU:HD13	1:C:159:HIS:CD2	2.35	0.62
1:M:79:TYR:HA	1:M:90:GLY:O	1.99	0.62
1:O:293:VAL:HG23	1:O:294:ASN:ND2	2.14	0.62
1:B:121:ASP:H	1:B:156:ASN:HD21	1.47	0.62
1:E:137:ASN:CG	1:E:140:SER:HB2	2.23	0.62
1:F:124:ARG:HB2	1:F:173:GLU:HG2	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:239:ASN:H	1:G:239:ASN:ND2	1.96	0.62
1:B:101:HIS:H	1:B:240:GLN:HE22	1.47	0.62
1:K:93:LEU:HD13	1:K:266:VAL:HG21	1.81	0.62
1:L:126:ILE:HB	1:L:169:LEU:HD23	1.80	0.62
1:M:157:PHE:CE1	1:M:186:LEU:HD22	2.35	0.62
1:N:93:LEU:HD13	1:N:266:VAL:HG21	1.81	0.62
1:P:118:PRO:HD3	1:P:124:ARG:NH2	2.15	0.62
1:B:115:SER:HB3	1:B:161:LEU:HB2	1.82	0.61
1:B:122:ILE:HD12	1:I:298:LEU:HD13	1.82	0.61
1:K:296:ASN:HD22	1:K:297:PRO:CD	2.12	0.61
1:L:144:LYS:HB2	1:L:144:LYS:HZ2	1.65	0.61
1:L:270:ALA:O	1:L:273:VAL:HG12	2.00	0.61
1:A:241:HIS:CG	1:A:289:LEU:HD11	2.35	0.61
1:I:60:PHE:HZ	1:K:60:PHE:HZ	1.48	0.61
1:P:109:MET:HB2	1:P:167:ALA:HB3	1.82	0.61
1:L:152:TYR:O	1:L:153:LEU:HG	2.00	0.61
1:N:103:VAL:CG2	1:N:173:GLU:HB2	2.29	0.61
1:D:49:LEU:HD11	1:G:49:LEU:HD11	1.82	0.61
1:D:243:LEU:C	1:D:243:LEU:HD12	2.25	0.61
1:H:202:GLU:OE2	1:H:233:VAL:HG12	1.99	0.61
1:L:241:HIS:HB2	1:L:269:MET:HB2	1.83	0.61
1:O:197:LEU:HD12	1:O:197:LEU:N	2.16	0.61
1:N:92:TYR:CZ	1:O:297:PRO:HG3	2.35	0.61
1:A:241:HIS:ND1	1:A:289:LEU:HD11	2.15	0.61
1:B:220:ILE:HD13	1:B:290:TYR:HA	1.83	0.61
1:D:82:LEU:CD1	1:D:90:GLY:HA3	2.30	0.61
1:J:273:VAL:HG13	1:J:273:VAL:O	2.00	0.61
1:K:152:TYR:HB2	1:K:210:LEU:HD21	1.80	0.61
1:K:204:PHE:CE1	1:K:223:MET:HE3	2.35	0.61
1:P:104:MET:HE3	1:P:172:PHE:CE1	2.35	0.61
1:D:126:ILE:HD12	1:D:126:ILE:O	2.01	0.61
1:F:47:PRO:HA	3:F:413:HOH:O	2.01	0.61
1:K:134:THR:HA	1:K:144:LYS:HA	1.82	0.61
1:P:82:LEU:HD11	1:P:90:GLY:HA3	1.83	0.61
1:P:224:ASP:OD2	1:P:286:ARG:CD	2.49	0.61
1:A:296:ASN:HD22	1:A:298:LEU:H	1.48	0.61
1:E:202:GLU:OE2	1:E:233:VAL:HG12	2.00	0.61
1:F:96:PRO:HD3	1:F:103:VAL:HG12	1.82	0.61
1:P:245:LEU:O	1:P:263:ALA:HA	2.00	0.61
1:O:247:GLU:HG2	1:O:286:ARG:HB3	1.82	0.61
1:B:125:LEU:HD13	1:B:125:LEU:C	2.26	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:204:PHE:CZ	1:G:223:MET:HE3	2.35	0.61
1:K:145:LEU:HD11	1:K:188:VAL:CG1	2.30	0.61
1:M:101:HIS:H	1:M:240:GLN:HE22	1.47	0.61
1:A:296:ASN:ND2	1:A:298:LEU:H	2.00	0.60
1:B:121:ASP:H	1:B:156:ASN:ND2	1.99	0.60
1:G:241:HIS:HD2	1:G:275:GLN:HE22	1.48	0.60
1:K:157:PHE:CZ	1:K:186:LEU:HD22	2.36	0.60
1:O:109:MET:HB3	1:O:113:SER:OG	2.00	0.60
1:O:204:PHE:HB3	1:O:225:PHE:CE1	2.36	0.60
1:H:245:LEU:HD23	1:H:262:GLN:C	2.26	0.60
1:L:249:GLN:HE21	1:N:56:ASP:CG	2.09	0.60
1:P:296:ASN:HD22	1:P:298:LEU:H	1.47	0.60
1:F:54:LEU:HD23	1:H:49:LEU:HD22	1.82	0.60
1:H:150:TYR:CE2	1:H:209:LEU:HB3	2.36	0.60
1:M:225:PHE:O	1:M:284:ARG:HB2	2.02	0.60
1:B:223:MET:CE	1:B:289:LEU:HD22	2.31	0.60
1:E:122:ILE:HD13	1:E:175:ARG:HA	1.82	0.60
1:F:224:ASP:OD1	1:F:286:ARG:HB2	2.01	0.60
1:J:40:ILE:HG22	1:J:41:TYR:CD2	2.36	0.60
1:K:137:ASN:N	1:K:137:ASN:HD22	1.98	0.60
1:O:137:ASN:ND2	1:O:141:SER:N	2.49	0.60
1:B:237:HIS:CE1	1:B:239:ASN:HB2	2.36	0.60
1:C:276:TRP:CH2	1:C:278:ALA:HB2	2.36	0.60
1:I:82:LEU:HD13	1:I:90:GLY:HA3	1.83	0.60
1:G:153:LEU:HD13	1:G:159:HIS:NE2	2.17	0.60
1:N:234:LYS:HE2	1:N:234:LYS:N	2.17	0.60
1:P:199:THR:HG21	1:P:204:PHE:CE1	2.36	0.60
1:I:72:ILE:N	1:I:72:ILE:HD12	2.17	0.60
1:O:151:ALA:HA	1:O:187:ILE:O	2.02	0.60
1:I:241:HIS:HB2	1:I:269:MET:HB2	1.83	0.60
1:I:252:TYR:HD1	1:I:277:TYR:CD1	2.19	0.60
1:L:62:ARG:HH22	1:L:265:ASP:CG	2.09	0.60
1:C:237:HIS:HB2	1:C:239:ASN:HD22	1.67	0.59
1:M:83:PRO:O	1:M:84:ASP:HB2	2.00	0.59
1:I:252:TYR:CE1	1:I:277:TYR:HB2	2.38	0.59
1:L:125:LEU:C	1:L:125:LEU:HD13	2.27	0.59
1:O:202:GLU:HG3	1:O:204:PHE:HE2	1.66	0.59
1:E:103:VAL:CG2	1:E:173:GLU:HB2	2.32	0.59
1:E:117:LEU:HD21	1:E:159:HIS:H	1.66	0.59
1:E:272:PHE:HE2	1:F:95:THR:HG1	1.50	0.59
1:K:126:ILE:HG12	1:K:161:LEU:HD11	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:204:PHE:CE1	1:G:223:MET:HE3	2.37	0.59
1:K:122:ILE:HD13	1:K:175:ARG:HA	1.84	0.59
1:A:101:HIS:O	1:A:174:ARG:HG3	2.03	0.59
1:F:208:LYS:HD3	1:F:221:HIS:NE2	2.17	0.59
1:L:121:ASP:H	1:L:156:ASN:ND2	1.97	0.59
1:L:150:TYR:CE2	1:L:209:LEU:HB3	2.37	0.59
1:L:179:LEU:HD22	1:L:295:ARG:HD3	1.84	0.59
1:M:125:LEU:HD13	1:M:126:ILE:N	2.18	0.59
1:C:74:PRO:C	1:C:76:SER:H	2.10	0.59
1:G:153:LEU:HD13	1:G:159:HIS:CE1	2.38	0.59
1:M:137:ASN:HD22	1:M:137:ASN:N	1.97	0.59
1:I:279:ALA:O	1:I:280:LEU:HD23	2.02	0.59
1:K:64:VAL:CG1	1:K:66:LYS:HE3	2.33	0.59
1:P:226:GLN:HB2	1:P:229:GLU:CD	2.28	0.59
1:D:103:VAL:HG23	1:D:173:GLU:HB2	1.84	0.59
1:H:87:ASN:HD21	1:H:110:LYS:HB2	1.65	0.59
1:I:164:VAL:HG23	1:I:165:GLU:H	1.67	0.59
1:K:64:VAL:HG11	1:K:66:LYS:HE3	1.83	0.59
1:L:126:ILE:HD13	1:L:169:LEU:HD23	1.85	0.59
1:C:70:ALA:HB3	1:C:268:TRP:HB3	1.84	0.59
1:C:101:HIS:N	1:C:240:GLN:HE22	1.97	0.59
1:M:296:ASN:ND2	1:O:119:PRO:HG2	2.18	0.59
1:P:127:PHE:HB3	1:P:170:VAL:HG13	1.85	0.59
1:P:52:SER:O	1:P:55:GLN:HG2	2.03	0.59
1:P:243:LEU:HB3	1:P:289:LEU:CD1	2.32	0.59
1:H:52:SER:O	1:H:55:GLN:HG2	2.03	0.58
1:H:207:ARG:HB2	1:H:222:THR:HB	1.85	0.58
1:E:55:GLN:HA	3:E:418:HOH:O	2.04	0.58
1:F:184:THR:HB	1:F:216:TYR:CE1	2.38	0.58
1:J:150:TYR:CZ	1:J:209:LEU:HB3	2.37	0.58
1:J:180:GLY:HA3	3:J:419:HOH:O	2.02	0.58
1:M:130:GLU:O	1:M:167:ALA:HA	2.03	0.58
1:N:133:VAL:HG23	1:N:163:CYS:CB	2.31	0.58
1:P:83:PRO:O	1:P:84:ASP:HB2	2.03	0.58
1:B:241:HIS:CE1	1:B:289:LEU:HD21	2.38	0.58
1:D:243:LEU:HD12	1:D:244:LEU:N	2.17	0.58
1:G:134:THR:OG1	1:G:144:LYS:HD3	2.02	0.58
1:G:202:GLU:HB3	1:G:204:PHE:CE2	2.38	0.58
1:M:237:HIS:ND1	1:M:239:ASN:HB2	2.18	0.58
1:F:170:VAL:O	1:F:170:VAL:HG13	2.04	0.58
1:F:206:LEU:HD12	1:F:207:ARG:H	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:204:PHE:CE1	1:L:223:MET:HE3	2.38	0.58
1:N:126:ILE:CD1	1:N:151:ALA:HB3	2.33	0.58
1:A:272:PHE:HE2	1:J:95:THR:HG1	1.51	0.58
1:P:87:ASN:OD1	1:P:110:LYS:HE2	2.03	0.58
1:F:296:ASN:HD22	1:F:298:LEU:H	1.50	0.58
1:K:218:PHE:HB2	1:K:290:TYR:HE1	1.69	0.58
1:P:92:TYR:CD1	1:P:105:TYR:HB3	2.39	0.58
1:A:126:ILE:HG22	1:A:171:VAL:HB	1.84	0.58
1:K:267:ILE:HG21	1:K:269:MET:HE2	1.86	0.58
1:N:95:THR:HG23	1:O:272:PHE:CZ	2.38	0.58
1:F:40:ILE:HD12	1:F:40:ILE:N	2.18	0.58
1:N:202:GLU:OE2	1:N:233:VAL:HG12	2.04	0.58
1:O:130:GLU:HA	3:O:419:HOH:O	2.04	0.58
1:P:84:ASP:HB3	3:P:415:HOH:O	2.02	0.58
1:P:145:LEU:HD22	1:P:149:SER:HB2	1.86	0.58
1:J:125:LEU:HD13	1:J:125:LEU:C	2.29	0.57
1:K:158:HIS:O	1:K:159:HIS:HB3	2.02	0.57
1:M:126:ILE:HD12	1:M:126:ILE:O	2.03	0.57
1:J:218:PHE:CD1	1:J:218:PHE:C	2.81	0.57
1:L:152:TYR:HB2	1:L:210:LEU:HD21	1.85	0.57
1:N:109:MET:HB2	1:N:167:ALA:HB3	1.86	0.57
1:N:199:THR:HG21	1:N:204:PHE:CE1	2.38	0.57
1:N:222:THR:HG21	1:N:286:ARG:HH11	1.68	0.57
1:O:227:PRO:HG3	1:O:283:THR:O	2.03	0.57
1:E:296:ASN:ND2	3:E:411:HOH:O	2.37	0.57
1:O:154:PRO:HB2	1:O:157:PHE:HB2	1.86	0.57
1:P:82:LEU:HD13	1:P:90:GLY:HA3	1.86	0.57
1:A:122:ILE:HD12	1:D:298:LEU:CD2	2.32	0.57
1:B:276:TRP:CH2	1:B:278:ALA:HB2	2.40	0.57
1:D:111:GLU:HA	1:D:164:VAL:O	2.05	0.57
1:L:109:MET:HB2	1:L:167:ALA:HB3	1.85	0.57
1:L:152:TYR:C	1:L:153:LEU:HG	2.29	0.57
1:N:135:LEU:HA	1:N:161:LEU:HD23	1.87	0.57
1:O:206:LEU:HD11	1:O:221:HIS:HB3	1.85	0.57
1:O:235:GLU:HB2	1:O:275:GLN:CG	2.34	0.57
1:N:234:LYS:HE2	1:N:234:LYS:H	1.69	0.57
1:P:243:LEU:HD23	1:P:289:LEU:HD13	1.85	0.57
1:I:49:LEU:HD22	1:K:54:LEU:HD23	1.87	0.57
1:J:82:LEU:HD13	1:J:90:GLY:HA3	1.86	0.57
1:O:82:LEU:O	1:O:85:TRP:HB2	2.03	0.57
1:J:141:SER:OG	1:J:142:SER:N	2.36	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:101:HIS:H	1:L:240:GLN:NE2	2.02	0.57
1:O:49:LEU:CD2	1:P:54:LEU:HD23	2.33	0.57
1:A:153:LEU:HD22	1:A:159:HIS:CG	2.40	0.57
1:F:208:LYS:HD3	1:F:221:HIS:CD2	2.39	0.57
1:K:101:HIS:H	1:K:240:GLN:HE22	1.53	0.57
1:M:153:LEU:HD13	1:M:159:HIS:CD2	2.40	0.57
1:C:186:LEU:O	1:C:187:ILE:HD13	2.05	0.57
1:I:243:LEU:HD12	1:I:243:LEU:C	2.30	0.57
1:B:85:TRP:CE3	1:B:115:SER:HA	2.40	0.56
1:N:130:GLU:HG2	1:N:131:GLY:N	2.19	0.56
1:A:152:TYR:HB3	1:A:187:ILE:HB	1.87	0.56
1:K:123:GLU:HG2	1:K:174:ARG:O	2.04	0.56
1:A:137:ASN:HD21	1:A:140:SER:N	2.03	0.56
1:B:150:TYR:CZ	1:B:209:LEU:HB3	2.40	0.56
1:G:243:LEU:HD13	1:G:287:TYR:HB2	1.88	0.56
1:I:186:LEU:HD12	1:I:187:ILE:N	2.20	0.56
1:I:227:PRO:HG3	1:I:283:THR:O	2.04	0.56
1:K:52:SER:O	1:K:55:GLN:HG2	2.05	0.56
1:K:82:LEU:O	1:K:85:TRP:HB2	2.05	0.56
1:K:126:ILE:HD12	1:K:126:ILE:C	2.29	0.56
1:L:83:PRO:O	1:L:85:TRP:HD1	1.88	0.56
1:O:192:ASP:OD1	1:O:193:LYS:HG2	2.05	0.56
1:O:202:GLU:CD	1:O:231:LEU:HD23	2.30	0.56
1:N:125:LEU:O	1:N:171:VAL:HG23	2.05	0.56
1:B:296:ASN:HD22	1:B:298:LEU:H	1.53	0.56
1:C:283:THR:HB	3:C:418:HOH:O	2.05	0.56
1:D:100:SER:HB2	1:D:240:GLN:NE2	2.20	0.56
1:I:49:LEU:HD22	1:K:54:LEU:CD2	2.36	0.56
1:I:209:LEU:O	1:I:210:LEU:HD23	2.06	0.56
1:K:125:LEU:O	1:K:125:LEU:HD13	2.06	0.56
1:A:268:TRP:CZ2	1:A:270:ALA:HB2	2.41	0.56
1:D:237:HIS:HB2	1:D:239:ASN:HD22	1.71	0.56
1:H:243:LEU:C	1:H:243:LEU:HD12	2.30	0.56
1:J:214:VAL:HG23	1:J:294:ASN:HB3	1.86	0.56
1:L:199:THR:HG21	1:L:204:PHE:CE1	2.40	0.56
1:M:153:LEU:HD13	1:M:159:HIS:NE2	2.21	0.56
1:N:40:ILE:HD13	1:N:147:VAL:HG11	1.88	0.56
1:F:243:LEU:HD12	1:F:244:LEU:N	2.20	0.56
1:H:186:LEU:O	1:H:187:ILE:HD13	2.05	0.56
1:M:127:PHE:HB3	1:M:170:VAL:CG1	2.36	0.56
1:A:63:SER:HA	1:A:71:LEU:O	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:72:ILE:H	1:N:72:ILE:HD12	1.70	0.56
1:G:253:ARG:HB3	1:G:276:TRP:HB3	1.88	0.56
1:J:102:PHE:HD2	1:J:240:GLN:HE21	1.54	0.56
1:B:243:LEU:HD12	1:B:243:LEU:C	2.31	0.56
1:E:96:PRO:HD3	1:E:103:VAL:HG12	1.87	0.56
1:K:127:PHE:HB3	1:K:170:VAL:HG13	1.87	0.56
1:N:124:ARG:HA	1:N:172:PHE:O	2.06	0.56
1:A:101:HIS:H	1:A:240:GLN:HE22	1.54	0.55
1:F:196:LEU:HD21	1:F:207:ARG:NH1	2.21	0.55
1:I:126:ILE:HD12	1:I:126:ILE:O	2.06	0.55
1:K:223:MET:O	1:K:286:ARG:HA	2.06	0.55
1:P:153:LEU:CD2	1:P:186:LEU:HD13	2.36	0.55
1:K:190:SER:O	1:K:193:LYS:N	2.37	0.55
1:M:104:MET:HE3	1:M:172:PHE:CZ	2.41	0.55
1:M:243:LEU:HG	1:M:267:ILE:HB	1.88	0.55
1:O:137:ASN:HD21	1:O:140:SER:HB3	1.70	0.55
1:D:50:SER:O	1:D:53:HIS:HB2	2.06	0.55
1:D:127:PHE:HB3	1:D:170:VAL:CG1	2.36	0.55
1:G:234:LYS:HE3	1:I:60:PHE:O	2.06	0.55
1:L:246:LEU:HD11	1:L:288:LEU:HB2	1.88	0.55
1:M:157:PHE:C	1:M:157:PHE:HD2	2.14	0.55
1:O:135:LEU:HB2	1:O:145:LEU:HD11	1.86	0.55
1:O:197:LEU:HD12	1:O:197:LEU:H	1.70	0.55
1:A:83:PRO:O	1:A:84:ASP:HB2	2.06	0.55
1:A:239:ASN:N	1:A:239:ASN:ND2	2.38	0.55
1:G:111:GLU:HA	1:G:164:VAL:O	2.07	0.55
1:K:145:LEU:HB3	1:K:149:SER:CB	2.37	0.55
1:N:296:ASN:ND2	1:N:298:LEU:H	2.03	0.55
1:C:40:ILE:HD13	1:C:147:VAL:HG11	1.88	0.55
1:D:126:ILE:HG12	1:D:161:LEU:HD11	1.89	0.55
1:P:128:VAL:CG2	1:P:149:SER:H	2.20	0.55
1:I:125:LEU:C	1:I:125:LEU:HD13	2.30	0.55
1:K:132:ALA:HB1	1:K:144:LYS:HE3	1.87	0.55
1:C:202:GLU:OE2	1:C:233:VAL:HG12	2.07	0.55
1:H:125:LEU:HD22	1:H:151:ALA:O	2.06	0.55
1:O:183:THR:HG22	1:O:184:THR:N	2.22	0.55
1:D:296:ASN:ND2	1:D:298:LEU:H	2.02	0.55
1:I:241:HIS:HB3	1:I:289:LEU:HD11	1.87	0.55
1:L:175:ARG:HH11	1:L:175:ARG:HG3	1.72	0.55
1:L:272:PHE:HZ	1:P:95:THR:HG23	1.71	0.55
1:M:120:GLN:HG3	1:M:156:ASN:HD21	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:218:PHE:CD1	1:M:218:PHE:C	2.85	0.55
1:O:204:PHE:CD1	1:O:223:MET:HG3	2.42	0.55
1:D:137:ASN:OD1	1:D:140:SER:N	2.40	0.55
1:I:119:PRO:HD2	1:I:122:ILE:HG13	1.88	0.55
1:J:126:ILE:HD13	1:J:161:LEU:CD1	2.36	0.55
1:L:205:GLU:HG3	1:L:224:ASP:HB2	1.87	0.55
1:O:271:PRO:O	1:O:272:PHE:HB2	2.07	0.55
1:P:126:ILE:C	1:P:126:ILE:HD12	2.32	0.55
1:D:202:GLU:OE2	1:D:233:VAL:HG12	2.07	0.54
1:J:176:TYR:HE2	1:J:178:TYR:HA	1.71	0.54
1:K:130:GLU:CB	1:K:168:THR:HB	2.26	0.54
1:K:185:GLU:HG3	1:K:185:GLU:O	2.05	0.54
1:N:196:LEU:H	1:N:196:LEU:CD2	2.20	0.54
1:O:70:ALA:HB3	1:O:268:TRP:HB3	1.89	0.54
1:G:96:PRO:HD3	1:G:103:VAL:HG12	1.90	0.54
1:H:204:PHE:CE1	1:H:223:MET:HE3	2.42	0.54
1:N:82:LEU:O	1:N:85:TRP:HB2	2.08	0.54
1:K:70:ALA:HB3	1:K:268:TRP:HB3	1.90	0.54
1:M:126:ILE:HD12	1:M:126:ILE:C	2.33	0.54
1:O:53:HIS:H	1:O:53:HIS:CD2	2.24	0.54
1:O:220:ILE:HG22	1:O:220:ILE:O	2.06	0.54
1:A:54:LEU:CD2	1:C:49:LEU:HD22	2.37	0.54
1:A:93:LEU:HD13	1:A:266:VAL:HG21	1.88	0.54
1:K:87:ASN:CG	1:K:110:LYS:HB2	2.33	0.54
1:M:121:ASP:H	1:M:156:ASN:ND2	2.05	0.54
1:A:54:LEU:HD23	1:C:49:LEU:HD22	1.89	0.54
1:C:93:LEU:HD11	1:C:106:LEU:HG	1.90	0.54
1:M:252:TYR:OH	1:M:269:MET:HE1	2.07	0.54
1:N:152:TYR:HB3	1:N:187:ILE:HB	1.89	0.54
1:P:94:ILE:O	1:P:103:VAL:HA	2.07	0.54
1:P:131:GLY:O	1:P:147:VAL:HG23	2.08	0.54
1:C:204:PHE:CE1	1:C:223:MET:HE3	2.42	0.54
1:H:90:GLY:HA2	1:H:106:LEU:O	2.07	0.54
1:H:119:PRO:HD2	1:H:122:ILE:HG13	1.89	0.54
1:L:153:LEU:HD13	1:L:159:HIS:CD2	2.42	0.54
1:M:206:LEU:HD12	1:M:207:ARG:H	1.72	0.54
1:O:92:TYR:HA	1:O:105:TYR:HB3	1.89	0.54
1:C:126:ILE:HD12	1:C:126:ILE:O	2.07	0.54
1:C:136:THR:HG22	1:C:142:SER:CB	2.26	0.54
1:F:127:PHE:HB3	1:F:170:VAL:CG1	2.38	0.54
1:G:118:PRO:HD3	1:G:124:ARG:CZ	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:218:PHE:HA	1:H:293:VAL:HG22	1.88	0.54
1:K:218:PHE:CG	1:K:290:TYR:HE1	2.25	0.54
1:N:92:TYR:CE1	1:O:297:PRO:HG3	2.43	0.54
1:D:154:PRO:HB3	1:D:184:THR:OG1	2.08	0.54
1:F:150:TYR:CD1	1:F:209:LEU:HD13	2.43	0.54
1:G:121:ASP:H	1:G:156:ASN:ND2	2.06	0.54
1:J:82:LEU:CD1	1:J:90:GLY:HA3	2.37	0.54
1:N:118:PRO:HD3	1:N:124:ARG:NH1	2.22	0.54
1:A:296:ASN:ND2	1:A:298:LEU:HB2	2.23	0.54
1:C:101:HIS:H	1:C:240:GLN:NE2	2.01	0.54
1:C:194:GLN:HB2	1:C:207:ARG:HD3	1.90	0.54
1:E:40:ILE:O	1:E:41:TYR:HB2	2.08	0.54
1:G:157:PHE:C	1:G:157:PHE:CD2	2.85	0.54
1:H:110:LYS:HB3	1:H:111:GLU:OE2	2.08	0.54
1:H:147:VAL:O	1:H:148:ASP:HB2	2.08	0.54
1:H:154:PRO:HG2	1:H:185:GLU:HA	1.89	0.54
1:N:222:THR:CG2	1:N:286:ARG:HH11	2.21	0.54
1:N:224:ASP:OD2	1:N:286:ARG:HB2	2.08	0.54
1:L:40:ILE:HD12	1:L:40:ILE:N	2.20	0.54
1:O:209:LEU:C	1:O:210:LEU:HD23	2.33	0.54
1:A:224:ASP:OD2	1:A:286:ARG:HD3	2.08	0.53
1:K:93:LEU:HD13	1:K:266:VAL:HG11	1.90	0.53
1:L:101:HIS:N	1:L:240:GLN:HE22	2.03	0.53
1:N:82:LEU:CD1	1:N:90:GLY:HA3	2.37	0.53
1:N:128:VAL:HA	1:N:169:LEU:HD23	1.89	0.53
1:C:185:GLU:O	1:C:187:ILE:HG12	2.09	0.53
1:D:126:ILE:HD12	1:D:126:ILE:C	2.33	0.53
1:F:128:VAL:HG23	1:F:149:SER:O	2.08	0.53
1:G:108:LYS:HG2	1:G:168:THR:HG23	1.89	0.53
1:G:136:THR:HG22	1:G:142:SER:CB	2.32	0.53
1:J:126:ILE:HD12	1:J:169:LEU:HD23	1.90	0.53
1:N:219:ASN:OD1	1:N:220:ILE:N	2.38	0.53
1:O:44:ALA:HB2	1:O:246:LEU:O	2.09	0.53
1:B:133:VAL:HG23	1:B:162:ASP:C	2.34	0.53
1:D:154:PRO:HG2	1:D:185:GLU:HA	1.88	0.53
1:K:208:LYS:HG2	1:K:221:HIS:CD2	2.43	0.53
1:L:237:HIS:HB2	1:L:239:ASN:ND2	2.23	0.53
1:L:296:ASN:HD22	1:L:297:PRO:CD	2.21	0.53
1:N:276:TRP:CH2	1:N:278:ALA:HB2	2.43	0.53
1:D:64:VAL:CG1	1:D:66:LYS:HE3	2.36	0.53
1:H:93:LEU:HD13	1:H:266:VAL:HG21	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:173:GLU:HB2	1:N:298:LEU:HD11	1.91	0.53
1:J:296:ASN:ND2	1:J:297:PRO:HD2	2.09	0.53
1:L:298:LEU:HD21	1:P:103:VAL:HG22	1.90	0.53
1:M:150:TYR:CZ	1:M:209:LEU:HB3	2.42	0.53
1:N:226:GLN:O	1:N:229:GLU:HG3	2.08	0.53
1:B:72:ILE:HD12	1:B:72:ILE:N	2.24	0.53
1:D:204:PHE:HB3	1:D:225:PHE:CE1	2.44	0.53
1:F:185:GLU:O	1:F:187:ILE:HG12	2.09	0.53
1:P:149:SER:HB3	3:P:427:HOH:O	2.09	0.53
1:A:147:VAL:HG23	3:A:440:HOH:O	2.09	0.53
1:B:129:VAL:O	1:B:129:VAL:HG12	2.07	0.53
1:I:127:PHE:HB3	1:I:170:VAL:HG12	1.90	0.53
1:K:151:ALA:HA	1:K:187:ILE:O	2.08	0.53
1:M:247:GLU:O	1:M:285:SER:HA	2.08	0.53
1:N:120:GLN:HA	1:N:156:ASN:HD21	1.74	0.53
1:P:246:LEU:O	1:P:263:ALA:HB1	2.09	0.53
1:B:226:GLN:NE2	1:B:284:ARG:HB3	2.24	0.53
1:D:196:LEU:HD21	1:D:207:ARG:NH2	2.24	0.53
1:J:93:LEU:HD13	1:J:266:VAL:HG21	1.90	0.53
1:J:152:TYR:C	1:J:153:LEU:HG	2.34	0.53
1:L:147:VAL:CG1	1:L:148:ASP:N	2.72	0.53
1:O:270:ALA:O	1:O:273:VAL:HG12	2.08	0.53
1:B:222:THR:HG23	1:B:286:ARG:HD2	1.89	0.53
1:F:153:LEU:HD13	1:F:159:HIS:NE2	2.24	0.53
1:G:222:THR:O	1:G:222:THR:HG22	2.08	0.53
1:H:101:HIS:O	1:H:174:ARG:HG3	2.09	0.53
1:O:204:PHE:CE1	1:O:223:MET:HG3	2.43	0.53
1:P:113:SER:O	1:P:162:ASP:HA	2.09	0.53
1:P:179:LEU:O	1:P:182:HIS:HB2	2.09	0.53
1:B:103:VAL:CG2	1:B:173:GLU:HB2	2.38	0.53
1:D:74:PRO:C	1:D:76:SER:H	2.17	0.53
1:M:82:LEU:O	1:M:85:TRP:HB2	2.08	0.53
1:N:218:PHE:CD1	1:N:218:PHE:C	2.86	0.53
1:O:88:THR:HG23	1:O:109:MET:HA	1.91	0.53
1:D:45:THR:HG21	1:D:130:GLU:OE2	2.09	0.53
1:H:133:VAL:HG21	1:H:161:LEU:HB3	1.90	0.53
1:J:102:PHE:HD2	1:J:240:GLN:NE2	2.07	0.53
1:K:150:TYR:CZ	1:K:209:LEU:HB3	2.43	0.53
1:M:124:ARG:CG	1:M:125:LEU:H	2.22	0.53
1:N:120:GLN:O	1:N:121:ASP:HB2	2.07	0.53
