



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 11, 2024 – 11:26 PM EDT

PDB ID : 1I0E
Title : CRYSTAL STRUCTURE OF CREATINE KINASE FROM HUMAN MUSCLE
Authors : Shen, Y.-Q.; Tang, L.; Zhou, H.-M.; Lin, Z.-J.
Deposited on : 2001-01-29
Resolution : 3.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

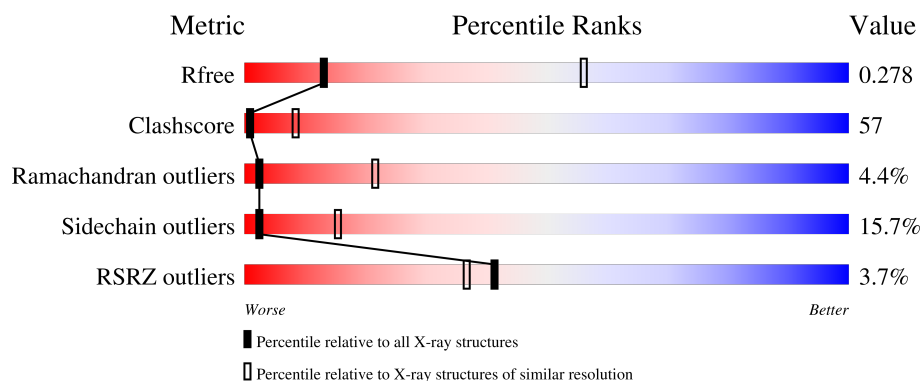
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

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	381	<div> <div>5%</div> <div> <div>38%</div> <div>44%</div> <div>13%</div> <div>• •</div> </div> </div>
1	B	381	<div> <div>3%</div> <div> <div>38%</div> <div>44%</div> <div>13%</div> <div>• •</div> </div> </div>
1	C	381	<div> <div>4%</div> <div> <div>38%</div> <div>44%</div> <div>13%</div> <div>• •</div> </div> </div>
1	D	381	<div> <div>3%</div> <div> <div>38%</div> <div>45%</div> <div>12%</div> <div>• •</div> </div> </div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 11608 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.

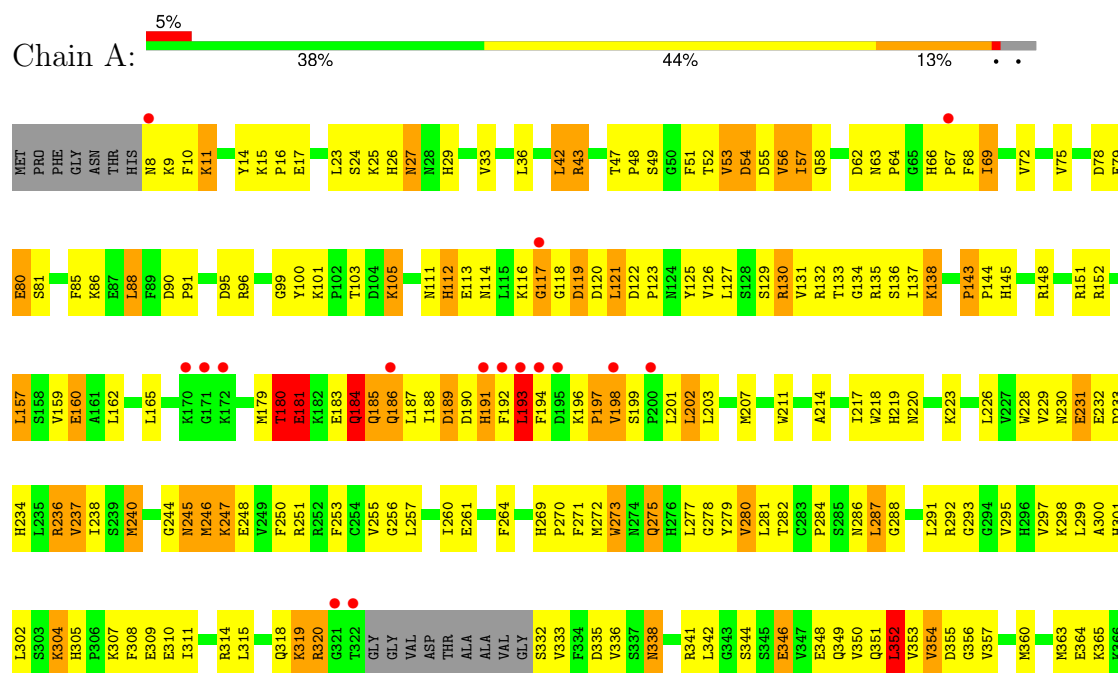
- Molecule 1 is a protein called CREATINE KINASE,M CHAIN.

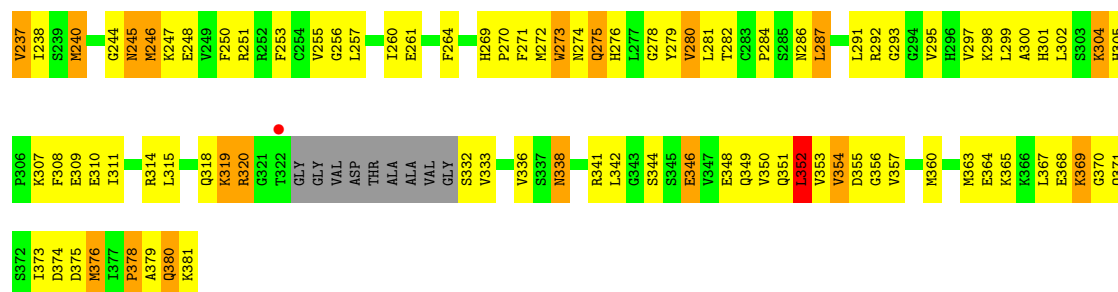
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	365	Total	C	N	O	S	0	0	0
			2902	1834	513	541	14			
1	B	365	Total	C	N	O	S	0	0	0
			2902	1834	513	541	14			
1	C	365	Total	C	N	O	S	0	0	0
			2902	1834	513	541	14			
1	D	365	Total	C	N	O	S	0	0	0
			2902	1834	513	541	14			

3 Residue-property plots

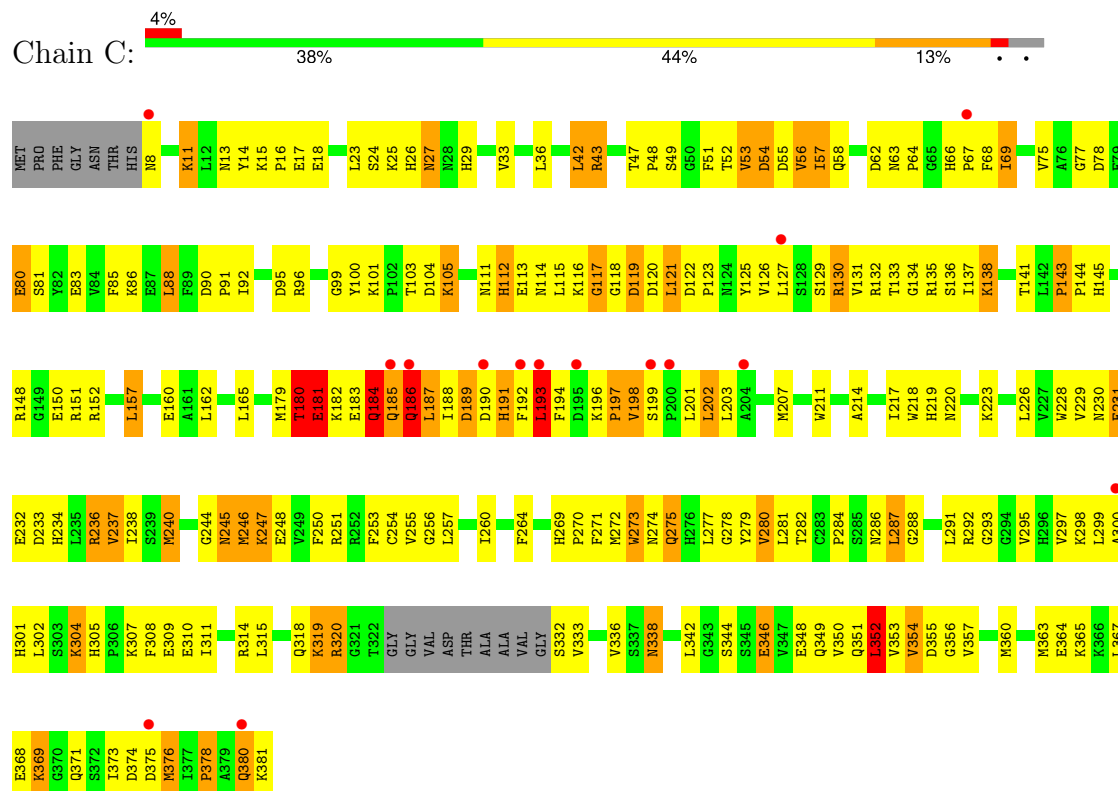
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

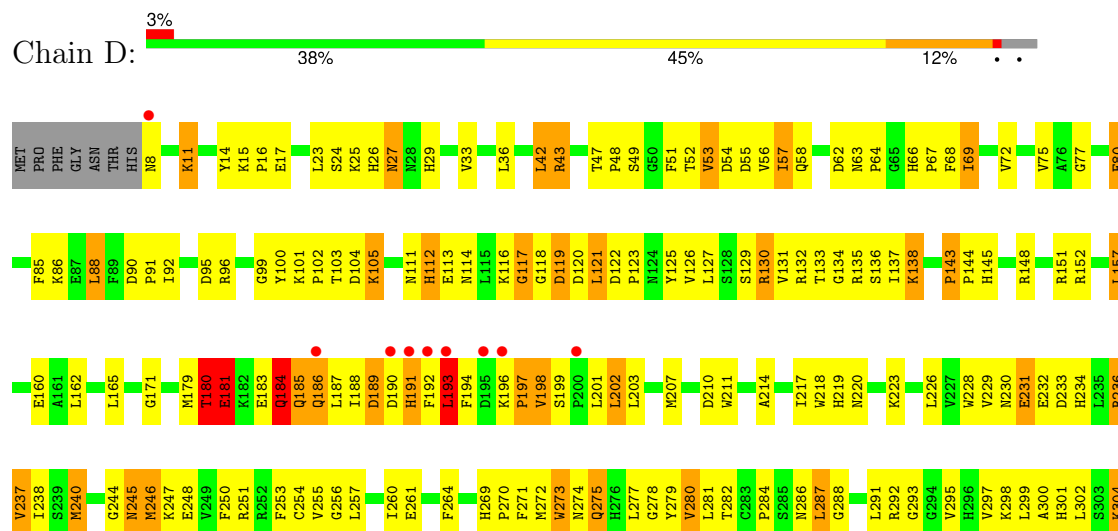


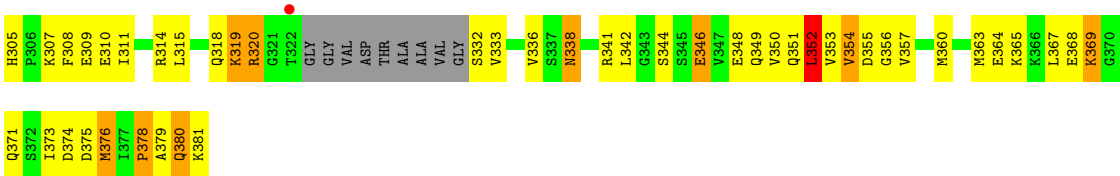


• Molecule 1: CREATINE KINASE,M CHAIN



• Molecule 1: CREATINE KINASE,M CHAIN





4 Data and refinement statistics

Property	Value	Source
Space group	P 31 1 2	Depositor
Cell constants a, b, c, α , β , γ	89.33Å 89.33Å 402.96Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	8.00 – 3.50 29.27 – 3.50	Depositor EDS
% Data completeness (in resolution range)	89.7 (8.00-3.50) 88.3 (29.27-3.50)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.17 (at 3.47Å)	Xtriage
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.211 , 0.287 0.210 , 0.278	Depositor DCC
R_{free} test set	2072 reflections (9.87%)	wwPDB-VP
Wilson B-factor (Å ²)	61.5	Xtriage
Anisotropy	0.214	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 84.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.052 for -h,-k,l	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	11608	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.52% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.40	0/2965	0.63	0/3992
1	B	0.46	0/2965	0.65	0/3992
1	C	0.42	0/2965	0.64	0/3992
1	D	0.43	0/2965	0.65	0/3992
All	All	0.43	0/11860	0.64	0/15968

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2902	0	2869	325	0
1	B	2902	0	2869	333	0
1	C	2902	0	2869	327	1
1	D	2902	0	2869	326	1
All	All	11608	0	11476	1311	1

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 57.

