



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 05:17 PM UTC

PDB ID : 3LIB / pdb_00003lib
Title : Crystal Structure of the extracellular domain of the putative histidine kinase mmHK1S-Z3
Authors : Zhang, Z.; Hendrickson, W.A.
Deposited on : 2010-01-24
Resolution : 2.99 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

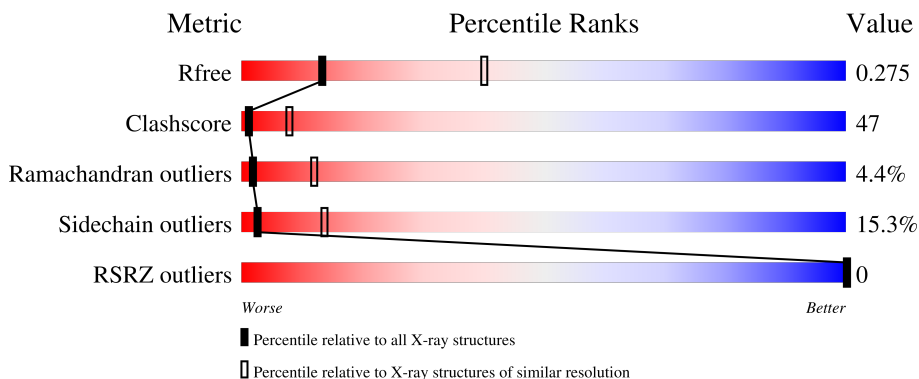
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.99 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.






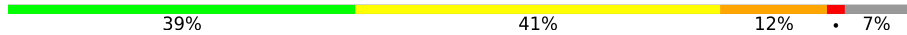
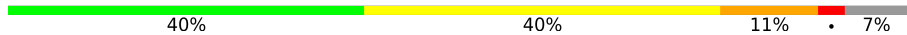
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	290	
1	B	290	
1	C	290	
1	D	290	
1	E	290	

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Mol	Chain	Length	Quality of chain
1	F	290	 48% 35% 10% • 7%
1	G	290	 44% 35% 12% • 7%
1	H	290	 35% 41% 14% • 8%
1	I	290	 39% 41% 12% • 7%
1	J	290	 40% 40% 11% • 7%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 21176 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 Hypothetical sensory transduction histidine kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	271	2122	1352	335	427	8	0	0	0
1	B	271	2122	1352	335	427	8	0	0	0
1	C	268	2092	1333	329	422	8	0	0	0
1	D	271	2122	1352	335	427	8	0	0	0
1	E	268	2094	1335	329	422	8	0	0	0
1	F	271	2122	1352	335	427	8	0	0	0
1	G	270	2113	1347	334	424	8	0	0	0
1	H	267	2086	1331	328	419	8	0	0	0
1	I	271	2122	1352	335	427	8	0	0	0
1	J	271	2122	1352	335	427	8	0	0	0

There are 90 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	30	MET	-	expression tag	UNP Q8PSW1
A	31	GLU	-	expression tag	UNP Q8PSW1
A	313	GLU	-	expression tag	UNP Q8PSW1
A	314	HIS	-	expression tag	UNP Q8PSW1
A	315	HIS	-	expression tag	UNP Q8PSW1
A	316	HIS	-	expression tag	UNP Q8PSW1
A	317	HIS	-	expression tag	UNP Q8PSW1
A	318	HIS	-	expression tag	UNP Q8PSW1
A	319	HIS	-	expression tag	UNP Q8PSW1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	30	MET	-	expression tag	UNP Q8PSW1
B	31	GLU	-	expression tag	UNP Q8PSW1
B	313	GLU	-	expression tag	UNP Q8PSW1
B	314	HIS	-	expression tag	UNP Q8PSW1
B	315	HIS	-	expression tag	UNP Q8PSW1
B	316	HIS	-	expression tag	UNP Q8PSW1
B	317	HIS	-	expression tag	UNP Q8PSW1
B	318	HIS	-	expression tag	UNP Q8PSW1
B	319	HIS	-	expression tag	UNP Q8PSW1
C	30	MET	-	expression tag	UNP Q8PSW1
C	31	GLU	-	expression tag	UNP Q8PSW1
C	313	GLU	-	expression tag	UNP Q8PSW1
C	314	HIS	-	expression tag	UNP Q8PSW1
C	315	HIS	-	expression tag	UNP Q8PSW1
C	316	HIS	-	expression tag	UNP Q8PSW1
C	317	HIS	-	expression tag	UNP Q8PSW1
C	318	HIS	-	expression tag	UNP Q8PSW1
C	319	HIS	-	expression tag	UNP Q8PSW1
D	30	MET	-	expression tag	UNP Q8PSW1
D	31	GLU	-	expression tag	UNP Q8PSW1
D	313	GLU	-	expression tag	UNP Q8PSW1
D	314	HIS	-	expression tag	UNP Q8PSW1
D	315	HIS	-	expression tag	UNP Q8PSW1
D	316	HIS	-	expression tag	UNP Q8PSW1
D	317	HIS	-	expression tag	UNP Q8PSW1
D	318	HIS	-	expression tag	UNP Q8PSW1
D	319	HIS	-	expression tag	UNP Q8PSW1
E	30	MET	-	expression tag	UNP Q8PSW1
E	31	GLU	-	expression tag	UNP Q8PSW1
E	313	GLU	-	expression tag	UNP Q8PSW1
E	314	HIS	-	expression tag	UNP Q8PSW1
E	315	HIS	-	expression tag	UNP Q8PSW1
E	316	HIS	-	expression tag	UNP Q8PSW1
E	317	HIS	-	expression tag	UNP Q8PSW1
E	318	HIS	-	expression tag	UNP Q8PSW1
E	319	HIS	-	expression tag	UNP Q8PSW1
F	30	MET	-	expression tag	UNP Q8PSW1
F	31	GLU	-	expression tag	UNP Q8PSW1
F	313	GLU	-	expression tag	UNP Q8PSW1
F	314	HIS	-	expression tag	UNP Q8PSW1
F	315	HIS	-	expression tag	UNP Q8PSW1
F	316	HIS	-	expression tag	UNP Q8PSW1

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Chain	Residue	Modelled	Actual	Comment	Reference
F	317	HIS	-	expression tag	UNP Q8PSW1
F	318	HIS	-	expression tag	UNP Q8PSW1
F	319	HIS	-	expression tag	UNP Q8PSW1
G	30	MET	-	expression tag	UNP Q8PSW1
G	31	GLU	-	expression tag	UNP Q8PSW1
G	313	GLU	-	expression tag	UNP Q8PSW1
G	314	HIS	-	expression tag	UNP Q8PSW1
G	315	HIS	-	expression tag	UNP Q8PSW1
G	316	HIS	-	expression tag	UNP Q8PSW1
G	317	HIS	-	expression tag	UNP Q8PSW1
G	318	HIS	-	expression tag	UNP Q8PSW1
G	319	HIS	-	expression tag	UNP Q8PSW1
H	30	MET	-	expression tag	UNP Q8PSW1
H	31	GLU	-	expression tag	UNP Q8PSW1
H	313	GLU	-	expression tag	UNP Q8PSW1
H	314	HIS	-	expression tag	UNP Q8PSW1
H	315	HIS	-	expression tag	UNP Q8PSW1
H	316	HIS	-	expression tag	UNP Q8PSW1
H	317	HIS	-	expression tag	UNP Q8PSW1
H	318	HIS	-	expression tag	UNP Q8PSW1
H	319	HIS	-	expression tag	UNP Q8PSW1
I	30	MET	-	expression tag	UNP Q8PSW1
I	31	GLU	-	expression tag	UNP Q8PSW1
I	313	GLU	-	expression tag	UNP Q8PSW1
I	314	HIS	-	expression tag	UNP Q8PSW1
I	315	HIS	-	expression tag	UNP Q8PSW1
I	316	HIS	-	expression tag	UNP Q8PSW1
I	317	HIS	-	expression tag	UNP Q8PSW1
I	318	HIS	-	expression tag	UNP Q8PSW1
I	319	HIS	-	expression tag	UNP Q8PSW1
J	30	MET	-	expression tag	UNP Q8PSW1
J	31	GLU	-	expression tag	UNP Q8PSW1
J	313	GLU	-	expression tag	UNP Q8PSW1
J	314	HIS	-	expression tag	UNP Q8PSW1
J	315	HIS	-	expression tag	UNP Q8PSW1
J	316	HIS	-	expression tag	UNP Q8PSW1
J	317	HIS	-	expression tag	UNP Q8PSW1
J	318	HIS	-	expression tag	UNP Q8PSW1
J	319	HIS	-	expression tag	UNP Q8PSW1

- Molecule 2 is POTASSIUM ION (CCD ID: K) (formula: K).

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

- Molecule 3 is water.

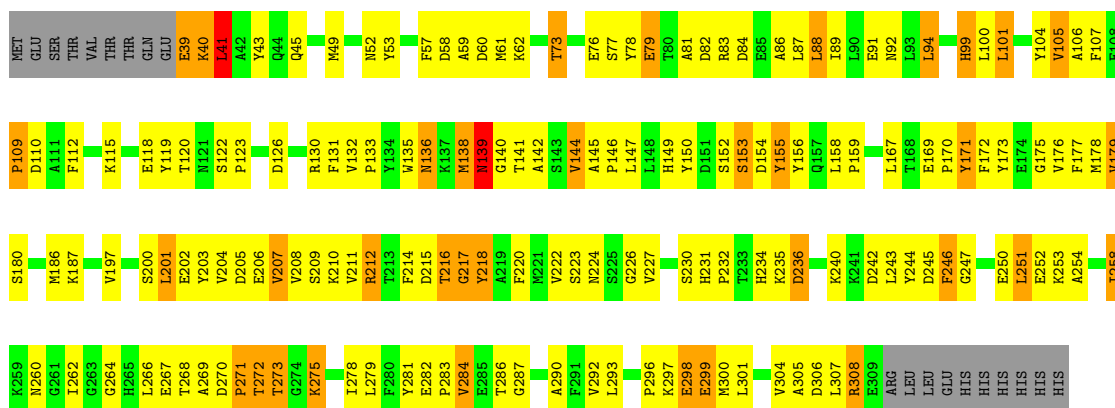
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	5	Total O 5 5	0	0
3	C	7	Total O 7 7	0	0
3	D	7	Total O 7 7	0	0
3	E	6	Total O 6 6	0	0
3	F	8	Total O 8 8	0	0
3	G	3	Total O 3 3	0	0
3	H	3	Total O 3 3	0	0
3	I	2	Total O 2 2	0	0
3	J	8	Total O 8 8	0	0

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.

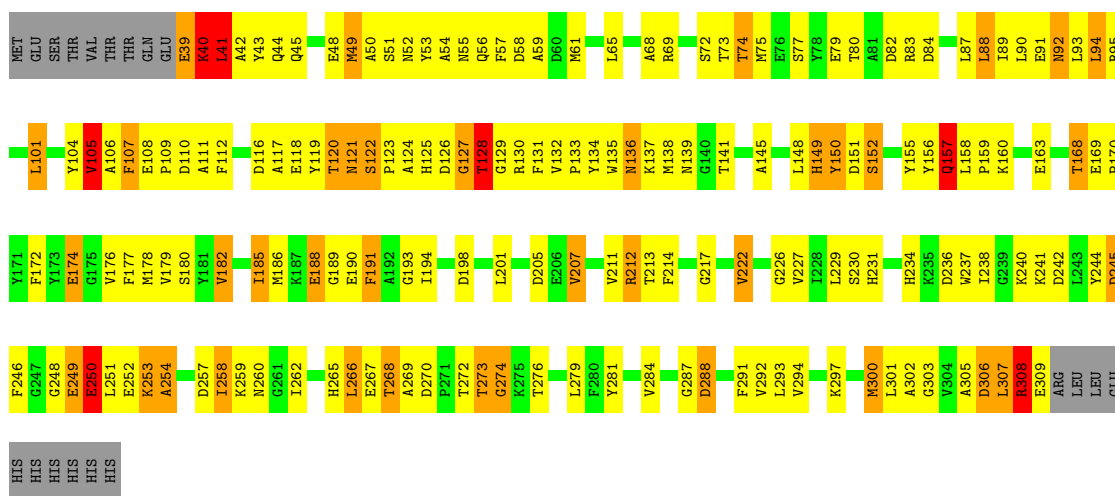
- Molecule 1: Hypothetical sensory transduction histidine kinase

Chain A: 



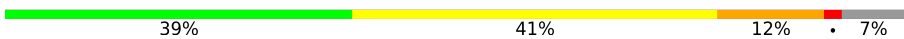
- Molecule 1: Hypothetical sensory transduction histidine kinase

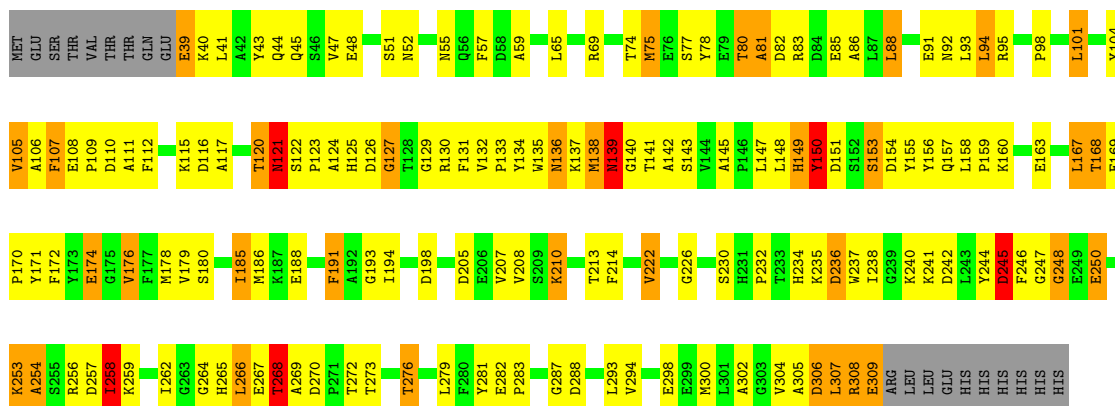
Chain B: 



- Molecule 1: Hypothetical sensory transduction histidine kinase

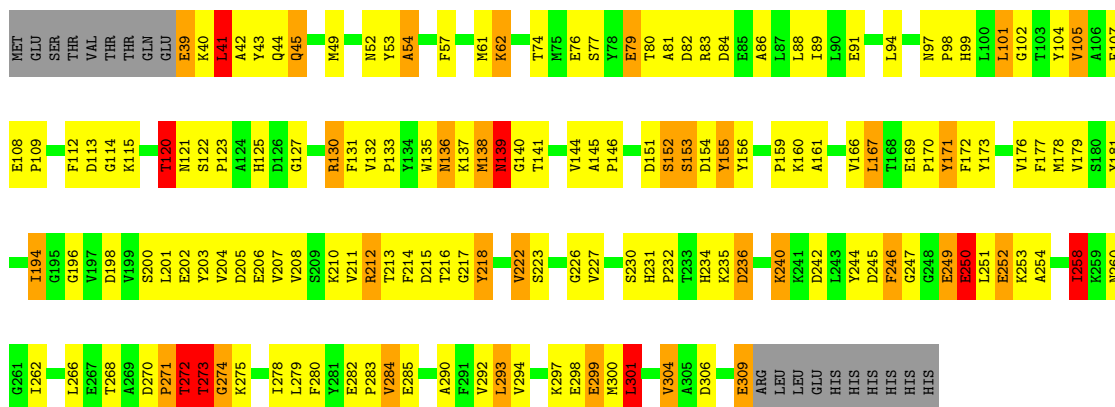
Chain C: 

Chain I:  39% 41% 12% 7%



● Molecule 1: Hypothetical sensory transduction histidine kinase

Chain J:  40% 40% 11% 7%



4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	129.52Å 129.52Å 404.73Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.72 – 2.99 46.72 – 2.99	Depositor EDS
% Data completeness (in resolution range)	99.3 (46.72-2.99) 99.4 (46.72-2.99)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.91 (at 3.01Å)	Xtrriage
Refinement program	REFMAC 5.5.0066	Depositor
R, R_{free}	0.197 , 0.272 0.202 , 0.275	Depositor DCC
R_{free} test set	3839 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	76.4	Xtrriage
Anisotropy	0.008	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 49.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.478 for h,-h-k,-l	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	21176	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.21% 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:
K

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	0.96	6/2172 (0.3%)	1.14	10/2950 (0.3%)
1	B	0.88	8/2172 (0.4%)	1.11	11/2950 (0.4%)
1	C	1.02	8/2142 (0.4%)	1.22	11/2910 (0.4%)
1	D	0.98	5/2172 (0.2%)	1.22	16/2950 (0.5%)
1	E	0.97	4/2144 (0.2%)	1.15	14/2913 (0.5%)
1	F	0.93	1/2172 (0.0%)	1.16	10/2950 (0.3%)
1	G	0.93	2/2163 (0.1%)	1.24	13/2938 (0.4%)
1	H	1.02	8/2136 (0.4%)	1.25	18/2902 (0.6%)
1	I	0.87	5/2172 (0.2%)	1.09	9/2950 (0.3%)
1	J	0.98	8/2172 (0.4%)	1.17	11/2950 (0.4%)
All	All	0.95	55/21617 (0.3%)	1.18	123/29363 (0.4%)

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	D	0	2

All (55) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	52	ASN	CG-OD1	6.37	1.35	1.23
1	C	139	ASN	CG-OD1	6.01	1.34	1.23
1	A	52	ASN	CG-OD1	5.96	1.34	1.23
1	H	45	GLN	CD-OE1	5.95	1.34	1.23
1	H	136	ASN	CG-OD1	5.92	1.34	1.23
1	C	92	ASN	CG-OD1	5.87	1.34	1.23
1	B	136	ASN	CG-OD1	5.86	1.34	1.23
1	A	99	HIS	ND1-CE1	5.86	1.38	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	99	HIS	ND1-CE1	5.82	1.38	1.32
1	F	278	ILE	CA-CB	-5.81	1.47	1.54
1	H	139	ASN	CG-OD1	5.81	1.34	1.23
1	A	45	GLN	CD-OE1	5.79	1.34	1.23
1	C	44	GLN	CD-OE1	5.78	1.34	1.23
1	H	157	GLN	CD-OE1	5.77	1.34	1.23
1	C	45	GLN	CD-OE1	5.73	1.34	1.23
1	E	136	ASN	CG-OD1	5.73	1.34	1.23
1	J	52	ASN	CG-OD1	5.71	1.34	1.23
1	C	52	ASN	CG-OD1	5.70	1.34	1.23
1	H	55	ASN	CG-OD1	5.69	1.34	1.23
1	D	44	GLN	CD-OE1	5.68	1.34	1.23
1	I	55	ASN	CG-OD1	5.66	1.34	1.23
1	B	55	ASN	CG-OD1	5.65	1.34	1.23
1	H	234	HIS	ND1-CE1	5.64	1.38	1.32
1	J	139	ASN	CG-OD1	5.64	1.34	1.23
1	C	55	ASN	CG-OD1	5.62	1.34	1.23
1	D	157	GLN	CD-OE1	5.62	1.34	1.23
1	J	45	GLN	CD-OE1	5.61	1.34	1.23
1	J	97	ASN	CG-ND2	-5.60	1.21	1.33
1	J	44	GLN	CD-OE1	5.59	1.34	1.23
1	B	45	GLN	CD-OE1	5.58	1.34	1.23
1	C	157	GLN	CD-OE1	5.56	1.34	1.23
1	C	136	ASN	CG-OD1	5.52	1.34	1.23
1	D	149	HIS	ND1-CE1	5.49	1.38	1.32
1	A	149	HIS	ND1-CE1	5.48	1.38	1.32
1	B	260	ASN	CG-OD1	5.46	1.33	1.23
1	I	136	ASN	CG-OD1	5.45	1.33	1.23
1	B	157	GLN	CD-OE1	5.38	1.33	1.23
1	I	52	ASN	CG-OD1	5.38	1.33	1.23
1	B	52	ASN	CG-OD1	5.37	1.33	1.23
1	E	234	HIS	ND1-CE1	5.37	1.38	1.32
1	I	139	ASN	CG-OD1	5.34	1.33	1.23
1	A	139	ASN	CG-OD1	5.32	1.33	1.23
1	H	92	ASN	CG-OD1	5.29	1.33	1.23
1	I	45	GLN	CD-OE1	5.28	1.33	1.23
1	J	258	ILE	CA-CB	5.24	1.61	1.54
1	B	56	GLN	CD-OE1	5.23	1.33	1.23
1	A	224	ASN	CG-OD1	5.21	1.33	1.23
1	B	92	ASN	CG-OD1	5.12	1.33	1.23
1	E	157	GLN	CD-OE1	5.12	1.33	1.23
1	G	157	GLN	CD-OE1	5.11	1.33	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	136	ASN	CG-OD1	5.11	1.33	1.23
1	G	56	GLN	CD-OE1	5.10	1.33	1.23
1	D	224	ASN	CG-OD1	5.09	1.33	1.23
1	H	92	ASN	CG-ND2	-5.07	1.22	1.33
1	D	157	GLN	CD-NE2	-5.05	1.22	1.33

All (123) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	45	GLN	N-CA-C	11.63	127.61	112.72
1	F	42	ALA	N-CA-C	-9.90	99.35	111.33
1	C	97	ASN	CA-C-N	8.96	129.86	119.47
1	C	97	ASN	C-N-CA	8.96	129.86	119.47
1	G	97	ASN	CA-C-N	8.92	130.99	119.84
1	G	97	ASN	C-N-CA	8.92	130.99	119.84
1	B	253	LYS	N-CA-C	-8.31	102.15	111.71
1	F	249	GLU	N-CA-C	-8.14	101.39	113.61
1	H	289	PHE	N-CA-C	-7.84	98.85	110.46
1	C	145	ALA	CA-C-N	-7.73	111.95	120.14
1	C	145	ALA	C-N-CA	-7.73	111.95	120.14
1	B	308	ARG	N-CA-C	-7.52	102.02	112.25
1	H	249	GLU	N-CA-C	-7.52	105.27	114.75
1	D	298	GLU	N-CA-C	7.50	122.66	112.68
1	F	136	ASN	N-CA-C	7.49	119.91	108.52
1	G	136	ASN	N-CA-C	7.19	121.20	109.85
1	A	73	THR	N-CA-C	-7.14	103.49	111.71
1	D	271	PRO	N-CA-C	-7.09	104.08	113.65
1	E	249	GLU	N-CA-C	-7.04	102.76	113.89
1	D	136	ASN	N-CA-C	7.01	120.38	109.52
1	F	250	GLU	N-CA-C	-6.99	104.01	112.54
1	D	169	GLU	N-CA-C	-6.83	100.66	110.08
1	B	44	GLN	N-CA-C	-6.76	103.84	111.07
1	H	105	VAL	N-CA-C	-6.73	99.47	108.35
1	J	217	GLY	N-CA-C	6.73	119.67	111.93
1	A	149	HIS	CB-CG-CD2	-6.72	122.47	131.20
1	B	107	PHE	N-CA-C	6.65	120.25	109.40
1	H	234	HIS	CB-CG-CD2	-6.65	122.55	131.20
1	E	234	HIS	CB-CG-CD2	-6.63	122.58	131.20
1	G	47	VAL	N-CA-C	-6.59	103.82	111.00
1	G	250	GLU	N-CA-C	-6.54	104.78	112.89
1	D	122	SER	CA-C-N	-6.52	112.94	119.92
1	D	122	SER	C-N-CA	-6.52	112.94	119.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	97	ASN	CA-C-N	6.49	127.95	119.84
1	H	97	ASN	C-N-CA	6.49	127.95	119.84
1	D	149	HIS	CB-CG-CD2	-6.45	122.81	131.20
1	I	145	ALA	CA-C-N	-6.44	114.00	120.31
1	I	145	ALA	C-N-CA	-6.44	114.00	120.31
1	A	41	LEU	N-CA-C	-6.39	105.47	113.20
1	H	136	ASN	N-CA-C	6.36	118.75	108.32
1	A	99	HIS	CB-CG-CD2	-6.34	122.96	131.20
1	D	47	VAL	N-CA-C	-6.33	104.58	110.53
1	I	250	GLU	N-CA-C	-6.29	104.47	111.71
1	J	99	HIS	CB-CG-CD2	-6.26	123.06	131.20
1	C	289	PHE	N-CA-C	-6.23	100.76	110.17
1	A	201	LEU	N-CA-C	-6.21	104.60	111.36
1	F	97	ASN	CA-C-N	6.21	125.89	119.56
1	F	97	ASN	C-N-CA	6.21	125.89	119.56
1	J	102	GLY	N-CA-C	6.21	119.34	111.09
1	D	107	PHE	N-CA-C	6.20	119.59	109.24
1	F	234	HIS	N-CA-C	6.14	118.38	110.65
1	E	250	GLU	N-CA-C	-6.11	105.88	113.15
1	J	252	GLU	N-CA-C	-6.05	104.01	111.40
1	D	97	ASN	CA-C-N	6.03	127.38	119.84
1	D	97	ASN	C-N-CA	6.03	127.38	119.84
1	I	253	LYS	N-CA-C	-6.02	104.62	111.07
1	H	183	SER	CA-C-N	6.00	125.97	119.78
1	H	183	SER	C-N-CA	6.00	125.97	119.78
1	J	145	ALA	CA-C-N	-5.92	113.87	119.85
1	J	145	ALA	C-N-CA	-5.92	113.87	119.85
1	G	214	PHE	CB-CA-C	-5.88	109.81	116.63
1	I	44	GLN	N-CA-C	-5.84	104.60	110.97
1	F	285	GLU	N-CA-C	5.83	117.64	111.28
1	F	107	PHE	N-CA-C	5.80	119.14	110.14
1	A	99	HIS	CB-CG-ND1	5.79	131.38	122.70
1	H	228	ILE	N-CA-C	5.78	116.46	108.84
1	B	306	ASP	N-CA-C	5.74	118.28	111.33
1	H	234	HIS	CB-CG-ND1	5.71	131.26	122.70
1	G	122	SER	CA-C-N	-5.67	114.42	120.03
1	G	122	SER	C-N-CA	-5.67	114.42	120.03
1	J	99	HIS	CB-CG-ND1	5.66	131.20	122.70
1	C	249	GLU	N-CA-C	-5.59	106.14	114.64
1	A	149	HIS	CB-CG-ND1	5.58	131.07	122.70
1	C	136	ASN	N-CA-C	5.58	117.59	108.55
1	E	234	HIS	CB-CG-ND1	5.57	131.06	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	105	VAL	N-CA-C	-5.57	100.45	108.42
1	I	258	ILE	N-CA-C	-5.57	105.07	110.42
1	F	274	GLY	N-CA-C	-5.56	100.00	113.18
1	D	149	HIS	CB-CG-ND1	5.53	131.00	122.70
1	A	136	ASN	N-CA-C	5.52	118.44	109.06
1	D	82	ASP	N-CA-C	5.51	117.28	108.41
1	C	250	GLU	N-CA-C	-5.48	105.40	111.71
1	H	214	PHE	CB-CA-C	-5.47	109.80	117.23
1	E	294	VAL	N-CA-C	5.39	115.85	107.28
1	B	55	ASN	N-CA-C	5.36	117.12	111.28
1	I	276	THR	N-CA-C	-5.36	101.74	110.20
1	H	72	SER	N-CA-C	5.34	117.11	111.28
1	H	178	MET	CB-CG-SD	-5.34	96.67	112.70
1	G	107	PHE	N-CA-C	5.31	118.06	109.40
1	D	60	ASP	N-CA-C	-5.31	105.54	112.23
1	B	105	VAL	N-CA-C	-5.30	100.23	108.81
1	G	45	GLN	CA-C-N	5.29	131.22	121.70
1	G	45	GLN	C-N-CA	5.29	131.22	121.70
1	B	207	VAL	CB-CA-C	-5.28	105.06	111.87
1	H	299	GLU	N-CA-C	-5.25	106.72	113.23
1	J	285	GLU	N-CA-C	5.24	117.40	111.11
1	A	217	GLY	N-CA-C	5.23	118.65	111.54
1	G	247	GLY	N-CA-C	5.19	125.48	113.18
1	H	246	PHE	N-CA-C	5.18	117.89	110.68
1	B	274	GLY	N-CA-C	-5.17	100.93	113.18
1	E	234	HIS	N-CA-C	5.14	117.50	108.56
1	A	211	VAL	N-CA-C	5.14	116.03	109.30
1	J	54	ALA	N-CA-C	-5.14	105.11	111.33
1	E	158	LEU	CA-C-N	-5.13	113.75	119.19
1	E	158	LEU	C-N-CA	-5.13	113.75	119.19
1	I	107	PHE	N-CA-C	5.13	117.77	109.40
1	E	285	GLU	CA-C-N	-5.13	114.28	121.72
1	E	285	GLU	C-N-CA	-5.13	114.28	121.72
1	H	179	VAL	CB-CA-C	5.13	118.40	110.50
1	C	214	PHE	CB-CA-C	-5.11	110.28	117.23
1	H	304	VAL	N-CA-C	-5.11	107.41	111.81
1	I	92	ASN	N-CA-C	5.09	116.83	111.28
1	B	145	ALA	CA-C-N	-5.08	114.11	120.51
1	B	145	ALA	C-N-CA	-5.08	114.11	120.51
1	J	194	ILE	N-CA-C	5.06	117.01	108.81
1	C	94	LEU	N-CA-C	-5.05	105.90	111.71
1	D	231	HIS	CA-C-N	5.04	124.83	119.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	231	HIS	C-N-CA	5.04	124.83	119.28
1	E	282	GLU	CA-C-N	5.03	124.79	119.76
1	E	282	GLU	C-N-CA	5.03	124.79	119.76
1	E	207	VAL	N-CA-C	5.02	115.24	110.42
1	J	138	MET	N-CA-C	5.02	118.89	112.87
1	E	302	ALA	N-CA-C	5.00	116.73	111.28