1:N:152:TYR:HE2	1:N:184:THR:HB	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:133:VAL:HA	1:P:163:CYS:CB	2.39	0.53
1:E:137:ASN:ND2	1:E:140:SER:HB2	2.24	0.52
1:O:294:ASN:O	1:O:295:ARG:NH1	2.40	0.52
1:A:121:ASP:H	1:A:156:ASN:ND2	2.06	0.52
1:M:224:ASP:OD2	1:M:286:ARG:HD2	2.08	0.52
1:C:87:ASN:ND2	1:C:110:LYS:HB2	2.25	0.52
1:F:118:PRO:HD3	1:F:124:ARG:CZ	2.39	0.52
1:I:170:VAL:HG13	1:I:170:VAL:O	2.10	0.52
1:J:297:PRO:HG3	1:K:92:TYR:CZ	2.43	0.52
1:P:64:VAL:HG11	1:P:66:LYS:HE3	1.89	0.52
1:P:101:HIS:H	1:P:240:GLN:HE22	1.57	0.52
1:G:62:ARG:HB2	1:G:73:THR:HG21	1.92	0.52
1:L:82:LEU:CD1	1:L:90:GLY:HA3	2.37	0.52
1:O:137:ASN:ND2	1:O:140:SER:HB3	2.24	0.52
1:B:150:TYR:CE2	1:B:209:LEU:HB3	2.45	0.52
1:C:40:ILE:HD12	1:C:40:ILE:N	2.25	0.52
1:C:208:LYS:HG2	1:C:221:HIS:CD2	2.44	0.52
1:J:153:LEU:HD13	1:J:159:HIS:NE2	2.24	0.52
1:B:127:PHE:HB3	1:B:170:VAL:HG13	1.92	0.52
1:F:253:ARG:NH1	1:L:61:THR:HG22	2.25	0.52
1:M:96:PRO:HD3	1:M:103:VAL:CG1	2.38	0.52
1:M:126:ILE:HG22	1:M:171:VAL:HB	1.92	0.52
1:N:204:PHE:CD1	1:N:204:PHE:C	2.88	0.52
1:A:93:LEU:HD11	1:A:106:LEU:HG	1.91	0.52
1:B:78:VAL:HG21	1:I:237:HIS:HD2	1.75	0.52
1:B:92:TYR:HA	1:B:105:TYR:HB3	1.92	0.52
1:D:87:ASN:HD21	1:D:110:LYS:HB2	1.75	0.52
1:L:243:LEU:HB2	1:L:289:LEU:CD1	2.39	0.52
1:N:296:ASN:HD22	1:N:298:LEU:H	1.57	0.52
1:O:125:LEU:HD13	1:O:126:ILE:N	2.25	0.52
1:P:54:LEU:HD22	1:P:60:PHE:CD2	2.44	0.52
1:P:204:PHE:CE1	1:P:223:MET:HE3	2.45	0.52
1:H:234:LYS:HE3	1:M:60:PHE:O	2.09	0.52
1:I:93:LEU:HD13	1:I:266:VAL:HG21	1.92	0.52
1:J:204:PHE:CE1	1:J:223:MET:HE3	2.45	0.52
1:M:290:TYR:C	1:M:290:TYR:CD2	2.87	0.52
1:N:100:SER:HA	1:N:240:GLN:HE22	1.74	0.52
1:O:155:PRO:O	1:O:156:ASN:HB2	2.09	0.52
1:P:70:ALA:HB3	1:P:268:TRP:HB3	1.91	0.52
1:P:207:ARG:HB3	1:P:222:THR:OG1	2.10	0.52
1:B:111:GLU:H	1:B:111:GLU:CD	2.18	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:127:PHE:CE1	1:G:209:LEU:HD11	2.45	0.52
1:J:135:LEU:HB2	1:J:145:LEU:CD1	2.38	0.52
1:N:68:ASP:OD2	1:N:273:VAL:HG23	2.10	0.52
1:K:196:LEU:HD21	1:K:207:ARG:NH2	2.25	0.52
1:M:122:ILE:HD13	1:M:175:ARG:HA	1.91	0.52
1:N:196:LEU:N	1:N:196:LEU:CD2	2.73	0.52
1:O:93:LEU:CD1	1:O:104:MET:HE2	2.40	0.52
1:O:243:LEU:HD12	1:O:244:LEU:N	2.25	0.52
1:K:152:TYR:C	1:K:153:LEU:HG	2.35	0.51
1:O:150:TYR:CD1	1:O:209:LEU:HD13	2.45	0.51
1:A:60:PHE:HZ	1:C:60:PHE:HZ	1.59	0.51
1:B:140:SER:O	1:B:141:SER:CB	2.58	0.51
1:E:90:GLY:HA2	1:E:106:LEU:O	2.11	0.51
1:L:137:ASN:OD1	1:L:137:ASN:O	2.28	0.51
1:M:204:PHE:CE1	1:M:223:MET:HG2	2.46	0.51
1:A:296:ASN:HD22	1:A:298:LEU:HB2	1.74	0.51
1:B:165:GLU:O	1:B:166:SER:HB3	2.10	0.51
1:C:100:SER:HB3	1:C:268:TRP:CH2	2.45	0.51
1:C:184:THR:HB	1:C:216:TYR:CE1	2.45	0.51
1:G:82:LEU:HD13	1:G:90:GLY:HA3	1.92	0.51
1:D:119:PRO:HG2	1:K:296:ASN:OD1	2.11	0.51
1:E:126:ILE:C	1:E:126:ILE:HD12	2.35	0.51
1:H:40:ILE:HD12	1:H:40:ILE:N	2.22	0.51
1:H:143:LYS:HD3	1:H:188:VAL:HG11	1.93	0.51
1:H:238:TYR:CE2	1:H:297:PRO:HB3	2.46	0.51
1:P:111:GLU:O	1:P:112:MET:HB2	2.10	0.51
1:E:147:VAL:O	1:E:148:ASP:HB2	2.11	0.51
1:G:150:TYR:CZ	1:G:209:LEU:HB3	2.46	0.51
1:K:123:GLU:HB3	1:K:155:PRO:HD3	1.91	0.51
1:O:197:LEU:CD1	1:O:207:ARG:HA	2.41	0.51
1:P:135:LEU:HA	1:P:161:LEU:HD23	1.92	0.51
1:P:243:LEU:C	1:P:243:LEU:HD12	2.35	0.51
1:C:126:ILE:HD12	1:C:126:ILE:C	2.35	0.51
1:N:93:LEU:CD1	1:N:266:VAL:HG21	2.40	0.51
1:N:121:ASP:H	1:N:156:ASN:ND2	2.08	0.51
1:N:205:GLU:O	1:N:223:MET:HA	2.11	0.51
1:G:101:HIS:N	1:G:240:GLN:HE22	2.07	0.51
1:I:101:HIS:H	1:I:240:GLN:HE22	1.58	0.51
1:J:147:VAL:O	1:J:148:ASP:HB2	2.10	0.51
1:L:202:GLU:HB3	1:L:204:PHE:CE2	2.46	0.51
1:L:207:ARG:HB2	1:L:222:THR:CG2	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:104:MET:HE3	1:M:172:PHE:HZ	1.73	0.51
1:M:224:ASP:OD2	1:M:286:ARG:CD	2.59	0.51
1:N:82:LEU:HD13	1:N:90:GLY:CA	2.38	0.51
1:A:202:GLU:OE2	1:A:233:VAL:HG12	2.10	0.51
1:I:105:TYR:CE1	1:I:171:VAL:CG1	2.94	0.51
1:K:170:VAL:HG13	1:K:170:VAL:O	2.11	0.51
1:L:93:LEU:HD12	1:L:104:MET:HE2	1.93	0.51
1:M:157:PHE:CE1	1:M:186:LEU:HB2	2.44	0.51
1:O:93:LEU:HD11	1:O:106:LEU:HG	1.93	0.51
1:F:214:VAL:HG13	1:F:215:ALA:N	2.26	0.51
1:J:63:SER:HA	1:J:71:LEU:O	2.11	0.51
1:J:66:LYS:HD2	1:J:69:HIS:CE1	2.46	0.51
1:M:115:SER:HB3	1:M:161:LEU:HB2	1.93	0.51
1:M:235:GLU:HB2	1:M:275:GLN:HG3	1.93	0.51
1:H:239:ASN:HD22	1:H:239:ASN:H	1.59	0.51
1:H:298:LEU:O	1:M:96:PRO:HG2	2.09	0.51
1:L:104:MET:HE1	1:L:266:VAL:HG13	1.92	0.51
1:L:197:LEU:HD22	1:L:208:LYS:HE3	1.93	0.51
1:M:41:TYR:HE2	1:M:247:GLU:OE1	1.93	0.51
1:M:145:LEU:CD2	1:M:149:SER:HB3	2.39	0.51
1:M:153:LEU:HD22	1:M:159:HIS:CG	2.46	0.51
1:M:179:LEU:CD2	1:M:214:VAL:HG22	2.40	0.51
1:O:130:GLU:HB3	1:O:168:THR:HB	1.93	0.51
1:O:146:THR:O	1:O:147:VAL:C	2.53	0.51
1:C:114:SER:HA	1:C:161:LEU:O	2.11	0.50
1:G:153:LEU:HD23	1:G:186:LEU:CD1	2.40	0.50
1:O:240:GLN:HB3	1:O:271:PRO:HG3	1.93	0.50
1:D:218:PHE:CD1	1:D:218:PHE:C	2.90	0.50
1:E:72:ILE:HD12	1:E:72:ILE:N	2.26	0.50
1:L:237:HIS:HB2	1:L:239:ASN:HD22	1.77	0.50
1:L:251:ILE:CD1	1:L:260:PRO:HA	2.38	0.50
1:M:118:PRO:HD3	1:M:124:ARG:CZ	2.42	0.50
1:E:82:LEU:HD23	1:E:85:TRP:CD2	2.46	0.50
1:E:196:LEU:O	1:E:197:LEU:HD23	2.11	0.50
1:J:114:SER:HA	1:J:161:LEU:O	2.11	0.50
1:J:207:ARG:HH11	1:J:207:ARG:HG3	1.75	0.50
1:M:127:PHE:O	1:M:170:VAL:HG12	2.10	0.50
1:M:155:PRO:O	1:M:156:ASN:HB2	2.10	0.50
1:M:227:PRO:HG2	1:M:282:LYS:O	2.11	0.50
1:O:149:SER:HA	1:O:189:GLY:O	2.12	0.50
1:F:252:TYR:OH	1:F:269:MET:HE1	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:184:THR:HG22	1:K:216:TYR:CD1	2.46	0.50
1:L:205:GLU:CG	1:L:224:ASP:HB2	2.41	0.50
1:N:199:THR:OG1	1:N:202:GLU:HB2	2.12	0.50
1:E:40:ILE:HD12	1:E:40:ILE:N	2.16	0.50
1:I:164:VAL:CG2	1:I:165:GLU:N	2.73	0.50
1:M:271:PRO:O	1:M:272:PHE:HB2	2.11	0.50
1:B:155:PRO:HG3	1:B:176:TYR:CD2	2.47	0.50
1:C:205:GLU:HB2	1:C:224:ASP:HB2	1.94	0.50
1:E:74:PRO:C	1:E:76:SER:H	2.19	0.50
1:E:125:LEU:HD13	1:E:125:LEU:C	2.37	0.50
1:F:222:THR:HG23	1:F:286:ARG:HD2	1.92	0.50
1:G:157:PHE:CZ	1:G:186:LEU:HD22	2.46	0.50
1:B:125:LEU:HD13	1:B:126:ILE:N	2.26	0.50
1:F:137:ASN:ND2	1:F:140:SER:N	2.59	0.50
1:L:193:LYS:O	1:L:194:GLN:C	2.55	0.50
1:L:298:LEU:HD23	1:P:103:VAL:HG13	1.94	0.50
1:N:40:ILE:HD12	1:N:40:ILE:N	2.27	0.50
1:N:133:VAL:O	1:N:145:LEU:N	2.41	0.50
1:N:133:VAL:CG2	1:N:163:CYS:HB2	2.38	0.50
1:N:199:THR:HG21	1:N:204:PHE:HE1	1.77	0.50
1:N:226:GLN:HB2	1:N:229:GLU:CD	2.37	0.50
1:J:150:TYR:CD1	1:J:209:LEU:HD13	2.47	0.50
1:K:88:THR:CG2	1:K:109:MET:HA	2.33	0.50
1:K:218:PHE:C	1:K:218:PHE:CD1	2.89	0.50
1:L:111:GLU:O	1:L:112:MET:C	2.54	0.50
1:N:243:LEU:HB3	1:N:289:LEU:CD1	2.42	0.50
1:O:53:HIS:CD2	1:O:53:HIS:N	2.80	0.50
1:O:260:PRO:HB3	1:P:58:PRO:O	2.11	0.50
1:P:96:PRO:HD3	1:P:103:VAL:HG13	1.94	0.50
1:P:128:VAL:HG23	1:P:128:VAL:O	2.11	0.50
1:G:82:LEU:CD1	1:G:90:GLY:HA3	2.42	0.49
1:H:111:GLU:HB3	3:H:443:HOH:O	2.12	0.49
1:I:94:ILE:O	1:I:103:VAL:HA	2.11	0.49
1:K:243:LEU:HG	1:K:267:ILE:HB	1.94	0.49
1:P:118:PRO:HB3	1:P:124:ARG:HH21	1.76	0.49
1:B:296:ASN:HD22	1:B:297:PRO:N	2.09	0.49
1:D:198:GLU:HG2	3:D:450:HOH:O	2.10	0.49
1:E:205:GLU:HB2	1:E:224:ASP:HB2	1.94	0.49
1:G:155:PRO:HG3	1:G:176:TYR:CD2	2.47	0.49
1:H:79:TYR:CD1	1:H:91:ALA:HB2	2.47	0.49
1:I:43:LYS:N	3:I:438:HOH:O	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:104:MET:HE3	1:I:172:PHE:CZ	2.47	0.49
1:J:86:THR:O	1:J:87:ASN:C	2.54	0.49
1:P:150:TYR:CZ	1:P:209:LEU:HB3	2.46	0.49
1:G:241:HIS:CD2	1:G:275:GLN:HE22	2.28	0.49
1:K:40:ILE:O	1:K:41:TYR:HB2	2.11	0.49
1:K:109:MET:SD	1:K:169:LEU:HD11	2.52	0.49
1:K:208:LYS:HE2	1:K:221:HIS:NE2	2.27	0.49
1:L:63:SER:HA	1:L:71:LEU:O	2.13	0.49
1:L:93:LEU:HD11	1:L:106:LEU:HG	1.95	0.49
1:M:204:PHE:CZ	1:M:223:MET:HE3	2.47	0.49
1:M:230:PHE:CD1	1:M:230:PHE:O	2.65	0.49
1:N:70:ALA:HB3	1:N:268:TRP:HB3	1.94	0.49
1:N:87:ASN:ND2	1:N:110:LYS:HB2	2.27	0.49
1:B:205:GLU:HB2	1:B:224:ASP:HB2	1.93	0.49
1:D:41:TYR:CZ	1:D:246:LEU:HD13	2.47	0.49
1:D:49:LEU:CD1	1:G:49:LEU:HD11	2.42	0.49
1:I:90:GLY:HA2	1:I:106:LEU:O	2.12	0.49
1:J:133:VAL:O	1:J:145:LEU:HB2	2.11	0.49
1:K:131:GLY:HA3	1:K:166:SER:O	2.13	0.49
1:L:196:LEU:HD11	1:L:207:ARG:NH2	2.27	0.49
1:N:243:LEU:O	1:N:266:VAL:HG13	2.12	0.49
1:B:125:LEU:C	1:B:125:LEU:CD1	2.85	0.49
1:B:296:ASN:ND2	1:B:298:LEU:H	2.11	0.49
1:D:154:PRO:HG2	1:D:185:GLU:CA	2.42	0.49
1:F:150:TYR:CG	1:F:209:LEU:HD13	2.48	0.49
1:G:120:GLN:HG3	1:G:156:ASN:HD21	1.77	0.49
1:H:239:ASN:H	1:H:239:ASN:ND2	2.08	0.49
1:I:150:TYR:CE1	1:I:209:LEU:HD22	2.47	0.49
1:I:243:LEU:HD12	1:I:244:LEU:N	2.27	0.49
1:P:95:THR:O	1:P:98:THR:HG23	2.13	0.49
1:P:121:ASP:N	1:P:156:ASN:ND2	2.36	0.49
1:P:153:LEU:HD22	1:P:157:PHE:CD2	2.47	0.49
1:B:83:PRO:O	1:B:84:ASP:HB2	2.12	0.49
1:C:73:THR:HG22	1:C:265:ASP:OD1	2.12	0.49
1:C:241:HIS:CE1	1:C:289:LEU:HD21	2.47	0.49
1:D:153:LEU:HD13	1:D:159:HIS:NE2	2.27	0.49
1:D:170:VAL:HG13	1:D:170:VAL:O	2.12	0.49
1:F:196:LEU:HD21	1:F:207:ARG:CZ	2.42	0.49
1:G:68:ASP:HB2	1:G:273:VAL:HB	1.94	0.49
1:H:94:ILE:O	1:H:103:VAL:HA	2.13	0.49
1:K:135:LEU:HA	1:K:161:LEU:HD23	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:209:LEU:HG	1:M:220:ILE:O	2.12	0.49
1:P:64:VAL:CG1	1:P:66:LYS:HE3	2.43	0.49
1:B:243:LEU:HD13	1:B:287:TYR:HB2	1.94	0.49
1:C:153:LEU:HD13	1:C:159:HIS:NE2	2.27	0.49
1:J:101:HIS:O	1:J:174:ARG:HG3	2.12	0.49
1:M:176:TYR:OH	1:M:215:ALA:O	2.18	0.49
1:P:111:GLU:HA	1:P:165:GLU:HA	1.95	0.49
1:P:127:PHE:HB3	1:P:170:VAL:CG1	2.43	0.49
1:P:137:ASN:C	1:P:140:SER:HA	2.37	0.49
1:G:243:LEU:HD21	1:G:252:TYR:CE1	2.47	0.49
1:P:64:VAL:HG11	1:P:66:LYS:CE	2.42	0.49
1:P:103:VAL:CG2	1:P:173:GLU:HB2	2.43	0.49
1:B:245:LEU:HD23	1:B:262:GLN:C	2.37	0.49
1:F:87:ASN:HD21	1:F:110:LYS:HB2	1.78	0.49
1:G:86:THR:HB	1:G:114:SER:OG	2.13	0.49
1:G:236:VAL:HG23	1:I:76:SER:HB3	1.94	0.49
1:H:210:LEU:HB3	1:H:211:PRO:CD	2.42	0.49
1:M:152:TYR:O	1:M:186:LEU:HD12	2.11	0.49
1:N:227:PRO:HD3	1:N:284:ARG:HA	1.95	0.49
1:P:82:LEU:HB3	1:P:85:TRP:HB2	1.94	0.49
1:F:63:SER:HA	1:F:71:LEU:O	2.13	0.49
1:F:296:ASN:ND2	1:F:298:LEU:HB2	2.28	0.49
1:H:207:ARG:HG3	1:H:207:ARG:HH11	1.78	0.49
1:H:243:LEU:HD12	1:H:244:LEU:N	2.27	0.49
1:K:152:TYR:HE2	1:K:184:THR:HB	1.77	0.49
1:L:245:LEU:HD12	1:L:287:TYR:HB3	1.95	0.49
1:M:198:GLU:HG3	1:M:200:PRO:HD3	1.94	0.49
1:M:241:HIS:HB2	1:M:269:MET:HB2	1.95	0.49
1:N:153:LEU:HD13	1:N:159:HIS:CD2	2.48	0.49
1:N:290:TYR:C	1:N:290:TYR:CD2	2.90	0.49
1:O:150:TYR:CE1	1:O:209:LEU:HD22	2.47	0.49
1:C:252:TYR:CE1	1:C:277:TYR:HB2	2.48	0.48
1:D:206:LEU:HD12	1:D:207:ARG:H	1.78	0.48
1:E:153:LEU:HD13	1:E:159:HIS:CE1	2.48	0.48
1:G:208:LYS:HZ2	1:G:212:MET:HE3	1.77	0.48
1:K:154:PRO:HG2	1:K:185:GLU:HA	1.94	0.48
1:B:155:PRO:O	1:B:156:ASN:HB2	2.13	0.48
1:C:208:LYS:HE2	1:C:221:HIS:NE2	2.28	0.48
1:E:133:VAL:HG13	1:E:145:LEU:HB2	1.94	0.48
1:G:153:LEU:HD13	1:G:159:HIS:CD2	2.48	0.48
1:I:125:LEU:O	1:I:171:VAL:HG23	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:40:ILE:N	1:K:40:ILE:CD1	2.73	0.48
1:K:296:ASN:HD22	1:K:297:PRO:N	2.09	0.48
1:L:155:PRO:O	1:L:156:ASN:HB2	2.11	0.48
1:L:272:PHE:CZ	1:P:95:THR:HG23	2.48	0.48
1:O:137:ASN:HD21	1:O:141:SER:N	2.05	0.48
1:A:234:LYS:HG2	1:J:61:THR:HB	1.94	0.48
1:B:154:PRO:HG2	1:B:185:GLU:HA	1.96	0.48
1:C:128:VAL:HG22	1:C:169:LEU:HD11	1.95	0.48
1:G:121:ASP:H	1:G:156:ASN:HD21	1.59	0.48
1:J:137:ASN:HB2	3:J:422:HOH:O	2.12	0.48
1:K:115:SER:OG	1:K:116:GLY:N	2.42	0.48
1:L:82:LEU:HD13	1:L:90:GLY:CA	2.38	0.48
1:M:157:PHE:CZ	1:M:186:LEU:HD22	2.47	0.48
1:N:126:ILE:CG1	1:N:151:ALA:HB3	2.43	0.48
1:N:243:LEU:C	1:N:243:LEU:HD12	2.37	0.48
1:O:121:ASP:H	1:O:156:ASN:HD21	1.61	0.48
1:P:40:ILE:O	1:P:41:TYR:C	2.57	0.48
1:A:164:VAL:HG22	3:A:427:HOH:O	2.12	0.48
1:C:127:PHE:HB3	1:C:170:VAL:HG13	1.95	0.48
1:E:150:TYR:CE1	1:E:209:LEU:HD22	2.49	0.48
1:F:54:LEU:CD2	1:H:49:LEU:HD22	2.44	0.48
1:F:70:ALA:HB3	1:F:268:TRP:HB3	1.94	0.48
1:H:296:ASN:HD21	1:H:298:LEU:HB2	1.74	0.48
1:J:179:LEU:O	1:J:180:GLY:C	2.56	0.48
1:J:206:LEU:HD12	1:J:207:ARG:N	2.28	0.48
1:J:207:ARG:HB2	1:J:222:THR:HB	1.93	0.48
1:K:277:TYR:CG	1:K:278:ALA:N	2.81	0.48
1:L:207:ARG:HD2	1:L:222:THR:HG21	1.96	0.48
1:M:243:LEU:C	1:M:243:LEU:CD1	2.85	0.48
1:O:121:ASP:H	1:O:156:ASN:ND2	2.11	0.48
1:O:202:GLU:HG3	1:O:204:PHE:CE2	2.48	0.48
1:O:241:HIS:HB2	1:O:269:MET:CB	2.35	0.48
1:P:244:LEU:HD12	1:P:265:ASP:O	2.12	0.48
1:B:101:HIS:H	1:B:240:GLN:NE2	2.10	0.48
1:B:296:ASN:HD22	1:B:296:ASN:C	2.21	0.48
1:I:125:LEU:HD13	1:I:126:ILE:N	2.29	0.48
1:J:70:ALA:HB3	1:J:268:TRP:HB3	1.95	0.48
1:L:254:LEU:HA	1:L:274:PRO:O	2.12	0.48
1:M:109:MET:HB3	1:M:113:SER:OG	2.13	0.48
1:M:184:THR:HB	1:M:216:TYR:CE1	2.49	0.48
1:P:153:LEU:CD1	1:P:159:HIS:CD2	2.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:VAL:CG1	1:A:66:LYS:HG3	2.44	0.48
1:E:240:GLN:HB3	1:E:271:PRO:HG3	1.96	0.48
1:G:62:ARG:NH2	1:G:265:ASP:OD1	2.46	0.48
1:G:297:PRO:HG3	1:I:92:TYR:CZ	2.48	0.48
1:K:81:PRO:O	1:K:83:PRO:HD3	2.13	0.48
1:L:234:LYS:HD2	1:L:234:LYS:N	2.29	0.48
1:L:247:GLU:O	1:L:285:SER:HA	2.13	0.48
1:M:157:PHE:HE1	1:M:186:LEU:HD22	1.79	0.48
1:M:204:PHE:CD1	1:M:223:MET:HG2	2.48	0.48
1:M:245:LEU:HA	1:M:287:TYR:HB3	1.95	0.48
1:P:156:ASN:ND2	1:P:156:ASN:N	2.60	0.48
1:A:240:GLN:HB3	1:A:271:PRO:HG3	1.95	0.48
1:F:120:GLN:O	1:F:121:ASP:HB2	2.12	0.48
1:H:85:TRP:CE3	1:H:115:SER:HA	2.48	0.48
1:O:103:VAL:HG22	1:O:173:GLU:HB2	1.96	0.48
1:O:252:TYR:CE1	1:O:277:TYR:HB2	2.49	0.48
1:B:174:ARG:NH1	1:B:217:ASP:O	2.46	0.48
1:F:137:ASN:HD21	1:F:140:SER:HB2	1.79	0.48
1:G:111:GLU:O	1:G:112:MET:C	2.56	0.48
1:G:146:THR:O	1:G:147:VAL:C	2.56	0.48
1:I:73:THR:HB	1:I:74:PRO:HD2	1.95	0.48
1:J:270:ALA:O	1:J:273:VAL:HG12	2.14	0.48
1:M:121:ASP:H	1:M:156:ASN:HD21	1.62	0.48
1:O:104:MET:HG3	1:O:172:PHE:CE1	2.49	0.48
1:A:243:LEU:HD12	1:A:243:LEU:C	2.39	0.48
1:C:243:LEU:HG	1:C:267:ILE:HB	1.94	0.48
1:I:207:ARG:HH11	1:I:207:ARG:HG3	1.78	0.48
1:K:84:ASP:O	1:K:116:GLY:HA3	2.14	0.48
1:N:60:PHE:O	1:O:234:LYS:HE3	2.14	0.48
1:N:153:LEU:HD13	1:N:159:HIS:CE1	2.48	0.48
1:K:218:PHE:CB	1:K:290:TYR:HE1	2.27	0.48
1:O:54:LEU:HD23	1:P:49:LEU:HD22	1.96	0.48
1:O:164:VAL:HG23	1:O:165:GLU:HG2	1.96	0.48
1:P:86:THR:O	1:P:87:ASN:C	2.56	0.48
1:P:243:LEU:HG	1:P:267:ILE:HB	1.95	0.48
1:A:166:SER:O	1:A:167:ALA:HB2	2.13	0.47
1:A:224:ASP:HA	1:A:285:SER:O	2.14	0.47
1:B:95:THR:HG23	1:I:272:PHE:HZ	1.79	0.47
1:B:126:ILE:C	1:B:126:ILE:HD12	2.38	0.47
1:D:64:VAL:HG12	1:D:66:LYS:HG3	1.96	0.47
1:D:82:LEU:HD13	1:D:90:GLY:CA	2.42	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:101:HIS:N	1:E:240:GLN:HE22	2.06	0.47
1:E:164:VAL:HG23	1:E:165:GLU:N	2.29	0.47
1:J:227:PRO:HD3	1:J:284:ARG:HA	1.96	0.47
1:K:103:VAL:HG22	1:K:173:GLU:HB2	1.95	0.47
1:K:152:TYR:CB	1:K:210:LEU:HD21	2.43	0.47
1:L:62:ARG:NH2	1:L:265:ASP:OD2	2.44	0.47
1:L:207:ARG:HG3	1:L:207:ARG:NH1	2.29	0.47
1:M:64:VAL:O	1:M:70:ALA:HA	2.14	0.47
1:E:111:GLU:HA	1:E:164:VAL:O	2.14	0.47
1:F:214:VAL:O	1:F:215:ALA:C	2.57	0.47
1:F:253:ARG:HD2	1:F:258:TRP:CZ2	2.49	0.47
1:F:276:TRP:CH2	1:F:278:ALA:HB2	2.48	0.47
1:L:196:LEU:HD12	1:L:196:LEU:N	2.28	0.47
1:P:258:TRP:HZ3	1:P:276:TRP:CZ3	2.32	0.47
1:B:54:LEU:HD23	1:J:49:LEU:HD22	1.95	0.47
1:D:227:PRO:HG3	1:D:283:THR:O	2.14	0.47
1:E:101:HIS:H	1:E:240:GLN:NE2	2.05	0.47
1:F:66:LYS:HB3	3:F:423:HOH:O	2.14	0.47
1:G:150:TYR:CE2	1:G:209:LEU:HB3	2.49	0.47
1:H:223:MET:O	1:H:286:ARG:HA	2.14	0.47
1:I:109:MET:O	1:I:166:SER:HA	2.15	0.47
1:J:253:ARG:HB3	1:J:276:TRP:HB3	1.96	0.47
1:O:49:LEU:CD2	1:P:57:LEU:HD12	2.42	0.47
1:O:140:SER:O	1:O:141:SER:CB	2.62	0.47
1:P:121:ASP:H	1:P:156:ASN:HD22	1.54	0.47
1:D:150:TYR:CE2	1:D:209:LEU:HB3	2.50	0.47
1:G:155:PRO:O	1:G:156:ASN:HB2	2.14	0.47
1:J:186:LEU:HD12	1:J:187:ILE:H	1.78	0.47
1:K:206:LEU:HD11	1:K:221:HIS:HB3	1.95	0.47
1:M:70:ALA:HB3	1:M:268:TRP:HB3	1.96	0.47
1:M:130:GLU:CD	1:M:131:GLY:N	2.73	0.47
1:M:222:THR:HG22	1:M:222:THR:O	2.13	0.47
1:O:82:LEU:HD23	1:O:85:TRP:CD2	2.49	0.47
1:E:87:ASN:ND2	1:E:110:LYS:HB2	2.29	0.47
1:E:128:VAL:HB	1:E:146:THR:O	2.14	0.47
1:H:132:ALA:HB1	1:H:144:LYS:HZ2	1.79	0.47
1:M:130:GLU:CB	1:M:168:THR:HB	2.45	0.47
1:N:113:SER:O	1:N:162:ASP:HA	2.14	0.47
1:B:49:LEU:HD22	1:J:54:LEU:HD23	1.97	0.47
1:D:93:LEU:HD13	1:D:266:VAL:HG21	1.95	0.47
1:D:100:SER:HB2	1:D:240:GLN:HE22	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:272:PHE:HE2	1:F:95:THR:OG1	1.97	0.47
1:F:55:GLN:HA	3:F:443:HOH:O	2.15	0.47
1:I:206:LEU:HD12	1:I:207:ARG:H	1.79	0.47
1:J:82:LEU:HD13	1:J:90:GLY:CA	2.44	0.47
1:K:85:TRP:HZ3	1:K:109:MET:HE3	1.79	0.47
1:L:126:ILE:HD13	1:L:169:LEU:CD2	2.44	0.47
1:P:87:ASN:OD1	1:P:87:ASN:C	2.58	0.47
