



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:51 PM UTC

PDB ID : 3CIA / pdb_00003cia
Title : Crystal structure of cold-aminopeptidase from Colwellia psychrerythraea
Authors : Bauvois, C.; Jacquamet, L.; Borel, F.; Ferrer, J.-L.
Deposited on : 2008-03-11
Resolution : 2.70 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

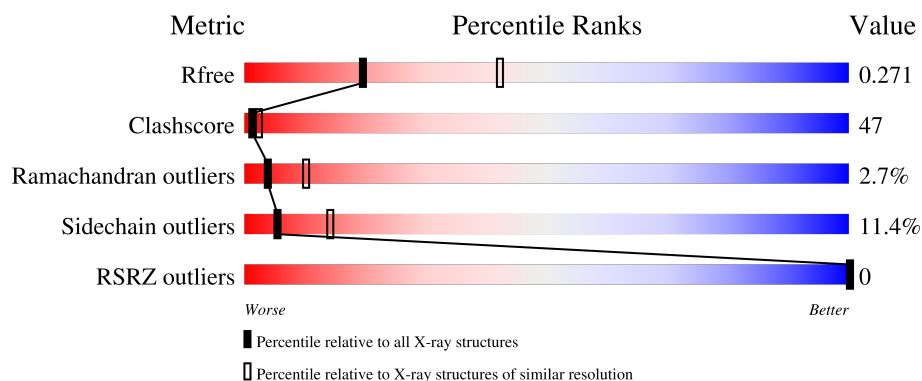
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	605	 31% 47% 17% . .
1	B	605	 30% 48% 15% . .
1	C	605	 30% 51% 13% . .
1	D	605	 30% 48% 16% . .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 19608 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 cold-active aminopeptidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	587	Total	C	N	O	S	0	0	0
			4708	3023	780	892	13			
1	B	581	Total	C	N	O	S	0	0	0
			4651	2987	770	882	12			
1	C	581	Total	C	N	O	S	0	0	0
			4657	2993	770	882	12			
1	D	582	Total	C	N	O	S	0	0	0
			4669	2999	772	886	12			

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		
2	B	1	Total	Zn	0	0
			1	1		
2	C	1	Total	Zn	0	0
			1	1		
2	D	1	Total	Zn	0	0
			1	1		

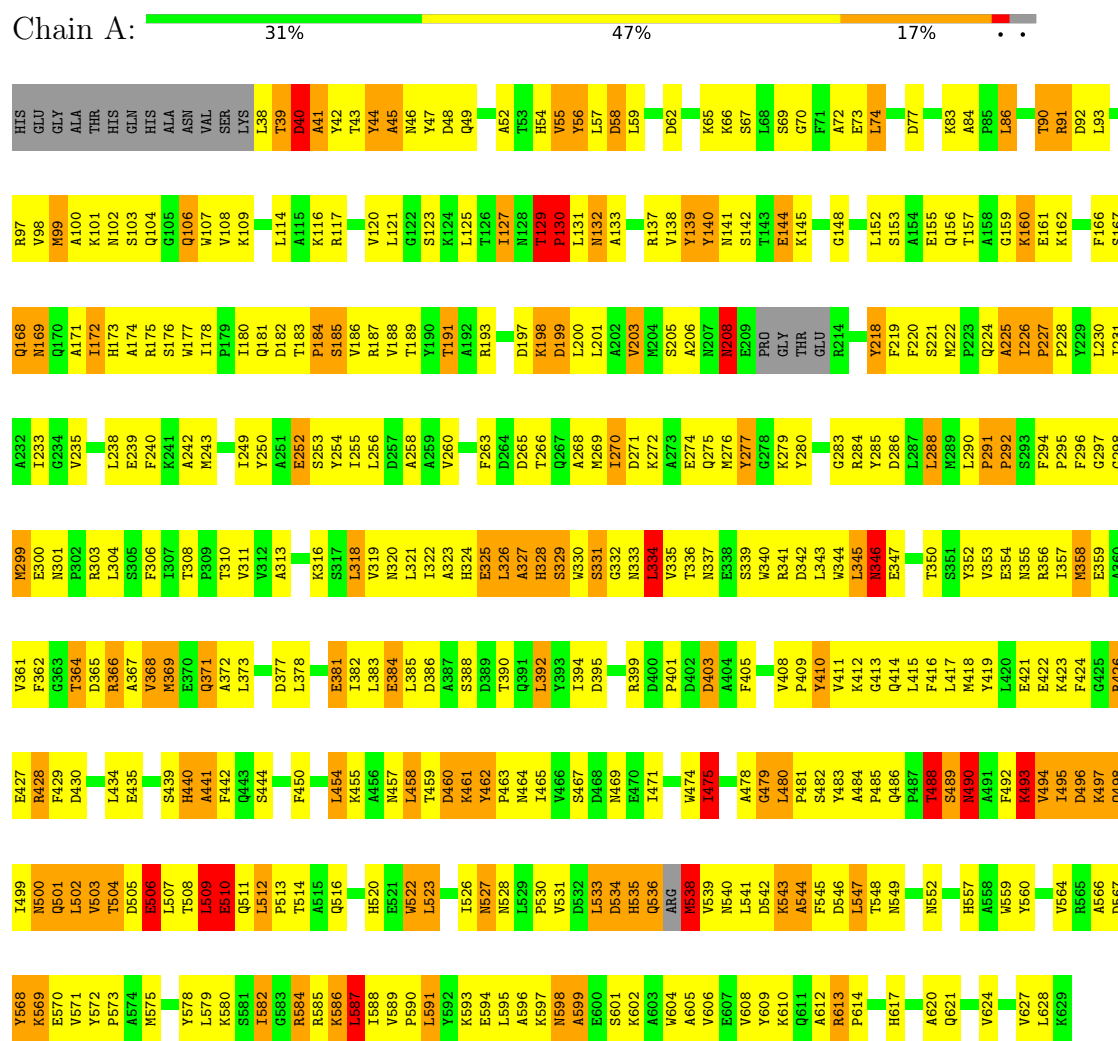
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	331	Total	O	0	0
			331	331		
3	B	154	Total	O	0	0
			154	154		
3	C	156	Total	O	0	0
			156	156		
3	D	278	Total	O	0	0
			278	278		

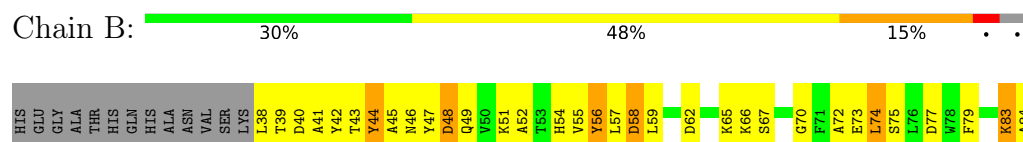
3 Residue-property plots

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.

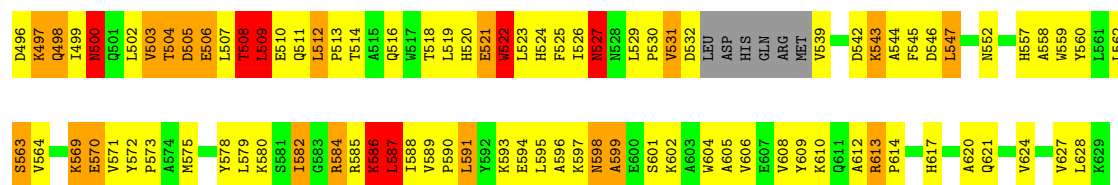
- Molecule 1: cold-active aminopeptidase



- Molecule 1: cold-active aminopeptidase

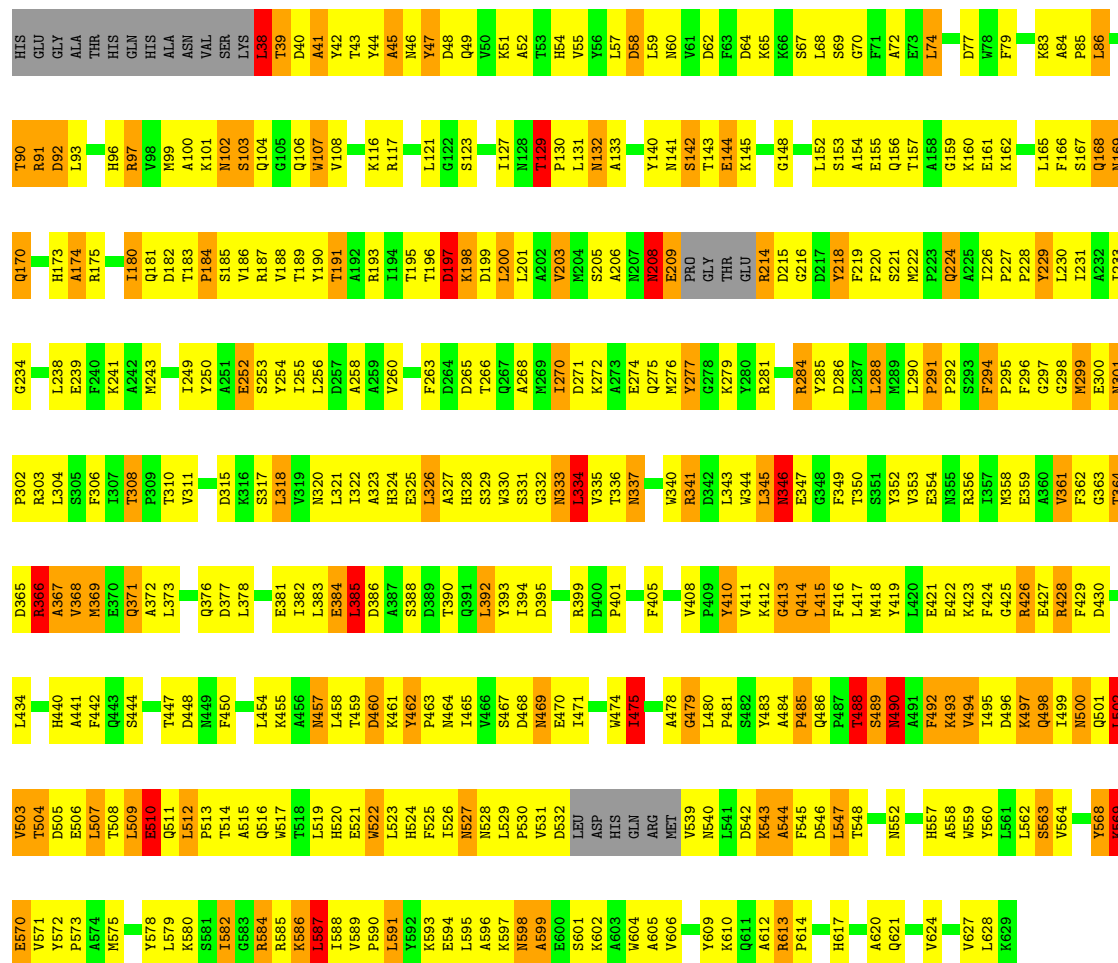






• Molecule 1: cold-active aminopeptidase

Chain D: 30% 48% 16%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	81.37Å 87.10Å 116.36Å 88.83° 70.68° 88.43°	Depositor
Resolution (Å)	46.68 – 2.70 46.68 – 2.70	Depositor EDS
% Data completeness (in resolution range)	97.3 (46.68-2.70) 97.3 (46.68-2.70)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.36 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.2	Depositor
R, R_{free}	0.249 , 0.270 0.250 , 0.271	Depositor DCC
R_{free} test set	4034 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	25.0	Xtriage
Anisotropy	0.165	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 39.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.039 for h,-k,h-l 0.186 for -h,k,-l 0.021 for -h,-k,-h+l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	19608	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.85% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	1.53	49/4823 (1.0%)	1.46	73/6555 (1.1%)
1	B	1.51	45/4764 (0.9%)	1.45	76/6476 (1.2%)
1	C	1.53	33/4771 (0.7%)	1.43	68/6485 (1.0%)
1	D	1.51	40/4783 (0.8%)	1.49	84/6501 (1.3%)
All	All	1.52	167/19141 (0.9%)	1.46	301/26017 (1.2%)

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	0	7
1	B	0	3
1	C	0	2
1	D	0	5
All	All	0	17

All (167) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	500	ASN	C-N	-30.81	0.90	1.33
1	D	208	ASN	C-N	12.06	1.50	1.33
1	D	97	ARG	C-N	11.42	1.48	1.33
1	B	168	GLN	C-O	-10.97	1.10	1.23
1	A	127	ILE	CA-CB	-10.69	1.41	1.54
1	D	127	ILE	CA-CB	-10.05	1.42	1.54
1	C	508	THR	C-N	-9.77	1.20	1.33
1	A	168	GLN	C-O	-9.74	1.11	1.23
1	D	168	GLN	C-O	-9.70	1.12	1.23
1	D	100	ALA	C-O	-9.07	1.12	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	168	GLN	CA-C	-8.98	1.42	1.53
1	D	478	ALA	CA-CB	-8.78	1.39	1.53
1	C	168	GLN	C-O	-8.70	1.13	1.23
1	B	98	VAL	C-O	-8.67	1.15	1.24
1	A	227	PRO	CA-C	8.51	1.60	1.52
1	A	346	ASN	CA-C	-8.43	1.45	1.53
1	B	100	ALA	C-O	-8.25	1.13	1.23
1	C	127	ILE	CA-CB	-8.14	1.44	1.54
1	B	372	ALA	CA-CB	-8.13	1.40	1.53
1	A	138	VAL	C-O	-8.06	1.15	1.24
1	D	168	GLN	CA-C	-7.93	1.44	1.53
1	B	72	ALA	CA-CB	-7.74	1.41	1.53
1	B	139	TYR	C-O	-7.51	1.15	1.24
1	B	168	GLN	CA-C	-7.33	1.44	1.53
1	C	98	VAL	C-O	-7.32	1.16	1.24
1	C	100	ALA	C-O	-7.27	1.14	1.23
1	B	227	PRO	CA-C	7.19	1.58	1.52
1	A	140	TYR	C-O	-7.15	1.15	1.23
1	D	521	GLU	CA-C	-7.07	1.43	1.52
1	A	72	ALA	CA-CB	-6.97	1.43	1.53
1	B	346	ASN	CA-C	-6.97	1.46	1.53
1	B	251	ALA	C-O	-6.94	1.16	1.24
1	D	494	VAL	CA-CB	-6.91	1.44	1.54
1	C	346	ASN	CA-C	-6.89	1.46	1.53
1	A	139	TYR	C-O	-6.87	1.15	1.24
1	B	367	ALA	CA-CB	-6.83	1.42	1.53
1	A	478	ALA	CA-CB	-6.82	1.42	1.53
1	B	84	ALA	CA-CB	-6.82	1.44	1.54
1	B	488	THR	CB-CG2	-6.78	1.30	1.52
1	A	127	ILE	N-CA	-6.78	1.38	1.46
1	B	127	ILE	CA-CB	-6.72	1.45	1.54
1	C	45	ALA	CA-CB	-6.72	1.42	1.53
1	D	521	GLU	C-O	-6.70	1.15	1.24
1	A	328	HIS	C-O	-6.69	1.16	1.24
1	D	140	TYR	CE1-CZ	-6.57	1.22	1.38
1	B	494	VAL	CA-CB	-6.57	1.44	1.54
1	A	137	ARG	C-O	-6.54	1.16	1.24
1	C	478	ALA	CA-CB	-6.54	1.43	1.53
1	D	346	ASN	CA-C	-6.51	1.47	1.53
1	C	278	GLY	C-O	6.49	1.30	1.24
1	B	140	TYR	C-O	-6.48	1.16	1.23
1	D	72	ALA	C-O	-6.45	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	333	ASN	CA-CB	-6.44	1.42	1.53
1	A	172	ILE	C-N	6.40	1.43	1.33
1	C	140	TYR	CE1-CZ	-6.38	1.23	1.38
1	C	227	PRO	CA-C	6.38	1.58	1.52
1	C	72	ALA	CA-CB	-6.35	1.42	1.53
1	A	100	ALA	C-O	-6.30	1.16	1.23
1	D	252	GLU	C-O	6.23	1.32	1.24
1	A	167	SER	CA-C	-6.20	1.44	1.52
1	A	494	VAL	CA-CB	-6.20	1.45	1.54
1	A	55	VAL	CA-CB	-6.19	1.45	1.54
1	D	140	TYR	CD2-CE2	-6.18	1.20	1.38
1	C	268	ALA	C-O	6.15	1.31	1.24
1	D	167	SER	CA-C	-6.12	1.44	1.52
1	B	89	ASP	C-O	-6.11	1.16	1.23
1	B	368	VAL	C-O	-6.08	1.17	1.24
1	C	99	MET	C-O	-6.03	1.16	1.23
1	C	84	ALA	CA-CB	-6.03	1.45	1.54
1	C	252	GLU	C-O	6.02	1.32	1.24
1	A	441	ALA	CA-CB	-6.02	1.44	1.53
1	A	72	ALA	C-O	-6.02	1.16	1.24
1	C	168	GLN	CA-C	-6.01	1.46	1.53
1	D	72	ALA	CA-CB	-6.01	1.44	1.53
1	B	129	THR	C-O	-5.99	1.16	1.24
1	B	229	TYR	C-O	5.97	1.31	1.24
1	A	498	GLN	C-O	-5.91	1.17	1.24
1	B	169	ASN	C-O	-5.89	1.16	1.24
1	B	97	ARG	C-O	-5.88	1.16	1.24
1	D	129	THR	C-O	-5.85	1.16	1.24
1	A	45	ALA	C-O	-5.83	1.17	1.24
1	D	127	ILE	N-CA	-5.83	1.39	1.46
1	A	488	THR	CB-CG2	-5.83	1.33	1.52
1	B	56	TYR	N-CA	-5.76	1.39	1.46
1	D	334	LEU	C-O	-5.76	1.16	1.24
1	A	169	ASN	C-O	-5.73	1.16	1.24
1	C	129	THR	C-O	-5.70	1.17	1.24
1	C	55	VAL	CA-CB	-5.70	1.46	1.54
1	A	120	VAL	CA-CB	5.68	1.61	1.54
1	A	291	PRO	C-O	5.68	1.30	1.24
1	C	169	ASN	C-O	-5.66	1.16	1.24
1	D	47	TYR	N-CA	-5.64	1.38	1.46
1	A	58	ASP	CA-C	5.63	1.59	1.53
1	A	129	THR	C-O	-5.62	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	127	ILE	N-CA	-5.62	1.39	1.46
1	B	202	ALA	CA-CB	-5.61	1.44	1.53
1	B	386	ASP	C-O	-5.60	1.17	1.23
1	D	447	THR	C-O	-5.60	1.17	1.24
1	A	252	GLU	C-O	5.59	1.31	1.24
1	B	106	GLN	C-O	-5.58	1.17	1.24
1	D	200	LEU	C-N	5.56	1.41	1.33
1	A	99	MET	C-O	-5.55	1.16	1.23
1	D	100	ALA	CA-C	-5.54	1.46	1.52
1	D	91	ARG	C-O	5.53	1.30	1.24
1	C	148	GLY	C-O	-5.53	1.20	1.24
1	C	251	ALA	C-O	-5.52	1.18	1.24
1	A	56	TYR	N-CA	-5.51	1.39	1.46
1	B	169	ASN	C-N	-5.50	1.25	1.33
1	A	225	ALA	C-O	-5.49	1.17	1.24
1	B	368	VAL	CA-CB	-5.49	1.47	1.54
1	A	423	LYS	C-O	-5.48	1.17	1.24
1	B	521	GLU	C-O	-5.47	1.16	1.24
1	D	414	GLN	C-O	5.47	1.30	1.24
1	D	47	TYR	C-O	-5.47	1.16	1.24
1	B	120	VAL	CA-CB	5.47	1.61	1.54
1	C	194	ILE	CA-CB	5.46	1.60	1.54
1	D	337	ASN	C-O	-5.46	1.17	1.23
1	B	94	VAL	C-O	-5.44	1.18	1.24
1	A	440	HIS	CA-C	-5.43	1.45	1.52
1	C	127	ILE	N-CA	-5.43	1.39	1.46
1	B	493	LYS	N-CA	-5.42	1.39	1.46
1	B	48	ASP	N-CA	-5.41	1.39	1.46
1	C	423	LYS	C-O	-5.40	1.17	1.24
1	D	423	LYS	C-O	-5.40	1.17	1.24
1	A	242	ALA	CA-CB	5.39	1.61	1.53
1	B	529	LEU	C-O	5.39	1.30	1.23
1	A	327	ALA	CA-CB	-5.38	1.44	1.53
1	A	493	LYS	N-CA	-5.37	1.39	1.46
1	C	521	GLU	C-O	-5.37	1.15	1.24
1	A	334	LEU	CA-C	-5.35	1.45	1.52
1	B	333	ASN	CA-CB	-5.33	1.44	1.53
1	C	242	ALA	CA-CB	5.29	1.61	1.53
1	C	334	LEU	C-O	-5.29	1.17	1.24
1	D	45	ALA	C-O	-5.25	1.17	1.23
1	C	202	ALA	CA-CB	-5.25	1.45	1.53
1	D	385	LEU	C-O	-5.25	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	490	ASN	C-O	-5.25	1.17	1.24
1	C	192	ALA	C-O	-5.24	1.17	1.23
1	A	130	PRO	CA-C	-5.24	1.46	1.52
1	A	495	ILE	C-O	-5.24	1.18	1.24
1	B	521	GLU	CA-C	-5.20	1.45	1.52
1	A	167	SER	N-CA	-5.20	1.39	1.45
1	A	226	ILE	CA-CB	-5.18	1.47	1.54
1	A	334	LEU	C-O	-5.18	1.17	1.24
1	B	58	ASP	C-O	-5.17	1.16	1.23
1	D	498	GLN	C-O	-5.17	1.18	1.24
1	A	419	TYR	C-O	-5.15	1.18	1.24
1	B	140	TYR	CE1-CZ	-5.14	1.25	1.38
1	B	95	ILE	C-O	-5.14	1.17	1.24
1	A	493	LYS	C-O	-5.13	1.16	1.23
1	D	170	GLN	C-O	-5.12	1.18	1.24
1	A	84	ALA	CA-CB	-5.11	1.46	1.54
1	C	418	MET	C-O	-5.08	1.17	1.24
1	D	169	ASN	C-O	-5.08	1.17	1.24
1	B	140	TYR	CG-CD1	-5.08	1.28	1.39
1	B	367	ALA	C-O	-5.08	1.17	1.24
1	C	431	ALA	CA-CB	5.08	1.61	1.53
1	B	164	PHE	N-CA	-5.08	1.39	1.46
1	B	317	SER	C-O	5.08	1.30	1.24
1	D	393	TYR	C-O	-5.07	1.16	1.23
1	D	448	ASP	C-O	-5.07	1.18	1.24
1	B	334	LEU	C-O	-5.05	1.18	1.24
1	D	107	TRP	C-O	-5.05	1.17	1.23
1	A	98	VAL	C-O	-5.04	1.18	1.24
1	D	169	ASN	C-N	-5.04	1.26	1.33
1	A	528	ASN	CA-C	-5.03	1.46	1.52
1	A	185	SER	CA-C	-5.00	1.45	1.52