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	297	LYS	Peptide
1	D	298	GLU	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2122	0	2022	203	0
1	B	2122	0	2022	213	0
1	C	2092	0	1985	256	0
1	D	2122	0	2022	202	0
1	E	2094	0	1991	165	0
1	F	2122	0	2022	149	0
1	G	2113	0	2016	196	0
1	H	2086	0	1988	224	0
1	I	2122	0	2022	186	0
1	J	2122	0	2022	233	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	J	1	0	0	0	0
3	A	5	0	0	1	0
3	C	7	0	0	3	0
3	D	7	0	0	0	0
3	E	6	0	0	0	0
3	F	8	0	0	1	0
3	G	3	0	0	0	0
3	H	3	0	0	0	0
3	I	2	0	0	0	0
3	J	8	0	0	0	0
All	All	21176	0	20112	1951	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 47.

All (1951) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:41:LEU:CD2	1:D:42:ALA:H	1.17	1.56
1:D:39:GLU:N	1:D:40:LYS:CG	1.71	1.50
1:C:270:ASP:CB	1:C:271:PRO:HA	1.32	1.44
1:E:39:GLU:N	1:E:40:LYS:HB3	1.31	1.42
1:D:41:LEU:CD2	1:D:42:ALA:N	1.77	1.41
1:A:39:GLU:HA	1:A:40:LYS:CB	1.41	1.39
1:D:41:LEU:HD22	1:D:42:ALA:N	1.05	1.35
1:F:39:GLU:CA	1:F:40:LYS:HB2	1.60	1.32
1:F:39:GLU:HA	1:F:40:LYS:CB	1.54	1.31
1:H:231:HIS:ND1	1:H:232:PRO:HD2	1.48	1.28
1:C:270:ASP:CB	1:C:271:PRO:CA	2.14	1.26
1:C:39:GLU:HB3	1:C:40:LYS:CB	1.64	1.25
1:D:41:LEU:O	1:D:43:TYR:N	1.70	1.23
1:C:91:GLU:HG3	1:C:135:TRP:CE2	1.75	1.21
1:A:39:GLU:OE2	1:A:40:LYS:HD3	1.07	1.21
1:B:307:LEU:CD2	1:B:307:LEU:N	2.05	1.19
1:E:273:THR:HG23	1:E:274:GLY:N	1.41	1.19
1:E:273:THR:CG2	1:E:274:GLY:H	1.50	1.18
1:G:136:ASN:OD1	1:G:138:MET:HB2	1.43	1.18
1:C:91:GLU:HG3	1:C:135:TRP:CZ2	1.78	1.18
1:A:39:GLU:CA	1:A:40:LYS:HB2	1.72	1.17
1:J:214:PHE:CD2	1:J:299:GLU:HB3	1.79	1.17
1:D:298:GLU:N	1:D:299:GLU:HB2	1.60	1.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:273:THR:HG21	1:E:275:LYS:CG	1.76	1.15
1:H:39:GLU:HA	1:H:41:LEU:H	1.02	1.14
1:I:39:GLU:N	1:I:40:LYS:HB2	1.62	1.14
1:J:273:THR:OG1	1:J:274:GLY:N	1.70	1.14
1:C:277:VAL:HG12	1:C:296:PRO:HA	1.21	1.14
1:I:75:MET:HE2	1:I:75:MET:HA	1.23	1.14
1:E:273:THR:HG21	1:E:275:LYS:HG3	1.29	1.13
1:E:273:THR:HG21	1:E:275:LYS:CD	1.78	1.13
1:E:43:TYR:O	1:E:45:GLN:N	1.82	1.12
1:J:249:GLU:HB2	1:J:252:GLU:N	1.64	1.12
1:C:270:ASP:HB3	1:C:271:PRO:HA	1.16	1.12
1:A:308:ARG:HG2	1:A:308:ARG:HH11	1.00	1.12
1:C:39:GLU:HB3	1:C:40:LYS:HB3	1.25	1.11
1:J:245:ASP:O	1:J:247:GLY:N	1.82	1.11
1:E:273:THR:HG21	1:E:275:LYS:HD2	1.32	1.11
1:G:43:TYR:CD1	1:G:300:MET:HE2	1.86	1.11
1:B:307:LEU:N	1:B:307:LEU:HD22	1.63	1.10
1:C:270:ASP:HB2	1:C:271:PRO:CA	1.80	1.10
1:E:77:SER:HB3	1:F:88:LEU:HD13	1.15	1.10
1:A:173:TYR:HB3	1:A:178:MET:HE3	1.28	1.10
1:B:249:GLU:O	1:B:251:LEU:N	1.85	1.10
1:D:39:GLU:N	1:D:40:LYS:HG3	0.77	1.10
1:G:270:ASP:OD2	1:G:273:THR:HG23	1.48	1.09
1:J:249:GLU:CG	1:J:252:GLU:HB2	1.82	1.09
1:A:298:GLU:OE1	1:H:121:ASN:HB3	1.54	1.07
1:C:272:THR:O	1:C:273:THR:HB	1.53	1.07
1:D:298:GLU:H	1:D:299:GLU:HB2	0.94	1.07
1:I:270:ASP:OD2	1:I:273:THR:HG23	1.51	1.07
1:A:39:GLU:OE2	1:A:40:LYS:CD	2.02	1.07
1:C:120:THR:O	1:C:121:ASN:HB2	1.51	1.07
1:J:249:GLU:CB	1:J:252:GLU:H	1.65	1.07
1:J:173:TYR:HB3	1:J:178:MET:CE	1.82	1.06
1:J:309:GLU:N	1:J:309:GLU:OE2	1.88	1.06
1:H:39:GLU:N	1:H:39:GLU:OE2	1.88	1.06
1:A:43:TYR:CE1	1:A:300:MET:HE1	1.90	1.06
1:A:260:ASN:HB2	1:A:262:ILE:HD12	1.36	1.06
1:I:222:VAL:HG13	1:I:226:GLY:HA2	1.33	1.06
1:F:273:THR:HG21	1:F:275:LYS:HB3	1.37	1.06
1:J:249:GLU:HA	1:J:250:GLU:HG3	1.36	1.06
1:F:273:THR:CG2	1:F:274:GLY:H	1.64	1.06
1:H:39:GLU:N	1:H:40:LYS:HB2	1.71	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:39:GLU:N	1:H:39:GLU:CD	2.14	1.05
1:J:298:GLU:HA	1:J:301:LEU:CD2	1.86	1.05
1:F:273:THR:HG23	1:F:275:LYS:N	1.71	1.05
1:J:40:LYS:O	1:J:42:ALA:N	1.89	1.05
1:B:240:LYS:HE2	1:B:240:LYS:HA	1.35	1.05
1:H:91:GLU:HG3	1:H:135:TRP:CE2	1.92	1.04
1:J:249:GLU:CA	1:J:250:GLU:HG3	1.87	1.04
1:F:273:THR:HG23	1:F:275:LYS:H	1.16	1.04
1:J:297:LYS:C	1:J:301:LEU:HD22	1.83	1.04
1:J:249:GLU:HG3	1:J:252:GLU:HB2	1.10	1.03
1:J:251:LEU:HD23	1:J:266:LEU:CD1	1.88	1.03
1:F:301:LEU:HA	1:F:304:VAL:CG2	1.88	1.03
1:H:250:GLU:HB3	1:H:266:LEU:CD2	1.89	1.03
1:B:222:VAL:HG13	1:B:226:GLY:HA2	1.39	1.02
1:C:273:THR:CG2	1:C:275:LYS:HG3	1.88	1.02
1:G:40:LYS:HA	1:G:42:ALA:H	1.24	1.02
1:H:91:GLU:HG3	1:H:135:TRP:CZ2	1.94	1.02
1:I:306:ASP:O	1:I:308:ARG:N	1.93	1.02
1:A:308:ARG:HH11	1:A:308:ARG:CG	1.73	1.02
1:G:272:THR:HG22	1:G:273:THR:H	1.19	1.02
1:B:307:LEU:HD23	1:B:307:LEU:H	1.24	1.02
1:F:273:THR:HG23	1:F:274:GLY:N	1.59	1.02
1:G:43:TYR:CE1	1:G:300:MET:HE2	1.93	1.02
1:D:41:LEU:HD22	1:D:42:ALA:CA	1.90	1.01
1:D:135:TRP:CE2	1:D:144:VAL:HG23	1.94	1.01
1:D:270:ASP:OD1	1:D:277:VAL:CG2	2.07	1.01
1:J:214:PHE:HB3	1:J:299:GLU:HG2	1.40	1.01
1:C:270:ASP:OD2	1:C:274:GLY:HA2	1.59	1.01
1:H:231:HIS:ND1	1:H:232:PRO:CD	2.22	1.01
1:D:39:GLU:N	1:D:39:GLU:OE1	1.93	1.01
1:D:298:GLU:HG3	1:D:299:GLU:CG	1.91	1.00
1:F:273:THR:HG23	1:F:274:GLY:H	0.85	1.00
1:J:91:GLU:HB2	1:J:135:TRP:CE2	1.96	1.00
1:C:270:ASP:HB2	1:C:271:PRO:HA	1.01	1.00
1:E:273:THR:CG2	1:E:275:LYS:HD2	1.92	1.00
1:B:120:THR:O	1:B:121:ASN:HB2	1.61	0.99
1:E:278:ILE:HD12	1:E:278:ILE:N	1.77	0.99
1:H:231:HIS:CE1	1:H:232:PRO:HD2	1.98	0.98
1:J:249:GLU:HB2	1:J:252:GLU:H	0.82	0.98
1:H:136:ASN:OD1	1:H:138:MET:HB2	1.63	0.98
1:I:122:SER:HB2	1:I:123:PRO:HD2	1.41	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:135:TRP:CD2	1:G:144:VAL:HG23	1.99	0.98
1:J:298:GLU:HA	1:J:301:LEU:HD23	1.45	0.98
1:F:300:MET:O	1:F:304:VAL:HG22	1.61	0.98
1:B:39:GLU:N	1:B:39:GLU:OE2	1.97	0.98
1:C:178:MET:HE1	3:C:8:HOH:O	1.63	0.97
1:E:39:GLU:N	1:E:40:LYS:CB	2.27	0.97
1:I:309:GLU:C	1:I:309:GLU:OE1	2.07	0.97
1:J:173:TYR:HB3	1:J:178:MET:HE3	1.42	0.97
1:G:43:TYR:CD1	1:G:300:MET:CE	2.47	0.97
1:C:270:ASP:HB3	1:C:271:PRO:CA	1.83	0.97
1:D:270:ASP:OD1	1:D:277:VAL:HG21	1.62	0.97
1:A:173:TYR:HB3	1:A:178:MET:CE	1.95	0.97
1:G:272:THR:HG22	1:G:273:THR:N	1.77	0.96
1:A:231:HIS:ND1	1:A:232:PRO:HD2	1.79	0.96
1:B:191:PHE:O	1:B:191:PHE:HD2	1.49	0.96
1:H:250:GLU:C	1:H:266:LEU:HD11	1.91	0.96
1:A:39:GLU:HA	1:A:40:LYS:CG	1.95	0.95
1:F:41:LEU:C	1:F:41:LEU:HD12	1.91	0.95
1:D:273:THR:OG1	1:D:274:GLY:HA2	1.64	0.95
1:A:91:GLU:HG3	1:A:135:TRP:CZ2	2.00	0.95
1:C:39:GLU:HB3	1:C:40:LYS:HB2	1.46	0.95
1:I:205:ASP:HA	1:I:230:SER:HB2	1.47	0.95
1:G:273:THR:HG21	1:G:275:LYS:HE3	1.48	0.94
1:A:39:GLU:CA	1:A:40:LYS:CB	2.33	0.94
1:E:273:THR:HG23	1:E:275:LYS:H	1.28	0.94
1:J:300:MET:CA	1:J:301:LEU:HB2	1.97	0.94
1:G:135:TRP:CE2	1:G:144:VAL:HG23	2.00	0.94
1:I:191:PHE:HD2	1:I:191:PHE:O	1.49	0.94
1:D:39:GLU:CA	1:D:40:LYS:HG3	1.97	0.94
1:F:41:LEU:C	1:F:41:LEU:CD1	2.40	0.94
1:J:240:LYS:HE2	1:J:240:LYS:HA	1.49	0.94
1:A:43:TYR:HE1	1:A:300:MET:HE1	1.31	0.94
1:C:160:LYS:HG3	1:C:191:PHE:CE2	2.02	0.94
1:C:132:VAL:HG23	1:C:132:VAL:O	1.65	0.94
1:F:303:GLY:O	1:F:307:LEU:HG	1.68	0.93
1:C:39:GLU:CB	1:C:40:LYS:HB3	1.96	0.93
1:B:48:GLU:O	1:B:51:SER:HB3	1.69	0.93
1:H:39:GLU:HA	1:H:41:LEU:N	1.82	0.93
1:J:298:GLU:CA	1:J:301:LEU:CD2	2.47	0.93
1:J:231:HIS:ND1	1:J:232:PRO:HD2	1.82	0.93
1:J:260:ASN:HB2	1:J:262:ILE:HD12	1.49	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:188:GLU:HG3	1:E:188:GLU:O	1.69	0.92
1:I:191:PHE:O	1:I:191:PHE:CD2	2.23	0.92
1:I:307:LEU:HD11	1:J:41:LEU:HD21	1.50	0.92
1:F:234:HIS:CE1	1:F:272:THR:HG23	2.04	0.92
1:C:277:VAL:HG12	1:C:296:PRO:CA	1.98	0.92
1:F:222:VAL:HG12	1:F:290:ALA:HB3	1.50	0.92
1:J:271:PRO:O	1:J:273:THR:N	2.02	0.91
1:B:69:ARG:HG2	1:B:69:ARG:HH11	1.31	0.91
1:D:277:VAL:HG12	1:D:296:PRO:HA	1.50	0.91
1:H:250:GLU:HB3	1:H:266:LEU:HD21	1.52	0.91
1:D:39:GLU:HA	1:D:40:LYS:HB2	1.53	0.91
1:C:163:GLU:HB3	1:E:259:LYS:NZ	1.85	0.91
1:F:49:MET:HE2	1:F:293:LEU:HD11	1.52	0.91
1:G:39:GLU:CA	1:G:40:LYS:HB2	1.99	0.90
1:J:298:GLU:CA	1:J:301:LEU:HD22	2.00	0.90
1:J:297:LYS:O	1:J:301:LEU:HD22	1.71	0.90
1:A:58:ASP:OD2	1:A:286:THR:HG23	1.71	0.90
1:D:309:GLU:OE1	1:D:309:GLU:HA	1.72	0.90
1:I:39:GLU:N	1:I:39:GLU:OE2	2.03	0.90
1:E:204:VAL:O	1:E:208:VAL:HG23	1.72	0.90
1:D:265:HIS:O	1:D:266:LEU:HD23	1.72	0.90
1:J:79:GLU:HA	1:J:79:GLU:OE2	1.70	0.90
1:E:77:SER:CB	1:F:88:LEU:HD13	2.02	0.89
1:E:273:THR:HG23	1:E:275:LYS:N	1.86	0.89
1:J:298:GLU:N	1:J:301:LEU:HD22	1.87	0.89
1:G:122:SER:HB2	1:G:123:PRO:HD2	1.52	0.89
1:E:247:GLY:O	1:E:248:GLY:O	1.91	0.88
1:J:300:MET:N	1:J:301:LEU:HB2	1.88	0.88
1:D:296:PRO:O	1:D:299:GLU:HB3	1.73	0.88
1:E:302:ALA:N	1:E:303:GLY:HA3	1.87	0.88
1:G:205:ASP:HA	1:G:230:SER:HB2	1.56	0.88
1:I:75:MET:HE2	1:I:75:MET:CA	2.04	0.88
1:J:249:GLU:HA	1:J:251:LEU:H	1.38	0.88
1:C:273:THR:HG21	1:C:275:LYS:HG3	1.53	0.88
1:E:117:ALA:O	1:E:120:THR:HG22	1.74	0.88
1:H:273:THR:OG1	1:H:275:LYS:HG2	1.74	0.88
1:E:39:GLU:CA	1:E:40:LYS:HB3	2.03	0.88
1:G:245:ASP:O	1:G:247:GLY:N	2.07	0.87
1:H:117:ALA:O	1:H:120:THR:HG22	1.74	0.87
1:D:58:ASP:OD2	1:D:286:THR:HG23	1.73	0.87
1:G:39:GLU:N	1:G:40:LYS:HB2	1.90	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:43:TYR:HA	1:H:300:MET:HE1	1.55	0.87
1:G:218:TYR:CD2	1:G:232:PRO:HG2	2.10	0.87
1:F:139:ASN:O	1:F:141:THR:N	2.07	0.87
1:B:191:PHE:O	1:B:191:PHE:CD2	2.27	0.87
1:J:245:ASP:C	1:J:247:GLY:N	2.32	0.87
1:I:191:PHE:CD2	1:I:191:PHE:C	2.53	0.86
1:C:231:HIS:ND1	1:C:232:PRO:HD2	1.90	0.86
1:D:177:PHE:CZ	1:D:240:LYS:HD2	2.10	0.86
1:B:248:GLY:O	1:B:249:GLU:HB2	1.73	0.86
1:H:275:LYS:HB3	1:H:275:LYS:NZ	1.90	0.86
1:A:305:ALA:HA	1:A:308:ARG:HH12	1.40	0.86
1:G:77:SER:OG	1:H:92:ASN:OD1	1.92	0.86
1:E:48:GLU:HG3	1:F:48:GLU:HG3	1.57	0.86
1:G:43:TYR:CE1	1:G:300:MET:CE	2.57	0.86
1:C:120:THR:O	1:C:121:ASN:CB	2.24	0.86
1:A:308:ARG:HG2	1:A:308:ARG:NH1	1.83	0.86
1:B:177:PHE:HB3	1:B:201:LEU:HD12	1.56	0.86
1:F:42:ALA:HB3	1:F:300:MET:HE1	1.56	0.86
1:I:136:ASN:OD1	1:I:138:MET:HB2	1.76	0.86
1:D:41:LEU:HD23	1:D:42:ALA:N	1.91	0.86
1:E:58:ASP:OD1	1:E:286:THR:HG23	1.74	0.86
1:E:172:PHE:CZ	1:E:175:GLY:HA2	2.09	0.85
1:F:234:HIS:HE1	1:F:272:THR:HG23	1.41	0.85
1:A:296:PRO:HB2	1:A:299:GLU:HG3	1.56	0.85
1:B:191:PHE:CD2	1:B:191:PHE:C	2.54	0.85
1:H:247:GLY:O	1:H:248:GLY:O	1.94	0.85
1:E:273:THR:CG2	1:E:275:LYS:HG3	2.05	0.85
1:A:231:HIS:CE1	1:A:232:PRO:HD2	2.10	0.85
1:I:39:GLU:CA	1:I:40:LYS:HB2	2.06	0.85
1:B:128:THR:OG1	1:B:130:ARG:HG3	1.77	0.85
1:D:135:TRP:CD2	1:D:144:VAL:HG23	2.11	0.85
1:B:104:TYR:HE2	1:B:198:ASP:OD2	1.60	0.84
1:G:58:ASP:OD2	1:G:286:THR:HG23	1.76	0.84
1:H:39:GLU:CA	1:H:41:LEU:H	1.88	0.84
1:A:260:ASN:CB	1:A:262:ILE:HD12	2.07	0.84
1:F:273:THR:CG2	1:F:275:LYS:H	1.89	0.84
1:I:306:ASP:C	1:I:308:ARG:H	1.85	0.84
1:C:273:THR:HG23	1:C:275:LYS:HG3	1.59	0.84
1:H:214:PHE:HE2	1:H:300:MET:HA	1.43	0.84
1:B:83:ARG:O	1:B:87:LEU:HD12	1.77	0.84
1:J:249:GLU:HG3	1:J:252:GLU:CB	2.03	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:273:THR:HG23	1:C:275:LYS:CG	2.08	0.83
1:C:277:VAL:CG1	1:C:296:PRO:HA	2.06	0.83
1:E:88:LEU:HD13	1:F:77:SER:HB3	1.57	0.83
1:G:120:THR:O	1:G:121:ASN:HB2	1.77	0.83
1:J:156:TYR:O	1:J:159:PRO:HD2	1.77	0.83
1:C:278:ILE:HG22	1:C:280:PHE:CE1	2.12	0.83
1:I:222:VAL:CG1	1:I:226:GLY:HA2	2.08	0.83
1:F:204:VAL:O	1:F:208:VAL:HG23	1.77	0.83
1:B:163:GLU:HB3	1:B:186:MET:CE	2.09	0.83
1:E:273:THR:HG23	1:E:274:GLY:H	0.68	0.83
1:H:188:GLU:O	1:H:188:GLU:HG2	1.76	0.83
1:F:41:LEU:HD12	1:F:42:ALA:N	1.94	0.83
1:G:272:THR:HG22	1:G:273:THR:HG22	1.58	0.83
1:A:39:GLU:HA	1:A:40:LYS:HB2	0.84	0.82
1:D:39:GLU:CA	1:D:40:LYS:CB	2.57	0.82
1:D:39:GLU:N	1:D:39:GLU:CD	2.36	0.82
1:A:136:ASN:HD22	1:A:138:MET:HB2	1.42	0.82
1:A:77:SER:OG	1:B:92:ASN:OD1	1.97	0.82
1:I:120:THR:HG23	1:I:120:THR:O	1.78	0.82
1:D:270:ASP:O	1:D:274:GLY:HA3	1.80	0.82
1:F:122:SER:HB2	1:F:123:PRO:HD2	1.62	0.82
1:E:273:THR:CG2	1:E:275:LYS:H	1.92	0.82
1:J:139:ASN:O	1:J:141:THR:HG22	1.78	0.82
1:J:173:TYR:CB	1:J:178:MET:HE3	2.10	0.82
1:C:136:ASN:OD1	1:C:138:MET:HB2	1.79	0.81
1:C:273:THR:CG2	1:C:275:LYS:CG	2.57	0.81
1:D:136:ASN:OD1	1:D:138:MET:HB2	1.79	0.81
1:D:298:GLU:HG3	1:D:299:GLU:HG2	1.62	0.81
1:G:273:THR:HG21	1:G:275:LYS:CE	2.09	0.81
1:H:240:LYS:HA	1:H:240:LYS:CE	2.11	0.81
1:G:273:THR:OG1	1:G:274:GLY:N	2.08	0.81
1:G:213:THR:O	1:G:217:GLY:HA3	1.81	0.81
1:B:39:GLU:HB3	1:B:40:LYS:O	1.80	0.81
1:C:91:GLU:HG3	1:C:135:TRP:CH2	2.15	0.81
1:D:91:GLU:OE1	1:D:135:TRP:CZ2	2.34	0.81
1:H:39:GLU:N	1:H:40:LYS:HD2	1.95	0.81
1:J:122:SER:HB2	1:J:123:PRO:HD2	1.61	0.81
1:J:260:ASN:CB	1:J:262:ILE:HD12	2.10	0.81
1:C:205:ASP:HA	1:C:230:SER:HB2	1.62	0.81
1:D:270:ASP:OD1	1:D:277:VAL:HG22	1.79	0.81
1:C:121:ASN:O	1:C:122:SER:HB2	1.79	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:39:GLU:N	1:I:39:GLU:CD	2.32	0.81
1:C:218:TYR:CD2	1:C:232:PRO:HG2	2.16	0.81
1:H:174:GLU:OE2	1:H:174:GLU:HA	1.77	0.81
1:B:257:ASP:HB3	1:B:262:ILE:O	1.81	0.80
1:B:39:GLU:CB	1:B:40:LYS:O	2.30	0.80
1:I:120:THR:O	1:I:121:ASN:HB2	1.80	0.80
1:A:41:LEU:HD11	1:B:307:LEU:CD1	2.11	0.80
1:C:91:GLU:CG	1:C:135:TRP:CZ2	2.62	0.80
1:F:298:GLU:H	1:F:298:GLU:CD	1.90	0.80
1:B:246:PHE:O	1:B:251:LEU:HD13	1.82	0.80
1:C:119:TYR:O	1:C:121:ASN:N	2.14	0.80
1:H:214:PHE:CE2	1:H:300:MET:HA	2.17	0.80
1:D:107:PHE:O	1:D:130:ARG:HD2	1.82	0.80
1:H:39:GLU:N	1:H:40:LYS:CB	2.45	0.80
1:I:43:TYR:O	1:I:47:VAL:HG23	1.80	0.80
1:J:298:GLU:O	1:J:301:LEU:HB3	1.80	0.80
1:D:208:VAL:O	1:D:211:VAL:HG23	1.81	0.80
1:E:273:THR:CG2	1:E:274:GLY:N	2.17	0.80
1:E:278:ILE:N	1:E:278:ILE:CD1	2.44	0.80
1:I:258:ILE:HG13	1:I:259:LYS:N	1.95	0.80
1:J:300:MET:CB	1:J:301:LEU:HB2	2.12	0.79
1:B:101:LEU:O	1:B:101:LEU:HD22	1.81	0.79
1:H:246:PHE:O	1:H:251:LEU:HD12	1.83	0.79
1:D:296:PRO:HB2	1:D:299:GLU:HG3	1.64	0.79
1:F:222:VAL:CG1	1:F:290:ALA:HB3	2.11	0.79
1:J:249:GLU:OE1	1:J:249:GLU:N	2.14	0.79
1:H:83:ARG:NH1	1:H:113:ASP:OD2	2.16	0.79
1:A:298:GLU:O	1:A:300:MET:N	2.16	0.79
1:A:203:TYR:O	1:A:207:VAL:HG23	1.83	0.79
1:F:203:TYR:O	1:F:207:VAL:HG23	1.83	0.79
1:H:91:GLU:HG3	1:H:135:TRP:CH2	2.18	0.79
1:B:120:THR:O	1:B:120:THR:HG23	1.82	0.79
1:D:178:MET:HE3	1:D:198:ASP:OD1	1.83	0.79
1:H:95:ARG:NH1	1:J:253:LYS:HG3	1.98	0.79
1:E:234:HIS:NE2	1:E:272:THR:HG23	1.97	0.78
1:C:91:GLU:HG3	1:C:135:TRP:CD2	2.18	0.78
1:A:91:GLU:HG3	1:A:135:TRP:CE2	2.18	0.78
1:C:174:GLU:HA	1:C:174:GLU:OE2	1.84	0.78
1:I:270:ASP:OD2	1:I:273:THR:CG2	2.31	0.78
1:A:244:TYR:CE2	1:A:252:GLU:HG2	2.19	0.78
1:B:95:ARG:CZ	1:D:253:LYS:HB3	2.13	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:177:PHE:HB3	1:C:201:LEU:HD12	1.64	0.78
1:E:203:TYR:O	1:E:207:VAL:HG23	1.83	0.78
1:H:278:ILE:HG21	1:H:280:PHE:CE1	2.19	0.78
1:A:39:GLU:OE2	1:A:39:GLU:N	2.17	0.78
1:D:39:GLU:HA	1:D:40:LYS:CB	2.13	0.78
1:C:174:GLU:OE2	1:C:174:GLU:CA	2.32	0.78
1:G:173:TYR:HB3	1:G:178:MET:HE3	1.66	0.78
1:H:277:VAL:HG12	1:H:296:PRO:HA	1.64	0.78
1:B:163:GLU:HB3	1:B:186:MET:HE2	1.65	0.77
1:D:270:ASP:HB3	1:D:272:THR:HG22	1.67	0.77
1:J:177:PHE:HB3	1:J:201:LEU:HD12	1.66	0.77
1:H:278:ILE:CG2	1:H:280:PHE:CE1	2.67	0.77
1:J:215:ASP:HB2	1:J:299:GLU:OE2	1.84	0.77
1:G:89:ILE:HD13	1:H:74:THR:HG23	1.66	0.77
1:I:75:MET:HA	1:I:75:MET:CE	2.10	0.77
1:I:83:ARG:NH1	1:I:125:HIS:CD2	2.52	0.77
1:E:278:ILE:HD11	1:E:297:LYS:HD3	1.66	0.77
1:E:85:GLU:OE1	1:F:79:GLU:HB2	1.83	0.77
1:F:139:ASN:O	1:F:141:THR:HG22	1.85	0.77
1:G:277:VAL:HG12	1:G:296:PRO:HA	1.67	0.77
1:J:156:TYR:C	1:J:159:PRO:HD2	2.10	0.77
1:A:79:GLU:HA	1:A:79:GLU:OE2	1.84	0.76
1:H:132:VAL:HG23	1:H:132:VAL:O	1.81	0.76
1:J:91:GLU:HB2	1:J:135:TRP:NE1	1.99	0.76
1:G:135:TRP:CE2	1:G:144:VAL:CG2	2.67	0.76
1:D:80:THR:O	1:D:80:THR:HG22	1.85	0.76
1:H:130:ARG:O	1:H:132:VAL:HG13	1.86	0.76
1:B:246:PHE:O	1:B:251:LEU:CD1	2.34	0.76
1:E:132:VAL:HG23	1:E:147:LEU:H	1.51	0.76
1:G:39:GLU:HA	1:G:40:LYS:HB2	1.67	0.76
1:H:57:PHE:O	1:H:61:MET:HG3	1.85	0.76
1:G:271:PRO:O	1:G:272:THR:C	2.29	0.76
1:J:245:ASP:C	1:J:247:GLY:H	1.94	0.76
1:C:213:THR:HG21	1:C:295:VAL:HG23	1.67	0.76
1:I:256:ARG:HG3	1:I:256:ARG:HH11	1.50	0.76
1:F:107:PHE:O	1:F:130:ARG:HD2	1.86	0.75
1:H:277:VAL:CG1	1:H:296:PRO:HA	2.16	0.75
1:C:125:HIS:O	1:C:146:PRO:HG2	1.86	0.75
1:A:231:HIS:ND1	1:A:232:PRO:CD	2.49	0.75
1:F:43:TYR:O	1:F:45:GLN:N	2.20	0.75
1:E:188:GLU:O	1:E:188:GLU:CG	2.33	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:120:THR:O	1:G:120:THR:HG23	1.86	0.75
1:H:122:SER:HB2	1:H:123:PRO:HD2	1.69	0.75
1:B:222:VAL:CG1	1:B:226:GLY:HA2	2.16	0.75
1:D:94:LEU:HD13	1:D:137:LYS:HE3	1.69	0.75
1:D:260:ASN:HB2	1:D:262:ILE:HD12	1.69	0.75
1:F:273:THR:HG21	1:F:275:LYS:CE	2.16	0.75
1:C:270:ASP:HB3	1:C:271:PRO:C	2.12	0.74
1:H:160:LYS:HG3	1:H:191:PHE:CE2	2.22	0.74
1:J:250:GLU:O	1:J:253:LYS:HB2	1.85	0.74
1:A:136:ASN:ND2	1:A:138:MET:HB2	2.01	0.74
1:E:277:VAL:C	1:E:278:ILE:HD12	2.11	0.74
1:H:188:GLU:O	1:H:188:GLU:CG	2.33	0.74
1:E:132:VAL:HG23	1:E:132:VAL:O	1.86	0.74
1:H:91:GLU:HG3	1:H:135:TRP:CD2	2.23	0.74
1:A:305:ALA:HA	1:A:308:ARG:NH1	2.02	0.74
1:F:41:LEU:O	1:F:41:LEU:HD13	1.87	0.74
1:H:105:VAL:HG13	1:H:107:PHE:HE1	1.52	0.74
1:H:95:ARG:CZ	1:J:253:LYS:HG3	2.17	0.74
1:I:149:HIS:C	1:I:151:ASP:H	1.96	0.74
1:C:91:GLU:CG	1:C:135:TRP:CE2	2.66	0.74
1:A:91:GLU:HG3	1:A:135:TRP:CH2	2.23	0.74
1:A:246:PHE:HB3	1:A:251:LEU:HD12	1.69	0.74
1:C:92:ASN:OD1	1:D:77:SER:OG	2.06	0.74
1:D:39:GLU:N	1:D:40:LYS:CB	2.51	0.74
1:H:80:THR:HG22	1:H:82:ASP:H	1.51	0.74
1:D:139:ASN:C	1:D:141:THR:H	1.95	0.74
1:E:41:LEU:O	1:E:42:ALA:C	2.31	0.74
1:E:167:LEU:HD23	1:E:287:GLY:HA3	1.70	0.74
