



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 12, 2024 – 01:01 PM EDT

PDB ID : 2VL0
Title : X-ray structure of a pentameric ligand gated ion channel from *Erwinia chrysanthemi* (ELIC)
Authors : Hilf, R.J.C.; Dutzler, R.
Deposited on : 2008-01-07
Resolution : 3.30 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:

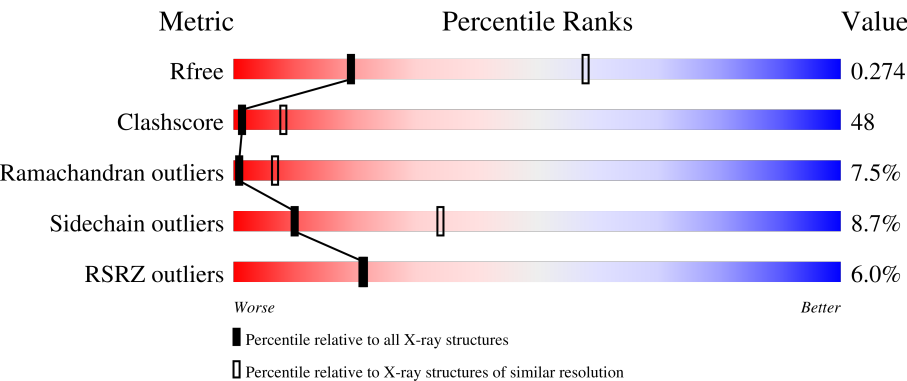
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation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

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.30 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	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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	321	<div><div>8%</div><div><div></div><div>33%</div><div>52%</div><div>9%</div><div>• 5%</div></div></div>
1	B	321	<div><div>4%</div><div><div></div><div>32%</div><div>53%</div><div>9%</div><div>• 5%</div></div></div>
1	C	321	<div><div>3%</div><div><div></div><div>31%</div><div>53%</div><div>11%</div><div>• 5%</div></div></div>
1	D	321	<div><div>6%</div><div><div></div><div>34%</div><div>51%</div><div>10%</div><div>• 5%</div></div></div>
1	E	321	<div><div>4%</div><div><div></div><div>34%</div><div>50%</div><div>10%</div><div>• 5%</div></div></div>

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Mol	Chain	Length	Quality of chain
1	F	321	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>6%33%52%9%• 5%</div></div>
1	G	321	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>6%35%50%10%• 5%</div></div>
1	H	321	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>7%35%50%10%• 5%</div></div>
1	I	321	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>7%35%50%10%• 5%</div></div>
1	J	321	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>5%35%51%9%• 5%</div></div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 25010 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 Cys-loop ligand-gated ion channel.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	306	Total	C	N	O	S	0	0	0
			2501	1631	415	449	6			
1	B	306	Total	C	N	O	S	0	0	0
			2501	1631	415	449	6			
1	C	306	Total	C	N	O	S	0	0	0
			2501	1631	415	449	6			
1	D	306	Total	C	N	O	S	0	0	0
			2501	1631	415	449	6			
1	E	306	Total	C	N	O	S	0	0	0
			2501	1631	415	449	6			
1	F	306	Total	C	N	O	S	0	0	0
			2501	1631	415	449	6			
1	G	306	Total	C	N	O	S	0	0	0
			2501	1631	415	449	6			
1	H	306	Total	C	N	O	S	0	0	0
			2501	1631	415	449	6			
1	I	306	Total	C	N	O	S	0	0	0
			2501	1631	415	449	6			
1	J	306	Total	C	N	O	S	0	0	0
			2501	1631	415	449	6			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	288	ASN	MET	conflict	UNP P0C7B7
B	288	ASN	MET	conflict	UNP P0C7B7
C	288	ASN	MET	conflict	UNP P0C7B7
D	288	ASN	MET	conflict	UNP P0C7B7
E	288	ASN	MET	conflict	UNP P0C7B7
F	288	ASN	MET	conflict	UNP P0C7B7
G	288	ASN	MET	conflict	UNP P0C7B7
H	288	ASN	MET	conflict	UNP P0C7B7
I	288	ASN	MET	conflict	UNP P0C7B7

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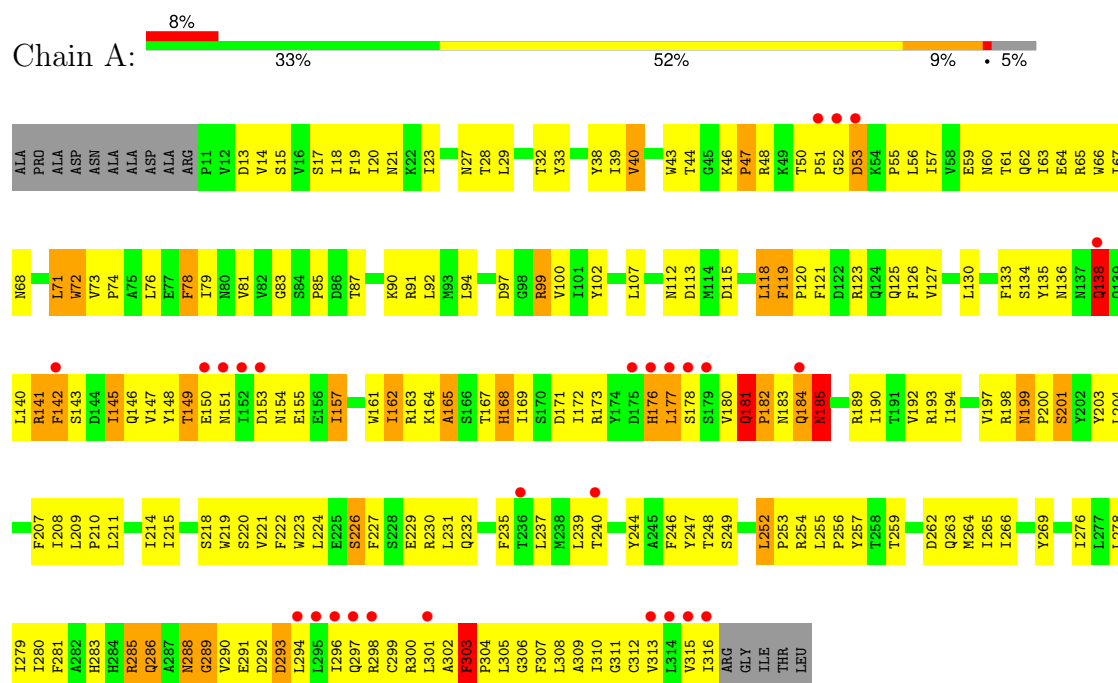
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Chain	Residue	Modelled	Actual	Comment	Reference
J	288	ASN	MET	conflict	UNP P0C7B7

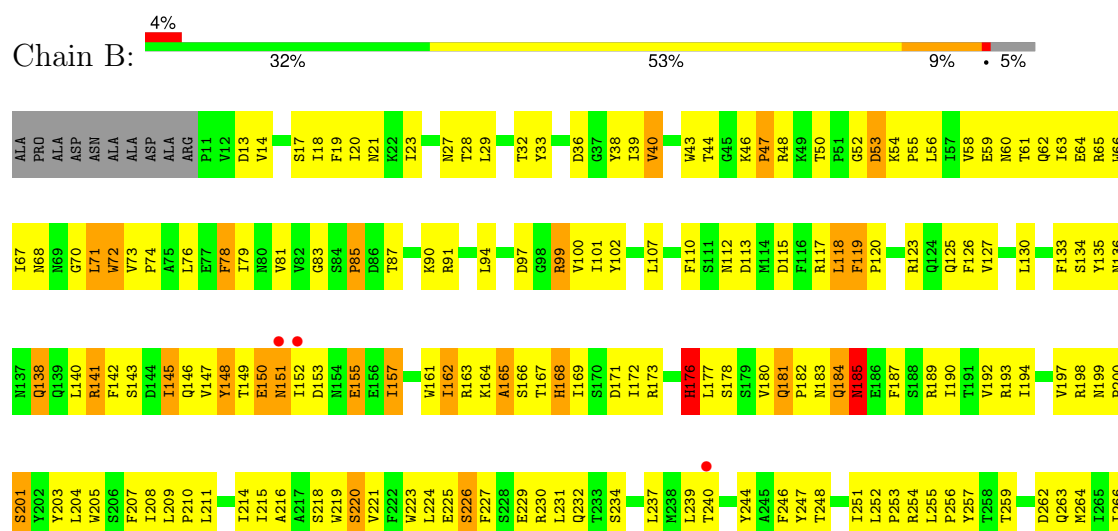
3 Residue-property plots

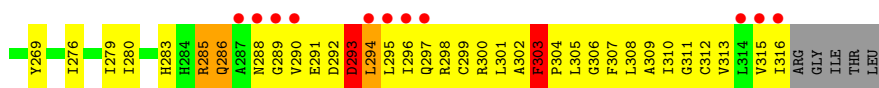
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Cys-loop ligand-gated ion channel