All (301) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	97	ARG	O-C-N	13.88	141.24	122.78
1	A	498	GLN	N-CA-C	10.58	124.14	111.33
1	C	523	LEU	N-CA-C	-10.56	100.89	113.88
1	D	208	ASN	CA-C-N	-10.51	102.78	121.70
1	D	208	ASN	C-N-CA	-10.51	102.78	121.70
1	B	462	TYR	CA-C-N	10.41	130.36	119.85
1	B	462	TYR	C-N-CA	10.41	130.36	119.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	402	ASP	CB-CA-C	-10.26	93.13	109.13
1	D	203	VAL	CB-CA-C	10.20	126.06	110.55
1	D	539	VAL	N-CA-CB	-10.14	94.26	111.50
1	C	539	VAL	N-CA-CB	-10.12	94.30	111.50
1	C	498	GLN	N-CA-C	9.95	122.13	111.28
1	C	522	TRP	N-CA-C	-9.94	99.54	114.64
1	A	208	ASN	O-C-N	-9.91	111.92	123.22
1	C	598	ASN	N-CA-C	-9.74	90.96	107.23
1	B	498	GLN	N-CA-C	9.54	121.68	111.28
1	A	323	ALA	N-CA-C	-9.53	100.77	111.82
1	B	197	ASP	CB-CA-C	9.53	129.37	109.65
1	A	598	ASN	N-CA-C	-9.41	91.20	107.20
1	B	44	TYR	N-CA-C	-9.18	102.08	113.28
1	A	510	GLU	N-CA-C	-9.07	101.24	114.39
1	B	200	LEU	N-CA-C	-9.01	95.30	109.72
1	D	462	TYR	CA-C-N	8.95	128.89	119.85
1	D	462	TYR	C-N-CA	8.95	128.89	119.85
1	D	345	LEU	N-CA-C	-8.92	102.39	113.18
1	A	345	LEU	N-CA-C	-8.89	102.34	113.01
1	C	219	PHE	N-CA-C	-8.84	94.03	109.06
1	B	219	PHE	N-CA-C	-8.81	94.09	109.06
1	B	345	LEU	N-CA-C	-8.66	102.62	113.01
1	D	219	PHE	N-CA-C	-8.66	93.37	108.69
1	A	219	PHE	N-CA-C	-8.60	93.00	108.48
1	A	527	ASN	N-CA-C	8.59	120.72	111.36
1	D	498	GLN	N-CA-C	8.58	121.71	111.33
1	C	294	PHE	CA-C-N	8.56	128.26	119.19
1	C	294	PHE	C-N-CA	8.56	128.26	119.19
1	D	598	ASN	N-CA-C	-8.55	92.95	107.23
1	B	598	ASN	N-CA-C	-8.52	93.01	107.23
1	B	403	ASP	N-CA-CB	-8.49	94.86	110.32
1	D	522	TRP	N-CA-C	-8.47	103.13	113.97
1	D	323	ALA	N-CA-C	-8.34	102.14	111.82
1	A	462	TYR	CA-C-N	8.33	128.28	120.03
1	A	462	TYR	C-N-CA	8.33	128.28	120.03
1	A	599	ALA	N-CA-CB	-8.25	96.54	110.49
1	A	489	SER	N-CA-CB	-8.24	97.80	110.65
1	A	369	MET	N-CA-C	-8.23	102.68	112.89
1	A	277	TYR	N-CA-C	8.23	123.54	113.17
1	C	323	ALA	N-CA-C	-8.22	101.58	111.69
1	A	410	TYR	N-CA-C	8.17	120.10	111.03
1	B	544	ALA	N-CA-CB	-8.17	98.14	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	465	ILE	N-CA-C	-8.15	104.55	111.56
1	D	544	ALA	N-CA-CB	-8.09	98.24	109.98
1	B	215	ASP	N-CA-C	8.08	119.87	111.14
1	B	403	ASP	N-CA-C	8.03	122.51	112.87
1	A	522	TRP	N-CA-C	-7.98	104.02	114.31
1	D	294	PHE	CA-C-N	7.91	127.98	119.28
1	D	294	PHE	C-N-CA	7.91	127.98	119.28
1	C	462	TYR	CA-C-N	7.90	127.83	119.85
1	C	462	TYR	C-N-CA	7.90	127.83	119.85
1	D	168	GLN	CB-CA-C	-7.90	100.92	111.82
1	A	544	ALA	N-CA-CB	-7.88	98.55	109.98
1	B	599	ALA	N-CA-CB	-7.87	97.19	110.49
1	C	544	ALA	N-CA-CB	-7.84	98.61	109.98
1	A	168	GLN	CB-CA-C	-7.82	101.03	111.82
1	D	493	LYS	N-CA-C	-7.81	104.28	113.88
1	B	323	ALA	N-CA-C	-7.78	102.42	112.23
1	D	277	TYR	N-CA-C	7.78	122.97	113.17
1	A	523	LEU	N-CA-C	-7.78	103.93	113.50
1	B	168	GLN	CB-CA-C	-7.76	101.11	111.82
1	A	208	ASN	CB-CA-C	-7.75	97.64	110.19
1	A	294	PHE	CA-C-N	7.75	127.65	119.05
1	A	294	PHE	C-N-CA	7.75	127.65	119.05
1	C	489	SER	N-CA-CB	-7.72	98.61	110.65
1	B	489	SER	N-CA-CB	-7.70	98.64	110.65
1	C	168	GLN	CB-CA-C	-7.69	101.21	111.82
1	C	413	GLY	N-CA-C	-7.69	105.13	114.66
1	D	599	ALA	N-CA-CB	-7.64	97.57	110.49
1	B	277	TYR	N-CA-C	7.63	122.78	113.17
1	B	191	THR	N-CA-C	-7.62	97.45	109.50
1	B	488	THR	N-CA-C	-7.62	96.11	109.06
1	C	391	GLN	O-C-N	-7.58	114.39	122.96
1	D	410	TYR	N-CA-C	7.56	119.42	111.03
1	B	403	ASP	CB-CA-C	-7.40	94.00	110.21
1	D	413	GLY	N-CA-C	-7.36	105.53	114.66
1	C	599	ALA	N-CA-CB	-7.35	98.07	110.49
1	C	369	MET	N-CA-C	-7.34	103.59	112.54
1	D	501	GLN	N-CA-C	-7.31	95.23	110.80
1	B	415	LEU	N-CA-C	-7.29	103.36	111.82
1	D	489	SER	N-CA-CB	-7.26	99.18	110.65
1	A	291	PRO	CA-C-N	7.24	128.89	119.84
1	A	291	PRO	C-N-CA	7.24	128.89	119.84
1	A	186	VAL	N-CA-C	7.23	118.30	107.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	44	TYR	N-CA-C	-7.19	104.48	113.18
1	C	277	TYR	N-CA-C	7.18	122.22	113.17
1	C	488	THR	N-CA-C	-7.17	96.88	109.06
1	C	215	ASP	N-CA-C	-7.14	103.57	111.36
1	B	522	TRP	N-CA-C	-7.09	105.16	114.31
1	A	569	LYS	N-CA-C	-7.07	104.74	113.15
1	D	198	LYS	CB-CA-C	-7.02	99.96	109.71
1	A	189	THR	N-CA-C	-7.01	99.55	110.42
1	A	488	THR	N-CA-C	-6.96	97.22	109.06
1	D	369	MET	N-CA-C	-6.96	104.05	112.54
1	D	186	VAL	N-CA-C	6.95	117.88	107.80
1	A	506	GLU	N-CA-C	-6.95	102.08	111.87
1	D	291	PRO	CA-C-N	6.94	128.52	119.84
1	D	291	PRO	C-N-CA	6.94	128.52	119.84
1	C	191	THR	N-CA-C	-6.92	98.57	109.50
1	B	208	ASN	CB-CA-C	-6.91	96.97	110.10
1	B	92	ASP	N-CA-C	-6.88	100.11	109.54
1	C	584	ARG	N-CA-C	-6.87	99.65	109.96
1	A	475	ILE	N-CA-C	6.86	123.39	113.16
1	C	186	VAL	N-CA-C	6.84	117.72	107.80
1	C	258	ALA	N-CA-C	-6.84	103.61	112.23
1	B	189	THR	N-CA-C	-6.80	100.45	110.52
1	D	584	ARG	N-CA-C	-6.79	99.77	109.96
1	A	533	LEU	N-CA-C	-6.76	105.56	113.88
1	B	349	PHE	N-CA-C	6.75	119.50	111.33
1	B	186	VAL	N-CA-C	6.69	117.50	107.80
1	C	345	LEU	N-CA-C	-6.66	104.41	112.54
1	D	208	ASN	CB-CA-C	-6.65	98.77	109.75
1	C	189	THR	N-CA-C	-6.65	100.12	110.42
1	D	97	ARG	CA-C-N	-6.65	113.75	122.99
1	D	97	ARG	C-N-CA	-6.65	113.75	122.99
1	A	191	THR	N-CA-C	-6.62	99.05	109.50
1	C	539	VAL	N-CA-C	-6.61	92.49	111.00
1	C	475	ILE	N-CA-C	6.61	123.00	113.16
1	B	492	PHE	N-CA-C	-6.58	104.19	111.82
1	C	341	ARG	N-CA-C	-6.54	105.33	113.38
1	D	460	ASP	N-CA-C	-6.47	105.68	113.97
1	C	492	PHE	N-CA-C	-6.46	104.32	111.82
1	D	44	TYR	N-CA-C	-6.45	104.90	112.89
1	B	490	ASN	N-CA-C	6.44	121.93	111.37
1	B	294	PHE	CA-C-N	6.43	126.19	119.05
1	B	294	PHE	C-N-CA	6.43	126.19	119.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	92	ASP	N-CA-CB	-6.42	99.64	110.49
1	B	480	LEU	CA-C-N	6.42	127.86	119.84
1	B	480	LEU	C-N-CA	6.42	127.86	119.84
1	A	92	ASP	N-CA-C	-6.41	97.14	110.80
1	D	474	TRP	N-CA-C	6.40	117.92	111.07
1	D	475	ILE	N-CA-C	6.39	122.68	113.16
1	D	174	ALA	N-CA-C	-6.36	104.44	111.82
1	B	475	ILE	N-CA-C	6.35	122.62	113.16
1	D	195	THR	O-C-N	6.34	130.62	123.27
1	A	494	VAL	CB-CA-C	-6.34	102.79	112.05
1	D	200	LEU	O-C-N	6.29	131.21	123.10
1	A	493	LYS	N-CA-C	-6.27	106.17	113.88
1	C	102	ASN	N-CA-C	6.25	117.95	110.19
1	A	203	VAL	CB-CA-C	6.25	121.90	110.71
1	C	486	GLN	CA-C-N	6.24	126.27	119.90
1	C	486	GLN	C-N-CA	6.24	126.27	119.90
1	A	460	ASP	N-CA-C	-6.22	106.29	114.31
1	A	587	LEU	N-CA-CB	-6.19	100.03	110.49
1	A	584	ARG	N-CA-C	-6.18	100.89	110.10
1	B	587	LEU	N-CA-CB	-6.18	100.05	110.49
1	C	75	SER	N-CA-C	-6.14	98.89	108.90
1	A	535	HIS	N-CA-C	-6.12	105.45	113.17
1	A	474	TRP	N-CA-C	6.11	118.44	111.11
1	C	132	ASN	N-CA-C	6.11	120.32	112.86
1	A	486	GLN	CA-C-N	6.09	126.11	119.90
1	A	486	GLN	C-N-CA	6.09	126.11	119.90
1	D	92	ASP	N-CA-C	-6.09	97.84	110.80
1	C	106	GLN	O-C-N	-6.08	116.09	123.27
1	D	539	VAL	N-CA-C	-6.07	94.02	111.00
1	B	406	SER	N-CA-C	6.05	120.08	109.80
1	D	195	THR	CA-C-N	-6.00	112.04	123.32
1	D	195	THR	C-N-CA	-6.00	112.04	123.32
1	A	106	GLN	O-C-N	-6.00	116.21	123.29
1	C	308	THR	CA-C-N	6.00	125.62	119.56
1	C	308	THR	C-N-CA	6.00	125.62	119.56
1	D	102	ASN	N-CA-C	5.99	117.61	110.19
1	B	91	ARG	CB-CA-C	5.98	122.33	110.42
1	B	357	ILE	CB-CA-C	-5.98	102.89	112.16
1	A	258	ALA	N-CA-C	-5.97	104.34	111.69
1	A	410	TYR	CB-CA-C	-5.97	101.69	110.95
1	D	191	THR	N-CA-C	-5.96	100.09	109.50
1	B	265	ASP	N-CA-C	-5.95	105.99	113.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	291	PRO	CA-C-N	5.95	127.28	119.84
1	C	291	PRO	C-N-CA	5.95	127.28	119.84
1	D	200	LEU	N-CA-C	5.95	119.36	110.14
1	B	431	ALA	N-CA-C	-5.93	104.73	111.14
1	D	367	ALA	N-CA-C	5.93	118.23	111.11
1	C	114	LEU	N-CA-C	-5.93	97.49	107.99
1	D	200	LEU	CA-C-N	-5.93	114.04	122.94
1	D	200	LEU	C-N-CA	-5.93	114.04	122.94
1	A	91	ARG	CB-CA-C	5.92	122.20	110.42
1	B	96	HIS	N-CA-C	-5.92	106.09	113.55
1	D	488	THR	N-CA-C	-5.91	99.02	109.06
1	B	258	ALA	N-CA-C	-5.87	104.47	111.69
1	B	568	TYR	N-CA-C	-5.87	101.44	109.71
1	C	357	ILE	CB-CA-C	-5.86	103.08	112.16
1	B	523	LEU	N-CA-C	-5.83	105.26	112.90
1	B	75	SER	N-CA-C	-5.81	99.43	108.90
1	C	493	LYS	N-CA-C	-5.80	106.33	113.41
1	C	91	ARG	CB-CA-C	5.78	121.92	110.42
1	D	587	LEU	N-CA-CB	-5.77	100.73	110.49
1	C	494	VAL	CB-CA-C	-5.77	103.63	112.05
1	D	229	TYR	N-CA-C	-5.76	106.09	113.01
1	B	382	ILE	N-CA-C	-5.76	104.75	110.62
1	B	584	ARG	N-CA-C	-5.75	101.53	110.10
1	B	197	ASP	N-CA-C	-5.74	102.91	110.43
1	C	208	ASN	CB-CA-C	-5.73	99.22	110.10
1	A	218	TYR	N-CA-C	-5.72	100.81	109.85
1	A	184	PRO	N-CA-C	-5.72	107.00	114.03
1	C	47	TYR	CB-CA-C	5.71	121.59	110.57
1	C	307	ILE	N-CA-C	5.71	116.81	108.53
1	D	91	ARG	CB-CA-C	5.71	121.79	110.42
1	D	490	ASN	N-CA-C	5.71	120.73	111.37
1	A	461	LYS	N-CA-C	-5.70	105.15	111.36
1	A	168	GLN	N-CA-C	5.69	119.15	107.37
1	A	357	ILE	CB-CA-C	-5.68	103.36	112.16
1	C	216	GLY	N-CA-C	-5.67	107.18	115.63
1	C	86	LEU	N-CA-C	-5.66	99.50	108.73
1	B	486	GLN	CA-C-N	5.66	126.91	119.84
1	B	486	GLN	C-N-CA	5.66	126.91	119.84
1	C	419	TYR	N-CA-C	-5.66	104.73	111.69
1	B	123	SER	N-CA-C	5.62	117.89	108.73
1	B	404	ALA	N-CA-CB	-5.61	101.58	109.94
1	D	469	ASN	N-CA-C	-5.60	105.56	112.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	410	TYR	CB-CA-C	-5.59	102.28	110.95
1	B	270	ILE	CB-CA-C	-5.58	103.22	112.26
1	C	168	GLN	N-CA-C	5.58	118.91	107.37
1	C	425	GLY	N-CA-C	-5.57	106.05	112.29
1	A	270	ILE	CB-CA-C	-5.57	103.08	112.16
1	D	341	ARG	N-CA-C	-5.57	106.53	113.38
1	A	169	ASN	N-CA-C	5.56	119.70	113.02
1	D	184	PRO	N-CA-C	-5.56	107.19	114.03
1	D	415	LEU	N-CA-C	-5.56	105.31	111.71
1	A	325	GLU	N-CA-C	-5.52	106.39	113.23
1	D	189	THR	N-CA-C	-5.51	101.87	110.42
1	B	425	GLY	N-CA-C	-5.51	106.12	112.29
1	D	568	TYR	N-CA-C	-5.50	101.95	109.71
1	C	527	ASN	N-CA-C	5.49	119.51	112.26
1	D	83	LYS	CB-CA-C	-5.47	100.89	109.70
1	D	308	THR	CA-C-N	5.46	125.08	119.56
1	D	308	THR	C-N-CA	5.46	125.08	119.56
1	B	570	GLU	N-CA-C	5.46	118.74	111.75
1	C	270	ILE	CB-CA-C	-5.45	103.43	112.26
1	C	44	TYR	N-CA-C	-5.44	106.14	112.89
1	A	490	ASN	N-CA-C	5.44	120.29	111.37
1	B	198	LYS	N-CA-C	-5.44	102.95	110.35
1	A	346	ASN	CB-CA-C	-5.42	102.29	112.00
1	D	96	HIS	CA-C-N	5.42	131.26	122.53
1	D	96	HIS	C-N-CA	5.42	131.26	122.53
1	B	494	VAL	CB-CA-C	-5.41	104.14	112.05
1	B	460	ASP	N-CA-C	-5.41	107.05	113.97
1	B	174	ALA	N-CA-C	-5.40	105.47	111.36
1	D	270	ILE	CB-CA-C	-5.39	103.37	112.16
1	A	539	VAL	N-CA-C	-5.39	107.59	112.12
1	C	229	TYR	N-CA-C	-5.38	106.55	113.01
1	B	399	ARG	N-CA-C	5.38	117.63	110.53
1	C	383	LEU	N-CA-C	5.37	116.82	111.07
1	B	106	GLN	O-C-N	-5.37	116.93	123.27
1	B	461	LYS	N-CA-C	-5.36	105.52	111.36
1	D	168	GLN	N-CA-C	5.35	118.44	107.37
1	B	474	TRP	N-CA-C	5.33	116.78	111.07
1	A	381	GLU	CB-CA-C	-5.33	101.78	110.85
1	C	92	ASP	N-CA-C	-5.33	99.44	110.80
1	D	494	VAL	CB-CA-C	-5.33	104.27	112.05
1	C	587	LEU	N-CA-CB	-5.32	101.50	110.49
1	B	83	LYS	CB-CA-C	-5.31	100.90	109.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	218	TYR	N-CA-C	-5.31	101.46	109.85
1	B	341	ARG	N-CA-C	-5.29	106.87	113.38
1	A	86	LEU	N-CA-C	-5.29	99.16	108.20
1	C	410	TYR	CB-CA-C	-5.29	102.75	110.95
1	D	86	LEU	N-CA-C	-5.28	99.17	108.20
1	B	420	LEU	N-CA-C	-5.26	106.13	112.54
1	A	358	MET	CG-SD-CE	5.23	112.41	100.90
1	D	132	ASN	N-CA-C	5.23	118.93	112.24
1	B	411	VAL	CB-CA-C	-5.22	105.24	112.24
1	D	301	ASN	N-CA-C	-5.22	101.69	109.42
1	C	570	GLU	N-CA-C	5.22	118.43	111.75
1	A	132	ASN	N-CA-C	5.21	118.91	112.24
1	C	96	HIS	N-CA-C	-5.21	105.99	112.93
1	A	47	TYR	CB-CA-C	5.21	120.62	110.57
1	A	403	ASP	N-CA-C	-5.20	105.31	110.97
1	B	168	GLN	N-CA-C	5.19	118.12	107.37
1	B	200	LEU	N-CA-CB	5.19	119.96	111.08
1	D	366	ARG	CA-C-N	5.19	127.55	120.54
1	D	366	ARG	C-N-CA	5.19	127.55	120.54
1	D	489	SER	CA-C-N	-5.19	112.94	121.19
1	D	489	SER	C-N-CA	-5.19	112.94	121.19
1	A	114	LEU	N-CA-C	-5.19	98.81	107.99
1	C	415	LEU	N-CA-C	-5.16	105.77	111.71
1	A	83	LYS	CB-CA-C	-5.15	101.41	109.70
1	C	92	ASP	N-CA-CB	-5.13	101.82	110.49
1	A	480	LEU	CA-C-N	5.13	125.81	120.12
1	A	480	LEU	C-N-CA	5.13	125.81	120.12
1	D	349	PHE	N-CA-C	5.13	116.87	111.28
1	A	227	PRO	CA-C-N	5.09	126.21	119.84
1	A	227	PRO	C-N-CA	5.09	126.21	119.84
1	D	584	ARG	CB-CA-C	5.09	118.04	109.89
1	C	490	ASN	N-CA-C	5.07	119.69	111.37
1	A	92	ASP	N-CA-CB	-5.07	101.93	110.49
1	D	218	TYR	N-CA-C	-5.06	101.86	109.85
1	D	457	ASN	N-CA-C	5.05	121.19	113.61
1	C	265	ASP	N-CA-C	-5.04	107.16	113.72
1	D	570	GLU	N-CA-C	5.04	117.51	111.71
1	B	308	THR	CA-C-N	5.02	124.63	119.56
1	B	308	THR	C-N-CA	5.02	124.63	119.56
1	B	493	LYS	N-CA-C	-5.01	107.72	113.88
1	B	404	ALA	N-CA-C	5.01	117.12	111.11
1	D	258	ALA	N-CA-C	-5.01	105.90	111.36

There are no chirality outliers.

All (17) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	197	ASP	Peptide
1	A	208	ASN	Mainchain
1	A	40	ASP	Peptide
1	A	506	GLU	Peptide
1	A	535	HIS	Peptide
1	A	538	MET	Peptide
1	A	568	TYR	Peptide
1	B	402	ASP	Peptide
1	B	404	ALA	Peptide
1	B	539	VAL	Peptide
1	C	500	ASN	Mainchain
1	C	527	ASN	Peptide
1	D	197	ASP	Peptide
1	D	208	ASN	Mainchain
1	D	214	ARG	Peptide
1	D	38	LEU	Peptide
1	D	510	GLU	Peptide

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	4708	0	4594	433	0
1	B	4651	0	4543	426	1
1	C	4657	0	4549	413	1
1	D	4669	0	4560	453	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	331	0	0	23	0
3	B	154	0	0	8	1
3	C	156	0	0	13	2
3	D	278	0	0	27	1
All	All	19608	0	18246	1718	3

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 47.