1:B:148:LEU:O	1:B:149:HIS:HB2	1.86	0.74
1:D:214:PHE:CD1	1:D:295:VAL:HG13	2.23	0.74
1:J:120:THR:HG23	1:J:120:THR:O	1.87	0.74
1:J:231:HIS:CE1	1:J:232:PRO:HD2	2.23	0.74
1:F:306:ASP:O	1:F:309:GLU:OE2	2.06	0.73
1:G:218:TYR:HD2	1:G:232:PRO:HG2	1.53	0.73
1:C:231:HIS:ND1	1:C:232:PRO:CD	2.51	0.73
1:G:100:LEU:HD22	1:G:197:VAL:HB	1.70	0.73
1:J:300:MET:N	1:J:301:LEU:CB	2.51	0.73
1:E:83:ARG:HD2	1:E:113:ASP:OD1	1.88	0.73
1:J:249:GLU:CG	1:J:252:GLU:CB	2.63	0.73
1:B:61:MET:CE	1:B:284:VAL:HG11	2.19	0.73
1:C:278:ILE:CG2	1:C:280:PHE:CE1	2.72	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:246:PHE:HB3	1:A:251:LEU:CD1	2.18	0.73
1:D:273:THR:OG1	1:D:274:GLY:CA	2.37	0.73
1:F:273:THR:HG21	1:F:275:LYS:CB	2.17	0.73
1:A:139:ASN:O	1:A:141:THR:HG22	1.89	0.73
1:J:251:LEU:CD2	1:J:266:LEU:CD1	2.67	0.73
1:B:107:PHE:O	1:B:130:ARG:HD2	1.88	0.73
1:D:296:PRO:O	1:D:299:GLU:CB	2.36	0.73
1:J:49:MET:HE3	1:J:53:TYR:HE1	1.54	0.73
1:A:298:GLU:OE1	1:H:121:ASN:CB	2.35	0.72
1:F:273:THR:HG21	1:F:275:LYS:HE2	1.70	0.72
1:J:122:SER:HB2	1:J:123:PRO:CD	2.19	0.72
1:J:231:HIS:ND1	1:J:232:PRO:CD	2.52	0.72
1:J:251:LEU:HD23	1:J:266:LEU:HD11	1.69	0.72
1:C:250:GLU:O	1:C:266:LEU:HD11	1.88	0.72
1:J:57:PHE:O	1:J:61:MET:HG3	1.88	0.72
1:D:91:GLU:HB2	1:D:135:TRP:NE1	2.04	0.72
1:I:104:TYR:HD2	1:I:134:TYR:CE2	2.08	0.72
1:I:309:GLU:C	1:I:309:GLU:CD	2.56	0.72
1:F:301:LEU:HA	1:F:304:VAL:HG23	1.70	0.72
1:E:136:ASN:OD1	1:E:138:MET:HB2	1.88	0.72
1:H:240:LYS:HA	1:H:240:LYS:HE2	1.72	0.72
1:A:154:ASP:O	1:A:156:TYR:N	2.23	0.72
1:B:69:ARG:HG2	1:B:69:ARG:NH1	2.04	0.72
1:C:267:GLU:OE1	1:C:297:LYS:NZ	2.19	0.72
1:F:122:SER:CB	1:F:123:PRO:HD2	2.19	0.72
1:H:82:ASP:OD1	1:H:84:ASP:HB2	1.90	0.72
1:H:91:GLU:CG	1:H:135:TRP:CZ2	2.72	0.72
1:J:300:MET:HB2	1:J:301:LEU:HB2	1.70	0.72
1:H:240:LYS:HE2	1:H:240:LYS:CA	2.19	0.72
1:C:75:MET:HE2	1:C:105:VAL:HG21	1.71	0.71
1:D:39:GLU:CA	1:D:40:LYS:CG	2.60	0.71
1:B:104:TYR:CE2	1:B:198:ASP:OD2	2.43	0.71
1:B:185:ILE:HG13	1:B:194:ILE:N	2.05	0.71
1:C:139:ASN:C	1:C:141:THR:H	1.99	0.71
1:C:273:THR:HG23	1:C:275:LYS:H	1.53	0.71
1:J:240:LYS:HA	1:J:240:LYS:CE	2.19	0.71
1:B:205:ASP:HA	1:B:230:SER:HB2	1.71	0.71
1:E:43:TYR:O	1:E:44:GLN:C	2.34	0.71
1:J:171:TYR:N	1:J:171:TYR:CD1	2.57	0.71
1:A:43:TYR:CD1	1:A:300:MET:HE1	2.25	0.71
1:B:39:GLU:CA	1:B:40:LYS:O	2.39	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:250:GLU:HG3	1:D:266:LEU:HD13	1.73	0.71
1:J:249:GLU:HA	1:J:251:LEU:N	2.05	0.71
1:A:298:GLU:O	1:A:301:LEU:N	2.23	0.71
1:C:231:HIS:CE1	1:C:232:PRO:HD2	2.26	0.71
1:D:41:LEU:CG	1:D:42:ALA:H	2.02	0.71
1:G:204:VAL:O	1:G:208:VAL:HG23	1.90	0.71
1:B:148:LEU:O	1:B:149:HIS:CB	2.38	0.71
1:C:75:MET:CE	1:C:105:VAL:HG21	2.21	0.71
1:H:136:ASN:OD1	1:H:138:MET:CB	2.39	0.71
1:I:168:THR:HG23	1:I:180:SER:O	1.91	0.70
1:J:171:TYR:N	1:J:171:TYR:HD1	1.89	0.70
1:A:218:TYR:N	1:A:218:TYR:CD1	2.57	0.70
1:H:238:ILE:HG22	1:H:238:ILE:O	1.92	0.70
1:J:139:ASN:O	1:J:141:THR:N	2.23	0.70
1:J:214:PHE:HD2	1:J:299:GLU:HB3	1.47	0.70
1:G:80:THR:HG22	1:G:80:THR:O	1.88	0.70
1:H:109:PRO:CD	1:H:130:ARG:HD3	2.22	0.70
1:H:124:ALA:O	1:H:146:PRO:HB3	1.91	0.70
1:D:218:TYR:CD2	1:D:232:PRO:HG2	2.27	0.70
1:G:222:VAL:HG12	1:G:290:ALA:HB3	1.74	0.70
1:A:39:GLU:CA	1:A:40:LYS:CG	2.66	0.70
1:H:174:GLU:OE2	1:H:174:GLU:CA	2.39	0.70
1:G:245:ASP:C	1:G:247:GLY:N	2.48	0.70
1:J:120:THR:O	1:J:120:THR:CG2	2.38	0.70
1:G:272:THR:CG2	1:G:273:THR:H	1.98	0.70
1:H:139:ASN:O	1:H:141:THR:N	2.18	0.70
1:C:139:ASN:O	1:C:141:THR:N	2.23	0.70
1:D:95:ARG:CZ	1:E:253:LYS:HD2	2.22	0.70
1:J:278:ILE:HG22	1:J:280:PHE:CE1	2.26	0.70
1:B:250:GLU:HA	1:B:253:LYS:HE2	1.72	0.70
1:D:205:ASP:HA	1:D:230:SER:HB2	1.74	0.70
1:H:277:VAL:HG12	1:H:296:PRO:CA	2.21	0.70
1:J:154:ASP:O	1:J:156:TYR:N	2.25	0.70
1:J:240:LYS:HE2	1:J:240:LYS:CA	2.21	0.70
1:F:301:LEU:HA	1:F:304:VAL:HG22	1.72	0.69
1:A:107:PHE:O	1:A:130:ARG:NH1	2.25	0.69
1:B:272:THR:O	1:B:272:THR:HG22	1.92	0.69
1:F:109:PRO:N	1:F:130:ARG:HD3	2.07	0.69
1:D:298:GLU:HG3	1:D:299:GLU:HG3	1.72	0.69
1:A:205:ASP:HA	1:A:230:SER:HB2	1.75	0.69
1:B:74:THR:O	1:B:77:SER:N	2.25	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:218:TYR:CD2	1:F:232:PRO:HG2	2.27	0.69
1:H:120:THR:O	1:H:121:ASN:HB2	1.93	0.69
1:J:173:TYR:HB3	1:J:178:MET:HE2	1.73	0.69
1:J:214:PHE:CD2	1:J:299:GLU:CB	2.70	0.69
1:C:39:GLU:CB	1:C:40:LYS:CB	2.56	0.69
1:C:82:ASP:OD1	1:C:84:ASP:HB2	1.92	0.69
1:H:109:PRO:HD3	1:H:130:ARG:HD3	1.74	0.69
1:H:250:GLU:CB	1:H:266:LEU:CD1	2.70	0.69
1:A:43:TYR:HE1	1:A:300:MET:CE	2.05	0.69
1:B:83:ARG:NH1	1:B:125:HIS:CD2	2.61	0.69
1:C:188:GLU:HB3	1:E:252:GLU:OE2	1.93	0.69
1:D:91:GLU:HB2	1:D:135:TRP:CE2	2.28	0.69
1:E:116:ASP:OD2	1:E:130:ARG:HG2	1.92	0.69
1:F:49:MET:HE1	1:F:213:THR:OG1	1.91	0.69
1:F:273:THR:CG2	1:F:275:LYS:HB3	2.19	0.69
1:A:250:GLU:HB2	1:A:266:LEU:HD22	1.75	0.69
1:B:39:GLU:N	1:B:39:GLU:CD	2.51	0.69
1:B:83:ARG:HH11	1:B:125:HIS:CD2	2.11	0.69
1:B:110:ASP:H	1:B:116:ASP:CG	2.01	0.69
1:C:278:ILE:HD12	1:C:300:MET:CE	2.23	0.69
1:E:222:VAL:CG2	1:E:290:ALA:HB3	2.22	0.69
1:B:306:ASP:C	1:B:307:LEU:HD22	2.18	0.68
1:C:132:VAL:O	1:C:132:VAL:CG2	2.41	0.68
1:D:248:GLY:O	1:D:251:LEU:HB2	1.93	0.68
1:J:249:GLU:HA	1:J:250:GLU:CG	2.17	0.68
1:I:65:LEU:O	1:I:69:ARG:HG3	1.94	0.68
1:I:83:ARG:HH11	1:I:125:HIS:CD2	2.09	0.68
1:C:272:THR:O	1:C:272:THR:HG23	1.93	0.68
1:H:65:LEU:O	1:H:69:ARG:HG3	1.93	0.68
1:G:273:THR:CG2	1:G:275:LYS:HE3	2.21	0.68
1:G:305:ALA:O	1:G:308:ARG:HG3	1.93	0.68
1:B:82:ASP:C	1:B:82:ASP:OD1	2.36	0.68
1:G:139:ASN:C	1:G:141:THR:H	2.00	0.68
1:H:301:LEU:O	1:H:304:VAL:HG23	1.93	0.68
1:J:271:PRO:C	1:J:273:THR:H	2.02	0.68
1:B:39:GLU:HA	1:B:40:LYS:CB	2.24	0.68
1:C:214:PHE:CE2	1:C:300:MET:HA	2.29	0.68
1:G:221:MET:HE3	1:G:229:LEU:HD12	1.75	0.68
1:B:43:TYR:CD1	1:B:300:MET:HE3	2.28	0.68
1:J:254:ALA:O	1:J:258:ILE:HG23	1.94	0.68
1:C:267:GLU:HG2	1:C:278:ILE:HG12	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:105:VAL:HG13	1:H:107:PHE:CE1	2.30	0.67
1:J:222:VAL:HA	1:J:227:VAL:O	1.94	0.67
1:C:124:ALA:C	1:C:146:PRO:HG3	2.19	0.67
1:D:302:ALA:O	1:D:305:ALA:HB3	1.94	0.67
1:F:278:ILE:CD1	1:F:300:MET:HG3	2.24	0.67
1:G:45:GLN:H	1:G:46:SER:HB2	1.59	0.67
1:A:218:TYR:CD2	1:A:232:PRO:HG2	2.29	0.67
1:E:43:TYR:C	1:E:45:GLN:N	2.52	0.67
1:H:231:HIS:CD2	1:H:237:TRP:HE3	2.13	0.67
1:C:222:VAL:HG22	1:C:226:GLY:HA2	1.77	0.67
1:D:139:ASN:O	1:D:141:THR:N	2.27	0.67
1:J:101:LEU:O	1:J:101:LEU:HD22	1.94	0.67
1:J:167:LEU:HD22	1:J:181:TYR:CE2	2.29	0.67
1:A:214:PHE:HB3	1:A:299:GLU:OE1	1.94	0.67
1:G:272:THR:CG2	1:G:273:THR:N	2.49	0.67
1:I:74:THR:O	1:I:77:SER:N	2.26	0.67
1:J:173:TYR:CB	1:J:178:MET:CE	2.67	0.67
1:H:83:ARG:HH11	1:H:113:ASP:CG	2.02	0.67
1:C:131:PHE:CE1	1:C:133:PRO:HG3	2.29	0.67
1:D:132:VAL:HG23	1:D:132:VAL:O	1.93	0.67
1:H:105:VAL:CG1	1:H:107:PHE:HE1	2.08	0.67
1:I:267:GLU:C	1:I:268:THR:HG22	2.20	0.67
1:D:165:ASP:OD1	1:D:183:SER:OG	2.09	0.67
1:D:174:GLU:HA	1:D:174:GLU:OE2	1.94	0.67
1:F:58:ASP:OD1	1:F:286:THR:HG23	1.95	0.67
1:H:151:ASP:O	1:H:152:SER:HB3	1.93	0.67
1:G:122:SER:HB2	1:G:123:PRO:CD	2.25	0.66
1:H:275:LYS:HB3	1:H:275:LYS:HZ3	1.59	0.66
1:J:218:TYR:CD1	1:J:218:TYR:N	2.62	0.66
1:G:135:TRP:HZ3	1:G:142:ALA:O	1.78	0.66
1:I:265:HIS:O	1:I:266:LEU:HD23	1.96	0.66
1:F:43:TYR:CE1	1:F:300:MET:HE2	2.30	0.66
1:F:123:PRO:O	1:F:124:ALA:HB3	1.95	0.66
1:G:185:ILE:HG13	1:G:193:GLY:C	2.21	0.66
1:I:105:VAL:HG12	1:I:133:PRO:HD2	1.77	0.66
1:J:213:THR:HG21	1:J:293:LEU:HD21	1.77	0.66
1:F:41:LEU:CD1	1:F:41:LEU:O	2.44	0.66
1:D:41:LEU:C	1:D:43:TYR:N	2.54	0.66
1:G:214:PHE:CD1	1:G:295:VAL:HG13	2.31	0.66
1:J:245:ASP:O	1:J:246:PHE:C	2.38	0.66
1:B:157:GLN:HA	1:B:157:GLN:HE21	1.59	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:120:THR:O	1:D:120:THR:HG23	1.96	0.66
1:C:74:THR:HG23	1:D:89:ILE:HG12	1.78	0.66
1:J:105:VAL:CG1	1:J:107:PHE:CE1	2.79	0.66
1:I:57:PHE:HE2	1:I:207:VAL:CG1	2.09	0.66
1:D:41:LEU:CD2	1:D:42:ALA:CA	2.62	0.65
1:E:222:VAL:HG23	1:E:290:ALA:HB3	1.78	0.65
1:F:244:TYR:CE2	1:F:252:GLU:HG3	2.31	0.65
1:D:120:THR:O	1:D:121:ASN:HB2	1.94	0.65
1:B:40:LYS:O	1:B:42:ALA:N	2.24	0.65
1:H:275:LYS:HB3	1:H:275:LYS:HZ2	1.60	0.65
1:I:107:PHE:O	1:I:130:ARG:HD2	1.96	0.65
1:I:155:TYR:O	1:I:159:PRO:HG2	1.96	0.65
1:I:307:LEU:HD11	1:J:41:LEU:CD2	2.23	0.65
1:C:110:ASP:OD1	1:C:114:GLY:C	2.39	0.65
1:G:80:THR:O	1:G:82:ASP:N	2.29	0.65
1:H:109:PRO:HD3	1:H:130:ARG:CD	2.26	0.65
1:B:61:MET:HE1	1:B:284:VAL:HG11	1.78	0.65
1:C:115:LYS:O	1:C:116:ASP:C	2.39	0.65
1:I:39:GLU:N	1:I:40:LYS:CB	2.52	0.65
1:D:177:PHE:CE1	1:D:240:LYS:HD2	2.32	0.65
1:G:165:ASP:C	1:G:166:VAL:HG23	2.21	0.65
1:F:205:ASP:HA	1:F:230:SER:HB2	1.79	0.65
1:F:139:ASN:C	1:F:141:THR:H	2.01	0.65
1:H:130:ARG:C	1:H:132:VAL:HG13	2.22	0.65
1:H:158:LEU:HB2	1:H:159:PRO:HD3	1.79	0.65
1:H:212:ARG:HH22	1:I:235:LYS:HZ2	1.45	0.65
1:H:185:ILE:HG13	1:H:193:GLY:O	1.97	0.65
1:I:131:PHE:CE1	1:I:133:PRO:HG3	2.32	0.65
1:J:105:VAL:HG11	1:J:107:PHE:HE1	1.61	0.65
1:J:136:ASN:OD1	1:J:138:MET:HB2	1.96	0.65
1:J:297:LYS:HD2	1:J:301:LEU:HD13	1.78	0.65
1:A:39:GLU:N	1:A:40:LYS:HD3	2.12	0.64
1:C:273:THR:HG21	1:C:275:LYS:CG	2.25	0.64
1:J:113:ASP:O	1:J:115:LYS:HG3	1.97	0.64
1:B:259:LYS:O	1:B:259:LYS:HG2	1.96	0.64
1:C:41:LEU:HD23	1:C:44:GLN:OE1	1.97	0.64
1:D:135:TRP:CE2	1:D:144:VAL:CG2	2.78	0.64
1:G:248:GLY:O	1:G:251:LEU:HB2	1.97	0.64
1:A:308:ARG:CG	1:A:308:ARG:NH1	2.42	0.64
1:D:300:MET:O	1:D:303:GLY:HA3	1.98	0.64
1:E:276:THR:O	1:E:297:LYS:CB	2.46	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:83:ARG:O	1:F:87:LEU:HD12	1.97	0.64
1:J:204:VAL:O	1:J:208:VAL:HG23	1.98	0.64
1:D:237:TRP:CD1	1:D:241:LYS:HD2	2.33	0.64
1:F:270:ASP:OD2	1:F:272:THR:HB	1.98	0.64
1:D:96:ASP:HB2	1:E:256:ARG:HH22	1.62	0.64
1:E:298:GLU:O	1:E:301:LEU:HB3	1.98	0.64
1:H:250:GLU:HB3	1:H:266:LEU:HD22	1.78	0.64
1:I:110:ASP:H	1:I:116:ASP:CG	2.05	0.64
1:J:249:GLU:CA	1:J:250:GLU:CG	2.73	0.64
1:G:182:VAL:HG12	1:G:183:SER:N	2.10	0.64
1:F:244:TYR:HE2	1:F:252:GLU:HG3	1.63	0.64
1:J:249:GLU:CA	1:J:251:LEU:H	2.10	0.64
1:D:80:THR:O	1:D:81:ALA:C	2.40	0.64
1:H:75:MET:HE2	1:H:105:VAL:HG21	1.79	0.64
1:H:250:GLU:CB	1:H:266:LEU:HD11	2.28	0.64
1:J:105:VAL:CG1	1:J:107:PHE:HE1	2.11	0.64
1:H:278:ILE:HG21	1:H:280:PHE:CZ	2.33	0.64
1:I:257:ASP:HB3	1:I:262:ILE:O	1.98	0.64
1:A:169:GLU:HB3	1:A:170:PRO:HD2	1.79	0.63
1:B:122:SER:HB2	1:B:123:PRO:HD2	1.80	0.63
1:D:158:LEU:O	1:D:162:THR:HG23	1.97	0.63
1:A:244:TYR:CD2	1:A:252:GLU:HG2	2.34	0.63
1:B:136:ASN:OD1	1:B:138:MET:HB2	1.98	0.63
1:B:267:GLU:OE1	1:B:297:LYS:HE3	1.97	0.63
1:H:42:ALA:C	1:H:300:MET:HE2	2.23	0.63
1:B:110:ASP:OD1	1:B:116:ASP:HB2	1.98	0.63
1:E:136:ASN:OD1	1:E:138:MET:CB	2.46	0.63
1:I:85:GLU:O	1:I:86:ALA:C	2.41	0.63
1:J:39:GLU:HG2	1:J:40:LYS:N	2.14	0.63
1:J:83:ARG:HG3	1:J:112:PHE:HE1	1.64	0.63
1:G:40:LYS:N	1:G:41:LEU:HB3	2.14	0.63
1:G:253:LYS:HB3	1:I:95:ARG:CZ	2.29	0.63
1:J:298:GLU:CA	1:J:301:LEU:HD23	2.18	0.63
1:B:185:ILE:HG13	1:B:193:GLY:C	2.23	0.63
1:H:126:ASP:O	1:H:127:GLY:C	2.41	0.63
1:H:250:GLU:HB2	1:H:266:LEU:HD13	1.81	0.63
1:A:139:ASN:O	1:A:141:THR:N	2.30	0.63
1:C:260:ASN:CB	1:C:262:ILE:HD12	2.29	0.63
1:G:279:LEU:CD2	1:G:294:VAL:HG22	2.28	0.63
1:H:110:ASP:OD1	1:H:114:GLY:C	2.42	0.63
1:I:308:ARG:HA	1:I:309:GLU:C	2.24	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:VAL:HG22	1:A:226:GLY:HA2	1.81	0.63
1:B:307:LEU:N	1:B:307:LEU:HD23	1.85	0.63
1:J:177:PHE:HB3	1:J:201:LEU:CD1	2.28	0.63
1:G:43:TYR:HD1	1:G:300:MET:CE	2.09	0.62
1:H:250:GLU:HB3	1:H:266:LEU:CD1	2.29	0.62
1:D:299:GLU:O	1:D:302:ALA:CB	2.46	0.62
1:I:135:TRP:CZ3	1:I:143:SER:HA	2.34	0.62
1:I:160:LYS:HG2	1:I:160:LYS:O	2.00	0.62
1:A:244:TYR:HE2	1:A:252:GLU:HG2	1.63	0.62
1:C:250:GLU:H	1:C:250:GLU:CD	2.07	0.62
1:E:300:MET:O	1:E:304:VAL:HG23	1.98	0.62
1:I:259:LYS:HG2	1:I:259:LYS:O	1.99	0.62
1:A:62:LYS:HD3	1:B:59:ALA:HB1	1.81	0.62
1:B:120:THR:O	1:B:121:ASN:CB	2.43	0.62
1:C:121:ASN:O	1:C:122:SER:CB	2.46	0.62
1:D:41:LEU:CD2	1:D:41:LEU:C	2.67	0.62
1:D:222:VAL:CG1	1:D:258:ILE:HD13	2.30	0.62
1:D:298:GLU:CA	1:D:299:GLU:HB2	2.28	0.62
1:E:40:LYS:HD2	1:E:40:LYS:O	1.99	0.62
1:G:43:TYR:C	1:G:45:GLN:H	2.08	0.62
1:F:172:PHE:CZ	1:F:175:GLY:HA2	2.35	0.62
1:G:176:VAL:HG13	1:G:178:MET:HE2	1.81	0.62
1:B:53:TYR:O	1:B:54:ALA:C	2.42	0.62
1:B:306:ASP:C	1:B:308:ARG:H	2.08	0.62
1:C:269:ALA:HA	1:C:276:THR:HA	1.82	0.62
1:G:40:LYS:HA	1:G:42:ALA:N	2.07	0.62
1:I:91:GLU:HB2	1:I:135:TRP:NE1	2.15	0.62
1:I:105:VAL:HG12	1:I:133:PRO:CD	2.30	0.62
1:B:149:HIS:C	1:B:151:ASP:H	2.05	0.62
1:B:212:ARG:NH1	1:C:212:ARG:NH2	2.47	0.62
1:C:213:THR:HG22	1:C:217:GLY:HA3	1.82	0.62
1:E:164:LYS:O	1:E:166:VAL:HG23	1.99	0.62
1:E:254:ALA:O	1:E:258:ILE:HG23	2.00	0.62
1:G:120:THR:O	1:G:120:THR:CG2	2.47	0.62
1:B:248:GLY:O	1:B:249:GLU:CB	2.45	0.61
1:C:256:ARG:HD3	3:C:321:HOH:O	2.00	0.61
1:E:79:GLU:O	1:E:81:ALA:N	2.33	0.61
1:I:91:GLU:HB2	1:I:135:TRP:CE2	2.35	0.61
1:C:213:THR:HG21	1:C:295:VAL:CG2	2.30	0.61
1:B:188:GLU:C	1:B:190:GLU:H	2.08	0.61
1:C:306:ASP:N	1:C:306:ASP:OD1	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:222:VAL:HG12	1:D:290:ALA:HB3	1.81	0.61
1:D:249:GLU:O	1:D:249:GLU:HG3	2.00	0.61
1:E:48:GLU:CG	1:F:48:GLU:HG3	2.30	0.61
1:E:172:PHE:CE2	1:E:175:GLY:HA2	2.34	0.61
1:G:80:THR:O	1:G:81:ALA:C	2.43	0.61
1:G:218:TYR:HD2	1:G:232:PRO:CG	2.13	0.61
1:G:306:ASP:O	1:G:308:ARG:N	2.33	0.61
1:D:41:LEU:C	1:D:43:TYR:H	2.03	0.61
1:D:85:GLU:O	1:D:89:ILE:HD12	2.00	0.61
1:E:274:GLY:O	1:E:275:LYS:C	2.44	0.61
1:I:185:ILE:HG13	1:I:193:GLY:C	2.26	0.61
1:E:41:LEU:C	1:E:43:TYR:N	2.58	0.61
1:B:84:ASP:HA	1:B:87:LEU:HD12	1.83	0.61
1:F:43:TYR:O	1:F:44:GLN:C	2.44	0.61
1:H:231:HIS:CD2	1:H:237:TRP:CE3	2.88	0.61
1:A:57:PHE:O	1:A:61:MET:HG3	2.01	0.61
1:B:105:VAL:HG12	1:B:133:PRO:HD2	1.81	0.61
1:G:165:ASP:C	1:G:166:VAL:CG2	2.73	0.61
1:I:265:HIS:HA	1:I:279:LEU:O	2.00	0.61
1:F:254:ALA:O	1:F:258:ILE:HG23	2.00	0.61
1:G:306:ASP:C	1:G:308:ARG:H	2.08	0.61
1:J:120:THR:OG1	1:J:127:GLY:O	2.17	0.61
1:I:234:HIS:CE1	1:I:272:THR:HG23	2.36	0.61
1:I:108:GLU:O	1:I:111:ALA:CB	2.49	0.61
1:A:214:PHE:HE2	1:A:299:GLU:O	1.83	0.60
1:E:41:LEU:O	1:E:43:TYR:N	2.34	0.60
1:A:173:TYR:CB	1:A:178:MET:HE3	2.16	0.60
1:E:43:TYR:C	1:E:45:GLN:H	2.10	0.60
1:H:216:THR:OG1	1:H:299:GLU:OE2	2.20	0.60
1:I:57:PHE:HE2	1:I:207:VAL:HG12	1.65	0.60
1:A:105:VAL:CG1	1:A:107:PHE:HE1	2.13	0.60
1:C:163:GLU:HB3	1:E:259:LYS:HZ3	1.64	0.60
1:G:135:TRP:CD2	1:G:144:VAL:CG2	2.81	0.60
1:I:104:TYR:HD2	1:I:134:TYR:HE2	1.49	0.60
1:A:245:ASP:C	1:A:247:GLY:H	2.07	0.60
1:B:177:PHE:CZ	1:B:240:LYS:HD2	2.37	0.60
1:E:228:ILE:HD12	1:E:241:LYS:O	2.01	0.60
1:F:79:GLU:HA	1:F:79:GLU:OE2	2.01	0.60
1:H:275:LYS:NZ	1:H:275:LYS:CB	2.60	0.60
1:J:249:GLU:C	1:J:250:GLU:CG	2.74	0.60
1:J:300:MET:CA	1:J:301:LEU:CB	2.78	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:104:TYR:HB3	1:F:134:TYR:HD2	1.66	0.60
1:C:172:PHE:CZ	1:C:175:GLY:HA2	2.36	0.60
1:F:211:VAL:HG12	1:F:212:ARG:N	2.15	0.60
1:H:91:GLU:CG	1:H:135:TRP:CE2	2.80	0.60
1:D:105:VAL:HG13	1:D:107:PHE:HE1	1.65	0.60
1:F:250:GLU:O	1:F:266:LEU:HD11	2.02	0.60
1:G:271:PRO:O	1:G:272:THR:O	2.20	0.60
1:G:307:LEU:N	1:G:307:LEU:HD23	2.17	0.60
1:H:185:ILE:HG13	1:H:193:GLY:C	2.26	0.60
1:C:150:TYR:HB3	1:C:155:TYR:OH	2.01	0.60
1:D:43:TYR:CE1	1:D:300:MET:HE2	2.37	0.60
1:E:117:ALA:O	1:E:120:THR:CG2	2.49	0.60
1:F:117:ALA:O	1:F:120:THR:HG22	2.01	0.60
1:I:106:ALA:HB3	1:I:194:ILE:HG12	1.84	0.60
1:A:105:VAL:HG11	1:A:107:PHE:HE1	1.67	0.60
1:D:94:LEU:HD11	1:D:137:LYS:HG3	1.84	0.60
1:H:42:ALA:C	1:H:300:MET:CE	2.75	0.60
1:H:130:ARG:NH2	1:H:150:TYR:HE1	2.00	0.60
1:H:273:THR:OG1	1:H:274:GLY:N	2.34	0.60
1:H:278:ILE:HG22	1:H:280:PHE:CE1	2.37	0.60
1:I:120:THR:O	1:I:121:ASN:CB	2.50	0.60
1:A:171:TYR:N	1:A:171:TYR:CD1	2.70	0.59
1:C:247:GLY:O	1:C:248:GLY:O	2.19	0.59
1:E:276:THR:O	1:E:297:LYS:HB3	2.02	0.59
1:G:104:TYR:OH	1:G:180:SER:HB3	2.01	0.59
1:H:171:TYR:OH	1:H:178:MET:HE3	2.02	0.59
1:I:59:ALA:HB1	1:J:62:LYS:HD2	1.84	0.59
1:J:54:ALA:O	1:J:284:VAL:HG22	2.02	0.59
1:J:82:ASP:C	1:J:82:ASP:OD1	2.45	0.59
1:J:278:ILE:CG2	1:J:280:PHE:CE1	2.85	0.59
1:D:250:GLU:CG	1:D:266:LEU:HD13	2.32	0.59
1:F:172:PHE:CE2	1:F:175:GLY:HA2	2.37	0.59
1:A:101:LEU:O	1:A:101:LEU:HD22	2.01	0.59
1:B:281:TYR:HB3	1:B:292:VAL:HG22	1.84	0.59
1:C:185:ILE:HD11	1:C:194:ILE:O	2.01	0.59
1:G:101:LEU:HD23	1:G:101:LEU:O	2.02	0.59
1:H:106:ALA:HB3	1:H:194:ILE:HG12	1.84	0.59
1:D:105:VAL:HG13	1:D:107:PHE:CE1	2.37	0.59
1:D:105:VAL:CG1	1:D:107:PHE:HE1	2.15	0.59
1:E:301:LEU:HD23	1:E:301:LEU:C	2.26	0.59
1:F:42:ALA:CB	1:F:300:MET:HE1	2.31	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:249:GLU:HB2	1:J:251:LEU:N	2.17	0.59
1:J:270:ASP:OD2	1:J:273:THR:HG23	2.03	0.59
1:C:130:ARG:O	1:C:132:VAL:HG13	2.02	0.59
1:D:245:ASP:O	1:D:246:PHE:HD2	1.85	0.59
1:F:116:ASP:OD2	1:F:130:ARG:HG2	2.02	0.59
1:I:256:ARG:HG3	1:I:256:ARG:NH1	2.14	0.59
1:J:154:ASP:O	1:J:155:TYR:C	2.46	0.59
1:J:167:LEU:C	1:J:167:LEU:HD12	2.26	0.59
1:A:250:GLU:H	1:A:250:GLU:CD	2.09	0.59
1:D:265:HIS:C	1:D:266:LEU:HD23	2.27	0.59
1:H:212:ARG:NH1	1:I:232:PRO:O	2.36	0.59
1:I:147:LEU:O	1:I:150:TYR:CE2	2.56	0.59
1:B:168:THR:HG23	1:B:180:SER:O	2.01	0.59