All (1311) 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:344:SER:HB2	1:D:349:GLN:HE21	1.12	1.14
1:B:105:LYS:HZ3	1:B:105:LYS:HA	1.09	1.14
1:C:344:SER:HB2	1:C:349:GLN:HE21	1.10	1.11
1:B:344:SER:HB2	1:B:349:GLN:HE21	1.11	1.10
1:B:181:GLU:HA	1:B:185:GLN:H	1.19	1.08
1:A:344:SER:HB2	1:A:349:GLN:HE21	1.13	1.07
1:D:105:LYS:HZ2	1:D:105:LYS:HA	1.13	1.07
1:C:187:LEU:HA	1:C:192:PHE:HD2	1.19	1.07
1:A:187:LEU:HA	1:A:192:PHE:HD2	1.20	1.07
1:B:187:LEU:HA	1:B:192:PHE:HD2	1.20	1.07
1:D:187:LEU:HA	1:D:192:PHE:HD2	1.20	1.06
1:A:181:GLU:HA	1:A:185:GLN:H	1.15	1.05
1:D:181:GLU:HA	1:D:185:GLN:H	1.17	1.04
1:C:105:LYS:HZ2	1:C:105:LYS:HA	1.20	1.03
1:C:181:GLU:HA	1:C:185:GLN:H	1.19	1.03
1:A:105:LYS:HA	1:A:105:LYS:HZ2	1.16	1.02
1:A:181:GLU:N	1:A:184:GLN:HB2	1.79	0.97
1:D:275:GLN:HE21	1:D:275:GLN:N	1.62	0.97
1:C:275:GLN:HE21	1:C:275:GLN:N	1.63	0.96
1:B:275:GLN:HE21	1:B:275:GLN:N	1.63	0.95
1:B:376:MET:HE2	1:B:376:MET:H	1.30	0.95
1:B:105:LYS:HZ3	1:B:105:LYS:CA	1.80	0.94
1:A:275:GLN:H	1:A:275:GLN:HE21	0.95	0.94
1:D:181:GLU:N	1:D:184:GLN:HB2	1.82	0.94
1:B:181:GLU:N	1:B:184:GLN:HB2	1.83	0.93
1:C:181:GLU:N	1:C:184:GLN:HB2	1.82	0.93
1:C:193:LEU:HA	1:C:217:ILE:HG13	1.51	0.92
1:D:193:LEU:HA	1:D:217:ILE:HG13	1.51	0.92
1:A:275:GLN:HE21	1:A:275:GLN:N	1.67	0.91
1:D:376:MET:HE2	1:D:376:MET:H	1.32	0.91
1:A:193:LEU:HA	1:A:217:ILE:HG13	1.51	0.91
1:A:376:MET:HE2	1:A:376:MET:H	1.36	0.90
1:B:275:GLN:HE21	1:B:275:GLN:H	0.91	0.90
1:B:193:LEU:HA	1:B:217:ILE:HG13	1.53	0.89
1:C:130:ARG:HB3	1:C:240:MET:HB2	1.53	0.89
1:D:275:GLN:HE21	1:D:275:GLN:H	0.89	0.89
1:D:130:ARG:HB3	1:D:240:MET:HB2	1.55	0.88
1:D:180:THR:C	1:D:184:GLN:HB2	1.93	0.88
1:A:130:ARG:HB3	1:A:240:MET:HB2	1.56	0.88
1:C:275:GLN:HE21	1:C:275:GLN:H	0.92	0.88
1:D:66:HIS:HD2	1:D:69:ILE:HG22	1.39	0.88
1:A:180:THR:C	1:A:184:GLN:HB2	1.94	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:194:PHE:HB3	1:D:228:TRP:CE2	2.10	0.87
1:A:23:LEU:HA	1:A:26:HIS:HD2	1.38	0.87
1:B:275:GLN:H	1:B:275:GLN:NE2	1.73	0.87
1:B:194:PHE:HB3	1:B:228:TRP:CE2	2.10	0.87
1:C:23:LEU:HA	1:C:26:HIS:HD2	1.37	0.87
1:D:275:GLN:H	1:D:275:GLN:NE2	1.72	0.87
1:C:66:HIS:HD2	1:C:69:ILE:HG22	1.40	0.86
1:B:23:LEU:HA	1:B:26:HIS:HD2	1.39	0.86
1:B:130:ARG:HB3	1:B:240:MET:HB2	1.57	0.86
1:B:180:THR:C	1:B:184:GLN:HB2	1.96	0.86
1:C:275:GLN:H	1:C:275:GLN:NE2	1.73	0.86
1:B:66:HIS:HD2	1:B:69:ILE:HG22	1.41	0.86
1:C:376:MET:H	1:C:376:MET:HE2	1.39	0.86
1:D:105:LYS:HA	1:D:105:LYS:NZ	1.91	0.86
1:A:66:HIS:HD2	1:A:69:ILE:HG22	1.41	0.85
1:B:187:LEU:HA	1:B:192:PHE:CD2	2.10	0.85
1:D:187:LEU:HA	1:D:192:PHE:CD2	2.11	0.85
1:B:314:ARG:HD3	1:B:376:MET:O	1.77	0.84
1:C:194:PHE:HB3	1:C:228:TRP:CE2	2.11	0.84
1:D:23:LEU:HA	1:D:26:HIS:HD2	1.43	0.84
1:A:194:PHE:HB3	1:A:228:TRP:CE2	2.12	0.84
1:B:105:LYS:HA	1:B:105:LYS:NZ	1.91	0.84
1:C:180:THR:C	1:C:184:GLN:HB2	1.97	0.84
1:A:181:GLU:HA	1:A:185:GLN:N	1.93	0.84
1:D:105:LYS:HZ2	1:D:105:LYS:CA	1.89	0.83
1:A:187:LEU:HA	1:A:192:PHE:CD2	2.10	0.83
1:C:314:ARG:HD3	1:C:376:MET:O	1.79	0.83
1:B:315:LEU:HB3	1:B:381:LYS:O	1.79	0.83
1:A:314:ARG:HD3	1:A:376:MET:O	1.79	0.83
1:A:105:LYS:HZ2	1:A:105:LYS:CA	1.92	0.83
1:D:16:PRO:HG2	1:D:17:GLU:OE2	1.79	0.83
1:B:355:ASP:HB3	1:B:381:LYS:HG2	1.61	0.82
1:D:314:ARG:HD3	1:D:376:MET:O	1.79	0.82
1:B:121:LEU:HD13	1:B:126:VAL:HG21	1.59	0.82
1:C:187:LEU:HA	1:C:192:PHE:CD2	2.09	0.82
1:B:376:MET:SD	1:B:376:MET:N	2.52	0.82
1:C:355:ASP:HB3	1:C:381:LYS:HG2	1.62	0.81
1:D:355:ASP:HB3	1:D:381:LYS:HG2	1.61	0.81
1:A:315:LEU:HB3	1:A:381:LYS:O	1.80	0.81
1:B:16:PRO:HG2	1:B:17:GLU:OE2	1.81	0.81
1:A:16:PRO:HG2	1:A:17:GLU:OE2	1.81	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:26:HIS:ND1	1:C:64:PRO:HA	1.96	0.81
1:C:344:SER:HB2	1:C:349:GLN:NE2	1.94	0.81
1:D:315:LEU:HB3	1:D:381:LYS:O	1.80	0.81
1:A:355:ASP:HB3	1:A:381:LYS:HG2	1.62	0.80
1:C:121:LEU:HD13	1:C:126:VAL:HG21	1.63	0.80
1:D:26:HIS:ND1	1:D:64:PRO:HA	1.96	0.80
1:B:181:GLU:HA	1:B:185:GLN:N	1.97	0.80
1:D:121:LEU:HD13	1:D:126:VAL:HG21	1.61	0.80
1:C:105:LYS:HA	1:C:105:LYS:NZ	1.96	0.80
1:C:181:GLU:HA	1:C:185:GLN:N	1.97	0.80
1:D:344:SER:HB2	1:D:349:GLN:NE2	1.96	0.80
1:B:16:PRO:HD3	1:B:43:ARG:HH12	1.47	0.80
1:D:181:GLU:HA	1:D:185:GLN:N	1.96	0.79
1:A:26:HIS:ND1	1:A:64:PRO:HA	1.98	0.79
1:C:315:LEU:HB3	1:C:381:LYS:O	1.81	0.79
1:C:105:LYS:HZ2	1:C:105:LYS:CA	1.96	0.79
1:C:376:MET:SD	1:C:376:MET:N	2.56	0.79
1:A:105:LYS:HA	1:A:105:LYS:NZ	1.95	0.79
1:A:121:LEU:HD13	1:A:126:VAL:HG21	1.64	0.79
1:B:184:GLN:NE2	1:B:188:ILE:HD11	1.99	0.78
1:A:237:VAL:HG11	1:A:257:LEU:HD21	1.65	0.78
1:D:16:PRO:HD3	1:D:43:ARG:HH12	1.49	0.77
1:A:275:GLN:H	1:A:275:GLN:NE2	1.77	0.77
1:C:16:PRO:HG2	1:C:17:GLU:OE2	1.84	0.77
1:C:237:VAL:HG11	1:C:257:LEU:HD21	1.64	0.77
1:C:48:PRO:HD2	1:C:80:GLU:HG3	1.67	0.77
1:D:48:PRO:HD2	1:D:80:GLU:HG3	1.66	0.77
1:A:48:PRO:HD2	1:A:80:GLU:HG3	1.67	0.76
1:B:183:GLU:O	1:B:187:LEU:HD23	1.85	0.76
1:C:23:LEU:HA	1:C:26:HIS:CD2	2.20	0.76
1:B:26:HIS:ND1	1:B:64:PRO:HA	2.01	0.76
1:C:301:HIS:HA	1:C:304:LYS:HG2	1.67	0.76
1:B:344:SER:HB2	1:B:349:GLN:NE2	1.95	0.76
1:B:237:VAL:HG11	1:B:257:LEU:HD21	1.67	0.76
1:C:183:GLU:O	1:C:187:LEU:HD23	1.85	0.76
1:A:16:PRO:HD3	1:A:43:ARG:HH12	1.52	0.75
1:A:183:GLU:O	1:A:187:LEU:HD23	1.85	0.75
1:A:53:VAL:O	1:A:57:ILE:HG23	1.86	0.75
1:C:130:ARG:HB3	1:C:240:MET:CB	2.17	0.75
1:A:301:HIS:HA	1:A:304:LYS:HG2	1.67	0.74
1:D:183:GLU:O	1:D:187:LEU:HD23	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:193:LEU:HA	1:B:217:ILE:CG1	2.17	0.74
1:B:301:HIS:HA	1:B:304:LYS:HG2	1.69	0.74
1:C:184:GLN:NE2	1:C:188:ILE:HD11	2.03	0.74
1:B:66:HIS:ND1	1:B:67:PRO:HD2	2.02	0.74
1:C:356:GLY:HA2	1:C:381:LYS:HB3	1.69	0.74
1:A:344:SER:HB2	1:A:349:GLN:NE2	1.98	0.74
1:B:23:LEU:HA	1:B:26:HIS:CD2	2.22	0.74
1:B:356:GLY:HA2	1:B:381:LYS:HB3	1.69	0.74
1:C:66:HIS:ND1	1:C:67:PRO:HD2	2.03	0.74
1:A:23:LEU:HA	1:A:26:HIS:CD2	2.22	0.74
1:D:66:HIS:ND1	1:D:67:PRO:HD2	2.02	0.74
1:D:237:VAL:HG11	1:D:257:LEU:HD21	1.67	0.74
1:D:194:PHE:HB3	1:D:228:TRP:CZ2	2.23	0.74
1:A:127:LEU:HD11	1:A:333:VAL:HG11	1.69	0.74
1:A:376:MET:SD	1:A:376:MET:N	2.61	0.74
1:D:356:GLY:HA2	1:D:381:LYS:HB3	1.70	0.74
1:A:356:GLY:HA2	1:A:381:LYS:HB3	1.68	0.73
1:B:194:PHE:HB3	1:B:228:TRP:CZ2	2.23	0.73
1:D:130:ARG:HB3	1:D:240:MET:CB	2.17	0.73
1:D:301:HIS:HA	1:D:304:LYS:HG2	1.69	0.73
1:C:197:PRO:O	1:C:202:LEU:HB2	1.88	0.73
1:A:66:HIS:ND1	1:A:67:PRO:HD2	2.03	0.73
1:B:48:PRO:HD2	1:B:80:GLU:HG3	1.70	0.73
1:C:53:VAL:HG22	1:C:85:PHE:HE1	1.54	0.73
1:C:16:PRO:HD3	1:C:43:ARG:HH12	1.53	0.73
1:B:53:VAL:O	1:B:57:ILE:HG23	1.88	0.73
1:D:376:MET:SD	1:D:376:MET:N	2.62	0.73
1:A:130:ARG:HB3	1:A:240:MET:CB	2.17	0.73
1:A:184:GLN:NE2	1:A:188:ILE:HD11	2.03	0.73
1:A:53:VAL:HG22	1:A:85:PHE:HE1	1.54	0.73
1:D:184:GLN:NE2	1:D:188:ILE:HD11	2.03	0.73
1:C:53:VAL:O	1:C:57:ILE:HG23	1.88	0.72
1:D:193:LEU:HA	1:D:217:ILE:CG1	2.18	0.72
1:A:197:PRO:O	1:A:202:LEU:HB2	1.90	0.72
1:D:197:PRO:O	1:D:202:LEU:HB2	1.89	0.72
1:C:193:LEU:HA	1:C:217:ILE:CG1	2.19	0.72
1:B:197:PRO:O	1:B:202:LEU:HB2	1.89	0.72
1:B:127:LEU:HD11	1:B:333:VAL:HG11	1.70	0.72
1:A:307:LYS:O	1:A:311:ILE:HG13	1.90	0.72
1:A:194:PHE:HB3	1:A:228:TRP:CZ2	2.25	0.71
1:B:130:ARG:HB3	1:B:240:MET:CB	2.19	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:23:LEU:HA	1:D:26:HIS:CD2	2.25	0.71
1:B:375:ASP:HB2	1:B:376:MET:HE2	1.72	0.71
1:A:134:GLY:O	1:A:135:ARG:NH1	2.22	0.71
1:A:193:LEU:HA	1:A:217:ILE:CG1	2.19	0.71
1:B:229:VAL:HG12	1:B:230:ASN:ND2	2.05	0.71
1:D:116:LYS:N	1:D:351:GLN:HE22	1.87	0.71
1:A:116:LYS:N	1:A:351:GLN:HE22	1.88	0.71
1:C:127:LEU:HD11	1:C:333:VAL:HG11	1.71	0.71
1:C:198:VAL:HA	1:C:203:LEU:HD11	1.73	0.71
1:D:375:ASP:HB2	1:D:376:MET:HE2	1.73	0.70
1:B:380:GLN:CD	1:B:381:LYS:H	1.93	0.70
1:C:194:PHE:HB3	1:C:228:TRP:CZ2	2.25	0.70
1:B:184:GLN:HE22	1:B:188:ILE:HD11	1.55	0.70
1:D:53:VAL:HG22	1:D:85:PHE:HE1	1.56	0.70
1:D:53:VAL:O	1:D:57:ILE:HG23	1.90	0.70
1:D:127:LEU:HD11	1:D:333:VAL:HG11	1.72	0.70
1:C:367:LEU:HD21	1:C:373:ILE:HD13	1.73	0.70
1:D:367:LEU:HD21	1:D:373:ILE:HD13	1.73	0.70
1:D:380:GLN:CD	1:D:381:LYS:H	1.94	0.70
1:C:307:LYS:O	1:C:311:ILE:HG13	1.92	0.70
1:A:138:LYS:HB2	1:A:138:LYS:NZ	2.07	0.70
1:A:305:HIS:CD2	1:A:373:ILE:HD11	2.26	0.70
1:C:229:VAL:HG12	1:C:230:ASN:ND2	2.06	0.70
1:D:307:LYS:O	1:D:311:ILE:HG13	1.92	0.70
1:C:116:LYS:N	1:C:351:GLN:HE22	1.89	0.70
1:B:198:VAL:HA	1:B:203:LEU:HD11	1.74	0.69
1:B:16:PRO:HD3	1:B:43:ARG:NH1	2.07	0.69
1:D:248:GLU:OE2	1:D:251:ARG:HD3	1.92	0.69
1:B:116:LYS:N	1:B:351:GLN:HE22	1.90	0.69
1:B:193:LEU:CA	1:B:217:ILE:HG13	2.22	0.69
1:D:229:VAL:HG12	1:D:230:ASN:ND2	2.08	0.69
1:C:369:LYS:HB2	1:C:369:LYS:NZ	2.07	0.69
1:B:376:MET:H	1:B:376:MET:CE	2.04	0.69
1:C:192:PHE:CZ	1:C:223:LYS:HD3	2.28	0.69
1:C:305:HIS:CD2	1:C:373:ILE:HD11	2.27	0.69
1:D:193:LEU:CA	1:D:217:ILE:HG13	2.22	0.69
1:D:138:LYS:HB2	1:D:138:LYS:NZ	2.07	0.69
1:D:299:LEU:HD13	1:D:302:LEU:HD23	1.75	0.69
1:A:229:VAL:HG12	1:A:230:ASN:ND2	2.08	0.69
1:B:369:LYS:HB2	1:B:369:LYS:NZ	2.08	0.69
1:B:53:VAL:HG22	1:B:85:PHE:HE1	1.58	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:134:GLY:O	1:D:135:ARG:NH1	2.26	0.68
1:D:369:LYS:HB2	1:D:369:LYS:NZ	2.09	0.68
1:D:305:HIS:CD2	1:D:373:ILE:HD11	2.27	0.68
1:C:299:LEU:HD13	1:C:302:LEU:HD23	1.73	0.68
1:D:192:PHE:CZ	1:D:223:LYS:HD3	2.28	0.68
1:B:192:PHE:CZ	1:B:223:LYS:HD3	2.28	0.68
1:C:184:GLN:HE22	1:C:188:ILE:HD11	1.59	0.68
1:D:181:GLU:CD	1:D:181:GLU:H	1.97	0.68
1:D:184:GLN:HE22	1:D:188:ILE:HD11	1.58	0.68
1:A:380:GLN:CD	1:A:381:LYS:H	1.97	0.68
1:B:91:PRO:O	1:B:95:ASP:HB2	1.94	0.68
1:A:192:PHE:CZ	1:A:223:LYS:HD3	2.29	0.68
1:B:134:GLY:O	1:B:135:ARG:NH1	2.27	0.68
1:B:248:GLU:OE2	1:B:251:ARG:HD3	1.92	0.68
1:B:138:LYS:HB2	1:B:138:LYS:NZ	2.08	0.68
1:B:186:GLN:HE21	1:B:187:LEU:N	1.91	0.68
1:C:193:LEU:CA	1:C:217:ILE:HG13	2.23	0.68
1:D:91:PRO:O	1:D:95:ASP:HB2	1.94	0.68
1:A:369:LYS:HB2	1:A:369:LYS:NZ	2.09	0.68
1:A:198:VAL:HA	1:A:203:LEU:HD11	1.75	0.67
1:B:151:ARG:HG2	1:B:214:ALA:HB3	1.76	0.67
1:C:186:GLN:HE21	1:C:187:LEU:N	1.92	0.67
1:C:380:GLN:CD	1:C:381:LYS:H	1.96	0.67
1:A:299:LEU:HD13	1:A:302:LEU:HD23	1.74	0.67
1:D:198:VAL:HA	1:D:203:LEU:HD11	1.75	0.67
1:A:193:LEU:CA	1:A:217:ILE:HG13	2.22	0.67
1:A:367:LEU:HD21	1:A:373:ILE:HD13	1.75	0.67
1:B:105:LYS:CA	1:B:105:LYS:NZ	2.55	0.67
1:C:192:PHE:HD1	1:C:226:LEU:HD21	1.60	0.67
1:D:292:ARG:HA	1:D:338:ASN:HD21	1.60	0.67
1:D:16:PRO:HD3	1:D:43:ARG:NH1	2.09	0.67
1:D:43:ARG:O	1:D:43:ARG:HG3	1.94	0.67
1:D:66:HIS:CD2	1:D:69:ILE:HG22	2.27	0.66
1:A:186:GLN:HE21	1:A:187:LEU:N	1.93	0.66
1:B:193:LEU:HA	1:B:217:ILE:CD1	2.26	0.66
1:B:305:HIS:CD2	1:B:373:ILE:HD11	2.29	0.66
1:C:138:LYS:NZ	1:C:138:LYS:HB2	2.08	0.66
1:B:367:LEU:HD21	1:B:373:ILE:HD13	1.75	0.66
1:C:91:PRO:O	1:C:95:ASP:HB2	1.96	0.66
1:C:157:LEU:HD22	1:C:264:PHE:CE2	2.31	0.66
1:B:116:LYS:H	1:B:351:GLN:HE22	1.43	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:248:GLU:OE2	1:C:251:ARG:HD3	1.96	0.66
1:C:355:ASP:CB	1:C:381:LYS:HG2	2.26	0.66
1:D:186:GLN:HE21	1:D:187:LEU:N	1.94	0.66
1:B:375:ASP:HB2	1:B:376:MET:CE	2.26	0.66
1:C:53:VAL:HG22	1:C:85:PHE:CE1	2.30	0.66
1:B:43:ARG:O	1:B:43:ARG:HG3	1.96	0.65
1:A:53:VAL:HG22	1:A:85:PHE:CE1	2.30	0.65
1:A:292:ARG:HA	1:A:338:ASN:HD21	1.59	0.65
1:A:43:ARG:O	1:A:43:ARG:HG3	1.96	0.65
1:B:237:VAL:O	1:B:238:ILE:HD12	1.96	0.65
1:B:307:LYS:O	1:B:311:ILE:HG13	1.96	0.65
1:C:184:GLN:O	1:C:188:ILE:N	2.30	0.65
1:D:151:ARG:HG2	1:D:214:ALA:HB3	1.79	0.65
