



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 06:46 AM UTC

PDB ID : 4ATW / pdb_00004atw
Title : The crystal structure of Arabinofuranosidase
Authors : Dumbrepatil, A.; Song, H.-N.; Jung, T.-Y.; Kim, T.-J.; Woo, E.-J.
Deposited on : 2012-05-10
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

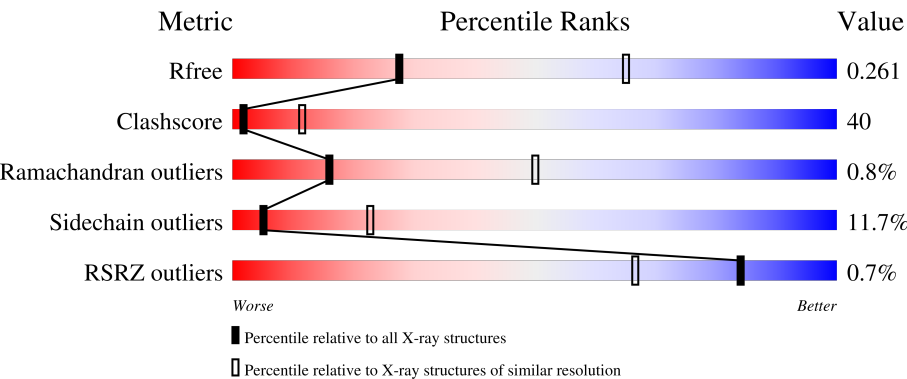
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	482	47%39%11%.
1	B	482	% 48%39%11%.
1	C	482	46%40%12%.
1	D	482	% 48%38%12%.
1	E	482	% 46%43%10%.

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Mol	Chain	Length	Quality of chain
1	F	482	% 48% 39% 10% .

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 23256 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 ALPHA-L-ARABINOFURANOSIDASE DOMAIN PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	481	Total	C	N	O	S	0	0	0
			3876	2486	646	729	15			
1	B	481	Total	C	N	O	S	0	0	0
			3876	2486	646	729	15			
1	C	481	Total	C	N	O	S	0	0	0
			3876	2486	646	729	15			
1	D	481	Total	C	N	O	S	0	0	0
			3876	2486	646	729	15			
1	E	481	Total	C	N	O	S	0	0	0
			3876	2486	646	729	15			
1	F	481	Total	C	N	O	S	0	0	0
			3876	2486	646	729	15			

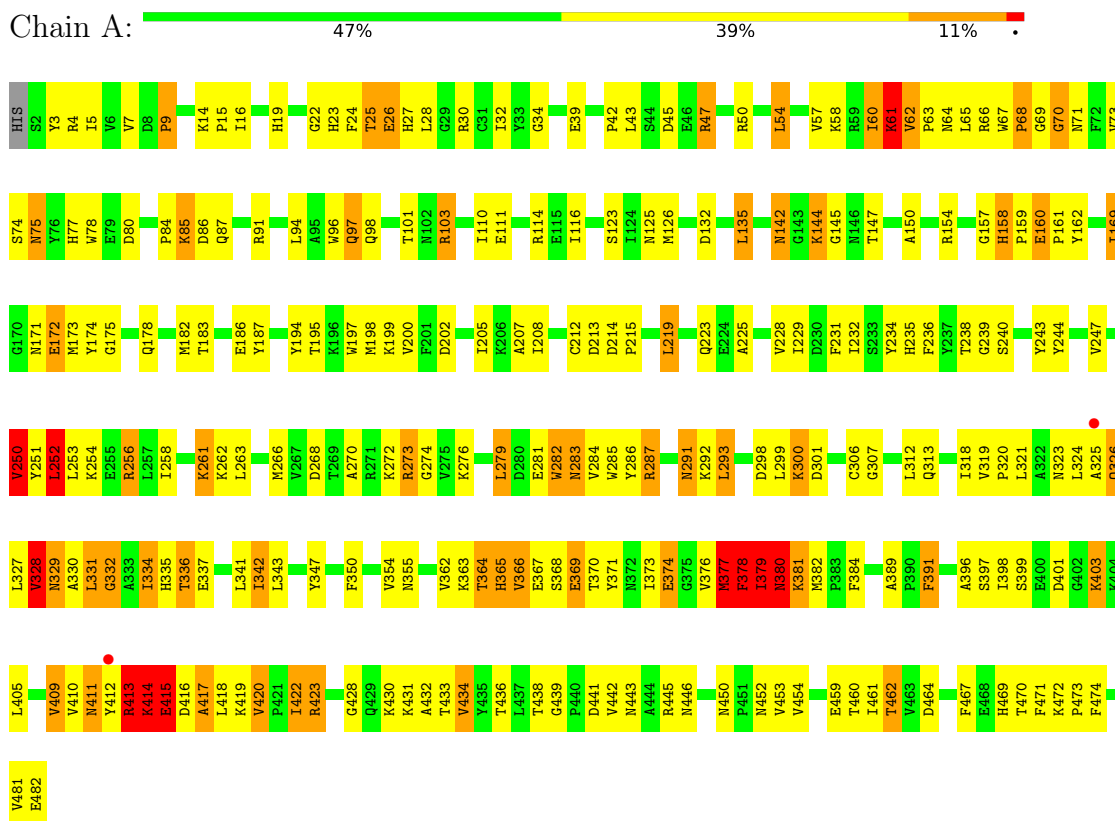
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	HIS	-	expression tag	UNP G4FHJ5
B	1	HIS	-	expression tag	UNP G4FHJ5
C	1	HIS	-	expression tag	UNP G4FHJ5
D	1	HIS	-	expression tag	UNP G4FHJ5
E	1	HIS	-	expression tag	UNP G4FHJ5
F	1	HIS	-	expression tag	UNP G4FHJ5

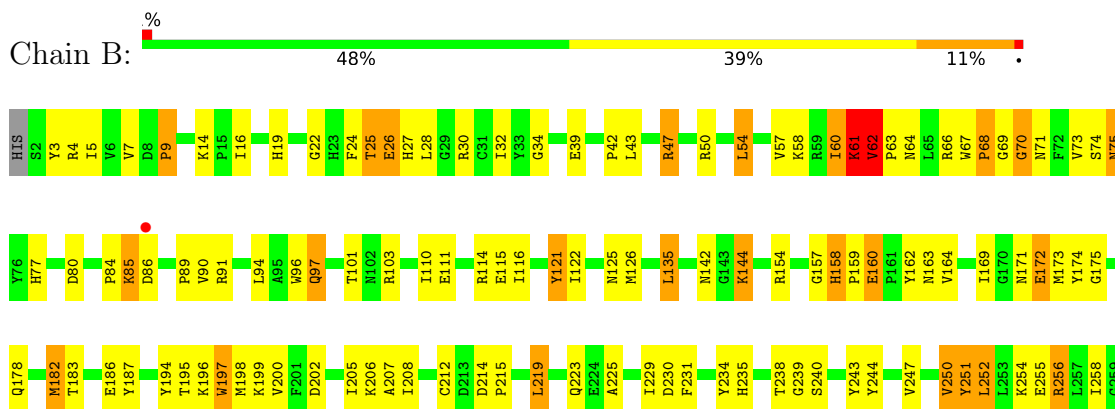
3 Residue-property plots

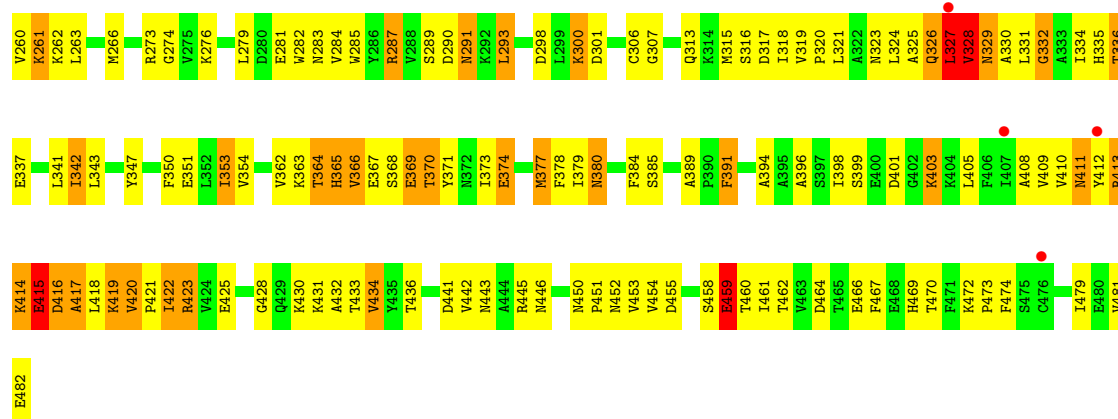
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: ALPHA-L-ARABINOFURANOSIDASE DOMAIN PROTEIN



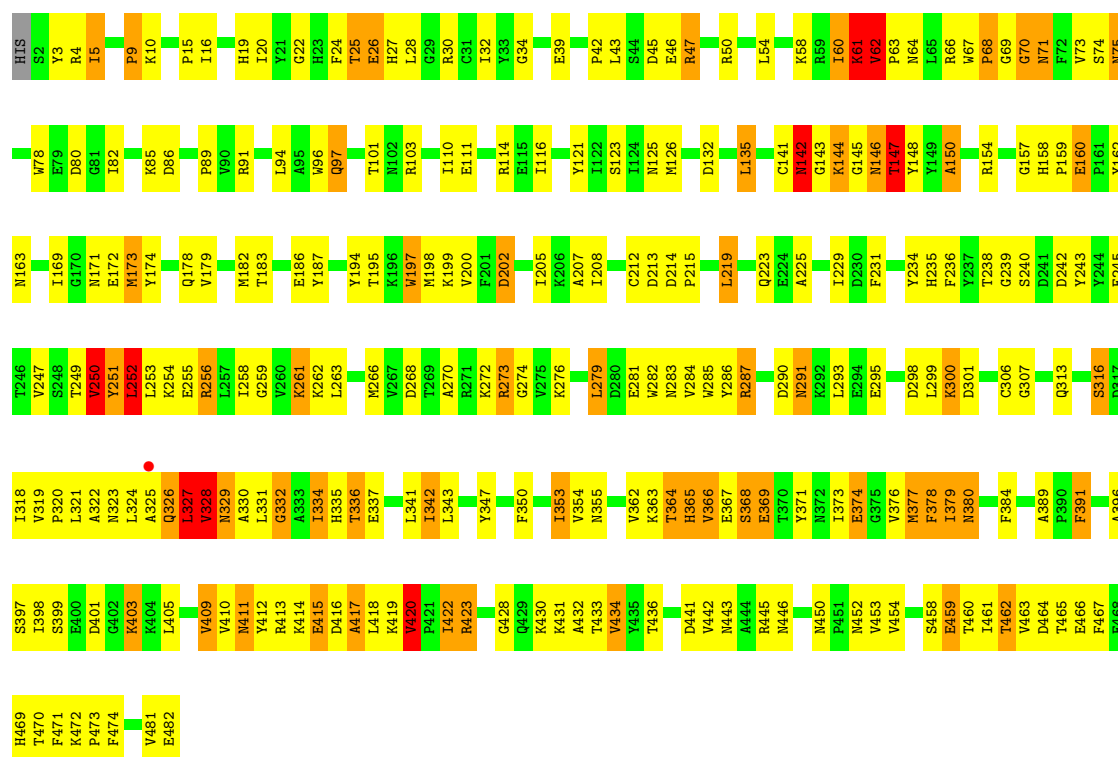
• Molecule 1: ALPHA-L-ARABINOFURANOSIDASE DOMAIN PROTEIN





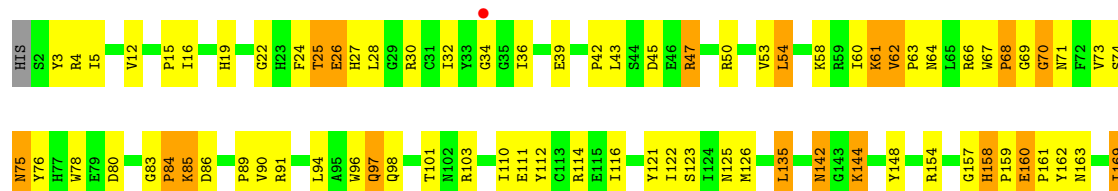
• Molecule 1: ALPHA-L-ARABINOFURANOSIDASE DOMAIN PROTEIN

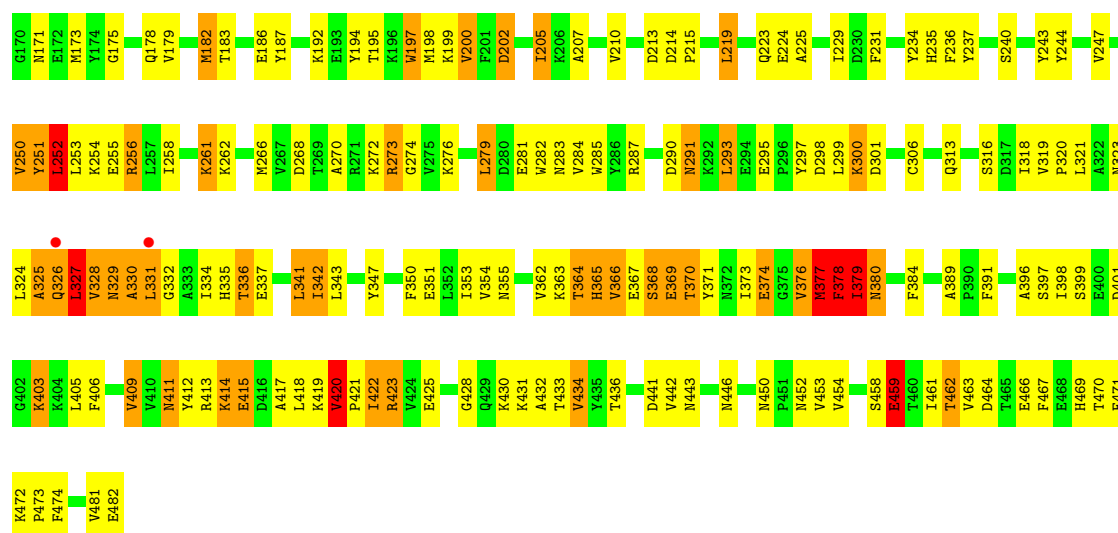
Chain C: 46% 40% 12%



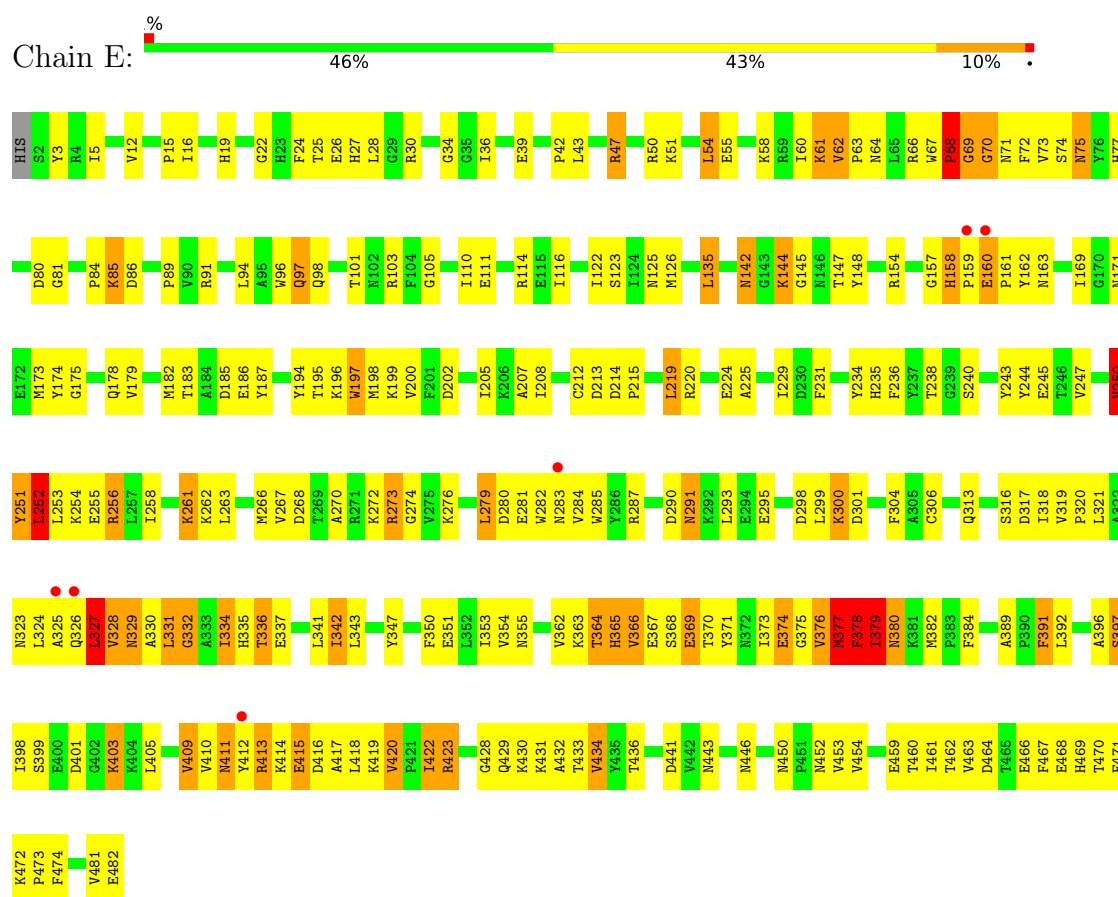
• Molecule 1: ALPHA-L-ARABINOFURANOSIDASE DOMAIN PROTEIN

Chain D: 48% 38% 12%

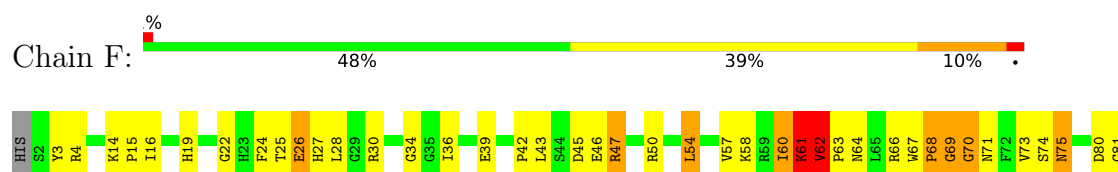


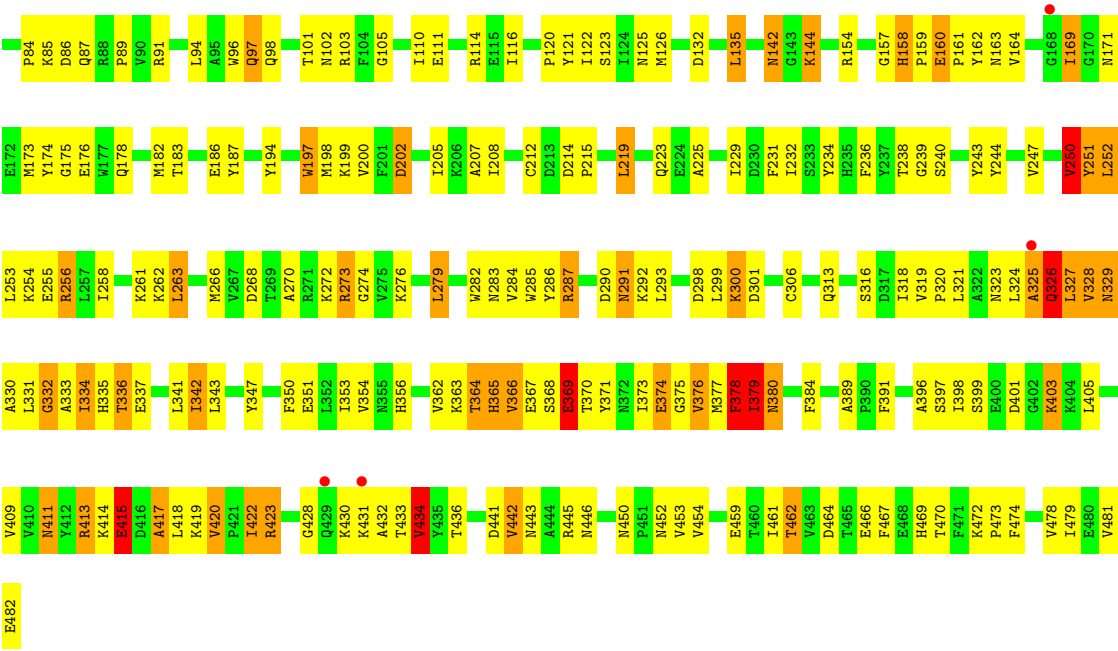


- Molecule 1: ALPHA-L-ARABINOFURANOSIDASE DOMAIN PROTEIN



- Molecule 1: ALPHA-L-ARABINOFURANOSIDASE DOMAIN PROTEIN





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	103.71Å 161.54Å 112.60Å 90.00° 106.30° 90.00°	Depositor
Resolution (Å)	29.94 – 3.00 29.94 – 3.00	Depositor EDS
% Data completeness (in resolution range)	84.5 (29.94-3.00) 84.4 (29.94-3.00)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.24 (at 3.00Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.227 , 0.262 0.227 , 0.261	Depositor DCC
R_{free} test set	4430 reflections (6.60%)	wwPDB-VP
Wilson B-factor (Å ²)	45.1	Xtriage
Anisotropy	0.271	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 36.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	23256	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.39% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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	1.21	25/3971 (0.6%)	1.42	66/5383 (1.2%)
1	B	0.91	9/3971 (0.2%)	1.37	48/5383 (0.9%)
1	C	1.29	28/3971 (0.7%)	1.35	48/5383 (0.9%)
1	D	1.42	44/3971 (1.1%)	1.44	71/5383 (1.3%)
1	E	1.01	21/3971 (0.5%)	1.32	49/5383 (0.9%)
1	F	0.91	14/3971 (0.4%)	1.31	52/5383 (1.0%)
All	All	1.14	141/23826 (0.6%)	1.37	334/32298 (1.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	1
1	B	0	1
1	C	0	1
1	D	0	2
1	E	0	1
1	F	0	3
All	All	1	9

All (141) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	26	GLU	C-N	-30.02	0.93	1.33
1	A	328	VAL	CA-CB	-28.43	1.15	1.54
1	D	378	PHE	C-O	-22.06	1.07	1.24
1	A	377	MET	C-O	-20.59	0.98	1.24
1	C	328	VAL	CA-CB	-20.37	1.26	1.54
1	C	26	GLU	C-N	-20.34	1.06	1.33
1	C	147	THR	C-O	-19.68	1.00	1.23
1	E	376	VAL	CA-CB	-19.34	1.22	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	368	SER	C-O	-18.73	1.00	1.23
1	F	376	VAL	CA-CB	-18.24	1.26	1.54
1	C	147	THR	N-CA	-16.84	1.24	1.46
1	A	328	VAL	C-O	-16.52	1.04	1.24
1	D	377	MET	N-CA	-16.49	1.26	1.46
1	B	328	VAL	C-O	-15.85	1.05	1.24
1	D	377	MET	C-O	-15.83	1.02	1.24
1	D	370	THR	CA-CB	-15.78	1.30	1.53
1	E	378	PHE	CA-C	-15.66	1.31	1.52
1	D	328	VAL	CA-CB	-15.64	1.32	1.54
1	D	327	LEU	C-O	-14.83	1.05	1.24
1	F	376	VAL	C-O	-14.69	1.04	1.23
1	B	26	GLU	C-N	-14.67	1.14	1.33
1	E	378	PHE	C-O	-14.64	1.05	1.24
1	C	414	LYS	C-O	-13.97	1.06	1.24
1	C	329	ASN	CA-C	-13.68	1.35	1.52
1	A	378	PHE	C-O	-13.29	1.08	1.23
1	B	328	VAL	CA-CB	-13.28	1.36	1.54
1	C	329	ASN	C-O	-13.13	1.04	1.23
1	D	377	MET	CA-C	-13.13	1.35	1.52
1	D	376	VAL	C-O	-12.71	1.09	1.23
1	A	26	GLU	C-N	-12.62	1.17	1.33
1	D	328	VAL	C-O	-12.49	1.10	1.24
1	D	377	MET	SD-CE	-12.41	1.48	1.79
1	D	376	VAL	CA-CB	-12.30	1.38	1.54
1	D	369	GLU	N-CA	-12.18	1.30	1.46
1	A	328	VAL	CB-CG1	-12.09	1.12	1.52
1	C	328	VAL	CA-C	-11.41	1.38	1.52
1	D	370	THR	C-O	-11.14	1.07	1.23
1	C	328	VAL	N-CA	-11.06	1.32	1.46
1	A	378	PHE	CE2-CZ	-10.86	1.06	1.38
1	D	370	THR	CA-C	-10.77	1.37	1.53
1	C	147	THR	CA-CB	-10.70	1.35	1.53
1	E	377	MET	C-O	-10.64	1.09	1.24
1	C	329	ASN	CG-OD1	-10.58	1.03	1.23
1	E	376	VAL	C-O	-10.32	1.12	1.23
1	D	328	VAL	CB-CG2	-10.28	1.18	1.52
1	D	327	LEU	CG-CD1	-10.06	1.19	1.52
1	D	327	LEU	CG-CD2	-9.92	1.19	1.52
1	F	369	GLU	C-O	-9.82	1.09	1.23
1	D	328	VAL	CB-CG1	-9.76	1.20	1.52
1	A	377	MET	SD-CE	-9.75	1.55	1.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	370	THR	CB-CG2	-9.73	1.20	1.52
1	B	328	VAL	CA-C	-9.69	1.40	1.52
1	D	329	ASN	C-O	-9.66	1.11	1.24
1	D	377	MET	CA-CB	-9.60	1.39	1.53
1	E	377	MET	N-CA	-9.46	1.36	1.46
1	C	147	THR	CB-CG2	-9.44	1.21	1.52
1	E	376	VAL	N-CA	-9.43	1.35	1.46
1	E	378	PHE	CE2-CZ	-9.38	1.10	1.38
1	A	328	VAL	CB-CG2	-9.38	1.21	1.52
1	E	376	VAL	CA-C	-9.33	1.41	1.52
1	D	368	SER	C-N	-9.16	1.21	1.33
1	B	328	VAL	CB-CG2	-9.07	1.22	1.52
1	C	414	LYS	CB-CG	-8.94	1.25	1.52
1	F	376	VAL	CB-CG2	-8.66	1.24	1.52
1	D	378	PHE	CA-C	-8.63	1.42	1.53
1	D	377	MET	CB-CG	-8.59	1.26	1.52
1	D	370	THR	CB-OG1	-8.53	1.30	1.43
1	C	414	LYS	N-CA	-8.51	1.35	1.46
1	D	328	VAL	CA-C	-8.48	1.41	1.52
1	D	376	VAL	CB-CG2	-8.44	1.24	1.52
1	C	147	THR	CA-C	-8.43	1.41	1.52
1	C	328	VAL	CB-CG2	-8.38	1.24	1.52
1	D	377	MET	CG-SD	-8.27	1.60	1.80
1	D	369	GLU	CA-C	-8.26	1.42	1.52
1	E	378	PHE	CA-CB	-8.26	1.39	1.53
1	A	378	PHE	CD1-CE1	-8.23	1.14	1.38
1	D	376	VAL	N-CA	-8.20	1.36	1.46
1	C	329	ASN	CG-ND2	-8.13	1.16	1.33
1	E	377	MET	SD-CE	-8.13	1.59	1.79
1	E	378	PHE	CG-CD1	-8.00	1.22	1.38
1	A	415	GLU	CA-CB	-7.85	1.44	1.53
1	C	414	LYS	CA-CB	-7.79	1.40	1.53
1	E	377	MET	CA-C	-7.66	1.43	1.53
1	A	377	MET	N-CA	-7.65	1.36	1.46
1	A	378	PHE	CD2-CE2	-7.59	1.15	1.38
1	B	328	VAL	CB-CG1	-7.56	1.27	1.52
1	F	376	VAL	CA-C	-7.47	1.42	1.53
1	C	147	THR	C-N	-7.46	1.23	1.33
1	C	414	LYS	CD-CE	-7.23	1.30	1.52
1	A	328	VAL	N-CA	-7.20	1.37	1.46
1	D	378	PHE	CA-CB	-7.19	1.45	1.54
1	D	327	LEU	CA-C	-7.16	1.42	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	328	VAL	N-CA	-7.13	1.37	1.46
1	A	378	PHE	CG-CD1	-7.05	1.24	1.38
1	F	376	VAL	CB-CG1	-7.02	1.29	1.52
1	D	378	PHE	CD2-CE2	-6.96	1.17	1.38
1	C	328	VAL	CB-CG1	-6.92	1.29	1.52
1	A	377	MET	CG-SD	-6.91	1.63	1.80
1	D	376	VAL	CA-C	-6.81	1.44	1.52
1	C	414	LYS	CE-NZ	-6.77	1.29	1.49
1	D	327	LEU	C-N	-6.74	1.25	1.33
1	A	378	PHE	CE1-CZ	-6.68	1.18	1.38
1	E	377	MET	CG-SD	-6.66	1.64	1.80
1	E	378	PHE	C-N	-6.65	1.24	1.33
1	F	434	VAL	CA-CB	6.61	1.62	1.54
1	F	369	GLU	CB-CG	-6.55	1.32	1.52
1	F	369	GLU	C-N	-6.51	1.25	1.33
1	E	375	GLY	C-N	-6.47	1.25	1.33
1	B	182	MET	SD-CE	-6.46	1.63	1.79
1	E	378	PHE	N-CA	-6.46	1.37	1.46
1	C	368	SER	CA-C	-6.43	1.44	1.52
1	D	378	PHE	CE1-CZ	-6.41	1.19	1.38
1	F	369	GLU	CD-OE1	-6.41	1.13	1.25
1	A	378	PHE	CA-C	-6.27	1.44	1.53
1	C	173	MET	SD-CE	6.27	1.95	1.79
1	A	377	MET	CA-C	-6.12	1.44	1.52
1	A	378	PHE	CG-CD2	-6.07	1.26	1.38
1	D	328	VAL	N-CA	-6.06	1.37	1.46
1	E	378	PHE	CE1-CZ	-6.02	1.20	1.38
1	D	377	MET	C-N	-5.90	1.27	1.33
1	A	328	VAL	C-N	-5.83	1.25	1.33
1	F	369	GLU	CG-CD	-5.78	1.37	1.52
1	E	376	VAL	CB-CG1	-5.76	1.33	1.52
1	A	377	MET	CB-CG	-5.71	1.35	1.52
1	C	368	SER	CA-CB	-5.69	1.43	1.54
1	B	434	VAL	CA-CB	5.69	1.61	1.54
1	D	378	PHE	CD1-CE1	-5.64	1.21	1.38
1	E	377	MET	CB-CG	-5.63	1.35	1.52
1	C	329	ASN	CB-CG	-5.58	1.38	1.52
1	D	376	VAL	CB-CG1	-5.56	1.34	1.52
1	A	9	PRO	N-CD	-5.55	1.40	1.47
1	A	377	MET	CA-CB	-5.34	1.44	1.53
1	F	369	GLU	CA-CB	-5.24	1.44	1.53
1	C	414	LYS	CA-C	-5.20	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	378	PHE	CD1-CE1	-5.20	1.23	1.38
1	D	15	PRO	N-CD	-5.16	1.40	1.47
1	A	377	MET	C-N	-5.10	1.26	1.33
1	D	369	GLU	CD-OE1	-5.09	1.15	1.25
1	E	378	PHE	CG-CD2	-5.08	1.28	1.38
1	F	369	GLU	N-CA	-5.04	1.38	1.47
1	D	182	MET	SD-CE	-5.03	1.67	1.79