1:G:253:LYS:HD3	1:I:95:ARG:NH1	2.18	0.59
1:H:167:LEU:HD11	1:H:179:VAL:HG13	1.84	0.59
1:H:205:ASP:HA	1:H:230:SER:HB2	1.85	0.59
1:J:169:GLU:HB3	1:J:170:PRO:HD2	1.84	0.59
1:A:91:GLU:CG	1:A:135:TRP:CZ2	2.82	0.59
1:C:101:LEU:O	1:C:101:LEU:HD22	2.01	0.59
1:C:131:PHE:CD1	1:C:133:PRO:HD3	2.38	0.59
1:G:41:LEU:O	1:G:41:LEU:HD13	2.03	0.59
1:G:45:GLN:N	1:G:46:SER:HB2	2.17	0.59
1:E:43:TYR:O	1:E:46:SER:N	2.36	0.59
1:E:48:GLU:HG3	1:F:48:GLU:CG	2.32	0.59
1:G:270:ASP:OD2	1:G:273:THR:CG2	2.37	0.59
1:B:163:GLU:CD	1:B:186:MET:HE1	2.28	0.59
1:E:79:GLU:O	1:E:80:THR:C	2.45	0.59
1:I:149:HIS:C	1:I:151:ASP:N	2.59	0.59
1:J:249:GLU:CA	1:J:251:LEU:N	2.65	0.59
1:F:136:ASN:OD1	1:F:138:MET:HB2	2.03	0.58
1:G:249:GLU:HG2	1:G:249:GLU:O	2.02	0.58
1:H:208:VAL:HG11	1:H:230:SER:OG	2.03	0.58
1:B:117:ALA:O	1:B:120:THR:HG22	2.03	0.58
1:C:265:HIS:HA	1:C:279:LEU:O	2.03	0.58
1:J:177:PHE:CZ	1:J:240:LYS:HD2	2.38	0.58
1:B:75:MET:HE2	1:B:75:MET:HA	1.85	0.58
1:B:158:LEU:HB2	1:B:159:PRO:HD3	1.86	0.58
1:C:297:LYS:HE2	1:C:301:LEU:HD11	1.84	0.58
1:A:82:ASP:OD1	1:A:84:ASP:N	2.33	0.58
1:A:270:ASP:HB3	1:A:273:THR:O	2.04	0.58
1:I:75:MET:CA	1:I:75:MET:CE	2.76	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:231:HIS:ND1	1:D:232:PRO:HD2	2.19	0.58
1:I:258:ILE:HD12	1:I:258:ILE:C	2.29	0.58
1:B:249:GLU:C	1:B:251:LEU:N	2.61	0.58
1:C:126:ASP:O	1:C:127:GLY:C	2.45	0.58
1:F:270:ASP:HB3	1:F:273:THR:HG22	1.86	0.58
1:G:270:ASP:OD1	1:G:271:PRO:N	2.37	0.58
1:G:305:ALA:HA	1:G:308:ARG:NH1	2.19	0.58
1:B:39:GLU:HA	1:B:40:LYS:O	2.04	0.58
1:C:125:HIS:O	1:C:146:PRO:CG	2.52	0.58
1:I:48:GLU:O	1:I:51:SER:HB3	2.04	0.58
1:A:254:ALA:O	1:A:258:ILE:HG23	2.04	0.58
1:B:108:GLU:O	1:B:111:ALA:CB	2.52	0.58
1:B:120:THR:O	1:B:120:THR:CG2	2.52	0.58
1:B:177:PHE:HZ	1:B:240:LYS:HD2	1.68	0.58
1:A:104:TYR:OH	1:A:180:SER:HB3	2.03	0.57
1:A:218:TYR:N	1:A:218:TYR:HD1	1.99	0.57
1:J:249:GLU:C	1:J:250:GLU:HG3	2.29	0.57
1:A:222:VAL:HG23	1:A:227:VAL:O	2.03	0.57
1:A:262:ILE:CD1	1:C:98:PRO:HG3	2.34	0.57
1:C:214:PHE:HE2	1:C:300:MET:HA	1.69	0.57
1:F:211:VAL:CG1	1:F:212:ARG:N	2.67	0.57
1:G:136:ASN:HD22	1:G:136:ASN:H	1.51	0.57
1:H:131:PHE:C	1:H:132:VAL:CG1	2.77	0.57
1:B:155:TYR:O	1:B:159:PRO:HG2	2.04	0.57
1:C:91:GLU:CG	1:C:135:TRP:CH2	2.86	0.57
1:C:278:ILE:HD12	1:C:300:MET:HE2	1.86	0.57
1:F:306:ASP:O	1:F:309:GLU:HG3	2.03	0.57
1:I:120:THR:O	1:I:120:THR:CG2	2.49	0.57
1:J:249:GLU:O	1:J:249:GLU:CD	2.48	0.57
1:D:39:GLU:CA	1:D:40:LYS:HB2	2.22	0.57
1:E:83:ARG:HD3	1:E:119:TYR:CZ	2.39	0.57
1:H:109:PRO:HD3	1:H:130:ARG:NH1	2.20	0.57
1:J:171:TYR:HD1	1:J:171:TYR:H	1.53	0.57
1:B:104:TYR:HE2	1:B:198:ASP:CG	2.12	0.57
1:D:177:PHE:HZ	1:D:240:LYS:HD2	1.64	0.57
1:A:145:ALA:HB1	1:A:146:PRO:HD2	1.85	0.57
1:B:302:ALA:O	1:B:305:ALA:HB3	2.05	0.57
1:E:122:SER:CB	1:E:123:PRO:HD2	2.34	0.57
1:H:173:TYR:O	1:H:174:GLU:C	2.48	0.57
1:A:245:ASP:C	1:A:247:GLY:N	2.56	0.57
1:I:104:TYR:HE2	1:I:198:ASP:CG	2.12	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:VAL:CG1	1:A:107:PHE:CE1	2.88	0.57
1:A:262:ILE:HG12	1:C:98:PRO:HG3	1.85	0.57
1:B:108:GLU:O	1:B:111:ALA:HB3	2.05	0.57
1:I:108:GLU:HB2	1:I:111:ALA:HB2	1.86	0.57
1:F:308:ARG:O	1:F:309:GLU:C	2.48	0.57
1:H:39:GLU:N	1:H:40:LYS:CD	2.68	0.57
1:J:105:VAL:HG13	1:J:107:PHE:CE1	2.40	0.57
1:C:240:LYS:HE2	1:C:240:LYS:HA	1.85	0.57
1:C:260:ASN:HB2	1:C:262:ILE:HD12	1.87	0.57
1:E:123:PRO:O	1:E:124:ALA:HB3	2.05	0.57
1:A:214:PHE:HD2	1:A:299:GLU:HB3	1.68	0.56
1:E:39:GLU:CA	1:E:40:LYS:CB	2.82	0.56
1:G:139:ASN:C	1:G:141:THR:N	2.63	0.56
1:H:43:TYR:HA	1:H:300:MET:CE	2.32	0.56
1:H:157:GLN:HA	1:H:157:GLN:OE1	2.05	0.56
1:J:203:TYR:O	1:J:207:VAL:HG23	2.05	0.56
1:C:295:VAL:HG11	1:C:300:MET:HG3	1.87	0.56
1:G:104:TYR:CZ	1:G:196:GLY:HA3	2.39	0.56
1:G:185:ILE:HG13	1:G:193:GLY:O	2.05	0.56
1:H:250:GLU:HB2	1:H:266:LEU:CD1	2.34	0.56
1:A:122:SER:HB2	1:A:123:PRO:HD2	1.85	0.56
1:B:108:GLU:HA	1:B:130:ARG:NH1	2.20	0.56
1:B:251:LEU:C	1:B:254:ALA:HB3	2.30	0.56
1:D:122:SER:HB3	1:D:123:PRO:HD2	1.85	0.56
1:F:273:THR:HG21	1:F:275:LYS:CD	2.35	0.56
1:F:273:THR:CG2	1:F:275:LYS:N	2.53	0.56
1:G:101:LEU:C	1:G:101:LEU:CD2	2.78	0.56
1:G:151:ASP:HA	1:G:157:GLN:OE1	2.06	0.56
1:H:57:PHE:O	1:H:61:MET:CG	2.52	0.56
1:H:123:PRO:O	1:H:124:ALA:HB3	2.05	0.56
1:I:105:VAL:O	1:I:133:PRO:HD2	2.05	0.56
1:I:106:ALA:O	1:I:193:GLY:HA3	2.05	0.56
1:J:205:ASP:HA	1:J:230:SER:HB2	1.86	0.56
1:J:249:GLU:CB	1:J:251:LEU:N	2.68	0.56
1:J:249:GLU:N	1:J:250:GLU:HG3	2.21	0.56
1:H:119:TYR:O	1:H:120:THR:C	2.48	0.56
1:I:108:GLU:O	1:I:111:ALA:HB3	2.05	0.56
1:A:264:GLY:C	1:A:281:TYR:CE2	2.84	0.56
1:B:234:HIS:CE1	1:B:272:THR:HG23	2.40	0.56
1:D:302:ALA:HB3	1:D:303:GLY:CA	2.36	0.56
1:F:160:LYS:HG3	1:F:191:PHE:CE2	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:104:TYR:CD2	1:I:134:TYR:CE2	2.93	0.56
1:D:95:ARG:NE	1:E:253:LYS:HD2	2.21	0.56
1:E:89:ILE:HD13	1:F:74:THR:HG23	1.88	0.56
1:E:132:VAL:O	1:E:132:VAL:CG2	2.54	0.56
1:G:253:LYS:HD3	1:I:95:ARG:HH12	1.71	0.56
1:I:153:SER:O	1:I:157:GLN:HG2	2.06	0.56
1:J:172:PHE:HB2	1:J:177:PHE:CE2	2.40	0.56
1:J:260:ASN:CB	1:J:262:ILE:CD1	2.83	0.56
1:C:273:THR:HG23	1:C:275:LYS:HG2	1.87	0.56
1:E:65:LEU:O	1:E:69:ARG:HG3	2.06	0.56
1:E:122:SER:CB	1:E:123:PRO:CD	2.84	0.56
1:G:43:TYR:O	1:G:45:GLN:N	2.39	0.56
1:G:206:GLU:OE1	1:G:206:GLU:C	2.48	0.56
1:J:154:ASP:C	1:J:156:TYR:N	2.62	0.56
1:J:173:TYR:CD2	1:J:178:MET:HE1	2.39	0.56
1:A:120:THR:HG23	1:A:120:THR:O	2.06	0.56
1:C:296:PRO:O	1:C:297:LYS:C	2.48	0.56
1:E:296:PRO:HB2	1:E:299:GLU:HG3	1.88	0.56
1:H:234:HIS:HB2	1:H:237:TRP:CE3	2.41	0.56
1:J:251:LEU:CD2	1:J:266:LEU:HD12	2.36	0.56
1:A:41:LEU:CD1	1:B:307:LEU:CD1	2.84	0.56
1:A:222:VAL:HA	1:A:227:VAL:O	2.06	0.56
1:E:169:GLU:OE2	1:E:225:SER:OG	2.24	0.56
1:G:246:PHE:HB3	1:G:251:LEU:CD1	2.35	0.56
1:J:246:PHE:HB3	1:J:251:LEU:CD1	2.36	0.56
1:C:186:MET:CE	1:C:191:PHE:HD1	2.19	0.56
1:E:41:LEU:HD22	1:E:44:GLN:OE1	2.06	0.56
1:G:43:TYR:C	1:G:45:GLN:N	2.63	0.56
1:G:101:LEU:O	1:G:101:LEU:CD2	2.54	0.56
1:A:39:GLU:OE2	1:A:39:GLU:CA	2.54	0.55
1:B:57:PHE:HE2	1:B:207:VAL:CG1	2.19	0.55
1:C:132:VAL:HG23	1:C:147:LEU:H	1.71	0.55
1:D:104:TYR:OH	1:D:180:SER:HB3	2.06	0.55
1:J:245:ASP:O	1:J:247:GLY:CA	2.54	0.55
1:F:176:VAL:HA	3:F:6:HOH:O	2.05	0.55
1:E:165:ASP:C	1:E:166:VAL:HG23	2.31	0.55
1:G:91:GLU:HB2	1:G:135:TRP:NE1	2.21	0.55
1:H:80:THR:HG22	1:H:82:ASP:N	2.21	0.55
1:J:40:LYS:C	1:J:42:ALA:N	2.63	0.55
1:A:156:TYR:C	1:A:159:PRO:HD2	2.31	0.55
1:B:163:GLU:HB3	1:B:186:MET:HE1	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:105:VAL:HG13	1:C:107:PHE:CE1	2.41	0.55
1:C:158:LEU:HB2	1:C:159:PRO:HD3	1.87	0.55
1:F:270:ASP:C	1:F:272:THR:H	2.14	0.55
1:J:104:TYR:CZ	1:J:196:GLY:HA3	2.41	0.55
1:A:131:PHE:CE1	1:A:133:PRO:HG3	2.41	0.55
1:C:163:GLU:HB3	1:E:259:LYS:HZ1	1.69	0.55
1:D:83:ARG:HG2	1:D:112:PHE:HE1	1.70	0.55
1:G:139:ASN:O	1:G:141:THR:N	2.28	0.55
1:G:270:ASP:OD1	1:G:270:ASP:C	2.49	0.55
1:H:250:GLU:O	1:H:266:LEU:HD11	2.06	0.55
1:C:171:TYR:CZ	1:C:178:MET:HE3	2.41	0.55
1:D:124:ALA:HB2	1:D:144:VAL:HG11	1.89	0.55
1:E:83:ARG:HD3	1:E:119:TYR:CE1	2.41	0.55
1:H:122:SER:HB2	1:H:123:PRO:CD	2.36	0.55
1:I:156:TYR:O	1:I:159:PRO:HD2	2.06	0.55
1:I:258:ILE:CG1	1:I:259:LYS:N	2.68	0.55
1:A:39:GLU:N	1:A:40:LYS:CD	2.70	0.55
1:G:41:LEU:O	1:G:41:LEU:CD1	2.54	0.55
1:H:277:VAL:HG12	1:H:295:VAL:C	2.32	0.55
1:J:40:LYS:C	1:J:42:ALA:H	2.14	0.55
1:A:297:LYS:O	1:A:297:LYS:HD2	2.06	0.55
1:D:299:GLU:O	1:D:302:ALA:HB2	2.07	0.55
1:E:273:THR:CG2	1:E:275:LYS:CG	2.66	0.55
1:F:123:PRO:O	1:F:124:ALA:CB	2.55	0.55
1:A:260:ASN:CB	1:A:262:ILE:CD1	2.82	0.55
1:B:149:HIS:C	1:B:151:ASP:N	2.58	0.55
1:H:222:VAL:HG12	1:H:290:ALA:HB3	1.89	0.55
1:C:57:PHE:O	1:C:61:MET:CG	2.55	0.54
1:D:273:THR:CB	1:D:274:GLY:HA2	2.37	0.54
1:F:182:VAL:HG11	1:F:194:ILE:HD12	1.89	0.54
1:H:185:ILE:HD11	1:H:194:ILE:O	2.07	0.54
1:J:297:LYS:O	1:J:301:LEU:CD2	2.51	0.54
1:F:167:LEU:HD23	1:F:287:GLY:HA3	1.88	0.54
1:G:266:LEU:HD23	1:G:266:LEU:H	1.72	0.54
1:J:153:SER:HB3	1:J:155:TYR:CD1	2.42	0.54
1:J:169:GLU:OE2	1:J:223:SER:OG	2.24	0.54
1:A:215:ASP:N	1:A:299:GLU:OE1	2.36	0.54
1:C:171:TYR:OH	1:C:178:MET:HE3	2.07	0.54
1:E:130:ARG:NH2	1:E:150:TYR:HE1	2.04	0.54
1:E:273:THR:HG22	1:E:275:LYS:HD2	1.86	0.54
1:B:240:LYS:HE2	1:B:240:LYS:CA	2.18	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:104:TYR:CZ	1:D:196:GLY:HA3	2.42	0.54
1:D:296:PRO:HB2	1:D:299:GLU:CG	2.36	0.54
1:D:298:GLU:N	1:D:299:GLU:CB	2.52	0.54
1:E:273:THR:CG2	1:E:275:LYS:CD	2.63	0.54
1:I:242:ASP:OD2	1:I:245:ASP:OD2	2.26	0.54
1:C:187:LYS:HG3	1:C:192:ALA:HB2	1.89	0.54
1:I:122:SER:HB2	1:I:123:PRO:CD	2.26	0.54
1:J:177:PHE:CB	1:J:201:LEU:HD12	2.35	0.54
1:J:249:GLU:CB	1:J:252:GLU:N	2.42	0.54
1:B:188:GLU:O	1:B:190:GLU:N	2.39	0.54
1:C:254:ALA:O	1:C:258:ILE:HG23	2.08	0.54
1:F:301:LEU:HD23	1:F:304:VAL:HG21	1.90	0.54
1:G:93:LEU:HD23	1:H:73:THR:HG21	1.89	0.54
1:B:213:THR:CG2	1:B:217:GLY:HA3	2.38	0.54
1:C:248:GLY:HA3	1:C:250:GLU:OE2	2.08	0.54
1:E:187:LYS:O	1:E:188:GLU:HG2	2.08	0.54
1:G:45:GLN:CA	1:G:46:SER:HB2	2.38	0.54
1:A:250:GLU:OE1	1:A:250:GLU:N	2.30	0.54
1:A:305:ALA:C	1:A:307:LEU:H	2.16	0.54
1:C:109:PRO:HD3	1:C:130:ARG:NH1	2.23	0.54
1:D:49:MET:HE1	1:D:213:THR:OG1	2.08	0.54
1:H:136:ASN:OD1	1:H:138:MET:HE2	2.08	0.54
1:A:167:LEU:HD23	1:A:287:GLY:HA3	1.90	0.54
1:C:80:THR:O	1:C:81:ALA:C	2.51	0.54
1:C:115:LYS:C	1:C:117:ALA:N	2.63	0.54
1:C:222:VAL:CG2	1:C:226:GLY:HA2	2.38	0.54
1:E:139:ASN:O	1:E:141:THR:N	2.33	0.54
1:G:137:LYS:HA	1:G:141:THR:O	2.08	0.54
1:G:266:LEU:HD23	1:G:266:LEU:N	2.22	0.54
1:I:108:GLU:HB2	1:I:111:ALA:CB	2.38	0.54
1:D:90:LEU:HD11	1:D:105:VAL:HB	1.90	0.53
1:G:136:ASN:OD1	1:G:138:MET:HE2	2.08	0.53
1:H:49:MET:O	1:H:50:ALA:C	2.50	0.53
1:A:270:ASP:OD1	1:A:271:PRO:N	2.41	0.53
1:C:79:GLU:HA	1:C:79:GLU:OE2	2.09	0.53
1:F:120:THR:O	1:F:121:ASN:HB2	2.08	0.53
1:G:107:PHE:O	1:G:130:ARG:HD2	2.08	0.53
1:H:109:PRO:HD3	1:H:130:ARG:CZ	2.38	0.53
1:H:185:ILE:N	1:H:193:GLY:O	2.33	0.53
1:J:298:GLU:C	1:J:301:LEU:CD2	2.82	0.53
1:B:40:LYS:C	1:B:42:ALA:H	2.12	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:273:THR:CG2	1:G:275:LYS:CE	2.83	0.53
1:I:213:THR:HG21	1:I:293:LEU:HD21	1.91	0.53
1:J:309:GLU:H	1:J:309:GLU:CD	2.15	0.53
1:A:154:ASP:O	1:A:155:TYR:C	2.52	0.53
1:A:275:LYS:HB3	1:H:122:SER:HB3	1.91	0.53
1:B:265:HIS:HA	1:B:279:LEU:O	2.09	0.53
1:C:115:LYS:O	1:C:117:ALA:N	2.42	0.53
1:D:94:LEU:CD1	1:D:137:LYS:HE3	2.36	0.53
1:B:230:SER:HA	1:B:238:ILE:HG12	1.90	0.53
1:C:49:MET:O	1:C:50:ALA:C	2.50	0.53
1:C:61:MET:HB2	1:C:286:THR:OG1	2.09	0.53
1:C:222:VAL:HG13	1:C:290:ALA:HB3	1.89	0.53
1:E:273:THR:CG2	1:E:275:LYS:N	2.62	0.53
1:J:214:PHE:HD2	1:J:299:GLU:CB	2.18	0.53
1:B:104:TYR:HB3	1:B:134:TYR:HD2	1.74	0.53
1:G:213:THR:O	1:G:217:GLY:CA	2.53	0.53
1:I:43:TYR:CD1	1:I:300:MET:HE3	2.44	0.53
1:I:157:GLN:OE1	1:I:157:GLN:HA	2.09	0.53
1:A:49:MET:HE3	1:A:53:TYR:HE1	1.74	0.53
1:B:108:GLU:HA	1:B:130:ARG:HH11	1.73	0.53
1:C:277:VAL:HA	1:C:297:LYS:H	1.72	0.53
1:E:122:SER:OG	1:E:123:PRO:HD2	2.09	0.53
1:F:43:TYR:HE1	1:F:300:MET:HE2	1.73	0.53
1:H:105:VAL:CG1	1:H:107:PHE:CE1	2.89	0.53
1:J:120:THR:O	1:J:121:ASN:HB2	2.09	0.53
1:A:281:TYR:CD2	1:A:281:TYR:N	2.77	0.53
1:C:256:ARG:HH22	1:F:92:ASN:CG	2.17	0.53
1:E:83:ARG:NH2	1:E:129:GLY:O	2.42	0.53
1:F:63:ALA:O	1:F:67:ILE:HG13	2.09	0.53
1:G:145:ALA:HB1	1:G:146:PRO:HD2	1.91	0.53
1:J:94:LEU:HD11	1:J:137:LYS:HG3	1.91	0.53
1:J:207:VAL:O	1:J:210:LYS:CG	2.56	0.53
1:B:69:ARG:NH1	1:B:69:ARG:CG	2.70	0.52
1:C:88:LEU:HD22	1:C:92:ASN:OD1	2.10	0.52
1:E:79:GLU:C	1:E:81:ALA:N	2.63	0.52
1:A:205:ASP:OD2	1:A:209:SER:OG	2.25	0.52
1:D:80:THR:O	1:D:80:THR:CG2	2.55	0.52
1:D:97:ASN:HB2	1:D:100:LEU:HD12	1.92	0.52
1:E:297:LYS:O	1:E:300:MET:HB2	2.08	0.52
1:F:268:THR:HG23	1:F:269:ALA:N	2.24	0.52
1:C:163:GLU:CB	1:E:259:LYS:NZ	2.68	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:42:ALA:HB3	1:G:300:MET:HE1	1.91	0.52
1:B:127:GLY:O	1:B:129:GLY:N	2.43	0.52
1:H:177:PHE:HB3	1:H:201:LEU:HD12	1.89	0.52
1:I:159:PRO:O	1:I:163:GLU:N	2.40	0.52
1:B:159:PRO:O	1:B:163:GLU:N	2.42	0.52
1:D:169:GLU:OE2	1:D:169:GLU:HA	2.08	0.52
1:G:306:ASP:C	1:G:308:ARG:N	2.67	0.52
1:H:278:ILE:HG22	1:H:280:PHE:CD1	2.45	0.52
1:A:41:LEU:CD1	1:B:307:LEU:HD11	2.39	0.52
1:A:59:ALA:HA	1:B:59:ALA:HA	1.91	0.52
1:G:79:GLU:C	1:G:81:ALA:H	2.17	0.52
1:G:91:GLU:HB2	1:G:135:TRP:CE2	2.44	0.52
1:H:302:ALA:C	1:H:304:VAL:H	2.18	0.52
1:I:104:TYR:HB3	1:I:134:TYR:HD2	1.74	0.52
1:A:218:TYR:HD1	1:A:218:TYR:H	1.56	0.52
1:B:186:MET:SD	1:B:191:PHE:HB2	2.50	0.52
1:B:240:LYS:HA	1:B:240:LYS:CE	2.21	0.52
1:C:248:GLY:CA	1:C:250:GLU:OE2	2.58	0.52
1:D:80:THR:O	1:D:82:ASP:N	2.42	0.52
1:G:272:THR:HG22	1:G:273:THR:CG2	2.34	0.52
1:I:247:GLY:O	1:I:248:GLY:O	2.27	0.52
1:J:39:GLU:O	1:J:304:VAL:HG21	2.10	0.52
1:J:107:PHE:O	1:J:130:ARG:NH1	2.40	0.52
1:C:185:ILE:N	1:C:193:GLY:O	2.39	0.52
1:E:83:ARG:HH11	1:E:113:ASP:CG	2.15	0.52
1:G:188:GLU:HG3	1:G:188:GLU:O	2.10	0.52
1:H:170:PRO:HG3	1:H:229:LEU:HD21	1.90	0.52
1:B:95:ARG:NH1	1:D:253:LYS:HB3	2.25	0.52
1:C:105:VAL:HG13	1:C:107:PHE:HE1	1.74	0.52
1:I:150:TYR:H	1:I:150:TYR:HD2	1.48	0.52
1:D:214:PHE:HD1	1:D:295:VAL:HG13	1.71	0.52
1:D:215:ASP:HB2	1:D:299:GLU:OE2	2.09	0.52
1:D:299:GLU:O	1:D:302:ALA:HB3	2.09	0.52
1:H:125:HIS:N	1:H:125:HIS:HD1	2.07	0.52
1:H:139:ASN:N	1:H:139:ASN:OD1	2.43	0.52
1:A:105:VAL:O	1:A:133:PRO:HD2	2.11	0.51
1:B:89:ILE:O	1:B:90:LEU:C	2.51	0.51
1:B:272:THR:O	1:B:272:THR:CG2	2.57	0.51
1:D:115:LYS:HD3	1:D:118:GLU:OE2	2.10	0.51
1:G:128:THR:C	1:G:130:ARG:H	2.18	0.51
1:I:158:LEU:N	1:I:159:PRO:CD	2.72	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:298:GLU:O	1:J:301:LEU:HD23	2.10	0.51
1:B:39:GLU:HA	1:B:40:LYS:HB3	1.92	0.51
1:B:90:LEU:HD13	1:B:104:TYR:HA	1.90	0.51
1:D:41:LEU:O	1:D:43:TYR:HB2	2.11	0.51
1:D:153:SER:HB2	1:D:155:TYR:CD1	2.45	0.51
1:F:148:LEU:HD12	1:F:174:GLU:OE2	2.10	0.51
1:G:83:ARG:HG2	1:G:112:PHE:HE1	1.74	0.51
1:I:258:ILE:HG13	1:I:259:LYS:H	1.71	0.51
1:A:156:TYR:O	1:A:159:PRO:HD2	2.10	0.51
1:A:214:PHE:CE2	1:A:299:GLU:O	2.61	0.51
1:B:265:HIS:O	1:B:266:LEU:HD23	2.10	0.51
1:B:268:THR:HG23	1:B:269:ALA:O	2.11	0.51
1:A:278:ILE:HD11	1:A:297:LYS:HD3	1.93	0.51
1:B:39:GLU:HA	1:B:40:LYS:C	2.35	0.51
1:C:273:THR:HG23	1:C:275:LYS:N	2.22	0.51
1:D:271:PRO:CD	1:D:272:THR:H	2.24	0.51
1:D:272:THR:HG22	1:D:273:THR:HG23	1.93	0.51
1:E:300:MET:O	1:E:304:VAL:N	2.43	0.51
1:G:123:PRO:O	1:G:124:ALA:HB3	2.11	0.51
1:G:245:ASP:O	1:G:246:PHE:C	2.51	0.51
1:I:156:TYR:C	1:I:159:PRO:HD2	2.35	0.51
1:A:250:GLU:CD	1:A:250:GLU:N	2.67	0.51
1:C:174:GLU:OE2	1:C:174:GLU:N	2.42	0.51
1:D:119:TYR:O	1:D:121:ASN:N	2.43	0.51
1:F:265:HIS:HA	1:F:279:LEU:O	2.10	0.51
1:H:72:SER:O	1:H:76:GLU:HG3	2.10	0.51
1:D:41:LEU:CD2	1:D:42:ALA:HA	2.40	0.51
1:G:177:PHE:HZ	1:G:240:LYS:HD2	1.76	0.51
1:G:218:TYR:CD2	1:G:232:PRO:CG	2.88	0.51
1:A:267:GLU:OE1	1:A:297:LYS:NZ	2.44	0.51
1:C:270:ASP:OD2	1:C:274:GLY:CA	2.46	0.51
1:F:298:GLU:CD	1:F:298:GLU:N	2.65	0.51
1:G:136:ASN:OD1	1:G:138:MET:CE	2.59	0.51
1:I:309:GLU:OE1	1:I:309:GLU:O	2.29	0.51
1:C:85:GLU:O	1:C:86:ALA:C	2.54	0.51
1:E:205:ASP:HA	1:E:230:SER:HB2	1.92	0.51
1:F:105:VAL:O	1:F:133:PRO:HD2	2.10	0.51
1:H:91:GLU:HG3	1:H:135:TRP:CZ3	2.45	0.51
1:H:91:GLU:CG	1:H:135:TRP:CH2	2.91	0.51
1:I:117:ALA:O	1:I:120:THR:HG22	2.10	0.51
1:J:222:VAL:HG22	1:J:226:GLY:C	2.35	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:GLU:CB	1:A:40:LYS:HB2	2.38	0.51
1:A:154:ASP:C	1:A:156:TYR:N	2.66	0.51
1:A:203:TYR:CE2	1:A:207:VAL:HG21	2.46	0.51
1:C:169:GLU:HB3	1:C:170:PRO:CD	2.40	0.51
1:C:278:ILE:HD12	1:C:300:MET:HE1	1.91	0.51
1:A:83:ARG:HG2	1:A:112:PHE:HE1	1.76	0.51
1:A:105:VAL:HG13	1:A:107:PHE:CE1	2.46	0.51
1:A:279:LEU:HD22	1:A:292:VAL:HG11	1.93	0.51
1:B:83:ARG:O	1:B:87:LEU:CD1	2.53	0.51
1:C:76:GLU:HG3	1:C:185:ILE:HG23	1.93	0.51
1:C:139:ASN:OD1	1:C:139:ASN:N	2.43	0.51
1:D:41:LEU:O	1:D:43:TYR:CA	2.55	0.51
1:D:91:GLU:OE1	1:D:135:TRP:HZ2	1.93	0.51
1:F:43:TYR:O	1:F:46:SER:N	2.42	0.51
1:F:266:LEU:O	1:F:278:ILE:HG23	2.11	0.51
1:A:298:GLU:C	1:A:300:MET:N	2.69	0.50
1:B:157:GLN:O	1:B:160:LYS:N	2.44	0.50
1:D:139:ASN:C	1:D:141:THR:N	2.61	0.50
1:D:154:ASP:N	1:D:154:ASP:OD1	2.44	0.50
1:J:74:THR:O	1:J:77:SER:N	2.44	0.50
1:J:246:PHE:HB3	1:J:251:LEU:HD12	1.93	0.50
1:J:249:GLU:N	1:J:249:GLU:CD	2.68	0.50
1:J:272:THR:O	1:J:273:THR:HG22	2.10	0.50
1:D:136:ASN:H	1:D:136:ASN:HD22	1.59	0.50
1:E:80:THR:O	1:E:81:ALA:C	2.53	0.50
1:E:269:ALA:O	1:E:271:PRO:HD3	2.11	0.50
1:E:106:ALA:HB3	1:E:194:ILE:HG12	1.93	0.50
1:F:43:TYR:C	1:F:45:GLN:N	2.70	0.50
1:J:218:TYR:N	1:J:218:TYR:HD1	2.07	0.50
1:A:106:ALA:HB2	1:A:147:LEU:HD12	1.93	0.50
1:A:218:TYR:CD2	1:A:232:PRO:CG	2.95	0.50
1:B:126:ASP:O	1:B:127:GLY:C	2.54	0.50
1:B:230:SER:O	1:B:231:HIS:HB2	2.11	0.50
1:B:287:GLY:O	1:B:288:ASP:C	2.54	0.50
1:C:186:MET:HE1	1:C:191:PHE:HD1	1.76	0.50
1:D:272:THR:CG2	1:D:273:THR:HG23	2.41	0.50
1:I:110:ASP:N	1:I:116:ASP:OD2	2.37	0.50
1:J:82:ASP:OD1	1:J:84:ASP:N	2.44	0.50
1:J:279:LEU:HD23	1:J:294:VAL:HG22	1.93	0.50
1:A:109:PRO:HA	1:A:130:ARG:HD3	1.92	0.50
1:G:188:GLU:O	1:G:188:GLU:CG	2.59	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:241:LYS:HA	1:H:245:ASP:OD2	2.10	0.50