1:C:66:HIS:CD2	1:C:69:ILE:HG22	2.28	0.65
1:C:184:GLN:HA	1:C:193:LEU:HD13	1.78	0.65
1:D:129:SER:HB3	1:D:295:VAL:HG12	1.79	0.65
1:A:184:GLN:HE22	1:A:188:ILE:HD11	1.60	0.65
1:A:311:ILE:O	1:A:315:LEU:HG	1.96	0.65
1:D:355:ASP:CB	1:D:381:LYS:HG2	2.26	0.65
1:A:181:GLU:CD	1:A:181:GLU:H	1.99	0.65
1:A:272:MET:HG3	1:A:280:VAL:HG22	1.79	0.65
1:C:43:ARG:HG3	1:C:43:ARG:O	1.98	0.64
1:C:275:GLN:N	1:C:275:GLN:NE2	2.40	0.64
1:A:179:MET:CE	1:A:187:LEU:HG	2.27	0.64
1:C:134:GLY:O	1:C:135:ARG:NH1	2.28	0.64
1:C:292:ARG:HA	1:C:338:ASN:HD21	1.62	0.64
1:D:105:LYS:NZ	1:D:105:LYS:CA	2.57	0.64
1:A:91:PRO:O	1:A:95:ASP:HB2	1.98	0.64
1:A:129:SER:HB3	1:A:295:VAL:HG12	1.80	0.64
1:B:184:GLN:HA	1:B:193:LEU:HD13	1.78	0.64
1:B:199:SER:HG	1:B:202:LEU:H	1.46	0.64
1:C:132:ARG:HB3	1:C:238:ILE:HD11	1.79	0.64
1:C:181:GLU:CD	1:C:181:GLU:H	2.00	0.64
1:C:151:ARG:HG2	1:C:214:ALA:HB3	1.80	0.64
1:D:116:LYS:H	1:D:351:GLN:HE22	1.45	0.64
1:D:184:GLN:O	1:D:188:ILE:N	2.31	0.64
1:D:184:GLN:HA	1:D:193:LEU:HD13	1.79	0.64
1:A:376:MET:H	1:A:376:MET:CE	2.10	0.64
1:B:299:LEU:HD13	1:B:302:LEU:HD23	1.78	0.64
1:A:16:PRO:HD3	1:A:43:ARG:NH1	2.11	0.64
1:A:66:HIS:CD2	1:A:69:ILE:HG22	2.29	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:248:GLU:OE2	1:A:251:ARG:HD3	1.96	0.64
1:B:179:MET:CE	1:B:187:LEU:HG	2.28	0.64
1:B:192:PHE:HD1	1:B:226:LEU:HD21	1.63	0.64
1:C:16:PRO:HD3	1:C:43:ARG:NH1	2.11	0.64
1:C:122:ASP:CG	1:C:125:TYR:HD1	2.02	0.64
1:C:311:ILE:O	1:C:315:LEU:HG	1.97	0.64
1:A:181:GLU:OE1	1:A:184:GLN:HB3	1.98	0.63
1:A:355:ASP:CB	1:A:381:LYS:HG2	2.27	0.63
1:B:66:HIS:CD2	1:B:69:ILE:HG22	2.28	0.63
1:D:53:VAL:HG22	1:D:85:PHE:CE1	2.32	0.63
1:D:192:PHE:HD1	1:D:226:LEU:HD21	1.62	0.63
1:C:63:ASN:OD1	1:C:201:LEU:HA	1.97	0.63
1:C:348:GLU:O	1:C:352:LEU:HD23	1.98	0.63
1:B:196:LYS:C	1:B:198:VAL:H	2.01	0.63
1:A:122:ASP:CG	1:A:125:TYR:HD1	2.02	0.63
1:A:180:THR:HA	1:A:184:GLN:HG3	1.80	0.63
1:B:251:ARG:O	1:B:255:VAL:HG23	1.98	0.63
1:C:180:THR:HA	1:C:184:GLN:HG3	1.80	0.63
1:C:237:VAL:O	1:C:238:ILE:HD12	1.98	0.63
1:A:151:ARG:HG2	1:A:214:ALA:HB3	1.79	0.63
1:D:179:MET:CE	1:D:187:LEU:HG	2.29	0.63
1:D:185:GLN:HG2	1:D:189:ASP:OD2	1.99	0.63
1:A:192:PHE:HD1	1:A:226:LEU:HD21	1.63	0.63
1:B:292:ARG:HA	1:B:338:ASN:HD21	1.62	0.63
1:C:251:ARG:O	1:C:255:VAL:HG23	1.97	0.63
1:D:122:ASP:CG	1:D:125:TYR:HD1	2.02	0.63
1:A:197:PRO:HB3	1:A:202:LEU:HD23	1.81	0.63
1:B:185:GLN:HG2	1:B:189:ASP:OD2	1.99	0.63
1:C:129:SER:HB3	1:C:295:VAL:HG12	1.80	0.63
1:C:116:LYS:H	1:C:351:GLN:HE22	1.46	0.63
1:D:275:GLN:N	1:D:275:GLN:NE2	2.39	0.63
1:A:251:ARG:O	1:A:255:VAL:HG23	1.99	0.62
1:A:348:GLU:O	1:A:352:LEU:HD23	1.99	0.62
1:B:181:GLU:CD	1:B:181:GLU:H	2.01	0.62
1:D:180:THR:HA	1:D:184:GLN:HG3	1.81	0.62
1:A:199:SER:HG	1:A:202:LEU:H	1.47	0.62
1:A:363:MET:O	1:A:367:LEU:HD23	1.99	0.62
1:A:354:VAL:CG2	1:A:355:ASP:N	2.62	0.62
1:B:355:ASP:CB	1:B:381:LYS:HG2	2.28	0.62
1:D:179:MET:HG3	1:D:183:GLU:HG2	1.81	0.62
1:B:179:MET:HG3	1:B:183:GLU:HG2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:180:THR:HA	1:B:184:GLN:HG3	1.81	0.62
1:D:192:PHE:HZ	1:D:223:LYS:HD3	1.65	0.62
1:D:256:GLY:O	1:D:260:ILE:HG12	1.99	0.62
1:D:237:VAL:O	1:D:238:ILE:HD12	2.00	0.62
1:B:272:MET:HG3	1:B:280:VAL:HG22	1.81	0.62
1:C:376:MET:H	1:C:376:MET:CE	2.09	0.62
1:D:63:ASN:OD1	1:D:201:LEU:HA	1.99	0.62
1:A:132:ARG:HB3	1:A:238:ILE:HD11	1.80	0.62
1:B:63:ASN:OD1	1:B:201:LEU:HA	2.00	0.62
1:B:157:LEU:HD22	1:B:264:PHE:CE2	2.34	0.62
1:A:237:VAL:O	1:A:238:ILE:HD12	1.99	0.62
1:A:300:ALA:HA	1:A:332:SER:OG	1.99	0.62
1:B:53:VAL:HG22	1:B:85:PHE:CE1	2.34	0.62
1:B:122:ASP:CG	1:B:125:TYR:HD1	2.04	0.62
1:B:197:PRO:HB3	1:B:202:LEU:HD23	1.82	0.62
1:B:348:GLU:O	1:B:352:LEU:HD23	2.00	0.62
1:A:185:GLN:HG2	1:A:189:ASP:OD2	1.99	0.61
1:C:185:GLN:HG2	1:C:189:ASP:OD2	2.00	0.61
1:C:165:LEU:HD11	1:C:260:ILE:CD1	2.30	0.61
1:A:184:GLN:HA	1:A:193:LEU:HD13	1.80	0.61
1:A:165:LEU:HD11	1:A:260:ILE:CD1	2.30	0.61
1:A:179:MET:HG3	1:A:183:GLU:HG2	1.82	0.61
1:A:181:GLU:HB3	1:A:185:GLN:HB3	1.83	0.61
1:D:165:LEU:HD11	1:D:260:ILE:CD1	2.30	0.61
1:D:311:ILE:O	1:D:315:LEU:HG	2.00	0.61
1:A:284:PRO:HA	1:A:287:LEU:HD22	1.83	0.61
1:B:184:GLN:O	1:B:188:ILE:N	2.31	0.61
1:B:376:MET:HE2	1:B:376:MET:N	2.09	0.61
1:C:179:MET:HG3	1:C:183:GLU:HG2	1.83	0.61
1:C:185:GLN:HA	1:C:188:ILE:HB	1.83	0.61
1:D:52:THR:O	1:D:55:ASP:HB2	2.00	0.61
1:B:275:GLN:N	1:B:275:GLN:NE2	2.41	0.61
1:B:354:VAL:CG2	1:B:355:ASP:N	2.63	0.61
1:C:183:GLU:O	1:C:187:LEU:N	2.33	0.61
1:A:183:GLU:O	1:A:187:LEU:N	2.32	0.61
1:B:52:THR:O	1:B:55:ASP:HB2	2.01	0.61
1:D:199:SER:C	1:D:201:LEU:H	2.03	0.61
1:D:376:MET:HE2	1:D:376:MET:N	2.11	0.61
1:A:116:LYS:H	1:A:351:GLN:HE22	1.48	0.60
1:B:237:VAL:HG11	1:B:257:LEU:CD2	2.30	0.60
1:C:348:GLU:O	1:C:351:GLN:HB3	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:188:ILE:HG22	1:D:189:ASP:N	2.16	0.60
1:D:251:ARG:O	1:D:255:VAL:HG23	2.01	0.60
1:D:348:GLU:O	1:D:352:LEU:HD23	2.00	0.60
1:B:129:SER:HB3	1:B:295:VAL:HG12	1.81	0.60
1:D:162:LEU:HB3	1:D:218:TRP:NE1	2.16	0.60
1:B:199:SER:C	1:B:201:LEU:H	2.03	0.60
1:D:196:LYS:C	1:D:198:VAL:H	2.03	0.60
1:A:162:LEU:HB3	1:A:218:TRP:NE1	2.16	0.60
1:A:187:LEU:O	1:A:192:PHE:N	2.35	0.60
1:A:193:LEU:HA	1:A:217:ILE:CD1	2.32	0.60
1:B:187:LEU:O	1:B:192:PHE:N	2.34	0.60
1:B:315:LEU:HD22	1:B:381:LYS:CB	2.31	0.60
1:C:356:GLY:O	1:C:360:MET:HG2	2.00	0.60
1:A:196:LYS:C	1:A:198:VAL:H	2.02	0.60
1:B:165:LEU:HD11	1:B:260:ILE:CD1	2.32	0.60
1:A:231:GLU:OE1	1:A:236:ARG:HD3	2.02	0.60
1:A:376:MET:HE2	1:A:376:MET:N	2.14	0.60
1:B:192:PHE:CE1	1:B:223:LYS:HB3	2.36	0.60
1:C:181:GLU:OE1	1:C:184:GLN:HB3	2.01	0.60
1:C:193:LEU:HA	1:C:217:ILE:CD1	2.31	0.60
1:A:52:THR:O	1:A:55:ASP:HB2	2.02	0.60
1:A:199:SER:C	1:A:201:LEU:H	2.04	0.60
1:D:192:PHE:CE1	1:D:223:LYS:HB3	2.36	0.60
1:A:63:ASN:OD1	1:A:201:LEU:HA	2.02	0.60
1:A:119:ASP:CG	1:A:120:ASP:H	2.04	0.60
1:A:348:GLU:O	1:A:351:GLN:HB3	2.02	0.60
1:D:187:LEU:O	1:D:192:PHE:N	2.35	0.60
1:A:192:PHE:HZ	1:A:223:LYS:HD3	1.67	0.60
1:A:192:PHE:CE1	1:A:223:LYS:HB3	2.36	0.60
1:B:151:ARG:HG2	1:B:214:ALA:CB	2.32	0.60
1:B:181:GLU:HB3	1:B:185:GLN:HB3	1.84	0.60
1:C:192:PHE:CE1	1:C:223:LYS:HB3	2.36	0.60
1:B:311:ILE:O	1:B:315:LEU:HG	2.01	0.60
1:C:69:ILE:HG23	1:C:69:ILE:O	2.01	0.60
1:A:184:GLN:O	1:A:188:ILE:N	2.32	0.59
1:D:151:ARG:HG2	1:D:214:ALA:CB	2.32	0.59
1:A:356:GLY:O	1:A:360:MET:HG2	2.02	0.59
1:C:196:LYS:C	1:C:198:VAL:H	2.03	0.59
1:A:349:GLN:O	1:A:353:VAL:HG23	2.02	0.59
1:B:284:PRO:HA	1:B:287:LEU:HD22	1.83	0.59
1:D:181:GLU:OE1	1:D:184:GLN:HB3	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:348:GLU:O	1:D:351:GLN:HB3	2.02	0.59
1:C:349:GLN:O	1:C:353:VAL:HG23	2.03	0.59
1:B:119:ASP:CG	1:B:120:ASP:H	2.04	0.59
1:B:132:ARG:HB3	1:B:238:ILE:HD11	1.83	0.59
1:A:293:GLY:H	1:A:338:ASN:ND2	2.01	0.59
1:B:256:GLY:O	1:B:260:ILE:HG12	2.02	0.59
1:D:375:ASP:HB2	1:D:376:MET:CE	2.32	0.59
1:C:118:GLY:HA2	1:C:354:VAL:HG21	1.85	0.59
1:C:199:SER:C	1:C:201:LEU:H	2.05	0.59
1:C:300:ALA:HA	1:C:332:SER:OG	2.03	0.59
1:B:162:LEU:HB3	1:B:218:TRP:NE1	2.18	0.59
1:C:179:MET:CE	1:C:187:LEU:HG	2.33	0.59
1:D:14:TYR:O	1:D:43:ARG:NH2	2.35	0.59
1:D:193:LEU:HA	1:D:217:ILE:CD1	2.32	0.59
1:D:310:GLU:O	1:D:314:ARG:HG3	2.02	0.59
1:D:237:VAL:HG11	1:D:257:LEU:CD2	2.33	0.59
1:B:293:GLY:H	1:B:338:ASN:ND2	2.01	0.58
1:A:375:ASP:HB2	1:A:376:MET:CE	2.33	0.58
1:B:188:ILE:HG22	1:B:189:ASP:N	2.19	0.58
1:D:315:LEU:HD22	1:D:381:LYS:CB	2.33	0.58
1:D:376:MET:H	1:D:376:MET:CE	2.09	0.58
1:A:315:LEU:HD22	1:A:381:LYS:CB	2.33	0.58
1:C:52:THR:O	1:C:55:ASP:HB2	2.03	0.58
1:A:105:LYS:CA	1:A:105:LYS:NZ	2.62	0.58
1:A:256:GLY:O	1:A:260:ILE:HG12	2.02	0.58
1:B:181:GLU:OE1	1:B:184:GLN:HB3	2.03	0.58
1:C:137:ILE:HG23	1:C:269:HIS:HB3	1.86	0.58
1:B:187:LEU:HB3	1:B:192:PHE:HB2	1.86	0.58
1:D:231:GLU:OE1	1:D:236:ARG:HD3	2.03	0.58
1:B:185:GLN:HA	1:B:188:ILE:HB	1.85	0.58
1:C:192:PHE:HZ	1:C:223:LYS:HD3	1.66	0.58
1:C:315:LEU:HD22	1:C:381:LYS:CB	2.33	0.58
1:D:181:GLU:HB3	1:D:185:GLN:HB3	1.86	0.58
1:D:380:GLN:CD	1:D:381:LYS:N	2.57	0.58
1:B:380:GLN:CD	1:B:381:LYS:N	2.56	0.58
1:C:119:ASP:CG	1:C:120:ASP:H	2.07	0.58
1:C:217:ILE:HD12	1:C:228:TRP:CD1	2.39	0.58
1:A:237:VAL:HG11	1:A:257:LEU:CD2	2.32	0.58
1:D:132:ARG:HB3	1:D:238:ILE:HD11	1.85	0.58
1:D:183:GLU:O	1:D:187:LEU:N	2.33	0.58
1:D:354:VAL:CG2	1:D:355:ASP:N	2.66	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:369:LYS:HB2	1:B:369:LYS:HZ3	1.69	0.58
1:C:375:ASP:HB2	1:C:376:MET:CE	2.33	0.57
1:D:179:MET:O	1:D:180:THR:HB	2.03	0.57
1:A:137:ILE:HG23	1:A:269:HIS:HB3	1.85	0.57
1:A:157:LEU:HD22	1:A:264:PHE:CE2	2.39	0.57
1:D:197:PRO:HB3	1:D:202:LEU:HD23	1.86	0.57
1:D:300:ALA:HA	1:D:332:SER:OG	2.04	0.57
1:A:14:TYR:O	1:A:43:ARG:NH2	2.37	0.57
1:C:187:LEU:O	1:C:192:PHE:N	2.37	0.57
1:A:185:GLN:HA	1:A:188:ILE:HB	1.86	0.57
1:A:188:ILE:HG22	1:A:189:ASP:N	2.19	0.57
1:A:375:ASP:HB2	1:A:376:MET:HE2	1.86	0.57
1:B:363:MET:O	1:B:367:LEU:HD23	2.05	0.57
1:C:187:LEU:HB3	1:C:192:PHE:HB2	1.84	0.57
1:D:284:PRO:HA	1:D:287:LEU:HD22	1.86	0.57
1:D:356:GLY:O	1:D:360:MET:HG2	2.04	0.57
1:C:293:GLY:H	1:C:338:ASN:ND2	2.01	0.57
1:B:119:ASP:O	1:B:120:ASP:CG	2.43	0.57
1:B:183:GLU:O	1:B:187:LEU:N	2.32	0.57
1:B:192:PHE:HZ	1:B:223:LYS:HD3	1.67	0.57
1:C:363:MET:O	1:C:367:LEU:HD23	2.04	0.57
1:A:179:MET:HG3	1:A:183:GLU:CG	2.35	0.57
1:B:369:LYS:O	1:B:371:GLN:HG3	2.04	0.57
1:B:349:GLN:O	1:B:353:VAL:HG23	2.05	0.57
1:D:184:GLN:NE2	1:D:188:ILE:CD1	2.68	0.57
1:D:272:MET:HG3	1:D:280:VAL:HG22	1.87	0.57
1:A:151:ARG:HG2	1:A:214:ALA:CB	2.35	0.57
1:C:162:LEU:HB3	1:C:218:TRP:NE1	2.20	0.57
1:B:348:GLU:O	1:B:351:GLN:HB3	2.05	0.57
1:C:135:ARG:HD2	1:C:271:PHE:CD2	2.40	0.57
1:D:363:MET:O	1:D:367:LEU:HD23	2.05	0.56
1:A:197:PRO:O	1:A:199:SER:N	2.38	0.56
1:C:199:SER:OG	1:C:202:LEU:HD22	2.05	0.56
1:C:272:MET:HG3	1:C:280:VAL:HG22	1.87	0.56
1:D:157:LEU:HD22	1:D:264:PHE:CE2	2.40	0.56
1:B:194:PHE:H	1:B:217:ILE:HD11	1.69	0.56
1:B:197:PRO:O	1:B:199:SER:N	2.38	0.56
1:B:356:GLY:O	1:B:360:MET:HG2	2.06	0.56
1:C:130:ARG:NH2	1:C:292:ARG:HG2	2.20	0.56
1:C:181:GLU:HB3	1:C:185:GLN:HB3	1.86	0.56
1:C:256:GLY:O	1:C:260:ILE:HG12	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:376:MET:HE2	1:C:376:MET:N	2.17	0.56
1:D:49:SER:O	1:D:145:HIS:HE1	1.88	0.56
1:A:69:ILE:HG23	1:A:69:ILE:O	2.06	0.56
1:A:132:ARG:HG2	1:A:238:ILE:HG13	1.88	0.56
1:A:187:LEU:HB3	1:A:192:PHE:HB2	1.87	0.56
1:A:275:GLN:N	1:A:275:GLN:NE2	2.44	0.56
1:D:185:GLN:HA	1:D:188:ILE:HB	1.86	0.56
1:B:217:ILE:HD12	1:B:228:TRP:CD1	2.40	0.56
1:C:165:LEU:HD11	1:C:260:ILE:HD13	1.88	0.56
1:D:69:ILE:HG23	1:D:69:ILE:O	2.06	0.56
1:D:293:GLY:H	1:D:338:ASN:ND2	2.02	0.56
1:A:112:HIS:ND1	1:A:251:ARG:HG3	2.21	0.56
1:C:137:ILE:CG2	1:C:269:HIS:HB3	2.35	0.56
1:C:310:GLU:O	1:C:314:ARG:HG3	2.05	0.56
1:D:129:SER:HB2	1:D:246:MET:CE	2.36	0.56
1:D:349:GLN:O	1:D:353:VAL:HG23	2.05	0.56
1:B:66:HIS:HE2	1:B:68:PHE:HB2	1.71	0.56
1:B:231:GLU:OE1	1:B:236:ARG:HD3	2.05	0.56
1:C:354:VAL:CG2	1:C:355:ASP:N	2.69	0.56
1:D:137:ILE:HG23	1:D:269:HIS:HB3	1.88	0.56
1:A:62:ASP:O	1:A:64:PRO:HD3	2.06	0.56
1:B:14:TYR:O	1:B:43:ARG:NH2	2.39	0.56
1:B:179:MET:HG3	1:B:183:GLU:CG	2.36	0.56
1:C:237:VAL:HG11	1:C:257:LEU:CD2	2.34	0.56
1:D:217:ILE:HD12	1:D:228:TRP:CD1	2.40	0.56
1:D:298:LYS:CB	1:D:333:VAL:HG12	2.36	0.56
1:A:217:ILE:HD12	1:A:228:TRP:CD1	2.41	0.56
1:C:197:PRO:O	1:C:199:SER:N	2.38	0.56
1:D:118:GLY:HA2	1:D:354:VAL:HG21	1.88	0.55