All (334) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	377	MET	N-CA-C	20.54	143.56	112.54
1	B	329	ASN	N-CA-C	19.38	152.09	110.80
1	A	369	GLU	N-CA-C	-18.74	80.01	110.17
1	A	380	ASN	N-CA-C	-18.02	89.07	114.12
1	D	377	MET	N-CA-C	17.55	137.69	112.94
1	D	327	LEU	N-CA-C	17.04	133.32	112.87
1	D	25	THR	O-C-N	-16.79	101.31	123.14
1	D	325	ALA	N-CA-C	-16.40	88.04	110.35
1	A	379	ILE	CB-CA-C	-15.61	85.69	111.29
1	F	328	VAL	N-CA-CB	-15.61	85.48	111.23
1	E	327	LEU	N-CA-C	-15.42	87.11	108.86
1	B	60	ILE	N-CA-C	-14.40	84.39	107.28
1	C	378	PHE	N-CA-C	14.31	132.26	108.08
1	D	25	THR	CA-C-N	14.18	147.87	122.92
1	D	25	THR	C-N-CA	14.18	147.87	122.92
1	F	60	ILE	N-CA-C	-14.06	84.92	107.28
1	E	329	ASN	N-CA-C	13.92	131.79	112.45
1	B	328	VAL	N-CA-CB	-13.59	88.81	111.23
1	B	419	LYS	CB-CA-C	-13.38	87.66	110.81
1	C	328	VAL	N-CA-CB	-13.33	89.23	111.23
1	E	376	VAL	CB-CA-C	-13.30	87.82	110.30
1	A	60	ILE	N-CA-C	-13.24	86.22	107.28
1	F	287	ARG	N-CA-C	13.21	127.14	111.02
1	E	378	PHE	N-CA-CB	-13.05	88.44	110.49
1	B	329	ASN	N-CA-CB	-12.89	88.70	110.49
1	B	332	GLY	N-CA-C	12.85	126.40	111.36
1	F	369	GLU	CA-C-N	12.84	142.02	121.74
1	F	369	GLU	C-N-CA	12.84	142.02	121.74
1	D	328	VAL	CB-CA-C	-12.59	95.75	110.73
1	D	369	GLU	N-CA-C	-12.29	86.93	108.69
1	A	282	TRP	CB-CA-C	-12.22	95.30	110.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	370	THR	N-CA-CB	-12.05	91.23	110.39
1	B	142	ASN	N-CA-C	12.00	133.85	110.56
1	B	370	THR	N-CA-CB	-11.93	91.42	110.39
1	C	327	LEU	N-CA-C	11.91	128.18	113.17
1	A	377	MET	N-CA-C	11.85	136.05	110.80
1	C	25	THR	O-C-N	-11.60	108.29	123.14
1	D	370	THR	CB-CA-C	-11.24	89.17	112.44
1	E	369	GLU	N-CA-C	-11.21	88.41	108.02
1	E	142	ASN	N-CA-C	11.16	132.21	110.56
1	D	325	ALA	CB-CA-C	11.11	129.50	109.62
1	D	85	LYS	N-CA-C	-11.04	93.19	109.63
1	F	332	GLY	N-CA-C	11.04	124.27	111.36
1	B	415	GLU	CB-CA-C	-10.93	94.32	110.06
1	C	376	VAL	CB-CA-C	-10.93	96.22	111.19
1	C	9	PRO	CA-N-CD	-10.69	97.04	112.00
1	C	142	ASN	N-CA-C	10.66	125.93	107.28
1	B	369	GLU	CB-CA-C	-10.62	93.48	110.79
1	E	369	GLU	CB-CA-C	-10.61	93.66	110.74
1	A	142	ASN	N-CA-C	10.49	130.92	110.56
1	C	25	THR	CA-C-N	10.44	141.74	122.74
1	C	25	THR	C-N-CA	10.44	141.74	122.74
1	C	332	GLY	N-CA-C	10.42	123.55	111.36
1	B	328	VAL	CA-C-N	-10.40	101.68	121.54
1	B	328	VAL	C-N-CA	-10.40	101.68	121.54
1	E	69	GLY	N-CA-C	10.38	125.47	110.63
1	D	370	THR	N-CA-CB	-10.31	93.33	110.65
1	A	332	GLY	N-CA-C	10.28	123.39	111.36
1	D	84	PRO	CB-CA-C	10.23	128.44	111.56
1	C	420	VAL	N-CA-CB	-10.17	96.97	111.21
1	E	420	VAL	N-CA-CB	-10.15	97.00	111.21
1	A	420	VAL	N-CA-CB	-10.15	97.00	111.21
1	A	282	TRP	N-CA-C	10.10	125.06	107.49
1	E	332	GLY	N-CA-C	10.10	123.17	111.36
1	C	69	GLY	N-CA-C	10.09	125.06	110.63
1	A	9	PRO	CA-N-CD	-10.09	97.88	112.00
1	B	9	PRO	CA-N-CD	-9.88	98.17	112.00
1	D	69	GLY	N-CA-C	9.87	124.75	110.63
1	C	414	LYS	N-CA-C	9.84	123.23	111.82
1	A	69	GLY	N-CA-C	9.82	124.68	110.63
1	B	69	GLY	N-CA-C	9.80	123.72	110.69
1	B	369	GLU	N-CA-C	-9.71	90.80	107.99
1	C	142	ASN	CB-CA-C	-9.72	98.10	111.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	326	GLN	N-CA-CB	-9.65	94.18	110.49
1	A	292	LYS	N-CA-C	-9.58	102.16	114.04
1	D	420	VAL	N-CA-CB	-9.47	97.95	111.21
1	F	376	VAL	CB-CA-C	-9.40	98.31	111.19
1	F	292	LYS	N-CA-C	-9.32	100.78	113.18
1	A	379	ILE	N-CA-C	9.12	128.32	109.34
1	C	147	THR	CB-CA-C	9.07	124.06	109.90
1	B	420	VAL	N-CA-CB	-9.02	98.58	111.21
1	D	15	PRO	CA-N-CD	-9.02	99.37	112.00
1	C	15	PRO	CA-N-CD	-9.00	99.40	112.00
1	A	413	ARG	CB-CA-C	8.99	128.18	109.38
1	E	15	PRO	CA-N-CD	-8.96	99.45	112.00
1	F	142	ASN	N-CA-C	8.86	129.66	110.80
1	A	15	PRO	CA-N-CD	-8.85	99.61	112.00
1	A	25	THR	O-C-N	-8.80	111.87	123.14
1	C	287	ARG	N-CA-C	8.79	120.78	111.03
1	F	69	GLY	N-CA-C	8.77	123.17	110.63
1	A	169	ILE	N-CA-C	8.73	115.55	106.21
1	C	147	THR	OG1-CB-CG2	-8.69	91.92	109.30
1	D	142	ASN	N-CA-C	8.63	129.18	110.80
1	E	341	LEU	CB-CA-C	-8.51	91.36	110.07
1	B	175	GLY	N-CA-C	8.43	122.83	111.03
1	D	376	VAL	CB-CA-C	-8.32	95.90	111.30
1	D	379	ILE	N-CA-C	8.32	126.65	109.34
1	A	377	MET	O-C-N	-8.29	111.57	122.59
1	F	15	PRO	CA-N-CD	-8.21	100.50	112.00
1	A	413	ARG	N-CA-C	-8.16	96.61	109.50
1	D	341	LEU	CB-CA-C	-8.16	92.48	110.67
1	E	377	MET	N-CA-CB	-8.14	95.39	111.60
1	F	370	THR	N-CA-CB	-8.14	98.10	110.39
1	D	377	MET	CA-C-O	-8.12	109.90	119.48
1	F	169	ILE	N-CA-C	8.06	114.84	106.21
1	A	287	ARG	N-CA-C	7.99	119.89	111.03
1	D	326	GLN	N-CA-C	7.99	127.81	110.80
1	D	376	VAL	CA-C-N	-7.91	110.19	122.37
1	D	376	VAL	C-N-CA	-7.91	110.19	122.37
1	F	415	GLU	N-CA-CB	-7.88	98.20	111.20
1	B	327	LEU	N-CA-C	7.84	121.36	111.24
1	C	252	LEU	N-CA-C	-7.82	101.86	111.40
1	F	452	ASN	N-CA-C	7.81	122.93	112.30
1	C	328	VAL	N-CA-C	7.81	125.58	109.34
1	F	379	ILE	N-CA-CB	-7.79	98.37	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	327	LEU	N-CA-C	7.77	119.66	111.03
1	C	414	LYS	N-CA-CB	-7.76	98.25	110.28
1	A	25	THR	CA-C-N	7.74	136.82	122.74
1	A	25	THR	C-N-CA	7.74	136.82	122.74
1	D	379	ILE	CB-CA-C	-7.70	98.66	111.29
1	A	175	GLY	N-CA-C	7.68	121.78	111.03
1	A	70	GLY	N-CA-C	-7.66	95.02	113.18
1	D	326	GLN	CB-CA-C	-7.58	95.34	110.42
1	E	379	ILE	N-CA-C	7.55	125.05	109.34
1	E	70	GLY	N-CA-C	-7.50	95.39	113.18
1	C	377	MET	N-CA-CB	-7.40	98.95	111.31
1	D	327	LEU	CA-C-N	-7.39	112.91	123.11
1	D	327	LEU	C-N-CA	-7.39	112.91	123.11
1	F	378	PHE	CB-CA-C	7.38	125.11	110.42
1	F	376	VAL	N-CA-CB	-7.38	103.08	112.60
1	B	25	THR	CA-C-N	7.32	136.05	122.74
1	B	25	THR	C-N-CA	7.32	136.05	122.74
1	B	252	LEU	N-CA-C	-7.22	102.59	111.40
1	C	341	LEU	CB-CA-C	-7.21	94.58	110.67
1	F	341	LEU	CB-CA-C	-7.21	94.60	110.67
1	A	341	LEU	CB-CA-C	-7.16	94.70	110.67
1	A	329	ASN	N-CA-CB	7.15	122.57	110.49
1	A	283	ASN	N-CA-CB	-7.14	98.06	110.76
1	D	377	MET	N-CA-CB	-7.11	99.25	110.98
1	C	68	PRO	CA-C-N	-7.11	111.70	121.23
1	C	68	PRO	C-N-CA	-7.11	111.70	121.23
1	D	175	GLY	N-CA-C	7.10	120.97	111.03
1	E	327	LEU	N-CA-CB	7.09	123.16	111.31
1	B	341	LEU	CB-CA-C	-7.09	96.23	111.11
1	F	252	LEU	N-CA-C	-7.08	102.76	111.40
1	A	202	ASP	CA-C-N	7.08	127.06	119.28
1	A	202	ASP	C-N-CA	7.08	127.06	119.28
1	C	70	GLY	N-CA-C	-7.04	96.51	113.18
1	F	326	GLN	N-CA-CB	-7.01	98.58	110.50
1	E	175	GLY	N-CA-C	7.01	120.84	111.03
1	C	334	ILE	CB-CA-C	-7.00	102.85	111.32
1	A	252	LEU	N-CA-C	-6.97	102.90	111.40
1	D	252	LEU	N-CA-C	-6.96	102.91	111.40
1	D	169	ILE	N-CA-C	6.93	113.62	106.21
1	C	377	MET	CB-CA-C	6.92	128.27	111.65
1	A	331	LEU	N-CA-C	-6.90	102.79	111.90
1	F	286	TYR	CB-CA-C	6.88	124.11	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	391	PHE	N-CA-C	-6.85	104.73	113.23
1	B	70	GLY	N-CA-C	-6.84	96.96	113.18
1	F	415	GLU	N-CA-C	6.84	121.31	112.41
1	A	370	THR	N-CA-CB	-6.83	98.94	110.49
1	D	202	ASP	CA-C-N	6.82	127.39	119.47
1	D	202	ASP	C-N-CA	6.82	127.39	119.47
1	B	25	THR	O-C-N	-6.80	114.44	123.14
1	C	150	ALA	N-CA-C	-6.78	103.81	111.14
1	E	378	PHE	CA-C-N	-6.76	109.80	121.97
1	E	378	PHE	C-N-CA	-6.76	109.80	121.97
1	F	370	THR	N-CA-C	-6.72	99.32	109.60
1	B	459	GLU	N-CA-C	-6.70	96.95	107.73
1	E	252	LEU	N-CA-C	-6.68	103.25	111.40
1	C	202	ASP	CA-C-N	6.67	126.61	119.28
1	C	202	ASP	C-N-CA	6.67	126.61	119.28
1	F	376	VAL	N-CA-C	6.65	118.40	108.96
1	D	353	ILE	N-CA-C	6.64	119.39	111.09
1	D	70	GLY	N-CA-C	-6.63	97.47	113.18
1	D	331	LEU	N-CA-C	-6.63	96.68	110.80
1	E	202	ASP	CA-C-N	6.62	126.56	119.28
1	E	202	ASP	C-N-CA	6.62	126.56	119.28
1	F	329	ASN	N-CA-C	6.61	121.17	112.72
1	F	197	TRP	N-CA-C	-6.59	99.51	109.79
1	F	14	LYS	CA-C-N	-6.57	113.90	120.21
1	F	14	LYS	C-N-CA	-6.57	113.90	120.21
1	A	61	LYS	N-CA-CB	-6.56	99.41	110.49
1	D	273	ARG	N-CA-C	-6.54	99.87	110.20
1	B	61	LYS	N-CA-CB	-6.54	99.44	110.49
1	F	202	ASP	CA-C-N	6.53	127.04	119.47
1	F	202	ASP	C-N-CA	6.53	127.04	119.47
1	F	61	LYS	N-CA-CB	-6.50	99.51	110.49
1	A	414	LYS	CB-CA-C	-6.49	99.90	110.08
1	A	378	PHE	N-CA-C	6.48	118.42	109.54
1	D	459	GLU	N-CA-C	-6.46	97.80	108.07
1	B	419	LYS	N-CA-C	6.45	120.16	112.93
1	A	273	ARG	N-CA-C	-6.43	100.03	110.20
1	E	376	VAL	CA-C-N	-6.43	109.25	121.15
1	E	376	VAL	C-N-CA	-6.43	109.25	121.15
1	A	326	GLN	CB-CA-C	6.43	127.25	111.95
1	A	263	LEU	N-CA-C	-6.40	104.22	111.07
1	A	68	PRO	CA-C-N	-6.36	112.70	121.23
1	A	68	PRO	C-N-CA	-6.36	112.70	121.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	205	ILE	N-CA-C	6.34	117.37	110.21
1	C	353	ILE	N-CA-C	6.28	118.94	111.09
1	D	329	ASN	N-CA-C	6.25	124.12	110.80
1	B	273	ARG	N-CA-C	-6.25	100.33	110.20
1	A	84	PRO	CB-CA-C	6.24	119.38	111.39
1	F	175	GLY	N-CA-C	6.21	119.72	111.03
1	B	459	GLU	CB-CA-C	6.19	122.19	110.56
1	F	70	GLY	N-CA-C	-6.15	98.60	113.18
1	A	205	ILE	N-CA-C	6.14	117.97	109.80
1	C	328	VAL	CA-C-O	-6.12	113.13	120.78
1	B	353	ILE	N-CA-C	6.11	118.73	111.09
1	C	273	ARG	N-CA-C	-6.09	100.58	110.20
1	A	326	GLN	N-CA-CB	-6.08	101.05	111.21
1	E	213	ASP	N-CA-C	6.08	120.54	113.18
1	F	391	PHE	N-CA-C	-6.07	105.70	113.23
1	E	85	LYS	N-CA-C	-6.04	100.36	109.79
1	A	62	VAL	CA-C-N	6.02	127.37	119.84
1	A	62	VAL	C-N-CA	6.02	127.37	119.84
1	B	327	LEU	N-CA-CB	-6.02	101.22	110.07
1	C	391	PHE	N-CA-C	-6.00	105.79	113.23
1	E	391	PHE	N-CA-C	-5.99	105.80	113.23
1	E	62	VAL	CA-C-N	5.97	127.31	119.84
1	E	62	VAL	C-N-CA	5.97	127.31	119.84
1	E	329	ASN	N-CA-CB	-5.95	101.40	110.26
1	D	200	VAL	N-CA-C	-5.94	103.49	111.44
1	B	328	VAL	CB-CA-C	5.93	121.01	111.29
1	C	146	ASN	N-CA-CB	-5.90	101.59	110.91
1	F	325	ALA	N-CA-C	5.89	123.35	110.80
1	E	377	MET	CA-C-O	-5.88	113.40	119.51
1	A	378	PHE	CA-CB-CG	5.80	119.61	113.80
1	C	146	ASN	N-CA-C	5.77	119.09	112.57
1	F	62	VAL	CA-C-N	5.75	127.03	119.84
1	F	62	VAL	C-N-CA	5.75	127.03	119.84
1	D	62	VAL	CA-C-N	5.75	127.02	119.84
1	D	62	VAL	C-N-CA	5.75	127.02	119.84
1	E	84	PRO	CB-CA-C	5.74	118.73	111.39
1	B	62	VAL	CA-C-N	5.72	126.99	119.84
1	B	62	VAL	C-N-CA	5.72	126.99	119.84
1	F	462	THR	N-CA-C	-5.70	99.89	109.07
1	E	331	LEU	N-CA-C	-5.70	104.38	111.90
1	E	273	ARG	N-CA-C	-5.70	101.20	110.20
1	D	331	LEU	N-CA-CB	5.69	120.10	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	250	VAL	N-CA-C	-5.68	104.60	112.50
1	D	377	MET	CA-C-N	-5.65	110.88	121.95
1	D	377	MET	C-N-CA	-5.65	110.88	121.95
1	E	250	VAL	N-CA-C	-5.65	103.88	111.44
1	F	334	ILE	CB-CA-C	-5.62	104.52	111.32
1	B	85	LYS	N-CA-C	-5.60	101.03	109.60
1	C	145	GLY	N-CA-C	-5.58	102.72	112.55
1	D	213	ASP	N-CA-C	5.58	119.93	113.18
1	D	84	PRO	N-CA-C	-5.58	100.98	112.47
1	C	62	VAL	CA-C-N	5.57	126.80	119.84
1	C	62	VAL	C-N-CA	5.57	126.80	119.84
1	D	327	LEU	CA-CB-CG	5.56	135.76	116.30
1	F	417	ALA	N-CA-C	-5.56	101.81	110.42
1	F	369	GLU	N-CA-C	5.53	119.33	107.67
1	B	334	ILE	CB-CA-C	-5.52	104.64	111.32
1	D	328	VAL	CA-C-O	-5.51	114.91	120.31
1	D	197	TRP	N-CA-C	-5.50	99.08	110.80
1	E	420	VAL	N-CA-C	5.50	120.76	108.88
1	D	391	PHE	N-CA-C	-5.49	106.08	112.89
1	E	334	ILE	CB-CA-C	-5.49	104.67	111.32
1	C	60	ILE	N-CA-C	-5.49	98.79	106.53
1	A	417	ALA	N-CA-C	-5.48	101.92	110.42
1	A	391	PHE	N-CA-C	-5.45	106.48	113.23
1	D	378	PHE	CA-C-N	-5.44	112.17	121.97
1	D	378	PHE	C-N-CA	-5.44	112.17	121.97
1	E	353	ILE	N-CA-C	5.44	117.89	111.09
1	D	376	VAL	N-CA-C	5.43	115.51	108.35
1	E	377	MET	CA-C-N	-5.42	111.19	121.54
1	E	377	MET	C-N-CA	-5.42	111.19	121.54
1	E	197	TRP	N-CA-C	-5.40	99.29	110.80
1	F	263	LEU	N-CA-C	-5.40	105.29	111.07
1	F	84	PRO	CB-CA-C	5.39	118.29	111.39
1	B	60	ILE	CB-CA-C	5.37	117.98	110.99
1	B	455	ASP	N-CA-C	5.37	115.63	108.38
1	D	210	VAL	N-CA-C	5.36	115.91	108.84
1	F	273	ARG	N-CA-C	-5.35	101.75	110.20
1	D	378	PHE	O-C-N	-5.35	116.73	122.88
1	F	200	VAL	N-CA-C	-5.34	104.28	111.44
1	D	328	VAL	CG1-CB-CG2	-5.33	99.08	110.80
1	D	420	VAL	N-CA-C	5.32	120.38	108.88
1	D	459	GLU	CB-CA-C	5.31	119.16	110.03
1	B	287	ARG	N-CA-C	5.31	118.09	111.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	462	THR	N-CA-C	-5.30	100.60	109.24
1	E	98	GLN	N-CA-C	-5.29	101.03	109.07
1	D	330	ALA	N-CA-C	5.28	117.32	108.23
1	F	250	VAL	N-CA-C	-5.28	104.37	111.44
1	D	327	LEU	O-C-N	-5.28	115.42	122.43
1	A	78	TRP	N-CA-C	5.27	118.49	111.75
1	E	205	ILE	N-CA-C	5.26	116.16	110.21
1	C	197	TRP	N-CA-C	-5.25	99.61	110.80
1	D	68	PRO	CA-C-N	-5.25	114.19	121.23
1	D	68	PRO	C-N-CA	-5.25	114.19	121.23
1	C	213	ASP	N-CA-C	5.23	119.51	113.18
1	C	417	ALA	N-CA-C	-5.23	102.32	110.42
1	D	378	PHE	N-CA-CB	-5.23	103.09	110.51
1	B	417	ALA	N-CA-C	-5.22	102.79	110.52
1	D	377	MET	O-C-N	-5.22	115.88	122.19
1	B	197	TRP	N-CA-C	-5.20	99.73	110.80
1	F	232	ILE	N-CA-C	-5.20	100.08	107.77
1	F	98	GLN	N-CA-C	-5.19	101.18	109.07
1	D	250	VAL	N-CA-C	-5.18	104.62	111.09
1	C	20	ILE	N-CA-C	-5.18	105.45	113.16
1	A	328	VAL	N-CA-CB	5.17	119.76	111.23
1	A	85	LYS	N-CA-C	-5.16	99.80	110.80
1	A	103	ARG	N-CA-C	-5.16	106.93	113.18
1	D	98	GLN	N-CA-C	-5.16	101.23	109.07
1	A	150	ALA	N-CA-C	-5.15	105.58	111.14
1	A	334	ILE	CB-CA-C	-5.15	105.09	111.32
1	A	98	GLN	N-CA-C	-5.14	101.25	109.07
1	E	414	LYS	N-CA-C	5.14	118.70	112.23
1	B	14	LYS	CA-C-N	-5.14	115.44	120.52
1	B	14	LYS	C-N-CA	-5.14	115.44	120.52
1	B	202	ASP	CA-C-N	5.14	126.26	119.84
1	B	202	ASP	C-N-CA	5.14	126.26	119.84
1	D	462	THR	N-CA-C	-5.13	100.36	108.73
1	A	462	THR	N-CA-C	-5.11	100.18	108.52
1	E	280	ASP	N-CA-C	5.11	119.09	113.21
1	F	353	ILE	N-CA-C	5.11	117.48	111.09
1	A	370	THR	N-CA-C	-5.10	99.94	110.80
1	A	420	VAL	N-CA-C	5.10	119.89	108.88
1	B	84	PRO	CB-CA-C	5.08	117.90	111.39
1	E	68	PRO	CA-C-N	-5.06	114.45	121.23
1	E	68	PRO	C-N-CA	-5.06	114.45	121.23
1	A	60	ILE	CB-CA-C	5.05	117.56	110.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	78	TRP	N-CA-C	5.05	118.21	111.75
1	A	228	VAL	CB-CA-C	-5.04	105.89	110.63
1	F	375	GLY	O-C-N	-5.04	116.74	123.64
1	D	205	ILE	N-CA-C	5.04	116.50	109.80
1	A	232	ILE	N-CA-C	-5.03	100.28	107.78
1	A	14	LYS	CA-C-N	-5.01	115.56	120.52
1	A	14	LYS	C-N-CA	-5.01	115.56	120.52
1	C	250	VAL	N-CA-C	-5.01	105.02	112.04
1	A	415	GLU	CA-C-O	5.00	128.17	120.37

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	377	MET	CA

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	377	MET	Mainchain
1	B	251	TYR	Sidechain
1	C	251	TYR	Sidechain
1	D	251	TYR	Sidechain
1	D	327	LEU	Mainchain
1	E	251	TYR	Sidechain
1	F	251	TYR	Sidechain
1	F	369	GLU	Peptide,Mainchain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3876	0	3789	305	0
1	B	3876	0	3789	306	0
1	C	3876	0	3788	293	2
1	D	3876	0	3788	323	0
1	E	3876	0	3789	322	2
1	F	3876	0	3788	324	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	23256	0	22731	1828	2

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 40.