1:I:131:PHE:C	1:I:132:VAL:HG13	2.36	0.50
1:G:41:LEU:CD1	1:G:41:LEU:C	2.85	0.50
1:G:122:SER:CB	1:G:123:PRO:CD	2.90	0.50
1:G:165:ASP:O	1:G:166:VAL:HG22	2.11	0.50
1:I:104:TYR:HE2	1:I:198:ASP:OD2	1.95	0.50
1:B:82:ASP:OD1	1:B:83:ARG:N	2.44	0.50
1:D:204:VAL:O	1:D:208:VAL:HG23	2.12	0.50
1:D:107:PHE:O	1:D:130:ARG:CD	2.57	0.50
1:D:172:PHE:CZ	1:D:175:GLY:HA2	2.47	0.50
1:J:109:PRO:HA	1:J:130:ARG:HD3	1.94	0.50
1:A:82:ASP:OD1	1:A:82:ASP:C	2.55	0.50
1:C:43:TYR:CE1	1:C:300:MET:HE1	2.47	0.50
1:C:123:PRO:O	1:C:124:ALA:HB3	2.12	0.50
1:C:163:GLU:HG2	1:C:186:MET:HE1	1.93	0.50
1:G:43:TYR:CE1	1:G:300:MET:HE3	2.47	0.50
1:H:131:PHE:CE1	1:H:133:PRO:HG3	2.47	0.50
1:H:213:THR:O	1:H:214:PHE:HB2	2.10	0.50
1:I:282:GLU:OE2	1:I:283:PRO:HD2	2.11	0.50
1:J:309:GLU:N	1:J:309:GLU:CD	2.69	0.50
1:D:124:ALA:HB2	1:D:144:VAL:CG1	2.42	0.49
1:G:122:SER:CB	1:G:123:PRO:HD2	2.34	0.49
1:I:244:TYR:C	1:I:246:PHE:H	2.19	0.49
1:I:307:LEU:C	1:I:308:ARG:HG3	2.30	0.49
1:A:150:TYR:CD1	1:A:150:TYR:C	2.90	0.49
1:C:170:PRO:HG3	1:C:229:LEU:HD21	1.94	0.49
1:D:160:LYS:O	1:D:161:ALA:C	2.54	0.49
1:F:45:GLN:O	1:F:45:GLN:HG2	2.12	0.49
1:F:278:ILE:HD11	1:F:300:MET:HG3	1.93	0.49
1:G:245:ASP:C	1:G:247:GLY:H	2.20	0.49
1:J:108:GLU:HA	1:J:130:ARG:NH1	2.27	0.49
1:B:48:GLU:O	1:B:51:SER:CB	2.51	0.49
1:B:108:GLU:HB2	1:B:111:ALA:HB2	1.94	0.49
1:C:86:ALA:CB	1:C:131:PHE:CZ	2.95	0.49
1:G:136:ASN:OD1	1:G:138:MET:CB	2.37	0.49
1:G:262:ILE:CD1	1:I:98:PRO:HG3	2.41	0.49
1:I:123:PRO:O	1:I:124:ALA:HB3	2.12	0.49
1:B:65:LEU:HD12	1:B:65:LEU:O	2.13	0.49
1:C:65:LEU:O	1:C:69:ARG:HG3	2.12	0.49
1:C:256:ARG:NH2	1:F:92:ASN:CG	2.71	0.49
1:C:260:ASN:HB3	1:C:262:ILE:HD12	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:41:LEU:HD22	1:D:42:ALA:H	0.38	0.49
1:G:246:PHE:HB3	1:G:251:LEU:HD12	1.94	0.49
1:H:98:PRO:HG3	1:J:262:ILE:CD1	2.43	0.49
1:H:186:MET:CE	1:H:191:PHE:HD1	2.25	0.49
1:I:104:TYR:HD2	1:I:134:TYR:CD2	2.30	0.49
1:J:270:ASP:OD1	1:J:271:PRO:N	2.45	0.49
1:C:78:TYR:OH	1:C:85:GLU:HB3	2.13	0.49
1:C:295:VAL:O	1:C:295:VAL:HG12	2.12	0.49
1:H:139:ASN:C	1:H:141:THR:N	2.71	0.49
1:H:277:VAL:HG12	1:H:296:PRO:N	2.27	0.49
1:B:40:LYS:C	1:B:42:ALA:N	2.71	0.49
1:B:50:ALA:HA	1:B:293:LEU:HD12	1.94	0.49
1:C:222:VAL:CG1	1:C:290:ALA:HB3	2.43	0.49
1:D:185:ILE:HG13	1:D:193:GLY:C	2.38	0.49
1:G:165:ASP:O	1:G:166:VAL:CG2	2.60	0.49
1:G:172:PHE:CE2	1:G:175:GLY:HA2	2.47	0.49
1:G:215:ASP:HB2	1:G:299:GLU:CD	2.38	0.49
1:H:267:GLU:OE1	1:H:297:LYS:HD3	2.13	0.49
1:B:39:GLU:OE2	1:B:39:GLU:CA	2.60	0.49
1:C:208:VAL:HG11	1:C:220:PHE:HA	1.93	0.49
1:C:275:LYS:CB	1:C:275:LYS:NZ	2.76	0.49
1:H:254:ALA:O	1:H:258:ILE:HG23	2.13	0.49
1:I:112:PHE:CD1	1:I:131:PHE:CD2	3.00	0.49
1:B:49:MET:HG2	1:B:293:LEU:HD11	1.95	0.49
1:B:156:TYR:C	1:B:159:PRO:HD2	2.38	0.49
1:C:80:THR:O	1:C:80:THR:HG22	2.10	0.49
1:D:104:TYR:CE2	1:D:196:GLY:C	2.91	0.49
1:D:154:ASP:O	1:D:156:TYR:N	2.45	0.49
1:E:130:ARG:NH2	1:E:150:TYR:CE1	2.80	0.49
1:G:39:GLU:CA	1:G:40:LYS:CB	2.75	0.49
1:I:267:GLU:O	1:I:268:THR:HG22	2.11	0.49
1:B:297:LYS:O	1:B:301:LEU:HG	2.13	0.49
1:C:86:ALA:CB	1:C:131:PHE:HZ	2.25	0.49
1:D:185:ILE:HG13	1:D:193:GLY:O	2.13	0.49
1:E:75:MET:HB2	1:E:185:ILE:HD13	1.95	0.49
1:G:77:SER:CB	1:H:88:LEU:HD13	2.43	0.49
1:G:273:THR:OG1	1:G:275:LYS:HD2	2.13	0.49
1:H:275:LYS:HZ2	1:H:275:LYS:CB	2.24	0.49
1:I:120:THR:HA	1:I:129:GLY:HA3	1.94	0.49
1:I:167:LEU:C	1:I:167:LEU:HD12	2.38	0.49
1:J:125:HIS:O	1:J:146:PRO:HG3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:LYS:HD3	1:A:118:GLU:OE2	2.11	0.49
1:D:177:PHE:CE2	1:D:239:GLY:O	2.66	0.49
1:E:55:ASN:ND2	1:F:52:ASN:OD1	2.42	0.49
1:F:193:GLY:C	1:F:194:ILE:CG2	2.85	0.49
1:G:177:PHE:HB3	1:G:201:LEU:HD22	1.94	0.49
1:G:302:ALA:O	1:G:305:ALA:HB3	2.13	0.49
1:J:309:GLU:OE2	1:J:309:GLU:CA	2.59	0.49
1:A:173:TYR:CD2	1:A:178:MET:HE1	2.48	0.48
1:A:200:SER:O	1:A:204:VAL:HG23	2.12	0.48
1:B:148:LEU:O	1:B:149:HIS:CG	2.66	0.48
1:D:298:GLU:HG3	1:D:299:GLU:CB	2.42	0.48
1:H:169:GLU:HB3	1:H:170:PRO:HD2	1.93	0.48
1:I:185:ILE:HG13	1:I:194:ILE:CA	2.43	0.48
1:I:234:HIS:HB3	1:I:237:TRP:CD1	2.47	0.48
1:A:109:PRO:O	1:A:110:ASP:HB2	2.12	0.48
1:A:269:ALA:O	1:A:270:ASP:C	2.55	0.48
1:D:137:LYS:HA	1:D:141:THR:O	2.13	0.48
1:E:48:GLU:CG	1:F:48:GLU:CG	2.91	0.48
1:H:122:SER:CB	1:H:123:PRO:HD2	2.40	0.48
1:I:43:TYR:CE1	1:I:300:MET:HE3	2.48	0.48
1:I:150:TYR:CD2	1:I:150:TYR:N	2.68	0.48
1:J:300:MET:HB2	1:J:301:LEU:HD13	1.95	0.48
1:A:171:TYR:N	1:A:171:TYR:HD1	2.08	0.48
1:B:244:TYR:C	1:B:246:PHE:H	2.22	0.48
1:C:53:TYR:O	1:C:54:ALA:C	2.57	0.48
1:C:57:PHE:O	1:C:61:MET:HG2	2.13	0.48
1:C:130:ARG:NH2	1:C:150:TYR:HE1	2.12	0.48
1:C:187:LYS:HG3	1:C:192:ALA:CB	2.43	0.48
1:F:193:GLY:C	1:F:194:ILE:HG23	2.39	0.48
1:E:302:ALA:N	1:E:303:GLY:CA	2.69	0.48
1:H:130:ARG:NH2	1:H:150:TYR:CE1	2.81	0.48
1:I:57:PHE:CE2	1:I:207:VAL:HG12	2.48	0.48
1:J:242:ASP:OD2	1:J:242:ASP:C	2.56	0.48
1:J:260:ASN:HB3	1:J:262:ILE:CD1	2.43	0.48
1:B:148:LEU:C	1:B:149:HIS:CG	2.91	0.48
1:D:214:PHE:CD1	1:D:295:VAL:CG1	2.94	0.48
1:E:213:THR:HG22	1:E:217:GLY:HA3	1.94	0.48
1:I:108:GLU:OE2	1:I:160:LYS:HE3	2.14	0.48
1:I:185:ILE:HG13	1:I:194:ILE:N	2.29	0.48
1:I:254:ALA:O	1:I:258:ILE:HG23	2.14	0.48
1:B:79:GLU:O	1:B:80:THR:C	2.57	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:115:LYS:HB3	1:C:118:GLU:HG3	1.96	0.48
1:D:182:VAL:HG12	1:D:183:SER:N	2.27	0.48
1:J:151:ASP:O	1:J:152:SER:HB3	2.13	0.48
1:C:258:ILE:HG13	1:C:259:LYS:N	2.22	0.48
1:F:148:LEU:HD12	1:F:174:GLU:CD	2.39	0.48
1:H:98:PRO:HG3	1:J:262:ILE:HD11	1.94	0.48
1:H:273:THR:HG1	1:H:275:LYS:HG2	1.73	0.48
1:I:39:GLU:HA	1:I:40:LYS:HB2	1.93	0.48
1:B:250:GLU:C	1:B:252:GLU:H	2.22	0.48
1:C:70:THR:HB	1:D:70:THR:HG21	1.95	0.48
1:C:273:THR:C	1:C:275:LYS:H	2.21	0.48
1:F:122:SER:CB	1:F:123:PRO:CD	2.88	0.48
1:F:158:LEU:HA	1:F:158:LEU:HD23	1.56	0.48
1:J:105:VAL:HG11	1:J:107:PHE:CE1	2.44	0.48
1:A:83:ARG:HG2	1:A:112:PHE:CE1	2.49	0.48
1:D:79:GLU:C	1:D:81:ALA:H	2.21	0.48
1:D:188:GLU:CG	1:D:188:GLU:O	2.61	0.48
1:D:307:LEU:O	1:D:308:ARG:C	2.56	0.48
1:E:49:MET:HE2	1:E:293:LEU:HD11	1.96	0.48
1:E:119:TYR:O	1:E:120:THR:C	2.57	0.48
1:F:132:VAL:O	1:F:132:VAL:HG23	2.14	0.48
1:F:182:VAL:CG1	1:F:194:ILE:HD12	2.43	0.48
1:H:91:GLU:HG3	1:H:135:TRP:CE3	2.49	0.48
1:J:61:MET:SD	1:J:284:VAL:HG11	2.54	0.48
1:J:298:GLU:C	1:J:301:LEU:HD23	2.38	0.48
1:B:139:ASN:C	1:B:141:THR:H	2.21	0.48
1:B:237:TRP:CE2	1:B:241:LYS:NZ	2.82	0.48
1:D:68:ALA:O	1:D:69:ARG:C	2.57	0.48
1:D:145:ALA:HB1	1:D:146:PRO:HD2	1.94	0.48
1:H:208:VAL:HG21	1:H:221:MET:HG3	1.95	0.48
1:A:41:LEU:HD11	1:B:307:LEU:HD11	1.94	0.47
1:A:132:VAL:N	1:A:133:PRO:HD3	2.28	0.47
1:B:104:TYR:HD2	1:B:134:TYR:CE2	2.32	0.47
1:E:295:VAL:CG1	1:E:300:MET:HG2	2.44	0.47
1:G:272:THR:CG2	1:G:273:THR:HG22	2.37	0.47
1:J:251:LEU:HD23	1:J:266:LEU:HD13	1.85	0.47
1:B:279:LEU:CD2	1:B:294:VAL:HG22	2.45	0.47
1:C:218:TYR:CD2	1:C:232:PRO:CG	2.94	0.47
1:E:265:HIS:HA	1:E:279:LEU:O	2.14	0.47
1:H:125:HIS:O	1:H:146:PRO:HG3	2.13	0.47
1:C:112:PHE:CG	1:C:131:PHE:HD2	2.33	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:169:GLU:HB3	1:C:170:PRO:HD2	1.97	0.47
1:C:256:ARG:CD	3:C:321:HOH:O	2.61	0.47
1:I:150:TYR:HB2	1:I:156:TYR:CD1	2.49	0.47
1:I:154:ASP:OD2	1:I:158:LEU:HD11	2.14	0.47
1:J:98:PRO:HA	1:J:137:LYS:HZ3	1.79	0.47
1:A:135:TRP:HZ3	1:A:142:ALA:O	1.97	0.47
1:B:101:LEU:HD22	1:B:101:LEU:C	2.40	0.47
1:E:245:ASP:C	1:E:247:GLY:H	2.23	0.47
1:H:182:VAL:HG11	1:H:194:ILE:HD12	1.97	0.47
1:J:113:ASP:O	1:J:115:LYS:N	2.47	0.47
1:J:200:SER:O	1:J:204:VAL:HG23	2.14	0.47
1:C:75:MET:HE3	1:C:105:VAL:HG21	1.94	0.47
1:C:273:THR:CG2	1:C:275:LYS:HG2	2.43	0.47
1:D:214:PHE:CE1	1:D:295:VAL:HG11	2.49	0.47
1:G:172:PHE:CZ	1:G:175:GLY:HA2	2.50	0.47
1:B:72:SER:O	1:B:73:THR:C	2.57	0.47
1:B:279:LEU:HD22	1:B:294:VAL:HG22	1.97	0.47
1:C:105:VAL:CG1	1:C:107:PHE:HE1	2.27	0.47
1:E:245:ASP:C	1:E:247:GLY:N	2.73	0.47
1:H:68:ALA:O	1:H:69:ARG:C	2.56	0.47
1:J:49:MET:CE	1:J:53:TYR:HE1	2.24	0.47
1:J:234:HIS:O	1:J:235:LYS:C	2.57	0.47
1:A:39:GLU:CA	1:A:40:LYS:HG3	2.42	0.47
1:A:61:MET:SD	1:A:284:VAL:HG11	2.55	0.47
1:B:91:GLU:HB2	1:B:135:TRP:CE2	2.50	0.47
1:B:131:PHE:CE1	1:B:133:PRO:HG3	2.49	0.47
1:D:71:ILE:O	1:D:74:THR:HB	2.15	0.47
1:D:172:PHE:CE2	1:D:175:GLY:HA2	2.50	0.47
1:E:93:LEU:CD2	1:F:70:THR:HG23	2.45	0.47
1:E:93:LEU:HD21	1:F:70:THR:HG23	1.96	0.47
1:E:295:VAL:HG11	1:E:300:MET:HG2	1.96	0.47
1:F:240:LYS:HE3	1:F:240:LYS:HB3	1.61	0.47
1:G:43:TYR:HD1	1:G:300:MET:HE1	1.78	0.47
1:G:182:VAL:CG1	1:G:183:SER:N	2.76	0.47
1:H:212:ARG:NH2	1:I:235:LYS:HZ2	2.10	0.47
1:H:250:GLU:CB	1:H:266:LEU:HD13	2.42	0.47
1:J:234:HIS:O	1:J:236:ASP:N	2.48	0.47
1:A:251:LEU:HD23	1:A:266:LEU:CD1	2.45	0.47
1:F:85:GLU:O	1:F:89:ILE:HG13	2.15	0.47
1:G:154:ASP:N	1:G:154:ASP:OD1	2.47	0.47
1:G:249:GLU:O	1:G:249:GLU:CG	2.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:104:TYR:CD2	1:I:134:TYR:HE2	2.29	0.47
1:B:50:ALA:CA	1:B:293:LEU:HD12	2.45	0.47
1:B:130:ARG:NH2	1:B:150:TYR:CD1	2.83	0.47
1:B:160:LYS:HA	1:B:191:PHE:CE1	2.50	0.47
1:F:173:TYR:O	1:F:174:GLU:C	2.57	0.47
1:G:273:THR:HG21	1:G:275:LYS:HE2	1.94	0.47
1:I:88:LEU:HD13	1:J:77:SER:HB3	1.97	0.47
1:B:49:MET:HE2	1:B:49:MET:HB2	1.82	0.47
1:D:136:ASN:HD22	1:D:136:ASN:N	2.12	0.47
1:D:178:MET:CE	1:D:198:ASP:OD1	2.58	0.47
1:E:165:ASP:C	1:E:166:VAL:CG2	2.88	0.47
1:H:93:LEU:O	1:H:94:LEU:C	2.57	0.47
1:I:107:PHE:HB3	1:I:111:ALA:HB3	1.97	0.47
1:J:278:ILE:HD11	1:J:297:LYS:HD3	1.97	0.47
1:A:99:HIS:ND1	1:A:203:TYR:CE1	2.83	0.46
1:B:122:SER:CB	1:B:123:PRO:HD2	2.45	0.46
1:C:221:MET:HE3	1:C:221:MET:HB3	1.55	0.46
1:C:301:LEU:HA	1:C:304:VAL:HG23	1.96	0.46
1:D:188:GLU:O	1:D:188:GLU:HG3	2.14	0.46
1:E:107:PHE:O	1:E:130:ARG:HD2	2.15	0.46
1:H:101:LEU:O	1:H:101:LEU:HD22	2.15	0.46
1:H:103:THR:C	1:H:104:TYR:CD2	2.93	0.46
1:H:126:ASP:O	1:H:129:GLY:N	2.47	0.46
1:I:115:LYS:O	1:I:116:ASP:C	2.57	0.46
1:J:169:GLU:CB	1:J:170:PRO:HD2	2.43	0.46
1:B:39:GLU:CA	1:B:40:LYS:CB	2.92	0.46
1:B:131:PHE:C	1:B:132:VAL:HG13	2.40	0.46
1:C:119:TYR:O	1:C:120:THR:C	2.58	0.46
1:F:193:GLY:O	1:F:194:ILE:HG22	2.15	0.46
1:G:45:GLN:H	1:G:46:SER:CB	2.26	0.46
1:H:215:ASP:HB2	1:H:299:GLU:OE1	2.15	0.46
1:A:262:ILE:CG1	1:C:98:PRO:HG3	2.44	0.46
1:E:156:TYR:C	1:E:156:TYR:CD2	2.93	0.46
1:F:273:THR:CG2	1:F:274:GLY:N	2.33	0.46
1:H:53:TYR:O	1:H:54:ALA:C	2.58	0.46
1:I:222:VAL:HG13	1:I:226:GLY:CA	2.25	0.46
1:A:300:MET:O	1:A:304:VAL:HG23	2.16	0.46
1:B:106:ALA:HB3	1:B:194:ILE:HG12	1.96	0.46
1:C:97:ASN:HB2	1:C:100:LEU:HD12	1.97	0.46
1:C:278:ILE:HG22	1:C:280:PHE:CD1	2.49	0.46
1:D:108:GLU:O	1:D:111:ALA:CB	2.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:85:GLU:O	1:E:89:ILE:HG13	2.15	0.46
1:H:231:HIS:HD2	1:H:237:TRP:HE3	1.62	0.46
1:H:277:VAL:HG13	1:H:296:PRO:HA	1.96	0.46
1:A:73:THR:HG21	1:B:93:LEU:HD23	1.97	0.46
1:A:187:LYS:NZ	3:A:7:HOH:O	2.48	0.46
1:A:272:THR:C	1:A:273:THR:HG22	2.40	0.46
1:B:138:MET:CE	1:B:174:GLU:HG2	2.45	0.46
1:C:213:THR:O	1:C:217:GLY:HA3	2.15	0.46
1:D:136:ASN:OD1	1:D:138:MET:CB	2.58	0.46
1:D:272:THR:HG23	1:D:273:THR:HG22	1.97	0.46
1:F:247:GLY:HA3	1:F:251:LEU:HD12	1.98	0.46
1:G:80:THR:O	1:G:80:THR:CG2	2.59	0.46
1:J:83:ARG:HG3	1:J:112:PHE:CE1	2.46	0.46
1:J:98:PRO:HA	1:J:137:LYS:NZ	2.31	0.46
1:A:201:LEU:O	1:A:204:VAL:N	2.49	0.46
1:B:249:GLU:C	1:B:251:LEU:H	2.18	0.46
1:C:80:THR:O	1:C:80:THR:CG2	2.60	0.46
1:A:79:GLU:OE2	1:A:79:GLU:CA	2.60	0.46
1:A:222:VAL:HG12	1:A:290:ALA:O	2.15	0.46
1:C:57:PHE:O	1:C:61:MET:HG3	2.15	0.46
1:C:85:GLU:O	1:C:89:ILE:HG13	2.15	0.46
1:G:154:ASP:O	1:G:155:TYR:C	2.58	0.46
1:H:39:GLU:N	1:H:40:LYS:CG	2.79	0.46
1:H:80:THR:O	1:H:81:ALA:C	2.57	0.46
1:A:242:ASP:O	1:A:244:TYR:N	2.49	0.46
1:A:298:GLU:O	1:A:299:GLU:C	2.59	0.46
1:B:213:THR:HG23	1:B:217:GLY:HA3	1.98	0.46
1:D:109:PRO:N	1:D:130:ARG:HD3	2.31	0.46
1:D:231:HIS:O	1:D:235:LYS:HD3	2.15	0.46
1:E:78:TYR:OH	1:E:85:GLU:HB3	2.16	0.46
1:F:270:ASP:C	1:F:272:THR:N	2.70	0.46
1:A:41:LEU:HD11	1:B:307:LEU:HD12	1.95	0.46
1:E:131:PHE:CE1	1:E:133:PRO:HG3	2.51	0.46
1:G:77:SER:HB3	1:H:88:LEU:HD13	1.96	0.46
1:H:135:TRP:CD2	1:H:144:VAL:HB	2.51	0.46
1:I:171:TYR:N	1:I:171:TYR:CD1	2.84	0.46
1:I:237:TRP:O	1:I:238:ILE:C	2.57	0.46
1:B:57:PHE:HE2	1:B:207:VAL:HG11	1.80	0.46
1:B:109:PRO:HA	1:B:116:ASP:OD2	2.16	0.46
1:C:83:ARG:NH2	1:C:113:ASP:OD2	2.34	0.46
1:C:91:GLU:HG3	1:C:135:TRP:CZ3	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:120:THR:O	1:C:120:THR:HG23	2.16	0.46
1:C:130:ARG:C	1:C:132:VAL:HG13	2.41	0.46
1:C:208:VAL:HG21	1:C:221:MET:HG3	1.98	0.46
1:I:136:ASN:OD1	1:I:138:MET:HE2	2.16	0.46
1:I:147:LEU:O	1:I:150:TYR:CD2	2.69	0.46
1:J:79:GLU:O	1:J:80:THR:C	2.58	0.46
1:J:80:THR:O	1:J:81:ALA:HB3	2.16	0.46
1:A:99:HIS:ND1	1:A:203:TYR:HE1	2.14	0.45
1:C:139:ASN:C	1:C:141:THR:N	2.65	0.45
1:G:265:HIS:ND1	1:G:265:HIS:O	2.48	0.45
1:G:273:THR:OG1	1:G:275:LYS:HE2	2.15	0.45
1:H:182:VAL:HG12	1:H:194:ILE:HB	1.98	0.45
1:H:184:PRO:HB2	1:H:186:MET:HE2	1.98	0.45
1:I:57:PHE:HE2	1:I:207:VAL:HG11	1.80	0.45
1:A:88:LEU:HD22	1:A:92:ASN:OD1	2.16	0.45
1:D:43:TYR:CD1	1:D:300:MET:HE2	2.51	0.45
1:E:132:VAL:HG23	1:E:147:LEU:HB2	1.98	0.45
1:G:128:THR:C	1:G:130:ARG:N	2.72	0.45
1:H:98:PRO:HG3	1:J:262:ILE:HG12	1.97	0.45
1:H:296:PRO:O	1:H:297:LYS:C	2.57	0.45
1:J:215:ASP:H	1:J:299:GLU:HG2	1.81	0.45
1:C:134:TYR:O	1:C:136:ASN:ND2	2.46	0.45
1:G:75:MET:HE2	1:G:75:MET:HA	1.97	0.45
1:G:135:TRP:CE3	1:G:144:VAL:HG23	2.50	0.45
1:G:177:PHE:CZ	1:G:240:LYS:HD2	2.51	0.45
1:I:250:GLU:OE1	1:I:250:GLU:HA	2.15	0.45
1:J:214:PHE:HE2	1:J:299:GLU:O	1.98	0.45
1:A:258:ILE:HG22	1:A:281:TYR:CD1	2.51	0.45
1:B:91:GLU:HB2	1:B:135:TRP:NE1	2.32	0.45
1:B:117:ALA:O	1:B:120:THR:CG2	2.64	0.45
1:B:213:THR:HG22	1:B:217:GLY:C	2.41	0.45
1:B:308:ARG:O	1:B:309:GLU:HB2	2.17	0.45
1:E:83:ARG:CD	1:E:119:TYR:CE1	2.99	0.45
1:F:119:TYR:O	1:F:120:THR:C	2.60	0.45
1:H:120:THR:O	1:H:121:ASN:CB	2.62	0.45
1:H:246:PHE:O	1:H:251:LEU:CD1	2.60	0.45
1:I:185:ILE:HD11	1:I:194:ILE:C	2.42	0.45
1:C:91:GLU:CD	1:C:135:TRP:CZ2	2.94	0.45
1:G:154:ASP:O	1:G:156:TYR:N	2.49	0.45
1:H:117:ALA:O	1:H:120:THR:CG2	2.56	0.45
1:I:82:ASP:OD1	1:I:82:ASP:C	2.58	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:136:ASN:OD1	1:I:138:MET:CB	2.57	0.45
1:I:302:ALA:O	1:I:305:ALA:HB3	2.16	0.45
1:J:156:TYR:CD1	1:J:194:ILE:HD13	2.52	0.45
1:A:251:LEU:HD23	1:A:251:LEU:HA	1.72	0.45
1:B:130:ARG:NH2	1:B:150:TYR:HD1	2.15	0.45
1:C:182:VAL:HG12	1:C:194:ILE:HB	1.99	0.45
1:C:213:THR:CG2	1:C:295:VAL:CG2	2.95	0.45
1:D:128:THR:O	1:D:129:GLY:C	2.59	0.45
1:G:101:LEU:HD23	1:G:101:LEU:C	2.42	0.45
1:G:108:GLU:O	1:G:109:PRO:C	2.58	0.45
1:J:104:TYR:CE1	1:J:196:GLY:HA3	2.50	0.45
1:J:246:PHE:CD1	1:J:251:LEU:HD11	2.51	0.45
1:B:112:PHE:CE1	1:B:131:PHE:CD2	3.04	0.45
1:B:182:VAL:HG11	1:B:194:ILE:HD12	1.97	0.45
1:C:126:ASP:O	1:C:128:THR:N	2.50	0.45
1:D:272:THR:HG23	1:D:273:THR:CG2	2.47	0.45
1:E:218:TYR:CD2	1:E:232:PRO:HG2	2.52	0.45
1:I:126:ASP:O	1:I:127:GLY:C	2.59	0.45
1:J:113:ASP:C	1:J:115:LYS:H	2.24	0.45
1:A:240:LYS:HA	1:A:240:LYS:HE2	1.98	0.45
1:B:172:PHE:CG	1:B:172:PHE:O	2.69	0.45
1:C:110:ASP:OD1	1:C:114:GLY:O	2.34	0.45
1:E:298:GLU:HG2	1:E:299:GLU:N	2.31	0.45
1:A:126:ASP:OD2	1:A:126:ASP:N	2.50	0.45
1:A:169:GLU:CB	1:A:170:PRO:HD2	2.46	0.45
1:B:105:VAL:O	1:B:133:PRO:HD2	2.17	0.45
1:D:83:ARG:HD3	1:D:131:PHE:CD1	2.52	0.45
1:D:95:ARG:CZ	1:E:253:LYS:CD	2.93	0.45
1:E:88:LEU:HD23	1:E:88:LEU:HA	1.57	0.45
1:E:115:LYS:O	1:E:116:ASP:C	2.60	0.45
1:F:139:ASN:C	1:F:141:THR:N	2.65	0.45
1:G:49:MET:HE1	1:G:213:THR:OG1	2.17	0.45
1:G:275:LYS:HD2	1:G:275:LYS:N	2.31	0.45
1:G:279:LEU:HD21	1:G:294:VAL:HG22	1.99	0.45
1:I:264:GLY:HA3	1:I:281:TYR:CZ	2.52	0.45
1:J:213:THR:HG21	1:J:293:LEU:CD2	2.44	0.45
1:A:282:GLU:OE2	1:A:283:PRO:HD2	2.16	0.45
1:B:249:GLU:O	1:B:250:GLU:C	2.56	0.45
1:E:130:ARG:HH21	1:E:150:TYR:HE1	1.65	0.45
1:F:84:ASP:HA	1:F:87:LEU:HD12	1.99	0.45
1:F:270:ASP:O	1:F:272:THR:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:273:THR:OG1	1:G:275:LYS:CE	2.65	0.45
1:A:94:LEU:HD21	1:A:100:LEU:O	2.17	0.44
1:B:159:PRO:O	1:B:163:GLU:HA	2.17	0.44
1:B:254:ALA:O	1:B:258:ILE:HG23	2.17	0.44
1:D:308:ARG:HA	1:D:308:ARG:HE	1.81	0.44
1:E:275:LYS:HG3	1:E:275:LYS:H	1.55	0.44
1:G:221:MET:HE3	1:G:221:MET:HB3	1.81	0.44
1:I:86:ALA:CB	1:I:131:PHE:HE2	2.30	0.44
1:J:282:GLU:OE2	1:J:282:GLU:HA	2.17	0.44
1:A:208:VAL:HG11	1:A:220:PHE:HA	1.99	0.44
1:B:83:ARG:C	1:B:87:LEU:HD12	2.42	0.44
1:B:169:GLU:HB3	1:B:170:PRO:HD2	2.00	0.44
1:C:201:LEU:HD21	1:C:229:LEU:HD22	1.99	0.44
1:C:205:ASP:HB2	1:C:238:ILE:HD13	2.00	0.44
1:F:88:LEU:HA	1:F:88:LEU:HD23	1.67	0.44
1:H:153:SER:O	1:H:154:ASP:C	2.61	0.44
1:J:212:ARG:HA	1:J:212:ARG:HD3	1.71	0.44
1:A:173:TYR:HD2	1:A:178:MET:HE1	1.82	0.44
1:C:154:ASP:O	1:C:156:TYR:N	2.50	0.44
1:C:203:TYR:O	1:C:204:VAL:C	2.60	0.44
1:C:273:THR:O	1:C:275:LYS:N	2.47	0.44
1:F:307:LEU:O	1:F:308:ARG:C	2.61	0.44
1:G:270:ASP:OD1	1:G:272:THR:HB	2.17	0.44
1:H:150:TYR:HB3	1:H:155:TYR:OH	2.17	0.44
1:H:167:LEU:CD1	1:H:179:VAL:HG13	2.45	0.44
1:I:104:TYR:CE2	1:I:198:ASP:OD2	2.70	0.44
1:J:203:TYR:C	1:J:203:TYR:CD2	2.96	0.44
1:A:139:ASN:C	1:A:141:THR:N	2.76	0.44
1:A:177:PHE:HB3	1:A:201:LEU:HD12	1.99	0.44