1:D:181:GLU:N	1:D:181:GLU:CD	2.57	0.55
1:A:315:LEU:HD22	1:A:381:LYS:HB2	1.89	0.55
1:B:112:HIS:ND1	1:B:251:ARG:HG3	2.22	0.55
1:C:66:HIS:HE2	1:C:68:PHE:HB2	1.71	0.55
1:C:199:SER:HG	1:C:202:LEU:HB2	1.72	0.55
1:C:284:PRO:HA	1:C:287:LEU:HD22	1.88	0.55
1:D:119:ASP:CG	1:D:120:ASP:H	2.08	0.55
1:A:136:SER:HA	1:A:234:HIS:HB2	1.89	0.55
1:B:69:ILE:HG23	1:B:69:ILE:O	2.07	0.55
1:B:99:GLY:O	1:B:101:LYS:HD2	2.07	0.55
1:B:184:GLN:NE2	1:B:188:ILE:CD1	2.67	0.55
1:C:197:PRO:HB3	1:C:202:LEU:HD23	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:250:PHE:CD1	1:C:350:VAL:HG21	2.41	0.55
1:C:380:GLN:CD	1:C:381:LYS:N	2.60	0.55
1:D:197:PRO:O	1:D:199:SER:N	2.39	0.55
1:A:181:GLU:N	1:A:181:GLU:CD	2.60	0.55
1:B:315:LEU:HD22	1:B:381:LYS:HB2	1.88	0.55
1:B:353:VAL:O	1:B:357:VAL:HG23	2.05	0.55
1:C:188:ILE:HG22	1:C:189:ASP:N	2.22	0.55
1:C:231:GLU:OE1	1:C:236:ARG:HD3	2.05	0.55
1:C:369:LYS:O	1:C:371:GLN:HG3	2.06	0.55
1:D:179:MET:HG3	1:D:183:GLU:CG	2.36	0.55
1:B:137:ILE:HG23	1:B:269:HIS:HB3	1.88	0.55
1:B:135:ARG:HD2	1:B:271:PHE:CD2	2.42	0.55
1:B:162:LEU:HD13	1:B:218:TRP:CG	2.42	0.55
1:D:17:GLU:H	1:D:17:GLU:CD	2.10	0.55
1:B:118:GLY:HA2	1:B:354:VAL:HG21	1.89	0.55
1:B:201:LEU:HD22	1:B:202:LEU:CD1	2.36	0.55
1:D:135:ARG:HD2	1:D:271:PHE:CD2	2.42	0.55
1:B:376:MET:N	1:B:376:MET:CE	2.68	0.55
1:C:192:PHE:HA	1:C:226:LEU:CD2	2.37	0.55
1:C:353:VAL:O	1:C:357:VAL:HG23	2.07	0.55
1:D:192:PHE:HA	1:D:226:LEU:HD21	1.89	0.55
1:D:315:LEU:HD22	1:D:381:LYS:HB2	1.89	0.55
1:C:192:PHE:HA	1:C:226:LEU:HD21	1.89	0.54
1:A:310:GLU:O	1:A:314:ARG:HG3	2.08	0.54
1:A:380:GLN:CD	1:A:381:LYS:N	2.60	0.54
1:C:315:LEU:HD22	1:C:381:LYS:HB2	1.90	0.54
1:B:132:ARG:HG2	1:B:238:ILE:HG13	1.88	0.54
1:C:132:ARG:HG2	1:C:238:ILE:HG13	1.88	0.54
1:A:369:LYS:O	1:A:371:GLN:HG3	2.07	0.54
1:B:127:LEU:CD1	1:B:333:VAL:HG11	2.38	0.54
1:C:184:GLN:NE2	1:C:188:ILE:CD1	2.70	0.54
1:C:201:LEU:HD22	1:C:202:LEU:CD1	2.37	0.54
1:D:48:PRO:CD	1:D:80:GLU:HG3	2.34	0.54
1:D:187:LEU:HB3	1:D:192:PHE:HB2	1.88	0.54
1:D:250:PHE:CD1	1:D:350:VAL:HG21	2.43	0.54
1:A:66:HIS:HE2	1:A:68:PHE:HB2	1.72	0.54
1:A:179:MET:O	1:A:180:THR:HB	2.07	0.54
1:A:250:PHE:CD1	1:A:350:VAL:HG21	2.42	0.54
1:C:105:LYS:NZ	1:C:105:LYS:CA	2.62	0.54
1:A:130:ARG:NH2	1:A:292:ARG:HG2	2.22	0.54
1:C:88:LEU:O	1:C:88:LEU:HD22	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:66:HIS:HE2	1:D:68:PHE:HB2	1.72	0.54
1:D:99:GLY:O	1:D:101:LYS:HD2	2.07	0.54
1:C:48:PRO:CD	1:C:80:GLU:HG3	2.35	0.54
1:D:199:SER:HG	1:D:202:LEU:H	1.53	0.54
1:A:192:PHE:HA	1:A:226:LEU:HD21	1.89	0.54
1:D:148:ARG:O	1:D:152:ARG:HG3	2.08	0.54
1:A:129:SER:HB2	1:A:246:MET:CE	2.38	0.54
1:A:201:LEU:HD22	1:A:202:LEU:CD1	2.38	0.54
1:A:48:PRO:CD	1:A:80:GLU:HG3	2.36	0.53
1:C:148:ARG:O	1:C:152:ARG:HG3	2.07	0.53
1:C:151:ARG:HG2	1:C:214:ALA:CB	2.37	0.53
1:D:119:ASP:O	1:D:120:ASP:CG	2.46	0.53
1:A:69:ILE:C	1:A:69:ILE:HD13	2.29	0.53
1:C:14:TYR:O	1:C:43:ARG:NH2	2.41	0.53
1:A:24:SER:C	1:A:25:LYS:HD2	2.28	0.53
1:A:184:GLN:NE2	1:A:188:ILE:CD1	2.70	0.53
1:B:181:GLU:N	1:B:181:GLU:CD	2.61	0.53
1:C:136:SER:HA	1:C:234:HIS:HB2	1.90	0.53
1:C:179:MET:HG3	1:C:183:GLU:CG	2.38	0.53
1:D:369:LYS:O	1:D:371:GLN:HG3	2.08	0.53
1:A:119:ASP:O	1:A:120:ASP:CG	2.46	0.53
1:A:137:ILE:CG2	1:A:269:HIS:HB3	2.38	0.53
1:B:300:ALA:HA	1:B:332:SER:OG	2.08	0.53
1:C:112:HIS:ND1	1:C:251:ARG:HG3	2.24	0.53
1:D:369:LYS:HB2	1:D:369:LYS:HZ3	1.72	0.53
1:A:165:LEU:HD11	1:A:260:ILE:HD13	1.90	0.53
1:B:130:ARG:NH2	1:B:292:ARG:HG2	2.24	0.53
1:B:298:LYS:CB	1:B:333:VAL:HG12	2.39	0.53
1:A:118:GLY:HA2	1:A:354:VAL:HG21	1.91	0.53
1:A:192:PHE:HA	1:A:226:LEU:CD2	2.39	0.53
1:A:218:TRP:CE3	1:A:219:HIS:HA	2.44	0.53
1:A:353:VAL:O	1:A:357:VAL:HG23	2.08	0.53
1:C:118:GLY:CA	1:C:354:VAL:HG21	2.39	0.53
1:D:353:VAL:O	1:D:357:VAL:HG23	2.08	0.53
1:D:130:ARG:NH2	1:D:292:ARG:HG2	2.24	0.53
1:B:319:LYS:C	1:B:320:ARG:HD2	2.29	0.53
1:C:298:LYS:CB	1:C:333:VAL:HG12	2.39	0.53
1:A:183:GLU:C	1:A:187:LEU:HD23	2.30	0.53
1:A:319:LYS:C	1:A:320:ARG:HD2	2.30	0.53
1:B:380:GLN:OE1	1:B:381:LYS:N	2.42	0.53
1:A:369:LYS:HB2	1:A:369:LYS:HZ3	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:130:ARG:HH12	1:B:292:ARG:NH2	2.07	0.52
1:C:129:SER:HB2	1:C:246:MET:CE	2.39	0.52
1:D:69:ILE:C	1:D:69:ILE:HD13	2.30	0.52
1:D:136:SER:HA	1:D:234:HIS:HB2	1.91	0.52
1:D:194:PHE:H	1:D:217:ILE:HD11	1.73	0.52
1:A:26:HIS:CE1	1:A:64:PRO:HG3	2.43	0.52
1:A:135:ARG:HD2	1:A:271:PHE:CD2	2.44	0.52
1:A:273:TRP:HA	1:A:278:GLY:O	2.09	0.52
1:B:179:MET:O	1:B:180:THR:HB	2.09	0.52
1:C:201:LEU:HD22	1:C:202:LEU:HD12	1.91	0.52
1:D:112:HIS:ND1	1:D:251:ARG:HG3	2.24	0.52
1:A:99:GLY:O	1:A:101:LYS:HD2	2.10	0.52
1:B:137:ILE:CG2	1:B:269:HIS:HB3	2.39	0.52
1:B:201:LEU:HD22	1:B:202:LEU:HD12	1.90	0.52
1:B:218:TRP:CE3	1:B:219:HIS:HA	2.45	0.52
1:C:138:LYS:HB2	1:C:138:LYS:HZ2	1.72	0.52
1:D:201:LEU:HD22	1:D:202:LEU:CD1	2.40	0.52
1:A:148:ARG:O	1:A:152:ARG:HG3	2.08	0.52
1:B:49:SER:O	1:B:145:HIS:HE1	1.91	0.52
1:B:192:PHE:HA	1:B:226:LEU:HD21	1.91	0.52
1:C:183:GLU:C	1:C:187:LEU:HD23	2.30	0.52
1:C:218:TRP:CE3	1:C:219:HIS:HA	2.44	0.52
1:D:127:LEU:CD1	1:D:333:VAL:HG11	2.39	0.52
1:C:217:ILE:HG23	1:C:228:TRP:CD1	2.45	0.52
1:A:298:LYS:CB	1:A:333:VAL:HG12	2.40	0.52
1:B:136:SER:HA	1:B:234:HIS:HB2	1.91	0.52
1:B:192:PHE:HA	1:B:226:LEU:CD2	2.40	0.52
1:C:119:ASP:O	1:C:120:ASP:CG	2.47	0.52
1:D:273:TRP:HA	1:D:278:GLY:O	2.09	0.52
1:D:380:GLN:OE1	1:D:381:LYS:N	2.42	0.52
1:A:138:LYS:HB2	1:A:138:LYS:HZ2	1.73	0.52
1:C:273:TRP:HA	1:C:278:GLY:O	2.09	0.52
1:D:218:TRP:CE3	1:D:219:HIS:HA	2.44	0.52
1:A:88:LEU:O	1:A:88:LEU:HD22	2.09	0.52
1:B:310:GLU:O	1:B:314:ARG:HG3	2.10	0.52
1:D:192:PHE:HA	1:D:226:LEU:CD2	2.39	0.52
1:B:365:LYS:O	1:B:368:GLU:HB2	2.10	0.52
1:C:194:PHE:H	1:C:217:ILE:HD11	1.74	0.52
1:D:62:ASP:O	1:D:64:PRO:HD3	2.10	0.52
1:A:36:LEU:O	1:A:36:LEU:HD13	2.10	0.52
1:A:194:PHE:H	1:A:217:ILE:HD11	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:319:LYS:C	1:C:320:ARG:HD2	2.31	0.52
1:C:375:ASP:HB2	1:C:376:MET:HE2	1.92	0.52
1:B:88:LEU:HD22	1:B:88:LEU:O	2.10	0.51
1:B:148:ARG:O	1:B:152:ARG:HG3	2.10	0.51
1:C:190:ASP:HB3	1:C:192:PHE:CE2	2.44	0.51
1:B:380:GLN:OE1	1:B:381:LYS:HG3	2.10	0.51
1:D:130:ARG:NH2	1:D:132:ARG:HG3	2.25	0.51
1:D:319:LYS:C	1:D:320:ARG:HD2	2.29	0.51
1:B:111:ASN:HD21	1:B:113:GLU:HB2	1.75	0.51
1:D:194:PHE:HB3	1:D:228:TRP:CD2	2.46	0.51
1:D:380:GLN:OE1	1:D:381:LYS:HG3	2.11	0.51
1:A:49:SER:O	1:A:145:HIS:HE1	1.92	0.51
1:A:318:GLN:O	1:A:336:VAL:HA	2.11	0.51
1:B:69:ILE:HD13	1:B:69:ILE:C	2.30	0.51
1:C:185:GLN:CA	1:C:188:ILE:HB	2.40	0.51
1:D:137:ILE:CG2	1:D:269:HIS:HB3	2.41	0.51
1:A:199:SER:OG	1:A:202:LEU:HD22	2.09	0.51
1:C:130:ARG:HH12	1:C:292:ARG:NH2	2.08	0.51
1:C:318:GLN:O	1:C:336:VAL:HA	2.10	0.51
1:C:49:SER:O	1:C:145:HIS:HE1	1.93	0.51
1:C:62:ASP:O	1:C:64:PRO:HD3	2.10	0.51
1:C:365:LYS:O	1:C:368:GLU:HB2	2.10	0.51
1:D:88:LEU:O	1:D:88:LEU:HD22	2.10	0.51
1:D:201:LEU:HD22	1:D:202:LEU:HD12	1.93	0.51
1:A:66:HIS:NE2	1:A:68:PHE:HB2	2.26	0.51
1:A:201:LEU:HD22	1:A:202:LEU:HD12	1.92	0.51
1:B:103:THR:O	1:B:105:LYS:NZ	2.44	0.51
1:B:194:PHE:HB3	1:B:228:TRP:CD2	2.45	0.51
1:B:280:VAL:C	1:B:281:LEU:HD12	2.30	0.51
1:C:26:HIS:CE1	1:C:64:PRO:HG3	2.46	0.51
1:C:99:GLY:O	1:C:101:LYS:HD2	2.11	0.51
1:D:165:LEU:HD11	1:D:260:ILE:HD11	1.91	0.51
1:B:17:GLU:H	1:B:17:GLU:CD	2.13	0.51
1:B:183:GLU:C	1:B:187:LEU:HD23	2.30	0.51
1:C:133:THR:HG23	1:C:237:VAL:HG13	1.92	0.51
1:C:231:GLU:OE1	1:C:232:GLU:HG3	2.10	0.51
1:D:66:HIS:NE2	1:D:68:PHE:HB2	2.25	0.51
1:D:318:GLN:O	1:D:336:VAL:HA	2.11	0.51
1:B:250:PHE:CD1	1:B:350:VAL:HG21	2.46	0.51
1:D:194:PHE:CD2	1:D:228:TRP:CG	2.99	0.51
1:B:66:HIS:NE2	1:B:68:PHE:HB2	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:179:MET:HG2	1:C:180:THR:N	2.26	0.51
1:D:26:HIS:CE1	1:D:64:PRO:HG3	2.46	0.51
1:A:186:GLN:HE21	1:A:187:LEU:HD22	1.76	0.50
1:A:190:ASP:HB3	1:A:192:PHE:CE2	2.46	0.50
1:B:273:TRP:HB2	1:B:279:TYR:CD1	2.46	0.50
1:C:25:LYS:HE3	1:C:25:LYS:HA	1.93	0.50
1:C:186:GLN:HE21	1:C:187:LEU:HD22	1.76	0.50
1:C:194:PHE:HB3	1:C:228:TRP:CD2	2.45	0.50
1:C:273:TRP:HB2	1:C:279:TYR:CD1	2.46	0.50
1:D:42:LEU:HD13	1:D:53:VAL:HG21	1.93	0.50
1:A:42:LEU:HD13	1:A:53:VAL:HG21	1.93	0.50
1:A:130:ARG:HH12	1:A:292:ARG:NH2	2.09	0.50
1:B:186:GLN:HE21	1:B:187:LEU:HD22	1.76	0.50
1:D:376:MET:N	1:D:376:MET:CE	2.72	0.50
1:B:24:SER:C	1:B:25:LYS:HD2	2.31	0.50
1:B:165:LEU:HD11	1:B:260:ILE:HD13	1.93	0.50
1:B:231:GLU:OE1	1:B:232:GLU:HG3	2.11	0.50
1:D:201:LEU:C	1:D:201:LEU:HD23	2.32	0.50
1:D:273:TRP:HB2	1:D:279:TYR:CD1	2.46	0.50
1:D:365:LYS:O	1:D:368:GLU:HB2	2.11	0.50
1:A:127:LEU:CD1	1:A:333:VAL:HG11	2.39	0.50
1:B:25:LYS:HE3	1:B:25:LYS:HA	1.94	0.50
1:C:127:LEU:CD1	1:C:333:VAL:HG11	2.39	0.50
1:C:380:GLN:OE1	1:C:381:LYS:HG3	2.12	0.50
1:A:51:PHE:CE2	1:A:56:VAL:HG12	2.47	0.50
1:B:165:LEU:HD11	1:B:260:ILE:HD11	1.94	0.50
1:B:48:PRO:CD	1:B:80:GLU:HG3	2.39	0.50
1:B:129:SER:HB2	1:B:246:MET:CE	2.42	0.50
1:B:186:GLN:NE2	1:B:187:LEU:N	2.59	0.50
1:C:66:HIS:NE2	1:C:68:PHE:HB2	2.26	0.50
1:A:365:LYS:O	1:A:368:GLU:HB2	2.12	0.50
1:B:62:ASP:O	1:B:64:PRO:HD3	2.12	0.50
1:C:194:PHE:CD2	1:C:228:TRP:CG	3.00	0.50
1:A:132:ARG:CG	1:A:238:ILE:HG13	2.42	0.50
1:C:184:GLN:HA	1:C:193:LEU:CD1	2.42	0.50
1:C:315:LEU:HA	1:C:380:GLN:O	2.12	0.50
1:A:179:MET:HG2	1:A:180:THR:N	2.26	0.50
1:A:231:GLU:OE1	1:A:232:GLU:HG3	2.12	0.50
1:B:190:ASP:HB3	1:B:192:PHE:CE2	2.47	0.50
1:D:132:ARG:HB3	1:D:132:ARG:HH11	1.77	0.50
1:D:199:SER:OG	1:D:202:LEU:HD22	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:THR:HG23	1:A:237:VAL:HG13	1.93	0.49
1:A:162:LEU:HD13	1:A:218:TRP:CG	2.48	0.49
1:B:180:THR:O	1:B:183:GLU:CD	2.49	0.49
1:B:217:ILE:HD12	1:B:228:TRP:NE1	2.27	0.49
1:B:273:TRP:HA	1:B:278:GLY:O	2.12	0.49
1:B:346:GLU:O	1:B:350:VAL:HG23	2.12	0.49
1:C:132:ARG:CG	1:C:238:ILE:HG13	2.42	0.49
1:D:365:LYS:HA	1:D:368:GLU:OE2	2.12	0.49
1:A:144:PRO:HA	1:A:207:MET:HB3	1.94	0.49
1:B:138:LYS:HA	1:B:272:MET:CE	2.42	0.49
1:B:315:LEU:HA	1:B:380:GLN:O	2.12	0.49
1:C:23:LEU:CA	1:C:26:HIS:HD2	2.19	0.49
1:C:376:MET:N	1:C:376:MET:CE	2.73	0.49
1:A:346:GLU:O	1:A:350:VAL:HG23	2.13	0.49
1:A:376:MET:N	1:A:376:MET:CE	2.74	0.49
1:B:184:GLN:HA	1:B:193:LEU:CD1	2.42	0.49
1:C:69:ILE:HD13	1:C:69:ILE:C	2.33	0.49
1:D:25:LYS:HE3	1:D:25:LYS:HA	1.94	0.49
1:A:295:VAL:HG23	1:A:297:VAL:HG13	1.94	0.49
1:B:194:PHE:CD2	1:B:228:TRP:CG	3.00	0.49
1:D:280:VAL:C	1:D:281:LEU:HD12	2.33	0.49
1:D:338:ASN:HD22	1:D:338:ASN:H	1.59	0.49
1:A:380:GLN:OE1	1:A:381:LYS:N	2.46	0.49
1:B:185:GLN:CA	1:B:188:ILE:HB	2.42	0.49
1:B:305:HIS:CE1	1:B:307:LYS:HB2	2.48	0.49
1:C:117:GLY:C	1:C:119:ASP:N	2.64	0.49
1:A:132:ARG:HB3	1:A:132:ARG:HH11	1.78	0.49
1:A:194:PHE:HB3	1:A:228:TRP:CD2	2.46	0.49
1:A:217:ILE:HG23	1:A:228:TRP:CD1	2.48	0.49
1:A:273:TRP:HB2	1:A:279:TYR:CD1	2.48	0.49
1:C:17:GLU:CD	1:C:17:GLU:H	2.15	0.49
1:C:86:LYS:HG2	1:C:90:ASP:OD2	2.12	0.49
1:C:179:MET:O	1:C:180:THR:HB	2.12	0.49
1:C:186:GLN:NE2	1:C:187:LEU:N	2.60	0.49
1:D:27:ASN:OD1	1:D:67:PRO:HA	2.12	0.49
1:D:133:THR:HG23	1:D:237:VAL:HG13	1.94	0.49
1:D:183:GLU:C	1:D:187:LEU:HD23	2.32	0.49
1:D:315:LEU:HA	1:D:380:GLN:O	2.13	0.49
1:A:25:LYS:HA	1:A:25:LYS:HE3	1.95	0.49
1:A:27:ASN:OD1	1:A:67:PRO:HA	2.12	0.49
1:A:75:VAL:HB	1:A:282:THR:HG22	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:162:LEU:HD13	1:C:218:TRP:CG	2.47	0.49
1:C:380:GLN:OE1	1:C:381:LYS:N	2.46	0.49
1:A:130:ARG:NH2	1:A:132:ARG:HG3	2.28	0.49
1:B:181:GLU:C	1:B:183:GLU:N	2.66	0.49