1:B:164:VAL:HG23	3:B:433:HOH:O	2.14	0.47
1:D:152:TYR:HB3	1:D:187:ILE:HB	1.96	0.47
1:E:96:PRO:HD3	1:E:103:VAL:CG1	2.45	0.47
1:F:206:LEU:HD12	1:F:207:ARG:N	2.29	0.47
1:G:198:GLU:O	1:G:199:THR:HG23	2.15	0.47
1:H:298:LEU:HD13	1:M:122:ILE:HD12	1.97	0.47
1:J:233:VAL:O	1:J:235:GLU:N	2.45	0.47
1:L:204:PHE:CD1	1:L:223:MET:HE3	2.49	0.47
1:N:238:TYR:O	1:N:271:PRO:HB3	2.15	0.47
1:O:41:TYR:O	1:O:44:ALA:N	2.44	0.47
1:O:125:LEU:HD13	1:O:125:LEU:C	2.40	0.47
1:O:207:ARG:HB2	1:O:222:THR:HG1	1.76	0.47
1:P:108:LYS:NZ	1:P:168:THR:OG1	2.33	0.47
1:P:133:VAL:CB	1:P:163:CYS:HB3	2.43	0.47
1:F:39:PRO:HB2	1:F:42:TRP:HB2	1.97	0.47
1:G:127:PHE:HE1	1:G:209:LEU:HD11	1.80	0.47
1:G:153:LEU:HD23	1:G:186:LEU:HD11	1.97	0.47
1:G:186:LEU:O	1:G:187:ILE:HD13	2.15	0.47
1:G:208:LYS:HZ3	1:G:212:MET:HE3	1.77	0.47
1:G:246:LEU:CD1	1:G:288:LEU:HD13	2.38	0.47
1:I:105:TYR:CE1	1:I:171:VAL:HG11	2.50	0.47
1:L:60:PHE:HZ	1:N:60:PHE:HZ	1.62	0.47
1:M:237:HIS:CG	1:M:239:ASN:HD22	2.33	0.47
1:N:296:ASN:HD22	1:N:298:LEU:HB2	1.79	0.47
1:O:120:GLN:HG2	1:O:121:ASP:OD2	2.14	0.47
1:E:83:PRO:O	1:E:84:ASP:HB2	2.15	0.47
1:E:276:TRP:CH2	1:E:278:ALA:HB2	2.50	0.47
1:F:93:LEU:CD1	1:F:266:VAL:HG21	2.40	0.47
1:I:86:THR:O	1:I:113:SER:HB2	2.14	0.47
1:N:111:GLU:CD	1:N:111:GLU:H	2.23	0.47
1:P:176:TYR:CE2	1:P:178:TYR:HA	2.50	0.47
1:B:268:TRP:CZ2	1:B:270:ALA:HB2	2.50	0.47
1:F:140:SER:O	1:F:141:SER:HB3	2.15	0.47
1:F:270:ALA:O	1:F:273:VAL:HG12	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:298:LEU:HD23	1:F:298:LEU:C	2.40	0.47
1:H:121:ASP:HB2	1:H:175:ARG:NH1	2.30	0.47
1:H:125:LEU:HD13	1:H:125:LEU:C	2.40	0.47
1:H:127:PHE:HB3	1:H:170:VAL:CG1	2.45	0.47
1:H:243:LEU:HG	1:H:267:ILE:HB	1.97	0.47
1:M:257:ASN:ND2	3:M:422:HOH:O	2.46	0.47
1:N:39:PRO:O	1:N:42:TRP:HB2	2.15	0.47
1:O:111:GLU:HA	1:O:165:GLU:HA	1.96	0.47
1:O:276:TRP:CH2	1:O:278:ALA:HB2	2.50	0.47
1:P:92:TYR:CE1	1:P:105:TYR:CD2	3.02	0.47
1:P:296:ASN:ND2	1:P:298:LEU:H	2.12	0.47
1:B:153:LEU:HD13	1:B:159:HIS:NE2	2.29	0.46
1:F:50:SER:HB2	1:F:51:PRO:HD2	1.95	0.46
1:H:290:TYR:C	1:H:290:TYR:CD2	2.92	0.46
1:I:164:VAL:CG2	1:I:165:GLU:H	2.28	0.46
1:J:126:ILE:HD12	1:J:169:LEU:CD2	2.45	0.46
1:J:154:PRO:HB3	1:J:184:THR:OG1	2.15	0.46
1:N:224:ASP:OD2	1:N:286:ARG:HD3	2.14	0.46
1:P:133:VAL:HG22	1:P:134:THR:N	2.30	0.46
1:P:147:VAL:CG1	1:P:148:ASP:N	2.78	0.46
1:E:85:TRP:CE3	1:E:88:THR:HG21	2.51	0.46
1:G:50:SER:HB2	1:G:51:PRO:HD2	1.97	0.46
1:M:124:ARG:CG	1:M:125:LEU:N	2.78	0.46
1:O:41:TYR:CZ	1:O:246:LEU:HD13	2.50	0.46
1:O:53:HIS:ND1	1:P:53:HIS:CG	2.83	0.46
1:P:93:LEU:HD13	1:P:266:VAL:HG21	1.96	0.46
1:A:85:TRP:CE3	1:A:115:SER:HA	2.50	0.46
1:A:120:GLN:O	1:A:121:ASP:HB2	2.14	0.46
1:B:137:ASN:ND2	1:B:140:SER:HA	2.30	0.46
1:E:60:PHE:O	1:P:234:LYS:HE3	2.14	0.46
1:E:72:ILE:HG21	1:E:93:LEU:HD22	1.97	0.46
1:F:153:LEU:HD22	1:F:159:HIS:CG	2.50	0.46
1:F:243:LEU:HD13	1:F:287:TYR:HB2	1.98	0.46
1:P:82:LEU:O	1:P:85:TRP:HB2	2.15	0.46
1:P:133:VAL:HG23	1:P:163:CYS:CB	2.30	0.46
1:P:227:PRO:HB3	1:P:281:GLY:O	2.15	0.46
1:B:101:HIS:O	1:B:174:ARG:HG3	2.15	0.46
1:F:126:ILE:C	1:F:126:ILE:HD12	2.40	0.46
1:G:125:LEU:C	1:G:125:LEU:CD1	2.87	0.46
1:H:241:HIS:CE1	1:H:289:LEU:HD21	2.51	0.46
1:J:123:GLU:OE2	1:J:217:ASP:OD1	2.32	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:111:GLU:HA	1:K:164:VAL:O	2.15	0.46
1:L:147:VAL:HG12	1:L:148:ASP:H	1.80	0.46
1:M:125:LEU:C	1:M:125:LEU:CD1	2.89	0.46
1:O:197:LEU:HD11	1:O:207:ARG:HA	1.96	0.46
1:P:101:HIS:O	1:P:174:ARG:HG3	2.15	0.46
1:D:127:PHE:HB3	1:D:170:VAL:HG13	1.97	0.46
1:E:275:GLN:NE2	3:E:444:HOH:O	2.48	0.46
1:E:296:ASN:HD22	1:E:297:PRO:CD	2.17	0.46
1:G:297:PRO:HB2	1:I:95:THR:HG21	1.96	0.46
1:K:108:LYS:HG2	1:K:168:THR:OG1	2.15	0.46
1:L:298:LEU:HD23	1:P:103:VAL:CG1	2.46	0.46
1:O:293:VAL:HG23	1:O:294:ASN:HD22	1.79	0.46
1:C:204:PHE:CZ	1:C:223:MET:HE3	2.51	0.46
1:J:176:TYR:CE2	1:J:178:TYR:HA	2.50	0.46
1:J:208:LYS:HE2	1:J:221:HIS:CE1	2.51	0.46
1:O:163:CYS:C	3:O:416:HOH:O	2.58	0.46
1:B:225:PHE:HZ	1:B:231:LEU:HD21	1.81	0.46
1:G:72:ILE:HD12	1:G:72:ILE:N	2.30	0.46
1:I:126:ILE:HG22	1:I:171:VAL:HB	1.98	0.46
1:K:175:ARG:HG3	1:K:175:ARG:HH11	1.80	0.46
1:N:196:LEU:HD11	1:N:207:ARG:NH2	2.30	0.46
1:O:125:LEU:HD22	1:O:126:ILE:H	1.81	0.46
1:D:113:SER:HG	1:D:163:CYS:HB3	1.80	0.46
1:D:297:PRO:O	1:D:298:LEU:OXT	2.34	0.46
1:G:206:LEU:HA	1:G:222:THR:O	2.15	0.46
1:H:204:PHE:CZ	1:H:223:MET:HE3	2.51	0.46
1:J:101:HIS:C	1:J:101:HIS:CD2	2.93	0.46
1:K:113:SER:HB2	1:K:163:CYS:SG	2.56	0.46
1:K:267:ILE:CG2	1:K:269:MET:HE2	2.46	0.46
1:M:105:TYR:CE1	1:M:171:VAL:HG13	2.51	0.46
1:N:127:PHE:HB3	1:N:170:VAL:HG13	1.97	0.46
1:P:89:LEU:HG	1:P:110:LYS:HZ1	1.79	0.46
1:A:125:LEU:C	1:A:125:LEU:HD13	2.41	0.46
1:C:74:PRO:C	1:C:76:SER:N	2.71	0.46
1:D:85:TRP:CE3	1:D:88:THR:HG21	2.51	0.46
1:D:206:LEU:HD11	1:D:221:HIS:HB3	1.97	0.46
1:F:82:LEU:HD23	1:F:85:TRP:CD2	2.51	0.46
1:H:132:ALA:HB1	1:H:144:LYS:NZ	2.29	0.46
1:I:87:ASN:HD21	1:I:110:LYS:CB	2.26	0.46
1:L:268:TRP:CZ2	1:L:270:ALA:HB2	2.51	0.46
1:N:164:VAL:HG23	1:N:165:GLU:N	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:150:TYR:CE2	1:O:209:LEU:HB3	2.51	0.46
1:B:184:THR:HB	1:B:216:TYR:CE1	2.51	0.46
1:C:115:SER:HB3	1:C:161:LEU:HB2	1.96	0.46
1:D:90:GLY:HA2	1:D:106:LEU:O	2.16	0.46
1:F:123:GLU:O	1:F:173:GLU:HA	2.16	0.46
1:F:125:LEU:HD13	1:F:126:ILE:N	2.30	0.46
1:F:137:ASN:HD21	1:F:140:SER:CB	2.28	0.46
1:F:237:HIS:HB2	1:F:239:ASN:HD22	1.80	0.46
1:F:273:VAL:O	1:F:273:VAL:HG13	2.16	0.46
1:G:101:HIS:H	1:G:240:GLN:NE2	2.09	0.46
1:G:145:LEU:HB3	1:G:149:SER:CB	2.46	0.46
1:K:185:GLU:O	1:K:186:LEU:C	2.58	0.46
1:L:250:GLY:O	1:L:251:ILE:HD13	2.16	0.46
1:O:130:GLU:CD	1:O:131:GLY:N	2.74	0.46
1:P:121:ASP:CA	1:P:156:ASN:HD21	2.27	0.46
1:P:125:LEU:HD13	1:P:125:LEU:C	2.41	0.46
1:C:298:LEU:HD13	1:G:122:ILE:HD12	1.97	0.45
1:D:273:VAL:HG13	1:D:273:VAL:O	2.16	0.45
1:E:122:ILE:CD1	1:P:298:LEU:HD13	2.44	0.45
1:F:249:GLN:N	1:F:249:GLN:OE1	2.50	0.45
1:G:83:PRO:C	1:G:85:TRP:H	2.24	0.45
1:G:227:PRO:HG3	1:G:283:THR:O	2.16	0.45
1:H:82:LEU:HD22	1:H:90:GLY:CA	2.42	0.45
1:H:111:GLU:O	1:H:112:MET:C	2.58	0.45
1:K:92:TYR:HB2	3:K:420:HOH:O	2.14	0.45
1:K:136:THR:HG22	1:K:142:SER:OG	2.16	0.45
1:L:131:GLY:HA3	1:L:167:ALA:HA	1.98	0.45
1:N:133:VAL:HG23	1:N:163:CYS:CA	2.46	0.45
1:O:56:ASP:HA	3:O:415:HOH:O	2.16	0.45
1:A:298:LEU:O	1:J:96:PRO:HG2	2.16	0.45
1:G:62:ARG:HG3	1:G:62:ARG:HH11	1.82	0.45
1:H:237:HIS:CE1	1:H:239:ASN:HB2	2.51	0.45
1:L:277:TYR:CG	1:L:278:ALA:N	2.84	0.45
1:M:121:ASP:HA	1:M:155:PRO:HB2	1.98	0.45
1:M:252:TYR:OH	1:M:269:MET:CE	2.64	0.45
1:N:223:MET:O	1:N:286:ARG:HA	2.16	0.45
1:C:110:LYS:HB3	1:C:111:GLU:OE2	2.16	0.45
1:F:155:PRO:O	1:F:156:ASN:HB2	2.17	0.45
1:G:203:VAL:HG22	3:G:410:HOH:O	2.16	0.45
1:G:297:PRO:HG3	1:I:92:TYR:CE1	2.51	0.45
1:H:74:PRO:C	1:H:76:SER:H	2.24	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:187:ILE:HD12	1:J:211:PRO:CD	2.42	0.45
1:K:85:TRP:HA	1:K:115:SER:O	2.16	0.45
1:K:208:LYS:HE2	1:K:221:HIS:CE1	2.51	0.45
1:O:133:VAL:O	1:O:145:LEU:HB2	2.16	0.45
1:O:135:LEU:CB	1:O:145:LEU:HD11	2.47	0.45
1:D:109:MET:HB3	1:D:113:SER:OG	2.17	0.45
1:F:101:HIS:N	1:F:240:GLN:HE22	2.13	0.45
1:L:218:PHE:CD1	1:L:218:PHE:C	2.94	0.45
1:M:86:THR:O	1:M:87:ASN:C	2.60	0.45
1:M:240:GLN:HG3	1:M:240:GLN:O	2.17	0.45
1:N:100:SER:CA	1:N:240:GLN:HE22	2.30	0.45
1:P:238:TYR:O	1:P:271:PRO:HB3	2.17	0.45
1:A:49:LEU:H	1:A:262:GLN:HE22	1.63	0.45
1:F:131:GLY:HA3	1:F:166:SER:O	2.17	0.45
1:F:296:ASN:ND2	3:F:451:HOH:O	2.43	0.45
1:I:130:GLU:CA	1:I:147:VAL:HG22	2.38	0.45
1:J:102:PHE:CD2	1:J:240:GLN:NE2	2.80	0.45
1:M:295:ARG:O	1:M:296:ASN:C	2.60	0.45
1:O:40:ILE:HD13	1:O:147:VAL:CG1	2.32	0.45
1:O:63:SER:HA	1:O:71:LEU:O	2.16	0.45
1:O:202:GLU:OE1	1:O:231:LEU:HA	2.16	0.45
1:P:88:THR:OG1	1:P:109:MET:HA	2.16	0.45
1:H:298:LEU:CD1	1:M:122:ILE:HG21	2.47	0.45
1:I:125:LEU:HD22	1:I:126:ILE:H	1.82	0.45
1:M:93:LEU:CD1	1:M:266:VAL:HG21	2.44	0.45
1:M:273:VAL:HG13	1:M:273:VAL:O	2.15	0.45
1:O:273:VAL:HG13	1:O:273:VAL:O	2.17	0.45
1:A:226:GLN:HB2	1:A:229:GLU:HG3	1.99	0.45
1:E:56:ASP:OD2	1:M:48:THR:OG1	2.32	0.45
1:G:39:PRO:O	1:G:42:TRP:HB2	2.17	0.45
1:G:191:THR:O	1:G:207:ARG:HD3	2.16	0.45
1:I:238:TYR:C	1:I:238:TYR:CD2	2.95	0.45
1:K:150:TYR:CE1	1:K:209:LEU:HD22	2.51	0.45
1:O:72:ILE:HD12	1:O:72:ILE:N	2.32	0.45
1:O:104:MET:HE1	1:O:266:VAL:HG13	1.98	0.45
1:O:147:VAL:O	1:O:148:ASP:CB	2.49	0.45
1:O:284:ARG:HG3	1:O:285:SER:N	2.31	0.45
1:A:218:PHE:CD1	1:A:218:PHE:C	2.95	0.45
1:C:190:SER:O	1:C:191:THR:C	2.60	0.45
1:D:237:HIS:HB2	1:D:239:ASN:ND2	2.32	0.45
1:E:63:SER:HA	1:E:71:LEU:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:117:LEU:HD11	1:E:158:HIS:CD2	2.52	0.45
1:G:197:LEU:HD12	1:G:208:LYS:HE3	1.98	0.45
1:I:235:GLU:HB2	1:I:275:GLN:HG3	1.99	0.45
1:J:233:VAL:O	1:J:233:VAL:HG13	2.17	0.45
1:K:129:VAL:O	1:K:147:VAL:HG22	2.16	0.45
1:P:248:GLY:HA3	1:P:285:SER:HA	1.99	0.45
1:A:119:PRO:HB2	1:A:122:ILE:HG13	1.99	0.45
1:D:104:MET:HE3	1:D:172:PHE:CZ	2.51	0.45
1:E:109:MET:HB3	1:E:113:SER:OG	2.17	0.45
1:F:137:ASN:HD21	1:F:140:SER:N	2.13	0.45
1:G:126:ILE:O	1:G:150:TYR:HB2	2.17	0.45
1:G:150:TYR:CD1	1:G:209:LEU:HD13	2.51	0.45
1:H:103:VAL:CG1	1:N:298:LEU:HG	2.46	0.45
1:H:152:TYR:CE2	1:H:154:PRO:HG3	2.49	0.45
1:J:207:ARG:HG3	1:J:207:ARG:NH1	2.31	0.45
1:L:94:ILE:O	1:L:103:VAL:HA	2.17	0.45
1:L:101:HIS:CE1	1:L:292:ASP:HB3	2.52	0.45
1:L:126:ILE:C	1:L:126:ILE:HD12	2.42	0.45
1:M:52:SER:O	1:M:55:GLN:HG2	2.16	0.45
1:M:129:VAL:HG23	1:M:168:THR:O	2.17	0.45
1:N:89:LEU:HG	3:N:418:HOH:O	2.17	0.45
1:N:102:PHE:CD1	1:N:102:PHE:C	2.95	0.45
1:O:203:VAL:HG23	1:O:229:GLU:OE2	2.16	0.45
1:P:101:HIS:N	1:P:240:GLN:HE22	2.14	0.45
1:P:105:TYR:CE1	1:P:171:VAL:HG11	2.52	0.45
1:A:152:TYR:HB2	1:A:210:LEU:HD21	2.00	0.45
1:E:111:GLU:O	1:E:112:MET:C	2.58	0.45
1:I:196:LEU:O	1:I:197:LEU:HD23	2.17	0.45
1:J:105:TYR:CE2	1:J:171:VAL:HG22	2.52	0.45
1:M:292:ASP:O	1:M:293:VAL:HG13	2.16	0.45
1:A:121:ASP:H	1:A:156:ASN:HD21	1.65	0.44
1:A:150:TYR:CE2	1:A:209:LEU:HB3	2.52	0.44
1:D:125:LEU:C	1:D:125:LEU:CD1	2.89	0.44
1:E:223:MET:O	1:E:286:ARG:HA	2.16	0.44
1:F:154:PRO:HG2	1:F:185:GLU:HA	1.99	0.44
1:G:224:ASP:CG	1:G:286:ARG:HH11	2.25	0.44
1:H:83:PRO:O	1:H:84:ASP:HB2	2.16	0.44
1:I:52:SER:O	1:I:55:GLN:CG	2.65	0.44
1:J:90:GLY:HA2	1:J:106:LEU:O	2.16	0.44
1:L:40:ILE:H	1:L:40:ILE:CD1	2.26	0.44
1:L:243:LEU:HD23	1:L:269:MET:CE	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:222:THR:HG23	1:N:286:ARG:HD3	1.97	0.44
1:O:82:LEU:HD23	1:O:85:TRP:CE2	2.52	0.44
1:C:69:HIS:CD2	1:C:254:LEU:HD13	2.52	0.44
1:D:56:ASP:OD2	1:G:48:THR:OG1	2.26	0.44
1:E:152:TYR:HB3	1:E:187:ILE:HB	1.99	0.44
1:E:260:PRO:HB3	1:M:58:PRO:O	2.17	0.44
1:H:40:ILE:H	1:H:40:ILE:CD1	2.06	0.44
1:I:147:VAL:O	1:I:148:ASP:HB2	2.16	0.44
1:I:171:VAL:CG2	1:I:172:PHE:N	2.80	0.44
1:L:62:ARG:CB	1:L:73:THR:HG21	2.47	0.44
1:O:125:LEU:O	1:O:171:VAL:HG23	2.17	0.44
1:E:292:ASP:O	1:E:293:VAL:HG13	2.17	0.44
1:G:93:LEU:HD13	1:G:266:VAL:HG21	1.98	0.44
1:H:121:ASP:HB2	1:H:175:ARG:HH12	1.83	0.44
1:J:154:PRO:HD2	1:J:157:PHE:CG	2.52	0.44
1:M:124:ARG:HG2	1:M:125:LEU:N	2.32	0.44
1:M:287:TYR:HE1	1:M:289:LEU:HD22	1.82	0.44
1:O:199:THR:HG21	1:O:204:PHE:O	2.17	0.44
1:F:50:SER:HB2	1:F:51:PRO:CD	2.47	0.44
1:G:79:TYR:CD1	1:G:91:ALA:HB2	2.53	0.44
1:G:206:LEU:HD12	1:G:207:ARG:H	1.81	0.44
1:H:253:ARG:HB3	1:H:276:TRP:HB3	1.99	0.44
1:L:243:LEU:HB2	1:L:289:LEU:HD13	1.98	0.44
1:L:244:LEU:HD12	1:L:245:LEU:H	1.81	0.44
1:L:290:TYR:C	1:L:290:TYR:CD2	2.95	0.44
1:M:103:VAL:O	1:M:103:VAL:HG23	2.17	0.44
1:O:196:LEU:HD21	1:O:207:ARG:NH2	2.32	0.44
1:O:244:LEU:HD12	1:O:245:LEU:H	1.81	0.44
1:A:276:TRP:CH2	1:A:278:ALA:HB2	2.52	0.44
1:C:85:TRP:CE3	1:C:115:SER:HA	2.52	0.44
1:D:199:THR:HG21	1:D:204:PHE:CE1	2.52	0.44
1:E:94:ILE:CD1	1:E:268:TRP:HB2	2.48	0.44
1:F:223:MET:O	1:F:286:ARG:HA	2.18	0.44
1:F:296:ASN:HB2	3:F:442:HOH:O	2.17	0.44
1:G:145:LEU:HB3	1:G:149:SER:HB3	1.99	0.44
1:G:207:ARG:HB2	1:G:222:THR:CG2	2.48	0.44
1:J:127:PHE:HB3	1:J:170:VAL:CG1	2.46	0.44
1:J:204:PHE:HB3	1:J:225:PHE:CE1	2.53	0.44
1:J:231:LEU:HD12	1:J:276:TRP:HA	2.00	0.44
1:L:123:GLU:OE1	1:L:218:PHE:HE2	2.01	0.44
1:L:273:VAL:HG13	1:L:273:VAL:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:95:THR:HA	1:M:103:VAL:HG12	1.99	0.44
1:M:298:LEU:O	1:O:96:PRO:HG2	2.17	0.44
1:O:124:ARG:CG	1:O:125:LEU:N	2.80	0.44
1:O:179:LEU:O	1:O:180:GLY:C	2.59	0.44
1:P:148:ASP:O	1:P:148:ASP:OD1	2.35	0.44
1:A:174:ARG:NH1	1:A:217:ASP:O	2.50	0.44
1:D:150:TYR:CD1	1:D:209:LEU:HD13	2.53	0.44
1:E:194:GLN:HB2	1:E:207:ARG:HD3	1.98	0.44
1:F:74:PRO:C	1:F:76:SER:H	2.25	0.44
1:H:253:ARG:NH1	1:M:59:GLY:O	2.50	0.44
1:I:118:PRO:HD3	1:I:124:ARG:CZ	2.47	0.44
1:L:125:LEU:HD13	1:L:125:LEU:O	2.17	0.44
1:L:296:ASN:OD1	1:P:119:PRO:HG2	2.17	0.44
1:M:235:GLU:OE1	1:M:237:HIS:CD2	2.69	0.44
1:O:130:GLU:HB3	1:O:168:THR:CB	2.48	0.44
1:P:132:ALA:CB	1:P:146:THR:HA	2.47	0.44
1:D:83:PRO:O	1:D:85:TRP:HD1	2.01	0.44
1:E:133:VAL:CG1	1:E:145:LEU:HB2	2.48	0.44
1:E:218:PHE:HA	1:E:293:VAL:HG22	1.99	0.44
1:F:243:LEU:HG	1:F:267:ILE:HB	2.00	0.44
1:H:170:VAL:O	1:H:170:VAL:HG13	2.18	0.44
1:J:243:LEU:C	1:J:243:LEU:HD12	2.43	0.44
1:L:245:LEU:HD23	1:L:262:GLN:C	2.43	0.44
1:O:140:SER:O	1:O:141:SER:HB3	2.17	0.44
1:A:225:PHE:HB2	1:A:279:ALA:HB2	1.98	0.44
1:D:61:THR:HB	1:K:234:LYS:HG2	2.00	0.44
1:E:110:LYS:H	1:E:113:SER:HB3	1.83	0.44
1:H:125:LEU:HD23	1:H:152:TYR:HB2	2.00	0.44
1:I:86:THR:HB	1:I:114:SER:OG	2.18	0.44
1:I:290:TYR:CD2	1:I:290:TYR:C	2.95	0.44
1:J:133:VAL:HG23	1:J:162:ASP:O	2.18	0.44
1:J:170:VAL:O	1:J:170:VAL:CG1	2.66	0.44
1:K:101:HIS:N	1:K:240:GLN:HE22	2.16	0.44
1:L:240:GLN:HB3	1:L:271:PRO:HD3	1.98	0.44
1:M:145:LEU:HD22	1:M:149:SER:CB	2.44	0.44
1:O:43:LYS:HA	1:O:46:ASN:O	2.18	0.44
1:O:85:TRP:CD1	1:O:116:GLY:HA3	2.53	0.44
1:O:224:ASP:OD2	1:O:286:ARG:HD3	2.17	0.44
1:P:134:THR:O	1:P:161:LEU:HA	2.18	0.44
1:C:222:THR:O	1:C:222:THR:HG22	2.17	0.44
1:H:218:PHE:CA	1:H:293:VAL:HG22	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:126:ILE:HD12	1:I:126:ILE:C	2.43	0.44
1:M:154:PRO:HD2	1:M:157:PHE:CD1	2.37	0.44
1:M:211:PRO:C	1:M:213:SER:H	2.26	0.44
1:O:96:PRO:HD3	1:O:103:VAL:HG12	2.00	0.44
1:O:126:ILE:HB	1:O:169:LEU:HD23	1.99	0.44
1:P:119:PRO:HB2	1:P:122:ILE:CG1	2.48	0.44
1:E:108:LYS:HD3	1:E:168:THR:HG23	1.99	0.43
1:E:220:ILE:HD13	1:E:290:TYR:HA	1.99	0.43
1:F:218:PHE:CD1	1:F:218:PHE:C	2.96	0.43
1:G:87:ASN:OD1	1:G:110:LYS:HB2	2.18	0.43
1:H:245:LEU:HD12	1:H:287:TYR:HB3	2.00	0.43
1:K:84:ASP:O	1:K:116:GLY:CA	2.66	0.43
1:N:253:ARG:HG3	1:N:253:ARG:HH11	1.82	0.43
1:A:122:ILE:CD1	1:D:298:LEU:HD22	2.42	0.43
1:I:95:THR:O	1:I:98:THR:HG23	2.17	0.43
1:J:273:VAL:O	1:J:273:VAL:CG1	2.65	0.43
1:K:80:SER:O	1:K:90:GLY:N	2.44	0.43
1:K:148:ASP:O	1:K:148:ASP:OD2	2.36	0.43
1:L:103:VAL:HG22	1:L:173:GLU:HB2	2.00	0.43
1:M:128:VAL:HA	1:M:169:LEU:HD13	1.99	0.43
1:P:101:HIS:C	1:P:101:HIS:CD2	2.96	0.43
1:G:118:PRO:HD3	1:G:124:ARG:NH2	2.33	0.43
1:K:153:LEU:HD23	1:K:186:LEU:CD1	2.48	0.43
1:K:202:GLU:HG3	1:K:204:PHE:HE2	1.84	0.43
1:L:251:ILE:HD11	1:N:58:PRO:HB2	2.01	0.43
1:M:69:HIS:CD2	1:M:254:LEU:HD13	2.53	0.43
1:O:202:GLU:CD	1:O:232:ASN:H	2.26	0.43
1:O:208:LYS:HG2	1:O:221:HIS:CD2	2.54	0.43
1:P:118:PRO:CD	1:P:124:ARG:NH2	2.80	0.43
1:D:197:LEU:HD12	1:D:208:LYS:HG3	1.99	0.43
1:E:234:LYS:HD3	1:E:234:LYS:N	2.32	0.43
1:G:157:PHE:C	1:G:157:PHE:HD2	2.25	0.43
1:J:125:LEU:HD13	1:J:126:ILE:N	2.34	0.43
1:K:127:PHE:HB3	1:K:170:VAL:CG1	2.48	0.43
1:N:150:TYR:CE2	1:N:209:LEU:HB3	2.53	0.43
1:P:82:LEU:HD12	1:P:82:LEU:HA	1.68	0.43
1:P:120:GLN:O	1:P:121:ASP:HB2	2.18	0.43
1:B:101:HIS:N	1:B:240:GLN:HE22	2.12	0.43
1:E:179:LEU:O	1:E:180:GLY:C	2.61	0.43
1:F:235:GLU:HB2	1:F:275:GLN:HG3	2.01	0.43
1:F:243:LEU:C	1:F:243:LEU:CD1	2.86	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:103:VAL:HG22	1:G:173:GLU:HB2	2.00	0.43
1:I:202:GLU:OE1	1:I:231:LEU:HD23	2.18	0.43
1:J:277:TYR:CG	1:J:278:ALA:N	2.86	0.43
1:M:63:SER:HA	1:M:71:LEU:O	2.18	0.43
1:P:40:ILE:CD1	1:P:40:ILE:N	2.69	0.43
1:P:245:LEU:HD23	1:P:262:GLN:C	2.43	0.43
1:A:224:ASP:CG	1:A:286:ARG:HD3	2.44	0.43
1:B:83:PRO:O	1:B:85:TRP:HD1	2.02	0.43
1:B:253:ARG:NH1	1:C:61:THR:HG22	2.33	0.43
1:E:153:LEU:HD13	1:E:159:HIS:NE2	2.34	0.43
1:F:125:LEU:C	1:F:125:LEU:CD1	2.90	0.43
1:F:186:LEU:O	1:F:187:ILE:HD13	2.19	0.43
1:H:112:MET:C	3:H:444:HOH:O	2.61	0.43
1:H:273:VAL:O	1:H:273:VAL:HG13	2.18	0.43
1:I:207:ARG:HG3	1:I:207:ARG:NH1	2.34	0.43
1:J:284:ARG:HH22	1:J:286:ARG:CZ	2.30	0.43
1:K:296:ASN:ND2	1:K:297:PRO:HD2	2.30	0.43