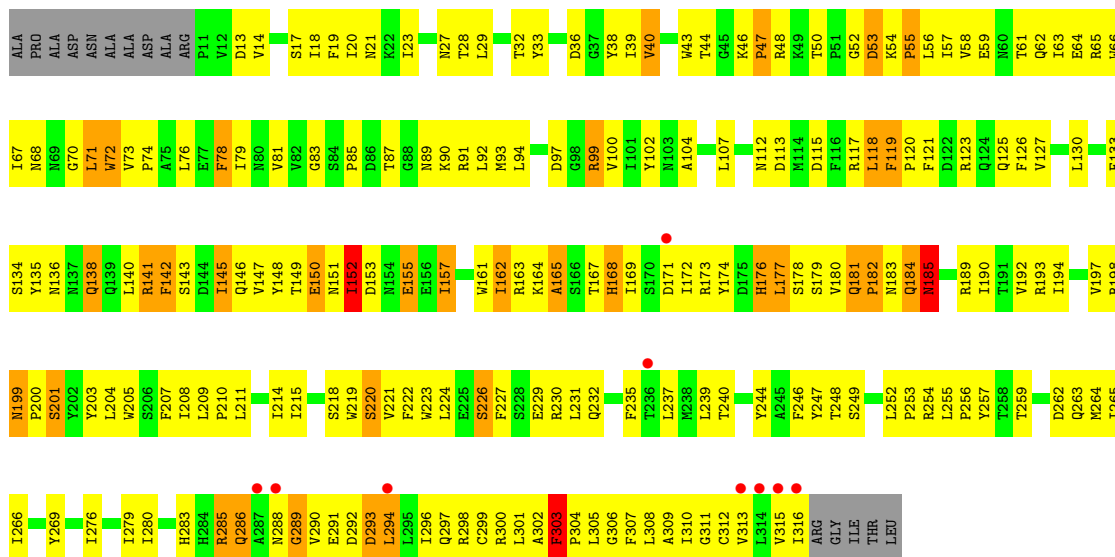


• Molecule 1: Cys-loop ligand-gated ion channel

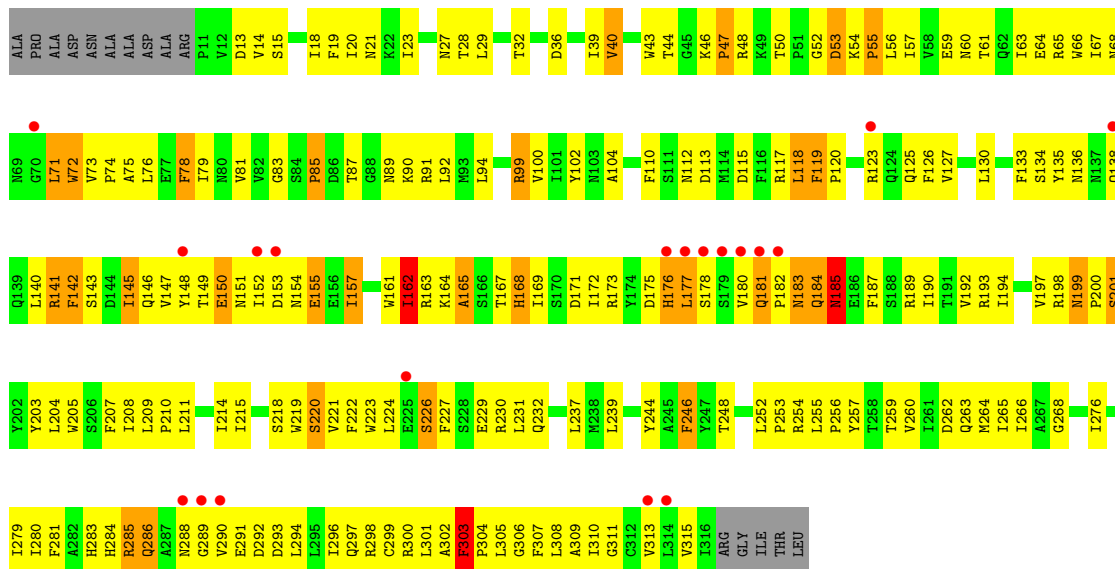




• Molecule 1: Cys-loop ligand-gated ion channel

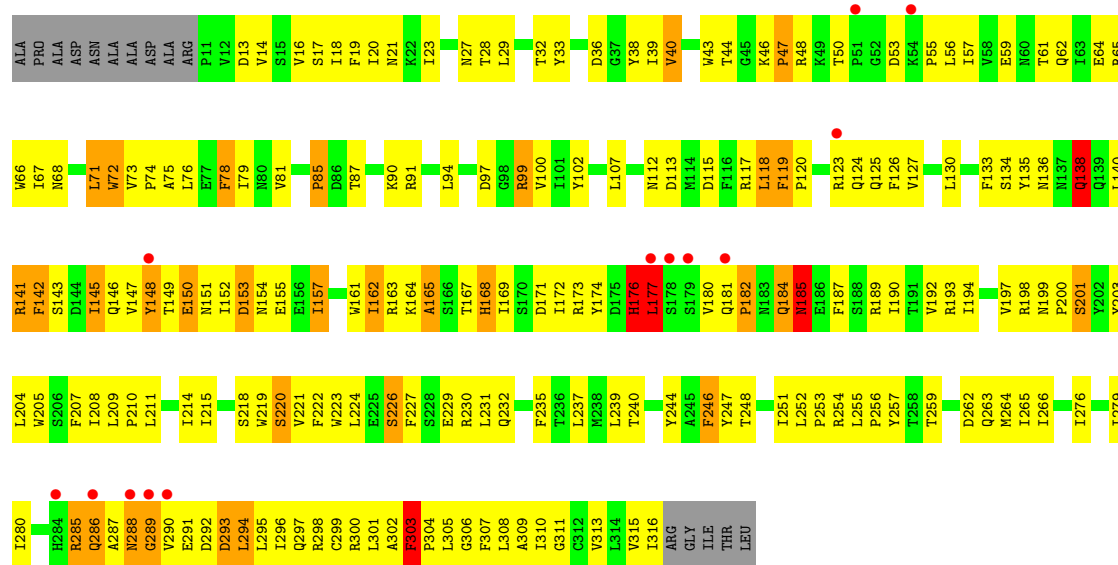


• Molecule 1: Cys-loop ligand-gated ion channel

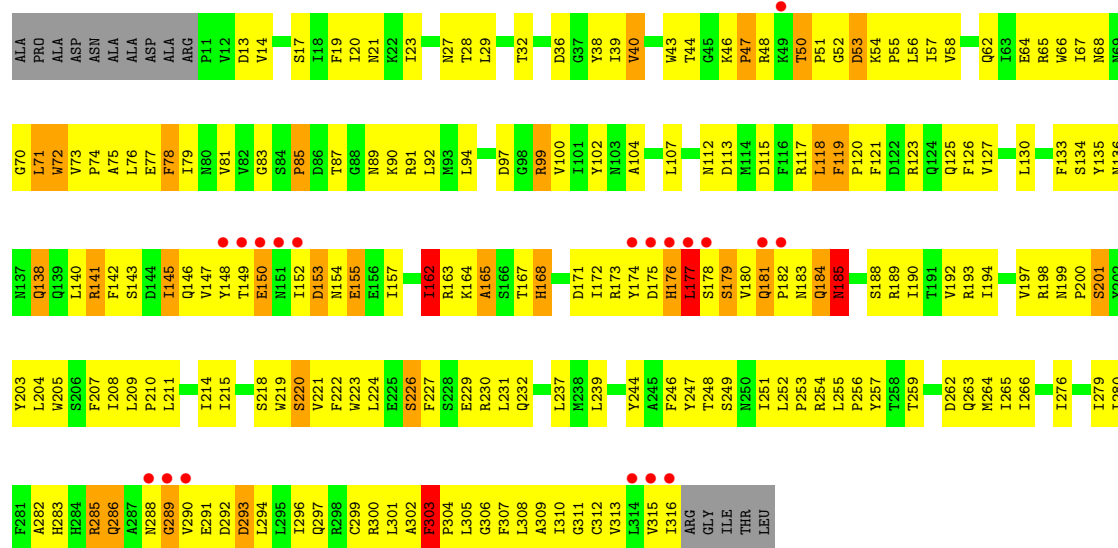


• Molecule 1: Cys-loop ligand-gated ion channel

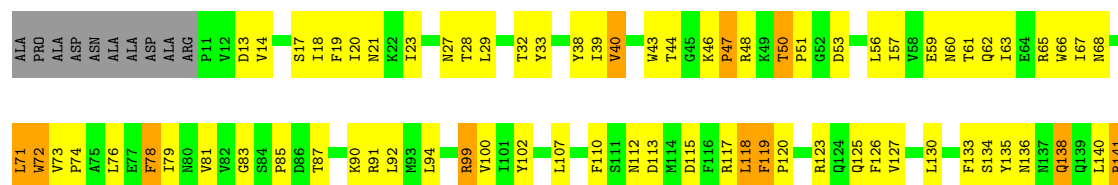


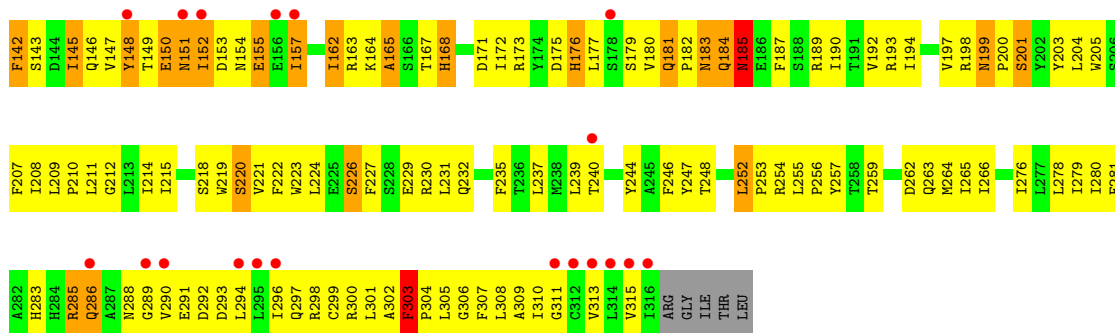


• Molecule 1: Cys-loop ligand-gated ion channel

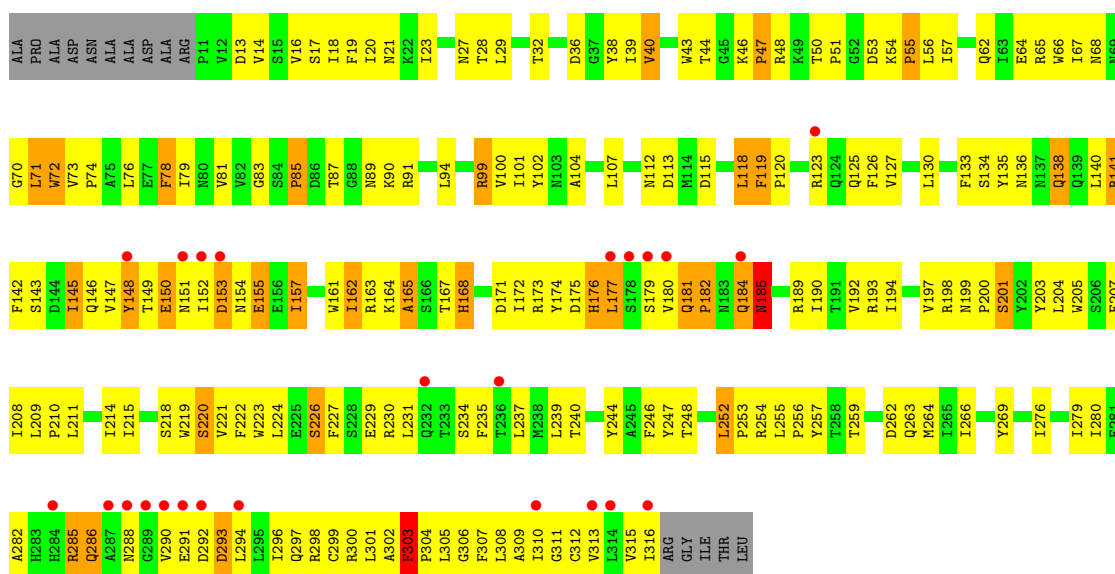


• Molecule 1: Cys-loop ligand-gated ion channel

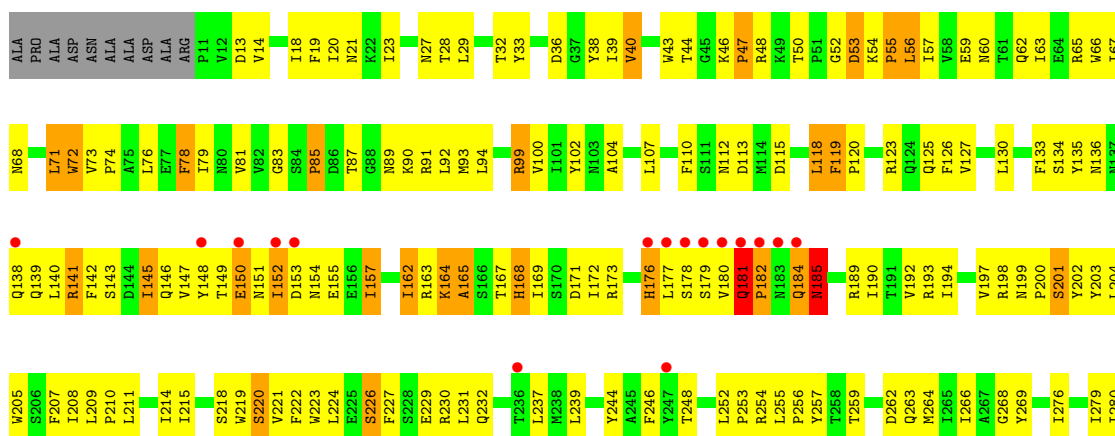




• Molecule 1: Cys-loop ligand-gated ion channel

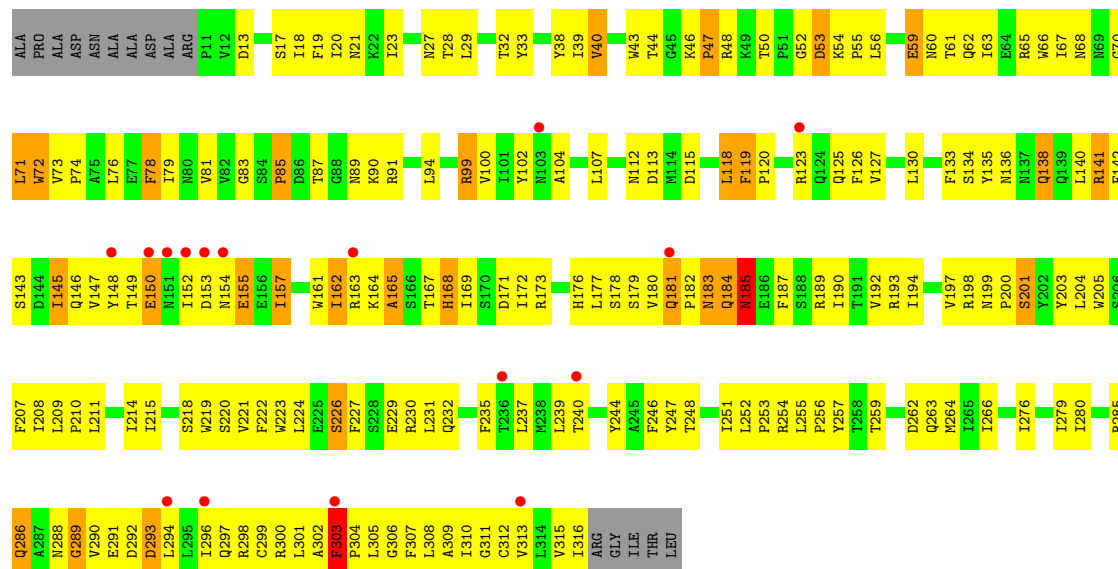


• Molecule 1: Cys-loop ligand-gated ion channel





• Molecule 1: Cys-loop ligand-gated ion channel



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	105.50Å 266.15Å 110.85Å 90.00° 109.52° 90.00°	Depositor
Resolution (Å)	29.93 – 3.30 39.63 – 3.11	Depositor EDS
% Data completeness (in resolution range)	99.8 (29.93-3.30) 84.0 (39.63-3.11)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.87 (at 3.12Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.263 , 0.274 0.262 , 0.274	Depositor DCC
R_{free} test set	4335 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	105.4	Xtriage
Anisotropy	0.263	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 63.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	25010	wwPDB-VP
Average B, all atoms (Å ²)	129.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.76% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.38	0/2569	0.67	2/3502 (0.1%)
1	B	0.39	0/2569	0.67	1/3502 (0.0%)
1	C	0.38	0/2569	0.67	1/3502 (0.0%)
1	D	0.39	0/2569	0.67	1/3502 (0.0%)
1	E	0.38	0/2569	0.66	1/3502 (0.0%)
1	F	0.38	0/2569	0.66	1/3502 (0.0%)
1	G	0.39	0/2569	0.67	1/3502 (0.0%)
1	H	0.38	0/2569	0.65	1/3502 (0.0%)
1	I	0.40	0/2569	0.66	1/3502 (0.0%)
1	J	0.39	0/2569	0.65	1/3502 (0.0%)
All	All	0.39	0/25690	0.66	11/35020 (0.0%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	138	GLN	N-CA-C	-5.86	95.17	111.00
1	H	138	GLN	N-CA-C	-5.72	95.55	111.00
1	C	138	GLN	N-CA-C	-5.71	95.57	111.00
1	E	138	GLN	N-CA-C	-5.71	95.57	111.00
1	B	138	GLN	N-CA-C	-5.68	95.65	111.00
1	A	138	GLN	N-CA-C	-5.64	95.76	111.00
1	J	138	GLN	N-CA-C	-5.63	95.79	111.00
1	I	138	GLN	N-CA-C	-5.62	95.82	111.00
1	D	138	GLN	N-CA-C	-5.62	95.83	111.00
1	A	149	THR	N-CA-C	-5.41	96.40	111.00
1	F	138	GLN	N-CA-C	-5.34	96.58	111.00

There are no chirality outliers.

There are no planarity outliers.

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	2501	0	2475	257	0
1	B	2501	0	2475	278	0
1	C	2501	0	2475	269	0
1	D	2501	0	2475	252	0
1	E	2501	0	2475	263	0
1	F	2501	0	2475	255	0
1	G	2501	0	2475	264	0
1	H	2501	0	2475	255	0
1	I	2501	0	2475	267	0
1	J	2501	0	2475	261	0
All	All	25010	0	24750	2374	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 48.