All (1828) 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:E:24:PHE:CD2	1:E:325:ALA:HB1	1.34	1.62
1:E:419:LYS:CG	1:E:470:THR:CG2	1.80	1.58
1:B:410:VAL:HG11	1:B:412:TYR:CZ	1.23	1.57
1:F:419:LYS:CG	1:F:470:THR:CG2	1.77	1.57
1:E:24:PHE:HD2	1:E:325:ALA:CB	1.17	1.57
1:C:419:LYS:CG	1:C:470:THR:CG2	1.83	1.53
1:F:24:PHE:HD2	1:F:325:ALA:CB	1.17	1.52
1:D:419:LYS:HG2	1:D:470:THR:CG2	1.40	1.51
1:E:24:PHE:CD2	1:E:325:ALA:CB	1.90	1.51
1:F:419:LYS:HG3	1:F:470:THR:CG2	1.37	1.51
1:D:419:LYS:CG	1:D:470:THR:CG2	1.89	1.50
1:A:419:LYS:CG	1:A:470:THR:CG2	1.92	1.47
1:F:24:PHE:CD2	1:F:325:ALA:CB	1.98	1.47
1:F:24:PHE:CD2	1:F:325:ALA:HB1	1.49	1.46
1:A:410:VAL:HG11	1:A:412:TYR:CZ	1.49	1.45
1:B:410:VAL:CG1	1:B:412:TYR:CZ	2.00	1.44
1:E:24:PHE:CB	1:E:325:ALA:HB2	1.49	1.40
1:B:410:VAL:HG11	1:B:412:TYR:CE2	1.55	1.40
1:E:419:LYS:HG2	1:E:470:THR:CG2	1.39	1.39
1:A:419:LYS:HG2	1:A:470:THR:CG2	1.47	1.39
1:C:419:LYS:HG3	1:C:470:THR:CG2	1.46	1.36
1:D:411:ASN:HD21	1:D:413:ARG:CB	1.39	1.35
1:C:419:LYS:HG2	1:C:470:THR:CG2	1.50	1.32
1:D:411:ASN:ND2	1:D:413:ARG:HB2	1.44	1.32
1:F:419:LYS:HG2	1:F:470:THR:CG2	1.48	1.29
1:E:24:PHE:HB3	1:E:325:ALA:CB	1.62	1.28
1:D:419:LYS:CG	1:D:470:THR:HG22	1.57	1.23
1:E:419:LYS:CG	1:E:470:THR:HG22	1.52	1.22
1:A:379:ILE:HG22	1:A:379:ILE:O	1.41	1.19
1:A:419:LYS:CG	1:A:470:THR:HG22	1.61	1.18
1:E:419:LYS:HG3	1:E:470:THR:CG2	1.51	1.17
1:A:410:VAL:CG1	1:A:412:TYR:CZ	2.26	1.17
1:A:419:LYS:HG3	1:A:470:THR:CG2	1.65	1.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:419:LYS:HG3	1:D:470:THR:CG2	1.65	1.16
1:F:481:VAL:HG22	1:F:482:GLU:H	1.12	1.15
1:B:285:TRP:CE2	1:B:379:ILE:HD11	1.81	1.14
1:F:326:GLN:NE2	1:F:330:ALA:HB3	1.59	1.14
1:B:410:VAL:CG1	1:B:412:TYR:CE1	2.30	1.14
1:F:419:LYS:CG	1:F:470:THR:HG22	1.49	1.14
1:A:410:VAL:HG11	1:A:412:TYR:CE1	1.82	1.13
1:A:239:GLY:O	1:A:377:MET:O	1.67	1.12
1:B:415:GLU:H	1:B:473:PRO:HB2	1.12	1.12
1:F:411:ASN:HD21	1:F:413:ARG:HB2	1.06	1.11
1:B:481:VAL:HG22	1:B:482:GLU:H	1.13	1.11
1:C:411:ASN:HD21	1:C:413:ARG:HB2	1.03	1.11
1:E:378:PHE:CD1	1:E:379:ILE:N	2.18	1.10
1:F:419:LYS:HG3	1:F:470:THR:HG21	1.29	1.10
1:C:481:VAL:HG22	1:C:482:GLU:H	1.14	1.10
1:F:24:PHE:CD2	1:F:325:ALA:HB2	1.85	1.10
1:E:24:PHE:CG	1:E:325:ALA:HB2	1.85	1.09
1:F:327:LEU:O	1:F:333:ALA:N	1.85	1.09
1:C:286:TYR:CB	1:C:378:PHE:O	2.00	1.09
1:F:326:GLN:HE22	1:F:330:ALA:HB3	0.98	1.08
1:C:419:LYS:HG3	1:C:470:THR:HG21	1.28	1.08
1:E:481:VAL:HG22	1:E:482:GLU:H	1.11	1.08
1:D:481:VAL:HG22	1:D:482:GLU:H	1.09	1.07
1:C:419:LYS:CG	1:C:470:THR:HG22	1.62	1.06
1:E:24:PHE:HB3	1:E:325:ALA:HB2	1.10	1.06
1:C:141:CYS:O	1:C:142:ASN:OD1	1.74	1.05
1:A:282:TRP:CD2	1:A:282:TRP:O	2.09	1.05
1:E:24:PHE:CG	1:E:325:ALA:CB	2.39	1.05
1:F:26:GLU:HB2	1:F:69:GLY:HA2	1.36	1.05
1:A:419:LYS:HG2	1:A:470:THR:HG23	1.11	1.04
1:A:481:VAL:HG22	1:A:482:GLU:H	1.14	1.04
1:D:135:LEU:HD21	1:F:94:LEU:HD21	1.38	1.04
1:D:414:LYS:O	1:D:473:PRO:HB2	1.57	1.03
1:E:419:LYS:HG3	1:E:470:THR:HG21	1.36	1.03
1:F:24:PHE:HB3	1:F:325:ALA:CA	1.88	1.03
1:D:419:LYS:HG2	1:D:470:THR:HG23	1.08	1.03
1:C:9:PRO:HD2	1:C:10:LYS:H	1.24	1.02
1:B:369:GLU:O	1:B:391:PHE:HD2	1.43	1.02
1:D:376:VAL:HG23	1:D:376:VAL:O	1.27	1.01
1:C:286:TYR:HB2	1:C:378:PHE:O	1.60	1.00
1:E:376:VAL:O	1:E:376:VAL:CG2	1.91	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:26:GLU:HB3	1:C:326:GLN:HE22	1.22	1.00
1:E:19:HIS:HD2	1:E:64:ASN:HD22	1.04	1.00
1:F:26:GLU:HB2	1:F:69:GLY:CA	1.90	1.00
1:A:419:LYS:HG3	1:A:470:THR:HG21	1.44	0.99
1:F:419:LYS:HG2	1:F:470:THR:HG23	1.01	0.99
1:F:362:VAL:O	1:F:364:THR:HG22	1.62	0.99
1:D:419:LYS:HG3	1:D:470:THR:HG21	1.43	0.98
1:E:24:PHE:HB3	1:E:325:ALA:CA	1.92	0.98
1:A:413:ARG:HD3	1:A:415:GLU:OE1	1.62	0.98
1:F:34:GLY:O	1:F:336:THR:HG21	1.63	0.98
1:E:328:VAL:HG12	1:E:329:ASN:H	1.28	0.98
1:C:328:VAL:HG12	1:C:329:ASN:N	1.77	0.98
1:C:411:ASN:ND2	1:C:413:ARG:HB2	1.77	0.98
1:D:24:PHE:O	1:D:326:GLN:HA	1.64	0.97
1:C:419:LYS:HG2	1:C:470:THR:HG23	0.98	0.97
1:C:327:LEU:HG	1:C:327:LEU:O	1.62	0.96
1:E:369:GLU:O	1:E:391:PHE:HD2	1.45	0.96
1:B:7:VAL:HG12	1:B:9:PRO:CD	1.94	0.96
1:A:410:VAL:CG1	1:A:412:TYR:CE2	2.48	0.96
1:F:239:GLY:O	1:F:377:MET:O	1.84	0.96
1:A:413:ARG:HD2	1:A:416:ASP:HB2	1.47	0.95
1:F:327:LEU:HG	1:F:328:VAL:HG23	1.45	0.95
1:C:26:GLU:HB3	1:C:326:GLN:NE2	1.81	0.95
1:F:71:ASN:HA	1:F:178:GLN:HE22	1.28	0.95
1:D:330:ALA:C	1:D:332:GLY:H	1.69	0.95
1:E:419:LYS:HG2	1:E:470:THR:HG23	0.97	0.95
1:A:380:ASN:HD22	1:A:380:ASN:N	1.60	0.95
1:B:391:PHE:CD1	1:B:413:ARG:HG3	2.02	0.95
1:B:7:VAL:HG12	1:B:9:PRO:HD3	1.45	0.95
1:B:410:VAL:CG1	1:B:412:TYR:CE2	2.37	0.95
1:E:19:HIS:CD2	1:E:64:ASN:HD22	1.83	0.95
1:C:247:VAL:O	1:C:250:VAL:HG12	1.66	0.95
1:C:19:HIS:HD2	1:C:64:ASN:HD22	1.11	0.94
1:C:446:ASN:HD21	1:C:454:VAL:H	1.13	0.94
1:C:286:TYR:HA	1:C:378:PHE:O	1.68	0.94
1:E:378:PHE:HD1	1:E:379:ILE:H	1.16	0.94
1:A:7:VAL:HG12	1:A:9:PRO:HD3	1.50	0.93
1:C:141:CYS:C	1:C:142:ASN:OD1	2.11	0.93
1:B:446:ASN:HD21	1:B:454:VAL:H	1.10	0.93
1:C:411:ASN:HD21	1:C:413:ARG:CB	1.81	0.93
1:A:380:ASN:H	1:A:380:ASN:ND2	1.67	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:326:GLN:HE22	1:F:330:ALA:CB	1.81	0.93
1:C:419:LYS:CG	1:C:470:THR:HG23	1.72	0.93
1:C:19:HIS:CD2	1:C:64:ASN:HD22	1.86	0.92
1:A:7:VAL:HG12	1:A:9:PRO:CD	1.99	0.92
1:A:19:HIS:HD2	1:A:64:ASN:HD22	1.07	0.92
1:C:24:PHE:HD2	1:C:325:ALA:O	1.50	0.92
1:E:446:ASN:HD21	1:E:454:VAL:H	1.13	0.92
1:C:60:ILE:HG13	1:C:60:ILE:O	1.68	0.92
1:D:376:VAL:O	1:D:376:VAL:CG2	2.05	0.92
1:B:378:PHE:HB3	1:B:380:ASN:ND2	1.84	0.92
1:D:411:ASN:ND2	1:D:413:ARG:H	1.68	0.92
1:C:369:GLU:O	1:C:391:PHE:HD2	1.51	0.92
1:D:19:HIS:HD2	1:D:64:ASN:HD22	1.12	0.92
1:B:34:GLY:O	1:B:336:THR:HG21	1.70	0.92
1:C:34:GLY:O	1:C:336:THR:HG21	1.70	0.91
1:C:286:TYR:CA	1:C:378:PHE:O	2.19	0.91
1:D:419:LYS:CG	1:D:470:THR:HG21	1.98	0.91
1:A:282:TRP:O	1:A:282:TRP:CE3	2.23	0.91
1:A:415:GLU:O	1:A:416:ASP:OD1	1.86	0.91
1:A:379:ILE:O	1:A:379:ILE:CG2	2.15	0.91
1:E:34:GLY:O	1:E:336:THR:HG21	1.71	0.91
1:E:376:VAL:O	1:E:376:VAL:HG23	1.10	0.91
1:F:411:ASN:ND2	1:F:413:ARG:HB2	1.86	0.91
1:E:411:ASN:HD21	1:E:413:ARG:HB2	1.34	0.91
1:B:410:VAL:HG12	1:B:412:TYR:CE1	2.06	0.90
1:D:326:GLN:NE2	1:D:330:ALA:HB3	1.86	0.90
1:E:328:VAL:HG12	1:E:329:ASN:N	1.86	0.90
1:F:282:TRP:CD1	1:F:323:ASN:O	2.25	0.90
1:F:19:HIS:HD2	1:F:64:ASN:HD22	1.17	0.90
1:D:411:ASN:ND2	1:D:413:ARG:N	2.19	0.90
1:F:327:LEU:HD23	1:F:327:LEU:H	1.36	0.90
1:D:330:ALA:C	1:D:332:GLY:N	2.25	0.90
1:D:411:ASN:HD21	1:D:413:ARG:HB2	0.75	0.90
1:F:24:PHE:HB3	1:F:325:ALA:HA	1.52	0.89
1:F:446:ASN:HD21	1:F:454:VAL:H	1.17	0.89
1:B:19:HIS:HD2	1:B:64:ASN:HD22	1.20	0.89
1:A:94:LEU:HD21	1:C:135:LEU:HD21	1.55	0.89
1:B:71:ASN:HA	1:B:178:GLN:HE22	1.38	0.89
1:F:481:VAL:HG22	1:F:482:GLU:N	1.85	0.89
1:A:328:VAL:HG12	1:A:329:ASN:N	1.84	0.89
1:F:415:GLU:H	1:F:415:GLU:CD	1.81	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:411:ASN:ND2	1:C:413:ARG:H	1.70	0.88
1:A:19:HIS:CD2	1:A:64:ASN:HD22	1.91	0.88
1:E:324:LEU:HD22	1:E:350:PHE:CE1	2.08	0.88
1:E:419:LYS:CG	1:E:470:THR:HG23	1.72	0.88
1:D:34:GLY:O	1:D:336:THR:HG21	1.72	0.87
1:F:419:LYS:CG	1:F:470:THR:HG23	1.69	0.87
1:B:415:GLU:N	1:B:473:PRO:HB2	1.90	0.87
1:E:94:LEU:HD21	1:F:135:LEU:HD21	1.56	0.87
1:A:378:PHE:CG	1:A:378:PHE:O	2.25	0.87
1:D:446:ASN:HD21	1:D:454:VAL:H	1.18	0.87
1:C:401:ASP:OD2	1:C:403:LYS:HG2	1.73	0.87
1:E:419:LYS:HG3	1:E:470:THR:HG22	1.24	0.87
1:D:325:ALA:HB1	1:D:331:LEU:HD13	1.56	0.86
1:A:30:ARG:HH12	1:A:336:THR:HG22	1.40	0.86
1:F:285:TRP:CE2	1:F:379:ILE:HD11	2.10	0.86
1:D:419:LYS:HG3	1:D:470:THR:HG22	1.35	0.86
1:B:378:PHE:HB3	1:B:380:ASN:HD21	1.38	0.86
1:D:401:ASP:OD2	1:D:403:LYS:HG2	1.75	0.86
1:A:135:LEU:HD21	1:B:94:LEU:HD21	1.58	0.86
1:D:47:ARG:HH11	1:D:47:ARG:HG3	1.40	0.86
1:E:481:VAL:HG22	1:E:482:GLU:N	1.90	0.86
1:F:419:LYS:HG3	1:F:470:THR:HG22	1.10	0.86
1:C:47:ARG:HG3	1:C:47:ARG:HH11	1.41	0.86
1:C:71:ASN:HA	1:C:178:GLN:HE22	1.39	0.86
1:B:62:VAL:HG11	1:B:116:ILE:HD12	1.58	0.86
1:D:481:VAL:HG22	1:D:482:GLU:N	1.87	0.86
1:E:54:LEU:O	1:E:58:LYS:HG3	1.76	0.86
1:A:380:ASN:HD22	1:A:380:ASN:H	0.86	0.85
1:E:247:VAL:O	1:E:250:VAL:HG12	1.76	0.85
1:A:446:ASN:HD21	1:A:454:VAL:H	1.21	0.85
1:A:481:VAL:HG22	1:A:482:GLU:N	1.91	0.85
1:B:410:VAL:HB	1:B:412:TYR:CE1	2.12	0.85
1:A:282:TRP:O	1:A:282:TRP:CG	2.26	0.85
1:B:362:VAL:O	1:B:364:THR:HG22	1.76	0.85
1:A:34:GLY:O	1:A:336:THR:HG21	1.75	0.85
1:B:481:VAL:HG22	1:B:482:GLU:N	1.92	0.85
1:A:401:ASP:OD2	1:A:403:LYS:HG2	1.76	0.85
1:C:9:PRO:HD2	1:C:10:LYS:N	1.91	0.85
1:E:401:ASP:OD2	1:E:403:LYS:HG2	1.75	0.85
1:D:19:HIS:CD2	1:D:64:ASN:HD22	1.95	0.85
1:D:326:GLN:HE21	1:D:330:ALA:HB3	1.42	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:71:ASN:HA	1:E:178:GLN:HE22	1.42	0.85
1:B:19:HIS:CD2	1:B:64:ASN:HD22	1.94	0.84
1:F:350:PHE:O	1:F:354:VAL:HG22	1.77	0.84
1:F:19:HIS:CD2	1:F:64:ASN:HD22	1.96	0.84
1:B:401:ASP:OD2	1:B:403:LYS:HG2	1.77	0.84
1:C:419:LYS:HG3	1:C:470:THR:HG22	1.27	0.84
1:D:26:GLU:HB3	1:D:326:GLN:OE1	1.75	0.84
1:D:42:PRO:HG2	1:D:43:LEU:HD12	1.60	0.83
1:F:401:ASP:OD2	1:F:403:LYS:HG2	1.77	0.83
1:D:334:ILE:HD11	1:D:347:TYR:CE2	2.12	0.83
1:E:328:VAL:O	1:E:332:GLY:HA3	1.77	0.83
1:F:24:PHE:HD2	1:F:325:ALA:HB1	0.68	0.83
1:A:368:SER:OG	1:A:369:GLU:O	1.95	0.83
1:D:71:ASN:HA	1:D:178:GLN:HE22	1.43	0.83
1:A:378:PHE:C	1:A:379:ILE:HG13	2.04	0.83
1:D:481:VAL:CG2	1:D:482:GLU:H	1.91	0.83
1:E:481:VAL:CG2	1:E:482:GLU:H	1.92	0.83
1:E:183:THR:OG1	1:E:186:GLU:HG3	1.78	0.83
1:E:324:LEU:HG	1:E:324:LEU:O	1.79	0.83
1:D:247:VAL:O	1:D:250:VAL:HG12	1.79	0.82
1:A:419:LYS:HG3	1:A:470:THR:HG22	1.35	0.82
1:E:362:VAL:O	1:E:364:THR:HG22	1.79	0.82
1:B:415:GLU:H	1:B:473:PRO:CB	1.91	0.82
1:B:481:VAL:CG2	1:B:482:GLU:H	1.92	0.82
1:F:62:VAL:HG11	1:F:116:ILE:HD12	1.61	0.82
1:A:71:ASN:HA	1:A:178:GLN:HE22	1.42	0.82
1:A:183:THR:OG1	1:A:186:GLU:HG3	1.80	0.81
1:A:481:VAL:CG2	1:A:482:GLU:H	1.93	0.81
1:E:419:LYS:CG	1:E:470:THR:HG21	1.96	0.81
1:B:247:VAL:O	1:B:250:VAL:HG12	1.80	0.81
1:E:378:PHE:CE1	1:E:379:ILE:HG13	2.15	0.81
1:F:481:VAL:CG2	1:F:482:GLU:H	1.91	0.81
1:D:325:ALA:CB	1:D:331:LEU:HD13	2.11	0.81
1:F:247:VAL:O	1:F:250:VAL:HG12	1.81	0.81
1:A:413:ARG:CD	1:A:415:GLU:OE1	2.28	0.81
1:A:419:LYS:CG	1:A:470:THR:HG21	2.02	0.81
1:D:411:ASN:HD22	1:D:413:ARG:H	1.27	0.81
1:F:24:PHE:CG	1:F:325:ALA:HB2	2.15	0.81
1:A:50:ARG:NH2	1:A:337:GLU:O	2.15	0.80
1:A:362:VAL:O	1:A:364:THR:HG22	1.82	0.80
1:C:326:GLN:HB3	1:C:330:ALA:O	1.81	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:410:VAL:CB	1:B:412:TYR:CE1	2.63	0.80
1:F:335:HIS:HB3	1:F:342:ILE:HG23	1.62	0.80
1:C:30:ARG:HH12	1:C:336:THR:HG22	1.46	0.80
1:B:369:GLU:O	1:B:391:PHE:CD2	2.34	0.80
1:B:410:VAL:HG12	1:B:412:TYR:CD1	2.16	0.80
1:D:362:VAL:O	1:D:364:THR:HG22	1.82	0.80
1:A:415:GLU:O	1:A:416:ASP:CG	2.25	0.80
1:D:157:GLY:C	1:D:158:HIS:HB2	2.07	0.79
1:C:362:VAL:O	1:C:364:THR:HG22	1.81	0.79
1:F:24:PHE:CB	1:F:325:ALA:HB2	2.12	0.79
1:A:335:HIS:HB3	1:A:342:ILE:HG23	1.64	0.79
1:D:411:ASN:CG	1:D:413:ARG:HB2	2.06	0.79
1:A:327:LEU:O	1:A:328:VAL:HG23	1.83	0.79
1:B:417:ALA:O	1:B:418:LEU:HD12	1.81	0.79
1:D:413:ARG:HG3	1:D:418:LEU:CD1	2.13	0.79
1:E:335:HIS:HB3	1:E:342:ILE:CG2	2.13	0.79
1:E:50:ARG:NH2	1:E:337:GLU:O	2.16	0.79
1:C:24:PHE:CD2	1:C:325:ALA:O	2.37	0.78
1:E:157:GLY:C	1:E:158:HIS:HB2	2.09	0.78
1:B:350:PHE:O	1:B:354:VAL:HG22	1.84	0.78
1:B:410:VAL:CB	1:B:412:TYR:CZ	2.65	0.78
1:F:47:ARG:HG3	1:F:47:ARG:HH11	1.49	0.78
1:A:157:GLY:C	1:A:158:HIS:HB2	2.08	0.78
1:E:42:PRO:HG2	1:E:43:LEU:HD12	1.66	0.78
1:F:411:ASN:ND2	1:F:413:ARG:H	1.81	0.78
1:F:4:ARG:HA	1:F:420:VAL:HG23	1.66	0.78
1:B:422:ILE:HD12	1:B:423:ARG:N	1.99	0.77
1:C:183:THR:OG1	1:C:186:GLU:HG3	1.83	0.77
1:D:413:ARG:O	1:D:473:PRO:HA	1.84	0.77
1:E:335:HIS:HB3	1:E:342:ILE:HG23	1.66	0.77
1:B:135:LEU:HD21	1:C:94:LEU:HD21	1.66	0.77
1:D:335:HIS:HB3	1:D:342:ILE:HG23	1.66	0.77
1:B:154:ARG:HG2	1:B:159:PRO:HA	1.66	0.77
1:C:239:GLY:O	1:C:377:MET:HA	1.84	0.77
1:C:350:PHE:O	1:C:354:VAL:HG22	1.85	0.77
1:A:42:PRO:HG2	1:A:43:LEU:HD12	1.67	0.77
1:F:369:GLU:O	1:F:369:GLU:HG2	1.84	0.77
1:A:247:VAL:O	1:A:250:VAL:HG12	1.84	0.77
1:A:350:PHE:O	1:A:354:VAL:HG22	1.84	0.77
1:D:50:ARG:NH2	1:D:337:GLU:O	2.18	0.77
1:A:47:ARG:HH11	1:A:47:ARG:HG3	1.49	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:239:GLY:O	1:B:377:MET:O	2.02	0.77
1:D:285:TRP:CE2	1:D:379:ILE:HD11	2.20	0.77
1:D:326:GLN:NE2	1:D:330:ALA:CB	2.48	0.77
1:E:47:ARG:HH11	1:E:47:ARG:HG3	1.50	0.77
1:A:378:PHE:O	1:A:379:ILE:HG13	1.83	0.77
1:D:62:VAL:HG11	1:D:116:ILE:HD12	1.67	0.77
1:D:144:LYS:H	1:D:144:LYS:HD3	1.49	0.77
1:B:285:TRP:NE1	1:B:379:ILE:HD11	1.99	0.76
1:F:157:GLY:C	1:F:158:HIS:HB2	2.10	0.76
1:A:378:PHE:O	1:A:379:ILE:CG1	2.33	0.76
1:E:369:GLU:O	1:E:391:PHE:CD2	2.34	0.76
1:A:335:HIS:HB3	1:A:342:ILE:CG2	2.15	0.76
1:D:417:ALA:O	1:D:418:LEU:HD12	1.85	0.76
1:A:62:VAL:HG11	1:A:116:ILE:HD12	1.67	0.76
1:A:318:ILE:HG13	1:A:319:VAL:HG23	1.68	0.76
1:C:101:THR:OG1	1:C:103:ARG:HG3	1.86	0.76
1:D:413:ARG:HG3	1:D:418:LEU:HD11	1.66	0.76
1:E:254:LYS:O	1:E:258:ILE:HG23	1.85	0.76
1:E:62:VAL:HG11	1:E:116:ILE:HD12	1.68	0.76
1:C:422:ILE:HD12	1:C:423:ARG:N	2.01	0.76
1:B:157:GLY:C	1:B:158:HIS:HB2	2.11	0.75
1:B:183:THR:OG1	1:B:186:GLU:HG3	1.85	0.75
1:D:335:HIS:HB3	1:D:342:ILE:CG2	2.16	0.75
1:F:16:ILE:HD13	1:F:313:GLN:HG3	1.67	0.75
1:A:410:VAL:HG12	1:A:412:TYR:CE2	2.20	0.75
1:E:24:PHE:CB	1:E:325:ALA:CB	2.28	0.75
1:B:285:TRP:CZ2	1:B:379:ILE:HD11	2.21	0.75
1:F:335:HIS:HB3	1:F:342:ILE:CG2	2.17	0.75
1:D:61:LYS:HE2	1:D:355:ASN:OD1	1.85	0.75
1:E:30:ARG:HH12	1:E:336:THR:HG22	1.50	0.75
1:A:417:ALA:O	1:A:418:LEU:HD12	1.86	0.75
1:A:154:ARG:HG2	1:A:159:PRO:HA	1.67	0.75
1:B:318:ILE:HG13	1:B:319:VAL:HG23	1.67	0.74
1:B:327:LEU:C	1:B:328:VAL:HG23	2.12	0.74
1:C:263:LEU:HG	1:F:266:MET:HE1	1.69	0.74
1:B:7:VAL:HG12	1:B:9:PRO:HD2	1.69	0.74
1:B:415:GLU:HG2	1:B:416:ASP:N	1.98	0.74
1:D:318:ILE:HG13	1:D:319:VAL:HG23	1.69	0.74
1:F:42:PRO:HG2	1:F:43:LEU:HD12	1.69	0.74
1:D:54:LEU:O	1:D:58:LYS:HG3	1.87	0.74
1:E:411:ASN:HD21	1:E:413:ARG:CB	1.99	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:154:ARG:HG2	1:F:159:PRO:HA	1.69	0.74
1:C:481:VAL:HG22	1:C:482:GLU:N	1.92	0.74
1:A:24:PHE:HD2	1:A:325:ALA:O	1.70	0.74
1:E:422:ILE:HD12	1:E:423:ARG:N	2.02	0.74
1:B:329:ASN:HD21	1:B:336:THR:HB	1.53	0.74
1:B:446:ASN:ND2	1:B:454:VAL:H	1.85	0.73
1:C:318:ILE:HG13	1:C:319:VAL:HG23	1.70	0.73
1:D:101:THR:OG1	1:D:103:ARG:HG3	1.88	0.73
1:E:24:PHE:HD2	1:E:325:ALA:HB1	0.64	0.73
1:E:61:LYS:HE2	1:E:355:ASN:OD1	1.88	0.73
1:E:154:ARG:HG2	1:E:159:PRO:HA	1.69	0.73
1:F:417:ALA:O	1:F:418:LEU:HD12	1.88	0.73
1:F:422:ILE:HD11	1:F:467:PHE:CE1	2.23	0.73
1:B:47:ARG:HH11	1:B:47:ARG:HG3	1.54	0.73
1:B:50:ARG:NH2	1:B:337:GLU:O	2.21	0.73
1:D:325:ALA:HB1	1:D:331:LEU:CD1	2.16	0.73
1:A:23:HIS:HB3	1:A:327:LEU:HD22	1.69	0.73
1:F:25:THR:HG23	1:F:25:THR:O	1.85	0.73
1:F:30:ARG:HH12	1:F:336:THR:HG22	1.52	0.73
1:B:197:TRP:HB3	1:C:94:LEU:HD23	1.70	0.73
1:A:410:VAL:CG1	1:A:412:TYR:CE1	2.62	0.73
1:D:350:PHE:O	1:D:354:VAL:HG22	1.88	0.73
1:F:24:PHE:HD2	1:F:325:ALA:CA	2.01	0.73
1:A:26:GLU:HB3	1:A:326:GLN:NE2	2.03	0.73
1:B:419:LYS:HA	1:B:470:THR:HG22	1.71	0.73
1:E:350:PHE:O	1:E:354:VAL:HG22	1.89	0.72
1:C:16:ILE:HD13	1:C:313:GLN:HG3	1.71	0.72
1:E:318:ILE:HG13	1:E:319:VAL:HG23	1.71	0.72
1:D:282:TRP:O	1:D:324:LEU:HD12	1.89	0.72
1:E:417:ALA:O	1:E:418:LEU:HD12	1.89	0.72
1:F:24:PHE:CG	1:F:325:ALA:CB	2.72	0.72
1:F:50:ARG:NH2	1:F:337:GLU:O	2.22	0.72
1:C:335:HIS:HB3	1:C:342:ILE:CG2	2.19	0.72
1:F:26:GLU:CB	1:F:69:GLY:HA2	2.18	0.72
1:B:291:ASN:HD22	1:B:291:ASN:H	1.34	0.71
1:C:422:ILE:HD11	1:C:467:PHE:CE2	2.25	0.71
1:C:481:VAL:CG2	1:C:482:GLU:H	1.96	0.71
1:F:413:ARG:O	1:F:474:PHE:N	2.23	0.71
1:D:422:ILE:HD12	1:D:423:ARG:N	2.03	0.71
1:E:94:LEU:HD23	1:F:197:TRP:HB3	1.71	0.71