All (1718) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:502:LEU:HD12	1:D:506:GLU:O	1.34	1.27
1:A:42:TYR:OH	1:A:399:ARG:O	1.53	1.26
1:A:503:VAL:O	1:A:504:THR:HG23	1.39	1.22
1:B:42:TYR:OH	1:B:399:ARG:O	1.59	1.19
1:A:42:TYR:CE2	1:A:401:PRO:HD3	1.80	1.17
1:C:509:LEU:HD23	1:C:509:LEU:H	1.11	1.15
1:C:502:LEU:HB2	1:C:506:GLU:HB2	1.25	1.15
1:B:144:GLU:H	1:B:144:GLU:CD	1.57	1.13
1:A:42:TYR:HE2	1:A:401:PRO:HD3	1.12	1.13
1:D:509:LEU:HG	1:D:510:GLU:N	1.59	1.12
1:C:144:GLU:CD	1:C:144:GLU:H	1.53	1.12
1:D:503:VAL:HG22	1:D:506:GLU:CG	1.79	1.12
1:D:503:VAL:HG22	1:D:506:GLU:CD	1.75	1.11
1:B:539:VAL:HG12	1:B:540:ASN:H	1.00	1.10
1:B:355:ASN:OD1	1:B:371:GLN:NE2	1.83	1.10
1:D:503:VAL:CG2	1:D:506:GLU:HG3	1.82	1.10
1:B:183:THR:HG22	1:B:185:SER:H	1.15	1.10
1:C:522:TRP:O	1:C:526:ILE:HG13	1.51	1.09
1:B:503:VAL:HG23	1:B:506:GLU:CG	1.81	1.09
1:B:523:LEU:O	1:B:527:ASN:HB2	1.51	1.08
1:D:503:VAL:C	1:D:506:GLU:HG3	1.77	1.07
1:A:504:THR:H	1:A:506:GLU:HB2	1.17	1.06
1:A:523:LEU:O	1:A:527:ASN:ND2	1.86	1.06
1:B:503:VAL:CG2	1:B:506:GLU:HG2	1.85	1.06
1:D:144:GLU:H	1:D:144:GLU:CD	1.57	1.06
1:D:525:PHE:O	1:D:529:LEU:HG	1.52	1.05
1:D:183:THR:HG22	1:D:185:SER:H	1.21	1.05
1:D:503:VAL:CA	1:D:506:GLU:HG3	1.84	1.05
1:C:503:VAL:O	1:C:504:THR:HG23	1.58	1.04
1:B:502:LEU:HG	1:B:507:LEU:HB2	1.39	1.04
1:D:503:VAL:C	1:D:506:GLU:CG	2.30	1.03
1:B:539:VAL:HG12	1:B:540:ASN:N	1.61	1.03
1:D:263:PHE:O	1:D:266:THR:HG23	1.57	1.03
1:A:183:THR:HG22	1:A:185:SER:H	1.18	1.02
1:D:503:VAL:HG22	1:D:506:GLU:HG3	1.34	1.02
1:D:503:VAL:C	1:D:504:THR:HG23	1.80	1.02
1:C:502:LEU:HD13	1:C:506:GLU:HB3	1.41	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:503:VAL:O	1:D:504:THR:HG23	1.58	1.02
1:D:543:LYS:HE3	1:D:543:LYS:O	1.57	1.02
1:C:502:LEU:CD1	1:C:506:GLU:HB3	1.91	1.01
1:C:405:PHE:HA	3:C:994:HOH:O	1.62	1.00
1:D:504:THR:N	1:D:506:GLU:HG2	1.76	1.00
1:C:368:VAL:HA	1:C:371:GLN:HG3	1.42	0.99
1:C:263:PHE:O	1:C:266:THR:HG23	1.62	0.99
1:C:509:LEU:H	1:C:509:LEU:CD2	1.76	0.99
1:D:560:TYR:HB3	1:D:575:MET:HE2	1.44	0.99
1:B:504:THR:HG23	1:B:504:THR:O	1.63	0.98
1:D:503:VAL:O	1:D:503:VAL:HG23	1.58	0.98
1:D:67:SER:HB2	1:D:142:SER:O	1.64	0.98
1:C:183:THR:HG22	1:C:185:SER:H	1.21	0.98
1:D:506:GLU:O	1:D:507:LEU:HB2	1.60	0.98
1:A:368:VAL:HA	1:A:371:GLN:HG3	1.43	0.98
1:C:157:THR:O	1:C:160:LYS:HE3	1.61	0.97
1:C:543:LYS:O	1:C:543:LYS:HE3	1.64	0.97
1:D:586:LYS:HG2	1:D:586:LYS:O	1.63	0.97
1:B:502:LEU:CG	1:B:507:LEU:HB2	1.94	0.97
1:A:263:PHE:O	1:A:266:THR:HG23	1.64	0.97
1:C:509:LEU:HD23	1:C:509:LEU:N	1.78	0.97
1:B:503:VAL:HG23	1:B:506:GLU:HG2	1.36	0.97
1:B:263:PHE:O	1:B:266:THR:HG23	1.65	0.96
1:B:502:LEU:CD1	1:B:507:LEU:HB2	1.95	0.96
1:B:157:THR:O	1:B:160:LYS:HE3	1.65	0.95
1:A:97:ARG:HH11	1:A:99:MET:HE3	1.31	0.95
1:C:503:VAL:C	1:C:504:THR:HG23	1.92	0.94
1:D:509:LEU:HG	1:D:510:GLU:H	1.30	0.94
1:A:586:LYS:O	1:A:586:LYS:HG2	1.65	0.94
1:A:157:THR:O	1:A:160:LYS:HE3	1.67	0.93
1:A:144:GLU:CD	1:A:144:GLU:H	1.76	0.93
1:C:97:ARG:HH11	1:C:99:MET:HE3	1.34	0.93
1:B:373:LEU:HD13	1:B:492:PHE:CZ	2.05	0.92
1:D:42:TYR:OH	1:D:399:ARG:O	1.86	0.92
1:B:400:ASP:HB3	1:B:403:ASP:HB2	1.52	0.92
1:B:510:GLU:H	1:B:510:GLU:CD	1.77	0.92
1:A:543:LYS:O	1:A:543:LYS:HE3	1.69	0.92
1:B:355:ASN:CG	1:B:371:GLN:HE21	1.78	0.92
1:B:67:SER:HB2	1:B:142:SER:O	1.71	0.90
1:C:560:TYR:HB3	1:C:575:MET:HE2	1.51	0.90
1:C:243:MET:HE2	1:C:249:ILE:HG13	1.52	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:157:THR:O	1:D:160:LYS:HE3	1.70	0.90
1:C:40:ASP:OD2	1:C:183:THR:HG23	1.72	0.90
1:B:543:LYS:O	1:B:543:LYS:HE3	1.72	0.90
1:C:507:LEU:HD11	3:C:971:HOH:O	1.70	0.90
1:A:361:VAL:HG23	1:A:362:PHE:CD1	2.06	0.90
1:B:341:ARG:HD2	1:B:394:ILE:O	1.72	0.89
1:B:522:TRP:O	1:B:526:ILE:HD13	1.72	0.89
1:B:586:LYS:HG2	1:B:586:LYS:O	1.71	0.89
1:D:522:TRP:O	1:D:526:ILE:HG13	1.73	0.89
1:C:67:SER:HB2	1:C:142:SER:O	1.71	0.89
1:B:522:TRP:O	1:B:526:ILE:HG23	1.71	0.89
1:C:144:GLU:CD	1:C:144:GLU:N	2.30	0.89
1:C:502:LEU:HB2	1:C:506:GLU:CB	2.03	0.88
1:C:361:VAL:HG23	1:C:362:PHE:CD1	2.08	0.88
1:A:582:ILE:CD1	1:A:587:LEU:HD23	2.04	0.88
1:B:560:TYR:HB3	1:B:575:MET:HE2	1.56	0.88
1:B:529:LEU:HD23	1:B:530:PRO:N	1.87	0.88
1:A:567:ASP:O	1:A:569:LYS:HD2	1.74	0.87
1:D:40:ASP:OD2	1:D:183:THR:HG23	1.75	0.86
1:A:530:PRO:O	1:A:533:LEU:HD13	1.75	0.86
1:D:153:SER:OG	1:D:155:GLU:HG2	1.75	0.86
1:A:523:LEU:O	1:A:527:ASN:HB2	1.75	0.86
1:A:500:ASN:HD22	1:A:500:ASN:N	1.70	0.86
1:C:97:ARG:HH11	1:C:99:MET:CE	1.89	0.86
1:A:67:SER:HB2	1:A:142:SER:O	1.76	0.85
1:D:500:ASN:HD22	1:D:500:ASN:H	1.23	0.85
1:D:361:VAL:HG23	1:D:362:PHE:CD1	2.12	0.85
1:B:502:LEU:HG	1:B:507:LEU:CB	2.05	0.84
1:B:144:GLU:CD	1:B:144:GLU:N	2.35	0.84
1:A:102:ASN:HB2	3:A:960:HOH:O	1.77	0.84
1:D:503:VAL:C	1:D:506:GLU:HG2	2.01	0.84
1:A:567:ASP:HB3	1:A:569:LYS:CE	2.08	0.84
1:B:373:LEU:HD13	1:B:492:PHE:CE2	2.12	0.84
1:C:464:ASN:HD22	1:D:241:LYS:HB3	1.42	0.83
1:D:296:PHE:HD2	3:D:970:HOH:O	1.60	0.83
1:D:503:VAL:CB	1:D:506:GLU:HG3	2.08	0.83
1:A:97:ARG:HH11	1:A:99:MET:CE	1.92	0.83
1:B:361:VAL:HG23	1:B:362:PHE:CD1	2.13	0.83
1:B:334:LEU:CD2	1:B:441:ALA:HA	2.08	0.83
1:C:586:LYS:O	1:C:586:LYS:HG2	1.76	0.83
1:A:198:LYS:O	1:A:199:ASP:HB2	1.77	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:243:MET:HE2	1:B:249:ILE:HG13	1.58	0.83
1:C:582:ILE:CD1	1:C:587:LEU:HD23	2.08	0.83
1:B:503:VAL:O	1:B:504:THR:HB	1.76	0.83
1:C:271:ASP:OD1	3:C:924:HOH:O	1.97	0.82
1:D:168:GLN:HE22	1:D:299:MET:HG2	1.44	0.82
1:D:405:PHE:O	3:D:761:HOH:O	1.96	0.82
1:D:584:ARG:O	1:D:588:ILE:HG12	1.78	0.82
1:A:40:ASP:OD2	1:A:183:THR:HG23	1.79	0.82
1:C:153:SER:OG	1:C:155:GLU:HG2	1.80	0.82
1:D:502:LEU:HD11	1:D:507:LEU:HD12	1.59	0.82
1:B:539:VAL:CG1	1:B:540:ASN:H	1.84	0.81
1:A:42:TYR:CE2	1:A:401:PRO:CD	2.61	0.81
1:B:198:LYS:O	1:B:199:ASP:HB2	1.79	0.81
1:D:341:ARG:HD2	1:D:394:ILE:O	1.80	0.81
1:A:560:TYR:HB3	1:A:575:MET:HE2	1.62	0.81
1:B:539:VAL:C	1:B:541:LEU:H	1.88	0.81
1:B:569:LYS:HD2	1:B:570:GLU:N	1.94	0.81
1:D:455:LYS:O	1:D:460:ASP:HB2	1.80	0.81
1:C:512:LEU:HB3	1:C:513:PRO:CD	2.11	0.80
1:A:243:MET:HE2	1:A:249:ILE:HG13	1.62	0.80
1:A:567:ASP:HB3	1:A:569:LYS:HE3	1.63	0.80
1:B:102:ASN:HB2	3:B:795:HOH:O	1.81	0.80
1:B:208:ASN:OD1	1:B:208:ASN:O	2.00	0.80
1:B:153:SER:OG	1:B:155:GLU:HG2	1.81	0.80
1:A:169:ASN:O	3:A:715:HOH:O	1.98	0.80
1:D:334:LEU:CD2	1:D:441:ALA:HA	2.12	0.80
1:D:144:GLU:CD	1:D:144:GLU:N	2.39	0.79
1:A:199:ASP:OD2	3:A:825:HOH:O	2.00	0.79
1:B:504:THR:O	1:B:504:THR:CG2	2.30	0.79
1:C:502:LEU:CB	1:C:506:GLU:HB2	2.10	0.79
1:D:489:SER:HB3	1:D:492:PHE:HB2	1.64	0.79
1:D:503:VAL:O	1:D:504:THR:CG2	2.30	0.79
1:A:153:SER:OG	1:A:155:GLU:HG2	1.83	0.79
1:A:503:VAL:H	1:A:506:GLU:HB3	1.48	0.79
1:B:547:LEU:H	1:B:547:LEU:HD12	1.47	0.79
1:A:341:ARG:HD2	1:A:394:ILE:O	1.81	0.79
1:D:168:GLN:HB3	3:D:737:HOH:O	1.82	0.79
1:B:368:VAL:CG1	1:B:368:VAL:O	2.30	0.78
1:B:509:LEU:HB2	1:B:510:GLU:OE2	1.83	0.78
1:C:208:ASN:O	1:C:208:ASN:OD1	2.01	0.78
1:D:296:PHE:CD2	3:D:970:HOH:O	2.35	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:508:THR:O	1:C:509:LEU:O	2.02	0.78
1:D:428:ARG:CD	3:D:956:HOH:O	2.32	0.78
1:C:418:MET:O	1:C:422:GLU:HG3	1.83	0.78
1:A:199:ASP:O	1:A:200:LEU:HD12	1.84	0.78
1:D:500:ASN:HD22	1:D:500:ASN:N	1.81	0.78
1:C:503:VAL:O	1:C:504:THR:CG2	2.30	0.78
1:D:295:PRO:HG2	1:D:296:PHE:HD1	1.49	0.78
1:D:424:PHE:O	3:D:873:HOH:O	2.02	0.78
1:C:168:GLN:HE22	1:C:299:MET:HG2	1.49	0.77
1:A:334:LEU:CD2	1:A:441:ALA:HA	2.14	0.77
1:A:101:LYS:O	3:A:981:HOH:O	2.03	0.77
1:C:341:ARG:HD2	1:C:394:ILE:O	1.84	0.77
1:C:419:TYR:CE1	3:C:976:HOH:O	2.37	0.77
1:B:547:LEU:HD12	1:B:547:LEU:N	2.00	0.77
1:A:424:PHE:O	3:A:866:HOH:O	2.02	0.76
1:D:503:VAL:CG2	1:D:506:GLU:CD	2.56	0.76
1:D:57:LEU:HB3	1:D:59:LEU:CD2	2.15	0.76
1:D:569:LYS:HD2	1:D:570:GLU:N	2.00	0.76
1:A:208:ASN:OD1	1:A:208:ASN:O	2.04	0.76
1:B:580:LYS:HA	1:B:612:ALA:HB2	1.67	0.76
1:D:503:VAL:CG2	1:D:503:VAL:O	2.29	0.76
1:A:405:PHE:O	3:A:732:HOH:O	2.04	0.76
1:A:502:LEU:HB2	1:A:506:GLU:O	1.85	0.76
1:B:271:ASP:OD1	3:B:763:HOH:O	2.02	0.76
1:B:381:GLU:O	1:B:385:LEU:HB2	1.84	0.76
1:A:168:GLN:HB3	3:A:703:HOH:O	1.84	0.76
1:A:523:LEU:C	1:A:527:ASN:HD22	1.93	0.76
1:A:144:GLU:CD	1:A:144:GLU:N	2.43	0.75
1:B:509:LEU:HD21	1:B:511:GLN:HB2	1.69	0.75
1:B:510:GLU:CD	1:B:510:GLU:N	2.42	0.75
1:B:569:LYS:HD2	1:B:570:GLU:H	1.50	0.75
1:C:358:MET:HE3	1:C:366:ARG:NH1	2.01	0.75
1:C:334:LEU:CD2	1:C:441:ALA:HA	2.17	0.75
1:B:582:ILE:CD1	1:B:587:LEU:HD23	2.17	0.75
1:C:492:PHE:O	1:C:495:ILE:HB	1.87	0.75
1:D:606:VAL:O	1:D:610:LYS:HD3	1.86	0.75
1:B:168:GLN:HE22	1:B:299:MET:HG2	1.51	0.75
1:B:418:MET:O	1:B:422:GLU:HG3	1.87	0.75
1:B:503:VAL:O	1:B:504:THR:CB	2.34	0.75
1:B:539:VAL:CG1	1:B:540:ASN:N	2.37	0.74
1:B:539:VAL:C	1:B:541:LEU:N	2.40	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:547:LEU:H	1:C:547:LEU:HD12	1.52	0.74
1:D:582:ILE:CD1	1:D:587:LEU:HD23	2.17	0.74
1:B:584:ARG:O	1:B:588:ILE:HG12	1.87	0.74
1:B:503:VAL:HB	1:B:506:GLU:OE1	1.87	0.74
1:C:543:LYS:O	1:C:543:LYS:CE	2.35	0.74
1:C:606:VAL:O	1:C:610:LYS:HD3	1.88	0.74
1:D:58:ASP:O	1:D:70:GLY:HA3	1.88	0.74
1:B:609:TYR:O	1:B:613:ARG:HB2	1.88	0.74
1:C:46:ASN:C	1:C:48:ASP:H	1.94	0.74
1:C:579:LEU:HD21	1:C:591:LEU:HD23	1.67	0.74
1:B:334:LEU:HD22	1:B:441:ALA:HA	1.70	0.74
1:B:606:VAL:O	1:B:610:LYS:HD3	1.87	0.74
1:A:503:VAL:O	1:A:504:THR:CG2	2.29	0.74
1:A:168:GLN:HG3	1:A:168:GLN:O	1.78	0.74
1:D:168:GLN:HG3	1:D:168:GLN:O	1.81	0.74
1:B:503:VAL:HG23	1:B:506:GLU:CD	2.13	0.73
1:C:381:GLU:O	1:C:385:LEU:HB2	1.88	0.73
1:C:290:LEU:HD21	1:C:306:PHE:HD2	1.53	0.73
1:C:569:LYS:HD2	1:C:570:GLU:N	2.02	0.73
1:D:543:LYS:O	1:D:543:LYS:CE	2.33	0.73
1:A:418:MET:O	1:A:422:GLU:HG3	1.89	0.73
1:A:584:ARG:O	1:A:588:ILE:HG12	1.87	0.73
1:A:543:LYS:O	1:A:543:LYS:CE	2.36	0.73
1:C:41:ALA:O	1:C:42:TYR:HB2	1.86	0.73
1:C:424:PHE:O	3:C:929:HOH:O	2.06	0.73
1:B:358:MET:HE3	1:B:366:ARG:NH1	2.05	0.72
1:A:533:LEU:O	1:A:536:GLN:N	2.18	0.72
1:A:606:VAL:O	1:A:610:LYS:HD3	1.89	0.72
1:C:295:PRO:HG2	1:C:296:PHE:HD1	1.52	0.72
1:D:169:ASN:O	3:D:746:HOH:O	2.06	0.72
1:B:102:ASN:HD21	1:B:106:GLN:HB2	1.54	0.72
1:A:501:GLN:HG2	1:A:508:THR:HG23	1.69	0.72
1:A:523:LEU:O	1:A:527:ASN:CB	2.37	0.72
1:B:290:LEU:HD21	1:B:306:PHE:HD2	1.55	0.72
1:A:580:LYS:HA	1:A:612:ALA:HB2	1.72	0.72
1:B:358:MET:HE3	1:B:366:ARG:HH12	1.54	0.72
1:D:243:MET:HE2	1:D:249:ILE:HG13	1.72	0.72
1:A:290:LEU:HD21	1:A:306:PHE:HD2	1.54	0.72
1:B:529:LEU:HD23	1:B:529:LEU:C	2.13	0.71
1:C:580:LYS:HA	1:C:612:ALA:HB2	1.70	0.71
1:D:358:MET:HE3	1:D:366:ARG:NH1	2.04	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:359:GLU:HG2	1:B:364:THR:HG22	1.72	0.71
1:C:582:ILE:HD11	1:C:584:ARG:HB3	1.71	0.71
1:D:418:MET:O	1:D:422:GLU:HG3	1.89	0.71
1:D:378:LEU:O	1:D:382:ILE:HG12	1.90	0.71
1:D:586:LYS:O	1:D:586:LYS:CG	2.35	0.71
1:A:295:PRO:HG2	1:A:296:PHE:HD1	1.55	0.71
1:C:527:ASN:OD1	1:C:558:ALA:HB1	1.90	0.71
1:B:46:ASN:C	1:B:48:ASP:H	1.98	0.71
1:C:168:GLN:HE22	1:C:299:MET:CG	2.03	0.71
1:D:580:LYS:HA	1:D:612:ALA:HB2	1.71	0.71
1:A:46:ASN:C	1:A:48:ASP:H	1.96	0.71
1:A:222:MET:SD	1:A:224:GLN:HB2	2.31	0.70
1:D:168:GLN:HE22	1:D:299:MET:CG	2.03	0.70
1:A:58:ASP:O	1:A:70:GLY:HA3	1.92	0.70
1:B:168:GLN:HG3	1:B:168:GLN:O	1.87	0.70
1:D:46:ASN:C	1:D:48:ASP:H	1.98	0.70
1:B:411:VAL:O	1:B:415:LEU:HG	1.90	0.70
1:C:503:VAL:HG23	1:C:506:GLU:HG2	1.73	0.70
1:D:42:TYR:CE2	1:D:401:PRO:HD3	2.26	0.70
1:B:503:VAL:HG23	1:B:506:GLU:OE1	1.91	0.70
1:B:543:LYS:O	1:B:543:LYS:CE	2.40	0.70
1:C:584:ARG:O	1:C:588:ILE:HG12	1.90	0.70
1:C:609:TYR:O	1:C:613:ARG:HB2	1.91	0.70
1:B:183:THR:HG22	1:B:185:SER:N	2.00	0.70
1:C:58:ASP:O	1:C:70:GLY:HA3	1.92	0.70
1:C:596:ALA:HA	1:C:602:LYS:HB2	1.73	0.70
1:D:290:LEU:HD21	1:D:306:PHE:HD2	1.56	0.70
1:C:57:LEU:HB3	1:C:59:LEU:CD2	2.22	0.69
1:A:378:LEU:O	1:A:382:ILE:HG12	1.92	0.69
1:A:411:VAL:O	1:A:415:LEU:HG	1.92	0.69
1:B:58:ASP:O	1:B:70:GLY:HA3	1.92	0.69
1:A:384:GLU:OE1	3:A:832:HOH:O	2.10	0.69
1:B:57:LEU:HB3	1:B:59:LEU:CD2	2.21	0.69
1:A:536:GLN:OE1	1:A:536:GLN:HA	1.90	0.69
1:A:547:LEU:HD12	1:A:547:LEU:H	1.57	0.69
1:A:568:TYR:C	1:A:570:GLU:H	2.00	0.69
1:B:507:LEU:HD23	1:B:507:LEU:C	2.18	0.69
1:C:598:ASN:HB3	1:C:601:SER:HB3	1.74	0.69
1:A:183:THR:HG22	1:A:185:SER:N	2.01	0.69
1:B:503:VAL:CB	1:B:506:GLU:OE1	2.40	0.69
1:B:509:LEU:H	1:B:509:LEU:CD2	2.06	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:455:LYS:O	1:C:460:ASP:HB2	1.93	0.69
1:B:503:VAL:HG21	1:B:506:GLU:HG2	1.72	0.69
1:A:101:LYS:HB3	1:A:101:LYS:HZ3	1.58	0.69
1:A:455:LYS:O	1:A:460:ASP:HB2	1.93	0.68
1:C:494:VAL:O	1:C:494:VAL:HG12	1.93	0.68
1:A:103:SER:N	3:A:960:HOH:O	2.16	0.68
1:C:101:LYS:HB3	1:C:101:LYS:HZ3	1.58	0.68
1:A:504:THR:N	1:A:506:GLU:HB2	1.99	0.68
1:C:168:GLN:HG3	1:C:168:GLN:O	1.89	0.68
1:C:180:ILE:HG12	1:C:181:GLN:H	1.58	0.68
1:B:101:LYS:HB3	1:B:101:LYS:HZ3	1.58	0.68
1:B:503:VAL:CG2	1:B:506:GLU:OE1	2.42	0.68
1:C:97:ARG:HD3	1:C:99:MET:HE3	1.76	0.68
1:C:547:LEU:HD12	1:C:547:LEU:N	2.09	0.68
1:A:168:GLN:HE22	1:A:299:MET:HG2	1.57	0.68
1:A:582:ILE:HD11	1:A:587:LEU:HD23	1.74	0.68
1:A:543:LYS:O	1:A:543:LYS:CD	2.40	0.68
1:D:197:ASP:HB3	1:D:198:LYS:O	1.93	0.68
1:C:358:MET:CE	1:C:366:ARG:HH12	2.06	0.68
1:D:502:LEU:HD12	1:D:507:LEU:HB2	1.74	0.68
1:A:392:LEU:HD23	1:A:475:ILE:HG22	1.74	0.68
1:D:369:MET:SD	1:D:520:HIS:HB2	2.33	0.68
1:A:547:LEU:HD12	1:A:547:LEU:N	2.09	0.68
1:B:509:LEU:H	1:B:509:LEU:HD22	1.58	0.68
1:A:538:MET:HG2	1:A:568:TYR:CG	2.29	0.67
1:D:97:ARG:HD3	1:D:99:MET:CE	2.24	0.67
1:A:492:PHE:O	1:A:495:ILE:HB	1.93	0.67
1:A:499:ILE:HG13	1:A:500:ASN:ND2	2.10	0.67
1:A:174:ALA:HB3	1:A:182:ASP:OD1	1.95	0.67
1:C:464:ASN:ND2	1:D:241:LYS:HD3	2.09	0.67
1:C:569:LYS:HD2	1:C:570:GLU:H	1.59	0.67
1:D:547:LEU:N	1:D:547:LEU:HD12	2.08	0.67
1:D:208:ASN:OD1	1:D:208:ASN:O	2.12	0.67
1:B:295:PRO:HG2	1:B:296:PHE:HD1	1.59	0.67
1:B:525:PHE:CD1	1:B:526:ILE:HG22	2.30	0.67
1:C:502:LEU:CB	1:C:506:GLU:CB	2.71	0.67
1:D:547:LEU:HD12	1:D:547:LEU:H	1.59	0.67
1:B:206:ALA:HB1	1:B:221:SER:C	2.20	0.67
1:C:596:ALA:HA	1:C:602:LYS:CB	2.23	0.67
1:D:609:TYR:O	1:D:613:ARG:HB2	1.95	0.67
1:D:582:ILE:HD11	1:D:584:ARG:HB3	1.75	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:400:ASP:HB3	1:B:403:ASP:CB	2.24	0.66
1:B:514:THR:HG21	1:B:545:PHE:CZ	2.29	0.66
1:D:359:GLU:HG2	1:D:364:THR:HG22	1.75	0.66
1:B:582:ILE:HD11	1:B:584:ARG:HB3	1.78	0.66
1:B:579:LEU:HD21	1:B:591:LEU:HD23	1.77	0.66
1:A:507:LEU:HD11	3:A:970:HOH:O	1.95	0.66
1:D:334:LEU:HD21	1:D:441:ALA:HA	1.76	0.66
1:B:509:LEU:CD2	1:B:509:LEU:N	2.59	0.66
1:D:224:GLN:OE1	3:D:792:HOH:O	2.14	0.66
1:D:509:LEU:CG	1:D:510:GLU:N	2.43	0.66
1:A:99:MET:HE1	1:A:109:LYS:HB2	1.77	0.66
1:C:334:LEU:HD22	1:C:441:ALA:HA	1.77	0.66
1:D:143:THR:HB	1:D:144:GLU:OE2	1.96	0.66
1:D:200:LEU:O	1:D:218:TYR:OH	2.13	0.66
1:B:358:MET:CE	1:B:366:ARG:HH12	2.08	0.66
1:D:368:VAL:HA	1:D:371:GLN:HG3	1.77	0.66
1:D:503:VAL:C	1:D:504:THR:CG2	2.54	0.66
1:B:540:ASN:OD1	1:B:541:LEU:N	2.29	0.65
1:C:586:LYS:O	1:C:586:LYS:CG	2.44	0.65
1:D:503:VAL:H	1:D:506:GLU:CB	2.09	0.65
1:D:411:VAL:O	1:D:415:LEU:HG	1.96	0.65
1:A:301:ASN:HB2	1:A:304:LEU:O	1.96	0.65
1:A:586:LYS:O	1:A:586:LYS:CG	2.39	0.65
1:B:272:LYS:HG3	1:B:361:VAL:HG12	1.78	0.65
1:B:455:LYS:O	1:B:460:ASP:HB2	1.95	0.65
1:B:529:LEU:HD23	1:B:530:PRO:CD	2.27	0.65
1:D:381:GLU:O	1:D:385:LEU:HB2	1.95	0.65
1:C:359:GLU:HG2	1:C:364:THR:HG22	1.78	0.65
1:B:539:VAL:O	1:B:541:LEU:N	2.30	0.65
1:C:272:LYS:HG3	1:C:361:VAL:HG12	1.79	0.65
1:A:500:ASN:HD22	1:A:500:ASN:H	1.45	0.65
1:B:489:SER:HB3	1:B:492:PHE:HB2	1.78	0.65
1:D:504:THR:N	1:D:506:GLU:CG	2.49	0.65
1:D:595:LEU:HD21	1:D:604:TRP:CE3	2.31	0.65
1:A:66:LYS:HB2	1:A:144:GLU:HB3	1.79	0.65
1:B:502:LEU:HD11	1:B:507:LEU:HB2	1.78	0.65
1:B:543:LYS:O	1:B:543:LYS:CD	2.44	0.65
1:C:514:THR:HG21	1:C:545:PHE:CZ	2.32	0.65
1:D:358:MET:CE	1:D:366:ARG:HH12	2.10	0.65
1:C:311:VAL:HG11	1:C:321:LEU:CD2	2.27	0.65
1:D:169:ASN:ND2	1:D:231:ILE:O	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:506:GLU:O	1:D:507:LEU:CB	2.35	0.65
1:A:144:GLU:N	1:A:144:GLU:OE2	2.30	0.64
1:A:198:LYS:O	1:A:199:ASP:CB	2.46	0.64
1:C:226:ILE:HD12	1:C:230:LEU:HB2	1.78	0.64
1:C:503:VAL:C	1:C:504:THR:CG2	2.64	0.64
1:A:52:ALA:O	1:A:188:VAL:HG12	1.97	0.64
1:D:209:GLU:HB3	3:D:768:HOH:O	1.96	0.64
1:D:579:LEU:HD21	1:D:591:LEU:HD23	1.79	0.64
1:A:57:LEU:HB3	1:A:59:LEU:CD2	2.28	0.64
1:A:534:ASP:OD1	3:A:1001:HOH:O	2.15	0.64
1:B:308:THR:O	1:B:311:VAL:HG22	1.98	0.64
1:D:457:ASN:O	1:D:461:LYS:HE2	1.98	0.64
1:A:359:GLU:HG2	1:A:364:THR:HG22	1.80	0.64
1:B:359:GLU:CG	1:B:364:THR:HG22	2.28	0.64
1:B:525:PHE:HD1	1:B:526:ILE:HG22	1.61	0.64
1:D:334:LEU:HD22	1:D:441:ALA:HA	1.78	0.64
1:A:514:THR:HG21	1:A:545:PHE:CZ	2.33	0.63
1:B:334:LEU:HD21	1:B:441:ALA:HA	1.78	0.63
1:A:102:ASN:HD21	1:A:106:GLN:HB2	1.62	0.63
1:A:222:MET:HE2	1:A:222:MET:HA	1.78	0.63
1:A:598:ASN:HB3	1:A:601:SER:HB3	1.80	0.63
1:B:369:MET:SD	1:B:520:HIS:HB2	2.38	0.63
1:C:222:MET:HE2	1:C:222:MET:HA	1.81	0.63
1:A:381:GLU:O	1:A:385:LEU:HB2	1.97	0.63
1:A:334:LEU:HD22	1:A:441:ALA:HA	1.78	0.63
1:A:369:MET:SD	1:A:520:HIS:HB2	2.39	0.63
1:B:129:THR:HG23	1:B:133:ALA:CB	2.29	0.63
1:B:159:GLY:O	1:B:160:LYS:HB2	1.99	0.63
1:B:311:VAL:HG11	1:B:321:LEU:CD2	2.29	0.63
1:A:97:ARG:HD3	1:A:99:MET:HE3	1.80	0.63
1:B:378:LEU:O	1:B:382:ILE:HG12	1.99	0.63
1:D:144:GLU:N	1:D:144:GLU:OE2	2.30	0.63
1:A:358:MET:HE3	1:A:366:ARG:NH1	2.13	0.62
1:B:392:LEU:HD23	1:B:475:ILE:HG22	1.81	0.62
1:B:492:PHE:CE1	1:B:520:HIS:O	2.51	0.62
1:C:183:THR:HG22	1:C:185:SER:N	2.05	0.62
1:C:40:ASP:O	1:C:43:THR:HG22	2.00	0.62
1:A:334:LEU:HD23	1:A:442:PHE:H	1.63	0.62
1:A:342:ASP:OD2	3:A:977:HOH:O	2.15	0.62
1:A:494:VAL:O	1:A:494:VAL:HG12	1.95	0.62
1:D:57:LEU:HB3	1:D:59:LEU:HD22	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:359:GLU:CG	1:D:364:THR:HG22	2.29	0.62
1:A:538:MET:HG2	1:A:568:TYR:CD2	2.33	0.62
1:B:52:ALA:O	1:B:188:VAL:HG12	1.99	0.62
1:C:369:MET:SD	1:C:520:HIS:HB2	2.39	0.62
1:D:43:THR:OG1	1:D:45:ALA:HB3	1.99	0.62
1:D:183:THR:HG22	1:D:185:SER:N	2.04	0.62
1:D:222:MET:HE2	1:D:222:MET:HA	1.79	0.62
1:D:503:VAL:CG2	1:D:506:GLU:CG	2.52	0.62
1:B:500:ASN:C	1:B:502:LEU:H	2.06	0.62
1:B:586:LYS:O	1:B:586:LYS:CG	2.43	0.62
1:C:40:ASP:OD1	1:C:41:ALA:O	2.17	0.62
1:B:514:THR:C	1:B:516:GLN:H	2.08	0.62
1:C:503:VAL:HB	1:C:506:GLU:OE1	1.99	0.62
1:A:90:THR:OG1	1:A:93:LEU:HD22	1.99	0.62
1:B:168:GLN:HE22	1:B:299:MET:CG	2.12	0.62
1:C:57:LEU:HD12	1:C:59:LEU:HD21	1.81	0.62
1:C:543:LYS:O	1:C:543:LYS:CD	2.48	0.62
1:D:503:VAL:N	1:D:506:GLU:HB2	2.14	0.62
1:C:102:ASN:HD21	1:C:106:GLN:HB2	1.65	0.62
1:C:311:VAL:HG11	1:C:321:LEU:HD23	1.81	0.62
1:C:419:TYR:CD1	3:C:976:HOH:O	2.53	0.62
1:A:276:MET:CE	1:A:356:ARG:HB3	2.30	0.62