All (2374) 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:I:150:GLU:HB2	1:I:153:ASP:HB3	1.21	1.17
1:G:288:ASN:OD1	1:G:291:GLU:HB2	1.47	1.14
1:H:150:GLU:HB2	1:H:153:ASP:HB3	1.28	1.10
1:E:150:GLU:HB2	1:E:153:ASP:HB3	1.18	1.09
1:B:164:LYS:HD3	1:I:163:ARG:HD2	1.39	1.05
1:H:140:LEU:HD13	1:H:190:ILE:HG13	1.38	1.05
1:C:140:LEU:HD13	1:C:190:ILE:HG13	1.36	1.05
1:F:140:LEU:HD13	1:F:190:ILE:HG13	1.38	1.04
1:B:140:LEU:HD13	1:B:190:ILE:HG13	1.38	1.04
1:G:140:LEU:HD13	1:G:190:ILE:HG13	1.36	1.03
1:J:140:LEU:HD13	1:J:190:ILE:HG13	1.40	1.03
1:D:140:LEU:HD13	1:D:190:ILE:HG13	1.40	1.03
1:F:150:GLU:HB2	1:F:153:ASP:HB3	1.38	1.02
1:D:164:LYS:NZ	1:D:165:ALA:H	1.59	1.01
1:B:164:LYS:HG2	1:I:163:ARG:HB3	1.41	1.00
1:E:140:LEU:HD13	1:E:190:ILE:HG13	1.43	1.00
1:A:140:LEU:HD13	1:A:190:ILE:HG13	1.40	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:164:LYS:HZ2	1:I:165:ALA:H	1.03	0.99
1:D:293:ASP:HB2	1:D:296:ILE:HG22	1.45	0.99
1:I:140:LEU:HD13	1:I:190:ILE:HG13	1.44	0.99
1:I:164:LYS:NZ	1:I:165:ALA:H	1.59	0.99
1:B:164:LYS:NZ	1:B:165:ALA:H	1.61	0.98
1:B:168:HIS:ND1	1:I:167:THR:HB	1.79	0.97
1:C:223:TRP:HE1	1:C:300:ARG:HB3	1.30	0.96
1:G:223:TRP:HE1	1:G:300:ARG:HB3	1.29	0.96
1:C:164:LYS:HZ2	1:C:165:ALA:H	0.97	0.96
1:J:223:TRP:HE1	1:J:300:ARG:HB3	1.31	0.95
1:J:181:GLN:HG3	1:J:182:PRO:HD3	1.46	0.95
1:A:223:TRP:HE1	1:A:300:ARG:HB3	1.30	0.94
1:D:150:GLU:HB2	1:D:153:ASP:HB3	1.49	0.94
1:H:223:TRP:HE1	1:H:300:ARG:HB3	1.31	0.94
1:G:293:ASP:HB2	1:G:296:ILE:HG22	1.50	0.94
1:J:293:ASP:HB2	1:J:296:ILE:HG22	1.51	0.93
1:A:164:LYS:NZ	1:A:165:ALA:H	1.65	0.93
1:F:198:ARG:O	1:F:200:PRO:HD3	1.68	0.93
1:I:164:LYS:HZ2	1:I:165:ALA:N	1.67	0.93
1:G:286:GLN:HB3	1:G:291:GLU:HB3	1.51	0.92
1:E:223:TRP:HE1	1:E:300:ARG:HB3	1.30	0.92
1:B:173:ARG:HH22	1:I:139:GLN:HE22	1.15	0.92
1:I:223:TRP:HE1	1:I:300:ARG:HB3	1.34	0.92
1:F:223:TRP:HE1	1:F:300:ARG:HB3	1.35	0.92
1:H:164:LYS:HZ2	1:H:165:ALA:H	0.95	0.92
1:H:164:LYS:NZ	1:H:165:ALA:H	1.66	0.92
1:C:177:LEU:HD11	1:C:185:ASN:HA	1.52	0.92
1:B:167:THR:HG22	1:B:168:HIS:H	1.35	0.92
1:H:162:ILE:HG22	1:H:163:ARG:H	1.35	0.91
1:J:164:LYS:NZ	1:J:165:ALA:H	1.68	0.91
1:F:164:LYS:NZ	1:F:165:ALA:H	1.67	0.91
1:B:150:GLU:CG	1:B:153:ASP:HB3	2.00	0.91
1:I:288:ASN:OD1	1:I:291:GLU:HB2	1.70	0.91
1:J:180:VAL:HG21	1:J:184:GLN:HB2	1.52	0.91
1:A:223:TRP:NE1	1:A:300:ARG:HB3	1.85	0.91
1:E:150:GLU:CB	1:E:153:ASP:HB3	2.00	0.91
1:G:223:TRP:NE1	1:G:300:ARG:HB3	1.86	0.91
1:H:286:GLN:HB3	1:H:291:GLU:HB3	1.52	0.91
1:D:223:TRP:HE1	1:D:300:ARG:HB3	1.35	0.91
1:C:294:LEU:HA	1:C:297:GLN:HE21	1.36	0.91
1:D:164:LYS:HZ2	1:D:165:ALA:N	1.69	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:162:ILE:HG22	1:E:163:ARG:H	1.36	0.91
1:A:162:ILE:HG22	1:A:163:ARG:H	1.35	0.90
1:H:223:TRP:NE1	1:H:300:ARG:HB3	1.86	0.90
1:H:149:THR:HG22	1:H:150:GLU:H	1.33	0.90
1:G:164:LYS:NZ	1:G:165:ALA:H	1.69	0.90
1:A:155:GLU:HB3	1:A:161:TRP:CD1	2.06	0.90
1:C:162:ILE:HG22	1:C:163:ARG:H	1.35	0.89
1:C:223:TRP:NE1	1:C:300:ARG:HB3	1.86	0.89
1:C:198:ARG:O	1:C:200:PRO:HD3	1.73	0.89
1:E:223:TRP:NE1	1:E:300:ARG:HB3	1.87	0.89
1:B:164:LYS:HZ1	1:B:165:ALA:N	1.69	0.89
1:J:223:TRP:NE1	1:J:300:ARG:HB3	1.87	0.89
1:H:167:THR:HG22	1:H:168:HIS:H	1.38	0.89
1:D:198:ARG:O	1:D:200:PRO:HD3	1.73	0.88
1:I:198:ARG:O	1:I:200:PRO:HD3	1.74	0.88
1:A:164:LYS:HZ2	1:A:165:ALA:N	1.70	0.88
1:D:177:LEU:CD1	1:D:185:ASN:HA	2.04	0.88
1:C:167:THR:HG22	1:C:168:HIS:H	1.38	0.88
1:F:294:LEU:HA	1:F:297:GLN:HE21	1.37	0.88
1:A:167:THR:HG22	1:A:168:HIS:H	1.39	0.88
1:D:177:LEU:HD12	1:D:185:ASN:HA	1.55	0.88
1:F:223:TRP:NE1	1:F:300:ARG:HB3	1.89	0.88
1:J:164:LYS:HZ2	1:J:165:ALA:H	1.20	0.88
1:F:164:LYS:HZ2	1:F:165:ALA:N	1.72	0.88
1:I:223:TRP:NE1	1:I:300:ARG:HB3	1.88	0.87
1:A:294:LEU:HA	1:A:297:GLN:HE21	1.37	0.87
1:I:294:LEU:HA	1:I:297:GLN:HE21	1.39	0.87
1:F:162:ILE:HG22	1:F:163:ARG:H	1.38	0.87
1:B:198:ARG:O	1:B:200:PRO:HD3	1.74	0.87
1:D:162:ILE:HG22	1:D:163:ARG:H	1.38	0.87
1:B:223:TRP:HE1	1:B:300:ARG:HB3	1.37	0.87
1:C:293:ASP:HB2	1:C:296:ILE:HG22	1.55	0.87
1:E:164:LYS:HZ2	1:E:165:ALA:H	1.21	0.86
1:G:150:GLU:CG	1:G:153:ASP:HB3	2.04	0.86
1:G:164:LYS:HZ2	1:G:165:ALA:H	1.17	0.86
1:C:293:ASP:HB2	1:C:296:ILE:CG2	2.05	0.86
1:D:285:ARG:HA	1:D:285:ARG:NE	1.88	0.86
1:E:293:ASP:HB2	1:E:296:ILE:HG22	1.56	0.86
1:H:145:ILE:HD12	1:H:145:ILE:H	1.38	0.86
1:J:123:ARG:HD2	1:J:197:VAL:HG22	1.57	0.86
1:J:167:THR:HG22	1:J:168:HIS:H	1.39	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:285:ARG:NE	1:C:285:ARG:HA	1.89	0.86
1:G:162:ILE:HG22	1:G:163:ARG:H	1.40	0.86
1:A:145:ILE:H	1:A:145:ILE:HD12	1.41	0.86
1:B:162:ILE:HG22	1:B:163:ARG:H	1.40	0.86
1:I:150:GLU:HG3	1:I:154:ASN:HB2	1.57	0.86
1:F:293:ASP:HB2	1:F:296:ILE:HG22	1.56	0.86
1:E:198:ARG:O	1:E:200:PRO:HD3	1.74	0.85
1:F:164:LYS:HZ2	1:F:165:ALA:H	0.88	0.85
1:H:293:ASP:HB2	1:H:296:ILE:HG22	1.58	0.85
1:A:198:ARG:O	1:A:200:PRO:HD3	1.76	0.85
1:B:223:TRP:NE1	1:B:300:ARG:HB3	1.91	0.85
1:I:72:TRP:CZ2	1:I:74:PRO:HG3	2.12	0.85
1:D:223:TRP:NE1	1:D:300:ARG:HB3	1.90	0.85
1:F:167:THR:HG22	1:F:168:HIS:H	1.40	0.85
1:J:288:ASN:OD1	1:J:291:GLU:HB2	1.76	0.85
1:D:293:ASP:HB2	1:D:296:ILE:CG2	2.06	0.85
1:E:167:THR:HG22	1:E:168:HIS:H	1.42	0.84
1:G:198:ARG:O	1:G:200:PRO:HD3	1.76	0.84
1:J:198:ARG:O	1:J:200:PRO:HD3	1.77	0.84
1:E:123:ARG:HD2	1:E:197:VAL:HG22	1.60	0.84
1:J:145:ILE:H	1:J:145:ILE:HD12	1.42	0.84
1:A:181:GLN:HG3	1:A:182:PRO:HD3	1.57	0.84
1:E:150:GLU:HB2	1:E:153:ASP:CB	2.06	0.84
1:C:164:LYS:NZ	1:C:165:ALA:H	1.74	0.84
1:D:167:THR:HG22	1:D:168:HIS:H	1.42	0.84
1:E:145:ILE:H	1:E:145:ILE:HD12	1.43	0.84
1:E:164:LYS:NZ	1:E:165:ALA:H	1.76	0.84
1:E:294:LEU:HA	1:E:297:GLN:HE21	1.41	0.84
1:B:150:GLU:HB2	1:B:153:ASP:HB3	1.58	0.84
1:H:198:ARG:O	1:H:200:PRO:HD3	1.78	0.84
1:A:150:GLU:HB3	1:A:153:ASP:HB2	1.59	0.84
1:B:164:LYS:HZ1	1:B:165:ALA:H	0.84	0.84
1:H:39:ILE:HD11	1:H:78:PHE:CZ	2.13	0.84
1:B:181:GLN:H	1:B:182:PRO:CD	1.92	0.83
1:B:145:ILE:H	1:B:145:ILE:HD12	1.41	0.83
1:D:164:LYS:HZ2	1:D:165:ALA:H	0.84	0.83
1:F:288:ASN:OD1	1:F:291:GLU:HB2	1.78	0.83
1:A:164:LYS:HZ2	1:A:165:ALA:H	0.86	0.83
1:A:294:LEU:HA	1:A:297:GLN:NE2	1.93	0.83
1:H:286:GLN:CB	1:H:291:GLU:HB3	2.08	0.83
1:C:145:ILE:HD12	1:C:145:ILE:H	1.44	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:150:GLU:HB3	1:C:153:ASP:CB	2.08	0.83
1:G:39:ILE:HD11	1:G:78:PHE:CZ	2.14	0.83
1:B:150:GLU:CB	1:B:153:ASP:HB3	2.09	0.83
1:G:145:ILE:H	1:G:145:ILE:HD12	1.43	0.83
1:A:39:ILE:HD11	1:A:78:PHE:CZ	2.14	0.83
1:C:180:VAL:HG21	1:C:184:GLN:HB2	1.59	0.83
1:I:180:VAL:HG21	1:I:184:GLN:HB2	1.59	0.82
1:A:288:ASN:CG	1:A:289:GLY:H	1.82	0.82
1:F:293:ASP:HB2	1:F:296:ILE:CG2	2.10	0.82
1:I:150:GLU:HG2	1:I:154:ASN:H	1.42	0.82
1:I:162:ILE:HG22	1:I:163:ARG:H	1.42	0.82
1:A:123:ARG:HD2	1:A:197:VAL:HG22	1.61	0.82
1:B:285:ARG:NE	1:B:285:ARG:HA	1.91	0.82
1:I:167:THR:HG22	1:I:168:HIS:H	1.44	0.82
1:I:145:ILE:H	1:I:145:ILE:HD12	1.43	0.82
1:B:150:GLU:HB2	1:B:153:ASP:CB	2.09	0.82
1:G:44:THR:HA	1:G:99:ARG:HA	1.62	0.82
1:J:39:ILE:HD11	1:J:78:PHE:CZ	2.15	0.81
1:J:293:ASP:HB2	1:J:296:ILE:CG2	2.10	0.81
1:C:123:ARG:HD2	1:C:197:VAL:HG22	1.62	0.81
1:G:167:THR:HG22	1:G:168:HIS:H	1.44	0.81
1:B:123:ARG:HD2	1:B:197:VAL:HG22	1.61	0.81
1:D:44:THR:HA	1:D:99:ARG:HA	1.62	0.81
1:D:72:TRP:CZ2	1:D:74:PRO:HG3	2.14	0.81
1:D:294:LEU:HA	1:D:297:GLN:HE21	1.44	0.81
1:H:164:LYS:HZ2	1:H:165:ALA:N	1.77	0.81
1:D:145:ILE:H	1:D:145:ILE:HD12	1.45	0.81
1:J:162:ILE:HG22	1:J:163:ARG:H	1.44	0.81
1:G:204:LEU:HD23	1:G:208:ILE:HG13	1.63	0.81
1:H:294:LEU:HA	1:H:297:GLN:HE21	1.45	0.81
1:D:91:ARG:HD2	1:E:134:SER:HB3	1.60	0.81
1:F:145:ILE:H	1:F:145:ILE:HD12	1.45	0.81
1:A:72:TRP:CZ2	1:A:74:PRO:HG3	2.16	0.80
1:E:39:ILE:HD11	1:E:78:PHE:CZ	2.17	0.80
1:F:177:LEU:H	1:F:177:LEU:HD12	1.46	0.80
1:G:150:GLU:HG2	1:G:153:ASP:HB3	1.60	0.80
1:E:313:VAL:HA	1:E:316:ILE:HG13	1.63	0.80
1:C:39:ILE:HD11	1:C:78:PHE:CZ	2.17	0.80
1:E:44:THR:HA	1:E:99:ARG:HA	1.63	0.80
1:D:150:GLU:HB2	1:D:153:ASP:CB	2.11	0.80
1:A:293:ASP:HB2	1:A:296:ILE:HG22	1.63	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:123:ARG:HD2	1:G:197:VAL:HG22	1.61	0.79
1:C:72:TRP:CZ2	1:C:74:PRO:HG3	2.16	0.79
1:F:123:ARG:HD2	1:F:197:VAL:HG22	1.65	0.79
1:H:154:ASN:O	1:H:155:GLU:HG3	1.82	0.79
1:B:224:LEU:HD21	1:C:231:LEU:HD22	1.65	0.79
1:I:123:ARG:HD2	1:I:197:VAL:HG22	1.63	0.79
1:F:256:PRO:HG2	1:F:257:TYR:HD2	1.48	0.79
1:G:256:PRO:HG2	1:G:257:TYR:HD2	1.48	0.79
1:B:173:ARG:HH22	1:I:139:GLN:NE2	1.80	0.79
1:E:256:PRO:HG2	1:E:257:TYR:HD2	1.48	0.79
1:G:91:ARG:HD2	1:H:134:SER:HB3	1.62	0.79
1:D:256:PRO:HG2	1:D:257:TYR:HD2	1.47	0.79
1:J:149:THR:HG22	1:J:150:GLU:H	1.45	0.79