1:A:422:ILE:HD12	1:A:423:ARG:N	2.04	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:7:VAL:CG1	1:B:9:PRO:HD3	2.20	0.71
1:B:414:LYS:O	1:B:415:GLU:CD	2.33	0.71
1:D:16:ILE:HD13	1:D:313:GLN:HG3	1.73	0.71
1:D:411:ASN:HD21	1:D:413:ARG:CA	2.03	0.71
1:C:283:ASN:HB2	1:C:325:ALA:HB2	1.73	0.71
1:D:144:LYS:HD3	1:D:144:LYS:N	2.05	0.71
1:F:24:PHE:HB3	1:F:325:ALA:CB	2.21	0.71
1:F:24:PHE:O	1:F:326:GLN:HB3	1.90	0.71
1:A:61:LYS:HE2	1:A:355:ASN:OD1	1.90	0.71
1:C:291:ASN:H	1:C:291:ASN:HD22	1.36	0.71
1:E:378:PHE:CG	1:E:379:ILE:N	2.54	0.71
1:B:254:LYS:O	1:B:258:ILE:HG23	1.91	0.71
1:A:24:PHE:O	1:A:326:GLN:HA	1.89	0.70
1:B:25:THR:HG23	1:B:25:THR:O	1.90	0.70
1:C:42:PRO:HG2	1:C:43:LEU:HD12	1.73	0.70
1:A:7:VAL:HG12	1:A:9:PRO:HD2	1.74	0.70
1:C:266:MET:HE1	1:F:263:LEU:HG	1.73	0.70
1:C:62:VAL:HG11	1:C:116:ILE:HD12	1.73	0.70
1:C:335:HIS:HB3	1:C:342:ILE:HG23	1.74	0.70
1:C:422:ILE:HD12	1:C:422:ILE:C	2.17	0.70
1:A:101:THR:OG1	1:A:103:ARG:HG3	1.91	0.70
1:B:158:HIS:C	1:B:159:PRO:N	2.49	0.70
1:B:414:LYS:O	1:B:414:LYS:HG2	1.91	0.70
1:F:419:LYS:CG	1:F:470:THR:HG21	1.96	0.70
1:C:417:ALA:O	1:C:418:LEU:HD12	1.91	0.70
1:D:291:ASN:HD22	1:D:291:ASN:H	1.37	0.70
1:F:328:VAL:HG12	1:F:329:ASN:N	2.05	0.70
1:B:415:GLU:N	1:B:473:PRO:CB	2.52	0.70
1:A:158:HIS:C	1:A:159:PRO:N	2.50	0.70
1:B:410:VAL:HG11	1:B:412:TYR:OH	1.87	0.70
1:C:328:VAL:HG12	1:C:329:ASN:H	1.57	0.70
1:E:24:PHE:CG	1:E:325:ALA:HB1	2.14	0.70
1:F:369:GLU:O	1:F:369:GLU:CG	2.33	0.70
1:D:36:ILE:HG23	1:D:328:VAL:HG21	1.73	0.69
1:E:24:PHE:HB3	1:E:325:ALA:HA	1.72	0.69
1:E:197:TRP:O	1:E:199:LYS:N	2.24	0.69
1:A:197:TRP:HB3	1:B:94:LEU:HD23	1.72	0.69
1:E:285:TRP:CE2	1:E:379:ILE:HD11	2.27	0.69
1:F:422:ILE:HD12	1:F:423:ARG:N	2.07	0.69
1:A:410:VAL:HG12	1:A:412:TYR:CD2	2.27	0.69
1:E:144:LYS:HD3	1:E:144:LYS:N	2.07	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:419:LYS:HG2	1:B:470:THR:CG2	2.22	0.69
1:E:25:THR:HG23	1:E:25:THR:O	1.91	0.69
1:A:234:TYR:OH	1:A:256:ARG:HG2	1.91	0.69
1:E:24:PHE:CD2	1:E:325:ALA:HB2	1.92	0.69
1:A:378:PHE:O	1:A:379:ILE:CB	2.39	0.69
1:B:54:LEU:O	1:B:58:LYS:HG3	1.92	0.69
1:C:50:ARG:NH2	1:C:337:GLU:O	2.24	0.69
1:F:70:GLY:O	1:F:73:VAL:HG12	1.93	0.69
1:A:7:VAL:CG1	1:A:9:PRO:HD3	2.23	0.69
1:A:414:LYS:O	1:A:473:PRO:CB	2.41	0.69
1:B:410:VAL:HG21	1:B:412:TYR:OH	1.92	0.69
1:D:379:ILE:HG22	1:D:379:ILE:O	1.92	0.69
1:A:422:ILE:HD11	1:A:467:PHE:CE2	2.28	0.69
1:B:42:PRO:HG2	1:B:43:LEU:HD12	1.74	0.69
1:C:197:TRP:O	1:C:199:LYS:N	2.24	0.68
1:E:422:ILE:HD11	1:E:467:PHE:CE1	2.28	0.68
1:F:329:ASN:HD21	1:F:336:THR:HB	1.58	0.68
1:C:432:ALA:HB2	1:C:481:VAL:HG23	1.76	0.68
1:D:234:TYR:OH	1:D:256:ARG:HG2	1.94	0.68
1:C:411:ASN:C	1:C:411:ASN:HD22	2.01	0.68
1:E:329:ASN:HD21	1:E:336:THR:HB	1.58	0.68
1:F:24:PHE:HB3	1:F:325:ALA:N	2.09	0.68
1:F:325:ALA:C	1:F:326:GLN:HG3	2.18	0.68
1:B:328:VAL:HG12	1:B:329:ASN:N	2.09	0.68
1:D:414:LYS:O	1:D:473:PRO:CB	2.36	0.68
1:A:24:PHE:CD2	1:A:325:ALA:O	2.47	0.68
1:D:411:ASN:HD22	1:D:411:ASN:C	2.02	0.68
1:F:110:ILE:HG13	1:F:162:TYR:CD2	2.29	0.68
1:A:291:ASN:H	1:A:291:ASN:HD22	1.41	0.68
1:B:422:ILE:HD11	1:B:467:PHE:CE2	2.28	0.68
1:C:411:ASN:HD22	1:C:413:ARG:H	1.38	0.68
1:D:328:VAL:O	1:D:329:ASN:HB2	1.92	0.68
1:B:16:ILE:HD13	1:B:313:GLN:HG3	1.76	0.68
1:B:335:HIS:HB3	1:B:342:ILE:HG23	1.76	0.68
1:C:182:MET:HE3	1:C:187:TYR:HD1	1.58	0.68
1:F:327:LEU:H	1:F:327:LEU:CD2	2.05	0.68
1:D:415:GLU:CD	1:D:415:GLU:H	2.02	0.67
1:E:245:GLU:OE1	1:E:376:VAL:HG22	1.95	0.67
1:D:154:ARG:HG2	1:D:159:PRO:HA	1.75	0.67
1:F:291:ASN:H	1:F:291:ASN:HD22	1.41	0.67
1:E:428:GLY:O	1:E:464:ASP:HA	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:54:LEU:O	1:F:58:LYS:HG3	1.93	0.67
1:B:194:TYR:O	1:B:198:MET:HB2	1.95	0.67
1:E:291:ASN:HD22	1:E:291:ASN:H	1.40	0.67
1:E:446:ASN:ND2	1:E:454:VAL:H	1.88	0.67
1:A:158:HIS:O	1:A:159:PRO:N	2.26	0.67
1:E:342:ILE:C	1:E:342:ILE:HD13	2.20	0.67
1:D:254:LYS:O	1:D:258:ILE:HG23	1.94	0.67
1:D:422:ILE:HD11	1:D:467:PHE:CE2	2.30	0.67
1:E:183:THR:HG1	1:E:186:GLU:HG3	1.59	0.67
1:A:182:MET:HE3	1:A:187:TYR:HD1	1.61	0.66
1:A:325:ALA:O	1:A:326:GLN:HG3	1.95	0.66
1:D:30:ARG:HH12	1:D:336:THR:HG22	1.60	0.66
1:E:24:PHE:HD2	1:E:325:ALA:HB3	1.46	0.66
1:B:335:HIS:HB3	1:B:342:ILE:CG2	2.25	0.66
1:B:26:GLU:HB3	1:B:326:GLN:NE2	2.10	0.66
1:E:250:VAL:HG13	1:E:251:TYR:CD2	2.30	0.66
1:B:62:VAL:CG1	1:B:116:ILE:HD12	2.25	0.66
1:F:183:THR:OG1	1:F:186:GLU:HG3	1.94	0.66
1:B:450:ASN:HB3	1:B:453:VAL:HG23	1.77	0.66
1:C:446:ASN:ND2	1:C:454:VAL:H	1.91	0.66
1:B:422:ILE:HD12	1:B:422:ILE:C	2.20	0.66
1:D:47:ARG:HG3	1:D:47:ARG:NH1	2.09	0.66
1:D:414:LYS:C	1:D:473:PRO:HB2	2.20	0.66
1:E:415:GLU:O	1:E:416:ASP:OD1	2.14	0.66
1:C:327:LEU:O	1:C:328:VAL:HG23	1.95	0.66
1:D:342:ILE:C	1:D:342:ILE:HD13	2.21	0.66
1:E:16:ILE:HD13	1:E:313:GLN:HG3	1.77	0.66
1:D:110:ILE:HG13	1:D:162:TYR:CD2	2.30	0.66
1:A:67:TRP:CD1	1:A:68:PRO:HA	2.31	0.66
1:F:101:THR:OG1	1:F:103:ARG:HG3	1.96	0.66
1:F:318:ILE:HG13	1:F:319:VAL:HG23	1.78	0.66
1:D:94:LEU:HD21	1:E:135:LEU:HD21	1.78	0.66
1:B:30:ARG:HH12	1:B:336:THR:HG22	1.61	0.65
1:E:36:ILE:HG23	1:E:328:VAL:HG21	1.78	0.65
1:B:197:TRP:O	1:B:199:LYS:N	2.28	0.65
1:E:251:TYR:HE2	1:E:412:TYR:HH	1.44	0.65
1:B:67:TRP:CD1	1:B:68:PRO:HA	2.32	0.65
1:B:182:MET:HE3	1:B:187:TYR:HD1	1.60	0.65
1:B:391:PHE:CD1	1:B:413:ARG:CG	2.78	0.65
1:E:287:ARG:NH2	1:E:301:ASP:OD2	2.26	0.65
1:E:450:ASN:HB3	1:E:453:VAL:HG23	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:362:VAL:HG22	1:A:396:ALA:O	1.96	0.65
1:D:194:TYR:O	1:D:198:MET:HB2	1.96	0.65
1:E:24:PHE:HB2	1:E:325:ALA:HB2	1.72	0.65
1:B:283:ASN:ND2	1:B:325:ALA:O	2.26	0.65
1:B:380:ASN:HD22	1:B:380:ASN:H	1.42	0.65
1:C:54:LEU:O	1:C:58:LYS:HG3	1.96	0.65
1:A:24:PHE:O	1:A:327:LEU:HD23	1.97	0.65
1:B:160:GLU:OE1	1:B:160:GLU:HA	1.95	0.65
1:C:282:TRP:O	1:C:324:LEU:HD12	1.96	0.65
1:C:39:GLU:OE2	1:C:103:ARG:HD3	1.96	0.65
1:C:369:GLU:O	1:C:391:PHE:CD2	2.43	0.65
1:F:419:LYS:CB	1:F:470:THR:HG22	2.26	0.65
1:A:182:MET:CE	1:A:187:TYR:HD1	2.10	0.65
1:D:368:SER:OG	1:D:369:GLU:N	2.26	0.65
1:F:234:TYR:OH	1:F:256:ARG:HG2	1.97	0.65
1:A:414:LYS:O	1:A:473:PRO:HB2	1.97	0.64
1:C:60:ILE:O	1:C:60:ILE:CG1	2.44	0.64
1:E:415:GLU:H	1:E:415:GLU:CD	2.05	0.64
1:B:158:HIS:O	1:B:159:PRO:N	2.30	0.64
1:B:250:VAL:HG13	1:B:251:TYR:CD2	2.32	0.64
1:E:26:GLU:HB2	1:E:69:GLY:HA2	1.78	0.64
1:E:411:ASN:HD22	1:E:411:ASN:C	2.05	0.64
1:F:24:PHE:CD2	1:F:325:ALA:CA	2.78	0.64
1:A:197:TRP:O	1:A:199:LYS:N	2.29	0.64
1:E:160:GLU:OE1	1:E:160:GLU:HA	1.95	0.64
1:C:450:ASN:HB3	1:C:453:VAL:HG23	1.79	0.64
1:D:450:ASN:HB3	1:D:453:VAL:HG23	1.79	0.64
1:E:431:LYS:NZ	1:E:462:THR:HG22	2.13	0.64
1:A:286:TYR:HA	1:A:379:ILE:HG13	1.79	0.64
1:C:157:GLY:C	1:C:158:HIS:HB2	2.21	0.64
1:C:410:VAL:CG1	1:C:412:TYR:CE1	2.80	0.64
1:F:26:GLU:HB2	1:F:69:GLY:HA3	1.77	0.64
1:A:380:ASN:N	1:A:380:ASN:ND2	2.31	0.64
1:A:54:LEU:O	1:A:58:LYS:HG3	1.98	0.64
1:D:158:HIS:C	1:D:159:PRO:N	2.56	0.64
1:E:110:ILE:HG13	1:E:162:TYR:CD2	2.32	0.64
1:E:182:MET:HE3	1:E:187:TYR:HD1	1.62	0.64
1:C:194:TYR:O	1:C:198:MET:HB2	1.97	0.64
1:C:287:ARG:NH2	1:C:301:ASP:OD2	2.28	0.64
1:E:432:ALA:HB2	1:E:481:VAL:HG23	1.80	0.64
1:F:24:PHE:CE2	1:F:325:ALA:HB1	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:182:MET:CE	1:C:187:TYR:HD1	2.11	0.63
1:A:16:ILE:HD13	1:A:313:GLN:HG3	1.80	0.63
1:F:285:TRP:CZ2	1:F:379:ILE:HD11	2.34	0.63
1:F:376:VAL:O	1:F:376:VAL:HG23	1.78	0.63
1:A:144:LYS:HD3	1:A:144:LYS:N	2.13	0.63
1:B:283:ASN:OD1	1:B:284:VAL:N	2.30	0.63
1:A:60:ILE:O	1:A:60:ILE:HG13	1.98	0.63
1:A:450:ASN:HB3	1:A:453:VAL:HG23	1.79	0.63
1:C:160:GLU:OE1	1:C:160:GLU:HA	1.98	0.63
1:D:183:THR:OG1	1:D:186:GLU:HG3	1.99	0.63
1:D:336:THR:CG2	1:D:337:GLU:N	2.62	0.63
1:E:70:GLY:O	1:E:73:VAL:HG12	1.98	0.63
1:E:158:HIS:C	1:E:159:PRO:N	2.57	0.63
1:E:274:GLY:O	1:E:276:LYS:HG3	1.99	0.63
1:C:254:LYS:O	1:C:258:ILE:HG23	1.98	0.63
1:A:160:GLU:OE1	1:A:160:GLU:HA	1.98	0.63
1:C:307:GLY:HA3	1:C:412:TYR:OH	1.99	0.63
1:A:446:ASN:ND2	1:A:454:VAL:H	1.94	0.63
1:B:234:TYR:OH	1:B:256:ARG:HG2	1.99	0.63
1:A:328:VAL:O	1:A:334:ILE:O	2.17	0.63
1:C:243:TYR:HA	1:C:300:LYS:HD2	1.81	0.63
1:F:24:PHE:HB3	1:F:325:ALA:HB2	1.81	0.63
1:F:160:GLU:OE1	1:F:160:GLU:HA	1.99	0.63
1:A:243:TYR:HA	1:A:300:LYS:HD2	1.81	0.62
1:E:101:THR:OG1	1:E:103:ARG:HG3	1.99	0.62
1:F:158:HIS:C	1:F:159:PRO:N	2.57	0.62
1:B:215:PRO:O	1:B:219:LEU:HB2	1.98	0.62
1:B:328:VAL:HG12	1:B:329:ASN:H	1.64	0.62
1:D:334:ILE:HG12	1:D:343:LEU:HD22	1.79	0.62
1:B:39:GLU:OE2	1:B:103:ARG:HD3	1.99	0.62
1:E:144:LYS:HD3	1:E:144:LYS:H	1.63	0.62
1:A:171:ASN:H	1:A:173:MET:HE2	1.65	0.62
1:F:450:ASN:HB3	1:F:453:VAL:HG23	1.81	0.62
1:A:286:TYR:HA	1:A:379:ILE:CG1	2.30	0.62
1:B:3:TYR:HA	1:B:367:GLU:O	2.00	0.62
1:B:417:ALA:C	1:B:418:LEU:HD12	2.24	0.62
1:D:282:TRP:O	1:D:282:TRP:CG	2.53	0.62
1:E:336:THR:CG2	1:E:337:GLU:N	2.62	0.62
1:E:378:PHE:O	1:E:379:ILE:C	2.30	0.62
1:A:419:LYS:CG	1:A:470:THR:HG23	1.91	0.62
1:D:419:LYS:HG2	1:D:470:THR:HG22	1.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:182:MET:CE	1:E:187:TYR:HD1	2.13	0.62
1:C:67:TRP:CD1	1:C:68:PRO:HA	2.35	0.62
1:C:419:LYS:CB	1:C:470:THR:HG22	2.29	0.62
1:D:432:ALA:HB2	1:D:481:VAL:HG23	1.81	0.62
1:E:285:TRP:O	1:E:378:PHE:CD1	2.53	0.62
1:A:328:VAL:HG12	1:A:329:ASN:H	1.60	0.62
1:D:160:GLU:OE1	1:D:160:GLU:HA	2.00	0.62
1:F:287:ARG:NH2	1:F:301:ASP:OD2	2.32	0.62
1:A:410:VAL:HB	1:A:412:TYR:CE2	2.35	0.61
1:B:144:LYS:HD3	1:B:144:LYS:N	2.14	0.61
1:B:364:THR:HG21	1:B:396:ALA:H	1.65	0.61
1:B:377:MET:HG2	1:B:384:PHE:HD2	1.65	0.61
1:C:9:PRO:CD	1:C:10:LYS:H	2.07	0.61
1:E:22:GLY:O	1:E:323:ASN:HA	2.00	0.61
1:E:243:TYR:HA	1:E:300:LYS:HD2	1.82	0.61
1:A:342:ILE:HD13	1:A:342:ILE:C	2.25	0.61
1:D:297:TYR:OH	1:D:331:LEU:HD23	2.01	0.61
1:E:194:TYR:O	1:E:198:MET:HB2	2.00	0.61
1:D:169:ILE:CD1	1:D:207:ALA:HB1	2.30	0.61
1:A:39:GLU:OE2	1:A:103:ARG:HD3	1.99	0.61
1:C:9:PRO:CD	1:C:10:LYS:N	2.63	0.61
1:B:22:GLY:O	1:B:323:ASN:HA	2.00	0.61
1:B:101:THR:OG1	1:B:103:ARG:HG3	1.99	0.61
1:B:414:LYS:O	1:B:415:GLU:CB	2.49	0.61
1:C:298:ASP:OD1	1:C:300:LYS:HB3	2.01	0.61
1:E:24:PHE:HD1	1:E:66:ARG:HB3	1.66	0.61
1:D:422:ILE:HD12	1:D:422:ILE:C	2.26	0.61
1:A:428:GLY:O	1:A:464:ASP:HA	2.00	0.61
1:B:328:VAL:O	1:B:332:GLY:HA3	2.00	0.61
1:C:342:ILE:HD13	1:C:342:ILE:C	2.26	0.61
1:D:250:VAL:HG13	1:D:251:TYR:CD2	2.36	0.61
1:D:411:ASN:ND2	1:D:413:ARG:CA	2.63	0.61
1:E:422:ILE:HD12	1:E:422:ILE:C	2.25	0.61
1:A:47:ARG:HG3	1:A:47:ARG:NH1	2.15	0.60
1:A:368:SER:OG	1:A:369:GLU:N	2.32	0.60
1:B:182:MET:CE	1:B:187:TYR:HD1	2.14	0.60
1:D:157:GLY:CA	1:D:158:HIS:HB2	2.31	0.60
1:B:197:TRP:HB3	1:C:94:LEU:CD2	2.31	0.60
1:F:328:VAL:O	1:F:334:ILE:O	2.19	0.60
1:C:274:GLY:O	1:C:276:LYS:HG3	2.02	0.60
1:B:428:GLY:O	1:B:464:ASP:HA	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:67:TRP:CD1	1:D:68:PRO:HA	2.36	0.60
1:E:415:GLU:CD	1:E:415:GLU:N	2.60	0.60
1:F:231:PHE:HE2	1:F:320:PRO:HG2	1.67	0.60
1:A:194:TYR:O	1:A:198:MET:HB2	2.02	0.60
1:E:327:LEU:HG	1:E:328:VAL:HG23	1.84	0.60
1:B:419:LYS:HG2	1:B:470:THR:HG22	1.82	0.60
1:F:144:LYS:HD3	1:F:144:LYS:N	2.17	0.60
1:F:254:LYS:O	1:F:258:ILE:HG23	2.00	0.60
1:A:70:GLY:O	1:A:73:VAL:HG12	2.00	0.60
1:B:231:PHE:HE2	1:B:320:PRO:HG2	1.66	0.60
1:D:411:ASN:HD22	1:D:413:ARG:N	1.91	0.60
1:F:67:TRP:CD1	1:F:68:PRO:HA	2.37	0.60
1:F:422:ILE:HD12	1:F:422:ILE:C	2.27	0.60
1:A:422:ILE:HD12	1:A:422:ILE:C	2.26	0.59
1:B:414:LYS:O	1:B:415:GLU:CG	2.49	0.59
1:E:24:PHE:CD2	1:E:325:ALA:HB3	2.26	0.59
1:E:47:ARG:HG3	1:E:47:ARG:NH1	2.14	0.59
1:C:336:THR:CG2	1:C:337:GLU:N	2.65	0.59
1:D:25:THR:O	1:D:25:THR:HG23	2.02	0.59
1:A:413:ARG:O	1:A:474:PHE:N	2.23	0.59
1:C:371:TYR:CD1	1:C:389:ALA:O	2.56	0.59
1:D:411:ASN:ND2	1:D:413:ARG:CB	2.22	0.59
1:F:26:GLU:HG3	1:F:27:HIS:N	2.17	0.59
1:D:75:ASN:C	1:D:75:ASN:HD22	2.08	0.59
1:E:234:TYR:OH	1:E:256:ARG:HG2	2.00	0.59
1:A:411:ASN:C	1:A:411:ASN:HD22	2.09	0.59
1:D:298:ASP:OD1	1:D:300:LYS:HB3	2.02	0.59
1:B:380:ASN:ND2	1:B:380:ASN:H	2.00	0.59
1:D:297:TYR:OH	1:D:331:LEU:CD2	2.51	0.59
1:E:283:ASN:OD1	1:E:284:VAL:N	2.34	0.59
1:A:250:VAL:HG13	1:A:251:TYR:CD2	2.38	0.59
1:B:342:ILE:C	1:B:342:ILE:HD13	2.26	0.59
1:D:414:LYS:HG2	1:D:415:GLU:N	2.16	0.59
1:F:169:ILE:CD1	1:F:207:ALA:HB1	2.33	0.59
1:F:182:MET:HE3	1:F:187:TYR:HD1	1.66	0.59
1:D:182:MET:HE3	1:D:187:TYR:HD1	1.67	0.59
1:D:417:ALA:C	1:D:418:LEU:HD12	2.27	0.59
1:E:362:VAL:O	1:E:363:LYS:C	2.45	0.59
1:A:197:TRP:HB3	1:B:94:LEU:CD2	2.33	0.59
1:C:410:VAL:HG11	1:C:412:TYR:CE1	2.38	0.59
1:D:231:PHE:HE2	1:D:320:PRO:HG2	1.68	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:378:PHE:CG	1:D:379:ILE:N	2.71	0.59
1:E:36:ILE:CG2	1:E:328:VAL:HG21	2.32	0.59
1:B:158:HIS:C	1:B:159:PRO:CA	2.76	0.59
1:B:287:ARG:NH2	1:B:301:ASP:OD2	2.35	0.59
1:D:158:HIS:O	1:D:159:PRO:N	2.36	0.59
1:F:24:PHE:CB	1:F:325:ALA:CB	2.78	0.59
1:C:231:PHE:HE2	1:C:320:PRO:HG2	1.68	0.58
1:D:334:ILE:HD11	1:D:347:TYR:CD2	2.37	0.58
1:E:169:ILE:CD1	1:E:207:ALA:HB1	2.33	0.58
1:E:362:VAL:HG22	1:E:396:ALA:O	2.02	0.58
1:F:411:ASN:HD22	1:F:413:ARG:H	1.50	0.58
1:C:74:SER:CB	1:C:178:GLN:HE21	2.15	0.58
1:F:327:LEU:HD23	1:F:327:LEU:N	2.12	0.58
1:E:91:ARG:HH11	1:E:91:ARG:HG3	1.68	0.58
1:E:231:PHE:HE2	1:E:320:PRO:HG2	1.67	0.58
1:A:80:ASP:OD2	1:A:91:ARG:NH1	2.36	0.58
1:C:67:TRP:CG	1:C:68:PRO:HA	2.39	0.58
1:D:75:ASN:C	1:D:75:ASN:ND2	2.60	0.58
1:E:24:PHE:CD1	1:E:66:ARG:HB3	2.38	0.58
1:E:70:GLY:HA2	1:E:171:ASN:OD1	2.04	0.58
1:E:380:ASN:HD22	1:E:380:ASN:N	2.00	0.58
1:F:411:ASN:HD22	1:F:411:ASN:C	2.10	0.58
1:C:26:GLU:CB	1:C:326:GLN:HE22	2.08	0.58
1:C:154:ARG:HG2	1:C:159:PRO:HA	1.85	0.58
1:D:169:ILE:HD11	1:D:207:ALA:HB1	1.86	0.58
1:D:197:TRP:O	1:D:199:LYS:N	2.34	0.58
1:D:282:TRP:O	1:D:282:TRP:CD2	2.57	0.58
1:D:419:LYS:CG	1:D:470:THR:HG23	1.90	0.58
1:D:419:LYS:CB	1:D:470:THR:HG22	2.32	0.58
1:E:67:TRP:CD1	1:E:68:PRO:HA	2.39	0.58
1:F:282:TRP:O	1:F:324:LEU:HD12	2.03	0.58
1:B:398:ILE:HG22	1:B:399:SER:O	2.03	0.58
1:D:24:PHE:O	1:D:326:GLN:CA	2.47	0.58
1:E:26:GLU:HG2	1:E:27:HIS:N	2.17	0.58
1:E:285:TRP:O	1:E:378:PHE:HD1	1.85	0.58
1:F:158:HIS:O	1:F:159:PRO:N	2.37	0.58
1:A:25:THR:O	1:A:25:THR:HG23	2.03	0.58
1:A:398:ILE:HG22	1:A:399:SER:O	2.03	0.58
1:B:57:VAL:O	1:B:60:ILE:O	2.21	0.58
1:B:243:TYR:HA	1:B:300:LYS:HD2	1.84	0.58
1:D:413:ARG:O	1:D:473:PRO:CA	2.51	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:364:THR:HG21	1:E:396:ALA:H	1.69	0.58
1:A:391:PHE:CD1	1:A:413:ARG:HG3	2.38	0.58
1:D:26:GLU:HA	1:D:68:PRO:O	2.04	0.58
1:F:243:TYR:HA	1:F:300:LYS:HD2	1.85	0.58
1:A:410:VAL:CB	1:A:412:TYR:CE2	2.87	0.57
1:D:431:LYS:NZ	1:D:462:THR:HG22	2.19	0.57
1:A:91:ARG:HH11	1:A:91:ARG:HG3	1.68	0.57
1:A:169:ILE:O	1:A:169:ILE:HG22	2.04	0.57
1:B:182:MET:HB3	1:B:186:GLU:HB2	1.86	0.57
1:D:80:ASP:OD2	1:D:91:ARG:NH1	2.37	0.57
1:A:3:TYR:HA	1:A:367:GLU:O	2.05	0.57
1:B:169:ILE:HG22	1:B:169:ILE:O	2.03	0.57
1:C:47:ARG:HG3	1:C:47:ARG:NH1	2.10	0.57
1:C:91:ARG:HG3	1:C:91:ARG:HH11	1.69	0.57
1:C:158:HIS:C	1:C:159:PRO:N	2.62	0.57
1:D:274:GLY:O	1:D:276:LYS:HG3	2.04	0.57
1:D:285:TRP:CZ2	1:D:379:ILE:HD11	2.40	0.57
1:F:398:ILE:HG22	1:F:399:SER:O	2.04	0.57
1:A:70:GLY:HA2	1:A:171:ASN:OD1	2.04	0.57
1:B:336:THR:CG2	1:B:337:GLU:N	2.66	0.57
1:D:270:ALA:O	1:D:273:ARG:O	2.23	0.57
1:D:285:TRP:HB2	1:D:331:LEU:HD21	1.86	0.57
1:F:274:GLY:O	1:F:276:LYS:HG3	2.04	0.57
1:D:3:TYR:HA	1:D:367:GLU:O	2.05	0.57
1:D:19:HIS:HD2	1:D:64:ASN:ND2	1.94	0.57
1:E:19:HIS:CD2	1:E:64:ASN:ND2	2.65	0.57
1:B:263:LEU:HG	1:E:266:MET:HE1	1.86	0.57
1:B:377:MET:HG2	1:B:384:PHE:CD2	2.40	0.57
1:D:380:ASN:ND2	1:D:380:ASN:H	2.03	0.57
1:F:22:GLY:O	1:F:323:ASN:HA	2.04	0.57
1:F:328:VAL:HA	1:F:334:ILE:O	2.04	0.57
1:B:411:ASN:HD22	1:B:411:ASN:C	2.11	0.57
1:D:252:LEU:HD21	1:D:256:ARG:CZ	2.35	0.57
1:E:80:ASP:OD2	1:E:91:ARG:NH1	2.38	0.57
1:E:157:GLY:CA	1:E:158:HIS:HB2	2.34	0.57
1:A:231:PHE:HE2	1:A:320:PRO:HG2	1.69	0.57
1:C:380:ASN:HD22	1:C:380:ASN:N	2.02	0.57
1:F:50:ARG:O	1:F:54:LEU:HB2	2.05	0.57
1:B:157:GLY:O	1:B:158:HIS:HB2	2.03	0.57