1:M:123:GLU:O	1:M:123:GLU:HG3	2.18	0.43
1:N:54:LEU:O	1:N:56:ASP:N	2.52	0.43
1:N:271:PRO:O	1:N:272:PHE:HB2	2.18	0.43
1:N:276:TRP:CZ2	1:N:278:ALA:HB2	2.54	0.43
1:P:199:THR:HB	1:P:202:GLU:HB2	2.01	0.43
1:A:39:PRO:N	3:A:454:HOH:O	2.51	0.43
1:D:239:ASN:ND2	1:D:239:ASN:N	2.64	0.43
1:D:243:LEU:HG	1:D:267:ILE:HB	2.01	0.43
1:E:282:LYS:HE3	3:H:427:HOH:O	2.18	0.43
1:G:101:HIS:C	1:G:101:HIS:CD2	2.96	0.43
1:H:218:PHE:C	1:H:218:PHE:CD1	2.97	0.43
1:I:52:SER:O	1:I:55:GLN:HG2	2.19	0.43
1:J:290:TYR:C	1:J:290:TYR:CD2	2.97	0.43
1:L:45:THR:HG22	1:L:45:THR:O	2.18	0.43
1:M:204:PHE:CE1	1:M:223:MET:HE3	2.53	0.43
1:M:262:GLN:O	1:M:263:ALA:C	2.59	0.43
1:M:267:ILE:HG22	1:M:268:TRP:N	2.33	0.43
1:A:234:LYS:HE3	1:J:60:PHE:O	2.18	0.43
1:E:144:LYS:O	1:E:145:LEU:HD23	2.19	0.43
1:F:111:GLU:H	1:F:111:GLU:HG2	1.56	0.43
1:G:207:ARG:HH11	1:G:207:ARG:HG3	1.83	0.43
1:I:105:TYR:CZ	1:I:171:VAL:HG11	2.54	0.43
1:K:110:LYS:O	1:K:111:GLU:C	2.61	0.43
1:L:124:ARG:CG	1:L:125:LEU:N	2.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:190:SER:O	1:L:194:GLN:HG2	2.18	0.43
1:N:43:LYS:HE2	1:N:48:THR:OG1	2.18	0.43
1:O:243:LEU:HD12	1:O:243:LEU:C	2.43	0.43
1:D:103:VAL:HG22	1:K:298:LEU:HD21	1.99	0.43
1:D:161:LEU:HD13	1:D:169:LEU:HD21	2.01	0.43
1:K:60:PHE:C	1:K:60:PHE:CD2	2.96	0.43
1:K:196:LEU:HD21	1:K:207:ARG:CZ	2.48	0.43
1:M:296:ASN:HD21	1:M:298:LEU:HB2	1.79	0.43
1:N:101:HIS:CD2	1:N:101:HIS:C	2.97	0.43
1:O:213:SER:HB3	1:O:216:TYR:CD2	2.54	0.43
1:O:253:ARG:HB3	1:O:276:TRP:HB3	2.00	0.43
1:P:133:VAL:HA	1:P:163:CYS:HB2	2.00	0.43
1:A:262:GLN:HG2	1:C:57:LEU:CD2	2.44	0.43
1:B:282:LYS:HE3	3:B:462:HOH:O	2.19	0.43
1:F:130:GLU:O	1:F:167:ALA:HA	2.18	0.43
1:I:64:VAL:HG11	1:I:259:TYR:OH	2.18	0.43
1:I:273:VAL:O	1:I:273:VAL:HG13	2.18	0.43
1:K:95:THR:O	1:K:98:THR:HG23	2.19	0.43
1:K:134:THR:HG23	1:K:144:LYS:CA	2.48	0.43
1:M:130:GLU:HB3	1:M:168:THR:H	1.84	0.43
1:N:237:HIS:CE1	1:N:239:ASN:HB2	2.54	0.43
1:O:104:MET:HE1	1:O:266:VAL:CG1	2.49	0.43
1:C:82:LEU:HD13	1:C:90:GLY:HA3	2.00	0.42
1:C:87:ASN:HD21	1:C:110:LYS:HB2	1.84	0.42
1:C:110:LYS:HA	1:C:110:LYS:HD3	1.88	0.42
1:D:254:LEU:HA	1:D:274:PRO:O	2.19	0.42
1:E:135:LEU:HD11	1:E:159:HIS:HB2	2.00	0.42
1:H:93:LEU:HD11	1:H:106:LEU:HG	2.01	0.42
1:I:86:THR:HB	1:I:114:SER:H	1.83	0.42
1:I:124:ARG:NE	1:I:173:GLU:OE2	2.52	0.42
1:K:82:LEU:HB3	1:K:85:TRP:CG	2.54	0.42
1:K:154:PRO:HB3	1:K:184:THR:OG1	2.19	0.42
1:L:82:LEU:HA	1:L:82:LEU:HD12	1.87	0.42
1:L:234:LYS:HE2	1:P:60:PHE:O	2.19	0.42
1:L:252:TYR:CE1	1:L:277:TYR:HB2	2.53	0.42
1:M:73:THR:HB	1:M:74:PRO:HD2	2.01	0.42
1:N:155:PRO:O	1:N:156:ASN:HB2	2.18	0.42
1:C:237:HIS:ND1	1:C:239:ASN:HB2	2.33	0.42
1:E:268:TRP:CZ2	1:E:270:ALA:HB2	2.54	0.42
1:H:122:ILE:CG2	1:N:298:LEU:HD13	2.48	0.42
1:H:207:ARG:HG3	1:H:207:ARG:NH1	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:220:ILE:HD13	1:I:290:TYR:HA	1.99	0.42
1:J:220:ILE:HD13	1:J:290:TYR:HA	2.00	0.42
1:K:270:ALA:O	1:K:273:VAL:HG12	2.18	0.42
1:L:152:TYR:CG	1:L:153:LEU:N	2.88	0.42
1:O:93:LEU:HD13	1:O:104:MET:CE	2.47	0.42
1:O:110:LYS:HA	1:O:110:LYS:HE2	2.01	0.42
1:P:128:VAL:HG22	1:P:149:SER:H	1.85	0.42
1:F:204:PHE:CD1	1:F:204:PHE:C	2.98	0.42
1:G:93:LEU:HD13	1:G:266:VAL:HG11	2.01	0.42
1:G:198:GLU:O	1:G:199:THR:CG2	2.67	0.42
1:I:208:LYS:HE2	1:I:221:HIS:CE1	2.54	0.42
1:J:208:LYS:HE2	1:J:221:HIS:NE2	2.34	0.42
1:L:124:ARG:HG2	1:L:125:LEU:N	2.34	0.42
1:L:207:ARG:HB2	1:L:222:THR:HG22	2.01	0.42
1:O:190:SER:O	1:O:191:THR:C	2.62	0.42
1:P:238:TYR:CZ	1:P:239:ASN:OD1	2.72	0.42
1:D:185:GLU:O	1:D:187:ILE:HG12	2.19	0.42
1:F:174:ARG:HG2	1:F:175:ARG:N	2.35	0.42
1:H:103:VAL:HG11	1:N:298:LEU:HG	2.01	0.42
1:K:54:LEU:HD12	1:K:75:GLU:HG3	2.01	0.42
1:L:106:LEU:HD23	1:L:170:VAL:HA	2.01	0.42
1:L:141:SER:OG	1:L:142:SER:N	2.52	0.42
1:N:129:VAL:HG23	1:N:170:VAL:HG12	2.01	0.42
1:O:266:VAL:C	1:O:267:ILE:HG13	2.45	0.42
1:A:152:TYR:C	1:A:153:LEU:HG	2.44	0.42
1:A:154:PRO:HG2	1:A:185:GLU:HA	2.00	0.42
1:D:137:ASN:HD21	1:D:140:SER:CB	2.26	0.42
1:E:93:LEU:HD13	1:E:266:VAL:HG11	2.00	0.42
1:F:153:LEU:HD13	1:F:159:HIS:CE1	2.55	0.42
1:J:169:LEU:N	1:J:169:LEU:HD12	2.34	0.42
1:K:125:LEU:HD13	1:K:125:LEU:C	2.43	0.42
1:O:100:SER:HB3	1:O:268:TRP:CH2	2.55	0.42
1:O:208:LYS:HE3	1:O:221:HIS:NE2	2.34	0.42
1:P:153:LEU:HD23	1:P:186:LEU:HD13	2.01	0.42
1:E:121:ASP:H	1:E:156:ASN:HD21	1.68	0.42
1:G:220:ILE:HA	1:G:289:LEU:O	2.20	0.42
1:H:128:VAL:HG22	1:H:169:LEU:HD11	2.01	0.42
1:J:214:VAL:O	1:J:214:VAL:HG22	2.20	0.42
1:K:88:THR:HG22	1:K:109:MET:CB	2.50	0.42
1:K:134:THR:HG23	1:K:144:LYS:HA	2.01	0.42
1:K:245:LEU:HD23	1:K:262:GLN:C	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:125:LEU:HD12	1:N:172:PHE:HD2	1.84	0.42
1:N:126:ILE:HD13	1:N:161:LEU:HD11	2.01	0.42
1:O:226:GLN:O	1:O:227:PRO:C	2.62	0.42
1:P:63:SER:HA	1:P:71:LEU:O	2.19	0.42
1:P:82:LEU:CB	1:P:85:TRP:HB2	2.49	0.42
1:P:153:LEU:HD22	1:P:157:PHE:CE2	2.55	0.42
1:P:191:THR:HG22	1:P:207:ARG:HH11	1.84	0.42
1:B:218:PHE:HA	1:B:293:VAL:HG22	2.01	0.42
1:C:206:LEU:HD12	1:C:207:ARG:H	1.83	0.42
1:D:83:PRO:O	1:D:84:ASP:HB2	2.19	0.42
1:E:125:LEU:HD13	1:E:126:ILE:N	2.34	0.42
1:F:158:HIS:ND1	1:F:158:HIS:C	2.78	0.42
1:G:237:HIS:CE1	1:G:239:ASN:HB2	2.55	0.42
1:I:165:GLU:HB3	1:I:166:SER:H	1.52	0.42
1:J:202:GLU:HA	1:J:232:ASN:HD22	1.85	0.42
1:K:164:VAL:HG23	1:K:165:GLU:H	1.85	0.42
1:O:133:VAL:HG22	1:O:134:THR:N	2.34	0.42
1:O:185:GLU:O	1:O:186:LEU:C	2.62	0.42
1:O:202:GLU:OE2	1:O:233:VAL:HG12	2.20	0.42
1:P:145:LEU:C	1:P:146:THR:O	2.61	0.42
1:B:100:SER:HA	1:B:240:GLN:HE22	1.85	0.42
1:H:133:VAL:HG23	1:H:162:ASP:C	2.45	0.42
1:J:155:PRO:C	1:J:157:PHE:H	2.27	0.42
1:J:168:THR:C	1:J:169:LEU:HD12	2.45	0.42
1:M:251:ILE:HD13	1:M:260:PRO:HA	2.01	0.42
1:N:73:THR:HG22	1:N:265:ASP:OD1	2.20	0.42
1:O:211:PRO:HB2	1:O:216:TYR:CE2	2.54	0.42
1:B:72:ILE:HG21	1:B:93:LEU:HD22	2.01	0.42
1:B:216:TYR:HA	3:B:443:HOH:O	2.20	0.42
1:E:218:PHE:CD1	1:E:218:PHE:C	2.98	0.42
1:F:175:ARG:NH1	1:F:175:ARG:HG3	2.35	0.42
1:J:153:LEU:HD22	1:J:159:HIS:CG	2.54	0.42
1:J:190:SER:HB3	1:J:193:LYS:HG3	2.01	0.42
1:M:85:TRP:CE3	1:M:115:SER:HA	2.55	0.42
1:M:88:THR:CG2	1:M:109:MET:HG2	2.50	0.42
1:N:132:ALA:HB1	1:N:144:LYS:HE3	2.01	0.42
1:O:131:GLY:HA3	1:O:166:SER:O	2.19	0.42
1:F:298:LEU:HG	1:L:103:VAL:HG13	2.01	0.42
1:G:127:PHE:CZ	1:G:288:LEU:HD11	2.54	0.42
1:G:154:PRO:HD2	1:G:157:PHE:CD1	2.54	0.42
1:H:196:LEU:HD22	1:H:205:GLU:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:250:GLY:HA3	1:H:278:ALA:O	2.20	0.42
1:K:56:ASP:O	1:K:58:PRO:HD3	2.20	0.42
1:L:62:ARG:HB2	1:L:73:THR:HG21	2.01	0.42
1:L:127:PHE:O	1:L:169:LEU:HA	2.19	0.42
1:G:172:PHE:O	1:G:173:GLU:HG3	2.20	0.41
1:H:72:ILE:HD13	1:H:93:LEU:O	2.20	0.41
1:H:288:LEU:HD12	1:H:288:LEU:HA	1.89	0.41
1:J:129:VAL:O	1:J:129:VAL:HG12	2.20	0.41
1:K:73:THR:OG1	1:K:75:GLU:OE2	2.38	0.41
1:M:141:SER:O	1:M:142:SER:HB3	2.19	0.41
1:M:208:LYS:CB	1:M:219:ASN:HD21	2.17	0.41
1:N:284:ARG:NH2	1:N:286:ARG:NH2	2.52	0.41
1:B:218:PHE:CD1	1:B:218:PHE:C	2.97	0.41
1:C:100:SER:HB3	1:C:268:TRP:CZ3	2.55	0.41
1:C:218:PHE:CD1	1:C:218:PHE:C	2.98	0.41
1:F:296:ASN:ND2	1:F:298:LEU:CB	2.82	0.41
1:G:114:SER:HA	1:G:161:LEU:O	2.19	0.41
1:G:135:LEU:HD23	1:G:143:LYS:HB2	2.01	0.41
1:G:151:ALA:HA	1:G:187:ILE:O	2.20	0.41
1:H:123:GLU:OE2	1:H:217:ASP:OD1	2.38	0.41
1:I:127:PHE:HB3	1:I:170:VAL:HG13	2.01	0.41
1:J:212:MET:O	1:J:213:SER:C	2.63	0.41
1:J:296:ASN:C	1:J:298:LEU:H	2.28	0.41
1:K:94:ILE:O	1:K:103:VAL:HA	2.20	0.41
1:M:276:TRP:CG	1:M:277:TYR:N	2.88	0.41
1:O:120:GLN:CG	1:O:121:ASP:OD2	2.68	0.41
1:B:69:HIS:HA	1:B:268:TRP:O	2.20	0.41
1:D:74:PRO:C	1:D:76:SER:N	2.76	0.41
1:E:253:ARG:HB3	1:E:276:TRP:HB3	2.02	0.41
1:F:224:ASP:OD1	1:F:286:ARG:CD	2.50	0.41
1:J:40:ILE:O	1:J:41:TYR:HB2	2.20	0.41
1:K:135:LEU:HD12	1:K:136:THR:H	1.86	0.41
1:M:243:LEU:HD12	1:M:244:LEU:N	2.34	0.41
1:N:82:LEU:HB3	1:N:85:TRP:CG	2.55	0.41
1:N:115:SER:CB	1:N:161:LEU:H	2.34	0.41
1:O:153:LEU:HD13	1:O:159:HIS:NE2	2.36	0.41
1:A:155:PRO:O	1:A:156:ASN:HB2	2.21	0.41
1:B:41:TYR:O	1:B:44:ALA:HB3	2.20	0.41
1:E:70:ALA:HB3	1:E:268:TRP:HB3	2.01	0.41
1:E:120:GLN:O	1:E:121:ASP:HB2	2.19	0.41
1:E:135:LEU:HD13	1:E:161:LEU:HD23	2.00	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:127:PHE:HB3	1:F:170:VAL:HG13	2.02	0.41
1:F:296:ASN:ND2	1:F:298:LEU:H	2.18	0.41
1:G:152:TYR:O	1:G:186:LEU:HD12	2.21	0.41
1:I:149:SER:HA	1:I:189:GLY:O	2.20	0.41
1:I:222:THR:HG23	1:I:286:ARG:HD2	2.02	0.41
1:J:294:ASN:O	1:J:295:ARG:HG2	2.21	0.41
1:K:96:PRO:C	1:K:98:THR:H	2.29	0.41
1:L:196:LEU:N	1:L:196:LEU:CD1	2.83	0.41
1:M:267:ILE:CG2	1:M:268:TRP:N	2.83	0.41
1:O:296:ASN:HD21	1:O:298:LEU:HD12	1.85	0.41
1:P:197:LEU:HD12	1:P:208:LYS:HG3	2.01	0.41
1:A:126:ILE:HD12	1:A:126:ILE:C	2.46	0.41
1:B:57:LEU:HD23	1:B:57:LEU:HA	1.95	0.41
1:B:209:LEU:O	1:B:210:LEU:HD23	2.19	0.41
1:E:273:VAL:O	1:E:273:VAL:HG13	2.19	0.41
1:F:94:ILE:O	1:F:103:VAL:HA	2.21	0.41
1:H:111:GLU:CD	1:H:111:GLU:N	2.70	0.41
1:I:220:ILE:HA	1:I:289:LEU:O	2.21	0.41
1:A:111:GLU:O	1:A:112:MET:C	2.64	0.41
1:D:74:PRO:O	1:D:76:SER:N	2.54	0.41
1:H:197:LEU:HD12	1:H:208:LYS:HG3	2.02	0.41
1:J:120:GLN:HG3	1:J:156:ASN:HD21	1.85	0.41
1:K:66:LYS:NZ	1:K:257:ASN:OD1	2.51	0.41
1:K:224:ASP:HA	1:K:285:SER:O	2.20	0.41
1:K:294:ASN:O	1:K:295:ARG:HG2	2.21	0.41
1:L:85:TRP:CE3	1:L:88:THR:HG21	2.55	0.41
1:M:221:HIS:HB2	1:M:289:LEU:HB3	2.02	0.41
1:N:92:TYR:HA	1:N:105:TYR:HB3	2.03	0.41
1:A:196:LEU:HD21	1:A:207:ARG:CZ	2.50	0.41
1:C:252:TYR:CD1	1:C:277:TYR:CD1	3.09	0.41
1:F:204:PHE:CE2	1:F:231:LEU:HD11	2.55	0.41
1:G:191:THR:HG22	1:G:207:ARG:HD2	2.01	0.41
1:I:83:PRO:O	1:I:85:TRP:HD1	2.02	0.41
1:J:137:ASN:ND2	1:J:140:SER:N	2.67	0.41
1:K:56:ASP:C	1:K:58:PRO:HD3	2.45	0.41
1:K:74:PRO:C	1:K:76:SER:H	2.29	0.41
1:K:79:TYR:HA	1:K:90:GLY:O	2.20	0.41
1:L:73:THR:HG1	1:L:75:GLU:CD	2.28	0.41
1:L:244:LEU:HD12	1:L:245:LEU:N	2.36	0.41
1:M:85:TRP:CD2	1:M:115:SER:HA	2.55	0.41
1:M:137:ASN:H	1:M:137:ASN:ND2	2.11	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:224:ASP:CG	1:M:286:ARG:HD2	2.45	0.41
1:N:100:SER:HB3	1:N:268:TRP:CH2	2.56	0.41
1:O:144:LYS:C	1:O:145:LEU:HG	2.46	0.41
1:P:117:LEU:HD11	1:P:158:HIS:CD2	2.55	0.41
1:D:298:LEU:O	1:D:298:LEU:HD23	2.20	0.41
1:E:237:HIS:HB2	1:E:239:ASN:HD22	1.86	0.41
1:E:243:LEU:HD23	1:E:269:MET:CE	2.50	0.41
1:G:241:HIS:HB2	1:G:269:MET:HB2	2.02	0.41
1:I:105:TYR:CZ	1:I:171:VAL:CG1	3.04	0.41
1:I:125:LEU:HD22	1:I:126:ILE:N	2.35	0.41
1:J:213:SER:C	1:J:215:ALA:H	2.29	0.41
1:K:113:SER:CB	1:K:163:CYS:SG	3.08	0.41
1:K:147:VAL:O	1:K:148:ASP:HB3	2.21	0.41
1:L:205:GLU:H	1:L:205:GLU:HG2	1.61	0.41
1:M:176:TYR:CE2	1:M:178:TYR:HA	2.56	0.41
1:B:142:SER:O	1:B:143:LYS:HD2	2.21	0.41
1:C:240:GLN:HB3	1:C:271:PRO:HG3	2.02	0.41
1:C:243:LEU:C	1:C:243:LEU:CD1	2.93	0.41
1:D:102:PHE:HD2	1:D:240:GLN:HE21	1.62	0.41
1:D:155:PRO:O	1:D:156:ASN:HB2	2.21	0.41
1:E:154:PRO:HG2	1:E:185:GLU:CA	2.49	0.41
1:E:235:GLU:HB2	1:E:275:GLN:HG3	2.03	0.41
1:F:83:PRO:C	1:F:85:TRP:H	2.28	0.41
1:G:108:LYS:HE2	1:G:168:THR:HG21	2.02	0.41
1:G:226:GLN:O	1:G:227:PRO:C	2.63	0.41
1:G:235:GLU:HB2	1:G:275:GLN:HG3	2.02	0.41
1:H:141:SER:HB2	1:H:142:SER:H	1.60	0.41
1:I:85:TRP:CD1	1:I:116:GLY:H	2.39	0.41
1:J:218:PHE:HE1	1:J:220:ILE:HG12	1.86	0.41
1:J:243:LEU:HD23	1:J:269:MET:CE	2.51	0.41
1:L:226:GLN:HB2	1:L:229:GLU:OE1	2.21	0.41
1:M:57:LEU:HA	1:M:57:LEU:HD23	1.81	0.41
1:M:107:ALA:N	1:M:169:LEU:O	2.46	0.41
1:N:108:LYS:NZ	1:N:168:THR:CG2	2.84	0.41
1:N:114:SER:HA	1:N:161:LEU:O	2.21	0.41
1:N:253:ARG:HG3	1:N:253:ARG:NH1	2.36	0.41
1:O:88:THR:CG2	1:O:109:MET:HG2	2.51	0.41
1:O:126:ILE:HD12	1:O:126:ILE:C	2.46	0.41
1:O:152:TYR:O	1:O:153:LEU:HD23	2.20	0.41
1:P:82:LEU:HB3	1:P:85:TRP:CG	2.56	0.41
1:P:123:GLU:O	1:P:173:GLU:HA	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:243:LEU:HD23	1:P:289:LEU:CD1	2.51	0.41
1:E:78:VAL:HG21	1:P:237:HIS:HD2	1.85	0.41
1:E:290:TYR:CD2	1:E:290:TYR:C	2.97	0.41
1:F:146:THR:O	1:F:147:VAL:C	2.64	0.41
1:H:113:SER:OG	1:H:163:CYS:HB3	2.20	0.41
1:H:197:LEU:HD12	1:H:208:LYS:HE3	2.03	0.41
1:H:205:GLU:HB2	1:H:224:ASP:HB2	2.03	0.41
1:H:206:LEU:HD12	1:H:207:ARG:H	1.86	0.41
1:I:40:ILE:O	1:I:41:TYR:HB2	2.20	0.41
1:I:153:LEU:HA	1:I:154:PRO:HD3	1.96	0.41
1:J:120:GLN:HA	1:J:156:ASN:ND2	2.36	0.41
1:J:121:ASP:H	1:J:156:ASN:ND2	2.19	0.41
1:J:207:ARG:HB2	1:J:222:THR:CG2	2.51	0.41
1:K:245:LEU:HD12	1:K:245:LEU:HA	1.90	0.41
1:L:134:THR:HG23	1:L:143:LYS:O	2.20	0.41
1:M:130:GLU:HB3	1:M:168:THR:HB	2.02	0.41
1:M:145:LEU:HB3	1:M:149:SER:HB2	2.02	0.41
1:O:207:ARG:O	1:O:221:HIS:HA	2.21	0.41
1:P:132:ALA:O	1:P:163:CYS:HB2	2.21	0.41
1:P:262:GLN:O	1:P:265:ASP:HB2	2.20	0.41
1:A:50:SER:HB2	1:A:51:PRO:CD	2.51	0.40
1:A:109:MET:HB2	1:A:167:ALA:HB3	2.04	0.40
1:A:199:THR:HB	1:A:202:GLU:HB2	2.03	0.40
1:C:298:LEU:HD21	3:G:426:HOH:O	2.21	0.40
1:D:85:TRP:CE3	1:D:115:SER:HA	2.56	0.40
1:E:123:GLU:HG2	1:E:174:ARG:O	2.20	0.40
1:E:146:THR:O	1:E:149:SER:HB2	2.21	0.40
1:E:185:GLU:O	1:E:187:ILE:HG12	2.21	0.40
1:E:285:SER:HB2	3:E:402:HOH:O	2.21	0.40
1:F:43:LYS:C	1:F:45:THR:N	2.77	0.40
1:G:262:GLN:O	1:G:263:ALA:C	2.63	0.40
1:H:122:ILE:HG21	1:N:298:LEU:HD13	2.03	0.40
1:I:197:LEU:O	1:I:199:THR:HG23	2.21	0.40
1:J:92:TYR:HA	1:J:105:TYR:HB3	2.03	0.40
1:K:259:TYR:HA	1:K:260:PRO:HD3	1.92	0.40
1:K:293:VAL:HG21	3:K:421:HOH:O	2.21	0.40
1:L:43:LYS:C	1:L:46:ASN:H	2.30	0.40
1:M:187:ILE:C	1:M:188:VAL:HG23	2.46	0.40
1:N:153:LEU:O	1:N:154:PRO:C	2.63	0.40
1:O:68:ASP:O	1:O:69:HIS:HB3	2.21	0.40
1:P:184:THR:HG22	1:P:215:ALA:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:247:GLU:O	1:A:285:SER:HA	2.21	0.40
1:C:271:PRO:O	1:C:272:PHE:HB2	2.20	0.40
1:E:82:LEU:HB3	1:E:85:TRP:HB2	2.03	0.40
1:E:82:LEU:HB2	1:E:88:THR:O	2.21	0.40
1:F:62:ARG:HD3	3:F:404:HOH:O	2.22	0.40
1:I:290:TYR:CD2	1:I:291:LYS:N	2.89	0.40
1:J:135:LEU:O	1:J:136:THR:HG23	2.20	0.40
1:K:96:PRO:C	1:K:98:THR:N	2.79	0.40
1:K:120:GLN:NE2	3:K:412:HOH:O	2.54	0.40
1:K:243:LEU:C	1:K:243:LEU:CD1	2.92	0.40
1:L:123:GLU:OE1	1:L:218:PHE:CE2	2.73	0.40
1:L:226:GLN:HB2	1:L:229:GLU:CD	2.45	0.40
1:N:214:VAL:O	1:N:215:ALA:C	2.64	0.40
1:O:155:PRO:O	1:O:156:ASN:CB	2.68	0.40
1:C:47:PRO:HA	3:C:407:HOH:O	2.20	0.40
1:C:272:PHE:HE2	1:G:95:THR:OG1	2.04	0.40
1:E:145:LEU:HD22	1:E:149:SER:HB3	2.03	0.40
1:F:253:ARG:HH12	1:L:61:THR:HG22	1.86	0.40
1:H:133:VAL:HG23	1:H:163:CYS:N	2.36	0.40
1:H:190:SER:O	1:H:191:THR:C	2.64	0.40
1:I:284:ARG:HD2	1:I:284:ARG:C	2.46	0.40
1:J:237:HIS:HD2	1:K:78:VAL:HG21	1.86	0.40
1:J:245:LEU:HD12	1:J:287:TYR:HB3	2.04	0.40
1:K:86:THR:N	1:K:114:SER:O	2.54	0.40
1:L:87:ASN:CG	1:L:110:LYS:HB2	2.46	0.40
1:L:147:VAL:CG1	1:L:148:ASP:H	2.32	0.40
1:L:243:LEU:CD1	1:L:287:TYR:HB2	2.45	0.40
1:M:86:THR:HB	1:M:114:SER:OG	2.21	0.40
1:M:276:TRP:CH2	1:M:278:ALA:HB2	2.56	0.40
1:O:95:THR:C	1:O:97:ALA:N	2.80	0.40
1:O:245:LEU:HD12	1:O:287:TYR:HB3	2.04	0.40
1:P:150:TYR:CD1	1:P:209:LEU:HD13	2.56	0.40
1:D:150:TYR:CG	1:D:209:LEU:HD13	2.56	0.40
1:E:243:LEU:HD12	1:E:243:LEU:O	2.19	0.40
1:F:233:VAL:O	1:F:233:VAL:HG13	2.21	0.40
1:G:218:PHE:CD1	1:G:218:PHE:C	3.00	0.40
1:H:80:SER:O	1:H:81:PRO:C	2.64	0.40
1:I:92:TYR:CE1	1:I:105:TYR:CD2	3.09	0.40
1:J:86:THR:O	1:J:113:SER:HB2	2.21	0.40
1:J:152:TYR:CG	1:J:153:LEU:N	2.89	0.40
1:J:279:ALA:O	1:J:280:LEU:HD23	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:109:MET:HB3	1:K:113:SER:HB3	2.03	0.40
1:M:191:THR:HG21	1:M:286:ARG:NH2	2.36	0.40
1:N:81:PRO:O	1:N:83:PRO:HD3	2.21	0.40
1:N:275:GLN:HE21	1:N:275:GLN:HB3	1.63	0.40
1:O:49:LEU:HD23	1:P:57:LEU:HD11	1.99	0.40
1:P:245:LEU:HD12	1:P:287:TYR:HB3	2.03	0.40
1:P:296:ASN:HA	1:P:297:PRO:HD2	1.84	0.40
1:A:43:LYS:HG2	3:A:430:HOH:O	2.22	0.40
1:C:82:LEU:HD12	1:C:82:LEU:HA	1.92	0.40
1:C:239:ASN:ND2	1:C:239:ASN:H	2.20	0.40
1:F:102:PHE:HE2	1:F:240:GLN:HE21	1.65	0.40
1:G:196:LEU:CD2	1:G:207:ARG:NH1	2.85	0.40
1:G:243:LEU:C	1:G:243:LEU:CD1	2.89	0.40
1:I:197:LEU:HD12	1:I:208:LYS:HG3	2.02	0.40
1:I:296:ASN:HD22	1:I:298:LEU:H	1.70	0.40
1:K:255:GLY:HA3	3:K:414:HOH:O	2.22	0.40
1:L:70:ALA:HB3	1:L:268:TRP:HB3	2.03	0.40
1:M:124:ARG:HG2	1:M:125:LEU:H	1.84	0.40
1:N:109:MET:HE2	1:N:113:SER:CB	2.52	0.40
1:N:115:SER:HB3	1:N:161:LEU:H	1.86	0.40
1:N:123:GLU:HG2	1:N:174:ARG:O	2.21	0.40
1:O:51:PRO:HG3	1:O:75:GLU:CA	2.52	0.40
1:P:95:THR:HA	1:P:103:VAL:HG12	2.04	0.40
1:P:110:LYS:HB3	1:P:111:GLU:OE1	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [\(i\)](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	254/266 (96%)	233 (92%)	18 (7%)	3 (1%)	10 20