1:B:318:GLN:O	1:B:336:VAL:HA	2.13	0.49
1:B:338:ASN:H	1:B:338:ASN:HD22	1.61	0.49
1:D:121:LEU:HD13	1:D:126:VAL:CG2	2.40	0.49
1:D:165:LEU:HD11	1:D:260:ILE:HD13	1.93	0.49
1:D:299:LEU:HD11	1:D:360:MET:HE3	1.95	0.49
1:B:27:ASN:OD1	1:B:67:PRO:HA	2.13	0.49
1:C:280:VAL:HA	1:C:287:LEU:CD1	2.43	0.49
1:B:314:ARG:NE	1:B:378:PRO:HD3	2.28	0.49
1:C:36:LEU:HD13	1:C:36:LEU:O	2.13	0.49
1:C:201:LEU:C	1:C:201:LEU:HD23	2.31	0.49
1:D:86:LYS:HG2	1:D:90:ASP:OD2	2.12	0.49
1:D:162:LEU:HD13	1:D:218:TRP:CG	2.48	0.49
1:D:181:GLU:O	1:D:185:GLN:NE2	2.45	0.49
1:D:185:GLN:CA	1:D:188:ILE:HB	2.43	0.49
1:A:184:GLN:HA	1:A:193:LEU:CD1	2.43	0.48
1:A:201:LEU:HD23	1:A:201:LEU:C	2.33	0.48
1:C:144:PRO:HA	1:C:207:MET:HB3	1.95	0.48
1:D:198:VAL:HA	1:D:203:LEU:CD1	2.43	0.48
1:D:346:GLU:O	1:D:350:VAL:HG23	2.13	0.48
1:A:17:GLU:CD	1:A:17:GLU:H	2.17	0.48
1:B:42:LEU:HD13	1:B:53:VAL:HG21	1.95	0.48
1:B:86:LYS:HG2	1:B:90:ASP:OD2	2.13	0.48
1:B:201:LEU:C	1:B:201:LEU:HD23	2.34	0.48
1:C:165:LEU:HD11	1:C:260:ILE:HD11	1.95	0.48
1:C:314:ARG:NE	1:C:378:PRO:HD3	2.28	0.48
1:D:190:ASP:HB3	1:D:192:PHE:CE2	2.48	0.48
1:A:194:PHE:CD2	1:A:228:TRP:CG	3.01	0.48
1:A:305:HIS:CE1	1:A:307:LYS:HB2	2.49	0.48
1:C:78:ASP:OD2	1:C:81:SER:OG	2.26	0.48
1:C:132:ARG:HB3	1:C:132:ARG:HH11	1.78	0.48
1:B:185:GLN:O	1:B:188:ILE:HB	2.12	0.48
1:B:314:ARG:O	1:B:378:PRO:HA	2.14	0.48
1:C:346:GLU:O	1:C:350:VAL:HG23	2.13	0.48
1:A:314:ARG:O	1:A:378:PRO:HA	2.13	0.48
1:A:315:LEU:HA	1:A:380:GLN:O	2.14	0.48
1:B:351:GLN:O	1:B:353:VAL:N	2.46	0.48
1:C:24:SER:C	1:C:25:LYS:HD2	2.33	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:LYS:HG2	1:A:90:ASP:OD2	2.14	0.48
1:B:8:ASN:ND2	1:B:58:GLN:HG2	2.29	0.48
1:B:51:PHE:CE2	1:B:56:VAL:HG12	2.49	0.48
1:B:132:ARG:HB3	1:B:132:ARG:HH11	1.79	0.48
1:C:180:THR:O	1:C:183:GLU:CD	2.52	0.48
1:A:380:GLN:OE1	1:A:381:LYS:HG3	2.13	0.48
1:C:27:ASN:OD1	1:C:67:PRO:HA	2.14	0.48
1:C:103:THR:O	1:C:105:LYS:NZ	2.45	0.48
1:D:188:ILE:CG1	1:D:193:LEU:HD21	2.44	0.48
1:D:231:GLU:OE1	1:D:232:GLU:HG3	2.14	0.48
1:B:179:MET:HG2	1:B:180:THR:N	2.28	0.48
1:B:220:ASN:OD1	1:B:223:LYS:N	2.45	0.48
1:C:132:ARG:HB3	1:C:238:ILE:CD1	2.44	0.48
1:D:75:VAL:HB	1:D:282:THR:HG22	1.95	0.48
1:A:280:VAL:C	1:A:281:LEU:HD12	2.34	0.48
1:C:185:GLN:O	1:C:188:ILE:HB	2.13	0.48
1:C:280:VAL:C	1:C:281:LEU:HD12	2.34	0.48
1:D:24:SER:C	1:D:25:LYS:HD2	2.33	0.48
1:D:217:ILE:HG23	1:D:228:TRP:CD1	2.48	0.48
1:B:130:ARG:NH2	1:B:132:ARG:HG3	2.28	0.48
1:C:111:ASN:HD21	1:C:113:GLU:HB2	1.79	0.48
1:D:36:LEU:HD13	1:D:36:LEU:O	2.14	0.48
1:D:101:LYS:C	1:D:103:THR:H	2.16	0.48
1:D:130:ARG:HH12	1:D:292:ARG:NH2	2.12	0.48
1:A:100:TYR:CZ	1:A:342:LEU:HD22	2.49	0.47
1:B:132:ARG:CG	1:B:238:ILE:HG13	2.42	0.47
1:C:299:LEU:HD11	1:C:360:MET:HE3	1.96	0.47
1:D:281:LEU:HD12	1:D:281:LEU:N	2.29	0.47
1:A:354:VAL:HG23	1:A:355:ASP:N	2.29	0.47
1:C:129:SER:CB	1:C:295:VAL:HG12	2.44	0.47
1:C:295:VAL:HG23	1:C:297:VAL:HG13	1.96	0.47
1:A:165:LEU:HD11	1:A:260:ILE:HD11	1.95	0.47
1:A:180:THR:O	1:A:183:GLU:CD	2.53	0.47
1:C:245:ASN:O	1:C:247:LYS:N	2.48	0.47
1:D:116:LYS:H	1:D:351:GLN:NE2	2.11	0.47
1:D:132:ARG:HG2	1:D:238:ILE:HG13	1.96	0.47
1:D:184:GLN:HA	1:D:193:LEU:CD1	2.43	0.47
1:D:194:PHE:HD2	1:D:228:TRP:CD1	2.32	0.47
1:B:117:GLY:C	1:B:119:ASP:N	2.66	0.47
1:B:138:LYS:HG2	1:B:270:PRO:O	2.15	0.47
1:B:253:PHE:CE1	1:B:257:LEU:HD11	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:281:LEU:HD12	1:B:281:LEU:N	2.30	0.47
1:D:100:TYR:CZ	1:D:342:LEU:HD22	2.49	0.47
1:D:186:GLN:HE21	1:D:187:LEU:HD22	1.78	0.47
1:A:179:MET:HE1	1:A:187:LEU:HG	1.96	0.47
1:A:181:GLU:O	1:A:185:GLN:NE2	2.47	0.47
1:A:199:SER:OG	1:A:202:LEU:HD13	2.14	0.47
1:B:133:THR:HG23	1:B:237:VAL:HG13	1.97	0.47
1:B:194:PHE:HD2	1:B:228:TRP:CD1	2.33	0.47
1:C:181:GLU:C	1:C:183:GLU:N	2.66	0.47
1:D:181:GLU:C	1:D:183:GLU:N	2.68	0.47
1:C:33:VAL:HG21	1:C:91:PRO:HG3	1.96	0.47
1:A:33:VAL:HG21	1:A:91:PRO:HG3	1.97	0.47
1:A:103:THR:O	1:A:105:LYS:NZ	2.47	0.47
1:A:338:ASN:HD22	1:A:338:ASN:H	1.63	0.47
1:B:33:VAL:HG21	1:B:91:PRO:HG3	1.97	0.47
1:B:123:PRO:C	1:B:125:TYR:H	2.18	0.47
1:B:181:GLU:O	1:B:185:GLN:NE2	2.47	0.47
1:B:196:LYS:O	1:B:198:VAL:N	2.42	0.47
1:B:199:SER:OG	1:B:202:LEU:HD22	2.15	0.47
1:C:33:VAL:HG21	1:C:91:PRO:CG	2.45	0.47
1:C:188:ILE:CG1	1:C:193:LEU:HD21	2.45	0.47
1:D:138:LYS:HB2	1:D:138:LYS:HZ2	1.78	0.47
1:A:138:LYS:HA	1:A:272:MET:CE	2.45	0.47
1:A:143:PRO:HG2	1:A:233:ASP:HA	1.96	0.47
1:A:185:GLN:CA	1:A:188:ILE:HB	2.44	0.47
1:B:217:ILE:HG23	1:B:228:TRP:CD1	2.49	0.47
1:B:351:GLN:C	1:B:353:VAL:H	2.18	0.47
1:C:42:LEU:HD13	1:C:53:VAL:HG21	1.97	0.47
1:C:351:GLN:O	1:C:353:VAL:N	2.48	0.47
1:D:104:ASP:C	1:D:105:LYS:HZ3	2.18	0.47
1:A:132:ARG:HB3	1:A:238:ILE:CD1	2.44	0.47
1:B:179:MET:HG2	1:B:184:GLN:HG2	1.97	0.47
1:C:199:SER:OG	1:C:202:LEU:HD13	2.15	0.47
1:C:220:ASN:OD1	1:C:223:LYS:N	2.48	0.47
1:C:351:GLN:C	1:C:353:VAL:H	2.19	0.47
1:D:179:MET:HE1	1:D:187:LEU:HG	1.97	0.47
1:A:181:GLU:C	1:A:183:GLU:N	2.66	0.47
1:B:144:PRO:HA	1:B:207:MET:HB3	1.96	0.47
1:B:186:GLN:NE2	1:B:187:LEU:HD22	2.30	0.47
1:C:338:ASN:HD22	1:C:338:ASN:H	1.62	0.47
1:A:179:MET:CG	1:A:180:THR:N	2.78	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:116:LYS:H	1:B:351:GLN:NE2	2.12	0.46
1:B:143:PRO:HG2	1:B:233:ASP:HA	1.97	0.46
1:C:113:GLU:O	1:C:115:LEU:N	2.47	0.46
1:C:181:GLU:O	1:C:185:GLN:NE2	2.48	0.46
1:D:118:GLY:CA	1:D:354:VAL:HG21	2.44	0.46
1:D:179:MET:HG2	1:D:184:GLN:HG2	1.97	0.46
1:C:314:ARG:O	1:C:378:PRO:HA	2.15	0.46
1:C:365:LYS:HA	1:C:368:GLU:OE2	2.15	0.46
1:D:103:THR:O	1:D:105:LYS:NZ	2.47	0.46
1:D:138:LYS:HG2	1:D:270:PRO:O	2.14	0.46
1:D:179:MET:HG2	1:D:180:THR:N	2.31	0.46
1:D:179:MET:CG	1:D:180:THR:N	2.78	0.46
1:A:129:SER:CB	1:A:295:VAL:HG12	2.43	0.46
1:B:75:VAL:HB	1:B:282:THR:HG22	1.97	0.46
1:C:181:GLU:N	1:C:181:GLU:CD	2.61	0.46
1:C:305:HIS:CE1	1:C:307:LYS:HB2	2.50	0.46
1:D:129:SER:CB	1:D:295:VAL:HG12	2.43	0.46
1:D:188:ILE:HG13	1:D:193:LEU:HD21	1.97	0.46
1:A:188:ILE:CG1	1:A:193:LEU:HD21	2.45	0.46
1:A:356:GLY:HA3	1:A:381:LYS:O	2.16	0.46
1:B:188:ILE:CG1	1:B:193:LEU:HD21	2.46	0.46
1:B:365:LYS:HA	1:B:368:GLU:OE2	2.16	0.46
1:C:75:VAL:HB	1:C:282:THR:HG22	1.96	0.46
1:C:130:ARG:NH2	1:C:132:ARG:HG3	2.30	0.46
1:C:198:VAL:HA	1:C:203:LEU:CD1	2.43	0.46
1:C:369:LYS:HB2	1:C:369:LYS:HZ3	1.76	0.46
1:C:8:ASN:ND2	1:C:58:GLN:HG2	2.31	0.46
1:D:199:SER:OG	1:D:202:LEU:HD13	2.15	0.46
1:A:117:GLY:C	1:A:119:ASP:N	2.67	0.46
1:B:179:MET:CG	1:B:180:THR:N	2.78	0.46
1:C:51:PHE:CE2	1:C:56:VAL:HG12	2.50	0.46
1:C:143:PRO:HG2	1:C:233:ASP:HA	1.97	0.46
1:C:179:MET:CG	1:C:180:THR:N	2.79	0.46
1:D:15:LYS:HB3	1:D:17:GLU:OE1	2.16	0.46
1:D:180:THR:O	1:D:183:GLU:CD	2.54	0.46
1:D:217:ILE:HD12	1:D:228:TRP:NE1	2.31	0.46
1:A:354:VAL:HG22	1:A:355:ASP:H	1.80	0.46
1:B:100:TYR:CZ	1:B:342:LEU:HD22	2.51	0.46
1:B:237:VAL:C	1:B:238:ILE:HD12	2.36	0.46
1:C:273:TRP:CE3	1:C:273:TRP:C	2.89	0.46
1:D:186:GLN:NE2	1:D:187:LEU:HD22	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:314:ARG:O	1:D:378:PRO:HA	2.16	0.46
1:D:117:GLY:C	1:D:119:ASP:N	2.65	0.46
1:A:185:GLN:O	1:A:188:ILE:HB	2.16	0.46
1:A:273:TRP:CE3	1:A:273:TRP:C	2.89	0.46
1:B:118:GLY:CA	1:B:354:VAL:HG21	2.46	0.46
1:B:341:ARG:HH11	1:B:341:ARG:HG2	1.80	0.46
1:C:100:TYR:CZ	1:C:342:LEU:HD22	2.51	0.46
1:C:138:LYS:HG2	1:C:270:PRO:O	2.16	0.46
1:C:291:LEU:HD23	1:C:291:LEU:C	2.36	0.46
1:D:196:LYS:O	1:D:198:VAL:N	2.48	0.46
1:D:273:TRP:CE3	1:D:273:TRP:C	2.89	0.46
1:A:186:GLN:NE2	1:A:187:LEU:HD22	2.31	0.45
1:B:199:SER:OG	1:B:202:LEU:HD13	2.17	0.45
1:B:299:LEU:HD11	1:B:360:MET:HE3	1.97	0.45
1:B:351:GLN:C	1:B:353:VAL:N	2.70	0.45
1:B:354:VAL:HG23	1:B:355:ASP:N	2.30	0.45
1:D:33:VAL:HG21	1:D:91:PRO:HG3	1.99	0.45
1:B:378:PRO:O	1:B:379:ALA:HB3	2.16	0.45
1:C:217:ILE:HD12	1:C:228:TRP:NE1	2.32	0.45
1:D:144:PRO:HA	1:D:207:MET:HB3	1.98	0.45
1:A:198:VAL:HA	1:A:203:LEU:CD1	2.44	0.45
1:A:281:LEU:HD12	1:A:281:LEU:N	2.32	0.45
1:A:351:GLN:O	1:A:353:VAL:N	2.50	0.45
1:B:133:THR:HG22	1:B:253:PHE:HE1	1.82	0.45
1:C:138:LYS:HA	1:C:272:MET:CE	2.45	0.45
1:C:186:GLN:NE2	1:C:187:LEU:HD22	2.31	0.45
1:C:194:PHE:HD2	1:C:228:TRP:CD1	2.34	0.45
1:C:315:LEU:O	1:C:381:LYS:OXT	2.35	0.45
1:C:351:GLN:C	1:C:353:VAL:N	2.70	0.45
1:A:220:ASN:OD1	1:A:223:LYS:N	2.48	0.45
1:B:47:THR:HB	1:B:48:PRO:HD2	1.99	0.45
1:B:112:HIS:CD2	1:B:112:HIS:H	2.33	0.45
1:B:198:VAL:HA	1:B:203:LEU:CD1	2.43	0.45
1:B:237:VAL:CG1	1:B:257:LEU:HD21	2.43	0.45
1:C:183:GLU:CA	1:C:187:LEU:HD23	2.46	0.45
1:A:33:VAL:HG21	1:A:91:PRO:CG	2.47	0.45
1:A:101:LYS:C	1:A:103:THR:H	2.20	0.45
1:A:194:PHE:HD2	1:A:228:TRP:CD1	2.35	0.45
1:A:299:LEU:HD11	1:A:360:MET:HE3	1.98	0.45
1:D:194:PHE:HD2	1:D:228:TRP:CG	2.35	0.45
1:D:253:PHE:CE1	1:D:257:LEU:HD11	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:138:LYS:HD3	1:B:270:PRO:HG2	1.98	0.45
1:B:354:VAL:HG22	1:B:355:ASP:H	1.81	0.45
1:D:138:LYS:HA	1:D:272:MET:CE	2.47	0.45
1:D:185:GLN:O	1:D:188:ILE:HB	2.17	0.45
1:A:122:ASP:HA	1:A:123:PRO:HD3	1.85	0.45
1:A:351:GLN:C	1:A:353:VAL:H	2.20	0.45
1:B:26:HIS:CE1	1:B:64:PRO:HG3	2.51	0.45
1:D:47:THR:HB	1:D:48:PRO:HD2	1.99	0.45
1:D:295:VAL:HG23	1:D:297:VAL:HG13	1.98	0.45
1:A:365:LYS:HA	1:A:368:GLU:OE2	2.17	0.45
1:C:141:THR:OG1	1:C:150:GLU:OE1	2.34	0.45
1:C:250:PHE:CE1	1:C:350:VAL:HG21	2.52	0.45
1:D:123:PRO:C	1:D:125:TYR:H	2.20	0.45
1:D:132:ARG:CG	1:D:238:ILE:HG13	2.47	0.45
1:C:134:GLY:O	1:C:135:ARG:HG2	2.17	0.45
1:C:356:GLY:CA	1:C:381:LYS:O	2.65	0.45
1:D:122:ASP:HA	1:D:123:PRO:HD3	1.85	0.45
1:A:112:HIS:H	1:A:112:HIS:CD2	2.35	0.44
1:A:250:PHE:CE1	1:A:350:VAL:HG21	2.52	0.44
1:B:33:VAL:HG21	1:B:91:PRO:CG	2.46	0.44
1:C:131:VAL:HG12	1:C:253:PHE:CE1	2.52	0.44
1:C:280:VAL:HA	1:C:287:LEU:HD11	1.98	0.44
1:C:369:LYS:HB2	1:C:369:LYS:HZ2	1.80	0.44
1:A:183:GLU:CA	1:A:187:LEU:HD23	2.47	0.44
1:B:101:LYS:C	1:B:103:THR:H	2.19	0.44
1:D:183:GLU:CA	1:D:187:LEU:HD23	2.47	0.44
1:D:218:TRP:CE3	1:D:218:TRP:C	2.90	0.44
1:A:138:LYS:HG2	1:A:270:PRO:O	2.18	0.44
1:A:253:PHE:CE1	1:A:257:LEU:HD11	2.52	0.44
1:A:314:ARG:NE	1:A:378:PRO:HD3	2.32	0.44
1:A:315:LEU:O	1:A:381:LYS:OXT	2.36	0.44
1:A:356:GLY:CA	1:A:381:LYS:O	2.65	0.44
1:B:132:ARG:HB3	1:B:238:ILE:CD1	2.47	0.44
1:C:138:LYS:HD3	1:C:270:PRO:HG2	1.99	0.44
1:A:123:PRO:C	1:A:125:TYR:H	2.20	0.44
1:A:363:MET:O	1:A:364:GLU:C	2.56	0.44
1:B:23:LEU:CA	1:B:26:HIS:HD2	2.20	0.44
1:D:143:PRO:HG2	1:D:233:ASP:HA	1.98	0.44
1:D:320:ARG:HD2	1:D:320:ARG:N	2.33	0.44
1:D:356:GLY:HA3	1:D:381:LYS:O	2.18	0.44
1:A:351:GLN:C	1:A:353:VAL:N	2.71	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:320:ARG:HD2	1:B:320:ARG:N	2.32	0.44
1:C:11:LYS:HE2	1:C:11:LYS:HA	1.99	0.44
1:C:123:PRO:C	1:C:125:TYR:H	2.20	0.44
1:C:356:GLY:HA3	1:C:381:LYS:O	2.17	0.44
1:D:196:LYS:HA	1:D:197:PRO:HD3	1.87	0.44
1:A:23:LEU:CA	1:A:26:HIS:HD2	2.20	0.44
1:A:186:GLN:NE2	1:A:187:LEU:N	2.62	0.44
1:A:280:VAL:HA	1:A:287:LEU:CD1	2.48	0.44
1:C:305:HIS:O	1:C:308:PHE:HB2	2.17	0.44
1:D:112:HIS:CD2	1:D:112:HIS:H	2.36	0.44
1:D:137:ILE:HD12	1:D:137:ILE:N	2.33	0.44
1:D:277:LEU:O	1:D:288:GLY:HA2	2.17	0.44
1:A:11:LYS:HA	1:A:11:LYS:HE2	1.98	0.44
1:B:112:HIS:CD2	1:B:112:HIS:N	2.86	0.44
1:B:193:LEU:CB	1:B:217:ILE:HG13	2.48	0.44
1:B:194:PHE:HD2	1:B:228:TRP:CG	2.36	0.44
1:B:380:GLN:NE2	1:B:381:LYS:H	2.13	0.44
1:D:378:PRO:O	1:D:379:ALA:HB3	2.18	0.44
1:A:319:LYS:HA	1:A:335:ASP:O	2.18	0.44
1:B:36:LEU:HD13	1:B:36:LEU:O	2.17	0.44
1:B:96:ARG:HG3	1:B:96:ARG:HH11	1.83	0.44
1:B:295:VAL:HG23	1:B:297:VAL:HG13	2.00	0.44