1:B:298:ASP:OD1	1:B:300:LYS:HB3	2.05	0.57
1:B:472:LYS:HB3	1:B:473:PRO:HD2	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:328:VAL:O	1:C:334:ILE:O	2.22	0.57
1:C:415:GLU:OE1	1:C:415:GLU:N	2.35	0.57
1:F:194:TYR:O	1:F:198:MET:HB2	2.04	0.57
1:C:169:ILE:O	1:C:169:ILE:HG22	2.05	0.56
1:C:126:MET:HE3	1:C:194:TYR:CD1	2.40	0.56
1:D:243:TYR:HA	1:D:300:LYS:HD2	1.87	0.56
1:A:336:THR:CG2	1:A:337:GLU:N	2.69	0.56
1:C:171:ASN:H	1:C:173:MET:HE2	1.70	0.56
1:C:411:ASN:ND2	1:C:413:ARG:N	2.50	0.56
1:C:431:LYS:HD3	1:C:462:THR:HG22	1.86	0.56
1:D:287:ARG:NH2	1:D:301:ASP:OD2	2.35	0.56
1:F:157:GLY:CA	1:F:158:HIS:HB2	2.35	0.56
1:E:154:ARG:HA	1:E:158:HIS:O	2.05	0.56
1:A:376:VAL:HG12	1:A:381:LYS:O	2.05	0.56
1:C:25:THR:HG23	1:C:25:THR:O	2.04	0.56
1:C:378:PHE:CE1	1:C:379:ILE:HG12	2.40	0.56
1:F:446:ASN:ND2	1:F:454:VAL:H	1.96	0.56
1:A:62:VAL:CG1	1:A:116:ILE:HD12	2.35	0.56
1:C:24:PHE:CD1	1:C:66:ARG:HB3	2.40	0.56
1:C:169:ILE:CD1	1:C:207:ALA:HB1	2.35	0.56
1:D:70:GLY:O	1:D:73:VAL:HG12	2.05	0.56
1:E:39:GLU:OE2	1:E:103:ARG:HD3	2.05	0.56
1:E:174:TYR:CE2	1:E:212:CYS:HB3	2.41	0.56
1:F:126:MET:HE3	1:F:194:TYR:CE1	2.41	0.56
1:F:415:GLU:CD	1:F:415:GLU:N	2.56	0.56
1:C:380:ASN:ND2	1:C:380:ASN:H	2.04	0.56
1:D:157:GLY:HA3	1:D:158:HIS:ND1	2.20	0.56
1:F:24:PHE:HD1	1:F:66:ARG:HB3	1.70	0.56
1:B:285:TRP:CZ2	1:B:379:ILE:CD1	2.89	0.56
1:C:362:VAL:HG11	1:C:398:ILE:CD1	2.36	0.56
1:F:342:ILE:HD13	1:F:342:ILE:C	2.30	0.56
1:A:274:GLY:O	1:A:276:LYS:HG3	2.06	0.56
1:B:70:GLY:O	1:B:73:VAL:HG12	2.06	0.56
1:B:158:HIS:CD2	1:B:158:HIS:N	2.73	0.56
1:B:378:PHE:CE1	1:B:379:ILE:HG13	2.40	0.56
1:C:283:ASN:CB	1:C:325:ALA:HB2	2.35	0.56
1:C:291:ASN:H	1:C:291:ASN:ND2	2.04	0.56
1:D:362:VAL:O	1:D:363:LYS:C	2.49	0.56
1:E:158:HIS:O	1:E:159:PRO:N	2.39	0.56
1:E:377:MET:O	1:E:378:PHE:HB2	2.06	0.56
1:F:414:LYS:HG3	1:F:442:VAL:HG11	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:362:VAL:O	1:B:363:LYS:C	2.48	0.56
1:C:417:ALA:C	1:C:418:LEU:HD12	2.31	0.56
1:D:24:PHE:CD1	1:D:66:ARG:HB3	2.41	0.56
1:D:428:GLY:O	1:D:464:ASP:HA	2.05	0.56
1:F:171:ASN:H	1:F:173:MET:HE2	1.70	0.56
1:D:39:GLU:OE2	1:D:103:ARG:HD3	2.06	0.55
1:D:179:VAL:HA	1:E:197:TRP:CZ2	2.41	0.55
1:E:328:VAL:HA	1:E:334:ILE:O	2.06	0.55
1:E:419:LYS:CB	1:E:470:THR:HG22	2.30	0.55
1:F:47:ARG:HG3	1:F:47:ARG:NH1	2.16	0.55
1:F:71:ASN:HA	1:F:178:GLN:NE2	2.11	0.55
1:A:461:ILE:CG2	1:A:462:THR:N	2.69	0.55
1:B:60:ILE:O	1:B:60:ILE:HG13	2.07	0.55
1:C:182:MET:HE3	1:C:187:TYR:CD1	2.38	0.55
1:C:419:LYS:CG	1:C:470:THR:HG21	1.96	0.55
1:C:431:LYS:NZ	1:C:462:THR:HG22	2.21	0.55
1:E:378:PHE:CD1	1:E:379:ILE:HG13	2.42	0.55
1:F:36:ILE:HG23	1:F:328:VAL:HG21	1.88	0.55
1:A:22:GLY:O	1:A:323:ASN:HA	2.06	0.55
1:B:291:ASN:H	1:B:291:ASN:ND2	2.03	0.55
1:C:3:TYR:HA	1:C:367:GLU:O	2.06	0.55
1:C:158:HIS:C	1:C:159:PRO:CA	2.79	0.55
1:C:413:ARG:O	1:C:474:PHE:N	2.37	0.55
1:D:446:ASN:ND2	1:D:454:VAL:H	1.96	0.55
1:F:327:LEU:HG	1:F:328:VAL:CG2	2.28	0.55
1:F:366:VAL:CG2	1:F:367:GLU:N	2.69	0.55
1:D:22:GLY:O	1:D:323:ASN:HA	2.06	0.55
1:A:362:VAL:O	1:A:363:LYS:C	2.47	0.55
1:D:126:MET:HE3	1:D:194:TYR:CE1	2.41	0.55
1:D:197:TRP:O	1:D:198:MET:HB2	2.07	0.55
1:E:182:MET:HE3	1:E:187:TYR:CD1	2.42	0.55
1:F:283:ASN:OD1	1:F:284:VAL:N	2.37	0.55
1:A:24:PHE:HD1	1:A:66:ARG:HB3	1.72	0.55
1:A:30:ARG:CB	1:A:329:ASN:HD22	2.19	0.55
1:A:182:MET:HE3	1:A:187:TYR:CD1	2.40	0.55
1:A:330:ALA:C	1:A:332:GLY:N	2.61	0.55
1:C:85:LYS:O	1:C:86:ASP:HB2	2.07	0.55
1:D:252:LEU:HD21	1:D:256:ARG:NH1	2.22	0.55
1:F:34:GLY:O	1:F:336:THR:CG2	2.45	0.55
1:F:262:LYS:O	1:F:266:MET:HG3	2.06	0.55
1:A:30:ARG:HB2	1:A:329:ASN:HD22	1.70	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:330:ALA:C	1:C:332:GLY:N	2.62	0.55
1:D:91:ARG:HH11	1:D:91:ARG:HG3	1.70	0.55
1:D:182:MET:HB3	1:D:186:GLU:HB2	1.88	0.55
1:E:336:THR:HG23	1:E:337:GLU:N	2.21	0.55
1:E:398:ILE:HG22	1:E:399:SER:O	2.06	0.55
1:A:67:TRP:CG	1:A:68:PRO:HA	2.41	0.55
1:B:75:ASN:ND2	1:B:75:ASN:C	2.65	0.55
1:D:90:VAL:O	1:E:147:THR:HA	2.07	0.55
1:D:157:GLY:O	1:D:158:HIS:HB2	2.07	0.55
1:E:3:TYR:HA	1:E:367:GLU:O	2.07	0.55
1:F:67:TRP:CG	1:F:68:PRO:HA	2.42	0.55
1:A:157:GLY:HA3	1:A:158:HIS:ND1	2.21	0.55
1:A:215:PRO:O	1:A:219:LEU:HB2	2.07	0.55
1:B:182:MET:HE3	1:B:187:TYR:CD1	2.41	0.55
1:C:398:ILE:HG22	1:C:399:SER:O	2.07	0.55
1:D:158:HIS:C	1:D:159:PRO:CA	2.80	0.55
1:D:24:PHE:HD1	1:D:66:ARG:HB3	1.71	0.55
1:A:3:TYR:OH	1:A:413:ARG:NH2	2.40	0.54
1:A:24:PHE:CD1	1:A:66:ARG:HB3	2.41	0.54
1:B:47:ARG:HG3	1:B:47:ARG:NH1	2.19	0.54
1:C:287:ARG:HB2	1:C:295:GLU:OE2	2.07	0.54
1:D:50:ARG:O	1:D:54:LEU:HB2	2.07	0.54
1:F:285:TRP:O	1:F:378:PHE:HB2	2.07	0.54
1:A:94:LEU:HD23	1:C:197:TRP:HB3	1.88	0.54
1:A:254:LYS:O	1:A:258:ILE:HG23	2.08	0.54
1:C:371:TYR:CE1	1:C:389:ALA:O	2.61	0.54
1:F:24:PHE:O	1:F:326:GLN:CB	2.56	0.54
1:E:70:GLY:HA2	1:E:171:ASN:CG	2.33	0.54
1:E:417:ALA:C	1:E:418:LEU:HD12	2.32	0.54
1:F:158:HIS:C	1:F:159:PRO:CA	2.80	0.54
1:F:197:TRP:O	1:F:198:MET:HB2	2.06	0.54
1:F:255:GLU:OE1	1:F:258:ILE:HD11	2.06	0.54
1:F:368:SER:OG	1:F:369:GLU:N	2.38	0.54
1:A:283:ASN:OD1	1:A:284:VAL:N	2.35	0.54
1:A:378:PHE:O	1:A:379:ILE:HB	2.07	0.54
1:B:431:LYS:NZ	1:B:462:THR:HG22	2.22	0.54
1:C:242:ASP:OD2	1:C:245:GLU:HG3	2.07	0.54
1:D:67:TRP:CG	1:D:68:PRO:HA	2.43	0.54
1:F:208:ILE:HD12	1:F:208:ILE:N	2.22	0.54
1:A:157:GLY:CA	1:A:158:HIS:HB2	2.36	0.54
1:B:373:ILE:HG12	1:B:374:GLU:N	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:195:THR:O	1:C:199:LYS:HB2	2.07	0.54
1:C:411:ASN:ND2	1:C:411:ASN:C	2.66	0.54
1:D:283:ASN:OD1	1:D:284:VAL:N	2.36	0.54
1:F:417:ALA:C	1:F:418:LEU:HD12	2.32	0.54
1:A:158:HIS:C	1:A:159:PRO:CA	2.81	0.54
1:A:431:LYS:NZ	1:A:462:THR:HG22	2.23	0.54
1:C:419:LYS:CA	1:C:470:THR:HG22	2.38	0.54
1:D:262:LYS:O	1:D:266:MET:HG3	2.07	0.54
1:D:413:ARG:O	1:D:474:PHE:N	2.37	0.54
1:E:73:VAL:HG21	1:E:123:SER:O	2.08	0.54
1:E:431:LYS:HD3	1:E:462:THR:HG22	1.89	0.54
1:F:380:ASN:HD22	1:F:380:ASN:N	2.04	0.54
1:A:19:HIS:HD2	1:A:64:ASN:ND2	1.91	0.54
1:B:289:SER:HB3	1:B:379:ILE:HG21	1.90	0.54
1:D:80:ASP:HB3	1:D:89:PRO:HG2	1.90	0.54
1:F:24:PHE:CD1	1:F:66:ARG:HB3	2.43	0.54
1:A:26:GLU:HB3	1:A:326:GLN:HE22	1.72	0.54
1:A:110:ILE:HG13	1:A:162:TYR:CD2	2.42	0.54
1:E:291:ASN:H	1:E:291:ASN:ND2	2.05	0.54
1:F:364:THR:HG21	1:F:396:ALA:H	1.72	0.54
1:B:26:GLU:HG2	1:B:27:HIS:N	2.23	0.54
1:C:259:GLY:HA2	1:F:262:LYS:HD3	1.90	0.54
1:C:336:THR:HG23	1:C:337:GLU:N	2.23	0.54
1:D:297:TYR:OH	1:D:331:LEU:HA	2.08	0.54
1:F:36:ILE:CG2	1:F:328:VAL:HG21	2.38	0.54
1:A:262:LYS:O	1:A:266:MET:HG3	2.08	0.54
1:D:380:ASN:HD22	1:D:380:ASN:N	2.04	0.54
1:E:343:LEU:HD13	1:E:347:TYR:CE1	2.43	0.54
1:F:182:MET:CE	1:F:187:TYR:HD1	2.20	0.54
1:B:28:LEU:HD22	1:B:330:ALA:CB	2.38	0.53
1:F:144:LYS:HD3	1:F:144:LYS:H	1.73	0.53
1:F:219:LEU:O	1:F:223:GLN:HB2	2.08	0.53
1:F:327:LEU:O	1:F:334:ILE:N	2.36	0.53
1:A:391:PHE:CE1	1:A:413:ARG:HG3	2.43	0.53
1:E:158:HIS:C	1:E:159:PRO:CA	2.81	0.53
1:F:26:GLU:CG	1:F:27:HIS:N	2.72	0.53
1:A:71:ASN:HA	1:A:178:GLN:NE2	2.20	0.53
1:A:373:ILE:HG12	1:A:374:GLU:N	2.23	0.53
1:C:431:LYS:CD	1:C:462:THR:HG22	2.37	0.53
1:D:197:TRP:HB3	1:F:94:LEU:HD23	1.89	0.53
1:D:215:PRO:O	1:D:219:LEU:HB2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:328:VAL:CG1	1:E:329:ASN:N	2.60	0.53
1:E:411:ASN:C	1:E:411:ASN:ND2	2.67	0.53
1:E:431:LYS:CD	1:E:462:THR:HG22	2.38	0.53
1:D:336:THR:HG23	1:D:337:GLU:N	2.23	0.53
1:E:197:TRP:C	1:E:199:LYS:H	2.16	0.53
1:A:142:ASN:O	1:A:161:PRO:HB2	2.09	0.53
1:A:144:LYS:HD3	1:A:144:LYS:H	1.73	0.53
1:B:144:LYS:HD3	1:B:144:LYS:H	1.73	0.53
1:B:410:VAL:CG1	1:B:412:TYR:CD2	2.91	0.53
1:E:26:GLU:CG	1:E:27:HIS:N	2.71	0.53
1:A:182:MET:HB3	1:A:186:GLU:HB2	1.91	0.53
1:E:50:ARG:O	1:E:54:LEU:HB2	2.08	0.53
1:A:431:LYS:HD3	1:A:462:THR:HG22	1.91	0.53
1:B:362:VAL:HG11	1:B:398:ILE:CD1	2.38	0.53
1:F:154:ARG:HA	1:F:158:HIS:O	2.08	0.53
1:A:225:ALA:HB1	1:A:229:ILE:HG23	1.90	0.53
1:A:328:VAL:CG1	1:A:329:ASN:N	2.43	0.53
1:B:208:ILE:N	1:B:208:ILE:HD12	2.24	0.53
1:D:334:ILE:HG23	1:D:343:LEU:HD23	1.91	0.53
1:E:28:LEU:HD22	1:E:330:ALA:CB	2.39	0.53
1:F:431:LYS:NZ	1:F:462:THR:HG22	2.23	0.53
1:B:431:LYS:HD3	1:B:462:THR:HG22	1.91	0.53
1:C:362:VAL:HG11	1:C:398:ILE:HD12	1.90	0.53
1:C:371:TYR:CZ	1:C:389:ALA:HB3	2.43	0.53
1:C:428:GLY:O	1:C:464:ASP:HA	2.09	0.53
1:E:67:TRP:CG	1:E:68:PRO:HA	2.43	0.53
1:F:291:ASN:HD22	1:F:291:ASN:N	2.03	0.53
1:A:283:ASN:HB2	1:A:325:ALA:HB2	1.91	0.53
1:A:287:ARG:NH2	1:A:301:ASP:OD2	2.36	0.53
1:A:405:LEU:HB3	1:A:481:VAL:CG1	2.39	0.53
1:C:126:MET:HE3	1:C:194:TYR:CE1	2.44	0.53
1:C:413:ARG:HD2	1:C:416:ASP:HB2	1.90	0.53
1:D:368:SER:OG	1:D:369:GLU:O	2.26	0.53
1:E:197:TRP:C	1:E:199:LYS:N	2.66	0.53
1:E:252:LEU:HD21	1:E:256:ARG:CZ	2.38	0.53
1:F:80:ASP:OD2	1:F:91:ARG:NH1	2.42	0.53
1:F:282:TRP:O	1:F:282:TRP:CG	2.62	0.53
1:F:356:HIS:HB3	1:F:478:VAL:HG11	1.91	0.53
1:A:307:GLY:HA2	1:A:412:TYR:OH	2.09	0.52
1:E:244:TYR:HA	1:E:247:VAL:HG22	1.90	0.52
1:F:91:ARG:HG3	1:F:91:ARG:HH11	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:157:GLY:HA3	1:F:158:HIS:ND1	2.24	0.52
1:A:423:ARG:O	1:A:423:ARG:HG3	2.09	0.52
1:C:291:ASN:HD22	1:C:291:ASN:N	1.99	0.52
1:D:373:ILE:HG12	1:D:374:GLU:N	2.25	0.52
1:F:39:GLU:OE2	1:F:103:ARG:HD3	2.09	0.52
1:F:250:VAL:HG13	1:F:251:TYR:CD2	2.44	0.52
1:A:19:HIS:CD2	1:A:64:ASN:ND2	2.69	0.52
1:A:158:HIS:CD2	1:A:158:HIS:N	2.77	0.52
1:B:67:TRP:CG	1:B:68:PRO:HA	2.45	0.52
1:B:75:ASN:C	1:B:75:ASN:HD22	2.16	0.52
1:C:410:VAL:HG12	1:C:412:TYR:CD1	2.44	0.52
1:D:182:MET:CE	1:D:187:TYR:HD1	2.22	0.52
1:E:19:HIS:HD2	1:E:64:ASN:ND2	1.89	0.52
1:A:157:GLY:O	1:A:158:HIS:HB2	2.09	0.52
1:B:74:SER:CB	1:B:178:GLN:HE21	2.22	0.52
1:B:419:LYS:CA	1:B:470:THR:HG22	2.38	0.52
1:C:262:LYS:O	1:C:266:MET:HG3	2.10	0.52
1:C:474:PHE:O	1:C:474:PHE:CD1	2.63	0.52
1:E:240:SER:O	1:E:300:LYS:HE3	2.09	0.52
1:A:298:ASP:OD1	1:A:300:LYS:HB3	2.09	0.52
1:D:142:ASN:O	1:D:161:PRO:CB	2.58	0.52
1:E:371:TYR:CD1	1:E:389:ALA:O	2.63	0.52
1:F:126:MET:HE3	1:F:194:TYR:CD1	2.45	0.52
1:C:80:ASP:HB3	1:C:89:PRO:HG2	1.92	0.52
1:C:415:GLU:N	1:C:415:GLU:CD	2.67	0.52
1:D:364:THR:HG21	1:D:396:ALA:H	1.75	0.52
1:D:398:ILE:HG22	1:D:399:SER:O	2.10	0.52
1:F:75:ASN:C	1:F:75:ASN:ND2	2.66	0.52
1:A:336:THR:HG23	1:A:337:GLU:N	2.24	0.52
1:B:110:ILE:HG13	1:B:162:TYR:CD2	2.45	0.52
1:C:70:GLY:HA2	1:C:171:ASN:CG	2.34	0.52
1:C:371:TYR:CE1	1:C:389:ALA:HB3	2.44	0.52
1:B:431:LYS:CD	1:B:462:THR:HG22	2.39	0.52
1:C:24:PHE:HD1	1:C:66:ARG:HB3	1.74	0.52
1:D:235:HIS:CD2	1:D:281:GLU:HB2	2.45	0.52
1:E:157:GLY:O	1:E:158:HIS:HB2	2.10	0.52
1:A:376:VAL:HG11	1:A:381:LYS:HB3	1.92	0.52
1:B:307:GLY:HA2	1:B:412:TYR:OH	2.09	0.52
1:D:380:ASN:H	1:D:380:ASN:HD22	1.57	0.52
1:E:75:ASN:ND2	1:E:75:ASN:C	2.68	0.52
1:E:197:TRP:HA	1:E:200:VAL:HG13	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:380:ASN:N	1:E:380:ASN:ND2	2.58	0.52
1:E:380:ASN:H	1:E:380:ASN:ND2	2.07	0.52
1:A:214:ASP:C	1:A:214:ASP:OD1	2.53	0.52
1:C:283:ASN:HB2	1:C:325:ALA:CB	2.39	0.52
1:C:474:PHE:O	1:C:474:PHE:HD1	1.93	0.52
1:D:461:ILE:CG2	1:D:462:THR:N	2.72	0.52
1:A:461:ILE:HG22	1:A:462:THR:N	2.25	0.51
1:C:110:ILE:HG13	1:C:162:TYR:CD2	2.45	0.51
1:C:225:ALA:HB1	1:C:229:ILE:HG23	1.92	0.51
1:E:75:ASN:C	1:E:75:ASN:HD22	2.18	0.51
1:F:3:TYR:HA	1:F:367:GLU:O	2.11	0.51
1:F:85:LYS:O	1:F:86:ASP:HB2	2.10	0.51
1:F:432:ALA:HB2	1:F:481:VAL:HG23	1.92	0.51
1:F:472:LYS:HB3	1:F:473:PRO:HD2	1.91	0.51
1:B:80:ASP:HB3	1:B:89:PRO:HG2	1.92	0.51
1:B:330:ALA:C	1:B:332:GLY:N	2.63	0.51
1:C:26:GLU:CB	1:C:326:GLN:NE2	2.66	0.51
1:F:380:ASN:N	1:F:380:ASN:ND2	2.58	0.51
1:A:126:MET:HE3	1:A:194:TYR:CE1	2.46	0.51
1:B:225:ALA:HB1	1:B:229:ILE:HG23	1.92	0.51
1:C:174:TYR:CE2	1:C:212:CYS:HB3	2.46	0.51
1:C:197:TRP:HA	1:C:200:VAL:HG13	1.91	0.51
1:C:262:LYS:HD2	1:F:258:ILE:HG13	1.92	0.51
1:E:291:ASN:HD22	1:E:291:ASN:N	2.04	0.51
1:E:373:ILE:HG12	1:E:374:GLU:N	2.26	0.51
1:B:80:ASP:OD2	1:B:91:ARG:NH1	2.43	0.51
1:E:298:ASP:OD1	1:E:300:LYS:HB3	2.10	0.51
1:E:299:LEU:HD21	1:E:474:PHE:CD1	2.45	0.51
1:F:285:TRP:NE1	1:F:379:ILE:HD11	2.25	0.51
1:A:219:LEU:O	1:A:223:GLN:HB2	2.10	0.51
1:B:380:ASN:HD22	1:B:380:ASN:N	2.01	0.51
1:C:252:LEU:HD21	1:C:256:ARG:CZ	2.40	0.51
1:D:74:SER:CB	1:D:178:GLN:HE21	2.22	0.51
1:D:419:LYS:CA	1:D:470:THR:HG22	2.41	0.51
1:E:157:GLY:HA3	1:E:158:HIS:ND1	2.25	0.51
1:E:366:VAL:CG2	1:E:367:GLU:N	2.73	0.51
1:F:282:TRP:HD1	1:F:323:ASN:O	1.87	0.51
1:B:423:ARG:HG3	1:B:423:ARG:O	2.10	0.51
1:D:326:GLN:HE22	1:D:330:ALA:CB	2.22	0.51
1:E:330:ALA:C	1:E:332:GLY:N	2.66	0.51
1:E:431:LYS:HZ3	1:E:462:THR:HG22	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:75:ASN:C	1:F:75:ASN:HD22	2.18	0.51
1:F:240:SER:O	1:F:300:LYS:HE3	2.11	0.51
1:F:327:LEU:CG	1:F:328:VAL:HG23	2.28	0.51
1:C:70:GLY:O	1:C:73:VAL:HG12	2.11	0.51
1:E:125:ASN:C	1:E:125:ASN:OD1	2.54	0.51
1:E:214:ASP:C	1:E:214:ASP:OD1	2.54	0.51
1:A:417:ALA:C	1:A:418:LEU:HD12	2.35	0.51
1:B:197:TRP:O	1:B:198:MET:HB2	2.10	0.51
1:B:262:LYS:O	1:B:266:MET:HG3	2.10	0.51
1:C:26:GLU:HA	1:C:68:PRO:O	2.10	0.51
1:D:142:ASN:O	1:D:161:PRO:HB2	2.10	0.51
1:E:461:ILE:CG2	1:E:462:THR:N	2.74	0.51
1:F:291:ASN:H	1:F:291:ASN:ND2	2.08	0.51
1:F:373:ILE:HG12	1:F:374:GLU:N	2.26	0.51
1:C:182:MET:HB3	1:C:186:GLU:HB2	1.92	0.51
1:E:182:MET:HB3	1:E:186:GLU:HB2	1.91	0.51
1:F:182:MET:HB3	1:F:186:GLU:HB2	1.93	0.51
1:A:85:LYS:O	1:A:86:ASP:HB2	2.11	0.51
1:A:410:VAL:HG11	1:A:412:TYR:OH	2.05	0.51
1:B:85:LYS:O	1:B:86:ASP:HB2	2.10	0.51
1:B:410:VAL:HG12	1:B:412:TYR:CG	2.45	0.51
1:B:474:PHE:O	1:B:474:PHE:CD1	2.64	0.51
1:C:250:VAL:HG13	1:C:251:TYR:CD2	2.46	0.51
1:D:19:HIS:CD2	1:D:64:ASN:ND2	2.73	0.51
1:D:83:GLY:C	1:D:84:PRO:O	2.52	0.51
1:E:74:SER:CB	1:E:178:GLN:HE21	2.24	0.51
1:E:287:ARG:HB2	1:E:295:GLU:OE2	2.11	0.51
1:C:285:TRP:CD1	1:C:285:TRP:C	2.88	0.50
1:E:169:ILE:HD11	1:E:207:ALA:HB1	1.93	0.50
1:F:57:VAL:O	1:F:60:ILE:O	2.29	0.50
1:F:244:TYR:HA	1:F:247:VAL:HG22	1.93	0.50
1:F:336:THR:CG2	1:F:337:GLU:N	2.74	0.50
1:F:414:LYS:O	1:F:473:PRO:HB2	2.11	0.50
1:A:235:HIS:CD2	1:A:281:GLU:HB2	2.46	0.50
1:A:450:ASN:C	1:A:452:ASN:H	2.20	0.50
1:C:70:GLY:HA2	1:C:171:ASN:OD1	2.11	0.50
1:D:342:ILE:HD13	1:D:343:LEU:N	2.27	0.50
1:E:179:VAL:HG22	1:F:197:TRP:CZ2	2.47	0.50
1:A:57:VAL:O	1:A:60:ILE:O	2.29	0.50
1:C:368:SER:OG	1:C:369:GLU:N	2.44	0.50
1:A:30:ARG:HB2	1:A:329:ASN:ND2	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:174:TYR:CE2	1:B:212:CYS:HB3	2.46	0.50
1:C:330:ALA:O	1:C:331:LEU:C	2.55	0.50
1:D:299:LEU:HD21	1:D:474:PHE:CD1	2.47	0.50
1:E:236:PHE:CG	1:E:253:LEU:HD13	2.46	0.50
1:F:384:PHE:CD1	1:F:384:PHE:C	2.90	0.50
1:B:291:ASN:HD22	1:B:291:ASN:N	1.98	0.50
1:C:22:GLY:O	1:C:323:ASN:HA	2.11	0.50
1:D:362:VAL:HG22	1:D:396:ALA:O	2.12	0.50
1:D:421:PRO:O	1:D:421:PRO:HG2	2.12	0.50
1:F:62:VAL:CG1	1:F:116:ILE:HD12	2.37	0.50
1:F:298:ASP:OD1	1:F:300:LYS:HB3	2.11	0.50
1:F:461:ILE:CG2	1:F:462:THR:N	2.73	0.50
1:A:384:PHE:CD1	1:A:384:PHE:C	2.89	0.50
1:B:252:LEU:HD23	1:B:252:LEU:C	2.37	0.50
1:D:158:HIS:CD2	1:D:158:HIS:N	2.80	0.50
1:D:434:VAL:O	1:D:434:VAL:HG23	2.11	0.50
1:B:342:ILE:HD13	1:B:343:LEU:N	2.27	0.50
1:D:169:ILE:CD1	1:D:195:THR:OG1	2.60	0.50
1:E:342:ILE:HD13	1:E:343:LEU:N	2.27	0.50
1:A:50:ARG:O	1:A:54:LEU:HB2	2.12	0.50
1:B:343:LEU:HD13	1:B:347:TYR:CE1	2.47	0.50
1:C:158:HIS:N	1:C:158:HIS:CD2	2.80	0.50
1:D:154:ARG:HA	1:D:158:HIS:O	2.11	0.50
1:D:318:ILE:CG1	1:D:319:VAL:HG23	2.41	0.50
1:E:85:LYS:O	1:E:86:ASP:HB2	2.12	0.50
1:F:415:GLU:N	1:F:415:GLU:OE1	2.39	0.50
1:B:432:ALA:HB2	1:B:481:VAL:HG23	1.94	0.50
1:C:283:ASN:OD1	1:C:284:VAL:N	2.41	0.50
1:C:380:ASN:HD22	1:C:380:ASN:H	1.57	0.50
1:D:214:ASP:C	1:D:214:ASP:OD1	2.55	0.50
1:D:482:GLU:OE1	1:D:482:GLU:O	2.30	0.50
1:E:279:LEU:HD22	1:E:282:TRP:HB3	1.94	0.50
1:F:239:GLY:N	1:F:377:MET:O	2.44	0.50
1:B:474:PHE:O	1:B:474:PHE:HD1	1.95	0.49
1:C:75:ASN:C	1:C:75:ASN:ND2	2.68	0.49
1:C:75:ASN:C	1:C:75:ASN:HD22	2.19	0.49
1:C:197:TRP:C	1:C:199:LYS:N	2.69	0.49
1:E:94:LEU:CD2	1:F:197:TRP:HB3	2.39	0.49