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	254/266 (96%)	238 (94%)	14 (6%)	2 (1%)	16	31
1	C	254/266 (96%)	238 (94%)	14 (6%)	2 (1%)	16	31
1	D	254/266 (96%)	235 (92%)	17 (7%)	2 (1%)	16	31
1	E	254/266 (96%)	240 (94%)	13 (5%)	1 (0%)	30	49
1	F	254/266 (96%)	234 (92%)	20 (8%)	0	100	100
1	G	254/266 (96%)	228 (90%)	24 (9%)	2 (1%)	16	31
1	H	254/266 (96%)	227 (89%)	26 (10%)	1 (0%)	30	49
1	I	254/266 (96%)	241 (95%)	11 (4%)	2 (1%)	16	31
1	J	254/266 (96%)	231 (91%)	21 (8%)	2 (1%)	16	31
1	K	254/266 (96%)	222 (87%)	20 (8%)	12 (5%)	2	2
1	L	254/266 (96%)	220 (87%)	26 (10%)	8 (3%)	3	5
1	M	254/266 (96%)	220 (87%)	30 (12%)	4 (2%)	7	14
1	N	254/266 (96%)	227 (89%)	23 (9%)	4 (2%)	7	14
1	O	254/266 (96%)	216 (85%)	32 (13%)	6 (2%)	4	8
1	P	254/266 (96%)	211 (83%)	32 (13%)	11 (4%)	2	2
All	All	4064/4256 (96%)	3661 (90%)	341 (8%)	62 (2%)	8	16