1:B:356:GLY:CA	1:B:381:LYS:O	2.66	0.44
1:C:104:ASP:C	1:C:105:LYS:HZ3	2.21	0.44
1:C:116:LYS:H	1:C:351:GLN:NE2	2.13	0.44
1:C:196:LYS:O	1:C:198:VAL:N	2.45	0.44
1:A:305:HIS:O	1:A:308:PHE:HB2	2.18	0.44
1:B:356:GLY:HA3	1:B:381:LYS:O	2.18	0.44
1:C:47:THR:HB	1:C:48:PRO:HD2	2.00	0.44
1:C:253:PHE:CE1	1:C:257:LEU:HD11	2.53	0.44
1:C:363:MET:O	1:C:364:GLU:C	2.57	0.44
1:D:33:VAL:HG21	1:D:91:PRO:CG	2.48	0.44
1:D:192:PHE:CZ	1:D:223:LYS:HB3	2.53	0.44
1:A:15:LYS:HB3	1:A:17:GLU:OE1	2.18	0.43
1:A:118:GLY:CA	1:A:354:VAL:HG21	2.47	0.43
1:A:197:PRO:CB	1:A:202:LEU:HD23	2.46	0.43
1:B:363:MET:O	1:B:364:GLU:C	2.56	0.43
1:C:237:VAL:C	1:C:238:ILE:HD12	2.39	0.43
1:D:51:PHE:CE2	1:D:77:GLY:N	2.86	0.43
1:D:138:LYS:HA	1:D:272:MET:HE1	1.99	0.43
1:D:194:PHE:CD1	1:D:231:GLU:HG3	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:GLN:HB3	1:A:184:GLN:HE21	1.59	0.43
1:B:280:VAL:HA	1:B:287:LEU:CD1	2.48	0.43
1:C:194:PHE:HD2	1:C:228:TRP:CG	2.35	0.43
1:C:274:ASN:OD1	1:C:274:ASN:C	2.57	0.43
1:D:245:ASN:O	1:D:247:LYS:N	2.51	0.43
1:A:218:TRP:CE3	1:A:218:TRP:C	2.92	0.43
1:B:196:LYS:C	1:B:198:VAL:N	2.71	0.43
1:B:274:ASN:OD1	1:B:274:ASN:C	2.56	0.43
1:D:356:GLY:CA	1:D:381:LYS:O	2.66	0.43
1:A:193:LEU:CB	1:A:217:ILE:HG13	2.48	0.43
1:A:194:PHE:CE1	1:A:211:TRP:CH2	3.06	0.43
1:A:217:ILE:HD12	1:A:228:TRP:NE1	2.33	0.43
1:A:237:VAL:CG1	1:A:257:LEU:HD21	2.44	0.43
1:B:23:LEU:HD23	1:B:26:HIS:CD2	2.53	0.43
1:D:193:LEU:CB	1:D:217:ILE:HG13	2.49	0.43
1:D:220:ASN:OD1	1:D:223:LYS:N	2.52	0.43
1:D:250:PHE:CE1	1:D:350:VAL:HG21	2.53	0.43
1:D:299:LEU:HD13	1:D:302:LEU:CD2	2.47	0.43
1:D:305:HIS:O	1:D:308:PHE:HB2	2.18	0.43
1:A:315:LEU:CB	1:A:381:LYS:O	2.60	0.43
1:A:341:ARG:HG2	1:A:341:ARG:HH11	1.82	0.43
1:B:129:SER:CB	1:B:295:VAL:HG12	2.47	0.43
1:A:47:THR:HB	1:A:48:PRO:HD2	2.00	0.43
1:A:277:LEU:O	1:A:288:GLY:HA2	2.19	0.43
1:B:253:PHE:CZ	1:B:257:LEU:HD11	2.53	0.43
1:C:179:MET:HG2	1:C:184:GLN:HG2	2.00	0.43
1:C:218:TRP:CE3	1:C:218:TRP:C	2.92	0.43
1:C:299:LEU:HD13	1:C:302:LEU:CD2	2.46	0.43
1:D:8:ASN:ND2	1:D:58:GLN:HG2	2.33	0.43
1:D:237:VAL:C	1:D:238:ILE:HD12	2.39	0.43
1:A:248:GLU:CD	1:A:251:ARG:HH11	2.22	0.43
1:A:293:GLY:N	1:A:338:ASN:ND2	2.67	0.43
1:B:135:ARG:HD2	1:B:271:PHE:CG	2.53	0.43
1:B:135:ARG:HG2	1:B:135:ARG:HH11	1.84	0.43
1:B:280:VAL:HA	1:B:287:LEU:HD11	2.01	0.43
1:D:96:ARG:HG3	1:D:96:ARG:HH11	1.83	0.43
1:D:315:LEU:O	1:D:381:LYS:OXT	2.37	0.43
1:D:380:GLN:NE2	1:D:381:LYS:H	2.15	0.43
1:A:193:LEU:N	1:A:193:LEU:HD23	2.33	0.43
1:B:134:GLY:O	1:B:135:ARG:HG2	2.19	0.43
1:B:183:GLU:CA	1:B:187:LEU:HD23	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:245:ASN:O	1:B:247:LYS:N	2.52	0.43
1:B:305:HIS:O	1:B:308:PHE:HB2	2.19	0.43
1:C:11:LYS:HA	1:C:11:LYS:CE	2.48	0.43
1:D:186:GLN:NE2	1:D:187:LEU:N	2.62	0.43
1:D:280:VAL:HA	1:D:287:LEU:CD1	2.48	0.43
1:D:305:HIS:CE1	1:D:307:LYS:HB2	2.53	0.43
1:A:116:LYS:H	1:A:351:GLN:NE2	2.14	0.43
1:B:117:GLY:O	1:B:118:GLY:C	2.56	0.43
1:B:194:PHE:CD1	1:B:231:GLU:HG3	2.54	0.43
1:D:250:PHE:CZ	1:D:254:CYS:SG	3.12	0.43
1:D:315:LEU:CB	1:D:381:LYS:O	2.61	0.43
1:A:11:LYS:HA	1:A:11:LYS:CE	2.49	0.43
1:A:122:ASP:CG	1:A:125:TYR:CD1	2.88	0.43
1:B:179:MET:HE1	1:B:193:LEU:HB3	2.01	0.43
1:B:193:LEU:N	1:B:193:LEU:HD23	2.33	0.43
1:B:315:LEU:HD22	1:B:381:LYS:HB3	2.01	0.43
1:C:23:LEU:HD23	1:C:26:HIS:CD2	2.54	0.43
1:C:112:HIS:H	1:C:112:HIS:CD2	2.35	0.43
1:D:11:LYS:HE2	1:D:11:LYS:HA	2.01	0.43
1:D:274:ASN:OD1	1:D:274:ASN:C	2.57	0.43
1:D:351:GLN:O	1:D:353:VAL:N	2.52	0.43
1:D:363:MET:O	1:D:364:GLU:C	2.57	0.43
1:A:192:PHE:CZ	1:A:223:LYS:HB3	2.54	0.42
1:B:250:PHE:CE1	1:B:350:VAL:HG21	2.54	0.42
1:C:101:LYS:C	1:C:103:THR:H	2.23	0.42
1:C:118:GLY:HA2	1:C:354:VAL:CG2	2.49	0.42
1:C:122:ASP:CG	1:C:125:TYR:CD1	2.88	0.42
1:C:248:GLU:CD	1:C:251:ARG:HH11	2.23	0.42
1:C:380:GLN:NE2	1:C:381:LYS:H	2.17	0.42
1:D:29:HIS:HB2	1:D:72:VAL:O	2.19	0.42
1:D:314:ARG:NE	1:D:378:PRO:HD3	2.34	0.42
1:A:75:VAL:HB	1:A:282:THR:CG2	2.49	0.42
1:A:237:VAL:C	1:A:238:ILE:HD12	2.40	0.42
1:A:320:ARG:HD2	1:A:320:ARG:N	2.33	0.42
1:B:104:ASP:C	1:B:105:LYS:HZ1	2.23	0.42
1:B:199:SER:C	1:B:201:LEU:N	2.71	0.42
1:C:15:LYS:HB3	1:C:17:GLU:OE1	2.19	0.42
1:C:320:ARG:HD2	1:C:320:ARG:N	2.34	0.42
1:D:351:GLN:C	1:D:353:VAL:H	2.22	0.42
1:A:111:ASN:HD21	1:A:113:GLU:HB2	1.84	0.42
1:A:159:VAL:O	1:A:160:GLU:C	2.57	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:354:VAL:HG23	1:D:355:ASP:N	2.33	0.42
1:B:137:ILE:HD12	1:B:137:ILE:N	2.34	0.42
1:B:162:LEU:HD22	1:B:218:TRP:CD2	2.54	0.42
1:B:179:MET:HE1	1:B:187:LEU:HG	2.00	0.42
1:C:83:GLU:O	1:C:86:LYS:HB2	2.20	0.42
1:C:250:PHE:CZ	1:C:254:CYS:SG	3.12	0.42
1:C:315:LEU:CB	1:C:381:LYS:O	2.62	0.42
1:D:351:GLN:C	1:D:353:VAL:N	2.73	0.42
1:A:54:ASP:O	1:A:58:GLN:HB2	2.20	0.42
1:A:179:MET:HG2	1:A:184:GLN:HG2	2.01	0.42
1:B:314:ARG:HG2	1:B:378:PRO:HG3	2.01	0.42
1:C:194:PHE:CD1	1:C:231:GLU:HG3	2.55	0.42
1:C:196:LYS:HB3	1:C:198:VAL:HG13	2.01	0.42
1:D:179:MET:CG	1:D:180:THR:H	2.32	0.42
1:A:138:LYS:HD3	1:A:270:PRO:HG2	2.01	0.42
1:A:188:ILE:HG13	1:A:193:LEU:HD21	2.02	0.42
1:A:194:PHE:HD2	1:A:228:TRP:CG	2.36	0.42
1:B:122:ASP:HA	1:B:123:PRO:HD3	1.85	0.42
1:B:291:LEU:C	1:B:291:LEU:HD23	2.40	0.42
1:C:113:GLU:C	1:C:115:LEU:H	2.22	0.42
1:D:11:LYS:HA	1:D:11:LYS:CE	2.50	0.42
1:D:53:VAL:C	1:D:55:ASP:N	2.72	0.42
1:D:151:ARG:NH2	1:D:210:ASP:OD2	2.52	0.42
1:A:196:LYS:O	1:A:198:VAL:N	2.44	0.42
1:A:380:GLN:NE2	1:A:381:LYS:H	2.17	0.42
1:C:184:GLN:HB3	1:C:184:GLN:HE21	1.57	0.42
1:C:198:VAL:HA	1:C:203:LEU:HD21	2.01	0.42
1:A:8:ASN:ND2	1:A:58:GLN:HG2	2.34	0.42
1:A:138:LYS:HB3	1:A:272:MET:HB3	2.01	0.42
1:A:291:LEU:HD23	1:A:291:LEU:C	2.40	0.42
1:B:192:PHE:CZ	1:B:223:LYS:HB3	2.55	0.42
1:C:121:LEU:HD13	1:C:126:VAL:CG2	2.41	0.42
1:D:138:LYS:HD3	1:D:270:PRO:HG2	2.01	0.42
1:D:194:PHE:CE1	1:D:211:TRP:CH2	3.08	0.42
1:D:198:VAL:HA	1:D:203:LEU:CG	2.50	0.42
1:D:248:GLU:CD	1:D:251:ARG:HH11	2.22	0.42
1:A:112:HIS:CD2	1:A:112:HIS:N	2.87	0.42
1:A:180:THR:N	1:A:183:GLU:OE1	2.53	0.42
1:B:183:GLU:HG2	1:B:184:GLN:N	2.35	0.42
1:B:248:GLU:CD	1:B:251:ARG:HH11	2.22	0.42
1:C:281:LEU:HD12	1:C:281:LEU:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:112:HIS:CD2	1:D:112:HIS:N	2.87	0.42
1:A:96:ARG:HG3	1:A:96:ARG:HH11	1.85	0.42
1:A:179:MET:HE1	1:A:193:LEU:HB3	2.01	0.42
1:A:245:ASN:O	1:A:247:LYS:N	2.53	0.42
1:B:198:VAL:HA	1:B:203:LEU:HD21	2.02	0.42
1:C:112:HIS:CD2	1:C:112:HIS:N	2.87	0.42
1:C:199:SER:CB	1:C:202:LEU:HD22	2.49	0.42
1:D:29:HIS:HB3	1:D:92:ILE:HG23	2.02	0.42
1:D:131:VAL:HG12	1:D:253:PHE:CE1	2.54	0.42
1:D:354:VAL:HG22	1:D:355:ASP:H	1.84	0.42
1:A:364:GLU:O	1:A:367:LEU:HB2	2.20	0.41
1:B:273:TRP:CE3	1:B:273:TRP:C	2.93	0.41
1:C:53:VAL:O	1:C:54:ASP:C	2.58	0.41
1:C:193:LEU:CB	1:C:217:ILE:HG13	2.49	0.41
1:D:111:ASN:HD21	1:D:113:GLU:HB2	1.84	0.41
1:D:135:ARG:HD2	1:D:271:PHE:CG	2.55	0.41
1:D:193:LEU:N	1:D:193:LEU:HD23	2.34	0.41
1:A:138:LYS:NZ	1:A:138:LYS:CB	2.81	0.41
1:A:198:VAL:HA	1:A:203:LEU:HD21	2.02	0.41
1:B:11:LYS:HA	1:B:11:LYS:CE	2.50	0.41
1:C:86:LYS:CG	1:C:90:ASP:OD2	2.69	0.41
1:C:199:SER:C	1:C:201:LEU:N	2.74	0.41
1:D:291:LEU:C	1:D:291:LEU:HD23	2.40	0.41
1:A:196:LYS:HB3	1:A:198:VAL:HG13	2.02	0.41
1:B:51:PHE:CE2	1:B:77:GLY:N	2.88	0.41
1:B:196:LYS:HB3	1:B:198:VAL:HG13	2.02	0.41
1:B:197:PRO:CB	1:B:202:LEU:HD23	2.48	0.41
1:B:354:VAL:HG22	1:B:355:ASP:N	2.35	0.41
1:C:51:PHE:CE2	1:C:77:GLY:N	2.88	0.41
1:C:193:LEU:HD23	1:C:193:LEU:N	2.35	0.41
1:C:199:SER:HG	1:C:202:LEU:H	1.64	0.41
1:C:277:LEU:O	1:C:288:GLY:HA2	2.20	0.41
1:D:186:GLN:O	1:D:190:ASP:HB2	2.21	0.41
1:A:9:LYS:HG3	1:A:10:PHE:H	1.85	0.41
1:A:194:PHE:CD1	1:A:231:GLU:HG3	2.55	0.41
1:A:354:VAL:HG22	1:A:355:ASP:N	2.35	0.41
1:B:15:LYS:HB3	1:B:17:GLU:OE1	2.21	0.41
1:C:78:ASP:HB3	1:C:141:THR:HG22	2.02	0.41
1:D:138:LYS:HB3	1:D:272:MET:HB3	2.02	0.41
1:D:196:LYS:HB3	1:D:198:VAL:HG13	2.02	0.41
1:D:341:ARG:HG2	1:D:341:ARG:HH11	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:GLU:HB2	1:A:272:MET:SD	2.60	0.41
1:A:131:VAL:HG12	1:A:253:PHE:CE1	2.55	0.41
1:A:135:ARG:HD2	1:A:271:PHE:CG	2.56	0.41
1:B:11:LYS:HA	1:B:11:LYS:HE2	2.01	0.41
1:B:274:ASN:OD1	1:B:276:HIS:N	2.48	0.41
1:C:196:LYS:HA	1:C:197:PRO:HD3	1.86	0.41
1:D:86:LYS:CG	1:D:90:ASP:OD2	2.69	0.41
1:D:199:SER:HG	1:D:202:LEU:HB2	1.85	0.41
1:B:261:GLU:HB2	1:B:271:PHE:CE2	2.56	0.41
1:C:96:ARG:HG3	1:C:96:ARG:HH11	1.85	0.41
1:A:26:HIS:HE1	1:A:64:PRO:HG3	1.85	0.41
1:B:113:GLU:O	1:B:115:LEU:N	2.53	0.41
1:B:180:THR:N	1:B:183:GLU:OE1	2.53	0.41
1:B:198:VAL:HA	1:B:203:LEU:CG	2.51	0.41
1:B:218:TRP:CE3	1:B:218:TRP:C	2.93	0.41
1:B:315:LEU:HD22	1:B:381:LYS:O	2.20	0.41
1:C:53:VAL:C	1:C:55:ASP:N	2.73	0.41
1:C:194:PHE:CE1	1:C:211:TRP:CH2	3.09	0.41
1:D:171:GLY:CA	1:D:220:ASN:HA	2.51	0.41
1:A:78:ASP:OD2	1:A:81:SER:OG	2.24	0.41
1:B:9:LYS:HG3	1:B:10:PHE:H	1.86	0.41
1:B:29:HIS:HB3	1:B:92:ILE:HG23	2.03	0.41
1:B:105:LYS:NZ	1:B:105:LYS:N	2.69	0.41
1:B:185:GLN:CD	1:B:186:GLN:N	2.74	0.41
1:C:13:ASN:HD22	1:C:13:ASN:HA	1.67	0.41
1:C:138:LYS:HB3	1:C:272:MET:HB3	2.02	0.41
1:C:198:VAL:HA	1:C:203:LEU:CG	2.51	0.41
1:C:293:GLY:N	1:C:338:ASN:ND2	2.68	0.41
1:D:261:GLU:HB2	1:D:271:PHE:CE2	2.55	0.41
1:A:29:HIS:HB2	1:A:72:VAL:O	2.20	0.41
1:A:196:LYS:C	1:A:198:VAL:N	2.72	0.41
1:A:198:VAL:HA	1:A:203:LEU:CG	2.51	0.41
1:A:261:GLU:HB2	1:A:271:PHE:CE2	2.56	0.41
1:B:53:VAL:C	1:B:55:ASP:N	2.72	0.41
1:B:54:ASP:O	1:B:58:GLN:HB2	2.21	0.41
1:B:171:GLY:CA	1:B:220:ASN:HA	2.51	0.41
1:B:196:LYS:HA	1:B:197:PRO:HD3	1.89	0.41
1:B:260:ILE:HG22	1:B:264:PHE:CD1	2.56	0.41
1:C:179:MET:HE1	1:C:193:LEU:HB3	2.03	0.41
1:C:190:ASP:CB	1:C:192:PHE:CE2	3.04	0.41
1:D:75:VAL:HB	1:D:282:THR:CG2	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:250:PHE:CG	1:D:250:PHE:O	2.73	0.41
1:A:137:ILE:HD12	1:A:137:ILE:N	2.36	0.41
1:B:101:LYS:C	1:B:103:THR:N	2.74	0.41
1:C:29:HIS:HB3	1:C:92:ILE:HG23	2.02	0.41
1:D:298:LYS:HB2	1:D:333:VAL:HG12	2.01	0.41
1:B:175:PRO:HG2	1:B:178:SER:OG	2.21	0.40
1:C:135:ARG:HD2	1:C:271:PHE:CG	2.56	0.40
1:C:196:LYS:C	1:C:198:VAL:N	2.73	0.40
1:D:100:TYR:CZ	1:D:105:LYS:O	2.75	0.40
1:D:196:LYS:C	1:D:198:VAL:N	2.74	0.40
1:D:197:PRO:CB	1:D:202:LEU:HD23	2.51	0.40
1:D:253:PHE:CZ	1:D:257:LEU:HD11	2.55	0.40
1:C:54:ASP:O	1:C:58:GLN:HB2	2.22	0.40
1:C:180:THR:O	1:C:182:LYS:N	2.54	0.40
1:C:185:GLN:CD	1:C:186:GLN:N	2.74	0.40
1:C:192:PHE:CZ	1:C:223:LYS:HB3	2.56	0.40
1:D:101:LYS:C	1:D:103:THR:N	2.74	0.40
1:D:184:GLN:HB3	1:D:184:GLN:HE21	1.58	0.40
1:D:185:GLN:CD	1:D:186:GLN:N	2.75	0.40
1:A:314:ARG:HG2	1:A:378:PRO:HG3	2.02	0.40
1:A:378:PRO:O	1:A:379:ALA:HB3	2.21	0.40
1:B:138:LYS:HA	1:B:272:MET:HE1	2.03	0.40
1:B:226:LEU:HD12	1:B:226:LEU:N	2.37	0.40
1:C:202:LEU:CD1	1:C:202:LEU:N	2.84	0.40
1:C:314:ARG:HG2	1:C:378:PRO:HG3	2.04	0.40
1:D:122:ASP:CG	1:D:125:TYR:CD1	2.89	0.40
1:D:138:LYS:NZ	1:D:138:LYS:CB	2.81	0.40
1:D:180:THR:N	1:D:183:GLU:OE1	2.55	0.40
1:A:24:SER:O	1:A:25:LYS:HD2	2.20	0.40
1:A:196:LYS:O	1:A:198:VAL:HG13	2.22	0.40
1:A:197:PRO:CA	1:A:202:LEU:HD23	2.51	0.40
1:B:131:VAL:HG12	1:B:253:PHE:CE1	2.56	0.40
1:B:193:LEU:N	1:B:193:LEU:CD2	2.84	0.40
1:B:315:LEU:O	1:B:381:LYS:OXT	2.39	0.40
1:D:132:ARG:HB3	1:D:238:ILE:CD1	2.49	0.40
1:A:193:LEU:N	1:A:193:LEU:CD2	2.84	0.40
1:A:299:LEU:HD13	1:A:302:LEU:CD2	2.46	0.40
1:B:187:LEU:CB	1:B:192:PHE:HB2	2.51	0.40
1:B:188:ILE:HG13	1:B:193:LEU:HD21	2.04	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:18:GLU:O	1:D:152:ARG:NH1[6_566]	1.99	0.21