1:A:579:LEU:HD21	1:A:591:LEU:HD23	1.82	0.62
1:B:368:VAL:O	1:B:368:VAL:HG12	1.99	0.62
1:C:277:TYR:OH	1:C:356:ARG:HG3	2.00	0.62
1:C:502:LEU:HD12	1:C:506:GLU:HB3	1.81	0.62
1:A:361:VAL:CG2	1:A:362:PHE:CD1	2.83	0.62
1:D:514:THR:HG21	1:D:545:PHE:CZ	2.35	0.62
1:A:334:LEU:CD2	1:A:442:PHE:H	2.13	0.61
1:B:518:THR:O	1:B:522:TRP:HD1	1.83	0.61
1:A:609:TYR:O	1:A:613:ARG:HB2	2.00	0.61
1:C:359:GLU:CG	1:C:364:THR:HG22	2.30	0.61
1:D:308:THR:O	1:D:311:VAL:HG22	2.00	0.61
1:C:55:VAL:HG12	1:C:57:LEU:HD22	1.81	0.61
1:B:494:VAL:O	1:B:494:VAL:HG12	1.96	0.61
1:C:205:SER:O	1:C:222:MET:HE3	2.00	0.61
1:B:499:ILE:C	1:B:501:GLN:H	2.08	0.61
1:C:200:LEU:O	1:C:218:TYR:OH	2.16	0.61
1:A:297:GLY:O	1:A:308:THR:HG22	2.00	0.61
1:A:494:VAL:O	1:A:498:GLN:HG3	2.01	0.61
1:D:596:ALA:HB1	1:D:602:LYS:HG3	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:184:PRO:HB2	1:B:337:ASN:O	2.01	0.61
1:C:596:ALA:HB1	1:C:602:LYS:HG3	1.82	0.61
1:D:327:ALA:HB3	1:D:350:THR:HG23	1.83	0.61
1:C:174:ALA:HB3	1:C:182:ASP:OD1	2.01	0.61
1:A:206:ALA:HB1	1:A:221:SER:C	2.25	0.61
1:B:499:ILE:O	1:B:501:GLN:N	2.34	0.61
1:D:596:ALA:HA	1:D:602:LYS:CB	2.31	0.61
1:A:352:TYR:CZ	1:A:429:PHE:HE2	2.19	0.61
1:C:42:TYR:HA	1:C:121:LEU:CD2	2.30	0.61
1:C:411:VAL:O	1:C:415:LEU:HG	2.00	0.61
1:D:334:LEU:CD2	1:D:442:PHE:H	2.14	0.61
1:D:503:VAL:O	1:D:504:THR:CB	2.46	0.61
1:A:334:LEU:HD21	1:A:441:ALA:HA	1.83	0.60
1:D:301:ASN:HB2	1:D:304:LEU:O	2.01	0.60
1:D:500:ASN:N	1:D:500:ASN:ND2	2.39	0.60
1:A:426:ARG:O	1:A:430:ASP:HB2	2.00	0.60
1:C:243:MET:HG2	1:C:260:VAL:HG13	1.83	0.60
1:C:308:THR:O	1:C:311:VAL:HG22	2.01	0.60
1:C:324:HIS:CE1	1:C:350:THR:HG22	2.36	0.60
1:C:464:ASN:ND2	1:D:241:LYS:HB3	2.15	0.60
1:C:503:VAL:O	1:C:504:THR:CB	2.49	0.60
1:A:595:LEU:HD21	1:A:604:TRP:CE3	2.36	0.60
1:A:567:ASP:HB3	1:A:569:LYS:NZ	2.15	0.60
1:D:271:ASP:O	1:D:275:GLN:HG3	2.01	0.60
1:C:373:LEU:HD13	1:C:492:PHE:CZ	2.36	0.60
1:D:503:VAL:N	1:D:506:GLU:HG3	2.16	0.60
1:A:180:ILE:HG12	1:A:181:GLN:H	1.66	0.60
1:A:457:ASN:O	1:A:461:LYS:HE2	2.02	0.60
1:C:464:ASN:HD21	1:D:241:LYS:HD3	1.67	0.60
1:A:168:GLN:O	1:A:168:GLN:CG	2.34	0.60
1:A:536:GLN:OE1	1:A:536:GLN:CA	2.49	0.60
1:B:222:MET:HA	1:B:222:MET:HE2	1.83	0.60
1:B:284:ARG:HD3	1:B:286:ASP:OD2	2.00	0.60
1:B:507:LEU:C	1:B:507:LEU:CD2	2.75	0.60
1:D:40:ASP:OD1	1:D:41:ALA:O	2.20	0.60
1:D:303:ARG:NH1	3:D:974:HOH:O	2.33	0.60
1:D:582:ILE:HG13	1:D:584:ARG:H	1.67	0.60
1:D:569:LYS:HD2	1:D:570:GLU:H	1.67	0.60
1:A:290:LEU:HD21	1:A:306:PHE:CD2	2.37	0.59
1:A:489:SER:HB3	1:A:492:PHE:HB2	1.83	0.59
1:B:492:PHE:O	1:B:495:ILE:HB	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:522:TRP:O	1:C:526:ILE:CG1	2.39	0.59
1:D:199:ASP:C	1:D:200:LEU:HD12	2.27	0.59
1:C:283:GLY:HA2	3:C:988:HOH:O	2.02	0.59
1:D:129:THR:HG23	1:D:133:ALA:CB	2.32	0.59
1:D:159:GLY:O	1:D:160:LYS:HB2	2.02	0.59
1:A:368:VAL:HA	1:A:371:GLN:CG	2.26	0.59
1:C:43:THR:OG1	1:C:45:ALA:HB3	2.01	0.59
1:C:169:ASN:ND2	1:C:231:ILE:O	2.36	0.59
1:C:391:GLN:OE1	1:C:476:PHE:O	2.19	0.59
1:C:578:TYR:OH	1:C:587:LEU:HG	2.03	0.59
1:A:54:HIS:CE1	1:A:191:THR:HG23	2.38	0.59
1:C:276:MET:CE	1:C:356:ARG:HB3	2.32	0.59
1:D:42:TYR:HA	1:D:121:LEU:CD2	2.33	0.59
1:A:42:TYR:HA	1:A:121:LEU:CD2	2.32	0.59
1:B:494:VAL:O	1:B:494:VAL:CG1	2.49	0.59
1:C:421:GLU:OE1	1:C:426:ARG:HD3	2.03	0.59
1:D:97:ARG:HD3	1:D:99:MET:HE2	1.84	0.59
1:D:199:ASP:O	1:D:200:LEU:HD12	2.03	0.59
1:A:543:LYS:O	1:A:543:LYS:HD2	2.03	0.59
1:D:90:THR:OG1	1:D:93:LEU:HD22	2.02	0.59
1:D:598:ASN:HB3	1:D:601:SER:HB3	1.83	0.59
1:D:55:VAL:HG22	1:D:74:LEU:HD13	1.84	0.59
1:A:46:ASN:C	1:A:48:ASP:N	2.60	0.59
1:A:501:GLN:HG2	1:A:508:THR:CG2	2.33	0.59
1:B:42:TYR:HA	1:B:121:LEU:CD2	2.33	0.59
1:B:605:ALA:CB	1:B:628:LEU:HD11	2.33	0.59
1:C:288:LEU:HB2	1:C:304:LEU:HD11	1.85	0.59
1:A:288:LEU:HB2	1:A:304:LEU:HD11	1.85	0.59
1:B:54:HIS:CE1	1:B:191:THR:HG23	2.37	0.59
1:B:334:LEU:CD2	1:B:442:PHE:H	2.16	0.59
1:C:102:ASN:C	1:C:104:GLN:H	2.09	0.59
1:A:169:ASN:ND2	1:A:231:ILE:O	2.36	0.58
1:A:523:LEU:O	1:A:527:ASN:CG	2.44	0.58
1:A:582:ILE:HD11	1:A:584:ARG:HB3	1.85	0.58
1:C:457:ASN:O	1:C:461:LYS:HE2	2.03	0.58
1:C:494:VAL:O	1:C:494:VAL:CG1	2.50	0.58
1:C:582:ILE:HG13	1:C:584:ARG:H	1.68	0.58
1:B:492:PHE:HE1	1:B:520:HIS:O	1.86	0.58
1:D:364:THR:O	1:D:368:VAL:HG13	2.03	0.58
1:B:503:VAL:HG23	1:B:506:GLU:CB	2.33	0.58
1:C:168:GLN:O	1:C:168:GLN:CG	2.44	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:249:ILE:HD12	1:D:260:VAL:HG22	1.85	0.58
1:D:38:LEU:HB2	1:D:39:THR:HG22	1.84	0.58
1:C:206:ALA:HB1	1:C:221:SER:C	2.29	0.58
1:C:368:VAL:HA	1:C:371:GLN:CG	2.27	0.58
1:D:494:VAL:O	1:D:494:VAL:HG12	1.98	0.58
1:A:320:ASN:HB3	1:A:358:MET:HE2	1.85	0.58
1:B:57:LEU:HD12	1:B:59:LEU:HD21	1.85	0.58
1:D:503:VAL:H	1:D:506:GLU:HB2	1.67	0.58
1:A:536:GLN:OE1	1:A:536:GLN:O	2.22	0.58
1:B:461:LYS:HE3	1:B:462:TYR:CE2	2.39	0.58
1:C:370:GLU:HG2	1:C:520:HIS:CD2	2.39	0.58
1:D:361:VAL:CG2	1:D:362:PHE:CD1	2.84	0.58
1:D:503:VAL:CA	1:D:506:GLU:CG	2.68	0.58
1:A:359:GLU:CG	1:A:364:THR:HG22	2.34	0.58
1:A:364:THR:O	1:A:368:VAL:HG13	2.04	0.58
1:B:42:TYR:CZ	1:B:399:ARG:O	2.55	0.58
1:B:43:THR:OG1	1:B:45:ALA:HB3	2.04	0.58
1:B:335:VAL:HG13	1:B:440:HIS:HB3	1.84	0.58
1:C:274:GLU:HG2	1:C:279:LYS:HA	1.86	0.58
1:C:373:LEU:HD13	1:C:492:PHE:CE2	2.39	0.58
1:D:180:ILE:HG12	1:D:181:GLN:H	1.67	0.58
1:C:254:TYR:CE2	1:C:255:ILE:HB	2.39	0.58
1:C:481:PRO:HD2	1:C:484:ALA:HB2	1.86	0.58
1:D:276:MET:CE	1:D:356:ARG:HB3	2.33	0.58
1:D:488:THR:HG22	1:D:488:THR:O	2.04	0.58
1:A:500:ASN:N	1:A:500:ASN:ND2	2.38	0.57
1:B:276:MET:CE	1:B:356:ARG:HB3	2.34	0.57
1:C:97:ARG:NH1	1:C:99:MET:CE	2.66	0.57
1:C:368:VAL:HG12	1:C:371:GLN:NE2	2.18	0.57
1:D:174:ALA:HB3	1:D:182:ASP:OD1	2.04	0.57
1:D:584:ARG:HD3	1:D:587:LEU:HD22	1.86	0.57
1:B:174:ALA:HB3	1:B:182:ASP:OD1	2.03	0.57
1:B:368:VAL:O	1:B:368:VAL:HG13	2.01	0.57
1:C:334:LEU:HD21	1:C:441:ALA:HA	1.85	0.57
1:C:507:LEU:CD2	1:C:508:THR:HG22	2.34	0.57
1:B:168:GLN:O	1:B:168:GLN:CG	2.44	0.57
1:B:298:GLY:C	1:B:325:GLU:OE2	2.47	0.57
1:C:284:ARG:HD3	1:C:286:ASP:OD2	2.03	0.57
1:C:320:ASN:HB3	1:C:358:MET:HE2	1.86	0.57
1:C:378:LEU:O	1:C:382:ILE:HG12	2.05	0.57
1:D:596:ALA:HA	1:D:602:LYS:HB2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:101:LYS:HB3	1:D:101:LYS:HZ3	1.69	0.57
1:A:277:TYR:OH	1:A:356:ARG:HG3	2.05	0.57
1:A:582:ILE:HG13	1:A:584:ARG:H	1.68	0.57
1:C:492:PHE:CD2	1:C:524:HIS:CD2	2.93	0.57
1:B:524:HIS:O	1:B:525:PHE:C	2.45	0.57
1:D:335:VAL:HG13	1:D:440:HIS:HB3	1.85	0.57
1:B:90:THR:OG1	1:B:93:LEU:HD22	2.05	0.57
1:C:594:GLU:HA	1:C:597:LYS:HD3	1.87	0.57
1:A:55:VAL:HG22	1:A:74:LEU:HD13	1.87	0.57
1:A:341:ARG:HH11	1:A:395:ASP:HA	1.70	0.57
1:B:332:GLY:HA2	1:B:346:ASN:OD1	2.05	0.57
1:D:334:LEU:HD23	1:D:442:PHE:H	1.70	0.57
1:A:332:GLY:C	1:A:336:THR:HG22	2.30	0.57
1:A:337:ASN:ND2	1:A:337:ASN:H	2.02	0.57
1:A:421:GLU:OE1	1:A:426:ARG:HD3	2.05	0.57
1:C:392:LEU:HD23	1:C:475:ILE:HG22	1.86	0.57
1:D:55:VAL:HG12	1:D:57:LEU:HD22	1.85	0.57
1:D:152:LEU:HD13	1:D:291:PRO:HG3	1.86	0.57
1:D:392:LEU:HD23	1:D:475:ILE:HG22	1.86	0.57
1:D:512:LEU:HB3	1:D:513:PRO:CD	2.35	0.57
1:A:568:TYR:O	1:A:570:GLU:N	2.38	0.57
1:B:332:GLY:C	1:B:336:THR:HG22	2.29	0.57
1:C:504:THR:O	1:C:505:ASP:HB2	2.05	0.57
1:D:107:TRP:NE1	3:D:706:HOH:O	2.27	0.57
1:D:324:HIS:CE1	1:D:350:THR:HG22	2.39	0.57
1:A:131:LEU:HD12	3:A:1016:HOH:O	2.05	0.56
1:D:97:ARG:HB2	3:D:709:HOH:O	2.04	0.56
1:A:522:TRP:O	1:A:526:ILE:HG13	2.05	0.56
1:B:301:ASN:HB2	1:B:304:LEU:O	2.05	0.56
1:A:336:THR:O	1:A:444:SER:HA	2.05	0.56
1:A:533:LEU:HD23	1:A:538:MET:HE3	1.87	0.56
1:B:290:LEU:HD21	1:B:306:PHE:CD2	2.38	0.56
1:C:199:ASP:O	1:C:200:LEU:HD12	2.05	0.56
1:C:283:GLY:N	3:C:988:HOH:O	2.38	0.56
1:C:361:VAL:CG2	1:C:362:PHE:CD1	2.86	0.56
1:D:57:LEU:HD12	1:D:59:LEU:HD21	1.86	0.56
1:D:311:VAL:HG11	1:D:321:LEU:CD2	2.35	0.56
1:D:373:LEU:HD13	1:D:492:PHE:CZ	2.40	0.56
1:D:503:VAL:N	1:D:506:GLU:CB	2.67	0.56
1:A:159:GLY:O	1:A:160:LYS:HB2	2.04	0.56
1:B:284:ARG:HG3	1:B:285:TYR:N	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:373:LEU:O	1:C:377:ASP:OD1	2.24	0.56
1:D:142:SER:OG	3:D:763:HOH:O	2.09	0.56
1:D:205:SER:O	1:D:222:MET:HE3	2.05	0.56
1:A:499:ILE:CG1	1:A:500:ASN:ND2	2.69	0.56
1:C:512:LEU:HB3	1:C:513:PRO:HD3	1.87	0.56
1:A:201:LEU:HD23	1:A:238:LEU:HB2	1.87	0.56
1:C:54:HIS:CE1	1:C:191:THR:HG23	2.40	0.56
1:C:271:ASP:O	1:C:275:GLN:HG3	2.06	0.56
1:C:519:LEU:HD13	1:C:519:LEU:C	2.29	0.56
1:D:514:THR:C	1:D:516:GLN:H	2.13	0.56
1:A:40:ASP:OD1	1:A:41:ALA:O	2.23	0.56
1:C:206:ALA:O	1:C:303:ARG:NH1	2.38	0.56
1:B:297:GLY:O	1:B:308:THR:HG22	2.06	0.56
1:C:294:PHE:CD1	1:C:295:PRO:HD2	2.41	0.56
1:B:129:THR:HG23	1:B:133:ALA:HB2	1.88	0.56
1:C:55:VAL:HG22	1:C:74:LEU:HD13	1.88	0.56
1:A:594:GLU:HA	1:A:597:LYS:HD3	1.88	0.56
1:C:593:LYS:HE2	1:C:627:VAL:HG11	1.88	0.56
1:D:153:SER:OG	1:D:156:GLN:HG3	2.06	0.56
1:D:332:GLY:HA2	1:D:346:ASN:OD1	2.06	0.56
1:C:90:THR:OG1	1:C:93:LEU:HD22	2.06	0.55
1:C:245:HIS:HD2	3:C:987:HOH:O	1.89	0.55
1:C:502:LEU:CD1	1:C:506:GLU:CB	2.77	0.55
1:D:243:MET:HG2	1:D:260:VAL:HG13	1.88	0.55
1:D:274:GLU:HG2	1:D:279:LYS:HA	1.87	0.55
1:D:494:VAL:O	1:D:494:VAL:CG1	2.48	0.55
1:D:496:ASP:O	1:D:499:ILE:HG12	2.06	0.55
1:D:502:LEU:CD1	1:D:507:LEU:HB2	2.36	0.55
1:B:529:LEU:C	1:B:529:LEU:CD2	2.79	0.55
1:D:337:ASN:ND2	1:D:337:ASN:H	2.03	0.55
1:D:504:THR:C	1:D:506:GLU:HG2	2.30	0.55
1:A:159:GLY:C	1:A:161:GLU:H	2.15	0.55
1:C:512:LEU:HB3	1:C:513:PRO:HD2	1.89	0.55
1:D:46:ASN:C	1:D:48:ASP:N	2.59	0.55
1:B:169:ASN:ND2	1:B:231:ILE:O	2.40	0.55
1:B:180:ILE:HG12	1:B:181:GLN:H	1.70	0.55
1:B:288:LEU:CB	1:B:304:LEU:HD11	2.37	0.55
1:B:547:LEU:H	1:B:547:LEU:CD1	2.17	0.55
1:C:529:LEU:HD23	1:C:562:LEU:HD21	1.88	0.55
1:D:405:PHE:HA	3:D:750:HOH:O	2.07	0.55
1:A:494:VAL:O	1:A:494:VAL:CG1	2.48	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:311:VAL:HG11	1:B:321:LEU:HD23	1.89	0.55
1:B:542:ASP:O	1:B:546:ASP:HA	2.07	0.55
1:C:65:LYS:O	1:C:144:GLU:OE1	2.25	0.55
1:C:129:THR:HG23	1:C:133:ALA:CB	2.36	0.55
1:D:52:ALA:O	1:D:188:VAL:HG12	2.07	0.55
1:D:557:HIS:HE1	1:D:590:PRO:HG2	1.71	0.55
1:A:298:GLY:C	1:A:325:GLU:OE2	2.49	0.55
1:B:324:HIS:CE1	1:B:350:THR:HG22	2.42	0.55
1:B:494:VAL:O	1:B:498:GLN:HG3	2.07	0.55
1:B:543:LYS:O	1:B:543:LYS:HD2	2.06	0.55
1:C:334:LEU:CD2	1:C:442:PHE:H	2.20	0.55
1:D:503:VAL:N	1:D:506:GLU:CG	2.70	0.55
1:D:284:ARG:HG3	1:D:285:TYR:N	2.21	0.55
1:D:492:PHE:O	1:D:495:ILE:HB	2.06	0.55
1:A:288:LEU:CB	1:A:304:LEU:HD11	2.36	0.55
1:B:208:ASN:OD1	1:B:208:ASN:C	2.50	0.55
1:B:503:VAL:CG2	1:B:506:GLU:CG	2.59	0.55
1:C:162:LYS:HE3	1:C:199:ASP:HB3	1.88	0.55
1:C:572:TYR:N	1:C:573:PRO:HD2	2.22	0.55
1:A:55:VAL:HG12	1:A:57:LEU:HD22	1.89	0.54
1:A:347:GLU:OE1	1:A:347:GLU:CA	2.55	0.54
1:A:373:LEU:HD13	1:A:492:PHE:CZ	2.42	0.54
1:C:130:PRO:O	1:C:131:LEU:C	2.48	0.54
1:D:578:TYR:OH	1:D:587:LEU:HG	2.08	0.54
1:D:596:ALA:CB	1:D:602:LYS:HG3	2.38	0.54
1:B:288:LEU:HB2	1:B:304:LEU:HD11	1.89	0.54
1:B:509:LEU:CD2	1:B:511:GLN:HB2	2.36	0.54
1:C:46:ASN:C	1:C:48:ASP:N	2.60	0.54
1:C:461:LYS:HE3	1:C:462:TYR:CE2	2.42	0.54
1:D:254:TYR:CE2	1:D:255:ILE:HB	2.42	0.54
1:A:514:THR:C	1:A:516:GLN:H	2.15	0.54
1:A:605:ALA:O	1:A:608:VAL:HG22	2.06	0.54
1:B:226:ILE:HD12	1:B:230:LEU:HB2	1.89	0.54
1:D:543:LYS:O	1:D:543:LYS:CD	2.56	0.54
1:C:496:ASP:O	1:C:499:ILE:HG12	2.06	0.54
1:D:106:GLN:O	1:D:108:VAL:HG13	2.07	0.54
1:D:328:HIS:HE1	1:D:347:GLU:OE1	1.91	0.54
1:D:542:ASP:O	1:D:546:ASP:HA	2.08	0.54
1:A:358:MET:CE	1:A:366:ARG:HH12	2.20	0.54
1:D:290:LEU:HD21	1:D:306:PHE:CD2	2.40	0.54
1:D:332:GLY:C	1:D:336:THR:HG22	2.32	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:347:GLU:HB3	1:B:410:TYR:CD2	2.41	0.54
1:C:42:TYR:OH	1:C:399:ARG:O	2.17	0.54
1:D:494:VAL:O	1:D:498:GLN:HG3	2.06	0.54
1:A:540:ASN:O	1:A:544:ALA:CB	2.56	0.54
1:B:205:SER:O	1:B:222:MET:HE3	2.07	0.54
1:C:298:GLY:C	1:C:325:GLU:OE2	2.51	0.54
1:D:206:ALA:HB1	1:D:221:SER:C	2.32	0.54
1:A:578:TYR:OH	1:A:587:LEU:HG	2.07	0.54
1:B:501:GLN:O	1:B:502:LEU:HB2	2.08	0.54
1:B:509:LEU:N	1:B:509:LEU:HD23	2.22	0.54
1:B:584:ARG:HD3	1:B:587:LEU:HD22	1.90	0.54
1:B:344:TRP:HH2	1:B:450:PHE:CE2	2.25	0.54
1:C:265:ASP:O	1:C:268:ALA:HB3	2.08	0.54
1:C:488:THR:O	1:C:488:THR:HG22	2.07	0.54
1:C:542:ASP:O	1:C:546:ASP:HA	2.08	0.54
1:D:102:ASN:C	1:D:104:GLN:H	2.15	0.54
1:A:205:SER:O	1:A:222:MET:HE3	2.07	0.54
1:A:498:GLN:C	1:A:500:ASN:N	2.65	0.54
1:C:494:VAL:O	1:C:498:GLN:HG3	2.06	0.54
1:C:585:ARG:O	1:C:587:LEU:N	2.38	0.54
1:D:524:HIS:O	1:D:528:ASN:HB2	2.07	0.54
1:A:57:LEU:HD12	1:A:59:LEU:HD21	1.90	0.53
1:A:531:VAL:O	1:A:531:VAL:HG12	2.08	0.53
1:B:320:ASN:HB3	1:B:358:MET:HE2	1.90	0.53
1:B:514:THR:C	1:B:516:GLN:N	2.66	0.53
1:B:582:ILE:HD11	1:B:587:LEU:HD23	1.90	0.53
1:C:341:ARG:HH11	1:C:395:ASP:HA	1.73	0.53
1:A:533:LEU:O	1:A:536:GLN:HB2	2.08	0.53
1:B:334:LEU:HD23	1:B:442:PHE:H	1.73	0.53
1:B:421:GLU:OE1	1:B:426:ARG:HD3	2.08	0.53
1:B:131:LEU:HD12	3:B:805:HOH:O	2.08	0.53
1:B:243:MET:HG2	1:B:260:VAL:HG13	1.90	0.53
1:C:595:LEU:HD21	1:C:604:TRP:CE3	2.42	0.53
1:D:596:ALA:HA	1:D:602:LYS:HA	1.91	0.53
1:A:308:THR:O	1:A:311:VAL:HG22	2.09	0.53
1:A:481:PRO:HD2	1:A:484:ALA:HB2	1.90	0.53
1:A:503:VAL:N	1:A:506:GLU:HB3	2.21	0.53
1:B:91:ARG:NH2	1:B:175:ARG:HD2	2.24	0.53
1:C:368:VAL:HG12	1:C:371:GLN:HE21	1.73	0.53
1:C:512:LEU:CB	1:C:513:PRO:CD	2.78	0.53
1:D:284:ARG:HD3	1:D:286:ASP:OD2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:284:ARG:NH1	1:D:286:ASP:OD1	2.35	0.53
1:C:152:LEU:HD13	1:C:291:PRO:HG3	1.90	0.53
1:C:300:GLU:O	1:C:300:GLU:HG2	2.08	0.53
1:C:498:GLN:HB3	1:C:512:LEU:CD2	2.39	0.53
1:C:514:THR:C	1:C:516:GLN:H	2.16	0.53
1:A:368:VAL:CA	1:A:371:GLN:HG3	2.30	0.53
1:B:201:LEU:HD23	1:B:238:LEU:HB2	1.90	0.53
1:B:378:LEU:HD21	1:B:480:LEU:HD21	1.91	0.53
1:D:288:LEU:HB2	1:D:304:LEU:HD11	1.90	0.53
1:D:421:GLU:OE1	1:D:426:ARG:HD3	2.08	0.53
1:A:405:PHE:HA	3:A:719:HOH:O	2.08	0.53
1:B:373:LEU:O	1:B:377:ASP:OD1	2.27	0.53
1:C:284:ARG:HG3	1:C:285:TYR:N	2.23	0.53
1:C:344:TRP:HH2	1:C:450:PHE:CE2	2.27	0.53
1:D:159:GLY:C	1:D:161:GLU:H	2.16	0.53
1:D:226:ILE:HD12	1:D:230:LEU:HB2	1.91	0.53
1:A:263:PHE:CD1	1:A:322:ILE:HG13	2.43	0.53
1:A:596:ALA:HA	1:A:602:LYS:CB	2.38	0.53
1:B:42:TYR:CD2	1:B:121:LEU:HD21	2.43	0.53
1:B:311:VAL:HG11	1:B:321:LEU:HD22	1.91	0.53
1:B:361:VAL:CG2	1:B:362:PHE:CD1	2.90	0.53
1:B:573:PRO:O	1:B:576:ALA:HB3	2.09	0.53
1:C:369:MET:HG3	1:C:492:PHE:CE1	2.44	0.53
1:D:184:PRO:HG3	1:D:340:TRP:CZ2	2.43	0.53
1:A:102:ASN:C	1:A:104:GLN:H	2.17	0.53
1:A:507:LEU:C	1:A:507:LEU:HD23	2.34	0.53
1:A:533:LEU:O	1:A:536:GLN:CB	2.57	0.53
1:A:485:PRO:HA	3:A:951:HOH:O	2.09	0.53
1:A:542:ASP:O	1:A:546:ASP:N	2.42	0.53
1:B:224:GLN:NE2	1:B:281:ARG:O	2.42	0.53
1:B:318:LEU:HD21	1:B:552:ASN:ND2	2.23	0.53
1:C:180:ILE:HG12	1:C:181:GLN:N	2.23	0.53
1:C:335:VAL:HG13	1:C:440:HIS:HB3	1.90	0.53
1:D:224:GLN:NE2	1:D:281:ARG:O	2.41	0.53
1:B:103:SER:N	3:B:795:HOH:O	2.22	0.52
1:B:159:GLY:C	1:B:161:GLU:H	2.17	0.52
1:A:324:HIS:CE1	1:A:350:THR:HG22	2.44	0.52
1:A:461:LYS:HE3	1:A:462:TYR:CE2	2.44	0.52
1:A:585:ARG:C	1:A:587:LEU:H	2.18	0.52
1:B:277:TYR:OH	1:B:356:ARG:HG3	2.09	0.52
1:C:239:GLU:HB2	1:C:256:LEU:HD22	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:284:ARG:HG3	1:A:285:TYR:N	2.24	0.52
1:B:542:ASP:HB2	1:B:559:TRP:HZ2	1.74	0.52
1:C:557:HIS:HE1	1:C:590:PRO:HG2	1.74	0.52
1:A:263:PHE:C	1:A:265:ASP:H	2.17	0.52
1:A:327:ALA:HB3	1:A:350:THR:HG23	1.91	0.52
1:B:249:ILE:HD12	1:B:260:VAL:HG22	1.90	0.52
1:B:254:TYR:CG	1:B:255:ILE:N	2.77	0.52
1:B:591:LEU:O	1:B:595:LEU:HB2	2.09	0.52
1:C:40:ASP:OD1	1:C:40:ASP:C	2.53	0.52
1:C:159:GLY:O	1:C:160:LYS:HB2	2.08	0.52
1:D:277:TYR:CE1	1:D:353:VAL:HG22	2.45	0.52
1:A:43:THR:OG1	1:A:45:ALA:HB3	2.10	0.52
1:B:274:GLU:HG2	1:B:279:LYS:HA	1.92	0.52
1:B:457:ASN:O	1:B:461:LYS:HE2	2.09	0.52
1:B:585:ARG:C	1:B:587:LEU:H	2.18	0.52
1:C:310:THR:HG21	1:C:582:ILE:HD12	1.91	0.52
1:D:129:THR:HG23	1:D:133:ALA:HB3	1.90	0.52
1:D:582:ILE:HD11	1:D:587:LEU:HD23	1.90	0.52
1:A:512:LEU:HB3	1:A:513:PRO:CD	2.40	0.52
1:B:295:PRO:HD3	1:B:617:HIS:HB2	1.91	0.52
1:C:378:LEU:HD21	1:C:480:LEU:HD21	1.90	0.52
1:C:386:ASP:O	1:C:388:SER:N	2.38	0.52
1:C:557:HIS:CE1	1:C:590:PRO:HG2	2.45	0.52
1:C:582:ILE:HD11	1:C:587:LEU:HD23	1.90	0.52
1:D:214:ARG:NH1	3:D:705:HOH:O	2.41	0.52
1:A:337:ASN:H	1:A:337:ASN:HD22	1.58	0.52
1:B:336:THR:O	1:B:444:SER:HA	2.10	0.52
1:B:373:LEU:HD13	1:B:492:PHE:HZ	1.69	0.52
1:C:101:LYS:HD2	1:C:107:TRP:CZ2	2.45	0.52
1:C:463:PRO:O	1:C:464:ASN:HB2	2.08	0.52
1:D:97:ARG:HH11	1:D:99:MET:CE	2.23	0.52
1:D:341:ARG:HH11	1:D:395:ASP:HA	1.75	0.52
1:A:596:ALA:HB1	1:A:602:LYS:HG3	1.92	0.52
1:B:598:ASN:HB3	1:B:601:SER:HB3	1.91	0.52
1:C:585:ARG:C	1:C:587:LEU:H	2.18	0.52
1:A:205:SER:OG	1:A:301:ASN:HB3	2.10	0.52
1:A:206:ALA:HA	1:A:222:MET:CE	2.40	0.52
1:B:426:ARG:O	1:B:430:ASP:HB2	2.09	0.52
1:B:459:THR:HG21	1:B:471:ILE:HD11	1.92	0.52
1:D:294:PHE:HE2	1:D:298:GLY:HA2	1.75	0.52
1:D:300:GLU:HG2	1:D:300:GLU:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:326:LEU:HD22	1:D:330:TRP:HZ3	1.74	0.52
1:D:467:SER:O	1:D:469:ASN:N	2.43	0.52
1:C:208:ASN:OD1	1:C:208:ASN:C	2.52	0.52
1:D:527:ASN:OD1	1:D:558:ALA:HB1	2.09	0.52
1:A:271:ASP:O	1:A:275:GLN:HG3	2.09	0.51
1:A:326:LEU:HD22	1:A:330:TRP:HZ3	1.75	0.51
1:B:596:ALA:HA	1:B:602:LYS:CB	2.40	0.51
1:C:90:THR:HG23	1:C:91:ARG:N	2.24	0.51
1:C:263:PHE:C	1:C:265:ASP:H	2.17	0.51
1:A:168:GLN:HE22	1:A:299:MET:CG	2.22	0.51
1:A:226:ILE:HD12	1:A:230:LEU:HB2	1.91	0.51
1:A:347:GLU:OE1	1:A:347:GLU:HA	2.08	0.51
1:A:496:ASP:O	1:A:499:ILE:HG12	2.09	0.51
1:A:540:ASN:O	1:A:544:ALA:HB3	2.10	0.51
1:B:130:PRO:O	1:B:131:LEU:C	2.52	0.51
1:B:557:HIS:HE1	1:B:590:PRO:HG2	1.76	0.51
1:C:159:GLY:C	1:C:161:GLU:H	2.18	0.51
1:C:180:ILE:CG1	1:C:181:GLN:H	2.22	0.51
1:D:378:LEU:HD13	1:D:411:VAL:HB	1.92	0.51
1:A:276:MET:HE3	1:A:356:ARG:HB3	1.91	0.51
1:C:168:GLN:NE2	1:C:299:MET:CG	2.73	0.51
1:D:358:MET:HE3	1:D:366:ARG:HH12	1.69	0.51
1:D:585:ARG:C	1:D:587:LEU:H	2.17	0.51
1:A:277:TYR:CE1	1:A:353:VAL:HG22	2.46	0.51
1:B:55:VAL:HG22	1:B:74:LEU:HD13	1.92	0.51
1:C:327:ALA:HB3	1:C:350:THR:HG23	1.92	0.51
1:C:530:PRO:C	1:C:532:ASP:H	2.19	0.51
1:D:295:PRO:HG2	1:D:296:PHE:CD1	2.36	0.51
1:A:228:PRO:C	1:A:230:LEU:H	2.18	0.51
1:A:311:VAL:HG11	1:A:321:LEU:CD2	2.41	0.51
1:C:435:GLU:O	1:C:439:SER:OG	2.27	0.51
1:D:344:TRP:HH2	1:D:450:PHE:CE2	2.29	0.51
1:A:208:ASN:OD1	1:A:208:ASN:C	2.53	0.51
1:B:46:ASN:C	1:B:48:ASP:N	2.61	0.51
1:C:52:ALA:O	1:C:188:VAL:HG12	2.10	0.51
1:C:106:GLN:O	1:C:108:VAL:HG13	2.11	0.51
1:C:263:PHE:CD1	1:C:322:ILE:HG13	2.46	0.51
1:C:596:ALA:HA	1:C:602:LYS:HA	1.93	0.51
1:D:40:ASP:HB3	1:D:47:TYR:OH	2.10	0.51
1:D:263:PHE:CD1	1:D:322:ILE:HG13	2.46	0.51