1:B:39:ILE:HD11	1:B:78:PHE:CZ	2.18	0.79
1:J:256:PRO:HG2	1:J:257:TYR:HD2	1.48	0.79
1:A:204:LEU:HD23	1:A:208:ILE:HG13	1.65	0.79
1:H:181:GLN:HG3	1:H:182:PRO:HD3	1.65	0.79
1:D:52:GLY:O	1:D:53:ASP:HB2	1.83	0.78
1:J:294:LEU:HA	1:J:297:GLN:HE21	1.46	0.78
1:D:123:ARG:HD2	1:D:197:VAL:HG22	1.65	0.78
1:E:204:LEU:HD23	1:E:208:ILE:HG13	1.63	0.78
1:F:44:THR:HA	1:F:99:ARG:HA	1.65	0.78
1:H:123:ARG:HD2	1:H:197:VAL:HG22	1.65	0.78
1:H:256:PRO:HG2	1:H:257:TYR:HD2	1.46	0.78
1:H:299:CYS:HB2	1:H:302:ALA:CB	2.13	0.78
1:J:286:GLN:HB3	1:J:291:GLU:HB3	1.63	0.78
1:A:44:THR:HA	1:A:99:ARG:HA	1.65	0.78
1:F:299:CYS:HB2	1:F:302:ALA:CB	2.14	0.78
1:I:44:THR:HA	1:I:99:ARG:HA	1.64	0.78
1:B:256:PRO:HG2	1:B:257:TYR:HD2	1.48	0.78
1:C:44:THR:HA	1:C:99:ARG:HA	1.64	0.78
1:F:72:TRP:CZ2	1:F:74:PRO:HG3	2.18	0.78
1:F:150:GLU:CB	1:F:153:ASP:HB3	2.14	0.78
1:E:299:CYS:HB2	1:E:302:ALA:CB	2.14	0.78
1:J:177:LEU:HD11	1:J:187:PHE:HE1	1.49	0.78
1:F:39:ILE:HD11	1:F:78:PHE:CZ	2.18	0.78
1:J:44:THR:HA	1:J:99:ARG:HA	1.65	0.77
1:A:256:PRO:HG2	1:A:257:TYR:HD2	1.47	0.77
1:B:181:GLN:H	1:B:182:PRO:HD3	1.49	0.77
1:B:204:LEU:HD23	1:B:208:ILE:HG13	1.66	0.77
1:F:294:LEU:HA	1:F:297:GLN:NE2	1.99	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:145:ILE:HG21	1:D:192:VAL:HG11	1.66	0.77
1:D:204:LEU:HD23	1:D:208:ILE:HG13	1.65	0.77
1:E:293:ASP:HB2	1:E:296:ILE:CG2	2.15	0.77
1:G:72:TRP:CZ2	1:G:74:PRO:HG3	2.20	0.77
1:C:218:SER:HA	1:C:237:LEU:HD21	1.67	0.77
1:C:256:PRO:HG2	1:C:257:TYR:HD2	1.47	0.77
1:E:294:LEU:HA	1:E:297:GLN:NE2	1.99	0.77
1:H:293:ASP:HB2	1:H:296:ILE:CG2	2.15	0.77
1:J:204:LEU:HD23	1:J:208:ILE:HG13	1.66	0.77
1:A:299:CYS:HB2	1:A:302:ALA:CB	2.14	0.77
1:B:299:CYS:HB2	1:B:302:ALA:CB	2.14	0.77
1:C:294:LEU:HA	1:C:297:GLN:NE2	1.97	0.77
1:I:150:GLU:CB	1:I:153:ASP:HB3	2.09	0.77
1:D:56:LEU:HD13	1:D:57:ILE:N	1.99	0.77
1:D:182:PRO:O	1:D:183:ASN:HB2	1.82	0.77
1:F:150:GLU:HB2	1:F:153:ASP:CB	2.15	0.77
1:G:294:LEU:HA	1:G:297:GLN:HE21	1.50	0.77
1:H:204:LEU:HD23	1:H:208:ILE:HG13	1.65	0.77
1:I:299:CYS:HB2	1:I:302:ALA:CB	2.15	0.76
1:B:164:LYS:HA	1:B:164:LYS:HZ2	1.49	0.76
1:D:39:ILE:HD11	1:D:78:PHE:CZ	2.21	0.76
1:D:299:CYS:HB2	1:D:302:ALA:CB	2.16	0.76
1:A:288:ASN:HD21	1:A:291:GLU:N	1.83	0.76
1:G:164:LYS:HZ2	1:G:165:ALA:N	1.83	0.76
1:G:299:CYS:HB2	1:G:302:ALA:CB	2.15	0.76
1:J:299:CYS:HB2	1:J:302:ALA:CB	2.16	0.76
1:D:294:LEU:HA	1:D:297:GLN:NE2	2.00	0.76
1:C:91:ARG:HD2	1:D:134:SER:HB3	1.68	0.76
1:I:39:ILE:HD11	1:I:78:PHE:CZ	2.21	0.76
1:I:204:LEU:HD23	1:I:208:ILE:HG13	1.67	0.76
1:J:227:PHE:HA	1:J:230:ARG:HH11	1.51	0.76
1:F:204:LEU:HD23	1:F:208:ILE:HG13	1.65	0.76
1:F:285:ARG:NE	1:F:285:ARG:HA	2.00	0.76
1:C:204:LEU:HD23	1:C:208:ILE:HG13	1.66	0.75
1:I:256:PRO:HG2	1:I:257:TYR:HD2	1.51	0.75
1:B:72:TRP:CZ2	1:B:74:PRO:HG3	2.20	0.75
1:D:177:LEU:HD11	1:D:187:PHE:HE1	1.52	0.75
1:E:72:TRP:CZ2	1:E:74:PRO:HG3	2.22	0.75
1:B:140:LEU:HD13	1:B:190:ILE:CG1	2.17	0.74
1:F:211:LEU:O	1:F:215:ILE:HG12	1.87	0.74
1:C:177:LEU:HD12	1:C:184:GLN:O	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:72:TRP:CZ2	1:H:74:PRO:HG3	2.21	0.74
1:A:51:PRO:HD2	1:A:56:LEU:HD23	1.69	0.74
1:H:91:ARG:CD	1:I:134:SER:HB3	2.18	0.74
1:H:91:ARG:HD2	1:I:134:SER:HB3	1.69	0.74
1:E:227:PHE:HA	1:E:230:ARG:HH11	1.52	0.74
1:G:181:GLN:HG2	1:G:182:PRO:HD3	1.69	0.74
1:C:288:ASN:OD1	1:C:291:GLU:HB2	1.88	0.74
1:H:44:THR:HA	1:H:99:ARG:HA	1.68	0.74
1:A:91:ARG:HD2	1:B:134:SER:HB3	1.70	0.74
1:B:44:THR:HA	1:B:99:ARG:HA	1.69	0.74
1:B:226:SER:O	1:B:230:ARG:HD3	1.88	0.74
1:A:145:ILE:HG21	1:A:192:VAL:HG11	1.68	0.74
1:G:140:LEU:HD13	1:G:190:ILE:CG1	2.15	0.74
1:G:294:LEU:HA	1:G:297:GLN:NE2	2.02	0.74
1:G:180:VAL:HG21	1:G:184:GLN:HB2	1.69	0.74
1:C:299:CYS:HB2	1:C:302:ALA:CB	2.17	0.74
1:J:162:ILE:N	1:J:162:ILE:HD12	2.02	0.74
1:C:227:PHE:HA	1:C:230:ARG:HH11	1.51	0.73
1:I:150:GLU:CG	1:I:154:ASN:H	2.00	0.73
1:D:150:GLU:CB	1:D:153:ASP:HB3	2.17	0.73
1:B:173:ARG:NH2	1:I:139:GLN:HE22	1.86	0.73
1:F:157:ILE:HD11	1:G:115:ASP:OD2	1.89	0.73
1:F:134:SER:HB3	1:J:91:ARG:HD2	1.71	0.73
1:H:256:PRO:HG2	1:H:257:TYR:CD2	2.23	0.73
1:D:180:VAL:HG21	1:D:184:GLN:HB2	1.69	0.73
1:J:177:LEU:HD12	1:J:185:ASN:HA	1.69	0.73
1:A:285:ARG:HA	1:A:285:ARG:NE	2.03	0.72
1:H:150:GLU:CB	1:H:153:ASP:HB3	2.14	0.72
1:B:215:ILE:O	1:B:218:SER:HB3	1.89	0.72
1:D:211:LEU:O	1:D:215:ILE:HG12	1.89	0.72
1:H:140:LEU:HD13	1:H:190:ILE:CG1	2.18	0.72
1:C:91:ARG:CD	1:D:134:SER:HB3	2.19	0.72
1:F:91:ARG:HD2	1:G:134:SER:HB3	1.69	0.72
1:G:91:ARG:HD2	1:H:134:SER:CB	2.20	0.72
1:A:162:ILE:HD12	1:A:162:ILE:N	2.05	0.72
1:D:145:ILE:HD13	1:D:165:ALA:HB1	1.70	0.72
1:E:218:SER:HA	1:E:237:LEU:HD21	1.72	0.72
1:I:293:ASP:HB2	1:I:296:ILE:HG22	1.72	0.72
1:A:293:ASP:HB2	1:A:296:ILE:CG2	2.19	0.72
1:B:288:ASN:OD1	1:B:291:GLU:HB2	1.90	0.72
1:A:227:PHE:HA	1:A:230:ARG:HH11	1.54	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:56:LEU:HD13	1:C:57:ILE:N	2.05	0.72
1:H:145:ILE:HG21	1:H:192:VAL:HG11	1.71	0.72
1:A:52:GLY:O	1:A:53:ASP:HB2	1.89	0.72
1:C:174:TYR:HB2	1:C:177:LEU:HD21	1.70	0.72
1:G:218:SER:HA	1:G:237:LEU:HD21	1.70	0.72
1:I:145:ILE:HG21	1:I:192:VAL:HG11	1.72	0.72
1:A:145:ILE:HD13	1:A:165:ALA:HB1	1.72	0.72
1:E:177:LEU:H	1:E:177:LEU:HD12	1.55	0.72
1:B:91:ARG:HD2	1:C:134:SER:HB3	1.72	0.72
1:B:223:TRP:CE3	1:C:280:ILE:HG22	2.24	0.72
1:C:211:LEU:O	1:C:215:ILE:HG12	1.90	0.72
1:F:149:THR:HG22	1:F:150:GLU:H	1.54	0.72
1:G:65:ARG:HD2	1:H:68:ASN:ND2	2.05	0.72
1:G:226:SER:O	1:G:230:ARG:HD3	1.89	0.71
1:C:256:PRO:HG2	1:C:257:TYR:CD2	2.25	0.71
1:E:164:LYS:HZ3	1:E:164:LYS:HA	1.55	0.71
1:H:181:GLN:H	1:H:182:PRO:CD	2.02	0.71
1:I:181:GLN:H	1:I:182:PRO:CD	2.03	0.71
1:J:145:ILE:HD13	1:J:165:ALA:HB1	1.71	0.71
1:E:226:SER:O	1:E:230:ARG:HD3	1.91	0.71
1:F:145:ILE:HD13	1:F:165:ALA:HB1	1.71	0.71
1:J:72:TRP:CZ2	1:J:74:PRO:HG3	2.25	0.71
1:A:256:PRO:HG2	1:A:257:TYR:CD2	2.26	0.71
1:F:68:ASN:ND2	1:J:65:ARG:HD2	2.05	0.71
1:D:231:LEU:HD12	1:D:280:ILE:HG12	1.73	0.71
1:E:294:LEU:HG	1:E:298:ARG:NH2	2.04	0.71
1:J:177:LEU:CD1	1:J:185:ASN:HA	2.21	0.71
1:J:181:GLN:HG3	1:J:182:PRO:CD	2.20	0.71
1:B:227:PHE:HA	1:B:230:ARG:HH11	1.55	0.71
1:G:56:LEU:HD13	1:G:57:ILE:N	2.05	0.71
1:B:119:PHE:HB3	1:B:120:PRO:HD3	1.71	0.71
1:H:218:SER:HA	1:H:237:LEU:HD21	1.71	0.71
1:I:227:PHE:HA	1:I:230:ARG:HH11	1.56	0.71
1:D:227:PHE:HA	1:D:230:ARG:HH11	1.56	0.71
1:H:157:ILE:HD11	1:I:115:ASP:OD2	1.91	0.71
1:J:226:SER:O	1:J:230:ARG:HD3	1.91	0.71
1:B:285:ARG:HA	1:B:285:ARG:CZ	2.20	0.71
1:H:162:ILE:N	1:H:162:ILE:HD12	2.06	0.71
1:I:224:LEU:HD21	1:J:231:LEU:HD22	1.73	0.71
1:J:182:PRO:O	1:J:183:ASN:HB2	1.89	0.71
1:E:211:LEU:O	1:E:215:ILE:HG12	1.90	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:145:ILE:HG21	1:J:192:VAL:HG11	1.70	0.70
1:B:247:TYR:HD1	1:C:246:PHE:HA	1.54	0.70
1:C:226:SER:O	1:C:230:ARG:HD3	1.91	0.70
1:E:231:LEU:HD12	1:E:280:ILE:HG12	1.73	0.70
1:D:91:ARG:CD	1:E:134:SER:HB3	2.20	0.70
1:F:256:PRO:HG2	1:F:257:TYR:CD2	2.26	0.70
1:G:285:ARG:HA	1:G:285:ARG:CZ	2.21	0.70
1:H:211:LEU:O	1:H:215:ILE:HG12	1.90	0.70
1:D:140:LEU:HD13	1:D:190:ILE:CG1	2.20	0.70
1:E:313:VAL:HG13	1:E:316:ILE:HD12	1.73	0.70
1:I:226:SER:O	1:I:230:ARG:HD3	1.92	0.70
1:A:231:LEU:HD12	1:A:280:ILE:HG12	1.74	0.70
1:E:256:PRO:HG2	1:E:257:TYR:CD2	2.26	0.70
1:F:218:SER:HA	1:F:237:LEU:HD21	1.73	0.70
1:H:227:PHE:HA	1:H:230:ARG:HH11	1.55	0.70
1:I:256:PRO:HG2	1:I:257:TYR:CD2	2.27	0.70
1:D:209:LEU:HB3	1:D:210:PRO:CD	2.22	0.70
1:J:162:ILE:HD12	1:J:162:ILE:H	1.56	0.70
1:J:164:LYS:HZ2	1:J:165:ALA:N	1.89	0.70
1:J:256:PRO:HG2	1:J:257:TYR:CD2	2.26	0.70
1:B:286:GLN:HG2	1:B:289:GLY:O	1.91	0.70
1:G:227:PHE:HA	1:G:230:ARG:HH11	1.55	0.70
1:I:145:ILE:HD13	1:I:165:ALA:HB1	1.73	0.70
1:B:256:PRO:HG2	1:B:257:TYR:CD2	2.26	0.69
1:D:162:ILE:HD12	1:D:162:ILE:H	1.57	0.69
1:I:293:ASP:HB2	1:I:296:ILE:CG2	2.22	0.69
1:G:293:ASP:HB2	1:G:296:ILE:CG2	2.20	0.69
1:D:226:SER:O	1:D:230:ARG:HD3	1.92	0.69
1:C:226:SER:HB3	1:C:229:GLU:HG3	1.75	0.69
1:J:211:LEU:O	1:J:215:ILE:HG12	1.92	0.69
1:E:145:ILE:HD13	1:E:165:ALA:HB1	1.73	0.69
1:F:215:ILE:O	1:F:218:SER:HB3	1.93	0.69
1:F:246:PHE:HA	1:J:247:TYR:HD1	1.57	0.69
1:F:286:GLN:HG2	1:F:289:GLY:O	1.93	0.69
1:F:293:ASP:O	1:F:296:ILE:HG22	1.92	0.69
1:D:164:LYS:HZ3	1:D:164:LYS:HA	1.58	0.69
1:D:218:SER:HA	1:D:237:LEU:HD21	1.73	0.69
1:E:294:LEU:HG	1:E:298:ARG:HH21	1.56	0.69
1:G:211:LEU:O	1:G:215:ILE:HG12	1.93	0.69
1:B:209:LEU:HB3	1:B:210:PRO:CD	2.23	0.69
1:D:256:PRO:HG2	1:D:257:TYR:CD2	2.27	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:134:SER:HB3	1:J:91:ARG:CD	2.23	0.69
1:G:162:ILE:HD12	1:G:162:ILE:N	2.07	0.69
1:B:211:LEU:O	1:B:215:ILE:HG12	1.92	0.69