1:B:446:ASN:HD21	1:B:454:VAL:N	1.93	0.49
1:C:423:ARG:HG3	1:C:423:ARG:O	2.11	0.49
1:E:324:LEU:HD22	1:E:350:PHE:HE1	1.72	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:74:SER:CB	1:F:178:GLN:HE21	2.25	0.49
1:A:132:ASP:OD2	1:B:77:HIS:CE1	2.65	0.49
1:C:236:PHE:CG	1:C:253:LEU:HD13	2.47	0.49
1:F:28:LEU:HD22	1:F:330:ALA:CB	2.43	0.49
1:F:169:ILE:HD11	1:F:207:ALA:HB1	1.94	0.49
1:C:73:VAL:O	1:C:125:ASN:HB2	2.11	0.49
1:C:270:ALA:O	1:C:273:ARG:O	2.30	0.49
1:A:432:ALA:HB2	1:A:481:VAL:HG23	1.93	0.49
1:B:28:LEU:HD23	1:B:28:LEU:C	2.37	0.49
1:D:334:ILE:HD11	1:D:347:TYR:HE2	1.69	0.49
1:F:428:GLY:O	1:F:464:ASP:HA	2.12	0.49
1:C:238:THR:O	1:C:284:VAL:HA	2.12	0.49
1:C:366:VAL:CG2	1:C:367:GLU:N	2.76	0.49
1:D:70:GLY:HA2	1:D:171:ASN:OD1	2.12	0.49
1:D:378:PHE:O	1:D:379:ILE:C	2.52	0.49
1:E:169:ILE:HG22	1:E:169:ILE:O	2.11	0.49
1:F:327:LEU:C	1:F:333:ALA:H	2.12	0.49
1:A:376:VAL:CG1	1:A:381:LYS:O	2.60	0.49
1:C:158:HIS:C	1:C:159:PRO:HA	2.37	0.49
1:E:423:ARG:HG3	1:E:423:ARG:O	2.11	0.49
1:F:252:LEU:HD12	1:F:384:PHE:CD1	2.48	0.49
1:F:411:ASN:ND2	1:F:411:ASN:C	2.71	0.49
1:B:91:ARG:HH11	1:B:91:ARG:HG3	1.78	0.49
1:B:169:ILE:CD1	1:B:207:ALA:HB1	2.43	0.49
1:B:328:VAL:O	1:B:332:GLY:CA	2.61	0.49
1:C:154:ARG:HA	1:C:158:HIS:O	2.12	0.49
1:D:96:TRP:C	1:D:97:GLN:HG3	2.37	0.49
1:D:126:MET:HE3	1:D:194:TYR:CD1	2.48	0.49
1:D:327:LEU:HG	1:D:328:VAL:HG23	1.94	0.49
1:D:472:LYS:HB3	1:D:473:PRO:HD2	1.95	0.49
1:A:431:LYS:HZ3	1:A:462:THR:HG22	1.78	0.49
1:B:252:LEU:HD13	1:B:377:MET:HE1	1.95	0.49
1:B:450:ASN:C	1:B:452:ASN:H	2.20	0.49
1:C:157:GLY:HA3	1:C:158:HIS:ND1	2.28	0.49
1:C:327:LEU:C	1:C:328:VAL:HG23	2.38	0.49
1:D:219:LEU:O	1:D:223:GLN:HB2	2.13	0.49
1:F:255:GLU:O	1:F:258:ILE:HG12	2.12	0.49
1:A:142:ASN:O	1:A:161:PRO:CB	2.61	0.49
1:B:347:TYR:C	1:B:347:TYR:CD1	2.90	0.49
1:C:28:LEU:HD22	1:C:330:ALA:CB	2.42	0.49
1:C:169:ILE:CD1	1:C:195:THR:OG1	2.61	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:171:ASN:H	1:D:173:MET:HE2	1.78	0.49
1:E:225:ALA:HB1	1:E:229:ILE:HG23	1.95	0.49
1:E:384:PHE:C	1:E:384:PHE:CD1	2.91	0.49
1:F:125:ASN:OD1	1:F:125:ASN:C	2.56	0.49
1:F:376:VAL:H	1:F:376:VAL:HG22	1.29	0.49
1:B:266:MET:HE1	1:E:263:LEU:HG	1.95	0.48
1:C:26:GLU:HG2	1:C:27:HIS:N	2.27	0.48
1:D:70:GLY:HA2	1:D:171:ASN:CG	2.37	0.48
1:D:225:ALA:HB1	1:D:229:ILE:HG23	1.95	0.48
1:F:70:GLY:HA2	1:F:171:ASN:OD1	2.12	0.48
1:F:343:LEU:HD13	1:F:347:TYR:CE1	2.47	0.48
1:A:75:ASN:C	1:A:75:ASN:ND2	2.71	0.48
1:A:261:LYS:C	1:A:261:LYS:CD	2.86	0.48
1:A:364:THR:HG21	1:A:396:ALA:H	1.78	0.48
1:B:26:GLU:CG	1:B:27:HIS:N	2.75	0.48
1:C:258:ILE:HG13	1:F:262:LYS:HD2	1.95	0.48
1:C:327:LEU:O	1:C:327:LEU:CG	2.45	0.48
1:F:70:GLY:HA2	1:F:171:ASN:CG	2.38	0.48
1:F:419:LYS:CA	1:F:470:THR:HG22	2.43	0.48
1:A:366:VAL:CG2	1:A:367:GLU:N	2.76	0.48
1:B:461:ILE:CG2	1:B:462:THR:N	2.75	0.48
1:C:343:LEU:HD13	1:C:347:TYR:CE1	2.49	0.48
1:E:330:ALA:O	1:E:331:LEU:C	2.57	0.48
1:E:335:HIS:O	1:E:342:ILE:HG22	2.13	0.48
1:F:380:ASN:ND2	1:F:380:ASN:H	2.11	0.48
1:C:147:THR:O	1:C:148:TYR:C	2.48	0.48
1:E:419:LYS:CA	1:E:470:THR:HG22	2.44	0.48
1:A:60:ILE:O	1:A:60:ILE:CG1	2.61	0.48
1:A:431:LYS:CD	1:A:462:THR:HG22	2.43	0.48
1:A:434:VAL:O	1:A:434:VAL:HG23	2.14	0.48
1:A:441:ASP:C	1:A:443:ASN:H	2.20	0.48
1:A:472:LYS:HB3	1:A:473:PRO:HD2	1.96	0.48
1:B:318:ILE:CG1	1:B:319:VAL:HG23	2.39	0.48
1:D:287:ARG:HB2	1:D:295:GLU:OE2	2.13	0.48
1:D:379:ILE:O	1:D:379:ILE:CG2	2.61	0.48
1:E:235:HIS:CD2	1:E:281:GLU:HB2	2.49	0.48
1:F:157:GLY:O	1:F:158:HIS:HB2	2.13	0.48
1:F:431:LYS:HD3	1:F:462:THR:HG22	1.94	0.48
1:C:450:ASN:C	1:C:452:ASN:H	2.22	0.48
1:D:22:GLY:HA2	1:D:63:PRO:HD2	1.96	0.48
1:D:73:VAL:HG21	1:D:123:SER:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:24:PHE:CB	1:F:325:ALA:HA	2.35	0.48
1:F:197:TRP:O	1:F:199:LYS:N	2.41	0.48
1:A:126:MET:HE3	1:A:194:TYR:CD1	2.49	0.48
1:A:197:TRP:O	1:A:198:MET:HB2	2.12	0.48
1:A:419:LYS:CB	1:A:470:THR:HG22	2.36	0.48
1:B:411:ASN:C	1:B:411:ASN:ND2	2.72	0.48
1:C:169:ILE:HD12	1:C:207:ALA:HB1	1.95	0.48
1:D:291:ASN:H	1:D:291:ASN:ND2	2.06	0.48
1:F:461:ILE:HD11	1:F:469:HIS:CE1	2.48	0.48
1:A:238:THR:O	1:A:284:VAL:HA	2.13	0.48
1:A:411:ASN:C	1:A:411:ASN:ND2	2.72	0.48
1:B:4:ARG:HH11	1:B:4:ARG:HG3	1.79	0.48
1:B:197:TRP:C	1:B:199:LYS:N	2.72	0.48
1:E:73:VAL:O	1:E:125:ASN:HB2	2.13	0.48
1:F:60:ILE:O	1:F:60:ILE:HG13	2.13	0.48
1:F:158:HIS:N	1:F:158:HIS:CD2	2.82	0.48
1:A:236:PHE:CG	1:A:253:LEU:HD13	2.49	0.47
1:B:70:GLY:HA2	1:B:171:ASN:CG	2.39	0.47
1:B:377:MET:SD	1:B:384:PHE:HB3	2.53	0.47
1:B:434:VAL:CG1	1:B:479:ILE:HG12	2.44	0.47
1:D:411:ASN:ND2	1:D:411:ASN:C	2.66	0.47
1:D:431:LYS:HD3	1:D:462:THR:HG22	1.96	0.47
1:F:279:LEU:HD22	1:F:282:TRP:HB3	1.95	0.47
1:B:125:ASN:C	1:B:125:ASN:OD1	2.57	0.47
1:B:410:VAL:HB	1:B:412:TYR:HE1	1.76	0.47
1:C:262:LYS:CD	1:F:258:ILE:HG13	2.44	0.47
1:D:144:LYS:N	1:D:144:LYS:CD	2.71	0.47
1:D:285:TRP:CD1	1:D:285:TRP:C	2.90	0.47
1:D:365:HIS:ND1	1:D:365:HIS:C	2.71	0.47
1:D:380:ASN:ND2	1:D:380:ASN:N	2.62	0.47
1:E:279:LEU:CD2	1:E:282:TRP:HB3	2.43	0.47
1:F:96:TRP:C	1:F:97:GLN:HG3	2.38	0.47
1:B:378:PHE:CG	1:B:379:ILE:N	2.81	0.47
1:D:384:PHE:CD1	1:D:384:PHE:C	2.92	0.47
1:F:70:GLY:O	1:F:71:ASN:C	2.57	0.47
1:F:182:MET:HE3	1:F:187:TYR:CD1	2.48	0.47
1:F:431:LYS:CD	1:F:462:THR:HG22	2.44	0.47
1:A:419:LYS:CA	1:A:470:THR:HG22	2.44	0.47
1:B:285:TRP:C	1:B:285:TRP:CD1	2.90	0.47
1:C:373:ILE:HG12	1:C:374:GLU:N	2.29	0.47
1:D:71:ASN:OD1	1:D:71:ASN:N	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:125:ASN:C	1:D:125:ASN:OD1	2.57	0.47
1:D:285:TRP:NE1	1:D:379:ILE:HD11	2.29	0.47
1:D:343:LEU:HD13	1:D:347:TYR:CE1	2.50	0.47
1:E:255:GLU:O	1:E:258:ILE:HG12	2.14	0.47
1:F:434:VAL:HG12	1:F:479:ILE:HG12	1.96	0.47
1:A:26:GLU:HG2	1:A:27:HIS:N	2.27	0.47
1:B:274:GLY:O	1:B:276:LYS:HG3	2.14	0.47
1:B:379:ILE:HG22	1:B:379:ILE:O	2.13	0.47
1:C:291:ASN:ND2	1:C:291:ASN:N	2.61	0.47
1:E:25:THR:O	1:E:25:THR:CG2	2.61	0.47
1:E:197:TRP:O	1:E:198:MET:HB2	2.14	0.47
1:B:24:PHE:CD1	1:B:66:ARG:HB3	2.50	0.47
1:B:244:TYR:HA	1:B:247:VAL:HG22	1.95	0.47
1:B:336:THR:HG23	1:B:337:GLU:N	2.29	0.47
1:C:197:TRP:O	1:C:198:MET:HB2	2.14	0.47
1:C:364:THR:HG21	1:C:396:ALA:H	1.80	0.47
1:E:158:HIS:N	1:E:158:HIS:CD2	2.83	0.47
1:F:252:LEU:HD21	1:F:256:ARG:CZ	2.45	0.47
1:B:197:TRP:HA	1:B:200:VAL:HG13	1.96	0.47
1:B:235:HIS:CD2	1:B:281:GLU:HB2	2.49	0.47
1:B:378:PHE:C	1:B:380:ASN:H	2.21	0.47
1:C:472:LYS:HB3	1:C:473:PRO:HD2	1.97	0.47
1:D:347:TYR:CD1	1:D:347:TYR:C	2.93	0.47
1:D:419:LYS:HE2	1:D:419:LYS:HB3	1.68	0.47
1:F:120:PRO:HG2	1:F:164:VAL:HG13	1.97	0.47
1:C:45:ASP:CG	1:C:46:GLU:N	2.71	0.47
1:C:464:ASP:O	1:C:466:GLU:N	2.47	0.47
1:D:268:ASP:O	1:D:272:LYS:HD3	2.15	0.47
1:E:285:TRP:CZ2	1:E:379:ILE:HD11	2.49	0.47
1:E:365:HIS:C	1:E:365:HIS:ND1	2.71	0.47
1:E:419:LYS:HE2	1:E:419:LYS:HB3	1.59	0.47
1:F:225:ALA:HB1	1:F:229:ILE:HG23	1.96	0.47
1:A:328:VAL:O	1:A:328:VAL:HG13	1.95	0.47
1:B:240:SER:O	1:B:300:LYS:HE3	2.14	0.47
1:C:27:HIS:CD2	1:C:32:ILE:HG13	2.50	0.47
1:C:464:ASP:C	1:C:466:GLU:N	2.71	0.47
1:D:197:TRP:C	1:D:199:LYS:N	2.72	0.47
1:E:142:ASN:O	1:E:161:PRO:HB2	2.15	0.47
1:F:252:LEU:HD21	1:F:256:ARG:NH1	2.30	0.47
1:F:268:ASP:O	1:F:272:LYS:HD3	2.15	0.47
1:F:330:ALA:C	1:F:332:GLY:N	2.67	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:LYS:O	1:A:87:GLN:N	2.43	0.47
1:B:378:PHE:CD1	1:B:379:ILE:N	2.80	0.47
1:B:384:PHE:CD1	1:B:384:PHE:C	2.93	0.47
1:C:50:ARG:O	1:C:54:LEU:HB2	2.15	0.47
1:D:169:ILE:HD13	1:D:195:THR:OG1	2.14	0.47
1:E:126:MET:HE3	1:E:194:TYR:CE1	2.49	0.47
1:E:362:VAL:HG11	1:E:398:ILE:CD1	2.45	0.47
1:F:142:ASN:O	1:F:161:PRO:HB2	2.15	0.47
1:C:235:HIS:CD2	1:C:281:GLU:HB2	2.50	0.46
1:C:419:LYS:HB3	1:C:419:LYS:HE2	1.70	0.46
1:D:244:TYR:HA	1:D:247:VAL:HG22	1.97	0.46
1:D:279:LEU:CD2	1:D:282:TRP:HB3	2.45	0.46
1:D:419:LYS:HA	1:D:470:THR:HG22	1.97	0.46
1:E:215:PRO:O	1:E:219:LEU:HB2	2.15	0.46
1:A:25:THR:HG22	1:A:66:ARG:O	2.15	0.46
1:B:378:PHE:C	1:B:380:ASN:N	2.71	0.46
1:C:268:ASP:O	1:C:272:LYS:HD3	2.16	0.46
1:C:419:LYS:HA	1:C:470:THR:HG22	1.98	0.46
1:D:94:LEU:HD23	1:E:197:TRP:HB3	1.97	0.46
1:F:445:ARG:HH11	1:F:445:ARG:HG3	1.79	0.46
1:F:461:ILE:HG22	1:F:462:THR:N	2.30	0.46
1:A:147:THR:HA	1:B:90:VAL:HG12	1.97	0.46
1:A:169:ILE:HD13	1:A:195:THR:OG1	2.15	0.46
1:A:197:TRP:C	1:A:199:LYS:N	2.73	0.46
1:A:252:LEU:HD21	1:A:256:ARG:CZ	2.45	0.46
1:C:215:PRO:HG3	1:F:266:MET:HB3	1.96	0.46
1:D:255:GLU:OE1	1:D:258:ILE:HD11	2.15	0.46
1:D:423:ARG:O	1:D:423:ARG:HG3	2.15	0.46
1:E:77:HIS:CE1	1:F:132:ASP:OD2	2.68	0.46
1:F:142:ASN:O	1:F:161:PRO:CB	2.64	0.46
1:A:25:THR:HB	1:A:65:LEU:HD11	1.98	0.46
1:A:70:GLY:HA2	1:A:171:ASN:CG	2.40	0.46
1:A:174:TYR:CE2	1:A:212:CYS:HB3	2.50	0.46
1:B:328:VAL:CG1	1:B:329:ASN:N	2.77	0.46
1:B:414:LYS:O	1:B:415:GLU:HB3	2.15	0.46
1:B:441:ASP:C	1:B:443:ASN:H	2.22	0.46
1:B:464:ASP:C	1:B:466:GLU:N	2.74	0.46
1:C:45:ASP:OD2	1:C:47:ARG:NH1	2.49	0.46
1:A:24:PHE:HB3	1:A:325:ALA:O	2.15	0.46
1:A:365:HIS:ND1	1:A:365:HIS:C	2.73	0.46
1:A:445:ARG:HG3	1:A:445:ARG:HH11	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:50:ARG:O	1:B:54:LEU:HB2	2.15	0.46
1:B:365:HIS:C	1:B:365:HIS:ND1	2.73	0.46
1:C:125:ASN:C	1:C:125:ASN:OD1	2.58	0.46
1:C:158:HIS:O	1:C:159:PRO:N	2.48	0.46
1:E:185:ASP:OD1	1:E:220:ARG:HD3	2.15	0.46
1:E:285:TRP:NE1	1:E:379:ILE:HD11	2.31	0.46
1:A:43:LEU:HD12	1:A:43:LEU:N	2.31	0.46
1:B:239:GLY:O	1:B:377:MET:HA	2.15	0.46
1:B:366:VAL:CG2	1:B:367:GLU:N	2.78	0.46
1:C:143:GLY:O	1:C:150:ALA:HB1	2.15	0.46
1:D:27:HIS:CD2	1:D:32:ILE:HG13	2.50	0.46
1:D:405:LEU:HG	1:D:406:PHE:N	2.29	0.46
1:D:409:VAL:HG21	1:D:471:PHE:CE2	2.50	0.46
1:D:461:ILE:HG22	1:D:462:THR:N	2.30	0.46
1:E:51:LYS:O	1:E:55:GLU:HG3	2.16	0.46
1:F:326:GLN:NE2	1:F:330:ALA:CB	2.52	0.46
1:F:378:PHE:O	1:F:379:ILE:C	2.59	0.46
1:A:239:GLY:O	1:A:377:MET:HA	2.15	0.46
1:B:24:PHE:HD1	1:B:66:ARG:HB3	1.80	0.46
1:B:154:ARG:HA	1:B:158:HIS:O	2.15	0.46
1:C:4:ARG:HG3	1:C:4:ARG:HH11	1.80	0.46
1:C:169:ILE:HD13	1:C:195:THR:OG1	2.15	0.46
1:D:291:ASN:HD22	1:D:291:ASN:N	1.98	0.46
1:B:5:ILE:HG22	1:B:366:VAL:HG23	1.97	0.46
1:B:126:MET:HE3	1:B:194:TYR:CE1	2.51	0.46
1:C:410:VAL:HG11	1:C:412:TYR:CZ	2.50	0.46
1:D:283:ASN:HB2	1:D:325:ALA:HB3	1.98	0.46
1:F:60:ILE:HG22	1:F:351:GLU:HA	1.97	0.46
1:F:327:LEU:HG	1:F:328:VAL:N	2.31	0.46
1:A:343:LEU:HD13	1:A:347:TYR:CE1	2.51	0.46
1:B:144:LYS:N	1:B:144:LYS:CD	2.78	0.46
1:D:157:GLY:HA3	1:D:158:HIS:HB2	1.97	0.46
1:D:330:ALA:O	1:D:332:GLY:N	2.49	0.46
1:D:441:ASP:C	1:D:443:ASN:H	2.24	0.46
1:F:80:ASP:HB3	1:F:89:PRO:HG2	1.98	0.46
1:F:362:VAL:HG22	1:F:396:ALA:O	2.16	0.46
1:F:431:LYS:HZ3	1:F:462:THR:HG22	1.81	0.46
1:F:434:VAL:CG1	1:F:479:ILE:HG12	2.46	0.46
1:A:96:TRP:C	1:A:97:GLN:HG3	2.41	0.46
1:A:410:VAL:CB	1:A:412:TYR:CZ	2.95	0.46
1:B:169:ILE:CD1	1:B:195:THR:OG1	2.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:255:GLU:O	1:D:258:ILE:HG12	2.15	0.46
1:D:342:ILE:C	1:D:342:ILE:CD1	2.89	0.46
1:D:434:VAL:O	1:D:434:VAL:CG2	2.63	0.46
1:A:307:GLY:CA	1:A:412:TYR:OH	2.63	0.45
1:B:329:ASN:ND2	1:B:336:THR:HB	2.27	0.45
1:B:368:SER:OG	1:B:369:GLU:N	2.50	0.45
1:C:279:LEU:HD22	1:C:282:TRP:HB3	1.99	0.45
1:C:362:VAL:O	1:C:363:LYS:C	2.59	0.45
1:C:445:ARG:HH11	1:C:445:ARG:HG3	1.81	0.45
1:D:73:VAL:O	1:D:125:ASN:HB2	2.16	0.45
1:E:27:HIS:HB2	1:E:72:PHE:CD2	2.50	0.45
1:E:240:SER:HB2	1:E:376:VAL:CG2	2.46	0.45
1:F:169:ILE:O	1:F:169:ILE:HG22	2.16	0.45
1:A:77:HIS:CE1	1:C:132:ASP:OD2	2.68	0.45
1:A:169:ILE:CD1	1:A:207:ALA:HB1	2.47	0.45
1:A:416:ASP:H	1:A:473:PRO:HB3	1.81	0.45
1:A:419:LYS:HE2	1:A:419:LYS:HB3	1.72	0.45
1:A:474:PHE:CD1	1:A:474:PHE:O	2.69	0.45
1:C:378:PHE:CG	1:C:379:ILE:N	2.84	0.45
1:D:36:ILE:CG2	1:D:328:VAL:HG21	2.43	0.45
1:D:158:HIS:C	1:D:159:PRO:HA	2.40	0.45
1:D:411:ASN:HD22	1:D:412:TYR:N	2.14	0.45
1:E:28:LEU:C	1:E:28:LEU:HD23	2.41	0.45
1:A:270:ALA:O	1:A:273:ARG:O	2.34	0.45
1:B:62:VAL:HA	1:B:63:PRO:HD3	1.75	0.45
1:E:94:LEU:HD23	1:F:197:TRP:CB	2.45	0.45
1:F:169:ILE:HD12	1:F:207:ALA:HB1	1.98	0.45
1:A:27:HIS:CD2	1:A:32:ILE:HG13	2.51	0.45
1:A:291:ASN:H	1:A:291:ASN:ND2	2.12	0.45
1:A:381:LYS:O	1:A:382:MET:C	2.60	0.45
1:B:158:HIS:C	1:B:159:PRO:HA	2.41	0.45
1:C:384:PHE:CD1	1:C:384:PHE:C	2.94	0.45
1:F:60:ILE:HA	1:F:354:VAL:HG21	1.97	0.45
1:B:47:ARG:NH2	1:B:115:GLU:OE1	2.49	0.45
1:B:282:TRP:O	1:B:282:TRP:CG	2.70	0.45
1:C:318:ILE:CG1	1:C:319:VAL:HG23	2.43	0.45
1:C:326:GLN:HG2	1:C:330:ALA:HB3	1.99	0.45
1:C:328:VAL:CG1	1:C:329:ASN:N	2.47	0.45
1:D:26:GLU:CB	1:D:326:GLN:OE1	2.56	0.45
1:D:169:ILE:O	1:D:169:ILE:HG22	2.17	0.45
1:E:262:LYS:O	1:E:266:MET:HG3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:450:ASN:C	1:E:452:ASN:H	2.25	0.45
1:F:25:THR:O	1:F:25:THR:CG2	2.56	0.45
1:F:243:TYR:CG	1:F:414:LYS:HD2	2.52	0.45
1:F:256:ARG:HH21	1:F:377:MET:HE1	1.82	0.45
1:F:362:VAL:O	1:F:363:LYS:C	2.59	0.45
1:A:47:ARG:HH11	1:A:47:ARG:CG	2.26	0.45
1:A:75:ASN:C	1:A:75:ASN:HD22	2.25	0.45
1:B:24:PHE:O	1:B:327:LEU:HB2	2.16	0.45
1:E:126:MET:HE3	1:E:194:TYR:CD1	2.51	0.45
1:E:231:PHE:HA	1:E:276:LYS:O	2.17	0.45
1:F:329:ASN:ND2	1:F:336:THR:HB	2.30	0.45
1:A:252:LEU:HD23	1:A:252:LEU:C	2.41	0.45
1:A:291:ASN:HD22	1:A:291:ASN:N	2.03	0.45
1:C:157:GLY:CA	1:C:158:HIS:HB2	2.47	0.45
1:C:163:ASN:CG	1:C:163:ASN:O	2.58	0.45
1:E:460:THR:HG22	1:E:461:ILE:N	2.32	0.45
1:F:4:ARG:HG3	1:F:4:ARG:HH11	1.82	0.45
1:F:376:VAL:O	1:F:376:VAL:CG2	2.44	0.45
1:A:30:ARG:NH1	1:A:336:THR:HG22	2.21	0.45
1:A:171:ASN:O	1:A:172:GLU:C	2.59	0.45
1:A:244:TYR:HA	1:A:247:VAL:HG22	1.98	0.45
1:C:26:GLU:CG	1:C:27:HIS:N	2.79	0.45
1:C:62:VAL:HA	1:C:63:PRO:HD3	1.71	0.45
1:C:347:TYR:CD1	1:C:347:TYR:C	2.94	0.45
1:C:461:ILE:CG2	1:C:462:THR:N	2.80	0.45
1:E:25:THR:HA	1:E:326:GLN:HG2	1.98	0.45
1:F:282:TRP:O	1:F:282:TRP:CD2	2.70	0.45
1:A:318:ILE:CG1	1:A:319:VAL:HG23	2.43	0.45
1:B:219:LEU:O	1:B:223:GLN:HB2	2.16	0.45
1:B:260:VAL:HA	1:B:263:LEU:HD12	1.97	0.45
1:B:416:ASP:N	1:B:473:PRO:HB3	2.32	0.45
1:C:73:VAL:HG21	1:C:123:SER:O	2.17	0.45
1:C:290:ASP:C	1:C:290:ASP:OD1	2.60	0.45
1:D:431:LYS:CD	1:D:462:THR:HG22	2.47	0.45
1:E:318:ILE:CG1	1:E:319:VAL:HG23	2.43	0.45
1:A:330:ALA:O	1:A:331:LEU:C	2.60	0.44
1:B:60:ILE:O	1:B:60:ILE:CG1	2.64	0.44
1:B:60:ILE:HG22	1:B:351:GLU:HA	1.98	0.44
1:B:252:LEU:HD21	1:B:256:ARG:CZ	2.47	0.44
1:B:261:LYS:CD	1:B:261:LYS:C	2.90	0.44
1:C:19:HIS:CD2	1:C:64:ASN:ND2	2.70	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:334:ILE:CG1	1:D:347:TYR:CD2	3.00	0.44
1:E:5:ILE:HG22	1:E:366:VAL:HG23	2.00	0.44
1:F:197:TRP:O	1:F:198:MET:CB	2.64	0.44
1:A:362:VAL:HG11	1:A:398:ILE:HG13	1.98	0.44
1:A:473:PRO:O	1:A:474:PHE:C	2.61	0.44
1:B:27:HIS:CD2	1:B:32:ILE:HG13	2.52	0.44
1:B:66:ARG:HA	1:B:121:TYR:O	2.17	0.44
1:D:45:ASP:OD2	1:D:47:ARG:NH1	2.49	0.44
1:D:179:VAL:HG22	1:E:197:TRP:CZ2	2.52	0.44
1:E:28:LEU:HD22	1:E:330:ALA:HB2	1.99	0.44
1:E:28:LEU:HD22	1:E:330:ALA:HB1	2.00	0.44
1:E:81:GLY:O	1:E:105:GLY:HA3	2.18	0.44
1:F:174:TYR:CE2	1:F:212:CYS:HB3	2.53	0.44
1:A:335:HIS:O	1:A:342:ILE:HG22	2.18	0.44
1:B:431:LYS:HZ3	1:B:462:THR:HG22	1.80	0.44
1:D:474:PHE:CD1	1:D:474:PHE:O	2.70	0.44
1:E:250:VAL:HG13	1:E:251:TYR:CE2	2.53	0.44
1:E:252:LEU:HD23	1:E:252:LEU:C	2.43	0.44
1:E:391:PHE:CD1	1:E:413:ARG:HD3	2.52	0.44
1:F:270:ALA:O	1:F:273:ARG:O	2.35	0.44
1:F:441:ASP:C	1:F:443:ASN:H	2.24	0.44
1:A:169:ILE:HD12	1:A:207:ALA:HB1	1.99	0.44
1:B:342:ILE:C	1:B:343:LEU:HD23	2.43	0.44
1:B:362:VAL:HG11	1:B:398:ILE:HD12	1.97	0.44
1:B:362:VAL:HG22	1:B:396:ALA:O	2.16	0.44
1:C:463:VAL:HB	1:C:467:PHE:CE2	2.53	0.44
1:D:4:ARG:HA	1:D:420:VAL:HG23	1.99	0.44
1:D:157:GLY:O	1:D:158:HIS:CB	2.66	0.44
1:D:197:TRP:HA	1:D:200:VAL:HG13	1.99	0.44
1:E:60:ILE:HG22	1:E:351:GLU:HA	2.00	0.44
1:E:392:LEU:HD12	1:E:410:VAL:O	2.18	0.44
1:E:464:ASP:C	1:E:466:GLU:N	2.75	0.44
1:F:202:ASP:O	1:F:205:ILE:HG12	2.16	0.44
1:F:403:LYS:O	1:F:403:LYS:HG3	2.17	0.44
1:A:28:LEU:HD23	1:A:28:LEU:C	2.43	0.44
1:B:70:GLY:HA2	1:B:171:ASN:OD1	2.18	0.44