1:D:272:LYS:HG3	1:D:361:VAL:HG12	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:297:GLY:O	1:D:308:THR:HG22	2.11	0.51
1:D:336:THR:O	1:D:444:SER:HA	2.10	0.51
1:D:428:ARG:HD3	3:D:956:HOH:O	2.02	0.51
1:D:254:TYR:CG	1:D:255:ILE:N	2.77	0.51
1:A:394:ILE:HD12	3:A:724:HOH:O	2.11	0.51
1:B:557:HIS:CE1	1:B:590:PRO:HG2	2.46	0.51
1:C:295:PRO:HG2	1:C:296:PHE:CD1	2.39	0.51
1:D:548:THR:OG1	1:D:571:VAL:HG12	2.11	0.51
1:A:249:ILE:HD12	1:A:260:VAL:HG22	1.93	0.51
1:A:284:ARG:NH1	1:A:286:ASP:OD1	2.40	0.51
1:C:454:LEU:HD23	1:C:454:LEU:O	2.10	0.51
1:A:392:LEU:HD23	1:A:475:ILE:CG2	2.40	0.51
1:B:529:LEU:HD23	1:B:530:PRO:HD2	1.93	0.51
1:D:38:LEU:CB	1:D:39:THR:HG22	2.41	0.51
1:D:373:LEU:O	1:D:377:ASP:OD1	2.28	0.51
1:D:591:LEU:O	1:D:595:LEU:HB2	2.11	0.51
1:C:57:LEU:HB3	1:C:59:LEU:HD22	1.94	0.50
1:C:197:ASP:C	1:C:198:LYS:O	2.51	0.50
1:C:328:HIS:HE1	1:C:347:GLU:OE1	1.94	0.50
1:A:162:LYS:HD3	1:A:200:LEU:CD1	2.41	0.50
1:C:144:GLU:N	1:C:144:GLU:OE2	2.30	0.50
1:C:336:THR:O	1:C:444:SER:HA	2.10	0.50
1:D:271:ASP:HA	3:D:951:HOH:O	2.10	0.50
1:A:373:LEU:O	1:A:377:ASP:OD1	2.30	0.50
1:A:548:THR:OG1	1:A:571:VAL:HG12	2.11	0.50
1:C:317:SER:OG	1:C:318:LEU:HD22	2.11	0.50
1:C:563:SER:CB	1:C:571:VAL:HG21	2.41	0.50
1:D:277:TYR:CD1	1:D:353:VAL:HG13	2.46	0.50
1:D:428:ARG:HG2	3:D:956:HOH:O	2.11	0.50
1:A:42:TYR:CE2	1:A:401:PRO:CG	2.94	0.50
1:B:205:SER:HB2	1:B:302:PRO:HG2	1.93	0.50
1:C:455:LYS:HA	1:C:459:THR:HB	1.94	0.50
1:C:514:THR:C	1:C:516:GLN:N	2.69	0.50
1:D:502:LEU:CD1	1:D:506:GLU:O	2.30	0.50
1:D:605:ALA:CB	1:D:628:LEU:HD11	2.42	0.50
1:A:129:THR:HG23	1:A:133:ALA:CB	2.41	0.50
1:A:148:GLY:CA	1:A:173:HIS:HB3	2.41	0.50
1:B:153:SER:O	1:B:157:THR:HG23	2.12	0.50
1:B:180:ILE:CG1	1:B:181:GLN:H	2.25	0.50
1:B:378:LEU:HD13	1:B:411:VAL:HB	1.92	0.50
1:B:392:LEU:HD23	1:B:475:ILE:CG2	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:596:ALA:CB	1:C:602:LYS:HG3	2.41	0.50
1:D:364:THR:HA	1:D:367:ALA:HB3	1.94	0.50
1:D:504:THR:O	1:D:506:GLU:OE2	2.30	0.50
1:A:97:ARG:NH1	1:A:99:MET:CE	2.68	0.50
1:A:503:VAL:HG23	1:A:506:GLU:HG2	1.93	0.50
1:A:584:ARG:HD3	1:A:587:LEU:HD22	1.93	0.50
1:B:162:LYS:HD3	1:B:200:LEU:CD1	2.41	0.50
1:C:332:GLY:HA2	1:C:346:ASN:OD1	2.12	0.50
1:D:467:SER:C	1:D:469:ASN:H	2.19	0.50
1:A:489:SER:O	1:A:490:ASN:C	2.52	0.50
1:A:605:ALA:CB	1:A:628:LEU:HD11	2.42	0.50
1:B:206:ALA:O	1:B:303:ARG:NH1	2.45	0.50
1:B:397:LYS:HA	3:B:798:HOH:O	2.12	0.50
1:B:500:ASN:C	1:B:502:LEU:N	2.68	0.50
1:D:489:SER:O	1:D:490:ASN:C	2.53	0.50
1:A:129:THR:HG23	1:A:133:ALA:HB3	1.94	0.50
1:A:274:GLU:HG2	1:A:279:LYS:HA	1.94	0.50
1:B:129:THR:HG23	1:B:133:ALA:HB3	1.93	0.50
1:C:46:ASN:O	1:C:48:ASP:N	2.45	0.50
1:C:129:THR:HG23	1:C:133:ALA:HB2	1.93	0.50
1:C:162:LYS:HD3	1:C:200:LEU:CD1	2.41	0.50
1:D:594:GLU:HA	1:D:597:LYS:HD3	1.94	0.50
1:B:57:LEU:HB3	1:B:59:LEU:HD22	1.93	0.50
1:C:143:THR:HB	1:C:144:GLU:OE2	2.11	0.50
1:C:596:ALA:HA	1:C:602:LYS:CA	2.41	0.50
1:D:481:PRO:HD2	1:D:484:ALA:HB2	1.94	0.50
1:B:184:PRO:HG3	1:B:340:TRP:CZ2	2.47	0.49
1:B:294:PHE:CD1	1:B:295:PRO:HD2	2.47	0.49
1:B:500:ASN:N	1:B:500:ASN:HD22	2.10	0.49
1:D:54:HIS:CE1	1:D:191:THR:HG23	2.47	0.49
1:D:416:PHE:CD1	1:D:416:PHE:O	2.65	0.49
1:A:54:HIS:HE1	1:A:191:THR:HG23	1.75	0.49
1:A:467:SER:C	1:A:469:ASN:H	2.19	0.49
1:B:206:ALA:HA	1:B:222:MET:CE	2.42	0.49
1:B:270:ILE:HG22	1:B:270:ILE:O	2.12	0.49
1:C:290:LEU:HD21	1:C:306:PHE:CD2	2.40	0.49
1:D:298:GLY:C	1:D:325:GLU:OE2	2.55	0.49
1:D:310:THR:HG21	1:D:582:ILE:HD12	1.94	0.49
1:D:414:GLN:O	1:D:418:MET:HG3	2.11	0.49
1:D:510:GLU:O	1:D:512:LEU:N	2.37	0.49
1:A:153:SER:HG	1:A:155:GLU:HG2	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:263:PHE:C	1:B:265:ASP:H	2.19	0.49
1:B:269:MET:HE1	1:B:319:VAL:CG1	2.42	0.49
1:B:582:ILE:HG13	1:B:584:ARG:H	1.78	0.49
1:D:326:LEU:CD2	1:D:326:LEU:O	2.60	0.49
1:A:239:GLU:HB2	1:A:256:LEU:HD22	1.94	0.49
1:A:269:MET:HE1	1:A:319:VAL:CG1	2.42	0.49
1:B:503:VAL:O	1:B:504:THR:CG2	2.61	0.49
1:B:578:TYR:OH	1:B:587:LEU:HG	2.11	0.49
1:C:301:ASN:HB2	1:C:304:LEU:O	2.12	0.49
1:C:396:LEU:O	1:C:399:ARG:NE	2.37	0.49
1:C:584:ARG:HD3	1:C:587:LEU:HD22	1.93	0.49
1:D:180:ILE:CG1	1:D:181:GLN:H	2.25	0.49
1:D:337:ASN:H	1:D:337:ASN:HD22	1.61	0.49
1:D:613:ARG:HB3	1:D:614:PRO:HD3	1.94	0.49
1:C:288:LEU:CB	1:C:304:LEU:HD11	2.43	0.49
1:D:277:TYR:OH	1:D:356:ARG:HG3	2.13	0.49
1:D:428:ARG:CG	3:D:956:HOH:O	2.60	0.49
1:A:596:ALA:HA	1:A:602:LYS:HB2	1.94	0.49
1:B:44:TYR:CD2	1:B:124:LYS:HB2	2.48	0.49
1:B:62:ASP:C	1:B:62:ASP:OD1	2.56	0.49
1:B:326:LEU:HD22	1:B:330:TRP:HZ3	1.78	0.49
1:B:580:LYS:HA	1:B:612:ALA:CB	2.39	0.49
1:C:153:SER:O	1:C:157:THR:HG23	2.13	0.49
1:A:57:LEU:HB3	1:A:59:LEU:HD22	1.93	0.49
1:A:284:ARG:HD3	1:A:286:ASP:OD2	2.13	0.49
1:C:504:THR:O	1:C:504:THR:OG1	2.30	0.49
1:C:507:LEU:HD23	1:C:508:THR:HG22	1.94	0.49
1:D:321:LEU:O	1:D:324:HIS:HB3	2.13	0.49
1:D:426:ARG:O	1:D:427:GLU:C	2.55	0.49
1:A:130:PRO:O	1:A:131:LEU:C	2.53	0.49
1:A:321:LEU:O	1:A:324:HIS:HB3	2.13	0.49
1:C:364:THR:O	1:C:368:VAL:HG13	2.13	0.49
1:D:130:PRO:O	1:D:131:LEU:C	2.53	0.49
1:D:168:GLN:NE2	1:D:299:MET:CG	2.73	0.49
1:D:463:PRO:O	1:D:464:ASN:HB2	2.13	0.49
1:A:180:ILE:HG12	1:A:181:GLN:N	2.28	0.49
1:A:359:GLU:HG3	1:A:364:THR:HA	1.94	0.49
1:C:152:LEU:HD13	1:C:291:PRO:CG	2.42	0.49
1:C:324:HIS:CE1	1:C:350:THR:CG2	2.95	0.49
1:C:332:GLY:C	1:C:336:THR:HG22	2.37	0.49
1:C:392:LEU:HD23	1:C:475:ILE:CG2	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:116:LYS:HD3	1:D:117:ARG:N	2.27	0.49
1:D:184:PRO:HB2	1:D:337:ASN:O	2.13	0.49
1:D:311:VAL:HG11	1:D:321:LEU:HD22	1.95	0.49
1:D:426:ARG:O	1:D:430:ASP:HB2	2.13	0.49
1:D:461:LYS:HE3	1:D:462:TYR:CE2	2.48	0.49
1:D:503:VAL:O	1:D:504:THR:OG1	2.29	0.49
1:D:514:THR:C	1:D:516:GLN:N	2.70	0.49
1:A:106:GLN:O	1:A:108:VAL:HG13	2.13	0.48
1:A:280:TYR:HH	1:A:285:TYR:HD1	1.59	0.48
1:B:605:ALA:HB1	1:B:628:LEU:HD11	1.94	0.48
1:C:54:HIS:HE1	1:C:191:THR:HG23	1.78	0.48
1:C:500:ASN:C	1:C:502:LEU:H	2.21	0.48
1:D:215:ASP:OD1	1:D:216:GLY:N	2.46	0.48
1:D:416:PHE:CD1	1:D:416:PHE:C	2.89	0.48
1:D:609:TYR:O	1:D:609:TYR:CG	2.65	0.48
1:A:62:ASP:C	1:A:62:ASP:OD1	2.56	0.48
1:A:254:TYR:CE2	1:A:255:ILE:HB	2.48	0.48
1:A:538:MET:HG3	1:A:538:MET:O	2.13	0.48
1:A:542:ASP:O	1:A:546:ASP:HA	2.14	0.48
1:C:503:VAL:O	1:C:504:THR:OG1	2.30	0.48
1:D:277:TYR:CE1	1:D:353:VAL:HG13	2.48	0.48
1:D:373:LEU:HD13	1:D:492:PHE:CE2	2.47	0.48
1:D:504:THR:O	1:D:504:THR:OG1	2.30	0.48
1:B:102:ASN:ND2	1:B:106:GLN:HB2	2.25	0.48
1:C:269:MET:HE1	1:C:319:VAL:CG1	2.44	0.48
1:D:557:HIS:CE1	1:D:590:PRO:HG2	2.47	0.48
1:A:184:PRO:HB2	1:A:337:ASN:O	2.13	0.48
1:A:272:LYS:HG3	1:A:361:VAL:HG12	1.96	0.48
1:B:55:VAL:HG12	1:B:57:LEU:HD22	1.96	0.48
1:B:428:ARG:HG3	1:B:462:TYR:CZ	2.48	0.48
1:B:455:LYS:HA	1:B:459:THR:HB	1.95	0.48
1:C:41:ALA:O	1:C:42:TYR:CB	2.57	0.48
1:C:542:ASP:HB2	1:C:559:TRP:HZ2	1.78	0.48
1:D:168:GLN:O	1:D:168:GLN:CG	2.38	0.48
1:A:493:LYS:O	1:A:497:LYS:HD2	2.14	0.48
1:B:315:ASP:O	1:B:316:LYS:HB2	2.12	0.48
1:B:595:LEU:HD21	1:B:604:TRP:CE3	2.49	0.48
1:C:184:PRO:HB2	1:C:337:ASN:O	2.14	0.48
1:C:276:MET:HE3	1:C:356:ARG:HB3	1.95	0.48
1:C:543:LYS:HD2	1:C:543:LYS:HA	1.45	0.48
1:D:347:GLU:OE1	1:D:347:GLU:CA	2.60	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:332:GLY:HA2	1:A:346:ASN:OD1	2.13	0.48
1:A:335:VAL:HG13	1:A:440:HIS:HB3	1.94	0.48
1:A:580:LYS:HA	1:A:612:ALA:CB	2.42	0.48
1:B:504:THR:O	1:B:505:ASP:CB	2.60	0.48
1:C:294:PHE:HE2	1:C:298:GLY:HA2	1.79	0.48
1:D:69:SER:HB3	1:D:141:ASN:HB2	1.95	0.48
1:D:74:LEU:N	1:D:74:LEU:HD22	2.28	0.48
1:D:347:GLU:OE1	1:D:347:GLU:HA	2.12	0.48
1:D:359:GLU:HG3	1:D:364:THR:HA	1.95	0.48
1:D:530:PRO:C	1:D:532:ASP:H	2.21	0.48
1:A:596:ALA:HA	1:A:602:LYS:HA	1.96	0.48
1:B:328:HIS:O	1:B:333:ASN:HB2	2.14	0.48
1:C:162:LYS:HD3	1:C:200:LEU:HD12	1.96	0.48
1:C:467:SER:C	1:C:469:ASN:H	2.20	0.48
1:C:613:ARG:N	1:C:614:PRO:HD2	2.28	0.48
1:D:102:ASN:HD21	1:D:106:GLN:HB2	1.79	0.48
1:D:294:PHE:CD1	1:D:295:PRO:HD2	2.49	0.48
1:D:392:LEU:HD23	1:D:475:ILE:CG2	2.43	0.48
1:D:596:ALA:HA	1:D:602:LYS:CA	2.44	0.48
1:A:533:LEU:HD22	1:A:538:MET:HE1	1.95	0.48
1:B:284:ARG:NH2	3:B:702:HOH:O	2.17	0.48
1:B:585:ARG:O	1:B:587:LEU:N	2.44	0.48
1:C:321:LEU:O	1:C:324:HIS:HB3	2.14	0.48
1:D:152:LEU:HD13	1:D:291:PRO:CG	2.44	0.48
1:D:376:GLN:HE22	1:D:524:HIS:CE1	2.30	0.48
1:A:103:SER:C	1:A:104:GLN:CG	2.87	0.48
1:C:283:GLY:CA	3:C:988:HOH:O	2.60	0.48
1:C:343:LEU:O	1:C:343:LEU:HD13	2.13	0.48
1:C:503:VAL:C	1:C:506:GLU:OE1	2.57	0.48
1:D:320:ASN:HB3	1:D:358:MET:HE2	1.95	0.48
1:D:384:GLU:OE1	3:D:843:HOH:O	2.20	0.48
1:D:510:GLU:C	1:D:512:LEU:H	2.21	0.48
1:A:42:TYR:HD2	1:A:172:ILE:HD13	1.79	0.48
1:A:585:ARG:O	1:A:587:LEU:N	2.41	0.48
1:B:46:ASN:O	1:B:48:ASP:N	2.47	0.48
1:B:228:PRO:C	1:B:230:LEU:H	2.21	0.48
1:B:352:TYR:CZ	1:B:429:PHE:HE2	2.32	0.48
1:B:579:LEU:HD23	1:B:588:ILE:HG22	1.96	0.48
1:C:241:LYS:HE3	3:C:985:HOH:O	2.14	0.48
1:C:359:GLU:HG3	1:C:364:THR:HA	1.96	0.48
1:C:525:PHE:O	1:C:529:LEU:HB2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:PRO:HG3	1:A:340:TRP:CZ2	2.48	0.47
1:A:243:MET:HG2	1:A:260:VAL:HG13	1.96	0.47
1:A:435:GLU:O	1:A:439:SER:OG	2.30	0.47
1:B:40:ASP:OD1	1:B:41:ALA:O	2.32	0.47
1:B:519:LEU:C	1:B:519:LEU:HD13	2.39	0.47
1:C:459:THR:HG21	1:C:471:ILE:HD11	1.96	0.47
1:D:206:ALA:HA	1:D:222:MET:CE	2.44	0.47
1:D:522:TRP:O	1:D:526:ILE:CG1	2.54	0.47
1:D:595:LEU:HD21	1:D:604:TRP:CZ3	2.49	0.47
1:A:91:ARG:NH2	1:A:175:ARG:HD2	2.29	0.47
1:A:328:HIS:HE1	1:A:347:GLU:OE1	1.98	0.47
1:A:378:LEU:HD21	1:A:480:LEU:HD21	1.95	0.47
1:A:416:PHE:CD1	1:A:416:PHE:C	2.86	0.47
1:B:300:GLU:O	1:B:300:GLU:HG2	2.13	0.47
1:B:514:THR:O	1:B:516:GLN:N	2.47	0.47
1:B:605:ALA:HB3	1:B:628:LEU:HD11	1.96	0.47
1:C:378:LEU:HD13	1:C:411:VAL:HB	1.95	0.47
1:D:39:THR:O	1:D:39:THR:OG1	2.30	0.47
1:D:46:ASN:O	1:D:48:ASP:N	2.47	0.47
1:D:288:LEU:CB	1:D:304:LEU:HD11	2.44	0.47
1:A:116:LYS:HD3	1:A:117:ARG:N	2.29	0.47
1:B:102:ASN:C	1:B:104:GLN:H	2.21	0.47
1:B:106:GLN:O	1:B:108:VAL:HG13	2.14	0.47
1:B:435:GLU:O	1:B:439:SER:OG	2.32	0.47
1:B:467:SER:C	1:B:469:ASN:H	2.22	0.47
1:B:493:LYS:O	1:B:497:LYS:HD2	2.14	0.47
1:B:504:THR:OG1	1:B:540:ASN:ND2	2.47	0.47
1:D:498:GLN:C	1:D:500:ASN:N	2.69	0.47
1:A:39:THR:O	1:A:339:SER:HB3	2.14	0.47
1:B:276:MET:HE1	1:B:356:ARG:HB3	1.96	0.47
1:B:488:THR:HG22	1:B:488:THR:O	2.11	0.47
1:B:596:ALA:HA	1:B:602:LYS:HA	1.95	0.47
1:C:297:GLY:O	1:C:308:THR:HG22	2.14	0.47
1:D:160:LYS:HD3	1:D:160:LYS:HA	1.70	0.47
1:A:326:LEU:CD2	1:A:326:LEU:O	2.61	0.47
1:A:344:TRP:HH2	1:A:450:PHE:CE2	2.30	0.47
1:B:42:TYR:HA	1:B:121:LEU:HD21	1.97	0.47
1:B:426:ARG:O	1:B:427:GLU:C	2.57	0.47
1:B:572:TYR:N	1:B:573:PRO:HD2	2.29	0.47
1:C:507:LEU:CD1	3:C:971:HOH:O	2.43	0.47
1:D:378:LEU:HD21	1:D:480:LEU:HD21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:579:LEU:HD23	1:D:588:ILE:HG22	1.97	0.47
1:A:298:GLY:HA2	1:A:306:PHE:O	2.15	0.47
1:B:328:HIS:C	1:B:330:TRP:N	2.73	0.47
1:B:498:GLN:C	1:B:500:ASN:N	2.70	0.47
1:D:129:THR:HG23	1:D:133:ALA:HB2	1.96	0.47
1:D:517:TRP:CH2	1:D:525:PHE:CD2	3.02	0.47
1:A:263:PHE:HB3	1:A:266:THR:CG2	2.44	0.47
1:A:328:HIS:C	1:A:330:TRP:N	2.71	0.47
1:A:613:ARG:HB3	1:A:614:PRO:HD3	1.96	0.47
1:B:327:ALA:HB3	1:B:350:THR:HG23	1.96	0.47
1:B:454:LEU:O	1:B:454:LEU:HD23	2.14	0.47
1:B:518:THR:O	1:B:522:TRP:CD1	2.66	0.47
1:B:543:LYS:HD2	1:B:543:LYS:HA	1.52	0.47
1:C:99:MET:HE1	1:C:109:LYS:HB2	1.96	0.47
1:C:276:MET:HE1	1:C:356:ARG:HB3	1.97	0.47
1:D:298:GLY:HA2	1:D:306:PHE:O	2.14	0.47
1:D:311:VAL:HG11	1:D:321:LEU:HD23	1.96	0.47
1:D:459:THR:HG21	1:D:471:ILE:HD11	1.97	0.47
1:A:361:VAL:HG23	1:A:362:PHE:HD1	1.72	0.47
1:C:498:GLN:C	1:C:500:ASN:N	2.72	0.47
1:D:352:TYR:CZ	1:D:429:PHE:HE2	2.32	0.47
1:D:428:ARG:HG3	1:D:462:TYR:CZ	2.49	0.47
1:D:498:GLN:C	1:D:500:ASN:H	2.22	0.47
1:A:39:THR:O	1:A:40:ASP:HB2	2.14	0.47
1:A:162:LYS:HD3	1:A:200:LEU:HD12	1.96	0.47
1:A:310:THR:HG21	1:A:582:ILE:HD12	1.96	0.47
1:B:542:ASP:O	1:B:546:ASP:N	2.48	0.47
1:C:184:PRO:HG3	1:C:340:TRP:CZ2	2.50	0.47
1:C:489:SER:HB3	1:C:492:PHE:HB2	1.97	0.47
1:D:166:PHE:HB2	1:D:306:PHE:HE2	1.80	0.47
1:D:252:GLU:O	1:D:253:SER:HB2	2.15	0.47
1:A:488:THR:O	1:A:488:THR:HG22	2.14	0.47
1:D:365:ASP:O	1:D:369:MET:HB2	2.15	0.47
1:D:509:LEU:CG	1:D:510:GLU:H	2.11	0.47
1:A:328:HIS:HA	1:A:331:SER:O	2.15	0.46
1:C:42:TYR:CD2	1:C:121:LEU:HD21	2.49	0.46
1:C:311:VAL:HG11	1:C:321:LEU:HD22	1.96	0.46
1:C:347:GLU:HB3	1:C:410:TYR:CD2	2.50	0.46
1:C:426:ARG:O	1:C:427:GLU:C	2.58	0.46
1:C:467:SER:C	1:C:469:ASN:N	2.73	0.46
1:D:413:GLY:O	1:D:417:LEU:HG	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:563:SER:CB	1:D:571:VAL:HG21	2.45	0.46
1:A:228:PRO:C	1:A:230:LEU:N	2.71	0.46
1:A:455:LYS:HA	1:A:459:THR:HB	1.96	0.46
1:A:543:LYS:HD2	1:A:543:LYS:HA	1.49	0.46
1:B:416:PHE:CD1	1:B:416:PHE:C	2.91	0.46
1:C:547:LEU:H	1:C:547:LEU:CD1	2.25	0.46
1:C:605:ALA:CB	1:C:628:LEU:HD11	2.46	0.46
1:A:46:ASN:O	1:A:48:ASP:N	2.48	0.46
1:A:325:GLU:HA	1:A:325:GLU:OE1	2.16	0.46
1:A:328:HIS:O	1:A:330:TRP:N	2.48	0.46
1:A:347:GLU:HB3	1:A:410:TYR:CD2	2.51	0.46
1:B:116:LYS:HD3	1:B:117:ARG:N	2.31	0.46
1:C:166:PHE:HB2	1:C:306:PHE:HE2	1.80	0.46
1:D:512:LEU:CB	1:D:513:PRO:CD	2.92	0.46
1:A:372:ALA:O	1:A:373:LEU:C	2.57	0.46
1:B:416:PHE:CD1	1:B:416:PHE:O	2.69	0.46
1:C:217:ASP:OD1	1:C:217:ASP:C	2.59	0.46
1:C:265:ASP:OD2	1:C:316:LYS:HD3	2.15	0.46
1:D:205:SER:HB2	1:D:302:PRO:HG2	1.97	0.46
1:A:295:PRO:HD3	1:A:617:HIS:HB2	1.97	0.46
1:A:459:THR:HG21	1:A:471:ILE:HD11	1.98	0.46
1:B:240:PHE:C	1:B:240:PHE:CD2	2.93	0.46
1:C:467:SER:O	1:C:469:ASN:N	2.49	0.46
1:C:510:GLU:O	1:C:512:LEU:N	2.47	0.46
1:D:208:ASN:OD1	1:D:208:ASN:C	2.58	0.46
1:D:328:HIS:O	1:D:330:TRP:N	2.49	0.46
1:A:276:MET:HE1	1:A:356:ARG:HB3	1.96	0.46
1:A:572:TYR:N	1:A:573:PRO:HD2	2.30	0.46
1:C:337:ASN:ND2	1:C:337:ASN:H	2.12	0.46
1:A:498:GLN:C	1:A:500:ASN:H	2.22	0.46
1:A:514:THR:C	1:A:516:GLN:N	2.73	0.46
1:A:596:ALA:CB	1:A:602:LYS:HG3	2.46	0.46
1:B:400:ASP:CB	1:B:403:ASP:HB2	2.34	0.46
1:B:596:ALA:HA	1:B:602:LYS:HB2	1.98	0.46
1:C:352:TYR:CZ	1:C:429:PHE:HE2	2.34	0.46
1:C:613:ARG:HB3	1:C:614:PRO:HD3	1.98	0.46
1:A:56:TYR:HB3	1:A:73:GLU:HB3	1.98	0.46
1:A:265:ASP:OD2	1:A:316:LYS:HD3	2.16	0.46
1:A:507:LEU:CD1	3:A:970:HOH:O	2.60	0.46
1:B:288:LEU:CD2	1:B:304:LEU:HD11	2.45	0.46
1:B:454:LEU:O	1:B:454:LEU:CD2	2.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:606:VAL:HG13	1:B:610:LYS:NZ	2.30	0.46
1:C:281:ARG:NH2	1:C:438:ASP:OD1	2.45	0.46
1:C:504:THR:O	1:C:505:ASP:CB	2.64	0.46
1:A:200:LEU:O	1:A:218:TYR:OH	2.28	0.46
1:A:254:TYR:CG	1:A:255:ILE:N	2.84	0.46
1:B:228:PRO:C	1:B:230:LEU:N	2.74	0.46
1:B:303:ARG:NH1	3:B:737:HOH:O	2.48	0.46
1:B:400:ASP:HA	1:B:401:PRO:HD3	1.74	0.46
1:C:201:LEU:HD23	1:C:238:LEU:HB2	1.97	0.46
1:C:426:ARG:O	1:C:430:ASP:HB2	2.16	0.46
1:D:166:PHE:HA	1:D:233:ILE:O	2.16	0.46
1:D:180:ILE:HG12	1:D:181:GLN:N	2.30	0.46
1:D:224:GLN:HG3	3:D:976:HOH:O	2.16	0.46
1:A:153:SER:OG	1:A:156:GLN:HG3	2.16	0.46
1:A:326:LEU:O	1:A:326:LEU:HD23	2.15	0.46
1:B:271:ASP:O	1:B:275:GLN:HG3	2.15	0.46
1:D:347:GLU:HB3	1:D:410:TYR:CD2	2.51	0.46
1:D:589:VAL:CG1	1:D:593:LYS:HE3	2.46	0.46
1:A:300:GLU:HG2	1:A:300:GLU:O	2.16	0.45
1:A:510:GLU:O	1:A:512:LEU:N	2.36	0.45
1:A:606:VAL:HG13	1:A:610:LYS:NZ	2.31	0.45
1:C:168:GLN:NE2	1:C:299:MET:HG3	2.32	0.45
1:C:270:ILE:O	1:C:270:ILE:HG22	2.16	0.45
1:C:328:HIS:C	1:C:330:TRP:N	2.74	0.45
1:C:526:ILE:O	1:C:529:LEU:HB3	2.16	0.45
1:D:467:SER:C	1:D:469:ASN:N	2.74	0.45
1:D:542:ASP:HB2	1:D:559:TRP:HZ2	1.81	0.45
1:D:547:LEU:N	1:D:547:LEU:CD1	2.79	0.45
1:D:613:ARG:HB3	1:D:614:PRO:CD	2.46	0.45
1:A:283:GLY:N	3:A:989:HOH:O	2.49	0.45
1:A:354:GLU:O	1:A:358:MET:HG2	2.15	0.45
1:A:481:PRO:O	1:A:482:SER:CB	2.62	0.45
1:B:503:VAL:O	1:B:504:THR:HG22	2.16	0.45
1:C:42:TYR:CE2	1:C:401:PRO:HD3	2.51	0.45
1:C:277:TYR:CD1	1:C:353:VAL:HG13	2.51	0.45
1:C:507:LEU:HD22	1:C:508:THR:HG22	1.98	0.45
1:C:518:THR:O	1:C:521:GLU:N	2.49	0.45
1:D:559:TRP:NE1	1:D:571:VAL:HG11	2.32	0.45
1:A:99:MET:CE	1:A:109:LYS:HB2	2.43	0.45
1:A:361:VAL:CG2	1:A:362:PHE:HD1	2.29	0.45
1:A:416:PHE:CD1	1:A:416:PHE:O	2.69	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:56:TYR:HB3	1:B:73:GLU:HB3	1.98	0.45
1:B:254:TYR:CE2	1:B:255:ILE:HB	2.51	0.45
1:B:295:PRO:HB3	1:B:617:HIS:HB3	1.98	0.45
1:B:326:LEU:HD23	1:B:326:LEU:O	2.16	0.45
1:B:332:GLY:C	1:B:336:THR:CG2	2.89	0.45
1:B:569:LYS:HA	1:B:572:TYR:CD1	2.51	0.45
1:C:160:LYS:HD3	1:C:160:LYS:HA	1.64	0.45
1:C:187:ARG:NH1	1:C:225:ALA:O	2.48	0.45
1:C:249:ILE:HD12	1:C:260:VAL:HA	1.99	0.45
1:C:324:HIS:ND1	1:C:350:THR:HG22	2.31	0.45
1:D:507:LEU:HB3	1:D:508:THR:H	1.63	0.45
1:D:582:ILE:CG1	1:D:584:ARG:H	2.29	0.45
1:B:372:ALA:O	1:B:373:LEU:C	2.57	0.45
1:B:500:ASN:O	1:B:502:LEU:N	2.49	0.45
1:B:520:HIS:ND1	1:B:520:HIS:N	2.65	0.45
1:B:539:VAL:O	1:B:540:ASN:C	2.59	0.45
1:C:42:TYR:HA	1:C:121:LEU:CD1	2.46	0.45
1:C:44:TYR:CD2	1:C:124:LYS:HB2	2.51	0.45
1:C:243:MET:CE	1:C:249:ILE:HG13	2.36	0.45
1:C:263:PHE:HB3	1:C:266:THR:CG2	2.47	0.45
1:D:270:ILE:O	1:D:270:ILE:HG22	2.15	0.45
1:D:568:TYR:CE2	1:D:571:VAL:HG13	2.51	0.45
1:A:42:TYR:HA	1:A:121:LEU:HD21	1.97	0.45
1:A:69:SER:HB3	1:A:141:ASN:CB	2.45	0.45
1:A:166:PHE:HA	1:A:233:ILE:O	2.15	0.45
1:A:252:GLU:O	1:A:253:SER:HB2	2.17	0.45
1:A:313:ALA:HB2	1:A:318:LEU:HD23	1.98	0.45
1:A:559:TRP:CZ2	1:A:568:TYR:CE1	3.05	0.45
1:B:263:PHE:CD1	1:B:322:ILE:HG13	2.51	0.45
1:B:484:ALA:O	1:B:485:PRO:C	2.59	0.45
1:B:542:ASP:O	1:B:546:ASP:CA	2.64	0.45
1:D:263:PHE:C	1:D:265:ASP:H	2.25	0.45
1:D:295:PRO:HD3	1:D:617:HIS:HB2	1.98	0.45
1:B:539:VAL:O	1:B:543:LYS:N	2.43	0.45
1:C:74:LEU:HD22	1:C:74:LEU:N	2.32	0.45
1:C:334:LEU:HD23	1:C:442:PHE:H	1.82	0.45
1:C:454:LEU:O	1:C:454:LEU:CD2	2.65	0.45
1:D:97:ARG:HD3	1:D:99:MET:HE3	1.97	0.45
1:A:311:VAL:HG11	1:A:321:LEU:HD22	1.99	0.45
1:A:394:ILE:O	1:A:394:ILE:HG23	2.16	0.45
1:B:137:ARG:HG2	1:B:139:TYR:CE2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:239:GLU:HB2	1:B:256:LEU:HD22	1.99	0.45
1:B:280:TYR:HH	1:B:285:TYR:HD1	1.64	0.45
1:B:561:LEU:O	1:B:565:ARG:HG3	2.17	0.45
1:C:116:LYS:HD3	1:C:117:ARG:N	2.31	0.45
1:C:339:SER:OG	1:C:342:ASP:OD2	2.29	0.45
1:D:239:GLU:HB2	1:D:256:LEU:HD22	1.98	0.45
1:D:328:HIS:C	1:D:330:TRP:N	2.71	0.45
1:A:152:LEU:HD13	1:A:291:PRO:HG3	1.98	0.45
1:A:175:ARG:HA	1:A:178:ILE:O	2.17	0.45
1:A:386:ASP:O	1:A:388:SER:N	2.47	0.45
1:A:591:LEU:O	1:A:595:LEU:HB2	2.16	0.45
1:A:595:LEU:HD21	1:A:604:TRP:CZ3	2.52	0.45
1:D:318:LEU:HD21	1:D:552:ASN:ND2	2.31	0.45
1:D:572:TYR:N	1:D:573:PRO:HD2	2.31	0.45
1:A:206:ALA:O	1:A:303:ARG:NH1	2.50	0.45
1:A:277:TYR:C	1:A:434:LEU:HD13	2.42	0.45
1:B:359:GLU:HG3	1:B:364:THR:HA	1.98	0.45
1:B:400:ASP:HB3	1:B:403:ASP:CG	2.41	0.45
1:B:530:PRO:C	1:B:532:ASP:H	2.25	0.45
1:C:62:ASP:C	1:C:62:ASP:OD1	2.59	0.45