1:F:227:PHE:HA	1:F:230:ARG:HH11	1.56	0.69
1:G:256:PRO:HG2	1:G:257:TYR:CD2	2.27	0.69
1:H:56:LEU:HD13	1:H:57:ILE:N	2.08	0.69
1:C:162:ILE:HD12	1:C:162:ILE:N	2.08	0.69
1:B:162:ILE:N	1:B:162:ILE:HD12	2.07	0.68
1:C:91:ARG:HD2	1:D:134:SER:CB	2.24	0.68
1:C:164:LYS:HZ2	1:C:165:ALA:N	1.82	0.68
1:H:215:ILE:O	1:H:218:SER:HB3	1.93	0.68
1:H:231:LEU:HD12	1:H:280:ILE:HG12	1.75	0.68
1:F:140:LEU:HD13	1:F:190:ILE:CG1	2.19	0.68
1:H:23:ILE:HG21	1:H:126:PHE:CD1	2.28	0.68
1:C:140:LEU:HD13	1:C:190:ILE:CG1	2.18	0.68
1:G:91:ARG:CD	1:H:134:SER:HB3	2.23	0.68
1:A:91:ARG:CD	1:B:134:SER:HB3	2.23	0.68
1:G:119:PHE:HB3	1:G:120:PRO:HD3	1.76	0.68
1:H:226:SER:O	1:H:230:ARG:HD3	1.93	0.68
1:D:145:ILE:HD13	1:D:165:ALA:CB	2.23	0.68
1:G:247:TYR:HD1	1:H:246:PHE:HA	1.59	0.68
1:I:285:ARG:HA	1:I:285:ARG:NE	2.08	0.68
1:B:91:ARG:HD2	1:C:134:SER:CB	2.24	0.68
1:D:162:ILE:HD12	1:D:162:ILE:N	2.08	0.68
1:I:162:ILE:HD12	1:I:162:ILE:N	2.08	0.68
1:J:180:VAL:CG2	1:J:184:GLN:HB2	2.23	0.68
1:A:211:LEU:O	1:A:215:ILE:HG12	1.93	0.68
1:A:218:SER:HA	1:A:237:LEU:HD21	1.76	0.68
1:C:224:LEU:HD21	1:D:231:LEU:HD22	1.73	0.68
1:E:145:ILE:HG21	1:E:192:VAL:HG11	1.73	0.68
1:G:209:LEU:HB3	1:G:210:PRO:CD	2.23	0.68
1:H:286:GLN:HA	1:H:291:GLU:OE1	1.93	0.68
1:I:215:ILE:O	1:I:218:SER:HB3	1.92	0.68
1:I:218:SER:HA	1:I:237:LEU:HD21	1.74	0.68
1:E:23:ILE:HG21	1:E:126:PHE:CD1	2.29	0.68
1:F:312:CYS:O	1:F:316:ILE:HG13	1.94	0.68
1:I:52:GLY:O	1:I:53:ASP:HB2	1.92	0.68
1:J:180:VAL:HG21	1:J:184:GLN:CB	2.22	0.68
1:B:91:ARG:CD	1:C:134:SER:HB3	2.23	0.68
1:D:283:HIS:O	1:D:286:GLN:HG3	1.94	0.68
1:F:182:PRO:HB2	1:F:184:GLN:HE22	1.59	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:28:THR:HB	1:J:255:LEU:HD21	1.76	0.68
1:I:294:LEU:HA	1:I:297:GLN:NE2	2.06	0.67
1:J:209:LEU:HB3	1:J:210:PRO:CD	2.24	0.67
1:F:224:LEU:HD21	1:G:231:LEU:HD22	1.75	0.67
1:J:154:ASN:O	1:J:155:GLU:HG3	1.94	0.67
1:C:150:GLU:OE1	1:C:150:GLU:HA	1.93	0.67
1:F:23:ILE:HG21	1:F:126:PHE:CD1	2.29	0.67
1:H:91:ARG:HD2	1:I:134:SER:CB	2.23	0.67
1:I:231:LEU:HD12	1:I:280:ILE:HG12	1.76	0.67
1:J:150:GLU:HB2	1:J:153:ASP:HB3	1.76	0.67
1:H:145:ILE:HD13	1:H:165:ALA:HB1	1.74	0.67
1:E:119:PHE:HB3	1:E:120:PRO:HD3	1.77	0.67
1:J:231:LEU:HD12	1:J:280:ILE:HG12	1.77	0.67
1:A:150:GLU:HB3	1:A:153:ASP:CB	2.24	0.67
1:B:23:ILE:HG21	1:B:126:PHE:CD1	2.30	0.67
1:B:145:ILE:HG21	1:B:192:VAL:HG11	1.76	0.67
1:C:177:LEU:CD1	1:C:185:ASN:HA	2.24	0.67
1:E:209:LEU:HB3	1:E:210:PRO:CD	2.24	0.67
1:J:218:SER:HA	1:J:237:LEU:HD21	1.74	0.67
1:B:167:THR:HG22	1:B:168:HIS:N	2.09	0.67
1:C:119:PHE:HB3	1:C:120:PRO:HD3	1.77	0.67
1:F:162:ILE:HD12	1:F:162:ILE:N	2.08	0.67
1:F:209:LEU:HB3	1:F:210:PRO:CD	2.25	0.67
1:G:145:ILE:HD13	1:G:165:ALA:HB1	1.75	0.67
1:G:145:ILE:HG21	1:G:192:VAL:HG11	1.77	0.67
1:G:231:LEU:HD12	1:G:280:ILE:HG12	1.77	0.67
1:I:211:LEU:O	1:I:215:ILE:HG12	1.95	0.67
1:C:145:ILE:HD13	1:C:165:ALA:HB1	1.75	0.67
1:D:215:ILE:O	1:D:218:SER:HB3	1.95	0.67
1:E:162:ILE:N	1:E:162:ILE:HD12	2.09	0.67
1:I:94:LEU:HD23	1:I:100:VAL:HG22	1.77	0.67
1:I:209:LEU:HB3	1:I:210:PRO:CD	2.24	0.67
1:B:140:LEU:HD22	1:B:190:ILE:HD11	1.77	0.67
1:E:292:ASP:O	1:E:294:LEU:N	2.28	0.67
1:H:150:GLU:HG2	1:H:154:ASN:H	1.60	0.67
1:H:157:ILE:HD11	1:I:115:ASP:CG	2.15	0.66
1:H:167:THR:HG22	1:H:168:HIS:N	2.10	0.66
1:J:286:GLN:CB	1:J:291:GLU:HB3	2.25	0.66
1:A:119:PHE:HB3	1:A:120:PRO:HD3	1.76	0.66
1:A:226:SER:O	1:A:230:ARG:HD3	1.95	0.66
1:H:28:THR:HB	1:H:255:LEU:HD21	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:72:TRP:HZ3	1:J:135:TYR:CZ	2.14	0.66
1:B:240:THR:OG1	1:C:239:LEU:HD23	1.96	0.66
1:F:162:ILE:HD12	1:F:162:ILE:H	1.61	0.66
1:F:226:SER:O	1:F:230:ARG:HD3	1.96	0.66
1:G:154:ASN:O	1:G:155:GLU:HG3	1.94	0.66
1:C:157:ILE:HD11	1:D:115:ASP:OD2	1.96	0.66
1:D:91:ARG:HD2	1:E:134:SER:CB	2.25	0.66
1:H:162:ILE:HD12	1:H:162:ILE:H	1.60	0.66
1:A:140:LEU:HD13	1:A:190:ILE:CG1	2.21	0.66
1:A:294:LEU:HG	1:A:298:ARG:HH21	1.61	0.66
1:C:181:GLN:H	1:C:182:PRO:CD	2.08	0.66
1:F:231:LEU:HD12	1:F:280:ILE:HG12	1.77	0.66
1:G:127:VAL:HG22	1:G:193:ARG:HG2	1.78	0.66
1:I:157:ILE:HD11	1:J:115:ASP:OD2	1.95	0.66
1:J:215:ILE:O	1:J:218:SER:HB3	1.95	0.66
1:A:28:THR:HB	1:A:255:LEU:HD21	1.76	0.66
1:C:23:ILE:HG21	1:C:126:PHE:CD1	2.31	0.66
1:C:215:ILE:O	1:C:218:SER:HB3	1.96	0.66
1:E:301:LEU:O	1:E:301:LEU:HD23	1.95	0.66
1:I:72:TRP:HZ3	1:I:135:TYR:CZ	2.14	0.66
1:E:145:ILE:HD13	1:E:165:ALA:CB	2.26	0.66
1:G:309:ALA:O	1:G:313:VAL:HG23	1.95	0.66
1:J:294:LEU:HA	1:J:297:GLN:NE2	2.10	0.66
1:C:231:LEU:HD12	1:C:280:ILE:HG12	1.77	0.66
1:H:180:VAL:HG21	1:H:184:GLN:HB2	1.77	0.66
1:J:286:GLN:HA	1:J:291:GLU:OE1	1.95	0.66
1:B:226:SER:HB3	1:B:229:GLU:HG3	1.77	0.65
1:G:162:ILE:HD12	1:G:162:ILE:H	1.59	0.65
1:G:215:ILE:O	1:G:218:SER:HB3	1.96	0.65
1:I:293:ASP:O	1:I:296:ILE:HG22	1.96	0.65
1:A:209:LEU:HB3	1:A:210:PRO:CD	2.26	0.65
1:C:145:ILE:HD13	1:C:165:ALA:CB	2.26	0.65
1:F:145:ILE:HD13	1:F:165:ALA:CB	2.25	0.65
1:G:72:TRP:HZ3	1:G:135:TYR:CZ	2.14	0.65
1:J:119:PHE:HB3	1:J:120:PRO:HD3	1.77	0.65
1:E:150:GLU:HG2	1:E:154:ASN:H	1.60	0.65
1:E:299:CYS:HB2	1:E:302:ALA:HB3	1.79	0.65
1:I:145:ILE:HD13	1:I:165:ALA:CB	2.27	0.65
1:A:288:ASN:OD1	1:A:291:GLU:HB3	1.96	0.65
1:B:65:ARG:HD2	1:C:68:ASN:ND2	2.11	0.65
1:B:231:LEU:HD12	1:B:280:ILE:HG12	1.76	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:172:ILE:HD13	1:G:189:ARG:HB3	1.79	0.65
1:H:294:LEU:HA	1:H:297:GLN:NE2	2.11	0.65
1:J:145:ILE:HD13	1:J:165:ALA:CB	2.27	0.65
1:I:226:SER:HB3	1:I:229:GLU:HG3	1.77	0.65
1:C:145:ILE:HG21	1:C:192:VAL:HG11	1.79	0.65
1:F:91:ARG:CD	1:G:134:SER:HB3	2.25	0.65
1:I:91:ARG:HD2	1:J:134:SER:HB3	1.77	0.65
1:A:150:GLU:CB	1:A:153:ASP:HB2	2.27	0.65
1:A:294:LEU:CA	1:A:297:GLN:HE21	2.08	0.65
1:C:209:LEU:HB3	1:C:210:PRO:CD	2.26	0.65
1:D:154:ASN:O	1:D:155:GLU:HG3	1.96	0.65
1:A:140:LEU:HD22	1:A:190:ILE:HD11	1.78	0.65
1:F:78:PHE:HB3	1:F:81:VAL:HG23	1.79	0.65
1:B:218:SER:HA	1:B:237:LEU:HD21	1.78	0.65
1:C:294:LEU:CA	1:C:297:GLN:HE21	2.10	0.65
1:J:167:THR:HG22	1:J:168:HIS:N	2.10	0.65
1:J:140:LEU:HD13	1:J:190:ILE:CG1	2.23	0.65
1:I:162:ILE:HD12	1:I:162:ILE:H	1.59	0.64
1:J:52:GLY:O	1:J:53:ASP:HB2	1.96	0.64
1:H:309:ALA:O	1:H:313:VAL:HG23	1.97	0.64
1:I:301:LEU:HD23	1:I:301:LEU:O	1.96	0.64
1:C:150:GLU:HB3	1:C:153:ASP:HB3	1.79	0.64
1:F:119:PHE:HB3	1:F:120:PRO:HD3	1.79	0.64
1:A:145:ILE:HD13	1:A:165:ALA:CB	2.27	0.64
1:C:28:THR:HB	1:C:255:LEU:HD21	1.79	0.64
1:C:301:LEU:O	1:C:301:LEU:HD23	1.97	0.64
1:E:72:TRP:HZ3	1:E:135:TYR:CZ	2.15	0.64
1:B:162:ILE:HD12	1:B:162:ILE:H	1.62	0.64
1:B:177:LEU:HD11	1:B:187:PHE:HE1	1.63	0.64
1:B:309:ALA:O	1:B:313:VAL:HG23	1.96	0.64
1:A:215:ILE:O	1:A:218:SER:HB3	1.98	0.64
1:D:28:THR:HB	1:D:255:LEU:HD21	1.79	0.64
1:E:182:PRO:HB2	1:E:184:GLN:HE22	1.63	0.64
1:F:309:ALA:O	1:F:313:VAL:HG23	1.97	0.64
1:H:149:THR:HG22	1:H:150:GLU:N	2.10	0.64
1:A:91:ARG:HD2	1:B:134:SER:CB	2.27	0.64
1:F:226:SER:HB3	1:F:229:GLU:HG3	1.79	0.64
1:J:181:GLN:H	1:J:182:PRO:CD	2.10	0.64
1:A:167:THR:HG22	1:A:168:HIS:N	2.10	0.64
1:F:134:SER:CB	1:J:91:ARG:HD2	2.26	0.64
1:I:290:VAL:O	1:I:290:VAL:HG12	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:309:ALA:O	1:J:313:VAL:HG23	1.97	0.64
1:A:72:TRP:HZ3	1:A:135:TYR:CZ	2.16	0.64
1:A:157:ILE:HD11	1:B:115:ASP:OD2	1.98	0.64
1:G:23:ILE:HG21	1:G:126:PHE:CD1	2.33	0.64
1:B:180:VAL:HG22	1:B:182:PRO:HD2	1.79	0.64
1:C:125:GLN:OE1	1:C:193:ARG:HD3	1.98	0.64
1:C:167:THR:HG22	1:C:168:HIS:N	2.10	0.64
1:C:299:CYS:HB2	1:C:302:ALA:HB3	1.80	0.64
1:C:309:ALA:O	1:C:313:VAL:HG23	1.98	0.64
1:G:164:LYS:HZ2	1:G:164:LYS:HA	1.63	0.64
1:A:134:SER:HB3	1:E:91:ARG:HD2	1.79	0.63
1:F:94:LEU:HD23	1:F:100:VAL:HG22	1.80	0.63
1:G:28:THR:HB	1:G:255:LEU:HD21	1.80	0.63
1:B:150:GLU:HG3	1:B:153:ASP:HB3	1.77	0.63
1:F:91:ARG:HD2	1:G:134:SER:CB	2.28	0.63
1:D:150:GLU:HG2	1:D:154:ASN:H	1.63	0.63
1:F:145:ILE:HG21	1:F:192:VAL:HG11	1.79	0.63
1:C:127:VAL:HG22	1:C:193:ARG:HG2	1.80	0.63
1:D:309:ALA:O	1:D:313:VAL:HG23	1.99	0.63
1:I:140:LEU:HD13	1:I:190:ILE:CG1	2.25	0.63
1:I:299:CYS:HB2	1:I:302:ALA:HB3	1.79	0.63
1:C:286:GLN:HG2	1:C:289:GLY:O	1.98	0.63
1:D:119:PHE:HB3	1:D:120:PRO:HD3	1.80	0.63
1:F:28:THR:HB	1:F:255:LEU:HD21	1.81	0.63
1:G:94:LEU:HD23	1:G:100:VAL:HG22	1.80	0.63
1:D:72:TRP:HZ3	1:D:135:TYR:CZ	2.16	0.63
1:E:226:SER:HB3	1:E:229:GLU:HG3	1.80	0.63
1:G:145:ILE:HD13	1:G:165:ALA:CB	2.28	0.63
1:H:119:PHE:HB3	1:H:120:PRO:HD3	1.80	0.63
1:I:180:VAL:CG2	1:I:184:GLN:HB2	2.29	0.63
1:J:178:SER:O	1:J:180:VAL:N	2.31	0.63
1:J:23:ILE:HG21	1:J:126:PHE:CD1	2.34	0.63
1:E:150:GLU:CG	1:E:154:ASN:H	2.11	0.63
1:H:155:GLU:HB3	1:H:161:TRP:CD1	2.34	0.63
1:H:224:LEU:HD21	1:I:231:LEU:HD22	1.81	0.63