1:B:171:ASN:O	1:B:172:GLU:C	2.61	0.44
1:B:325:ALA:HA	1:B:326:GLN:HA	1.75	0.44
1:B:446:ASN:HD22	1:B:446:ASN:N	2.15	0.44
1:D:318:ILE:HG13	1:D:319:VAL:CG2	2.44	0.44
1:E:24:PHE:O	1:E:326:GLN:HA	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:291:ASN:ND2	1:E:291:ASN:N	2.64	0.44
1:E:377:MET:O	1:E:377:MET:HG3	2.17	0.44
1:F:365:HIS:C	1:F:365:HIS:ND1	2.76	0.44
1:B:162:TYR:O	1:B:163:ASN:HB3	2.18	0.44
1:C:208:ILE:HD12	1:C:208:ILE:N	2.33	0.44
1:D:162:TYR:O	1:D:163:ASN:HB3	2.18	0.44
1:D:192:LYS:HE2	1:F:176:GLU:OE2	2.17	0.44
1:E:208:ILE:N	1:E:208:ILE:HD12	2.33	0.44
1:E:267:VAL:O	1:E:268:ASP:C	2.60	0.44
1:F:243:TYR:CB	1:F:414:LYS:HD2	2.48	0.44
1:A:145:GLY:O	1:A:154:ARG:NH2	2.50	0.44
1:A:240:SER:O	1:A:300:LYS:HE3	2.18	0.44
1:B:60:ILE:HA	1:B:354:VAL:HG21	2.00	0.44
1:B:418:LEU:O	1:B:470:THR:HA	2.18	0.44
1:D:463:VAL:HB	1:D:467:PHE:CE2	2.53	0.44
1:E:434:VAL:O	1:E:434:VAL:HG23	2.18	0.44
1:F:215:PRO:O	1:F:219:LEU:HB2	2.17	0.44
1:F:371:TYR:CD1	1:F:389:ALA:O	2.71	0.44
1:F:423:ARG:O	1:F:423:ARG:HG3	2.16	0.44
1:A:74:SER:CB	1:A:178:GLN:HE21	2.30	0.44
1:A:324:LEU:O	1:A:325:ALA:C	2.60	0.44
1:C:22:GLY:HA2	1:C:63:PRO:HD2	1.99	0.44
1:C:214:ASP:OD1	1:C:214:ASP:C	2.60	0.44
1:D:126:MET:HB2	1:D:173:MET:HE3	1.98	0.44
1:D:252:LEU:C	1:D:252:LEU:HD23	2.43	0.44
1:E:282:TRP:O	1:E:324:LEU:HD12	2.18	0.44
1:E:397:SER:O	1:E:405:LEU:HD12	2.17	0.44
1:E:472:LYS:HB3	1:E:473:PRO:HD2	1.99	0.44
1:F:24:PHE:CB	1:F:325:ALA:CA	2.78	0.44
1:F:197:TRP:C	1:F:199:LYS:N	2.76	0.44
1:F:342:ILE:HD13	1:F:343:LEU:N	2.33	0.44
1:B:197:TRP:O	1:B:198:MET:CB	2.65	0.44
1:B:255:GLU:O	1:B:258:ILE:HG12	2.18	0.44
1:B:410:VAL:CG2	1:B:412:TYR:OH	2.64	0.44
1:C:28:LEU:HD22	1:C:330:ALA:HB1	2.00	0.44
1:D:324:LEU:C	1:D:325:ALA:O	2.52	0.44
1:D:464:ASP:C	1:D:466:GLU:N	2.74	0.44
1:E:158:HIS:C	1:E:159:PRO:HA	2.42	0.44
1:E:377:MET:N	1:E:382:MET:O	2.47	0.44
1:B:250:VAL:HG13	1:B:251:TYR:CE2	2.53	0.43
1:B:405:LEU:HB3	1:B:481:VAL:CG1	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:74:SER:HB2	1:C:178:GLN:HE21	1.83	0.43
1:C:219:LEU:O	1:C:223:GLN:HB2	2.17	0.43
1:E:409:VAL:HG21	1:E:471:PHE:CE2	2.53	0.43
1:F:60:ILE:O	1:F:60:ILE:CG1	2.66	0.43
1:A:291:ASN:ND2	1:A:291:ASN:N	2.66	0.43
1:A:299:LEU:HD21	1:A:474:PHE:CD1	2.53	0.43
1:A:419:LYS:HG2	1:A:470:THR:HG22	1.38	0.43
1:B:126:MET:HE3	1:B:194:TYR:CD1	2.53	0.43
1:B:318:ILE:HG13	1:B:319:VAL:CG2	2.43	0.43
1:B:330:ALA:O	1:B:331:LEU:C	2.60	0.43
1:C:282:TRP:O	1:C:282:TRP:CG	2.71	0.43
1:D:250:VAL:HG13	1:D:251:TYR:CE2	2.54	0.43
1:D:371:TYR:CD1	1:D:389:ALA:O	2.72	0.43
1:B:373:ILE:CG1	1:B:374:GLU:N	2.80	0.43
1:D:251:TYR:HE2	1:D:412:TYR:HH	1.64	0.43
1:D:261:LYS:CD	1:D:261:LYS:C	2.91	0.43
1:D:458:SER:O	1:D:459:GLU:HB2	2.18	0.43
1:E:342:ILE:C	1:E:342:ILE:CD1	2.90	0.43
1:E:415:GLU:N	1:E:415:GLU:OE1	2.43	0.43
1:F:22:GLY:HA2	1:F:63:PRO:HD2	2.00	0.43
1:F:328:VAL:HA	1:F:334:ILE:HB	2.00	0.43
1:A:208:ILE:HD12	1:A:208:ILE:N	2.32	0.43
1:A:474:PHE:O	1:A:474:PHE:HD1	2.01	0.43
1:B:473:PRO:O	1:B:474:PHE:C	2.61	0.43
1:E:91:ARG:HH11	1:E:91:ARG:CG	2.31	0.43
1:F:85:LYS:O	1:F:87:GLN:N	2.49	0.43
1:A:380:ASN:HD22	1:A:381:LYS:N	2.16	0.43
1:A:409:VAL:HG21	1:A:471:PHE:CE1	2.54	0.43
1:B:28:LEU:HD22	1:B:330:ALA:HB2	1.98	0.43
1:B:122:ILE:HD12	1:B:164:VAL:HG21	2.01	0.43
1:C:16:ILE:HA	1:C:316:SER:OG	2.18	0.43
1:C:30:ARG:NH1	1:C:336:THR:HG22	2.24	0.43
1:C:405:LEU:HB3	1:C:481:VAL:CG1	2.48	0.43
1:D:377:MET:O	1:D:378:PHE:CB	2.54	0.43
1:E:251:TYR:HE2	1:E:412:TYR:CZ	2.37	0.43
1:F:285:TRP:CD1	1:F:285:TRP:C	2.92	0.43
1:F:434:VAL:O	1:F:434:VAL:HG23	2.19	0.43
1:C:261:LYS:C	1:C:261:LYS:CD	2.92	0.43
1:D:62:VAL:CG1	1:D:116:ILE:HD12	2.44	0.43
1:D:446:ASN:HD22	1:D:446:ASN:N	2.16	0.43
1:E:62:VAL:HA	1:E:63:PRO:HD3	1.74	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:VAL:HG21	1:A:123:SER:O	2.18	0.43
1:A:460:THR:HG22	1:A:461:ILE:N	2.33	0.43
1:B:157:GLY:O	1:B:158:HIS:CB	2.65	0.43
1:B:326:GLN:HB2	1:B:330:ALA:O	2.19	0.43
1:B:458:SER:O	1:B:459:GLU:HB2	2.18	0.43
1:C:252:LEU:HD23	1:C:252:LEU:C	2.43	0.43
1:C:255:GLU:O	1:C:258:ILE:HG12	2.18	0.43
1:D:182:MET:HE3	1:D:187:TYR:CD1	2.49	0.43
1:E:285:TRP:C	1:E:285:TRP:CD1	2.94	0.43
1:E:411:ASN:HD22	1:E:412:TYR:N	2.16	0.43
1:F:157:GLY:HA3	1:F:158:HIS:HB2	2.01	0.43
1:F:256:ARG:NH2	1:F:377:MET:HE1	2.34	0.43
1:F:291:ASN:N	1:F:291:ASN:ND2	2.64	0.43
1:B:206:LYS:HA	1:B:230:ASP:OD2	2.18	0.43
1:B:215:PRO:HG3	1:E:266:MET:HB3	2.01	0.43
1:B:434:VAL:HG12	1:B:479:ILE:HG12	2.01	0.43
1:C:5:ILE:HG22	1:C:366:VAL:HG23	2.01	0.43
1:D:279:LEU:HD22	1:D:282:TRP:HB3	1.99	0.43
1:F:73:VAL:O	1:F:125:ASN:HB2	2.18	0.43
1:F:238:THR:O	1:F:284:VAL:HA	2.19	0.43
1:F:279:LEU:CD2	1:F:282:TRP:HB3	2.49	0.43
1:A:283:ASN:HD22	1:A:325:ALA:HB3	1.83	0.43
1:C:365:HIS:C	1:C:365:HIS:ND1	2.76	0.43
1:D:53:VAL:HG22	1:D:341:LEU:HD11	2.01	0.43
1:E:142:ASN:O	1:E:161:PRO:CB	2.67	0.43
1:F:62:VAL:HA	1:F:63:PRO:HD3	1.77	0.43
1:A:26:GLU:CG	1:A:27:HIS:N	2.81	0.43
1:B:74:SER:HB2	1:B:178:GLN:HE21	1.84	0.43
1:B:96:TRP:C	1:B:97:GLN:HG3	2.43	0.43
1:D:331:LEU:O	1:D:332:GLY:C	2.61	0.43
1:D:411:ASN:OD1	1:D:413:ARG:HB2	2.19	0.43
1:E:67:TRP:O	1:E:122:ILE:HA	2.18	0.43
1:F:199:LYS:HE2	1:F:205:ILE:O	2.18	0.43
1:F:362:VAL:HG11	1:F:398:ILE:HD12	2.00	0.43
1:F:461:ILE:HD11	1:F:469:HIS:ND1	2.34	0.43
1:A:371:TYR:CD1	1:A:389:ALA:O	2.72	0.42
1:B:335:HIS:O	1:B:342:ILE:HG22	2.19	0.42
1:B:394:ALA:HB1	1:B:408:ALA:O	2.19	0.42
1:D:415:GLU:CD	1:D:415:GLU:N	2.71	0.42
1:E:96:TRP:C	1:E:97:GLN:HG3	2.44	0.42
1:F:411:ASN:ND2	1:F:413:ARG:N	2.60	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:ARG:CB	1:A:329:ASN:ND2	2.83	0.42
1:A:197:TRP:HA	1:A:200:VAL:HG13	2.00	0.42
1:B:197:TRP:CZ2	1:C:179:VAL:HG22	2.53	0.42
1:B:460:THR:HG22	1:B:461:ILE:N	2.34	0.42
1:C:126:MET:HB2	1:C:173:MET:HE3	2.00	0.42
1:C:202:ASP:O	1:C:205:ILE:HG12	2.18	0.42
1:C:234:TYR:OH	1:C:256:ARG:HG2	2.19	0.42
1:C:299:LEU:HD21	1:C:474:PHE:CD1	2.54	0.42
1:D:67:TRP:O	1:D:122:ILE:HA	2.19	0.42
1:E:461:ILE:HD11	1:E:469:HIS:CE1	2.54	0.42
1:F:418:LEU:O	1:F:470:THR:HA	2.18	0.42
1:A:197:TRP:O	1:A:198:MET:CB	2.66	0.42
1:B:157:GLY:CA	1:B:158:HIS:HB2	2.49	0.42
1:C:34:GLY:O	1:C:336:THR:CG2	2.56	0.42
1:C:171:ASN:O	1:C:172:GLU:C	2.63	0.42
1:D:28:LEU:HD23	1:D:28:LEU:C	2.43	0.42
1:D:148:TYR:CD1	1:D:148:TYR:C	2.96	0.42
1:D:362:VAL:HG11	1:D:398:ILE:CD1	2.50	0.42
1:E:214:ASP:HA	1:E:215:PRO:HD3	1.92	0.42
1:E:362:VAL:HG11	1:E:398:ILE:HD12	2.01	0.42
1:E:368:SER:OG	1:E:369:GLU:N	2.52	0.42
1:F:214:ASP:OD1	1:F:214:ASP:C	2.60	0.42
1:A:67:TRP:CE2	1:A:68:PRO:HB3	2.55	0.42
1:A:94:LEU:CD2	1:C:197:TRP:HB3	2.49	0.42
1:B:126:MET:HE2	1:B:182:MET:HE1	2.01	0.42
1:B:157:GLY:HA3	1:B:158:HIS:ND1	2.34	0.42
1:B:411:ASN:ND2	1:B:413:ARG:H	2.16	0.42
1:B:445:ARG:HH11	1:B:445:ARG:HG3	1.85	0.42
1:C:71:ASN:OD1	1:C:71:ASN:N	2.42	0.42
1:C:215:PRO:O	1:C:219:LEU:HB2	2.18	0.42
1:C:330:ALA:O	1:C:332:GLY:N	2.52	0.42
1:D:94:LEU:CD2	1:E:197:TRP:HB3	2.49	0.42
1:E:461:ILE:HG22	1:E:462:THR:N	2.34	0.42
1:F:236:PHE:CG	1:F:253:LEU:HD13	2.54	0.42
1:A:154:ARG:HA	1:A:158:HIS:O	2.19	0.42
1:B:28:LEU:HD22	1:B:330:ALA:HB1	2.00	0.42
1:B:371:TYR:CD1	1:B:389:ALA:O	2.72	0.42
1:B:461:ILE:HD11	1:B:469:HIS:ND1	2.34	0.42
1:C:61:LYS:HE2	1:C:355:ASN:OD1	2.19	0.42
1:D:240:SER:O	1:D:300:LYS:HE3	2.19	0.42
1:E:169:ILE:CD1	1:E:195:THR:OG1	2.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:347:TYR:CD1	1:A:347:TYR:C	2.98	0.42
1:C:245:GLU:O	1:C:249:THR:HG23	2.18	0.42
1:D:158:HIS:O	1:D:159:PRO:CA	2.68	0.42
1:E:347:TYR:CD1	1:E:347:TYR:C	2.98	0.42
1:F:45:ASP:CG	1:F:46:GLU:N	2.76	0.42
1:A:45:ASP:OD2	1:A:47:ARG:NH1	2.52	0.42
1:A:158:HIS:O	1:A:159:PRO:CA	2.68	0.42
1:B:362:VAL:HG11	1:B:398:ILE:HG13	2.02	0.42
1:E:148:TYR:CD1	1:E:148:TYR:C	2.98	0.42
1:E:179:VAL:HG22	1:F:197:TRP:CE2	2.54	0.42
1:E:299:LEU:HD21	1:E:474:PHE:HD1	1.84	0.42
1:E:378:PHE:HD1	1:E:379:ILE:N	1.84	0.42
1:F:158:HIS:O	1:F:159:PRO:CA	2.68	0.42
1:A:324:LEU:HD12	1:A:324:LEU:HA	1.91	0.42
1:D:62:VAL:HA	1:D:63:PRO:HD3	1.73	0.42
1:D:202:ASP:O	1:D:205:ILE:HG12	2.20	0.42
1:D:405:LEU:HB3	1:D:481:VAL:CG1	2.50	0.42
1:E:268:ASP:O	1:E:272:LYS:HD3	2.20	0.42
1:E:329:ASN:ND2	1:E:336:THR:HB	2.31	0.42
1:F:28:LEU:HD23	1:F:28:LEU:C	2.45	0.42
1:F:126:MET:HE2	1:F:182:MET:HE1	2.02	0.42
1:A:268:ASP:O	1:A:272:LYS:HD3	2.19	0.42
1:A:438:THR:HG23	1:A:439:GLY:N	2.35	0.42
1:C:96:TRP:C	1:C:97:GLN:HG3	2.43	0.42
1:C:441:ASP:C	1:C:443:ASN:H	2.28	0.42
1:D:473:PRO:O	1:D:474:PHE:C	2.61	0.42
1:E:250:VAL:HG11	1:E:412:TYR:OH	2.20	0.42
1:E:413:ARG:HG2	1:E:416:ASP:HB2	2.02	0.42
1:F:158:HIS:C	1:F:159:PRO:HA	2.45	0.42
1:F:252:LEU:HD23	1:F:252:LEU:C	2.45	0.42
1:B:169:ILE:HD13	1:B:195:THR:OG1	2.19	0.42
1:B:231:PHE:HA	1:B:276:LYS:O	2.19	0.42
1:D:75:ASN:OD1	1:D:94:LEU:HD13	2.20	0.42
1:E:224:GLU:OE1	1:E:224:GLU:HA	2.19	0.42
1:F:81:GLY:O	1:F:105:GLY:HA3	2.19	0.42
1:F:464:ASP:C	1:F:466:GLU:N	2.78	0.42
1:B:238:THR:O	1:B:284:VAL:HA	2.20	0.41
1:C:409:VAL:HG21	1:C:471:PHE:CE2	2.54	0.41
1:C:410:VAL:HG12	1:C:412:TYR:CE1	2.53	0.41
1:D:80:ASP:CG	1:D:91:ARG:HH12	2.28	0.41
1:D:112:TYR:O	1:D:116:ILE:HG12	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:380:ASN:HD22	1:F:380:ASN:C	2.27	0.41
1:B:70:GLY:O	1:B:71:ASN:C	2.63	0.41
1:B:196:LYS:C	1:B:197:TRP:O	2.60	0.41
1:B:197:TRP:CB	1:C:94:LEU:HD23	2.43	0.41
1:B:293:LEU:HD12	1:B:293:LEU:HA	1.82	0.41
1:B:370:THR:H	1:B:370:THR:HG23	1.38	0.41
1:F:330:ALA:O	1:F:331:LEU:C	2.62	0.41
1:A:285:TRP:O	1:A:378:PHE:HB2	2.19	0.41
1:A:286:TYR:HA	1:A:379:ILE:HG12	1.99	0.41
1:A:342:ILE:HD13	1:A:343:LEU:N	2.36	0.41
1:B:410:VAL:CB	1:B:412:TYR:OH	2.68	0.41
1:B:434:VAL:O	1:B:434:VAL:HG23	2.19	0.41
1:B:461:ILE:HG22	1:B:462:THR:N	2.35	0.41
1:D:224:GLU:OE1	1:D:224:GLU:HA	2.20	0.41
1:D:283:ASN:CB	1:D:325:ALA:HB3	2.50	0.41
1:E:157:GLY:HA3	1:E:158:HIS:HB2	2.02	0.41
1:E:238:THR:HG21	1:E:304:PHE:CE1	2.55	0.41
1:E:290:ASP:C	1:E:290:ASP:OD1	2.63	0.41
1:E:405:LEU:HB3	1:E:481:VAL:CG1	2.50	0.41
1:E:446:ASN:HD21	1:E:454:VAL:N	1.96	0.41
1:E:463:VAL:HB	1:E:467:PHE:CE1	2.55	0.41
1:E:481:VAL:CG2	1:E:482:GLU:N	2.62	0.41
1:F:28:LEU:HD22	1:F:330:ALA:HB2	2.01	0.41
1:F:110:ILE:HG13	1:F:162:TYR:CE2	2.55	0.41
1:F:411:ASN:ND2	1:F:413:ARG:CB	2.71	0.41
1:A:373:ILE:CG1	1:A:374:GLU:N	2.82	0.41
1:A:419:LYS:HA	1:A:470:THR:HG22	2.00	0.41
1:A:434:VAL:O	1:A:434:VAL:CG2	2.67	0.41
1:B:171:ASN:H	1:B:173:MET:HE2	1.85	0.41
1:C:458:SER:O	1:C:459:GLU:HB2	2.20	0.41
1:C:460:THR:HG22	1:C:461:ILE:N	2.34	0.41
1:E:144:LYS:N	1:E:144:LYS:CD	2.74	0.41
1:A:4:ARG:HH11	1:A:4:ARG:HG3	1.85	0.41
1:B:197:TRP:CE2	1:C:179:VAL:HG22	2.55	0.41
1:C:4:ARG:HA	1:C:420:VAL:HG23	2.02	0.41
1:C:157:GLY:O	1:C:158:HIS:HB2	2.19	0.41
1:E:22:GLY:HA2	1:E:63:PRO:HD2	2.02	0.41
1:F:397:SER:O	1:F:405:LEU:HD12	2.21	0.41
1:A:22:GLY:HA2	1:A:63:PRO:HD2	2.03	0.41
1:D:85:LYS:O	1:D:86:ASP:HB2	2.21	0.41
1:D:237:TYR:HE1	1:D:325:ALA:HB2	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:157:GLY:C	1:E:158:HIS:O	2.63	0.41
1:F:73:VAL:HG21	1:F:123:SER:O	2.20	0.41
1:F:446:ASN:N	1:F:446:ASN:HD22	2.18	0.41
1:A:250:VAL:HG13	1:A:251:TYR:CE2	2.56	0.41
1:C:28:LEU:HD23	1:C:28:LEU:C	2.45	0.41
1:C:431:LYS:HZ3	1:C:462:THR:HG22	1.83	0.41
1:C:434:VAL:O	1:C:434:VAL:HG23	2.20	0.41
1:D:91:ARG:HH11	1:D:91:ARG:CG	2.32	0.41
1:D:110:ILE:HG13	1:D:162:TYR:CE2	2.56	0.41
1:D:461:ILE:HD11	1:D:469:HIS:CE1	2.56	0.41
1:D:474:PHE:O	1:D:474:PHE:HD1	2.03	0.41
1:E:412:TYR:O	1:E:413:ARG:C	2.64	0.41
1:F:290:ASP:OD1	1:F:290:ASP:C	2.64	0.41
1:F:347:TYR:CD1	1:F:347:TYR:C	2.98	0.41
1:F:419:LYS:HE2	1:F:419:LYS:HB3	1.65	0.41
1:A:60:ILE:HA	1:A:354:VAL:HG21	2.03	0.41
1:B:158:HIS:O	1:B:159:PRO:CA	2.67	0.41
1:B:353:ILE:O	1:B:353:ILE:HG22	2.21	0.41
1:C:353:ILE:O	1:C:353:ILE:HG22	2.20	0.41
1:D:60:ILE:HG22	1:D:351:GLU:HA	2.01	0.41
1:D:285:TRP:HB2	1:D:331:LEU:CD2	2.48	0.41
1:E:461:ILE:HD11	1:E:469:HIS:ND1	2.36	0.41
1:F:61:LYS:H	1:F:61:LYS:HG2	1.01	0.41
1:F:231:PHE:HA	1:F:276:LYS:O	2.20	0.41
1:A:279:LEU:HD22	1:A:282:TRP:HB3	2.03	0.41
1:A:380:ASN:O	1:A:381:LYS:HB2	2.21	0.41
1:A:441:ASP:C	1:A:443:ASN:N	2.78	0.41
1:A:446:ASN:N	1:A:446:ASN:HD22	2.18	0.41
1:B:25:THR:O	1:B:25:THR:CG2	2.61	0.41
1:B:25:THR:HG22	1:B:66:ARG:O	2.21	0.41
1:C:71:ASN:HA	1:C:178:GLN:NE2	2.21	0.41
1:C:240:SER:O	1:C:300:LYS:HE3	2.21	0.41
1:C:279:LEU:O	1:C:322:ALA:HA	2.21	0.41
1:D:76:TYR:CE2	1:D:78:TRP:HA	2.55	0.41
1:D:231:PHE:HA	1:D:276:LYS:O	2.20	0.41
1:D:362:VAL:HG11	1:D:398:ILE:HD12	2.02	0.41
1:D:412:TYR:O	1:D:413:ARG:C	2.62	0.41
1:D:413:ARG:HG3	1:D:418:LEU:HD13	1.96	0.41
1:D:423:ARG:NH1	1:D:425:GLU:OE1	2.54	0.41
1:D:450:ASN:C	1:D:452:ASN:H	2.29	0.41
1:E:126:MET:HB2	1:E:173:MET:HE3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:197:TRP:O	1:E:198:MET:CB	2.69	0.41
1:E:261:LYS:C	1:E:261:LYS:CD	2.94	0.41
1:E:317:ASP:OD1	1:E:317:ASP:N	2.53	0.41
1:F:336:THR:HG23	1:F:337:GLU:N	2.36	0.41
1:A:293:LEU:HD12	1:A:293:LEU:HA	1.88	0.41
1:A:461:ILE:HD11	1:A:469:HIS:ND1	2.36	0.41
1:C:258:ILE:HG13	1:F:262:LYS:CD	2.50	0.41
1:D:43:LEU:HD12	1:D:43:LEU:N	2.35	0.41
1:D:158:HIS:O	1:D:159:PRO:HA	2.21	0.41
1:D:179:VAL:HG22	1:E:197:TRP:CE2	2.56	0.41
1:D:377:MET:HB3	1:D:384:PHE:CD2	2.56	0.41
1:D:378:PHE:HD2	1:D:380:ASN:ND2	2.19	0.41
1:E:429:GLN:HA	1:E:463:VAL:O	2.21	0.41
1:F:80:ASP:O	1:F:102:ASN:HB3	2.21	0.41
1:A:312:LEU:O	1:A:313:GLN:C	2.62	0.40
1:B:214:ASP:C	1:B:214:ASP:OD1	2.64	0.40
1:B:282:TRP:O	1:B:324:LEU:HD12	2.21	0.40
1:B:482:GLU:OE1	1:B:482:GLU:O	2.40	0.40
1:C:252:LEU:HD13	1:C:377:MET:HE1	2.04	0.40
1:D:197:TRP:C	1:D:199:LYS:H	2.25	0.40
1:D:411:ASN:HD21	1:D:413:ARG:CG	2.19	0.40
1:E:28:LEU:HD12	1:E:96:TRP:CZ2	2.56	0.40
1:E:94:LEU:HD23	1:F:197:TRP:CG	2.56	0.40
1:E:434:VAL:O	1:E:434:VAL:CG2	2.69	0.40
1:E:473:PRO:O	1:E:474:PHE:C	2.64	0.40
1:F:162:TYR:O	1:F:163:ASN:HB3	2.21	0.40
1:A:376:VAL:HB	1:A:381:LYS:CA	2.51	0.40
1:B:315:MET:O	1:B:317:ASP:N	2.54	0.40
1:B:423:ARG:HH11	1:B:425:GLU:CD	2.29	0.40
1:C:146:ASN:O	1:C:147:THR:C	2.62	0.40
1:C:318:ILE:HG13	1:C:319:VAL:CG2	2.48	0.40
1:D:197:TRP:O	1:D:198:MET:CB	2.66	0.40
1:D:366:VAL:CG2	1:D:367:GLU:N	2.83	0.40
1:E:252:LEU:HD12	1:E:384:PHE:CD1	2.57	0.40
1:F:253:LEU:O	1:F:253:LEU:HG	2.20	0.40
1:F:299:LEU:HD21	1:F:474:PHE:CD1	2.56	0.40
1:F:461:ILE:CD1	1:F:469:HIS:ND1	2.84	0.40
1:A:212:CYS:SG	1:A:213:ASP:N	2.94	0.40
1:B:290:ASP:C	1:B:290:ASP:OD1	2.63	0.40
1:C:158:HIS:O	1:C:159:PRO:HA	2.21	0.40
1:D:236:PHE:CG	1:D:253:LEU:HD13	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:291:ASN:ND2	1:D:291:ASN:N	2.61	0.40
1:D:293:LEU:HD12	1:D:293:LEU:HA	1.87	0.40
1:D:324:LEU:O	1:D:325:ALA:C	2.58	0.40
1:E:145:GLY:O	1:E:154:ARG:NH2	2.54	0.40
1:E:162:TYR:O	1:E:163:ASN:HB3	2.19	0.40
1:E:169:ILE:HD12	1:E:207:ALA:HB1	2.01	0.40
1:E:270:ALA:O	1:E:273:ARG:O	2.39	0.40
1:E:467:PHE:HD2	1:E:468:GLU:O	2.04	0.40
1:F:325:ALA:HA	1:F:326:GLN:HA	1.77	0.40
1:F:405:LEU:HB3	1:F:481:VAL:CG1	2.52	0.40
1:A:125:ASN:OD1	1:A:125:ASN:C	2.64	0.40
1:A:215:PRO:HB2	1:D:219:LEU:HD21	2.03	0.40
1:A:231:PHE:HA	1:A:276:LYS:O	2.20	0.40
1:A:283:ASN:CB	1:A:325:ALA:HB2	2.51	0.40
1:B:384:PHE:CD1	1:B:385:SER:N	2.90	0.40
1:B:421:PRO:O	1:B:421:PRO:HG2	2.21	0.40
1:C:461:ILE:HD11	1:C:469:HIS:ND1	2.36	0.40
1:E:62:VAL:CG1	1:E:116:ILE:HD12	2.46	0.40
1:E:80:ASP:HB3	1:E:89:PRO:HG2	2.04	0.40
1:E:196:LYS:C	1:E:197:TRP:O	2.61	0.40
1:E:240:SER:HB2	1:E:376:VAL:HG23	2.03	0.40
1:E:441:ASP:C	1:E:443:ASN:H	2.28	0.40
1:F:411:ASN:HD21	1:F:413:ARG:CB	1.99	0.40
1:A:414:LYS:O	1:A:473:PRO:HB3	2.20	0.40
1:B:373:ILE:HG12	1:B:374:GLU:H	1.87	0.40
1:C:82:ILE:HD13	1:C:82:ILE:HG21	1.87	0.40
1:D:4:ARG:HH11	1:D:4:ARG:HG3	1.86	0.40
1:D:26:GLU:HG2	1:D:27:HIS:N	2.36	0.40
1:D:290:ASP:OD1	1:D:290:ASP:C	2.63	0.40
1:E:195:THR:O	1:E:199:LYS:HB2	2.22	0.40
1:E:467:PHE:CD2	1:E:468:GLU:N	2.90	0.40
1:F:67:TRP:O	1:F:122:ILE:HA	2.21	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:144:LYS:CE	1:E:431:LYS:CE[1_556]	1.60	0.60
1:C:144:LYS:CE	1:E:431:LYS:NZ[1_556]	1.90	0.30