1:D:120:THR:O	1:D:120:THR:CG2	2.65	0.44
1:E:135:TRP:CE2	1:E:144:VAL:HB	2.53	0.44
1:G:39:GLU:HA	1:G:40:LYS:CB	2.34	0.44
1:G:108:GLU:HB2	1:G:111:ALA:HB2	2.00	0.44
1:H:125:HIS:N	1:H:125:HIS:ND1	2.63	0.44
1:H:131:PHE:C	1:H:132:VAL:HG13	2.41	0.44
1:H:132:VAL:N	1:H:133:PRO:HD3	2.32	0.44
1:H:139:ASN:C	1:H:141:THR:H	2.15	0.44
1:H:276:THR:OG1	1:H:297:LYS:HB3	2.18	0.44
1:B:105:VAL:HG12	1:B:133:PRO:CD	2.45	0.44
1:C:94:LEU:HD11	1:C:136:ASN:HA	1.99	0.44
1:C:240:LYS:HA	1:C:240:LYS:CE	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:213:THR:HG21	1:D:293:LEU:HD22	2.00	0.44
1:E:61:MET:SD	1:E:284:VAL:HG11	2.58	0.44
1:J:91:GLU:OE1	1:J:135:TRP:CZ2	2.71	0.44
1:J:203:TYR:O	1:J:206:GLU:HB3	2.18	0.44
1:J:234:HIS:C	1:J:236:ASP:N	2.75	0.44
1:J:252:GLU:O	1:J:253:LYS:C	2.60	0.44
1:A:262:ILE:HD11	1:C:98:PRO:HG3	2.00	0.44
1:B:178:MET:HE2	1:B:178:MET:HB3	1.83	0.44
1:G:43:TYR:O	1:G:46:SER:HB3	2.18	0.44
1:G:158:LEU:HD23	1:G:158:LEU:HA	1.80	0.44
1:G:275:LYS:HD2	1:G:275:LYS:H	1.83	0.44
1:H:97:ASN:CB	1:H:100:LEU:HD12	2.47	0.44
1:H:108:GLU:O	1:H:111:ALA:CB	2.65	0.44
1:H:108:GLU:O	1:H:111:ALA:HB3	2.17	0.44
1:J:213:THR:CG2	1:J:293:LEU:HD21	2.46	0.44
1:A:216:THR:OG1	1:A:299:GLU:OE2	2.28	0.44
1:B:53:TYR:HB3	1:B:291:PHE:CE1	2.52	0.44
1:B:188:GLU:C	1:B:190:GLU:N	2.76	0.44
1:B:213:THR:O	1:B:214:PHE:C	2.61	0.44
1:C:78:TYR:CE1	1:C:80:THR:HB	2.53	0.44
1:C:86:ALA:HB3	1:C:131:PHE:HZ	1.82	0.44
1:C:154:ASP:O	1:C:155:TYR:C	2.60	0.44
1:C:215:ASP:HB2	1:C:299:GLU:OE1	2.18	0.44
1:F:305:ALA:O	1:F:308:ARG:CB	2.66	0.44
1:H:293:LEU:HD23	1:H:293:LEU:HA	1.83	0.44
1:I:272:THR:O	1:I:272:THR:HG22	2.18	0.44
1:J:203:TYR:CE2	1:J:207:VAL:HG21	2.52	0.44
1:B:101:LEU:O	1:B:101:LEU:CD2	2.60	0.44
1:B:211:VAL:CG1	1:B:212:ARG:N	2.80	0.44
1:D:266:LEU:O	1:D:278:ILE:HA	2.18	0.44
1:F:39:GLU:HA	1:F:40:LYS:HB2	0.64	0.44
1:G:44:GLN:NE2	1:H:45:GLN:OE1	2.50	0.44
1:J:39:GLU:HG2	1:J:40:LYS:H	1.82	0.44
1:A:209:SER:HB3	1:A:232:PRO:HA	1.99	0.44
1:B:57:PHE:HE2	1:B:207:VAL:HG12	1.83	0.44
1:B:61:MET:SD	1:B:284:VAL:HG11	2.58	0.44
1:C:49:MET:HE2	1:C:293:LEU:HD11	1.99	0.44
1:D:57:PHE:CE2	1:D:208:VAL:HG22	2.53	0.44
1:D:154:ASP:C	1:D:156:TYR:N	2.73	0.44
1:D:299:GLU:OE1	1:D:299:GLU:HA	2.17	0.44
1:F:222:VAL:CG1	1:F:258:ILE:HD12	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:221:MET:HE3	1:H:221:MET:HB3	1.54	0.44
1:I:98:PRO:HA	1:I:137:LYS:NZ	2.33	0.44
1:I:207:VAL:O	1:I:210:LYS:HB2	2.17	0.44
1:J:218:TYR:CD2	1:J:232:PRO:HG2	2.53	0.44
1:C:181:TYR:N	1:C:181:TYR:CD1	2.86	0.43
1:D:273:THR:OG1	1:D:275:LYS:N	2.50	0.43
1:E:57:PHE:O	1:E:61:MET:HG3	2.18	0.43
1:E:122:SER:HB2	1:E:123:PRO:HD2	2.00	0.43
1:G:105:VAL:HG13	1:G:107:PHE:CE1	2.52	0.43
1:H:212:ARG:HH22	1:I:235:LYS:NZ	2.15	0.43
1:J:282:GLU:OE2	1:J:283:PRO:HD2	2.17	0.43
1:B:87:LEU:O	1:B:88:LEU:C	2.59	0.43
1:I:75:MET:HE1	1:I:78:TYR:CD2	2.53	0.43
1:I:148:LEU:HD12	1:I:174:GLU:OE2	2.17	0.43
1:J:53:TYR:O	1:J:54:ALA:C	2.61	0.43
1:A:253:LYS:HD3	1:C:95:ARG:NH2	2.34	0.43
1:C:250:GLU:HB2	1:C:266:LEU:HD13	2.00	0.43
1:C:272:THR:O	1:C:272:THR:CG2	2.64	0.43
1:C:295:VAL:CG1	1:C:300:MET:HG3	2.48	0.43
1:G:119:TYR:O	1:G:121:ASN:N	2.49	0.43
1:H:91:GLU:CD	1:H:135:TRP:CZ2	2.97	0.43
1:I:171:TYR:OH	1:I:180:SER:OG	2.30	0.43
1:I:208:VAL:C	1:I:210:LYS:H	2.25	0.43
1:J:166:VAL:HG12	1:J:167:LEU:N	2.33	0.43
1:J:207:VAL:O	1:J:210:LYS:HG3	2.17	0.43
1:J:231:HIS:ND1	1:J:232:PRO:N	2.65	0.43
1:J:244:TYR:HE2	1:J:252:GLU:HG2	1.83	0.43
1:J:279:LEU:HD22	1:J:292:VAL:HG11	1.99	0.43
1:A:135:TRP:CD2	1:A:144:VAL:HB	2.53	0.43
1:B:117:ALA:C	1:B:119:TYR:H	2.26	0.43
1:C:238:ILE:HG22	1:C:238:ILE:O	2.18	0.43
1:H:131:PHE:CD1	1:H:133:PRO:HD3	2.53	0.43
1:H:178:MET:CE	1:H:198:ASP:OD1	2.66	0.43
1:H:265:HIS:HA	1:H:279:LEU:O	2.18	0.43
1:I:81:ALA:HA	1:I:112:PHE:CE2	2.54	0.43
1:I:176:VAL:HG12	1:I:178:MET:HE2	1.99	0.43
1:I:186:MET:SD	1:I:191:PHE:HB2	2.58	0.43
1:J:300:MET:N	1:J:301:LEU:HB3	2.33	0.43
1:A:222:VAL:HG22	1:A:226:GLY:CA	2.47	0.43
1:B:201:LEU:HA	1:B:201:LEU:HD23	1.65	0.43
1:F:105:VAL:HG13	1:F:107:PHE:CE1	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:40:LYS:H	1:G:41:LEU:HB3	1.81	0.43
1:G:218:TYR:CE1	1:G:294:VAL:HG11	2.54	0.43
1:J:40:LYS:CG	1:J:41:LEU:H	2.32	0.43
1:A:86:ALA:O	1:A:87:LEU:C	2.60	0.43
1:B:101:LEU:HD23	1:B:101:LEU:HA	1.57	0.43
1:C:158:LEU:HB2	1:C:159:PRO:CD	2.49	0.43
1:D:154:ASP:O	1:D:155:TYR:C	2.60	0.43
1:F:167:LEU:HD11	1:F:179:VAL:HG13	1.99	0.43
1:G:214:PHE:CE1	1:G:295:VAL:CG1	3.02	0.43
1:I:86:ALA:CB	1:I:131:PHE:CE2	3.01	0.43
1:I:88:LEU:HD23	1:I:88:LEU:HA	1.76	0.43
1:I:149:HIS:O	1:I:151:ASP:N	2.51	0.43
1:J:43:TYR:C	1:J:45:GLN:N	2.72	0.43
1:J:131:PHE:CD1	1:J:133:PRO:HD3	2.53	0.43
1:A:119:TYR:O	1:A:120:THR:C	2.60	0.43
1:B:258:ILE:HG13	1:B:259:LYS:N	2.33	0.43
1:A:212:ARG:HG3	1:A:217:GLY:O	2.18	0.43
1:C:153:SER:O	1:C:154:ASP:C	2.62	0.43
1:C:170:PRO:HG2	1:C:227:VAL:HG11	2.00	0.43
1:C:208:VAL:HG11	1:C:230:SER:OG	2.18	0.43
1:C:276:THR:O	1:C:297:LYS:HB3	2.19	0.43
1:F:39:GLU:CA	1:F:40:LYS:CB	2.46	0.43
1:H:110:ASP:OD1	1:H:114:GLY:HA2	2.19	0.43
1:H:250:GLU:HB3	1:H:266:LEU:HD11	1.99	0.43
1:I:148:LEU:O	1:I:149:HIS:HB2	2.19	0.43
1:J:61:MET:HE3	1:J:167:LEU:HD21	2.01	0.43
1:J:177:PHE:HZ	1:J:240:LYS:HD2	1.80	0.43
1:B:110:ASP:N	1:B:116:ASP:OD2	2.49	0.43
1:C:130:ARG:HH21	1:C:150:TYR:HE1	1.66	0.43
1:D:148:LEU:HD12	1:D:148:LEU:HA	1.73	0.43
1:D:296:PRO:O	1:D:299:GLU:HB2	2.19	0.43
1:F:43:TYR:CD1	1:F:300:MET:HE2	2.54	0.43
1:G:253:LYS:HB3	1:I:95:ARG:NH1	2.32	0.43
1:I:83:ARG:HH12	1:I:125:HIS:CD2	2.36	0.43
1:I:169:GLU:HB3	1:I:170:PRO:HD2	2.01	0.43
1:I:287:GLY:O	1:I:288:ASP:C	2.61	0.43
1:J:160:LYS:O	1:J:161:ALA:C	2.62	0.43
1:A:169:GLU:OE2	1:A:170:PRO:HD2	2.18	0.43
1:A:171:TYR:CE2	1:A:173:TYR:HB2	2.53	0.43
1:B:68:ALA:O	1:B:69:ARG:C	2.62	0.43
1:B:151:ASP:O	1:B:152:SER:HB3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:249:GLU:HB2	1:B:250:GLU:OE2	2.18	0.43
1:C:216:THR:OG1	1:C:299:GLU:OE2	2.26	0.43
1:D:221:MET:HE3	1:D:221:MET:HB3	1.65	0.43
1:G:77:SER:HB3	1:H:88:LEU:HB3	2.01	0.43
1:J:122:SER:CB	1:J:123:PRO:CD	2.91	0.43
1:A:206:GLU:O	1:A:210:LYS:HG2	2.19	0.42
1:B:94:LEU:HD13	1:B:137:LYS:HE3	2.01	0.42
1:B:227:VAL:HA	1:B:242:ASP:HB3	2.01	0.42
1:C:132:VAL:N	1:C:133:PRO:HD3	2.34	0.42
1:D:218:TYR:N	1:D:218:TYR:CD1	2.86	0.42
1:E:178:MET:HE2	1:E:178:MET:HB3	1.72	0.42
1:I:101:LEU:HD23	1:I:101:LEU:HA	1.78	0.42
1:A:78:TYR:CE2	1:A:81:ALA:N	2.87	0.42
1:C:91:GLU:HG3	1:C:135:TRP:CE3	2.53	0.42
1:C:112:PHE:CD2	1:C:131:PHE:HD2	2.36	0.42
1:C:158:LEU:O	1:C:159:PRO:C	2.62	0.42
1:C:278:ILE:HG21	1:C:280:PHE:CE1	2.53	0.42
1:E:216:THR:OG1	1:E:299:GLU:OE2	2.36	0.42
1:F:120:THR:O	1:F:120:THR:HG23	2.19	0.42
1:J:139:ASN:C	1:J:141:THR:N	2.77	0.42
1:B:123:PRO:O	1:B:124:ALA:HB3	2.17	0.42
1:C:153:SER:HB3	1:C:155:TYR:CD1	2.54	0.42
1:C:295:VAL:HA	1:C:296:PRO:HD3	1.79	0.42
1:D:72:SER:C	1:D:74:THR:N	2.76	0.42
1:H:41:LEU:HD23	1:H:41:LEU:HA	1.80	0.42
1:I:109:PRO:CA	1:I:130:ARG:HD3	2.49	0.42
1:B:58:ASP:O	1:B:59:ALA:C	2.62	0.42
1:C:222:VAL:CG2	1:C:226:GLY:C	2.92	0.42
1:C:246:PHE:HB2	1:C:251:LEU:HD13	2.01	0.42
1:E:240:LYS:CA	1:E:240:LYS:HE2	2.50	0.42
1:F:115:LYS:O	1:F:116:ASP:C	2.58	0.42
1:G:245:ASP:O	1:G:247:GLY:CA	2.68	0.42
1:H:75:MET:CE	1:H:105:VAL:HG21	2.48	0.42
1:H:295:VAL:HA	1:H:296:PRO:HD3	1.83	0.42
1:A:212:ARG:HE	1:A:212:ARG:HB2	1.53	0.42
1:A:218:TYR:HD2	1:A:232:PRO:CG	2.32	0.42
1:A:231:HIS:HA	1:A:232:PRO:HD3	1.89	0.42
1:C:91:GLU:CD	1:C:135:TRP:CH2	2.98	0.42
1:C:160:LYS:HG3	1:C:191:PHE:CD2	2.53	0.42
1:C:296:PRO:HB2	1:C:299:GLU:HG3	2.01	0.42
1:D:107:PHE:HB3	1:D:111:ALA:HB3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:167:LEU:HD13	1:D:181:TYR:CD2	2.54	0.42
1:E:248:GLY:N	1:E:251:LEU:HD12	2.34	0.42
1:G:171:TYR:N	1:G:171:TYR:CD1	2.88	0.42
1:H:302:ALA:C	1:H:304:VAL:N	2.77	0.42
1:I:112:PHE:CE1	1:I:131:PHE:CD2	3.07	0.42
1:A:172:PHE:CE1	1:A:175:GLY:O	2.72	0.42
1:A:242:ASP:C	1:A:242:ASP:OD2	2.62	0.42
1:B:72:SER:C	1:B:74:THR:N	2.77	0.42
1:C:90:LEU:HD13	1:C:104:TYR:HA	2.02	0.42
1:C:105:VAL:CG1	1:C:107:PHE:CE1	3.03	0.42
1:D:298:GLU:CG	1:D:299:GLU:HB2	2.48	0.42
1:F:104:TYR:HE1	1:F:198:ASP:OD2	2.02	0.42
1:G:97:ASN:HB2	1:G:100:LEU:HD12	2.01	0.42
1:I:93:LEU:O	1:I:94:LEU:C	2.62	0.42
1:I:268:THR:OG1	1:I:269:ALA:N	2.53	0.42
1:B:213:THR:HG22	1:B:217:GLY:HA3	2.02	0.42
1:C:61:MET:HE3	1:C:61:MET:HB3	1.79	0.42
1:E:203:TYR:CE2	1:E:207:VAL:HG21	2.55	0.42
1:E:240:LYS:HA	1:E:240:LYS:CE	2.48	0.42
1:H:120:THR:O	1:H:120:THR:HG23	2.19	0.42
1:I:65:LEU:HG	1:I:69:ARG:HD2	2.02	0.42
1:I:130:ARG:NH2	1:I:150:TYR:CD1	2.88	0.42
1:I:293:LEU:C	1:I:293:LEU:HD23	2.45	0.42
1:J:104:TYR:CD2	1:J:104:TYR:N	2.87	0.42
1:A:246:PHE:CD1	1:A:251:LEU:HD11	2.55	0.42
1:B:201:LEU:HD21	1:B:229:LEU:HD22	2.01	0.42
1:B:273:THR:HB	1:B:274:GLY:H	1.77	0.42
1:C:46:SER:O	1:C:47:VAL:C	2.62	0.42
1:C:173:TYR:CB	1:C:178:MET:HE2	2.50	0.42
1:E:79:GLU:HB2	1:F:85:GLU:OE1	2.19	0.42
1:E:158:LEU:HA	1:E:158:LEU:HD23	1.35	0.42
1:E:301:LEU:C	1:E:303:GLY:HA3	2.42	0.42
1:G:105:VAL:CG1	1:G:107:PHE:HE1	2.33	0.42
1:G:273:THR:OG1	1:G:275:LYS:CD	2.67	0.42
1:H:241:LYS:HD2	1:H:245:ASP:OD2	2.20	0.42
1:I:241:LYS:HA	1:I:241:LYS:HD3	1.89	0.42
1:A:222:VAL:CG2	1:A:227:VAL:O	2.66	0.42
1:B:88:LEU:HD23	1:B:88:LEU:HA	1.68	0.42
1:B:245:ASP:OD2	1:B:245:ASP:N	2.52	0.42
1:E:201:LEU:HD23	1:E:201:LEU:HA	1.61	0.42
1:H:218:TYR:CD2	1:H:232:PRO:CG	3.03	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:139:ASN:OD1	1:I:139:ASN:N	2.52	0.42
1:J:40:LYS:O	1:J:43:TYR:N	2.46	0.42
1:J:86:ALA:O	1:J:89:ILE:HB	2.20	0.42
1:A:272:THR:C	1:A:273:THR:CG2	2.92	0.42
1:C:88:LEU:HD13	1:D:77:SER:HB3	2.02	0.42
1:C:216:THR:O	1:C:217:GLY:C	2.63	0.42
1:E:40:LYS:O	1:E:40:LYS:CD	2.67	0.42
1:E:171:TYR:N	1:E:171:TYR:CD1	2.88	0.42
1:F:305:ALA:O	1:F:308:ARG:HB3	2.20	0.42
1:G:89:ILE:CD1	1:H:74:THR:HG23	2.42	0.42
1:G:131:PHE:CD1	1:G:133:PRO:HD3	2.55	0.42
1:H:119:TYR:HB3	1:H:125:HIS:CD2	2.55	0.42
1:H:233:THR:OG1	1:H:234:HIS:HD2	2.02	0.42
1:I:80:THR:O	1:I:82:ASP:N	2.53	0.42
1:I:130:ARG:NH2	1:I:150:TYR:HD1	2.17	0.42
1:I:304:VAL:O	1:I:305:ALA:C	2.62	0.42
1:A:104:TYR:N	1:A:104:TYR:CD2	2.87	0.41
1:A:234:HIS:C	1:A:236:ASP:N	2.77	0.41
1:C:231:HIS:ND1	1:C:232:PRO:N	2.68	0.41
1:D:251:LEU:HD23	1:D:266:LEU:HD12	2.01	0.41
1:E:130:ARG:O	1:E:132:VAL:HG13	2.20	0.41
1:E:285:GLU:O	1:E:285:GLU:HG2	2.19	0.41
1:F:243:LEU:HD23	1:F:243:LEU:HA	1.82	0.41
1:G:214:PHE:CE1	1:G:295:VAL:HG13	2.55	0.41
1:B:156:TYR:O	1:B:159:PRO:HD2	2.21	0.41
1:B:234:HIS:HB3	1:B:237:TRP:CD1	2.55	0.41
1:F:79:GLU:O	1:F:80:THR:C	2.63	0.41
1:J:298:GLU:N	1:J:301:LEU:CD2	2.70	0.41
1:J:298:GLU:C	1:J:301:LEU:HD22	2.45	0.41
1:A:158:LEU:HD23	1:A:158:LEU:HA	1.80	0.41
1:A:231:HIS:CG	1:A:232:PRO:CD	3.03	0.41
1:C:300:MET:C	1:C:302:ALA:H	2.28	0.41
1:D:83:ARG:HG2	1:D:112:PHE:CE1	2.54	0.41
1:D:301:LEU:O	1:D:302:ALA:C	2.63	0.41
1:E:123:PRO:O	1:E:124:ALA:CB	2.68	0.41
1:E:276:THR:O	1:E:297:LYS:HB2	2.19	0.41
1:G:97:ASN:HA	1:G:98:PRO:HD2	1.69	0.41
1:G:104:TYR:CD2	1:G:104:TYR:N	2.88	0.41
1:G:262:ILE:HD13	1:I:98:PRO:HG3	2.02	0.41
1:H:278:ILE:HD12	1:H:300:MET:SD	2.60	0.41
1:I:83:ARG:HG2	1:I:112:PHE:HE1	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:168:THR:CG2	1:I:180:SER:HB2	2.50	0.41
1:I:293:LEU:HD23	1:I:294:VAL:N	2.35	0.41
1:J:104:TYR:CE2	1:J:198:ASP:OD2	2.73	0.41
1:J:135:TRP:CE2	1:J:144:VAL:HB	2.56	0.41
1:J:141:THR:HG23	1:J:141:THR:O	2.19	0.41
1:D:123:PRO:O	1:D:124:ALA:HB3	2.20	0.41
1:F:72:SER:O	1:F:73:THR:C	2.61	0.41
1:G:108:GLU:O	1:G:111:ALA:CB	2.67	0.41
1:G:258:ILE:HG21	1:G:258:ILE:HD13	1.62	0.41
1:H:46:SER:O	1:H:47:VAL:C	2.63	0.41
1:B:268:THR:HG23	1:B:269:ALA:N	2.35	0.41
1:D:91:GLU:HB2	1:D:135:TRP:CD1	2.55	0.41
1:D:135:TRP:NE1	1:D:144:VAL:CG2	2.84	0.41
1:D:244:TYR:CE2	1:D:252:GLU:HG2	2.55	0.41
1:E:104:TYR:OH	1:E:180:SER:HB3	2.20	0.41
1:E:156:TYR:CD2	1:E:156:TYR:O	2.73	0.41
1:F:186:MET:HE3	1:F:186:MET:HB3	1.84	0.41
1:F:302:ALA:O	1:F:306:ASP:CG	2.63	0.41
1:H:42:ALA:O	1:H:300:MET:HE3	2.21	0.41
1:H:97:ASN:HB2	1:H:100:LEU:HD12	2.03	0.41
1:A:122:SER:CB	1:A:123:PRO:HD2	2.50	0.41
1:A:244:TYR:CD2	1:A:252:GLU:CG	3.03	0.41
1:C:49:MET:HE1	1:C:213:THR:OG1	2.21	0.41
1:C:250:GLU:HG2	1:C:251:LEU:N	2.35	0.41
1:F:135:TRP:CE2	1:F:144:VAL:HB	2.55	0.41
1:G:106:ALA:O	1:G:193:GLY:HA3	2.21	0.41
1:A:101:LEU:O	1:A:101:LEU:CD2	2.67	0.41
1:A:112:PHE:CD1	1:A:131:PHE:CD2	3.09	0.41
1:C:122:SER:HA	1:C:123:PRO:HA	1.81	0.41
1:C:223:SER:O	1:C:258:ILE:HD11	2.20	0.41
1:F:201:LEU:HD23	1:F:201:LEU:HA	1.65	0.41
1:G:177:PHE:CE2	1:G:239:GLY:O	2.74	0.41
1:H:154:ASP:O	1:H:155:TYR:C	2.63	0.41
1:J:132:VAL:O	1:J:132:VAL:HG23	2.21	0.41
1:J:278:ILE:CD1	1:J:297:LYS:HD3	2.51	0.41
1:A:88:LEU:O	1:A:89:ILE:C	2.64	0.41
1:A:153:SER:HB3	1:A:155:TYR:CD1	2.56	0.41
1:C:256:ARG:HG3	1:C:256:ARG:NH1	2.35	0.41
1:D:222:VAL:HG22	1:D:227:VAL:O	2.21	0.41
1:D:231:HIS:NE2	1:D:237:TRP:HZ3	2.19	0.41
1:H:70:THR:O	1:H:71:ILE:C	2.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:132:VAL:N	1:H:133:PRO:CD	2.84	0.41
1:I:306:ASP:C	1:I:308:ARG:N	2.50	0.41
1:J:272:THR:C	1:J:273:THR:CG2	2.94	0.41
1:A:101:LEU:HD22	1:A:101:LEU:C	2.45	0.41
1:A:167:LEU:HD11	1:A:179:VAL:CG1	2.50	0.41
1:B:270:ASP:OD1	1:B:270:ASP:C	2.61	0.41
1:C:115:LYS:C	1:C:117:ALA:H	2.29	0.41
1:C:186:MET:HE1	1:C:191:PHE:CD1	2.54	0.41
1:C:270:ASP:HA	1:C:274:GLY:N	2.36	0.41
1:D:231:HIS:CD2	1:D:237:TRP:CE3	3.09	0.41
1:D:247:GLY:O	1:D:248:GLY:C	2.62	0.41
1:D:272:THR:CG2	1:D:273:THR:N	2.83	0.41
1:E:155:TYR:CD2	1:E:155:TYR:C	2.99	0.41
1:E:268:THR:HG23	1:E:269:ALA:N	2.35	0.41
1:H:172:PHE:CD1	1:H:177:PHE:CE2	3.08	0.41
1:H:186:MET:HE1	1:H:191:PHE:HB2	2.03	0.41
1:H:251:LEU:HD23	1:H:266:LEU:HD12	2.03	0.41
1:H:298:GLU:HA	1:H:301:LEU:HB2	2.02	0.41
1:I:135:TRP:HZ3	1:I:142:ALA:O	2.03	0.41
1:I:213:THR:O	1:I:214:PHE:C	2.64	0.41
1:C:41:LEU:O	1:C:42:ALA:C	2.63	0.41
1:C:41:LEU:C	1:C:43:TYR:N	2.74	0.41
1:C:63:ALA:O	1:C:66:ALA:HB3	2.20	0.41
1:C:131:PHE:C	1:C:132:VAL:CG1	2.94	0.41
1:C:240:LYS:HE2	1:C:240:LYS:CA	2.47	0.41
1:D:97:ASN:HA	1:D:98:PRO:HD2	1.84	0.41
1:D:135:TRP:HZ3	1:D:142:ALA:O	2.04	0.41
1:G:222:VAL:HG22	1:G:227:VAL:O	2.21	0.41
1:I:172:PHE:O	1:I:172:PHE:CG	2.74	0.41
1:J:40:LYS:O	1:J:41:LEU:C	2.59	0.41
1:J:81:ALA:HB1	1:J:113:ASP:HB3	2.02	0.41
1:J:214:PHE:CE2	1:J:299:GLU:O	2.74	0.41
1:A:235:LYS:H	1:A:235:LYS:HG2	1.53	0.40
1:A:308:ARG:HD3	1:A:308:ARG:HA	1.60	0.40
1:B:40:LYS:O	1:B:41:LEU:HG	2.20	0.40
1:B:158:LEU:CB	1:B:159:PRO:HD3	2.51	0.40
1:C:106:ALA:HB2	1:C:147:LEU:HD12	2.03	0.40
1:D:231:HIS:ND1	1:D:232:PRO:CD	2.84	0.40
1:E:41:LEU:O	1:E:43:TYR:C	2.65	0.40
1:G:79:GLU:C	1:G:81:ALA:N	2.78	0.40
1:G:128:THR:O	1:G:130:ARG:N	2.53	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:222:VAL:CG1	1:H:290:ALA:HB3	2.51	0.40
1:I:236:ASP:O	1:I:240:LYS:HG2	2.21	0.40
1:J:222:VAL:HG12	1:J:290:ALA:HB3	2.03	0.40
1:A:132:VAL:N	1:A:133:PRO:CD	2.85	0.40
1:D:47:VAL:HG23	1:D:280:PHE:HE2	1.85	0.40
1:E:186:MET:HE3	1:E:186:MET:HB3	1.95	0.40
1:E:205:ASP:O	1:E:206:GLU:C	2.64	0.40
1:E:241:LYS:HD2	1:E:245:ASP:OD2	2.21	0.40
1:G:112:PHE:CD1	1:G:131:PHE:CD2	3.10	0.40
1:G:153:SER:HB2	1:G:155:TYR:CD2	2.56	0.40
1:H:173:TYR:O	1:H:175:GLY:N	2.54	0.40
1:J:249:GLU:O	1:J:249:GLU:OE2	2.39	0.40
1:A:169:GLU:OE2	1:A:223:SER:OG	2.38	0.40
1:A:222:VAL:HG22	1:A:226:GLY:C	2.47	0.40
1:C:184:PRO:HB2	1:C:186:MET:CE	2.51	0.40
1:C:201:LEU:CD2	1:C:229:LEU:HD22	2.52	0.40
1:C:304:VAL:O	1:C:305:ALA:C	2.65	0.40
1:D:243:LEU:HD23	1:D:243:LEU:HA	1.81	0.40
1:F:222:VAL:HG23	1:F:227:VAL:O	2.21	0.40
1:A:76:GLU:HG2	1:A:186:MET:O	2.21	0.40
1:A:94:LEU:HD23	1:A:94:LEU:HA	1.73	0.40
1:B:211:VAL:HG12	1:B:212:ARG:N	2.35	0.40
1:B:303:GLY:O	1:B:306:ASP:HB2	2.21	0.40
1:F:218:TYR:O	1:F:293:LEU:HD23	2.21	0.40
1:F:278:ILE:HD11	1:F:297:LYS:HD2	2.03	0.40
1:G:167:LEU:HD11	1:G:179:VAL:HG13	2.02	0.40
1:H:63:ALA:O	1:H:66:ALA:HB3	2.21	0.40
1:J:207:VAL:O	1:J:210:LYS:HG2	2.21	0.40
1:A:73:THR:CG2	1:B:93:LEU:HD23	2.52	0.40
1:A:177:PHE:HB3	1:A:201:LEU:CD1	2.52	0.40
1:C:134:TYR:CE1	1:C:173:TYR:HE2	2.40	0.40
1:D:302:ALA:CB	1:D:303:GLY:CA	2.98	0.40
1:E:101:LEU:HG	1:E:200:SER:HB3	2.04	0.40
1:F:103:THR:O	1:F:104:TYR:HB3	2.20	0.40
1:F:193:GLY:O	1:F:194:ILE:CG2	2.68	0.40
1:F:282:GLU:HA	1:F:283:PRO:HD3	1.94	0.40
1:G:169:GLU:OE2	1:G:225:SER:OG	2.38	0.40
1:H:123:PRO:O	1:H:124:ALA:CB	2.70	0.40
1:H:172:PHE:HD1	1:H:177:PHE:CD2	2.38	0.40
1:I:86:ALA:HB3	1:I:131:PHE:CZ	2.57	0.40
1:I:138:MET:HB2	1:I:138:MET:HE2	1.79	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:186:MET:HE3	1:I:186:MET:HB3	1.90	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	269/290 (93%)	230 (86%)	29 (11%)	10 (4%)	2	15
1	B	269/290 (93%)	209 (78%)	46 (17%)	14 (5%)	1	9
1	C	266/290 (92%)	221 (83%)	33 (12%)	12 (4%)	2	12
1	D	269/290 (93%)	224 (83%)	34 (13%)	11 (4%)	2	13
1	E	266/290 (92%)	221 (83%)	34 (13%)	11 (4%)	2	13
1	F	269/290 (93%)	231 (86%)	30 (11%)	8 (3%)	3	19
1	G	268/290 (92%)	225 (84%)	28 (10%)	15 (6%)	1	8
1	H	265/290 (91%)	219 (83%)	37 (14%)	9 (3%)	3	17
1	I	269/290 (93%)	217 (81%)	38 (14%)	14 (5%)	1	9
1	J	269/290 (93%)	222 (82%)	32 (12%)	15 (6%)	1	8
All	All	2679/2900 (92%)	2219 (83%)	341 (13%)	119 (4%)	2	12