1:H:226:SER:HB3	1:H:229:GLU:HG3	1.79	0.63
1:A:23:ILE:HG21	1:A:126:PHE:CD1	2.33	0.62
1:F:72:TRP:HZ3	1:F:135:TYR:CZ	2.16	0.62
1:J:150:GLU:CG	1:J:153:ASP:HB3	2.29	0.62
1:D:140:LEU:HD22	1:D:190:ILE:HD11	1.82	0.62
1:H:154:ASN:O	1:H:155:GLU:CG	2.46	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:299:CYS:HB2	1:A:302:ALA:HB3	1.79	0.62
1:F:176:HIS:CD2	1:J:146:GLN:HE21	2.16	0.62
1:H:140:LEU:HD22	1:H:190:ILE:HD11	1.80	0.62
1:C:162:ILE:HD12	1:C:162:ILE:H	1.63	0.62
1:F:313:VAL:HG22	1:F:316:ILE:HD12	1.80	0.62
1:G:149:THR:HG22	1:G:150:GLU:H	1.64	0.62
1:G:294:LEU:HG	1:G:298:ARG:HH21	1.64	0.62
1:C:293:ASP:O	1:C:296:ILE:HG22	1.99	0.62
1:F:83:GLY:HA2	1:J:107:LEU:HD23	1.81	0.62
1:H:299:CYS:HB2	1:H:302:ALA:HB3	1.81	0.62
1:H:312:CYS:O	1:H:316:ILE:HG13	1.99	0.62
1:J:299:CYS:HB2	1:J:302:ALA:HB3	1.81	0.62
1:A:162:ILE:HD12	1:A:162:ILE:H	1.61	0.62
1:A:309:ALA:O	1:A:313:VAL:HG23	1.99	0.62
1:B:299:CYS:HB2	1:B:302:ALA:HB3	1.80	0.62
1:E:28:THR:HB	1:E:255:LEU:HD21	1.80	0.62
1:E:215:ILE:O	1:E:218:SER:HB3	2.00	0.62
1:F:299:CYS:HB2	1:F:302:ALA:HB3	1.81	0.62
1:G:315:VAL:O	1:G:315:VAL:HG12	1.99	0.62
1:E:162:ILE:HD12	1:E:162:ILE:H	1.63	0.62
1:H:299:CYS:HB2	1:H:302:ALA:HB2	1.81	0.62
1:I:182:PRO:HB2	1:I:184:GLN:HE22	1.62	0.62
1:B:164:LYS:CD	1:I:163:ARG:HD2	2.24	0.62
1:D:254:ARG:O	1:D:255:LEU:HD23	1.99	0.62
1:F:140:LEU:HD22	1:F:190:ILE:HD11	1.81	0.62
1:H:78:PHE:HB3	1:H:81:VAL:HG23	1.81	0.62
1:G:78:PHE:HB3	1:G:81:VAL:HG23	1.82	0.62
1:I:28:THR:HB	1:I:255:LEU:HD21	1.82	0.62
1:G:299:CYS:HB2	1:G:302:ALA:HB3	1.81	0.62
1:H:145:ILE:HD13	1:H:165:ALA:CB	2.30	0.62
1:A:226:SER:HB3	1:A:229:GLU:HG3	1.82	0.61
1:B:299:CYS:HB2	1:B:302:ALA:HB2	1.81	0.61
1:H:180:VAL:HG23	1:H:182:PRO:HD2	1.82	0.61
1:I:56:LEU:HD13	1:I:57:ILE:N	2.14	0.61
1:F:299:CYS:HB2	1:F:302:ALA:HB2	1.81	0.61
1:H:294:LEU:HG	1:H:298:ARG:NH2	2.15	0.61
1:B:107:LEU:HD23	1:C:83:GLY:HA2	1.82	0.61
1:B:177:LEU:HD12	1:B:185:ASN:HA	1.82	0.61
1:B:149:THR:HG22	1:B:150:GLU:H	1.64	0.61
1:D:299:CYS:HB2	1:D:302:ALA:HB3	1.81	0.61
1:A:231:LEU:HD22	1:E:224:LEU:HD21	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:145:ILE:HD13	1:B:165:ALA:HB1	1.83	0.61
1:B:147:VAL:HG23	1:B:165:ALA:HB2	1.81	0.61
1:B:293:ASP:O	1:B:295:LEU:N	2.34	0.61
1:D:91:ARG:HB2	1:E:133:PHE:HE2	1.64	0.61
1:E:309:ALA:O	1:E:313:VAL:HG23	2.01	0.61
1:H:72:TRP:HZ3	1:H:135:TYR:CZ	2.18	0.61
1:I:292:ASP:O	1:I:294:LEU:N	2.33	0.61
1:E:292:ASP:O	1:E:297:GLN:NE2	2.33	0.61
1:H:209:LEU:HB3	1:H:210:PRO:CD	2.30	0.61
1:B:180:VAL:CG2	1:B:182:PRO:HD2	2.30	0.61
1:C:180:VAL:CG2	1:C:184:GLN:HB2	2.31	0.61
1:E:167:THR:HG22	1:E:168:HIS:N	2.12	0.61
1:J:150:GLU:CB	1:J:153:ASP:HB3	2.31	0.61
1:B:313:VAL:HA	1:B:316:ILE:HD12	1.81	0.61
1:F:54:LYS:HB3	1:F:55:PRO:HD2	1.83	0.61
1:F:181:GLN:H	1:F:182:PRO:CD	2.13	0.61
1:G:140:LEU:HD22	1:G:190:ILE:HD11	1.82	0.61
1:G:285:ARG:HA	1:G:285:ARG:NE	2.16	0.61
1:I:309:ALA:O	1:I:313:VAL:HG23	2.01	0.61
1:J:294:LEU:HG	1:J:298:ARG:NH2	2.15	0.61
1:A:301:LEU:HD23	1:A:301:LEU:O	2.00	0.61
1:D:293:ASP:O	1:D:297:GLN:HG2	2.00	0.61
1:I:164:LYS:HZ2	1:I:164:LYS:HA	1.65	0.61
1:C:72:TRP:HZ3	1:C:135:TYR:CZ	2.19	0.60
1:D:23:ILE:HG21	1:D:126:PHE:CD1	2.36	0.60
1:G:172:ILE:CD1	1:G:189:ARG:HB3	2.31	0.60
1:G:224:LEU:HD21	1:H:231:LEU:HD22	1.82	0.60
1:H:127:VAL:HG22	1:H:193:ARG:HG2	1.83	0.60
1:I:140:LEU:HD22	1:I:190:ILE:HD11	1.83	0.60
1:J:301:LEU:HD23	1:J:301:LEU:O	2.00	0.60
1:A:254:ARG:O	1:A:255:LEU:HD23	2.01	0.60
1:B:127:VAL:HG22	1:B:193:ARG:HG2	1.82	0.60
1:B:185:ASN:HD22	1:B:185:ASN:N	1.99	0.60
1:B:290:VAL:O	1:B:290:VAL:HG12	2.01	0.60
1:D:294:LEU:CA	1:D:297:GLN:HE21	2.13	0.60
1:F:290:VAL:O	1:F:290:VAL:HG12	2.01	0.60
1:B:301:LEU:HD23	1:B:301:LEU:O	2.01	0.60
1:D:59:GLU:OE2	1:E:75:ALA:HB3	2.02	0.60
1:D:284:HIS:HA	1:D:286:GLN:HE21	1.66	0.60
1:E:180:VAL:CG2	1:E:184:GLN:HB2	2.31	0.60
1:J:149:THR:HG22	1:J:150:GLU:N	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:61:THR:HG21	1:H:64:GLU:HG3	1.81	0.60
1:I:119:PHE:HB3	1:I:120:PRO:HD3	1.83	0.60
1:J:127:VAL:HG22	1:J:193:ARG:HG2	1.82	0.60
1:D:157:ILE:HD11	1:E:115:ASP:OD2	2.02	0.60
1:F:19:PHE:CE2	1:F:146:GLN:HG3	2.37	0.60
1:A:65:ARG:HD2	1:B:68:ASN:ND2	2.17	0.60
1:A:185:ASN:N	1:A:185:ASN:HD22	2.00	0.60
1:D:167:THR:HG22	1:D:168:HIS:N	2.16	0.60
1:F:68:ASN:HA	1:J:65:ARG:NH1	2.17	0.60
1:G:185:ASN:HD22	1:G:185:ASN:N	1.98	0.60
1:G:226:SER:HB3	1:G:229:GLU:HG3	1.84	0.60
1:I:185:ASN:N	1:I:185:ASN:HD22	2.00	0.60
1:J:227:PHE:HA	1:J:230:ARG:NH1	2.16	0.60
1:A:134:SER:HB3	1:E:91:ARG:CD	2.31	0.60
1:A:162:ILE:HG22	1:A:163:ARG:N	2.13	0.60
1:D:226:SER:HB3	1:D:229:GLU:HG3	1.82	0.60
1:E:140:LEU:HD13	1:E:190:ILE:CG1	2.25	0.60
1:B:28:THR:HB	1:B:255:LEU:HD21	1.82	0.60
1:D:185:ASN:N	1:D:185:ASN:HD22	1.99	0.60
1:F:286:GLN:HB3	1:F:291:GLU:HB3	1.84	0.60
1:C:118:LEU:N	1:C:118:LEU:HD23	2.17	0.60
1:A:211:LEU:HD11	1:A:264:MET:HB3	1.83	0.60
1:A:246:PHE:HE2	1:E:246:PHE:CD2	2.19	0.60
1:C:227:PHE:HA	1:C:230:ARG:NH1	2.17	0.60
1:F:210:PRO:O	1:F:214:ILE:HG12	2.02	0.60
1:G:118:LEU:N	1:G:118:LEU:HD23	2.16	0.60
1:H:254:ARG:O	1:H:255:LEU:HD23	2.02	0.60
1:J:59:GLU:O	1:J:63:ILE:HG13	2.02	0.60
1:J:239:LEU:O	1:J:239:LEU:HD13	2.02	0.60
1:E:67:ILE:HD11	1:E:73:VAL:HG21	1.83	0.59
1:J:54:LYS:HB3	1:J:55:PRO:HD2	1.83	0.59
1:A:299:CYS:HB2	1:A:302:ALA:HB2	1.84	0.59
1:C:65:ARG:HD2	1:D:68:ASN:ND2	2.17	0.59
1:D:125:GLN:OE1	1:D:193:ARG:HD3	2.02	0.59
1:F:149:THR:HG22	1:F:150:GLU:OE1	2.01	0.59
1:F:285:ARG:HA	1:F:285:ARG:CZ	2.32	0.59
1:H:150:GLU:HB2	1:H:153:ASP:CB	2.19	0.59
1:H:301:LEU:O	1:H:301:LEU:HD23	2.02	0.59
1:B:177:LEU:CD1	1:B:185:ASN:HA	2.32	0.59
1:C:211:LEU:HD23	1:C:244:TYR:CD2	2.36	0.59
1:D:286:GLN:HG2	1:D:289:GLY:O	2.00	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:299:CYS:HB2	1:E:302:ALA:HB2	1.84	0.59
1:F:164:LYS:HA	1:F:164:LYS:HZ3	1.67	0.59
1:F:167:THR:HG22	1:F:168:HIS:N	2.12	0.59
1:J:150:GLU:HG3	1:J:153:ASP:HB3	1.84	0.59
1:D:147:VAL:HG23	1:D:165:ALA:HB2	1.84	0.59
1:H:164:LYS:HA	1:H:164:LYS:HZ3	1.68	0.59
1:B:294:LEU:HA	1:B:297:GLN:HE21	1.67	0.59
1:E:182:PRO:HB2	1:E:184:GLN:NE2	2.16	0.59
1:E:227:PHE:HA	1:E:230:ARG:NH1	2.16	0.59
1:E:288:ASN:OD1	1:E:291:GLU:HB2	2.01	0.59
1:F:185:ASN:HD22	1:F:185:ASN:N	2.00	0.59
1:H:211:LEU:HD23	1:H:244:TYR:CD2	2.37	0.59
1:B:145:ILE:HD13	1:B:165:ALA:CB	2.31	0.59
1:C:211:LEU:HD11	1:C:264:MET:HB3	1.85	0.59
1:F:246:PHE:HE2	1:J:246:PHE:CD2	2.21	0.59
1:C:52:GLY:O	1:C:53:ASP:HB2	2.02	0.59
1:D:162:ILE:HG22	1:D:163:ARG:N	2.15	0.59
1:D:303:PHE:O	1:D:307:PHE:HB2	2.02	0.59
1:G:182:PRO:HB2	1:G:184:GLN:HE22	1.68	0.59
1:H:145:ILE:HD12	1:H:145:ILE:N	2.14	0.59
1:H:252:LEU:HG	1:H:253:PRO:HD2	1.84	0.59
1:I:286:GLN:CB	1:I:291:GLU:HB3	2.33	0.59
1:A:286:GLN:HB2	1:A:288:ASN:OD1	2.02	0.59
1:B:72:TRP:HZ3	1:B:135:TYR:CZ	2.20	0.59
1:C:147:VAL:HG23	1:C:165:ALA:HB2	1.83	0.59
1:D:150:GLU:H	1:D:150:GLU:CD	2.06	0.59
1:G:99:ARG:NH1	1:H:179:SER:HB3	2.17	0.59
1:A:286:GLN:HA	1:A:291:GLU:OE2	2.02	0.59
1:D:59:GLU:O	1:D:63:ILE:HG13	2.02	0.59
1:E:262:ASP:O	1:E:266:ILE:HG12	2.03	0.59
1:G:299:CYS:HB2	1:G:302:ALA:HB2	1.84	0.59
1:I:91:ARG:CD	1:J:134:SER:HB3	2.32	0.59
1:J:211:LEU:HD23	1:J:244:TYR:CD2	2.38	0.59
1:A:246:PHE:HA	1:E:247:TYR:HD1	1.67	0.59
1:C:254:ARG:O	1:C:255:LEU:HD23	2.01	0.59
1:G:300:ARG:O	1:G:304:PRO:HG2	2.02	0.59
1:A:172:ILE:HD13	1:A:189:ARG:HB3	1.85	0.58
1:A:262:ASP:O	1:A:266:ILE:HG12	2.03	0.58
1:D:299:CYS:HB2	1:D:302:ALA:HB2	1.84	0.58
1:I:164:LYS:HZ2	1:I:164:LYS:CA	2.16	0.58
1:B:54:LYS:HB3	1:B:55:PRO:HD2	1.83	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:59:GLU:O	1:B:63:ILE:HG13	2.04	0.58
1:D:94:LEU:HD23	1:D:100:VAL:HG22	1.85	0.58
1:E:127:VAL:HG22	1:E:193:ARG:HG2	1.85	0.58
1:G:150:GLU:H	1:G:150:GLU:CD	2.05	0.58
1:H:185:ASN:HD22	1:H:185:ASN:N	2.00	0.58
1:I:303:PHE:O	1:I:307:PHE:HB2	2.04	0.58
1:J:21:ASN:HD21	1:J:38:TYR:HE1	1.51	0.58
1:J:254:ARG:O	1:J:255:LEU:HD23	2.03	0.58
1:A:211:LEU:HD23	1:A:244:TYR:CE2	2.38	0.58
1:A:224:LEU:HD21	1:B:231:LEU:HD22	1.85	0.58
1:B:167:THR:O	1:B:168:HIS:HB2	2.03	0.58
1:D:301:LEU:HD23	1:D:301:LEU:O	2.04	0.58
1:E:185:ASN:HD22	1:E:185:ASN:N	1.99	0.58
1:G:149:THR:HG22	1:G:150:GLU:OE1	2.04	0.58
1:A:211:LEU:HD23	1:A:244:TYR:CD2	2.38	0.58
1:C:303:PHE:O	1:C:307:PHE:HB2	2.04	0.58
1:F:211:LEU:HD23	1:F:244:TYR:CD2	2.39	0.58
1:H:180:VAL:CG2	1:H:182:PRO:HD2	2.34	0.58
1:E:177:LEU:HD11	1:E:185:ASN:CB	2.33	0.58
1:G:167:THR:HG22	1:G:168:HIS:N	2.16	0.58
1:H:211:LEU:HD11	1:H:264:MET:HB3	1.85	0.58
1:A:64:GLU:HG3	1:E:61:THR:HG21	1.86	0.58
1:A:227:PHE:HA	1:A:230:ARG:NH1	2.19	0.58
1:H:162:ILE:HG22	1:H:163:ARG:N	2.13	0.58
1:I:23:ILE:HG21	1:I:126:PHE:CD1	2.38	0.58
1:A:210:PRO:O	1:A:214:ILE:HG12	2.04	0.58