5.3 Torsion angles

5.3.1 Protein backbone

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	476/482 (99%)	409 (86%)	62 (13%)	5 (1%)	11	43
1	B	476/482 (99%)	409 (86%)	61 (13%)	6 (1%)	9	38
1	C	476/482 (99%)	410 (86%)	61 (13%)	5 (1%)	11	43
1	D	476/482 (99%)	403 (85%)	70 (15%)	3 (1%)	21	56
1	E	476/482 (99%)	407 (86%)	66 (14%)	3 (1%)	21	56
1	F	476/482 (99%)	406 (85%)	68 (14%)	2 (0%)	30	65
All	All	2856/2892 (99%)	2444 (86%)	388 (14%)	24 (1%)	16	50

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	328	VAL
1	A	379	ILE
1	B	172	GLU
1	C	465	THR
1	E	328	VAL
1	A	172	GLU
1	B	61	LYS
1	B	316	SER
1	C	61	LYS
1	D	316	SER
1	A	61	LYS
1	C	71	ASN
1	C	316	SER
1	E	316	SER
1	F	316	SER
1	B	328	VAL
1	E	379	ILE
1	F	442	VAL
1	C	442	VAL
1	D	442	VAL

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Mol	Chain	Res	Type
1	A	442	VAL
1	B	442	VAL
1	B	451	PRO
1	D	379	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	417/418 (100%)	368 (88%)	49 (12%)	5	22
1	B	417/418 (100%)	369 (88%)	48 (12%)	5	24
1	C	417/418 (100%)	367 (88%)	50 (12%)	5	22
1	D	417/418 (100%)	368 (88%)	49 (12%)	5	22
1	E	417/418 (100%)	369 (88%)	48 (12%)	5	24
1	F	417/418 (100%)	369 (88%)	48 (12%)	5	24
All	All	2502/2508 (100%)	2210 (88%)	292 (12%)	5	23

All (292) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ILE
1	A	47	ARG
1	A	54	LEU
1	A	61	LYS
1	A	75	ASN
1	A	97	GLN
1	A	111	GLU
1	A	114	ARG
1	A	135	LEU
1	A	144	LYS
1	A	158	HIS
1	A	160	GLU
1	A	219	LEU
1	A	250	VAL

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Mol	Chain	Res	Type
1	A	252	LEU
1	A	256	ARG
1	A	261	LYS
1	A	279	LEU
1	A	291	ASN
1	A	293	LEU
1	A	300	LYS
1	A	306	CYS
1	A	321	LEU
1	A	328	VAL
1	A	336	THR
1	A	342	ILE
1	A	364	THR
1	A	365	HIS
1	A	366	VAL
1	A	374	GLU
1	A	377	MET
1	A	378	PHE
1	A	380	ASN
1	A	381	LYS
1	A	397	SER
1	A	403	LYS
1	A	409	VAL
1	A	411	ASN
1	A	413	ARG
1	A	414	LYS
1	A	415	GLU
1	A	420	VAL
1	A	422	ILE
1	A	423	ARG
1	A	430	LYS
1	A	433	THR
1	A	434	VAL
1	A	436	THR
1	A	459	GLU
1	B	47	ARG
1	B	54	LEU
1	B	61	LYS
1	B	62	VAL
1	B	68	PRO
1	B	75	ASN
1	B	97	GLN

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Mol	Chain	Res	Type
1	B	111	GLU
1	B	114	ARG
1	B	121	TYR
1	B	135	LEU
1	B	144	LYS
1	B	158	HIS
1	B	160	GLU
1	B	219	LEU
1	B	250	VAL
1	B	256	ARG
1	B	261	LYS
1	B	279	LEU
1	B	291	ASN
1	B	293	LEU
1	B	300	LYS
1	B	306	CYS
1	B	321	LEU
1	B	326	GLN
1	B	327	LEU
1	B	336	THR
1	B	342	ILE
1	B	364	THR
1	B	365	HIS
1	B	366	VAL
1	B	374	GLU
1	B	377	MET
1	B	380	ASN
1	B	403	LYS
1	B	409	VAL
1	B	411	ASN
1	B	413	ARG
1	B	414	LYS
1	B	415	GLU
1	B	416	ASP
1	B	420	VAL
1	B	422	ILE
1	B	423	ARG
1	B	430	LYS
1	B	433	THR
1	B	436	THR
1	B	459	GLU
1	C	5	ILE

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Mol	Chain	Res	Type
1	C	47	ARG
1	C	61	LYS
1	C	62	VAL
1	C	75	ASN
1	C	97	GLN
1	C	111	GLU
1	C	114	ARG
1	C	121	TYR
1	C	135	LEU
1	C	142	ASN
1	C	144	LYS
1	C	147	THR
1	C	160	GLU
1	C	219	LEU
1	C	250	VAL
1	C	252	LEU
1	C	256	ARG
1	C	261	LYS
1	C	279	LEU
1	C	291	ASN
1	C	293	LEU
1	C	300	LYS
1	C	306	CYS
1	C	321	LEU
1	C	326	GLN
1	C	327	LEU
1	C	328	VAL
1	C	336	THR
1	C	342	ILE
1	C	364	THR
1	C	365	HIS
1	C	366	VAL
1	C	369	GLU
1	C	374	GLU
1	C	379	ILE
1	C	380	ASN
1	C	397	SER
1	C	403	LYS
1	C	409	VAL
1	C	411	ASN
1	C	415	GLU
1	C	420	VAL

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Mol	Chain	Res	Type
1	C	422	ILE
1	C	423	ARG
1	C	430	LYS
1	C	433	THR
1	C	434	VAL
1	C	436	THR
1	C	459	GLU
1	D	5	ILE
1	D	12	VAL
1	D	47	ARG
1	D	54	LEU
1	D	61	LYS
1	D	75	ASN
1	D	97	GLN
1	D	111	GLU
1	D	114	ARG
1	D	121	TYR
1	D	135	LEU
1	D	144	LYS
1	D	158	HIS
1	D	160	GLU
1	D	219	LEU
1	D	252	LEU
1	D	256	ARG
1	D	261	LYS
1	D	279	LEU
1	D	291	ASN
1	D	293	LEU
1	D	300	LYS
1	D	306	CYS
1	D	321	LEU
1	D	327	LEU
1	D	336	THR
1	D	342	ILE
1	D	364	THR
1	D	365	HIS
1	D	366	VAL
1	D	370	THR
1	D	374	GLU
1	D	377	MET
1	D	378	PHE
1	D	380	ASN

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Mol	Chain	Res	Type
1	D	397	SER
1	D	403	LYS
1	D	409	VAL
1	D	411	ASN
1	D	414	LYS
1	D	415	GLU
1	D	420	VAL
1	D	422	ILE
1	D	423	ARG
1	D	430	LYS
1	D	433	THR
1	D	434	VAL
1	D	436	THR
1	D	459	GLU
1	E	12	VAL
1	E	47	ARG
1	E	54	LEU
1	E	61	LYS
1	E	68	PRO
1	E	75	ASN
1	E	97	GLN
1	E	111	GLU
1	E	114	ARG
1	E	135	LEU
1	E	144	LYS
1	E	158	HIS
1	E	160	GLU
1	E	219	LEU
1	E	250	VAL
1	E	252	LEU
1	E	256	ARG
1	E	261	LYS
1	E	279	LEU
1	E	291	ASN
1	E	293	LEU
1	E	300	LYS
1	E	306	CYS
1	E	321	LEU
1	E	327	LEU
1	E	336	THR
1	E	342	ILE
1	E	364	THR

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Mol	Chain	Res	Type
1	E	365	HIS
1	E	366	VAL
1	E	374	GLU
1	E	377	MET
1	E	378	PHE
1	E	380	ASN
1	E	397	SER
1	E	403	LYS
1	E	409	VAL
1	E	411	ASN
1	E	413	ARG
1	E	415	GLU
1	E	420	VAL
1	E	422	ILE
1	E	423	ARG
1	E	430	LYS
1	E	433	THR
1	E	434	VAL
1	E	436	THR
1	E	459	GLU
1	F	26	GLU
1	F	47	ARG
1	F	54	LEU
1	F	61	LYS
1	F	62	VAL
1	F	68	PRO
1	F	75	ASN
1	F	97	GLN
1	F	111	GLU
1	F	114	ARG
1	F	121	TYR
1	F	135	LEU
1	F	144	LYS
1	F	158	HIS
1	F	160	GLU
1	F	219	LEU
1	F	250	VAL
1	F	256	ARG
1	F	261	LYS
1	F	279	LEU
1	F	291	ASN
1	F	293	LEU

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Mol	Chain	Res	Type
1	F	300	LYS
1	F	306	CYS
1	F	321	LEU
1	F	326	GLN
1	F	336	THR
1	F	342	ILE
1	F	364	THR
1	F	365	HIS
1	F	366	VAL
1	F	374	GLU
1	F	378	PHE
1	F	379	ILE
1	F	380	ASN
1	F	403	LYS
1	F	409	VAL
1	F	411	ASN
1	F	413	ARG
1	F	415	GLU
1	F	420	VAL
1	F	422	ILE
1	F	423	ARG
1	F	430	LYS
1	F	433	THR
1	F	434	VAL
1	F	436	THR
1	F	459	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (77) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	HIS
1	A	23	HIS
1	A	77	HIS
1	A	87	GLN
1	A	97	GLN
1	A	178	GLN
1	A	291	ASN
1	A	326	GLN
1	A	380	ASN
1	A	388	ASN
1	A	411	ASN
1	A	429	GLN

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Mol	Chain	Res	Type
1	A	446	ASN
1	A	452	ASN
1	B	19	HIS
1	B	77	HIS
1	B	87	GLN
1	B	97	GLN
1	B	178	GLN
1	B	291	ASN
1	B	380	ASN
1	B	388	ASN
1	B	411	ASN
1	B	429	GLN
1	B	446	ASN
1	B	452	ASN
1	C	19	HIS
1	C	77	HIS
1	C	87	GLN
1	C	97	GLN
1	C	178	GLN
1	C	291	ASN
1	C	326	GLN
1	C	380	ASN
1	C	388	ASN
1	C	411	ASN
1	C	429	GLN
1	C	446	ASN
1	C	452	ASN
1	D	19	HIS
1	D	77	HIS
1	D	87	GLN
1	D	97	GLN
1	D	178	GLN
1	D	291	ASN
1	D	380	ASN
1	D	388	ASN
1	D	411	ASN
1	D	429	GLN
1	D	446	ASN
1	D	452	ASN
1	E	19	HIS
1	E	77	HIS
1	E	87	GLN

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Mol	Chain	Res	Type
1	E	97	GLN
1	E	178	GLN
1	E	291	ASN
1	E	326	GLN
1	E	380	ASN
1	E	388	ASN
1	E	411	ASN
1	E	429	GLN
1	E	446	ASN
1	E	452	ASN
1	F	19	HIS
1	F	77	HIS
1	F	87	GLN
1	F	97	GLN
1	F	178	GLN
1	F	291	ASN
1	F	326	GLN
1	F	380	ASN
1	F	388	ASN
1	F	411	ASN
1	F	429	GLN
1	F	446	ASN
1	F	452	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	C	3
1	A	3
1	B	3
1	D	3
1	F	2
1	E	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	157:GLY	C	158:HIS	N	3.85
1	F	157:GLY	C	158:HIS	N	3.82
1	A	157:GLY	C	158:HIS	N	3.80
1	B	157:GLY	C	158:HIS	N	3.80
1	E	157:GLY	C	158:HIS	N	3.79
1	D	157:GLY	C	158:HIS	N	3.76
1	C	158:HIS	C	159:PRO	N	2.62
1	E	158:HIS	C	159:PRO	N	2.57
1	F	158:HIS	C	159:PRO	N	2.57
1	D	158:HIS	C	159:PRO	N	2.56
1	A	158:HIS	C	159:PRO	N	2.50
1	B	158:HIS	C	159:PRO	N	2.49
1	A	26:GLU	C	27:HIS	N	1.17
1	B	26:GLU	C	27:HIS	N	1.14
1	C	26:GLU	C	27:HIS	N	1.07
1	D	26:GLU	C	27:HIS	N	0.93

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	481/482 (99%)	-0.35	2 (0%) 88 76	14, 42, 75, 115	0
1	B	481/482 (99%)	-0.16	5 (1%) 79 59	15, 47, 92, 117	0
1	C	481/482 (99%)	-0.37	1 (0%) 91 83	17, 40, 66, 88	0
1	D	481/482 (99%)	-0.12	3 (0%) 85 69	17, 54, 85, 110	0
1	E	481/482 (99%)	0.26	6 (1%) 76 55	31, 67, 93, 115	0
1	F	481/482 (99%)	0.19	4 (0%) 82 64	33, 64, 91, 129	0
All	All	2886/2892 (99%)	-0.09	21 (0%) 84 66	14, 52, 88, 129	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	412	TYR	5.6
1	A	412	TYR	5.1
1	E	325	ALA	4.7
1	A	325	ALA	4.3
1	F	325	ALA	4.1
1	E	326	GLN	3.8
1	C	325	ALA	3.5
1	F	431	LYS	3.3
1	E	412	TYR	3.0
1	B	86	ASP	2.8
1	D	331	LEU	2.8
1	B	476	CYS	2.6
1	F	168	GLY	2.5
1	E	283	ASN	2.5
1	D	34	GLY	2.5
1	F	429	GLN	2.3
1	B	327	LEU	2.1
1	E	160	GLU	2.1
1	D	326	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	407	ILE	2.0
1	E	159	PRO	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.