All (62) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	141	SER
1	I	141	SER
1	K	115	SER
1	L	148	ASP
1	O	147	VAL
1	O	148	ASP
1	P	115	SER
1	P	146	THR
1	A	167	ALA
1	D	142	SER
1	K	159	HIS
1	K	186	LEU
1	K	214	VAL
1	M	142	SER
1	N	294	ASN
1	P	87	ASN
1	P	191	THR

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Mol	Chain	Res	Type
1	C	75	GLU
1	D	75	GLU
1	K	58	PRO
1	K	142	SER
1	K	165	GLU
1	L	142	SER
1	L	151	ALA
1	L	194	GLN
1	N	55	GLN
1	P	40	ILE
1	A	141	SER
1	C	119	PRO
1	E	75	GLU
1	H	119	PRO
1	I	112	MET
1	J	119	PRO
1	K	182	HIS
1	L	193	LYS
1	M	119	PRO
1	M	231	LEU
1	O	165	GLU
1	P	154	PRO
1	P	214	VAL
1	A	112	MET
1	G	182	HIS
1	K	111	GLU
1	K	164	VAL
1	P	109	MET
1	P	112	MET
1	P	211	PRO
1	G	119	PRO
1	J	214	VAL
1	K	75	GLU
1	K	203	VAL
1	N	81	PRO
1	N	154	PRO
1	O	154	PRO
1	P	141	SER
1	L	147	VAL
1	O	58	PRO
1	B	96	PRO
1	L	227	PRO