1:B:204:LEU:HA	1:B:208:ILE:HG12	1.85	0.58
1:D:78:PHE:HB3	1:D:81:VAL:HG23	1.85	0.58
1:F:127:VAL:HG22	1:F:193:ARG:HG2	1.84	0.58
1:F:147:VAL:HG23	1:F:165:ALA:HB2	1.84	0.58
1:I:286:GLN:HB3	1:I:291:GLU:HB3	1.85	0.58
1:C:185:ASN:HD22	1:C:185:ASN:N	2.02	0.58
1:F:303:PHE:O	1:F:307:PHE:HB2	2.04	0.58
1:G:125:GLN:OE1	1:G:193:ARG:HD3	2.04	0.58
1:H:290:VAL:O	1:H:290:VAL:HG12	2.04	0.58
1:E:294:LEU:CA	1:E:297:GLN:HE21	2.13	0.58
1:G:107:LEU:HD23	1:H:83:GLY:HA2	1.85	0.58
1:I:299:CYS:HB2	1:I:302:ALA:HB2	1.84	0.58
1:J:152:ILE:O	1:J:152:ILE:HG22	2.04	0.58
1:A:204:LEU:HA	1:A:208:ILE:HG12	1.86	0.58
1:F:118:LEU:N	1:F:118:LEU:HD23	2.19	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:147:VAL:HG23	1:G:165:ALA:HB2	1.86	0.58
1:G:293:ASP:O	1:G:297:GLN:HG2	2.04	0.58
1:J:125:GLN:OE1	1:J:193:ARG:HD3	2.03	0.58
1:J:185:ASN:HD22	1:J:185:ASN:N	2.02	0.58
1:J:259:THR:O	1:J:263:GLN:HG3	2.04	0.58
1:A:107:LEU:HD23	1:B:83:GLY:HA2	1.86	0.57
1:C:181:GLN:HG2	1:C:182:PRO:HD3	1.86	0.57
1:F:64:GLU:HG3	1:J:61:THR:HG21	1.85	0.57
1:F:301:LEU:O	1:F:301:LEU:HD23	2.03	0.57
1:A:59:GLU:O	1:A:63:ILE:HG13	2.03	0.57
1:D:211:LEU:HD11	1:D:264:MET:HB3	1.86	0.57
1:D:315:VAL:O	1:D:315:VAL:HG12	2.04	0.57
1:E:66:TRP:HB3	1:E:71:LEU:HD12	1.86	0.57
1:E:300:ARG:O	1:E:304:PRO:HG2	2.03	0.57
1:F:252:LEU:HG	1:F:253:PRO:HD2	1.87	0.57
1:H:118:LEU:HD23	1:H:118:LEU:N	2.19	0.57
1:A:303:PHE:O	1:A:307:PHE:HB2	2.05	0.57
1:B:150:GLU:O	1:B:150:GLU:HG2	2.05	0.57
1:E:180:VAL:HG21	1:E:184:GLN:HB2	1.86	0.57
1:A:300:ARG:O	1:A:304:PRO:HG2	2.04	0.57
1:G:87:THR:HG21	1:G:90:LYS:HE2	1.86	0.57
1:H:148:TYR:HH	1:I:176:HIS:CE1	2.19	0.57
1:H:300:ARG:O	1:H:304:PRO:HG2	2.04	0.57
1:I:91:ARG:HD2	1:J:134:SER:CB	2.33	0.57
1:I:93:MET:SD	1:J:178:SER:HB3	2.44	0.57
1:I:286:GLN:HA	1:I:291:GLU:OE1	2.05	0.57
1:A:252:LEU:HG	1:A:253:PRO:HD2	1.86	0.57
1:C:204:LEU:HA	1:C:208:ILE:HG12	1.86	0.57
1:C:290:VAL:HG12	1:C:290:VAL:O	2.05	0.57
1:F:87:THR:HG21	1:F:90:LYS:HE2	1.86	0.57
1:G:262:ASP:O	1:G:266:ILE:HG12	2.05	0.57
1:G:301:LEU:HD23	1:G:301:LEU:O	2.04	0.57
1:B:303:PHE:O	1:B:307:PHE:HB2	2.04	0.57
1:D:182:PRO:HB2	1:D:184:GLN:HE22	1.70	0.57
1:G:252:LEU:HG	1:G:253:PRO:HD2	1.86	0.57
1:H:51:PRO:HD2	1:H:56:LEU:HD23	1.86	0.57
1:H:211:LEU:HD23	1:H:244:TYR:CE2	2.39	0.57
1:I:59:GLU:O	1:I:63:ILE:HG13	2.05	0.57
1:J:226:SER:HB3	1:J:229:GLU:HG3	1.85	0.57
1:B:151:ASN:HD22	1:B:151:ASN:N	2.03	0.57
1:B:254:ARG:O	1:B:255:LEU:HD23	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:19:PHE:CE2	1:D:146:GLN:HG3	2.40	0.57
1:F:125:GLN:OE1	1:F:193:ARG:HD3	2.05	0.57
1:F:305:LEU:C	1:F:305:LEU:HD12	2.25	0.57
1:G:21:ASN:HD21	1:G:38:TYR:HE1	1.52	0.57
1:A:68:ASN:ND2	1:E:65:ARG:HD2	2.20	0.57
1:B:224:LEU:O	1:B:230:ARG:HD2	2.05	0.57
1:D:224:LEU:O	1:D:230:ARG:HD2	2.05	0.57
1:E:211:LEU:HD11	1:E:264:MET:HB3	1.85	0.57
1:J:312:CYS:O	1:J:316:ILE:HG13	2.03	0.57
1:B:19:PHE:CE2	1:B:146:GLN:HG3	2.40	0.57
1:D:262:ASP:O	1:D:266:ILE:HG12	2.04	0.57
1:E:285:ARG:NE	1:E:285:ARG:HA	2.19	0.57
1:G:59:GLU:O	1:G:63:ILE:HG13	2.05	0.57
1:J:94:LEU:HD23	1:J:100:VAL:HG22	1.87	0.57
1:A:150:GLU:HG3	1:A:153:ASP:HB2	1.87	0.57
1:B:172:ILE:CD1	1:B:189:ARG:HB3	2.35	0.57
1:E:78:PHE:HB3	1:E:81:VAL:HG23	1.87	0.57
1:G:19:PHE:CE2	1:G:146:GLN:HG3	2.40	0.57
1:G:204:LEU:HA	1:G:208:ILE:HG12	1.87	0.57
1:G:224:LEU:O	1:G:230:ARG:HD2	2.05	0.57
1:A:125:GLN:OE1	1:A:193:ARG:HD3	2.04	0.56
1:A:312:CYS:O	1:A:316:ILE:HG13	2.04	0.56
1:C:107:LEU:HD23	1:D:83:GLY:HA2	1.85	0.56
1:D:292:ASP:O	1:D:297:GLN:NE2	2.38	0.56
1:J:299:CYS:HB2	1:J:302:ALA:HB2	1.84	0.56
1:A:127:VAL:HG22	1:A:193:ARG:HG2	1.85	0.56
1:A:147:VAL:HG23	1:A:165:ALA:HB2	1.87	0.56
1:C:136:ASN:ND2	1:C:184:GLN:HA	2.20	0.56
1:D:204:LEU:HA	1:D:208:ILE:HG12	1.85	0.56
1:E:204:LEU:HA	1:E:208:ILE:HG12	1.87	0.56
1:G:150:GLU:HB2	1:G:153:ASP:HB3	1.87	0.56
1:G:150:GLU:CB	1:G:153:ASP:HB3	2.34	0.56
1:G:290:VAL:O	1:G:290:VAL:HG12	2.03	0.56
1:A:134:SER:CB	1:E:91:ARG:HD2	2.34	0.56
1:B:172:ILE:HD13	1:B:189:ARG:HB3	1.86	0.56
1:D:181:GLN:CG	1:D:182:PRO:HD3	2.35	0.56
1:E:140:LEU:HD22	1:E:190:ILE:HD11	1.85	0.56
1:F:204:LEU:HA	1:F:208:ILE:HG12	1.87	0.56
1:F:254:ARG:O	1:F:255:LEU:HD23	2.06	0.56
1:G:150:GLU:O	1:G:152:ILE:N	2.38	0.56
1:G:211:LEU:HD11	1:G:264:MET:HB3	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:78:PHE:HB3	1:H:81:VAL:CG2	2.35	0.56
1:I:118:LEU:N	1:I:118:LEU:HD23	2.20	0.56
1:E:293:ASP:O	1:E:296:ILE:HG22	2.05	0.56
1:G:227:PHE:HA	1:G:230:ARG:NH1	2.19	0.56
1:G:305:LEU:C	1:G:305:LEU:HD12	2.26	0.56
1:A:303:PHE:N	1:A:304:PRO:CD	2.69	0.56
1:B:262:ASP:O	1:B:266:ILE:HG12	2.04	0.56
1:C:283:HIS:O	1:C:286:GLN:HG3	2.06	0.56
1:D:286:GLN:HA	1:D:291:GLU:HB3	1.86	0.56
1:E:219:TRP:C	1:E:221:VAL:H	2.08	0.56
1:E:290:VAL:O	1:E:290:VAL:HG12	2.04	0.56
1:G:157:ILE:HD11	1:H:115:ASP:OD2	2.05	0.56
1:G:162:ILE:HG22	1:G:163:ARG:N	2.16	0.56
1:H:240:THR:OG1	1:I:239:LEU:HD23	2.06	0.56
1:J:149:THR:HG22	1:J:150:GLU:OE2	2.05	0.56
1:B:157:ILE:HD11	1:C:115:ASP:CG	2.26	0.56
1:C:288:ASN:CG	1:C:289:GLY:H	2.09	0.56
1:F:305:LEU:HD12	1:F:306:GLY:N	2.21	0.56
1:J:136:ASN:ND2	1:J:184:GLN:HA	2.20	0.56
1:A:305:LEU:C	1:A:305:LEU:HD12	2.26	0.56
1:B:315:VAL:O	1:B:315:VAL:HG12	2.06	0.56
1:C:19:PHE:CE2	1:C:146:GLN:HG3	2.41	0.56
1:D:288:ASN:OD1	1:D:291:GLU:HB2	2.05	0.56
1:E:94:LEU:HD23	1:E:100:VAL:HG22	1.87	0.56
1:F:262:ASP:O	1:F:266:ILE:HG12	2.05	0.56
1:G:292:ASP:O	1:G:297:GLN:NE2	2.37	0.56
1:A:118:LEU:N	1:A:118:LEU:HD23	2.20	0.56
1:C:211:LEU:HD23	1:C:244:TYR:CE2	2.41	0.56
1:C:303:PHE:N	1:C:304:PRO:CD	2.69	0.56
1:C:305:LEU:C	1:C:305:LEU:HD12	2.26	0.56
1:D:172:ILE:HD13	1:D:189:ARG:HB3	1.87	0.56
1:E:259:THR:O	1:E:263:GLN:HG3	2.06	0.56
1:G:167:THR:O	1:G:168:HIS:HB2	2.05	0.56
1:H:67:ILE:HD11	1:H:73:VAL:HG21	1.87	0.56
1:I:227:PHE:HA	1:I:230:ARG:NH1	2.20	0.56
1:B:118:LEU:N	1:B:118:LEU:HD23	2.21	0.56
1:C:67:ILE:HD11	1:C:73:VAL:HG21	1.88	0.56
1:C:294:LEU:HD12	1:C:297:GLN:NE2	2.20	0.56
1:E:172:ILE:N	1:E:172:ILE:HD12	2.20	0.56
1:I:237:LEU:HD13	1:J:235:PHE:CE2	2.41	0.56
1:D:227:PHE:HA	1:D:230:ARG:NH1	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:172:ILE:HD13	1:E:189:ARG:HB3	1.87	0.56
1:G:67:ILE:HD11	1:G:73:VAL:HG21	1.88	0.56
1:H:181:GLN:H	1:H:182:PRO:HD2	1.71	0.56
1:H:223:TRP:CE3	1:I:280:ILE:HG22	2.41	0.56
1:A:313:VAL:HA	1:A:316:ILE:HB	1.88	0.55
1:B:259:THR:O	1:B:263:GLN:HG3	2.05	0.55
1:E:280:ILE:HG22	1:E:280:ILE:O	2.06	0.55
1:F:172:ILE:HD13	1:F:189:ARG:HB3	1.88	0.55
1:J:180:VAL:HG22	1:J:182:PRO:HD2	1.86	0.55
1:B:303:PHE:N	1:B:304:PRO:CD	2.69	0.55
1:C:172:ILE:HD13	1:C:189:ARG:HB3	1.87	0.55
1:C:226:SER:HB3	1:C:229:GLU:CG	2.36	0.55
1:D:285:ARG:HA	1:D:285:ARG:CZ	2.35	0.55
1:G:219:TRP:C	1:G:221:VAL:H	2.10	0.55
1:B:147:VAL:CG2	1:B:165:ALA:HB2	2.37	0.55
1:B:300:ARG:O	1:B:304:PRO:HG2	2.06	0.55
1:C:176:HIS:CD2	1:C:176:HIS:N	2.74	0.55
1:C:292:ASP:O	1:C:294:LEU:N	2.39	0.55
1:E:211:LEU:HD23	1:E:244:TYR:CD2	2.42	0.55
1:G:136:ASN:ND2	1:G:184:GLN:HA	2.22	0.55
1:G:223:TRP:CE3	1:H:280:ILE:HG22	2.40	0.55
1:H:152:ILE:O	1:H:152:ILE:HG22	2.06	0.55
1:A:155:GLU:HB3	1:A:161:TRP:NE1	2.21	0.55
1:B:21:ASN:HD21	1:B:38:TYR:HE1	1.54	0.55
1:D:164:LYS:NZ	1:D:165:ALA:N	2.41	0.55
1:D:290:VAL:O	1:D:290:VAL:HG12	2.05	0.55
1:F:259:THR:O	1:F:263:GLN:HG3	2.06	0.55
1:H:182:PRO:HB2	1:H:184:GLN:HE22	1.72	0.55
1:I:167:THR:HG22	1:I:168:HIS:N	2.17	0.55
1:J:262:ASP:O	1:J:266:ILE:HG12	2.06	0.55
1:A:66:TRP:HB3	1:A:71:LEU:HD12	1.89	0.55
1:F:220:SER:HB2	1:G:280:ILE:CD1	2.35	0.55
1:F:239:LEU:O	1:F:239:LEU:HD13	2.06	0.55
1:H:227:PHE:HA	1:H:230:ARG:NH1	2.22	0.55
1:H:303:PHE:O	1:H:307:PHE:HB2	2.06	0.55
1:I:147:VAL:HG23	1:I:165:ALA:HB2	1.87	0.55
1:B:150:GLU:CG	1:B:150:GLU:O	2.55	0.55
1:B:227:PHE:HA	1:B:230:ARG:NH1	2.20	0.55
1:C:87:THR:HG21	1:C:90:LYS:HE2	1.89	0.55
1:D:259:THR:O	1:D:263:GLN:HG3	2.07	0.55
1:D:303:PHE:N	1:D:304:PRO:CD	2.69	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:303:PHE:N	1:E:304:PRO:CD	2.70	0.55
1:G:303:PHE:N	1:G:304:PRO:CD	2.70	0.55
1:I:107:LEU:HD23	1:J:83:GLY:HA2	1.89	0.55
1:I:172:ILE:HD13	1:I:189:ARG:HB3	1.88	0.55
1:J:150:GLU:HG3	1:J:154:ASN:H	1.72	0.55
1:G:294:LEU:CA	1:G:297:GLN:HE21	2.17	0.55
1:H:157:ILE:HD12	1:I:115:ASP:HA	1.88	0.55
1:H:303:PHE:N	1:H:304:PRO:CD	2.70	0.55
1:I:303:PHE:N	1:I:304:PRO:CD	2.70	0.55
1:J:315:VAL:O	1:J:315:VAL:HG12	2.06	0.55
1:B:205:TRP:O	1:C:266:ILE:HD12	2.07	0.55
1:D:285:ARG:NE	1:D:285:ARG:CA	2.67	0.55
1:E:210:PRO:O	1:E:214:ILE:HG12	2.06	0.55
1:E:315:VAL:O	1:E:315:VAL:HG12	2.06	0.55
1:H:285:ARG:NE	1:H:285:ARG:HA	2.21	0.55
1:I:204:LEU:HA	1:I:208:ILE:HG12	1.89	0.55
1:I:254:ARG:O	1:I:255:LEU:HD23	2.06	0.55
1:A:94:LEU:HD23	1:A:100:VAL:HG22	1.89	0.55