All (119) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	298	GLU
1	A	299	GLU
1	B	120	THR
1	B	149	HIS
1	B	188	GLU
1	B	250	GLU

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Mol	Chain	Res	Type
1	C	120	THR
1	C	121	ASN
1	C	248	GLY
1	C	270	ASP
1	C	273	THR
1	D	42	ALA
1	D	81	ALA
1	D	120	THR
1	D	121	ASN
1	D	302	ALA
1	E	43	TYR
1	E	44	GLN
1	E	248	GLY
1	F	43	TYR
1	F	44	GLN
1	G	81	ALA
1	G	121	ASN
1	G	246	PHE
1	G	272	THR
1	G	273	THR
1	H	152	SER
1	H	248	GLY
1	I	81	ALA
1	I	248	GLY
1	I	307	LEU
1	J	41	LEU
1	J	152	SER
1	J	246	PHE
1	J	272	THR
1	J	301	LEU
1	A	140	GLY
1	A	155	TYR
1	A	306	ASP
1	B	41	LEU
1	B	127	GLY
1	B	152	SER
1	B	249	GLU
1	C	80	THR
1	C	127	GLY
1	C	140	GLY
1	C	188	GLU
1	D	140	GLY

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Mol	Chain	Res	Type
1	D	152	SER
1	E	42	ALA
1	E	80	THR
1	E	140	GLY
1	F	140	GLY
1	F	248	GLY
1	G	44	GLN
1	G	140	GLY
1	G	271	PRO
1	G	307	LEU
1	H	127	GLY
1	H	140	GLY
1	H	238	ILE
1	I	120	THR
1	I	188	GLU
1	I	245	ASP
1	J	114	GLY
1	J	140	GLY
1	J	271	PRO
1	J	273	THR
1	A	40	LYS
1	A	243	LEU
1	B	128	THR
1	B	189	GLY
1	D	188	GLU
1	D	299	GLU
1	F	40	LYS
1	F	120	THR
1	F	124	ALA
1	G	188	GLU
1	G	274	GLY
1	H	120	THR
1	I	121	ASN
1	I	149	HIS
1	I	150	TYR
1	J	120	THR
1	J	211	VAL
1	J	250	GLU
1	J	306	ASP
1	B	254	ALA
1	B	288	ASP
1	D	41	LEU