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Mol	Chain	Res	Type
1	M	236	VAL
1	L	214	VAL
1	O	220	ILE

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	230/237 (97%)	217 (94%)	13 (6%)	18	39
1	B	230/237 (97%)	217 (94%)	13 (6%)	18	39
1	C	230/237 (97%)	219 (95%)	11 (5%)	23	46
1	D	230/237 (97%)	213 (93%)	17 (7%)	13	27
1	E	230/237 (97%)	217 (94%)	13 (6%)	18	39
1	F	230/237 (97%)	217 (94%)	13 (6%)	18	39
1	G	230/237 (97%)	211 (92%)	19 (8%)	10	22
1	H	230/237 (97%)	215 (94%)	15 (6%)	15	32
1	I	230/237 (97%)	216 (94%)	14 (6%)	17	35
1	J	230/237 (97%)	217 (94%)	13 (6%)	18	39
1	K	230/237 (97%)	210 (91%)	20 (9%)	9	21
1	L	230/237 (97%)	214 (93%)	16 (7%)	14	29
1	M	230/237 (97%)	212 (92%)	18 (8%)	11	24
1	N	230/237 (97%)	213 (93%)	17 (7%)	13	27
1	O	230/237 (97%)	207 (90%)	23 (10%)	7	15
1	P	230/237 (97%)	212 (92%)	18 (8%)	11	24
All	All	3680/3792 (97%)	3427 (93%)	253 (7%)	14	30