1:C:148:GLY:CA	1:C:173:HIS:HB3	2.47	0.45
1:C:205:SER:HB2	1:C:302:PRO:HG2	1.99	0.45
1:D:41:ALA:C	1:D:43:THR:H	2.25	0.45
1:D:51:LYS:HB2	1:D:79:PHE:CE1	2.51	0.45
1:D:198:LYS:O	1:D:199:ASP:HB2	2.16	0.45
1:D:201:LEU:HD23	1:D:238:LEU:HB2	1.98	0.45
1:D:495:ILE:O	1:D:499:ILE:HG23	2.17	0.45
1:A:97:ARG:HG3	1:A:139:TYR:CD2	2.52	0.45
1:A:270:ILE:O	1:A:270:ILE:HG22	2.17	0.45
1:B:414:GLN:O	1:B:418:MET:HG3	2.17	0.45
1:D:103:SER:C	1:D:104:GLN:HG3	2.42	0.45
1:D:526:ILE:O	1:D:562:LEU:HD22	2.17	0.45
1:A:265:ASP:O	1:A:268:ALA:HB3	2.16	0.44
1:B:180:ILE:HG12	1:B:181:GLN:N	2.32	0.44
1:C:365:ASP:O	1:C:369:MET:HB2	2.17	0.44
1:D:187:ARG:HG2	1:D:227:PRO:HD3	1.99	0.44
1:D:249:ILE:CD1	1:D:260:VAL:HA	2.47	0.44
1:D:290:LEU:HD11	1:D:306:PHE:HB3	2.00	0.44
1:D:373:LEU:HD21	1:D:523:LEU:HD12	1.98	0.44
1:D:455:LYS:HA	1:D:459:THR:HB	1.99	0.44
1:D:620:ALA:O	1:D:621:GLN:C	2.60	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:328:HIS:HE1	1:B:347:GLU:OE1	2.01	0.44
1:C:464:ASN:HD22	1:D:241:LYS:CB	2.19	0.44
1:D:418:MET:HE2	1:D:418:MET:HB3	1.82	0.44
1:D:543:LYS:HA	1:D:543:LYS:HD2	1.49	0.44
1:A:365:ASP:O	1:A:369:MET:HB2	2.16	0.44
1:A:495:ILE:HA	1:A:498:GLN:HE21	1.82	0.44
1:A:593:LYS:HE2	1:A:627:VAL:HG11	2.00	0.44
1:A:605:ALA:HB1	1:A:628:LEU:HD11	1.98	0.44
1:B:200:LEU:O	1:B:218:TYR:OH	2.28	0.44
1:B:263:PHE:HB3	1:B:266:THR:CG2	2.47	0.44
1:B:489:SER:O	1:B:490:ASN:C	2.58	0.44
1:C:228:PRO:C	1:C:230:LEU:N	2.75	0.44
1:C:311:VAL:HG21	1:C:321:LEU:HD23	2.00	0.44
1:C:395:ASP:O	1:C:399:ARG:NH2	2.51	0.44
1:D:484:ALA:O	1:D:485:PRO:C	2.61	0.44
1:A:613:ARG:HB3	1:A:614:PRO:CD	2.48	0.44
1:A:613:ARG:HD2	1:A:621:GLN:NE2	2.32	0.44
1:B:463:PRO:O	1:B:464:ASN:HB2	2.17	0.44
1:C:413:GLY:O	1:C:417:LEU:HG	2.17	0.44
1:C:580:LYS:HA	1:C:612:ALA:CB	2.42	0.44
1:D:60:ASN:O	1:D:68:LEU:HA	2.17	0.44
1:D:229:TYR:HA	3:D:746:HOH:O	2.18	0.44
1:D:276:MET:HE3	1:D:356:ARG:HB3	1.99	0.44
1:D:300:GLU:HG3	1:D:333:ASN:OD1	2.18	0.44
1:D:613:ARG:N	1:D:614:PRO:HD2	2.33	0.44
1:A:295:PRO:HG2	1:A:296:PHE:CD1	2.44	0.44
1:A:295:PRO:HD3	1:A:617:HIS:CB	2.48	0.44
1:B:54:HIS:HE1	1:B:191:THR:HG23	1.81	0.44
1:B:321:LEU:O	1:B:324:HIS:HB3	2.17	0.44
1:C:206:ALA:HA	1:C:222:MET:CE	2.48	0.44
1:C:277:TYR:CE1	1:C:353:VAL:HG22	2.52	0.44
1:D:372:ALA:O	1:D:373:LEU:C	2.61	0.44
1:D:497:LYS:O	1:D:500:ASN:ND2	2.50	0.44
1:A:427:GLU:HG3	1:A:428:ARG:CZ	2.48	0.44
1:A:467:SER:C	1:A:469:ASN:N	2.75	0.44
1:B:347:GLU:OE1	1:B:347:GLU:CA	2.66	0.44
1:C:228:PRO:C	1:C:230:LEU:H	2.25	0.44
1:D:354:GLU:O	1:D:358:MET:HG2	2.17	0.44
1:A:69:SER:HB3	1:A:141:ASN:HB2	1.98	0.44
1:A:101:LYS:HD2	1:A:107:TRP:CZ2	2.53	0.44
1:A:547:LEU:H	1:A:547:LEU:CD1	2.26	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:620:ALA:O	1:A:621:GLN:C	2.61	0.44
1:B:298:GLY:HA2	1:B:306:PHE:O	2.17	0.44
1:C:386:ASP:C	1:C:388:SER:H	2.25	0.44
1:D:228:PRO:C	1:D:230:LEU:N	2.74	0.44
1:B:341:ARG:HH11	1:B:395:ASP:HA	1.83	0.44
1:B:354:GLU:O	1:B:358:MET:HG2	2.18	0.44
1:C:137:ARG:HG2	1:C:139:TYR:CE2	2.53	0.44
1:C:464:ASN:HB3	1:D:241:LYS:HA	2.00	0.44
1:A:239:GLU:O	1:A:250:TYR:HA	2.17	0.44
1:A:240:PHE:CD2	1:A:240:PHE:C	2.96	0.44
1:A:510:GLU:C	1:A:512:LEU:H	2.21	0.44
1:B:471:ILE:O	1:B:475:ILE:HG12	2.18	0.44
1:B:502:LEU:HG	1:B:507:LEU:HB3	1.96	0.44
1:C:313:ALA:HB2	1:C:318:LEU:HD23	1.99	0.44
1:C:414:GLN:O	1:C:418:MET:HG3	2.18	0.44
1:C:543:LYS:CD	1:C:543:LYS:C	2.88	0.44
1:A:102:ASN:ND2	1:A:106:GLN:HB2	2.32	0.43
1:B:187:ARG:NH1	1:B:225:ALA:O	2.50	0.43
1:C:325:GLU:OE1	1:C:325:GLU:HA	2.17	0.43
1:C:564:VAL:HG23	1:C:572:TYR:OH	2.17	0.43
1:D:564:VAL:HG23	1:D:572:TYR:OH	2.18	0.43
1:A:102:ASN:CA	3:A:960:HOH:O	2.65	0.43
1:A:324:HIS:ND1	1:A:350:THR:HG22	2.32	0.43
1:A:463:PRO:O	1:A:464:ASN:HB2	2.18	0.43
1:B:265:ASP:O	1:B:268:ALA:HB3	2.17	0.43
1:B:295:PRO:HD3	1:B:617:HIS:CB	2.47	0.43
1:C:298:GLY:HA2	1:C:306:PHE:O	2.17	0.43
1:C:318:LEU:HD21	1:C:552:ASN:ND2	2.32	0.43
1:C:354:GLU:O	1:C:358:MET:HG2	2.18	0.43
1:A:201:LEU:O	1:A:235:VAL:HA	2.18	0.43
1:B:102:ASN:CB	3:B:795:HOH:O	2.55	0.43
1:B:252:GLU:O	1:B:253:SER:HB2	2.18	0.43
1:B:427:GLU:HG3	1:B:428:ARG:CZ	2.49	0.43
1:B:569:LYS:HA	1:B:572:TYR:CE1	2.53	0.43
1:C:526:ILE:O	1:C:529:LEU:CB	2.67	0.43
1:D:471:ILE:O	1:D:475:ILE:HG12	2.18	0.43
1:A:42:TYR:HE2	1:A:401:PRO:CD	2.02	0.43
1:A:249:ILE:HD12	1:A:260:VAL:HA	1.99	0.43
1:A:303:ARG:NH1	3:A:782:HOH:O	2.45	0.43
1:A:564:VAL:HG23	1:A:572:TYR:OH	2.18	0.43
1:B:83:LYS:HD2	1:D:363:GLY:HA2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:162:LYS:HD3	1:B:200:LEU:HD12	2.01	0.43
1:B:318:LEU:HD21	1:B:552:ASN:HD21	1.83	0.43
1:B:370:GLU:HG2	1:B:520:HIS:CD2	2.52	0.43
1:C:531:VAL:O	1:C:531:VAL:HG12	2.19	0.43
1:D:276:MET:HE1	1:D:356:ARG:HB3	1.97	0.43
1:A:300:GLU:HG3	1:A:333:ASN:OD1	2.19	0.43
1:A:458:LEU:HD23	1:A:458:LEU:HA	1.87	0.43
1:A:546:ASP:OD1	1:A:549:ASN:HB2	2.17	0.43
1:A:598:ASN:O	1:A:601:SER:N	2.51	0.43
1:B:214:ARG:HB3	1:B:215:ASP:H	1.45	0.43
1:B:227:PRO:HD2	1:B:230:LEU:HD12	2.01	0.43
1:B:343:LEU:O	1:B:343:LEU:HD13	2.18	0.43
1:C:51:LYS:HB2	1:C:79:PHE:CZ	2.53	0.43
1:C:102:ASN:ND2	1:C:106:GLN:HB2	2.31	0.43
1:D:197:ASP:O	1:D:216:GLY:HA3	2.18	0.43
1:D:486:GLN:NE2	1:D:486:GLN:HA	2.33	0.43
1:A:277:TYR:CE1	1:A:353:VAL:HG13	2.53	0.43
1:A:390:THR:HA	1:A:408:VAL:HG21	2.00	0.43
1:B:277:TYR:CE1	1:B:353:VAL:HG22	2.54	0.43
1:B:467:SER:O	1:B:469:ASN:N	2.51	0.43
1:C:42:TYR:HA	1:C:121:LEU:HD21	1.99	0.43
1:C:328:HIS:HA	1:C:331:SER:O	2.18	0.43
1:D:326:LEU:O	1:D:326:LEU:HD23	2.19	0.43
1:D:588:ILE:HG13	1:D:589:VAL:N	2.34	0.43
1:A:277:TYR:CD1	1:A:353:VAL:HG13	2.53	0.43
1:A:303:ARG:HD2	3:A:987:HOH:O	2.17	0.43
1:A:414:GLN:O	1:A:418:MET:HG3	2.18	0.43
1:A:467:SER:O	1:A:469:ASN:N	2.52	0.43
1:A:624:VAL:HA	1:A:627:VAL:HG22	2.00	0.43
1:B:481:PRO:C	1:B:483:TYR:H	2.26	0.43
1:B:609:TYR:O	1:B:609:TYR:CG	2.71	0.43
1:C:364:THR:HA	1:C:367:ALA:HB3	2.00	0.43
1:C:591:LEU:O	1:C:595:LEU:HB2	2.18	0.43
1:D:220:PHE:N	1:D:220:PHE:CD1	2.86	0.43
1:D:277:TYR:C	1:D:434:LEU:HD13	2.44	0.43
1:D:367:ALA:O	1:D:371:GLN:HG3	2.19	0.43
1:D:416:PHE:O	1:D:419:TYR:HB3	2.19	0.43
1:A:596:ALA:HA	1:A:602:LYS:CA	2.48	0.43
1:B:152:LEU:HD13	1:B:291:PRO:CG	2.48	0.43
1:B:166:PHE:HB2	1:B:306:PHE:HE2	1.82	0.43
1:C:372:ALA:O	1:C:373:LEU:C	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:620:ALA:O	1:C:621:GLN:C	2.61	0.43
1:D:92:ASP:OD1	1:D:145:LYS:HE2	2.19	0.43
1:A:153:SER:O	1:A:157:THR:HG23	2.18	0.43
1:A:160:LYS:HA	1:A:160:LYS:HD3	1.58	0.43
1:A:534:ASP:H	1:A:566:ALA:HB1	1.83	0.43
1:B:310:THR:HG21	1:B:582:ILE:HD12	2.00	0.43
1:B:563:SER:CB	1:B:571:VAL:HG21	2.48	0.43
1:C:465:ILE:N	1:C:465:ILE:HD12	2.34	0.43
1:C:543:LYS:O	1:C:543:LYS:HD2	2.19	0.43
1:D:42:TYR:HA	1:D:121:LEU:HD21	2.00	0.43
1:D:51:LYS:HB2	1:D:79:PHE:CZ	2.53	0.43
1:D:148:GLY:CA	1:D:173:HIS:HB3	2.48	0.43
1:D:290:LEU:CD1	1:D:306:PHE:HB3	2.48	0.43
1:D:390:THR:HA	1:D:408:VAL:HG21	2.00	0.43
1:D:481:PRO:C	1:D:483:TYR:H	2.27	0.43
1:D:613:ARG:HE	1:D:621:GLN:HB3	1.84	0.43
1:A:283:GLY:HA2	3:A:989:HOH:O	2.19	0.43
1:B:418:MET:HE2	1:B:418:MET:HB3	1.74	0.43
1:B:542:ASP:HB2	1:B:559:TRP:CZ2	2.53	0.43
1:B:588:ILE:HG13	1:B:589:VAL:N	2.32	0.43
1:C:547:LEU:N	1:C:547:LEU:CD1	2.81	0.43
1:C:589:VAL:CG1	1:C:593:LYS:HE3	2.49	0.43
1:A:542:ASP:O	1:A:546:ASP:CA	2.67	0.42
1:A:557:HIS:CE1	1:A:590:PRO:HG2	2.54	0.42
1:B:132:ASN:O	1:B:133:ALA:C	2.62	0.42
1:B:294:PHE:HE2	1:B:298:GLY:HA2	1.83	0.42
1:B:400:ASP:O	1:B:403:ASP:HB2	2.20	0.42
1:C:254:TYR:CG	1:C:255:ILE:N	2.86	0.42
1:A:220:PHE:N	1:A:220:PHE:CD1	2.87	0.42
1:A:596:ALA:O	1:A:597:LYS:HG3	2.20	0.42
1:C:42:TYR:HA	1:C:121:LEU:HD22	1.99	0.42
1:C:249:ILE:CD1	1:C:260:VAL:HA	2.48	0.42
1:C:315:ASP:O	1:C:316:LYS:HB2	2.19	0.42
1:D:290:LEU:HD22	1:D:294:PHE:CD1	2.54	0.42
1:A:180:ILE:CG1	1:A:181:GLN:H	2.32	0.42
1:A:426:ARG:O	1:A:427:GLU:C	2.62	0.42
1:A:508:THR:C	1:A:509:LEU:O	2.62	0.42
1:A:613:ARG:N	1:A:614:PRO:HD2	2.35	0.42
1:B:40:ASP:OD2	1:B:183:THR:HG23	2.20	0.42
1:B:160:LYS:HA	1:B:160:LYS:HD3	1.70	0.42
1:B:372:ALA:C	1:B:374:GLY:N	2.73	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:568:TYR:CE2	1:B:571:VAL:HG13	2.54	0.42
1:C:542:ASP:O	1:C:546:ASP:CA	2.67	0.42
1:D:42:TYR:CD2	1:D:121:LEU:HD21	2.55	0.42
1:D:345:LEU:HD21	1:D:450:PHE:CG	2.54	0.42
1:D:504:THR:CA	1:D:506:GLU:HG2	2.46	0.42
1:A:412:LYS:NZ	1:A:479:GLY:O	2.42	0.42
1:A:534:ASP:OD1	1:A:566:ALA:O	2.37	0.42
1:B:277:TYR:CD1	1:B:353:VAL:HG13	2.54	0.42
1:B:311:VAL:HG21	1:B:321:LEU:HD23	2.00	0.42
1:B:326:LEU:O	1:B:326:LEU:CD2	2.68	0.42
1:B:541:LEU:HD23	1:B:541:LEU:HA	1.89	0.42
1:C:416:PHE:CD1	1:C:416:PHE:C	2.96	0.42
1:D:165:LEU:O	1:D:234:GLY:HA2	2.20	0.42
1:D:263:PHE:HB3	1:D:266:THR:CG2	2.50	0.42
1:D:427:GLU:HG3	1:D:428:ARG:CZ	2.49	0.42
1:D:580:LYS:HA	1:D:612:ALA:CB	2.43	0.42
1:A:187:ARG:NH1	1:A:225:ALA:O	2.53	0.42
1:A:533:LEU:HD23	1:A:538:MET:CE	2.50	0.42
1:B:220:PHE:CD1	1:B:220:PHE:N	2.87	0.42
1:B:222:MET:SD	1:B:224:GLN:HB2	2.59	0.42
1:B:361:VAL:HG23	1:B:362:PHE:HD1	1.79	0.42
1:C:272:LYS:CG	1:C:361:VAL:HG12	2.49	0.42
1:C:370:GLU:CG	1:C:520:HIS:CD2	3.02	0.42
1:C:497:LYS:O	1:C:500:ASN:HB2	2.19	0.42
1:D:101:LYS:HD2	1:D:107:TRP:CZ2	2.55	0.42
1:D:317:SER:OG	1:D:318:LEU:HD22	2.19	0.42
1:A:93:LEU:HD11	1:A:176:SER:C	2.45	0.42
1:A:504:THR:H	1:A:506:GLU:CB	2.08	0.42
1:A:557:HIS:HE1	1:A:590:PRO:HG2	1.83	0.42
1:C:69:SER:HB3	1:C:141:ASN:HB2	2.02	0.42
1:C:277:TYR:CE1	1:C:353:VAL:HG13	2.55	0.42
1:C:328:HIS:O	1:C:333:ASN:HB2	2.19	0.42
1:C:416:PHE:O	1:C:419:TYR:HB3	2.19	0.42
1:D:239:GLU:O	1:D:250:TYR:HA	2.20	0.42
1:D:324:HIS:CE1	1:D:350:THR:CG2	3.02	0.42
1:D:624:VAL:HA	1:D:627:VAL:HG22	2.01	0.42
1:B:413:GLY:O	1:B:417:LEU:HG	2.19	0.42
1:B:416:PHE:O	1:B:419:TYR:HB3	2.19	0.42
1:B:543:LYS:CD	1:B:543:LYS:C	2.88	0.42
1:C:166:PHE:HA	1:C:233:ILE:O	2.20	0.42
1:C:240:PHE:CD2	1:C:240:PHE:C	2.97	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:315:ASP:OD1	1:C:317:SER:CB	2.68	0.42
1:D:168:GLN:HE21	1:D:170:GLN:HB3	1.84	0.42
1:D:295:PRO:HB3	1:D:617:HIS:HB3	2.01	0.42
1:D:502:LEU:H	1:D:502:LEU:HG	1.46	0.42
1:A:148:GLY:HA3	1:A:173:HIS:HB3	2.02	0.42
1:A:320:ASN:CA	1:A:358:MET:HE2	2.49	0.42
1:A:418:MET:HE2	1:A:418:MET:HB3	1.85	0.42
1:B:148:GLY:CA	1:B:173:HIS:HB3	2.49	0.42
1:B:180:ILE:CG1	1:B:181:GLN:N	2.82	0.42
1:B:498:GLN:C	1:B:500:ASN:H	2.27	0.42
1:B:608:VAL:C	1:B:610:LYS:N	2.78	0.42
1:C:97:ARG:NH1	1:C:99:MET:HE1	2.33	0.42
1:C:624:VAL:HA	1:C:627:VAL:HG22	2.01	0.42
1:D:102:ASN:C	1:D:104:GLN:N	2.78	0.42
1:D:394:ILE:HD12	3:D:754:HOH:O	2.19	0.42
1:D:467:SER:OG	1:D:470:GLU:OE2	2.29	0.42
1:A:291:PRO:HA	1:A:292:PRO:HD3	1.87	0.42
1:A:542:ASP:HB2	1:A:559:TRP:HZ2	1.85	0.42
1:A:567:ASP:C	1:A:569:LYS:HD2	2.41	0.42
1:B:276:MET:HE3	1:B:356:ARG:HB3	2.01	0.42
1:B:369:MET:HG2	1:B:492:PHE:CE1	2.55	0.42
1:C:129:THR:HG23	1:C:133:ALA:HB3	2.01	0.42
1:C:150:GLN:HG3	1:C:152:LEU:HG	2.02	0.42
1:C:361:VAL:CG2	1:C:362:PHE:HD1	2.30	0.42
1:C:520:HIS:ND1	1:C:520:HIS:N	2.67	0.42
1:C:582:ILE:CG1	1:C:584:ARG:H	2.32	0.42
1:D:228:PRO:C	1:D:230:LEU:H	2.26	0.42
1:D:304:LEU:HD12	1:D:306:PHE:CE1	2.55	0.42
1:D:392:LEU:HB2	1:D:475:ILE:HA	2.01	0.42
1:A:101:LYS:HG3	1:A:107:TRP:CE2	2.55	0.42
1:A:345:LEU:HD23	1:A:345:LEU:HA	1.88	0.42
1:A:566:ALA:O	1:A:567:ASP:HB2	2.20	0.42
1:B:101:LYS:HD2	1:B:107:TRP:CZ2	2.55	0.42
1:B:154:ALA:HA	1:B:162:LYS:O	2.20	0.42
1:B:159:GLY:C	1:B:161:GLU:N	2.77	0.42
1:B:192:ALA:HB1	1:B:194:ILE:HD11	2.02	0.42
1:B:496:ASP:O	1:B:499:ILE:HG12	2.20	0.42
1:B:499:ILE:C	1:B:501:GLN:N	2.72	0.42
1:B:546:ASP:OD1	1:B:549:ASN:HB2	2.20	0.42
1:C:159:GLY:C	1:C:161:GLU:N	2.77	0.42
1:C:542:ASP:O	1:C:546:ASP:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:90:THR:HG23	1:D:91:ARG:N	2.34	0.42
1:D:465:ILE:HD12	1:D:465:ILE:N	2.35	0.42
1:A:125:LEU:HD21	1:A:127:ILE:HD11	2.02	0.41
1:A:171:ALA:HB3	1:A:401:PRO:HB2	2.01	0.41
1:A:318:LEU:HD21	1:A:552:ASN:ND2	2.35	0.41
1:B:57:LEU:HB3	1:B:59:LEU:HD23	2.01	0.41
1:B:481:PRO:HD2	1:B:484:ALA:HB2	2.01	0.41
1:B:526:ILE:HG12	1:B:527:ASN:N	2.34	0.41
1:B:594:GLU:HA	1:B:597:LYS:HD3	2.01	0.41
1:C:481:PRO:O	1:C:482:SER:CB	2.68	0.41
1:D:54:HIS:HE1	1:D:191:THR:HG23	1.84	0.41
1:D:196:THR:OG1	1:D:218:TYR:HE1	2.03	0.41
1:D:332:GLY:C	1:D:336:THR:CG2	2.93	0.41
1:D:412:LYS:NZ	1:D:479:GLY:O	2.43	0.41
1:A:102:ASN:C	1:A:104:GLN:N	2.78	0.41
1:A:227:PRO:HA	1:A:228:PRO:HD3	1.92	0.41
1:A:313:ALA:HB2	1:A:318:LEU:CD2	2.50	0.41
1:A:343:LEU:O	1:A:343:LEU:HD13	2.20	0.41
1:A:454:LEU:CD2	1:A:454:LEU:O	2.69	0.41
1:C:304:LEU:HD12	1:C:306:PHE:CE1	2.55	0.41
1:C:356:ARG:HA	1:C:356:ARG:HD2	1.92	0.41
1:D:295:PRO:HD3	1:D:617:HIS:CB	2.50	0.41
1:D:519:LEU:C	1:D:519:LEU:HD13	2.45	0.41
1:A:74:LEU:N	1:A:74:LEU:HD22	2.35	0.41
1:A:328:HIS:C	1:A:330:TRP:H	2.28	0.41
1:A:332:GLY:C	1:A:336:THR:CG2	2.93	0.41
1:B:177:TRP:C	1:B:178:ILE:HG13	2.46	0.41
1:B:345:LEU:HD21	1:B:450:PHE:CG	2.55	0.41
1:D:90:THR:HG22	1:D:123:SER:O	2.20	0.41
1:D:132:ASN:O	1:D:133:ALA:C	2.64	0.41
1:D:154:ALA:HA	1:D:162:LYS:O	2.20	0.41
1:D:180:ILE:CG1	1:D:181:GLN:N	2.83	0.41
1:D:617:HIS:NE2	3:D:737:HOH:O	2.35	0.41
1:A:319:VAL:CG1	1:A:319:VAL:O	2.67	0.41
1:A:358:MET:CE	1:A:366:ARG:NH1	2.78	0.41
1:A:509:LEU:HB3	1:A:510:GLU:H	1.67	0.41
1:B:95:ILE:N	1:B:95:ILE:HD13	2.35	0.41
1:B:295:PRO:HG2	1:B:296:PHE:CD1	2.46	0.41
1:B:345:LEU:HD23	1:B:345:LEU:HA	1.88	0.41
1:B:596:ALA:HA	1:B:602:LYS:CA	2.50	0.41
1:C:104:GLN:HB2	1:C:106:GLN:HG3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:180:ILE:CG1	1:C:181:GLN:N	2.80	0.41
1:C:198:LYS:O	1:C:199:ASP:HB2	2.20	0.41
1:D:249:ILE:HD12	1:D:260:VAL:HA	2.02	0.41
1:D:512:LEU:HB3	1:D:513:PRO:HD3	2.02	0.41
1:D:568:TYR:CD2	1:D:571:VAL:HG13	2.55	0.41
1:D:605:ALA:HB3	1:D:628:LEU:HD11	2.01	0.41
1:A:132:ASN:O	1:A:133:ALA:C	2.64	0.41
1:A:399:ARG:HD2	1:A:403:ASP:OD2	2.20	0.41
1:B:593:LYS:HE2	1:B:627:VAL:HG11	2.02	0.41
1:C:222:MET:HE2	1:C:222:MET:CA	2.45	0.41
1:C:290:LEU:HD11	1:C:306:PHE:CD2	2.55	0.41
1:D:42:TYR:HA	1:D:121:LEU:HD22	2.01	0.41
1:D:156:GLN:NE2	3:D:800:HOH:O	2.54	0.41
1:D:265:ASP:O	1:D:268:ALA:HB3	2.20	0.41
1:D:302:PRO:O	1:D:303:ARG:HB2	2.20	0.41
1:A:44:TYR:CD2	3:A:713:HOH:O	2.57	0.41
1:A:428:ARG:HG3	1:A:462:TYR:CZ	2.54	0.41
1:A:512:LEU:CB	1:A:513:PRO:CD	2.98	0.41
1:B:66:LYS:HB2	1:B:144:GLU:HB3	2.03	0.41
1:B:373:LEU:HD12	1:B:373:LEU:HA	1.86	0.41
1:C:102:ASN:C	1:C:104:GLN:N	2.77	0.41
1:C:114:LEU:HD12	1:C:114:LEU:HA	1.94	0.41
1:C:295:PRO:HD3	1:C:617:HIS:HB2	2.02	0.41
1:C:326:LEU:HD22	1:C:330:TRP:HZ3	1.85	0.41
1:C:418:MET:HE2	1:C:418:MET:HB3	1.79	0.41
1:C:613:ARG:HD2	1:C:621:GLN:NE2	2.35	0.41
1:D:290:LEU:HD11	1:D:306:PHE:CB	2.51	0.41
1:D:425:GLY:HA3	3:D:873:HOH:O	2.20	0.41
1:D:613:ARG:HD2	1:D:621:GLN:NE2	2.35	0.41
1:A:140:TYR:N	1:A:140:TYR:CD1	2.89	0.41
1:A:152:LEU:HD13	1:A:291:PRO:CG	2.51	0.41
1:A:413:GLY:O	1:A:417:LEU:HG	2.21	0.41
1:B:168:GLN:HE21	1:B:170:GLN:HB3	1.86	0.41
1:B:568:TYR:CD2	1:B:571:VAL:HG13	2.56	0.41
1:C:214:ARG:HB3	1:C:215:ASP:H	1.34	0.41
1:C:290:LEU:CD1	1:C:306:PHE:HB3	2.51	0.41
1:C:495:ILE:HA	1:C:498:GLN:HE21	1.85	0.41
1:D:386:ASP:O	1:D:388:SER:N	2.45	0.41
1:A:177:TRP:C	1:A:178:ILE:HG13	2.46	0.41
1:B:372:ALA:C	1:B:374:GLY:H	2.29	0.41
1:C:40:ASP:HB3	1:C:47:TYR:OH	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:347:GLU:OE1	1:C:347:GLU:CA	2.69	0.41
1:D:43:THR:HG21	1:D:47:TYR:HE1	1.86	0.41
1:D:542:ASP:O	1:D:546:ASP:CA	2.68	0.41
1:A:329:SER:O	1:A:334:LEU:HB2	2.21	0.41
1:A:364:THR:HA	1:A:367:ALA:HB3	2.03	0.41
1:B:43:THR:HG21	1:B:47:TYR:HE1	1.86	0.41
1:B:228:PRO:HA	1:B:231:ILE:HG13	2.03	0.41
1:B:324:HIS:ND1	1:B:350:THR:HG22	2.36	0.41
1:B:376:GLN:OE1	1:B:524:HIS:CD2	2.74	0.41
1:B:392:LEU:HD13	1:B:412:LYS:HD3	2.03	0.41
1:B:531:VAL:CG1	1:B:565:ARG:HB3	2.51	0.41
1:B:564:VAL:HG23	1:B:572:TYR:OH	2.20	0.41
1:B:595:LEU:HD21	1:B:604:TRP:CZ3	2.56	0.41
1:B:624:VAL:HA	1:B:627:VAL:HG22	2.03	0.41
1:C:369:MET:CG	1:C:492:PHE:CE1	3.04	0.41
1:C:608:VAL:C	1:C:610:LYS:N	2.79	0.41
1:D:62:ASP:OD1	1:D:64:ASP:N	2.53	0.41
1:D:74:LEU:N	1:D:74:LEU:CD2	2.84	0.41
1:D:84:ALA:HA	1:D:85:PRO:HD3	1.95	0.41
1:D:91:ARG:NH2	1:D:175:ARG:HD2	2.36	0.41
1:D:190:TYR:CD1	1:D:222:MET:HB3	2.56	0.41
1:D:294:PHE:HA	1:D:295:PRO:HD2	1.88	0.41
1:D:517:TRP:HH2	1:D:525:PHE:CD2	2.39	0.41
1:D:540:ASN:O	1:D:544:ALA:CB	2.68	0.41
1:A:90:THR:HG23	1:A:91:ARG:N	2.35	0.41
1:A:129:THR:O	1:A:130:PRO:C	2.63	0.41
1:A:249:ILE:CD1	1:A:260:VAL:HA	2.50	0.41
1:A:344:TRP:HA	1:A:409:PRO:HB2	2.03	0.41
1:A:454:LEU:O	1:A:454:LEU:HD23	2.21	0.41
1:B:51:LYS:HB2	1:B:79:PHE:CZ	2.56	0.41
1:B:74:LEU:HD22	1:B:74:LEU:N	2.35	0.41
1:B:172:ILE:HA	1:B:182:ASP:OD2	2.21	0.41
1:B:608:VAL:C	1:B:610:LYS:H	2.29	0.41
1:C:62:ASP:OD1	1:C:64:ASP:N	2.54	0.41
1:C:177:TRP:C	1:C:178:ILE:HG13	2.46	0.41
1:C:313:ALA:HB2	1:C:318:LEU:CD2	2.51	0.41
1:C:440:HIS:O	1:C:443:GLN:HB2	2.21	0.41
1:C:454:LEU:CD2	1:C:454:LEU:C	2.94	0.41
1:C:579:LEU:HD23	1:C:588:ILE:HG22	2.03	0.41
1:C:609:TYR:O	1:C:609:TYR:CG	2.74	0.41
1:D:148:GLY:HA3	1:D:173:HIS:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:175:ARG:HH21	1:D:182:ASP:HB3	1.86	0.41
1:D:324:HIS:ND1	1:D:350:THR:HG22	2.35	0.41
1:D:547:LEU:H	1:D:547:LEU:CD1	2.29	0.41
1:A:144:GLU:OE2	1:A:145:LYS:N	2.53	0.40
1:A:162:LYS:HE3	1:A:199:ASP:HB3	2.03	0.40
1:A:297:GLY:HA2	1:A:308:THR:HG21	2.02	0.40
1:A:355:ASN:O	1:A:358:MET:HB2	2.22	0.40
1:A:471:ILE:O	1:A:475:ILE:HG12	2.21	0.40
1:B:297:GLY:HA2	1:B:308:THR:HG21	2.03	0.40
1:B:372:ALA:O	1:B:374:GLY:N	2.54	0.40
1:C:514:THR:O	1:C:516:GLN:N	2.53	0.40
1:C:527:ASN:OD1	1:C:558:ALA:CB	2.66	0.40
1:D:523:LEU:O	1:D:527:ASN:HB2	2.22	0.40
1:A:373:LEU:HD12	1:A:373:LEU:HA	1.85	0.40
1:B:90:THR:HG23	1:B:91:ARG:N	2.36	0.40
1:B:320:ASN:CA	1:B:358:MET:HE2	2.51	0.40
1:B:356:ARG:HA	1:B:356:ARG:HD2	1.90	0.40
1:B:386:ASP:O	1:B:388:SER:N	2.45	0.40
1:B:458:LEU:HD23	1:B:458:LEU:HA	1.91	0.40
1:C:498:GLN:C	1:C:500:ASN:H	2.28	0.40
1:D:296:PHE:CD1	1:D:296:PHE:N	2.88	0.40
1:A:481:PRO:C	1:A:483:TYR:H	2.29	0.40
1:A:534:ASP:HA	1:A:566:ALA:O	2.20	0.40
1:B:137:ARG:HH11	1:B:137:ARG:HD3	1.66	0.40
1:D:153:SER:HG	1:D:155:GLU:HG2	1.81	0.40
1:D:502:LEU:HD11	1:D:507:LEU:CD1	2.40	0.40
1:A:567:ASP:CB	1:A:569:LYS:HE3	2.43	0.40
1:A:588:ILE:HG13	1:A:589:VAL:N	2.36	0.40
1:B:288:LEU:HD22	1:B:304:LEU:HD11	2.03	0.40
1:B:569:LYS:CD	1:B:570:GLU:N	2.76	0.40
1:C:484:ALA:O	1:C:485:PRO:C	2.63	0.40
1:D:168:GLN:NE2	1:D:299:MET:HG3	2.35	0.40
1:A:290:LEU:HD12	1:A:290:LEU:N	2.37	0.40
1:B:582:ILE:CG1	1:B:583:GLY:N	2.82	0.40
1:B:605:ALA:O	1:B:608:VAL:HG22	2.21	0.40
1:C:337:ASN:H	1:C:337:ASN:HD22	1.70	0.40
1:C:425:GLY:HA3	3:C:929:HOH:O	2.21	0.40
1:D:315:ASP:OD1	1:D:317:SER:CB	2.70	0.40
1:D:328:HIS:HA	1:D:331:SER:O	2.21	0.40
1:D:373:LEU:HD12	1:D:373:LEU:HA	1.88	0.40
1:D:486:GLN:HG3	3:D:820:HOH:O	2.21	0.40