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Mol	Chain	Res	Type
1	E	120	THR
1	E	274	GLY
1	E	289	PHE
1	F	188	GLU
1	G	46	SER
1	G	80	THR
1	I	127	GLY
1	I	268	THR
1	J	274	GLY
1	A	152	SER
1	B	121	ASN
1	C	122	SER
1	C	217	GLY
1	H	137	LYS
1	I	80	THR
1	B	40	LYS
1	E	40	LYS
1	G	51	SER
1	I	140	GLY
1	I	254	ALA
1	J	155	TYR
1	A	271	PRO
1	G	175	GLY
1	H	109	PRO
1	D	129	GLY
1	C	238	ILE
1	A	109	PRO
1	E	89	ILE
1	H	122	SER

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	227/246 (92%)	195 (86%)	32 (14%)	3 16
1	B	227/246 (92%)	193 (85%)	34 (15%)	3 14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	223/246 (91%)	188 (84%)	35 (16%)	2	13
1	D	227/246 (92%)	190 (84%)	37 (16%)	2	12
1	E	224/246 (91%)	187 (84%)	37 (16%)	2	12
1	F	227/246 (92%)	199 (88%)	28 (12%)	4	21
1	G	226/246 (92%)	189 (84%)	37 (16%)	2	12
1	H	223/246 (91%)	186 (83%)	37 (17%)	2	12
1	I	227/246 (92%)	194 (86%)	33 (14%)	3	15
1	J	227/246 (92%)	191 (84%)	36 (16%)	2	13
All	All	2258/2460 (92%)	1912 (85%)	346 (15%)	3	14

All (346) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	GLU
1	A	41	LEU
1	A	60	ASP
1	A	79	GLU
1	A	88	LEU
1	A	94	LEU
1	A	101	LEU
1	A	105	VAL
1	A	138	MET
1	A	139	ASN
1	A	144	VAL
1	A	153	SER
1	A	171	TYR
1	A	176	VAL
1	A	179	VAL
1	A	197	VAL
1	A	202	GLU
1	A	207	VAL
1	A	212	ARG
1	A	216	THR
1	A	218	TYR
1	A	236	ASP
1	A	246	PHE
1	A	251	LEU
1	A	258	ILE
1	A	268	THR

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Mol	Chain	Res	Type
1	A	272	THR
1	A	273	THR
1	A	275	LYS
1	A	284	VAL
1	A	293	LEU
1	A	308	ARG
1	B	39	GLU
1	B	40	LYS
1	B	41	LEU
1	B	49	MET
1	B	74	THR
1	B	88	LEU
1	B	94	LEU
1	B	101	LEU
1	B	105	VAL
1	B	118	GLU
1	B	122	SER
1	B	128	THR
1	B	150	TYR
1	B	157	GLN
1	B	168	THR
1	B	174	GLU
1	B	176	VAL
1	B	179	VAL
1	B	182	VAL
1	B	185	ILE
1	B	191	PHE
1	B	212	ARG
1	B	222	VAL
1	B	236	ASP
1	B	245	ASP
1	B	250	GLU
1	B	258	ILE
1	B	266	LEU
1	B	268	THR
1	B	273	THR
1	B	276	THR
1	B	300	MET
1	B	307	LEU
1	B	308	ARG
1	C	39	GLU
1	C	44	GLN

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Mol	Chain	Res	Type
1	C	45	GLN
1	C	61	MET
1	C	65	LEU
1	C	88	LEU
1	C	94	LEU
1	C	101	LEU
1	C	105	VAL
1	C	132	VAL
1	C	138	MET
1	C	153	SER
1	C	167	LEU
1	C	174	GLU
1	C	179	VAL
1	C	181	TYR
1	C	182	VAL
1	C	183	SER
1	C	190	GLU
1	C	197	VAL
1	C	208	VAL
1	C	213	THR
1	C	228	ILE
1	C	236	ASP
1	C	256	ARG
1	C	258	ILE
1	C	267	GLU
1	C	273	THR
1	C	275	LYS
1	C	276	THR
1	C	277	VAL
1	C	295	VAL
1	C	300	MET
1	C	304	VAL
1	C	306	ASP
1	D	39	GLU
1	D	41	LEU
1	D	88	LEU
1	D	94	LEU
1	D	101	LEU
1	D	105	VAL
1	D	136	ASN
1	D	141	THR
1	D	144	VAL

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Mol	Chain	Res	Type
1	D	148	LEU
1	D	153	SER
1	D	154	ASP
1	D	163	GLU
1	D	164	LYS
1	D	169	GLU
1	D	176	VAL
1	D	179	VAL
1	D	180	SER
1	D	185	ILE
1	D	187	LYS
1	D	190	GLU
1	D	207	VAL
1	D	210	LYS
1	D	212	ARG
1	D	221	MET
1	D	222	VAL
1	D	249	GLU
1	D	250	GLU
1	D	251	LEU
1	D	258	ILE
1	D	266	LEU
1	D	272	THR
1	D	273	THR
1	D	275	LYS
1	D	298	GLU
1	D	308	ARG
1	D	309	GLU
1	E	39	GLU
1	E	41	LEU
1	E	77	SER
1	E	80	THR
1	E	83	ARG
1	E	88	LEU
1	E	94	LEU
1	E	101	LEU
1	E	105	VAL
1	E	120	THR
1	E	122	SER
1	E	132	VAL
1	E	152	SER
1	E	174	GLU

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Mol	Chain	Res	Type
1	E	176	VAL
1	E	179	VAL
1	E	185	ILE
1	E	187	LYS
1	E	201	LEU
1	E	207	VAL
1	E	216	THR
1	E	221	MET
1	E	228	ILE
1	E	230	SER
1	E	236	ASP
1	E	240	LYS
1	E	256	ARG
1	E	258	ILE
1	E	259	LYS
1	E	266	LEU
1	E	268	THR
1	E	275	LYS
1	E	278	ILE
1	E	286	THR
1	E	293	LEU
1	E	298	GLU
1	E	301	LEU
1	F	41	LEU
1	F	46	SER
1	F	60	ASP
1	F	77	SER
1	F	85	GLU
1	F	88	LEU
1	F	94	LEU
1	F	101	LEU
1	F	105	VAL
1	F	138	MET
1	F	152	SER
1	F	176	VAL
1	F	179	VAL
1	F	212	ARG
1	F	221	MET
1	F	240	LYS
1	F	250	GLU
1	F	258	ILE
1	F	266	LEU

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Mol	Chain	Res	Type
1	F	268	THR
1	F	275	LYS
1	F	276	THR
1	F	278	ILE
1	F	286	THR
1	F	293	LEU
1	F	298	GLU
1	F	304	VAL
1	F	308	ARG
1	G	39	GLU
1	G	41	LEU
1	G	44	GLN
1	G	46	SER
1	G	51	SER
1	G	52	ASN
1	G	88	LEU
1	G	94	LEU
1	G	101	LEU
1	G	105	VAL
1	G	120	THR
1	G	122	SER
1	G	130	ARG
1	G	136	ASN
1	G	144	VAL
1	G	153	SER
1	G	154	ASP
1	G	164	LYS
1	G	179	VAL
1	G	180	SER
1	G	185	ILE
1	G	201	LEU
1	G	206	GLU
1	G	210	LYS
1	G	212	ARG
1	G	213	THR
1	G	221	MET
1	G	222	VAL
1	G	236	ASP
1	G	246	PHE
1	G	251	LEU
1	G	258	ILE
1	G	272	THR

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Mol	Chain	Res	Type
1	G	273	THR
1	G	275	LYS
1	G	293	LEU
1	G	298	GLU
1	H	39	GLU
1	H	44	GLN
1	H	45	GLN
1	H	47	VAL
1	H	61	MET
1	H	83	ARG
1	H	88	LEU
1	H	94	LEU
1	H	101	LEU
1	H	105	VAL
1	H	109	PRO
1	H	120	THR
1	H	122	SER
1	H	132	VAL
1	H	139	ASN
1	H	141	THR
1	H	174	GLU
1	H	179	VAL
1	H	182	VAL
1	H	185	ILE
1	H	188	GLU
1	H	197	VAL
1	H	208	VAL
1	H	216	THR
1	H	222	VAL
1	H	225	SER
1	H	228	ILE
1	H	240	LYS
1	H	258	ILE
1	H	268	THR
1	H	273	THR
1	H	275	LYS
1	H	276	THR
1	H	277	VAL
1	H	293	LEU
1	H	295	VAL
1	H	301	LEU
1	I	39	GLU

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Mol	Chain	Res	Type
1	I	41	LEU
1	I	75	MET
1	I	88	LEU
1	I	94	LEU
1	I	101	LEU
1	I	105	VAL
1	I	121	ASN
1	I	138	MET
1	I	139	ASN
1	I	141	THR
1	I	150	TYR
1	I	153	SER
1	I	167	LEU
1	I	168	THR
1	I	174	GLU
1	I	176	VAL
1	I	179	VAL
1	I	185	ILE
1	I	191	PHE
1	I	210	LYS
1	I	222	VAL
1	I	236	ASP
1	I	245	ASP
1	I	253	LYS
1	I	258	ILE
1	I	266	LEU
1	I	268	THR
1	I	276	THR
1	I	298	GLU
1	I	306	ASP
1	I	308	ARG
1	I	309	GLU
1	J	39	GLU
1	J	41	LEU
1	J	62	LYS
1	J	76	GLU
1	J	79	GLU
1	J	88	LEU
1	J	101	LEU
1	J	105	VAL
1	J	120	THR
1	J	130	ARG

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Mol	Chain	Res	Type
1	J	139	ASN
1	J	153	SER
1	J	167	LEU
1	J	171	TYR
1	J	176	VAL
1	J	179	VAL
1	J	202	GLU
1	J	212	ARG
1	J	216	THR
1	J	218	TYR
1	J	222	VAL
1	J	236	ASP
1	J	240	LYS
1	J	249	GLU
1	J	250	GLU
1	J	258	ILE
1	J	268	THR
1	J	272	THR
1	J	273	THR
1	J	275	LYS
1	J	284	VAL
1	J	293	LEU
1	J	299	GLU
1	J	301	LEU
1	J	304	VAL
1	J	309	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	224	ASN
1	C	121	ASN
1	C	157	GLN
1	D	52	ASN
1	F	224	ASN
1	G	92	ASN
1	G	97	ASN
1	G	231	HIS
1	G	234	HIS
1	H	224	ASN
1	I	224	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 10 ligands modelled in this entry, 10 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	271/290 (93%)	-1.40	0 100 100	57, 74, 97, 127	0
1	B	271/290 (93%)	-1.30	0 100 100	62, 80, 102, 115	0
1	C	268/290 (92%)	-1.36	0 100 100	50, 70, 100, 113	0
1	D	271/290 (93%)	-1.37	0 100 100	20, 71, 97, 113	0
1	E	268/290 (92%)	-1.43	0 100 100	43, 66, 98, 119	0
1	F	271/290 (93%)	-1.42	0 100 100	42, 67, 96, 130	0
1	G	270/290 (93%)	-1.41	0 100 100	48, 71, 94, 107	0
1	H	267/290 (92%)	-1.37	0 100 100	51, 70, 97, 108	0
1	I	271/290 (93%)	-1.31	0 100 100	62, 80, 103, 113	0
1	J	271/290 (93%)	-1.40	0 100 100	58, 74, 97, 123	0
All	All	2699/2900 (93%)	-1.38	0 100 100	20, 73, 99, 130	0

There are no RSRZ outliers to report.

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(Å ²)	Q<0.9
2	K	B	10	1/1	0.98	0.12	130,130,130,130	0
2	K	D	5	1/1	0.98	0.10	131,131,131,131	0
2	K	E	6	1/1	0.98	0.06	104,104,104,104	0
2	K	G	4	1/1	0.98	0.08	122,122,122,122	0
2	K	H	7	1/1	0.98	0.10	119,119,119,119	0
2	K	I	9	1/1	0.98	0.09	113,113,113,113	0
2	K	A	1	1/1	0.99	0.08	91,91,91,91	0
2	K	C	3	1/1	0.99	0.11	112,112,112,112	0
2	K	F	8	1/1	0.99	0.07	107,107,107,107	0
2	K	J	2	1/1	0.99	0.08	85,85,85,85	0

6.5 Other polymers [i](#)

There are no such residues in this entry.