All (253) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	ILE

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Mol	Chain	Res	Type
1	A	125	LEU
1	A	153	LEU
1	A	169	LEU
1	A	171	VAL
1	A	222	THR
1	A	233	VAL
1	A	239	ASN
1	A	243	LEU
1	A	249	GLN
1	A	268	TRP
1	A	283	THR
1	A	286	ARG
1	B	82	LEU
1	B	111	GLU
1	B	125	LEU
1	B	143	LYS
1	B	170	VAL
1	B	171	VAL
1	B	197	LEU
1	B	222	THR
1	B	243	LEU
1	B	249	GLN
1	B	286	ARG
1	B	289	LEU
1	B	296	ASN
1	C	40	ILE
1	C	82	LEU
1	C	144	LYS
1	C	169	LEU
1	C	171	VAL
1	C	222	THR
1	C	243	LEU
1	C	249	GLN
1	C	283	THR
1	C	286	ARG
1	C	298	LEU
1	D	40	ILE
1	D	82	LEU
1	D	103	VAL
1	D	112	MET
1	D	125	LEU
1	D	134	THR

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Mol	Chain	Res	Type
1	D	153	LEU
1	D	171	VAL
1	D	199	THR
1	D	222	THR
1	D	239	ASN
1	D	243	LEU
1	D	247	GLU
1	D	249	GLN
1	D	286	ARG
1	D	296	ASN
1	D	298	LEU
1	E	76	SER
1	E	111	GLU
1	E	125	LEU
1	E	136	THR
1	E	165	GLU
1	E	166	SER
1	E	170	VAL
1	E	171	VAL
1	E	233	VAL
1	E	243	LEU
1	E	249	GLN
1	E	286	ARG
1	E	296	ASN
1	F	40	ILE
1	F	111	GLU
1	F	112	MET
1	F	153	LEU
1	F	171	VAL
1	F	192	ASP
1	F	203	VAL
1	F	222	THR
1	F	231	LEU
1	F	243	LEU
1	F	283	THR
1	F	286	ARG
1	F	289	LEU
1	G	40	ILE
1	G	45	THR
1	G	46	ASN
1	G	68	ASP
1	G	82	LEU

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Mol	Chain	Res	Type
1	G	111	GLU
1	G	133	VAL
1	G	135	LEU
1	G	164	VAL
1	G	169	LEU
1	G	171	VAL
1	G	183	THR
1	G	214	VAL
1	G	222	THR
1	G	239	ASN
1	G	243	LEU
1	G	249	GLN
1	G	286	ARG
1	G	288	LEU
1	H	40	ILE
1	H	82	LEU
1	H	111	GLU
1	H	134	THR
1	H	141	SER
1	H	153	LEU
1	H	169	LEU
1	H	171	VAL
1	H	239	ASN
1	H	243	LEU
1	H	247	GLU
1	H	249	GLN
1	H	286	ARG
1	H	296	ASN
1	H	298	LEU
1	I	40	ILE
1	I	49	LEU
1	I	82	LEU
1	I	137	ASN
1	I	148	ASP
1	I	171	VAL
1	I	185	GLU
1	I	186	LEU
1	I	191	THR
1	I	222	THR
1	I	243	LEU
1	I	249	GLN
1	I	286	ARG

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Mol	Chain	Res	Type
1	I	296	ASN
1	J	111	GLU
1	J	136	THR
1	J	141	SER
1	J	148	ASP
1	J	162	ASP
1	J	171	VAL
1	J	187	ILE
1	J	222	THR
1	J	243	LEU
1	J	249	GLN
1	J	285	SER
1	J	286	ARG
1	J	296	ASN
1	K	40	ILE
1	K	45	THR
1	K	75	GLU
1	K	82	LEU
1	K	86	THR
1	K	95	THR
1	K	96	PRO
1	K	111	GLU
1	K	113	SER
1	K	125	LEU
1	K	130	GLU
1	K	137	ASN
1	K	153	LEU
1	K	164	VAL
1	K	193	LYS
1	K	199	THR
1	K	218	PHE
1	K	222	THR
1	K	243	LEU
1	K	249	GLN
1	L	40	ILE
1	L	81	PRO
1	L	111	GLU
1	L	144	LYS
1	L	148	ASP
1	L	166	SER
1	L	170	VAL
1	L	171	VAL

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Mol	Chain	Res	Type
1	L	192	ASP
1	L	197	LEU
1	L	205	GLU
1	L	222	THR
1	L	243	LEU
1	L	249	GLN
1	L	286	ARG
1	L	298	LEU
1	M	86	THR
1	M	111	GLU
1	M	129	VAL
1	M	134	THR
1	M	137	ASN
1	M	144	LYS
1	M	163	CYS
1	M	165	GLU
1	M	169	LEU
1	M	171	VAL
1	M	198	GLU
1	M	222	THR
1	M	232	ASN
1	M	233	VAL
1	M	243	LEU
1	M	249	GLN
1	M	284	ARG
1	M	298	LEU
1	N	40	ILE
1	N	55	GLN
1	N	80	SER
1	N	82	LEU
1	N	84	ASP
1	N	130	GLU
1	N	133	VAL
1	N	134	THR
1	N	136	THR
1	N	185	GLU
1	N	196	LEU
1	N	205	GLU
1	N	243	LEU
1	N	249	GLN
1	N	252	TYR
1	N	275	GLN

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Mol	Chain	Res	Type
1	N	286	ARG
1	O	40	ILE
1	O	45	THR
1	O	56	ASP
1	O	75	GLU
1	O	88	THR
1	O	96	PRO
1	O	111	GLU
1	O	142	SER
1	O	143	LYS
1	O	148	ASP
1	O	166	SER
1	O	170	VAL
1	O	171	VAL
1	O	191	THR
1	O	197	LEU
1	O	214	VAL
1	O	219	ASN
1	O	223	MET
1	O	231	LEU
1	O	233	VAL
1	O	243	LEU
1	O	244	LEU
1	O	249	GLN
1	P	40	ILE
1	P	49	LEU
1	P	72	ILE
1	P	82	LEU
1	P	125	LEU
1	P	136	THR
1	P	146	THR
1	P	149	SER
1	P	156	ASN
1	P	170	VAL
1	P	183	THR
1	P	212	MET
1	P	222	THR
1	P	243	LEU
1	P	249	GLN
1	P	266	VAL
1	P	283	THR
1	P	296	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (130) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	77	HIS
1	A	156	ASN
1	A	221	HIS
1	A	239	ASN
1	A	240	GLN
1	A	249	GLN
1	A	262	GLN
1	A	296	ASN
1	B	87	ASN
1	B	120	GLN
1	B	137	ASN
1	B	156	ASN
1	B	194	GLN
1	B	226	GLN
1	B	239	ASN
1	B	240	GLN
1	B	262	GLN
1	B	296	ASN
1	C	53	HIS
1	C	55	GLN
1	C	87	ASN
1	C	221	HIS
1	C	239	ASN
1	C	240	GLN
1	C	249	GLN
1	C	262	GLN
1	C	296	ASN
1	D	46	ASN
1	D	137	ASN
1	D	156	ASN
1	D	158	HIS
1	D	239	ASN
1	D	240	GLN
1	D	294	ASN
1	D	296	ASN
1	E	156	ASN
1	E	239	ASN
1	E	240	GLN
1	E	296	ASN
1	F	46	ASN
1	F	137	ASN

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Mol	Chain	Res	Type
1	F	226	GLN
1	F	239	ASN
1	F	240	GLN
1	F	262	GLN
1	F	296	ASN
1	G	156	ASN
1	G	182	HIS
1	G	226	GLN
1	G	239	ASN
1	G	240	GLN
1	G	249	GLN
1	G	262	GLN
1	G	275	GLN
1	H	156	ASN
1	H	221	HIS
1	H	239	ASN
1	H	240	GLN
1	H	249	GLN
1	H	262	GLN
1	H	296	ASN
1	I	46	ASN
1	I	55	GLN
1	I	87	ASN
1	I	120	GLN
1	I	137	ASN
1	I	156	ASN
1	I	182	HIS
1	I	226	GLN
1	I	237	HIS
1	I	239	ASN
1	I	249	GLN
1	I	296	ASN
1	J	46	ASN
1	J	55	GLN
1	J	156	ASN
1	J	221	HIS
1	J	232	ASN
1	J	240	GLN
1	J	249	GLN
1	J	257	ASN
1	J	262	GLN
1	J	296	ASN

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Mol	Chain	Res	Type
1	K	87	ASN
1	K	120	GLN
1	K	156	ASN
1	K	194	GLN
1	K	221	HIS
1	K	240	GLN
1	K	249	GLN
1	K	296	ASN
1	L	120	GLN
1	L	137	ASN
1	L	156	ASN
1	L	239	ASN
1	L	240	GLN
1	L	296	ASN
1	M	87	ASN
1	M	137	ASN
1	M	156	ASN
1	M	239	ASN
1	M	240	GLN
1	M	249	GLN
1	M	257	ASN
1	M	262	GLN
1	M	296	ASN
1	N	156	ASN
1	N	194	GLN
1	N	239	ASN
1	N	240	GLN
1	N	294	ASN
1	N	296	ASN
1	O	55	GLN
1	O	101	HIS
1	O	137	ASN
1	O	156	ASN
1	O	219	ASN
1	O	221	HIS
1	O	240	GLN
1	O	262	GLN
1	O	294	ASN
1	O	296	ASN
1	P	46	ASN
1	P	156	ASN
1	P	158	HIS

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Mol	Chain	Res	Type
1	P	232	ASN
1	P	237	HIS
1	P	240	GLN
1	P	249	GLN
1	P	296	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	-0.05	1 (0%) 88 86	20, 32, 47, 64	0
1	B	258/266 (96%)	-0.00	4 (1%) 70 67	18, 33, 47, 55	0
1	C	258/266 (96%)	-0.02	5 (1%) 66 62	18, 32, 50, 63	0
1	D	258/266 (96%)	-0.08	0 100 100	19, 34, 47, 62	0
1	E	258/266 (96%)	0.08	1 (0%) 88 86	19, 37, 53, 65	0
1	F	258/266 (96%)	0.12	1 (0%) 88 86	24, 38, 50, 66	0
1	G	258/266 (96%)	0.32	5 (1%) 66 62	22, 41, 58, 70	0
1	H	258/266 (96%)	0.15	4 (1%) 70 67	24, 38, 54, 66	0
1	I	258/266 (96%)	0.31	2 (0%) 82 80	24, 41, 53, 66	0
1	J	258/266 (96%)	0.46	4 (1%) 70 67	27, 44, 57, 73	0
1	K	258/266 (96%)	0.65	15 (5%) 29 25	26, 46, 63, 70	0
1	L	258/266 (96%)	0.42	3 (1%) 76 73	33, 47, 58, 65	0
1	M	258/266 (96%)	0.63	9 (3%) 47 42	27, 48, 61, 67	0
1	N	258/266 (96%)	0.43	4 (1%) 70 67	26, 46, 59, 66	0
1	O	258/266 (96%)	0.64	8 (3%) 51 47	31, 50, 59, 71	0
1	P	258/266 (96%)	0.66	6 (2%) 61 57	28, 52, 64, 67	0
All	All	4128/4256 (96%)	0.30	72 (1%) 69 65	18, 41, 58, 73	0

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	P	39	PRO	3.9
1	B	140	SER	3.5
1	L	136	THR	3.4
1	O	39	PRO	3.3
1	K	141	SER	3.2

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Mol	Chain	Res	Type	RSRZ
1	H	140	SER	3.1
1	N	40	ILE	3.1
1	K	145	LEU	3.1
1	J	141	SER	2.9
1	O	40	ILE	2.8
1	K	164	VAL	2.7
1	K	199	THR	2.7
1	L	135	LEU	2.7
1	K	169	LEU	2.6
1	P	164	VAL	2.6
1	G	164	VAL	2.6
1	P	40	ILE	2.6
1	G	140	SER	2.5
1	N	65	TYR	2.5
1	I	39	PRO	2.5
1	K	89	LEU	2.5
1	B	141	SER	2.5
1	K	83	PRO	2.5
1	F	40	ILE	2.5
1	B	40	ILE	2.4
1	I	40	ILE	2.4
1	P	142	SER	2.4
1	O	82	LEU	2.4
1	C	140	SER	2.4
1	B	39	PRO	2.3
1	E	141	SER	2.3
1	M	140	SER	2.3
1	M	40	ILE	2.3
1	G	179	LEU	2.3
1	L	39	PRO	2.3
1	M	164	VAL	2.3
1	O	141	SER	2.3
1	C	40	ILE	2.3
1	O	214	VAL	2.3
1	J	134	THR	2.2
1	O	131	GLY	2.2
1	M	186	LEU	2.2
1	M	141	SER	2.2
1	K	86	THR	2.2
1	H	141	SER	2.2
1	K	81	PRO	2.2
1	C	199	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	M	252	TYR	2.2
1	J	140	SER	2.2
1	C	198	GLU	2.2
1	K	131	GLY	2.1
1	K	136	THR	2.1
1	P	246	LEU	2.1
1	K	105	TYR	2.1
1	O	149	SER	2.1
1	P	166	SER	2.1
1	K	112	MET	2.1
1	H	198	GLU	2.1
1	O	220	ILE	2.1
1	M	163	CYS	2.1
1	M	158	HIS	2.1
1	N	116	GLY	2.1
1	A	65	TYR	2.1
1	C	65	TYR	2.1
1	N	161	LEU	2.0
1	H	40	ILE	2.0
1	M	110	LYS	2.0
1	G	39	PRO	2.0
1	K	147	VAL	2.0
1	J	135	LEU	2.0
1	G	65	TYR	2.0
1	K	140	SER	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
2	MN	L	301	1/1	0.96	0.07	46,46,46,46	0
2	MN	C	301	1/1	0.97	0.04	30,30,30,30	0
2	MN	D	301	1/1	0.97	0.07	30,30,30,30	0
2	MN	E	301	1/1	0.97	0.05	29,29,29,29	0
2	MN	J	301	1/1	0.97	0.09	51,51,51,51	0
2	MN	A	301	1/1	0.97	0.08	33,33,33,33	0
2	MN	O	301	1/1	0.97	0.04	47,47,47,47	0
2	MN	H	301	1/1	0.98	0.06	36,36,36,36	0
2	MN	M	301	1/1	0.98	0.04	48,48,48,48	0
2	MN	B	301	1/1	0.98	0.09	32,32,32,32	0
2	MN	K	301	1/1	0.99	0.07	40,40,40,40	0
2	MN	F	301	1/1	0.99	0.03	36,36,36,36	0
2	MN	I	301	1/1	0.99	0.06	34,34,34,34	0
2	MN	N	301	1/1	0.99	0.05	41,41,41,41	0
2	MN	G	301	1/1	0.99	0.06	34,34,34,34	0
2	MN	P	301	1/1	0.99	0.10	44,44,44,44	0

6.5 Other polymers [i](#)

There are no such residues in this entry.