All (3) 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:B:97:ARG:NH1	1:C:217:ASP:OD1[1_545]	1.80	0.40
3:C:946:HOH:O	3:D:797:HOH:O[1_565]	2.03	0.17
3:B:712:HOH:O	3:C:856:HOH:O[1_545]	2.19	0.01

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	581/605 (96%)	484 (83%)	81 (14%)	16 (3%)	4	9
1	B	575/605 (95%)	481 (84%)	81 (14%)	13 (2%)	5	13
1	C	575/605 (95%)	478 (83%)	84 (15%)	13 (2%)	5	13
1	D	576/605 (95%)	482 (84%)	74 (13%)	20 (4%)	3	6
All	All	2307/2420 (95%)	1925 (83%)	320 (14%)	62 (3%)	4	10

All (62) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	40	ASP
1	A	41	ALA
1	A	509	LEU
1	A	511	GLN
1	B	504	THR
1	B	509	LEU
1	B	540	ASN
1	C	509	LEU
1	D	507	LEU
1	D	509	LEU
1	D	511	GLN
1	D	586	LYS
1	A	198	LYS

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Mol	Chain	Res	Type
1	A	329	SER
1	A	504	THR
1	A	586	LYS
1	A	599	ALA
1	B	500	ASN
1	B	501	GLN
1	B	586	LYS
1	C	504	THR
1	C	511	GLN
1	C	586	LYS
1	D	329	SER
1	D	502	LEU
1	D	504	THR
1	A	479	GLY
1	B	515	ALA
1	B	599	ALA
1	C	103	SER
1	D	41	ALA
1	D	468	ASP
1	A	496	ASP
1	A	587	LEU
1	C	479	GLY
1	C	563	SER
1	C	587	LEU
1	D	197	ASP
1	D	563	SER
1	D	569	LYS
1	D	587	LEU
1	A	292	PRO
1	B	292	PRO
1	B	502	LEU
1	B	587	LEU
1	C	500	ASN
1	C	599	ALA
1	D	292	PRO
1	D	479	GLY
1	A	199	ASP
1	A	502	LEU
1	A	534	ASP
1	C	292	PRO
1	C	531	VAL
1	D	103	SER