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	361/381 (95%)	281 (78%)	64 (18%)	16 (4%)	2	21
1	B	361/381 (95%)	284 (79%)	61 (17%)	16 (4%)	2	21
1	C	361/381 (95%)	279 (77%)	66 (18%)	16 (4%)	2	21
1	D	361/381 (95%)	281 (78%)	64 (18%)	16 (4%)	2	21
All	All	1444/1524 (95%)	1125 (78%)	255 (18%)	64 (4%)	2	21

All (64) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	119	ASP
1	A	181	GLU
1	A	198	VAL
1	B	119	ASP
1	B	181	GLU
1	B	198	VAL
1	C	119	ASP
1	C	181	GLU
1	C	198	VAL
1	D	119	ASP
1	D	181	GLU
1	D	198	VAL
1	A	184	GLN
1	A	246	MET
1	B	117	GLY
1	B	184	GLN
1	B	246	MET

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Mol	Chain	Res	Type
1	C	117	GLY
1	C	184	GLN
1	C	246	MET
1	D	117	GLY
1	D	184	GLN
1	A	117	GLY
1	A	191	HIS
1	A	193	LEU
1	A	352	LEU
1	B	191	HIS
1	B	352	LEU
1	C	114	ASN
1	C	191	HIS
1	C	352	LEU
1	D	180	THR
1	D	191	HIS
1	D	193	LEU
1	D	246	MET
1	D	352	LEU
1	A	180	THR
1	A	231	GLU
1	A	378	PRO
1	B	114	ASN
1	B	180	THR
1	B	193	LEU
1	B	231	GLU
1	C	180	THR
1	C	193	LEU
1	C	231	GLU
1	C	378	PRO
1	D	114	ASN
1	D	231	GLU
1	A	114	ASN
1	A	197	PRO
1	B	197	PRO
1	B	378	PRO
1	C	186	GLN
1	C	197	PRO
1	D	197	PRO
1	D	378	PRO
1	A	244	GLY
1	B	244	GLY

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Mol	Chain	Res	Type
1	B	370	GLY
1	C	244	GLY
1	D	102	PRO
1	D	244	GLY
1	A	370	GLY

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	318/335 (95%)	268 (84%)	50 (16%)	2	15
1	B	318/335 (95%)	268 (84%)	50 (16%)	2	15
1	C	318/335 (95%)	267 (84%)	51 (16%)	2	14
1	D	318/335 (95%)	269 (85%)	49 (15%)	2	16
All	All	1272/1340 (95%)	1072 (84%)	200 (16%)	2	15

All (200) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	LYS
1	A	27	ASN
1	A	42	LEU
1	A	43	ARG
1	A	53	VAL
1	A	54	ASP
1	A	56	VAL
1	A	57	ILE
1	A	69	ILE
1	A	80	GLU
1	A	88	LEU
1	A	105	LYS
1	A	112	HIS
1	A	121	LEU
1	A	130	ARG
1	A	138	LYS

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Mol	Chain	Res	Type
1	A	143	PRO
1	A	157	LEU
1	A	160	GLU
1	A	180	THR
1	A	181	GLU
1	A	184	GLN
1	A	185	GLN
1	A	186	GLN
1	A	189	ASP
1	A	191	HIS
1	A	193	LEU
1	A	202	LEU
1	A	236	ARG
1	A	237	VAL
1	A	240	MET
1	A	245	ASN
1	A	247	LYS
1	A	273	TRP
1	A	275	GLN
1	A	280	VAL
1	A	286	ASN
1	A	287	LEU
1	A	304	LYS
1	A	309	GLU
1	A	319	LYS
1	A	320	ARG
1	A	338	ASN
1	A	346	GLU
1	A	352	LEU
1	A	354	VAL
1	A	369	LYS
1	A	374	ASP
1	A	376	MET
1	A	380	GLN
1	B	11	LYS
1	B	27	ASN
1	B	42	LEU
1	B	43	ARG
1	B	53	VAL
1	B	54	ASP
1	B	56	VAL
1	B	57	ILE

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Mol	Chain	Res	Type
1	B	69	ILE
1	B	80	GLU
1	B	88	LEU
1	B	105	LYS
1	B	112	HIS
1	B	121	LEU
1	B	130	ARG
1	B	138	LYS
1	B	143	PRO
1	B	157	LEU
1	B	160	GLU
1	B	180	THR
1	B	181	GLU
1	B	184	GLN
1	B	185	GLN
1	B	186	GLN
1	B	187	LEU
1	B	189	ASP
1	B	191	HIS
1	B	193	LEU
1	B	202	LEU
1	B	236	ARG
1	B	237	VAL
1	B	240	MET
1	B	245	ASN
1	B	273	TRP
1	B	275	GLN
1	B	280	VAL
1	B	286	ASN
1	B	287	LEU
1	B	304	LYS
1	B	309	GLU
1	B	319	LYS
1	B	320	ARG
1	B	338	ASN
1	B	346	GLU
1	B	352	LEU
1	B	354	VAL
1	B	369	LYS
1	B	374	ASP
1	B	376	MET
1	B	380	GLN

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Mol	Chain	Res	Type
1	C	11	LYS
1	C	27	ASN
1	C	42	LEU
1	C	43	ARG
1	C	53	VAL
1	C	54	ASP
1	C	56	VAL
1	C	57	ILE
1	C	69	ILE
1	C	80	GLU
1	C	88	LEU
1	C	105	LYS
1	C	112	HIS
1	C	121	LEU
1	C	130	ARG
1	C	138	LYS
1	C	143	PRO
1	C	157	LEU
1	C	160	GLU
1	C	180	THR
1	C	181	GLU
1	C	184	GLN
1	C	185	GLN
1	C	186	GLN
1	C	187	LEU
1	C	189	ASP
1	C	191	HIS
1	C	193	LEU
1	C	202	LEU
1	C	236	ARG
1	C	237	VAL
1	C	240	MET
1	C	245	ASN
1	C	247	LYS
1	C	273	TRP
1	C	275	GLN
1	C	280	VAL
1	C	286	ASN
1	C	287	LEU
1	C	304	LYS
1	C	309	GLU
1	C	319	LYS

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Mol	Chain	Res	Type
1	C	320	ARG
1	C	338	ASN
1	C	346	GLU
1	C	352	LEU
1	C	354	VAL
1	C	369	LYS
1	C	374	ASP
1	C	376	MET
1	C	380	GLN
1	D	11	LYS
1	D	27	ASN
1	D	42	LEU
1	D	43	ARG
1	D	53	VAL
1	D	54	ASP
1	D	56	VAL
1	D	57	ILE
1	D	69	ILE
1	D	80	GLU
1	D	88	LEU
1	D	105	LYS
1	D	112	HIS
1	D	121	LEU
1	D	130	ARG
1	D	138	LYS
1	D	143	PRO
1	D	157	LEU
1	D	160	GLU
1	D	180	THR
1	D	181	GLU
1	D	184	GLN
1	D	185	GLN
1	D	186	GLN
1	D	189	ASP
1	D	191	HIS
1	D	193	LEU
1	D	202	LEU
1	D	236	ARG
1	D	237	VAL
1	D	240	MET
1	D	245	ASN
1	D	273	TRP

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Mol	Chain	Res	Type
1	D	275	GLN
1	D	280	VAL
1	D	286	ASN
1	D	287	LEU
1	D	304	LYS
1	D	309	GLU
1	D	319	LYS
1	D	320	ARG
1	D	338	ASN
1	D	346	GLU
1	D	352	LEU
1	D	354	VAL
1	D	369	LYS
1	D	374	ASP
1	D	376	MET
1	D	380	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (71) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	ASN
1	A	13	ASN
1	A	26	HIS
1	A	27	ASN
1	A	111	ASN
1	A	114	ASN
1	A	145	HIS
1	A	163	ASN
1	A	184	GLN
1	A	186	GLN
1	A	219	HIS
1	A	230	ASN
1	A	245	ASN
1	A	275	GLN
1	A	301	HIS
1	A	338	ASN
1	A	349	GLN
1	A	351	GLN
1	B	8	ASN
1	B	13	ASN
1	B	26	HIS
1	B	111	ASN

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Mol	Chain	Res	Type
1	B	114	ASN
1	B	145	HIS
1	B	163	ASN
1	B	184	GLN
1	B	186	GLN
1	B	230	ASN
1	B	245	ASN
1	B	275	GLN
1	B	301	HIS
1	B	338	ASN
1	B	349	GLN
1	B	351	GLN
1	C	8	ASN
1	C	13	ASN
1	C	26	HIS
1	C	27	ASN
1	C	111	ASN
1	C	114	ASN
1	C	145	HIS
1	C	163	ASN
1	C	184	GLN
1	C	186	GLN
1	C	219	HIS
1	C	245	ASN
1	C	275	GLN
1	C	296	HIS
1	C	301	HIS
1	C	338	ASN
1	C	349	GLN
1	C	351	GLN
1	D	8	ASN
1	D	13	ASN
1	D	26	HIS
1	D	27	ASN
1	D	111	ASN
1	D	114	ASN
1	D	145	HIS
1	D	163	ASN
1	D	184	GLN
1	D	186	GLN
1	D	219	HIS
1	D	230	ASN

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Mol	Chain	Res	Type
1	D	245	ASN
1	D	275	GLN
1	D	296	HIS
1	D	301	HIS
1	D	338	ASN
1	D	349	GLN
1	D	351	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	365/381 (95%)	-0.17	18 (4%) 29 26	6, 46, 93, 100	0
1	B	365/381 (95%)	-0.51	11 (3%) 50 44	2, 23, 85, 100	0
1	C	365/381 (95%)	-0.28	15 (4%) 37 33	5, 42, 93, 100	0
1	D	365/381 (95%)	-0.40	10 (2%) 54 48	2, 31, 83, 100	0
All	All	1460/1524 (95%)	-0.34	54 (3%) 41 37	2, 36, 91, 100	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	193	LEU	6.7
1	A	322	THR	6.4
1	A	200	PRO	6.0
1	D	200	PRO	5.9
1	A	195	ASP	5.8
1	D	193	LEU	5.4
1	D	195	ASP	5.2
1	C	193	LEU	5.1
1	C	200	PRO	4.1
1	A	194	PHE	4.0
1	B	190	ASP	3.7
1	C	204	ALA	3.5
1	D	8	ASN	3.4
1	A	192	PHE	3.3
1	B	8	ASN	3.2
1	D	192	PHE	3.1
1	D	196	LYS	3.1
1	B	322	THR	2.9
1	C	190	ASP	2.9
1	A	198	VAL	2.8
1	C	186	GLN	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	190	ASP	2.7
1	B	193	LEU	2.7
1	A	372	SER	2.7
1	B	195	ASP	2.7
1	B	189	ASP	2.7
1	C	67	PRO	2.7
1	B	200	PRO	2.6
1	C	195	ASP	2.6
1	C	192	PHE	2.6
1	C	199	SER	2.6
1	B	192	PHE	2.6
1	B	199	SER	2.5
1	A	170	LYS	2.5
1	A	186	GLN	2.5
1	C	127	LEU	2.5
1	C	185	GLN	2.4
1	D	322	THR	2.4
1	A	8	ASN	2.4
1	B	204	ALA	2.4
1	C	380	GLN	2.4
1	A	380	GLN	2.3
1	D	186	GLN	2.3
1	A	321	GLY	2.3
1	A	171	GLY	2.2
1	A	191	HIS	2.2
1	A	67	PRO	2.1
1	C	300	ALA	2.1
1	C	8	ASN	2.1
1	B	186	GLN	2.1
1	A	172	LYS	2.0
1	C	375	ASP	2.0
1	D	191	HIS	2.0
1	A	117	GLY	2.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.