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Mol	Chain	Res	Type
1	D	515	ALA
1	D	599	ALA
1	B	180	ILE
1	B	531	VAL
1	C	180	ILE
1	D	531	VAL
1	D	180	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	502/517 (97%)	448 (89%)	54 (11%)	6	16
1	B	495/517 (96%)	433 (88%)	62 (12%)	4	11
1	C	496/517 (96%)	442 (89%)	54 (11%)	6	16
1	D	498/517 (96%)	441 (89%)	57 (11%)	5	14
All	All	1991/2068 (96%)	1764 (89%)	227 (11%)	5	14

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

Mol	Chain	Res	Type
1	A	38	LEU
1	A	39	THR
1	A	49	GLN
1	A	65	LYS
1	A	74	LEU
1	A	77	ASP
1	A	86	LEU
1	A	90	THR
1	A	123	SER
1	A	129	THR
1	A	130	PRO
1	A	144	GLU
1	A	160	LYS
1	A	193	ARG

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Mol	Chain	Res	Type
1	A	203	VAL
1	A	288	LEU
1	A	299	MET
1	A	318	LEU
1	A	326	LEU
1	A	331	SER
1	A	334	LEU
1	A	346	ASN
1	A	364	THR
1	A	366	ARG
1	A	368	VAL
1	A	371	GLN
1	A	383	LEU
1	A	384	GLU
1	A	392	LEU
1	A	426	ARG
1	A	428	ARG
1	A	454	LEU
1	A	458	LEU
1	A	475	ILE
1	A	488	THR
1	A	490	ASN
1	A	493	LYS
1	A	497	LYS
1	A	500	ASN
1	A	501	GLN
1	A	503	VAL
1	A	505	ASP
1	A	506	GLU
1	A	509	LEU
1	A	510	GLU
1	A	512	LEU
1	A	536	GLN
1	A	538	MET
1	A	541	LEU
1	A	543	LYS
1	A	547	LEU
1	A	582	ILE
1	A	591	LEU
1	A	613	ARG
1	B	38	LEU
1	B	39	THR

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Mol	Chain	Res	Type
1	B	49	GLN
1	B	65	LYS
1	B	74	LEU
1	B	77	ASP
1	B	86	LEU
1	B	90	THR
1	B	97	ARG
1	B	123	SER
1	B	129	THR
1	B	130	PRO
1	B	144	GLU
1	B	193	ARG
1	B	198	LYS
1	B	200	LEU
1	B	215	ASP
1	B	288	LEU
1	B	299	MET
1	B	318	LEU
1	B	326	LEU
1	B	331	SER
1	B	334	LEU
1	B	346	ASN
1	B	361	VAL
1	B	364	THR
1	B	368	VAL
1	B	371	GLN
1	B	373	LEU
1	B	383	LEU
1	B	384	GLU
1	B	392	LEU
1	B	403	ASP
1	B	406	SER
1	B	426	ARG
1	B	428	ARG
1	B	454	LEU
1	B	458	LEU
1	B	475	ILE
1	B	485	PRO
1	B	488	THR
1	B	490	ASN
1	B	492	PHE
1	B	493	LYS

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Mol	Chain	Res	Type
1	B	495	ILE
1	B	497	LYS
1	B	500	ASN
1	B	503	VAL
1	B	506	GLU
1	B	507	LEU
1	B	509	LEU
1	B	510	GLU
1	B	526	ILE
1	B	527	ASN
1	B	541	LEU
1	B	543	LYS
1	B	547	LEU
1	B	569	LYS
1	B	582	ILE
1	B	586	LYS
1	B	591	LEU
1	B	613	ARG
1	C	38	LEU
1	C	39	THR
1	C	49	GLN
1	C	65	LYS
1	C	74	LEU
1	C	77	ASP
1	C	82	ASN
1	C	86	LEU
1	C	90	THR
1	C	129	THR
1	C	142	SER
1	C	144	GLU
1	C	193	ARG
1	C	215	ASP
1	C	222	MET
1	C	224	GLN
1	C	288	LEU
1	C	299	MET
1	C	318	LEU
1	C	326	LEU
1	C	334	LEU
1	C	346	ASN
1	C	361	VAL
1	C	364	THR

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Mol	Chain	Res	Type
1	C	368	VAL
1	C	371	GLN
1	C	383	LEU
1	C	384	GLU
1	C	385	LEU
1	C	392	LEU
1	C	426	ARG
1	C	454	LEU
1	C	458	LEU
1	C	475	ILE
1	C	482	SER
1	C	488	THR
1	C	490	ASN
1	C	493	LYS
1	C	497	LYS
1	C	503	VAL
1	C	505	ASP
1	C	506	GLU
1	C	508	THR
1	C	509	LEU
1	C	512	LEU
1	C	522	TRP
1	C	527	ASN
1	C	543	LYS
1	C	547	LEU
1	C	569	LYS
1	C	582	ILE
1	C	586	LYS
1	C	591	LEU
1	C	613	ARG
1	D	38	LEU
1	D	39	THR
1	D	49	GLN
1	D	58	ASP
1	D	65	LYS
1	D	74	LEU
1	D	77	ASP
1	D	86	LEU
1	D	90	THR
1	D	129	THR
1	D	142	SER
1	D	144	GLU

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Mol	Chain	Res	Type
1	D	193	ARG
1	D	203	VAL
1	D	209	GLU
1	D	224	GLN
1	D	284	ARG
1	D	288	LEU
1	D	299	MET
1	D	318	LEU
1	D	326	LEU
1	D	334	LEU
1	D	343	LEU
1	D	346	ASN
1	D	361	VAL
1	D	364	THR
1	D	366	ARG
1	D	368	VAL
1	D	371	GLN
1	D	383	LEU
1	D	384	GLU
1	D	385	LEU
1	D	392	LEU
1	D	426	ARG
1	D	428	ARG
1	D	454	LEU
1	D	458	LEU
1	D	475	ILE
1	D	485	PRO
1	D	488	THR
1	D	490	ASN
1	D	492	PHE
1	D	493	LYS
1	D	497	LYS
1	D	500	ASN
1	D	502	LEU
1	D	503	VAL
1	D	505	ASP
1	D	510	GLU
1	D	512	LEU
1	D	527	ASN
1	D	543	LYS
1	D	547	LEU
1	D	569	LYS

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Mol	Chain	Res	Type
1	D	582	ILE
1	D	591	LEU
1	D	613	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (75) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	104	GLN
1	A	168	GLN
1	A	207	ASN
1	A	246	GLN
1	A	301	ASN
1	A	324	HIS
1	A	337	ASN
1	A	379	ASN
1	A	391	GLN
1	A	414	GLN
1	A	486	GLN
1	A	498	GLN
1	A	500	ASN
1	A	511	GLN
1	A	524	HIS
1	A	528	ASN
1	A	549	ASN
1	A	621	GLN
1	B	104	GLN
1	B	106	GLN
1	B	132	ASN
1	B	168	GLN
1	B	207	ASN
1	B	208	ASN
1	B	301	ASN
1	B	324	HIS
1	B	371	GLN
1	B	376	GLN
1	B	379	ASN
1	B	391	GLN
1	B	486	GLN
1	B	498	GLN
1	B	500	ASN
1	B	524	HIS
1	B	549	ASN

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Mol	Chain	Res	Type
1	B	557	HIS
1	B	621	GLN
1	C	104	GLN
1	C	106	GLN
1	C	132	ASN
1	C	168	GLN
1	C	207	ASN
1	C	301	ASN
1	C	324	HIS
1	C	337	ASN
1	C	379	ASN
1	C	391	GLN
1	C	414	GLN
1	C	457	ASN
1	C	464	ASN
1	C	469	ASN
1	C	486	GLN
1	C	498	GLN
1	C	501	GLN
1	C	524	HIS
1	C	549	ASN
1	C	557	HIS
1	D	128	ASN
1	D	132	ASN
1	D	168	GLN
1	D	207	ASN
1	D	246	GLN
1	D	301	ASN
1	D	324	HIS
1	D	337	ASN
1	D	379	ASN
1	D	391	GLN
1	D	414	GLN
1	D	457	ASN
1	D	486	GLN
1	D	498	GLN
1	D	500	ASN
1	D	511	GLN
1	D	549	ASN
1	D	598	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	C	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	508:THR	C	509:LEU	N	1.20
1	C	500:ASN	C	501:GLN	N	0.90

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	587/605 (97%)	-1.63	0 100 100	7, 25, 67, 83	0
1	B	581/605 (96%)	-1.60	0 100 100	9, 25, 74, 87	0
1	C	581/605 (96%)	-1.59	0 100 100	7, 27, 74, 86	0
1	D	582/605 (96%)	-1.59	0 100 100	8, 27, 76, 89	0
All	All	2331/2420 (96%)	-1.60	0 100 100	7, 26, 73, 89	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	ZN	B	701	1/1	0.98	0.04	24,24,24,24	1
2	ZN	A	701	1/1	0.99	0.03	9,9,9,9	1
2	ZN	C	701	1/1	0.99	0.02	15,15,15,15	1
2	ZN	D	701	1/1	1.00	0.04	28,28,28,28	1

6.5 Other polymers [i](#)

There are no such residues in this entry.