1:B:211:LEU:HD23	1:B:244:TYR:CD2	2.42	0.55
1:D:181:GLN:HG2	1:D:182:PRO:HD3	1.88	0.55
1:F:211:LEU:HD23	1:F:244:TYR:CE2	2.42	0.55
1:H:305:LEU:C	1:H:305:LEU:HD12	2.27	0.55
1:I:19:PHE:CE2	1:I:146:GLN:HG3	2.41	0.55
1:A:290:VAL:O	1:A:290:VAL:HG12	2.06	0.55
1:B:78:PHE:HB3	1:B:81:VAL:HG23	1.89	0.55
1:B:155:GLU:HB3	1:B:161:TRP:CD1	2.42	0.55
1:B:219:TRP:C	1:B:221:VAL:H	2.10	0.55
1:E:136:ASN:ND2	1:E:184:GLN:HA	2.22	0.55
1:F:313:VAL:HA	1:F:316:ILE:HD12	1.88	0.55
1:G:147:VAL:O	1:G:149:THR:N	2.40	0.55
1:G:211:LEU:HD23	1:G:244:TYR:CD2	2.42	0.55
1:H:172:ILE:HD13	1:H:189:ARG:HB3	1.88	0.55
1:H:262:ASP:O	1:H:266:ILE:HG12	2.07	0.55
1:J:155:GLU:HB3	1:J:161:TRP:CD1	2.42	0.55
1:J:172:ILE:HD13	1:J:189:ARG:HB3	1.88	0.55
1:J:280:ILE:HG22	1:J:280:ILE:O	2.07	0.55
1:B:226:SER:HB3	1:B:229:GLU:CG	2.37	0.54
1:B:292:ASP:O	1:B:294:LEU:N	2.40	0.54
1:C:312:CYS:O	1:C:316:ILE:HG13	2.08	0.54
1:D:180:VAL:HG11	1:D:184:GLN:HB2	1.89	0.54
1:D:305:LEU:C	1:D:305:LEU:HD12	2.27	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:151:ASN:O	1:E:152:ILE:HD13	2.07	0.54
1:F:136:ASN:ND2	1:F:184:GLN:HA	2.22	0.54
1:F:227:PHE:HA	1:F:230:ARG:NH1	2.21	0.54
1:F:283:HIS:O	1:F:286:GLN:HG3	2.07	0.54
1:H:94:LEU:HD23	1:H:100:VAL:HG22	1.90	0.54
1:H:136:ASN:ND2	1:H:184:GLN:HA	2.22	0.54
1:H:259:THR:O	1:H:263:GLN:HG3	2.07	0.54
1:A:181:GLN:CG	1:A:182:PRO:HD3	2.35	0.54
1:F:162:ILE:HG22	1:F:163:ARG:N	2.15	0.54
1:F:303:PHE:N	1:F:304:PRO:CD	2.71	0.54
1:G:283:HIS:HA	1:G:292:ASP:OD1	2.06	0.54
1:H:107:LEU:HD23	1:I:83:GLY:HA2	1.88	0.54
1:H:125:GLN:OE1	1:H:193:ARG:HD3	2.08	0.54
1:J:140:LEU:HD22	1:J:190:ILE:HD11	1.88	0.54
1:A:78:PHE:HB3	1:A:81:VAL:HG23	1.89	0.54
1:A:219:TRP:C	1:A:221:VAL:H	2.11	0.54
1:A:285:ARG:NE	1:A:285:ARG:CA	2.71	0.54
1:B:286:GLN:HB3	1:B:291:GLU:HB3	1.88	0.54
1:C:219:TRP:C	1:C:221:VAL:H	2.09	0.54
1:D:300:ARG:O	1:D:304:PRO:HG2	2.07	0.54
1:E:313:VAL:HA	1:E:316:ILE:CG1	2.35	0.54
1:I:280:ILE:HG22	1:I:280:ILE:O	2.07	0.54
1:A:280:ILE:HD13	1:E:220:SER:HB2	1.90	0.54
1:D:219:TRP:C	1:D:221:VAL:H	2.11	0.54
1:F:219:TRP:C	1:F:221:VAL:H	2.11	0.54
1:G:210:PRO:O	1:G:214:ILE:HG12	2.08	0.54
1:H:149:THR:HG22	1:H:150:GLU:OE1	2.07	0.54
1:H:315:VAL:O	1:H:315:VAL:HG12	2.07	0.54
1:J:164:LYS:HZ2	1:J:164:LYS:HA	1.71	0.54
1:J:300:ARG:O	1:J:304:PRO:HG2	2.07	0.54
1:A:164:LYS:HZ3	1:A:164:LYS:HA	1.72	0.54
1:B:181:GLN:N	1:B:182:PRO:CD	2.65	0.54
1:C:211:LEU:CD1	1:C:264:MET:HB3	2.38	0.54
1:D:286:GLN:HB2	1:D:289:GLY:H	1.73	0.54
1:D:305:LEU:HD12	1:D:306:GLY:N	2.23	0.54
1:E:162:ILE:HG22	1:E:163:ARG:N	2.14	0.54
1:E:303:PHE:O	1:E:307:PHE:HB2	2.08	0.54
1:F:239:LEU:HD23	1:J:240:THR:OG1	2.07	0.54
1:J:219:TRP:C	1:J:221:VAL:H	2.10	0.54
1:C:230:ARG:HB3	1:C:279:ILE:HD13	1.89	0.54
1:C:315:VAL:O	1:C:315:VAL:HG12	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:294:LEU:CA	1:F:297:GLN:HE21	2.15	0.54
1:G:303:PHE:O	1:G:307:PHE:HB2	2.07	0.54
1:J:303:PHE:O	1:J:307:PHE:HB2	2.07	0.54
1:A:294:LEU:HG	1:A:298:ARG:NH2	2.23	0.54
1:C:140:LEU:HD22	1:C:190:ILE:HD11	1.89	0.54
1:C:150:GLU:HB3	1:C:153:ASP:HB2	1.89	0.54
1:E:118:LEU:N	1:E:118:LEU:HD23	2.22	0.54
1:E:147:VAL:HG23	1:E:165:ALA:HB2	1.90	0.54
1:J:230:ARG:HB3	1:J:279:ILE:HD13	1.90	0.54
1:J:294:LEU:HG	1:J:298:ARG:HH21	1.72	0.54
1:J:303:PHE:N	1:J:304:PRO:CD	2.71	0.54
1:A:288:ASN:OD1	1:A:291:GLU:CB	2.56	0.54
1:B:125:GLN:OE1	1:B:193:ARG:HD3	2.08	0.54
1:I:252:LEU:HG	1:I:253:PRO:HD2	1.90	0.54
1:D:118:LEU:N	1:D:118:LEU:HD23	2.23	0.54
1:I:300:ARG:O	1:I:304:PRO:HG2	2.07	0.54
1:A:306:GLY:O	1:A:310:ILE:HG13	2.08	0.54
1:B:112:ASN:OD1	1:B:113:ASP:N	2.41	0.54
1:B:280:ILE:HG22	1:B:280:ILE:O	2.08	0.54
1:C:162:ILE:HG22	1:C:163:ARG:N	2.14	0.54
1:C:311:GLY:O	1:C:315:VAL:HG23	2.08	0.54
1:E:125:GLN:OE1	1:E:193:ARG:HD3	2.08	0.54
1:G:259:THR:O	1:G:263:GLN:HG3	2.08	0.54
1:A:87:THR:HG21	1:A:90:LYS:HE2	1.90	0.53
1:B:167:THR:CG2	1:B:168:HIS:H	2.16	0.53
1:C:182:PRO:HB2	1:C:184:GLN:HE22	1.72	0.53
1:G:286:GLN:CB	1:G:291:GLU:HB3	2.33	0.53
1:H:87:THR:HG21	1:H:90:LYS:HE2	1.90	0.53
1:I:78:PHE:HB3	1:I:81:VAL:HG23	1.88	0.53
1:I:127:VAL:HG22	1:I:193:ARG:HG2	1.90	0.53
1:A:28:THR:HG21	1:A:253:PRO:HB2	1.90	0.53
1:B:150:GLU:HB2	1:B:153:ASP:HB2	1.86	0.53
1:C:299:CYS:HB2	1:C:302:ALA:HB2	1.88	0.53
1:E:149:THR:HG22	1:E:150:GLU:N	2.23	0.53
1:F:181:GLN:N	1:F:182:PRO:CD	2.72	0.53
1:H:305:LEU:HD12	1:H:306:GLY:N	2.24	0.53
1:I:262:ASP:O	1:I:266:ILE:HG12	2.07	0.53
1:I:305:LEU:C	1:I:305:LEU:HD12	2.29	0.53
1:B:94:LEU:HD23	1:B:100:VAL:HG22	1.88	0.53
1:B:211:LEU:HD11	1:B:264:MET:HB3	1.90	0.53
1:F:76:LEU:HB3	1:F:130:LEU:HD22	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:240:THR:OG1	1:H:239:LEU:HD23	2.09	0.53
1:G:254:ARG:O	1:G:255:LEU:HD23	2.08	0.53
1:H:66:TRP:HB3	1:H:71:LEU:HD12	1.90	0.53
1:H:280:ILE:HG22	1:H:280:ILE:O	2.08	0.53
1:I:178:SER:O	1:I:180:VAL:N	2.42	0.53
1:J:204:LEU:HA	1:J:208:ILE:HG12	1.89	0.53
1:A:293:ASP:O	1:A:296:ILE:HG22	2.08	0.53
1:B:305:LEU:C	1:B:305:LEU:HD12	2.28	0.53
1:C:276:ILE:O	1:C:280:ILE:HG13	2.08	0.53
1:C:305:LEU:HD12	1:C:306:GLY:N	2.23	0.53
1:D:181:GLN:H	1:D:182:PRO:CD	2.22	0.53
1:E:252:LEU:HG	1:E:253:PRO:HD2	1.90	0.53
1:I:181:GLN:H	1:I:182:PRO:HD3	1.70	0.53
1:A:27:ASN:HB3	1:A:32:THR:HB	1.91	0.53
1:C:239:LEU:HD13	1:C:239:LEU:O	2.08	0.53
1:G:149:THR:HG22	1:G:150:GLU:N	2.23	0.53
1:F:178:SER:O	1:F:180:VAL:N	2.35	0.53
1:F:220:SER:HB2	1:G:280:ILE:HD13	1.89	0.53
1:I:231:LEU:HD23	1:I:231:LEU:C	2.29	0.53
1:A:235:PHE:CD2	1:E:237:LEU:HD13	2.44	0.53
1:B:136:ASN:ND2	1:B:184:GLN:HA	2.24	0.53
1:I:211:LEU:HD11	1:I:264:MET:HB3	1.90	0.53
1:B:306:GLY:O	1:B:310:ILE:HG13	2.07	0.53
1:D:152:ILE:HG22	1:D:152:ILE:O	2.09	0.53
1:E:263:GLN:HA	1:E:266:ILE:HG12	1.91	0.53
1:F:66:TRP:HB3	1:F:71:LEU:HD12	1.91	0.53
1:I:286:GLN:HA	1:I:291:GLU:HB3	1.90	0.53
1:I:315:VAL:HG12	1:I:315:VAL:O	2.08	0.53
1:J:19:PHE:CE2	1:J:146:GLN:HG3	2.44	0.53
1:J:252:LEU:HG	1:J:253:PRO:HD2	1.91	0.53
1:B:172:ILE:N	1:B:172:ILE:HD12	2.24	0.53
1:E:305:LEU:HD12	1:E:305:LEU:C	2.29	0.53
1:F:149:THR:HG22	1:F:150:GLU:N	2.23	0.53
1:F:172:ILE:HD12	1:F:172:ILE:N	2.24	0.53
1:H:172:ILE:HD12	1:H:172:ILE:N	2.24	0.53
1:I:27:ASN:HB3	1:I:32:THR:HB	1.90	0.53
1:I:246:PHE:CD2	1:J:246:PHE:HE2	2.26	0.53
1:A:133:PHE:HE2	1:E:91:ARG:HB2	1.73	0.52
1:B:283:HIS:HA	1:B:292:ASP:OD1	2.09	0.52
1:C:172:ILE:HD12	1:C:172:ILE:N	2.24	0.52
1:C:247:TYR:HD1	1:D:246:PHE:HA	1.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:147:VAL:O	1:D:149:THR:N	2.35	0.52
1:D:211:LEU:HD23	1:D:244:TYR:CD2	2.44	0.52
1:I:219:TRP:C	1:I:221:VAL:H	2.11	0.52
1:B:210:PRO:O	1:B:214:ILE:HG12	2.08	0.52
1:G:211:LEU:CD1	1:G:264:MET:HB3	2.39	0.52
1:G:311:GLY:O	1:G:315:VAL:HG23	2.10	0.52
1:C:59:GLU:OE2	1:D:75:ALA:HB3	2.09	0.52
1:C:181:GLN:N	1:C:182:PRO:CD	2.72	0.52
1:G:20:ILE:HG13	1:G:194:ILE:HD11	1.92	0.52
1:G:181:GLN:H	1:G:182:PRO:CD	2.22	0.52
1:G:301:LEU:C	1:G:304:PRO:HD2	2.29	0.52
1:H:306:GLY:O	1:H:310:ILE:HG13	2.09	0.52
1:J:147:VAL:HG23	1:J:165:ALA:HB2	1.90	0.52
1:J:162:ILE:HG22	1:J:163:ARG:N	2.21	0.52
1:J:172:ILE:N	1:J:172:ILE:HD12	2.24	0.52
1:J:180:VAL:HG21	1:J:184:GLN:CG	2.38	0.52
1:A:239:LEU:O	1:A:239:LEU:HD13	2.10	0.52
1:A:247:TYR:HD1	1:B:246:PHE:HA	1.74	0.52
1:A:259:THR:O	1:A:263:GLN:HG3	2.09	0.52
1:D:210:PRO:O	1:D:214:ILE:HG12	2.09	0.52
1:E:230:ARG:HB3	1:E:279:ILE:HD13	1.91	0.52
1:H:28:THR:HB	1:H:255:LEU:CD2	2.38	0.52
1:H:293:ASP:O	1:H:296:ILE:HG22	2.10	0.52
1:I:210:PRO:O	1:I:214:ILE:HG12	2.10	0.52
1:I:263:GLN:HA	1:I:266:ILE:HG12	1.92	0.52
1:J:178:SER:O	1:J:180:VAL:HG12	2.09	0.52
1:B:67:ILE:HD11	1:B:73:VAL:HG21	1.91	0.52
1:B:312:CYS:O	1:B:316:ILE:HG13	2.10	0.52
1:C:112:ASN:OD1	1:C:113:ASP:N	2.43	0.52
1:D:145:ILE:HD12	1:D:145:ILE:N	2.21	0.52
1:D:155:GLU:HB3	1:D:161:TRP:CD1	2.45	0.52
1:E:28:THR:HG21	1:E:253:PRO:HB2	1.92	0.52
1:F:226:SER:HB3	1:F:229:GLU:CG	2.38	0.52
1:F:300:ARG:O	1:F:304:PRO:HG2	2.09	0.52
1:H:167:THR:O	1:H:168:HIS:HB2	2.09	0.52
1:I:226:SER:HB3	1:I:229:GLU:CG	2.38	0.52
1:J:211:LEU:HD11	1:J:264:MET:HB3	1.90	0.52
1:A:285:ARG:C	1:A:285:ARG:HD3	2.30	0.52
1:C:263:GLN:HA	1:C:266:ILE:HG12	1.90	0.52
1:D:127:VAL:HG22	1:D:193:ARG:HG2	1.92	0.52
1:F:286:GLN:HG2	1:F:289:GLY:C	2.30	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:112:ASN:OD1	1:G:113:ASP:N	2.43	0.52
1:G:305:LEU:HD12	1:G:306:GLY:N	2.24	0.52
1:J:150:GLU:HB2	1:J:153:ASP:CB	2.39	0.52
1:B:169:ILE:HB	1:I:168:HIS:ND1	2.24	0.52
1:B:252:LEU:HG	1:B:253:PRO:HD2	1.91	0.52
1:C:164:LYS:HA	1:C:164:LYS:HZ3	1.73	0.52
1:C:203:TYR:O	1:C:207:PHE:HB2	2.09	0.52
1:C:204:LEU:HA	1:C:208:ILE:CG1	2.40	0.52
1:C:286:GLN:HB3	1:C:291:GLU:HB3	1.92	0.52
1:I:220:SER:HB2	1:J:280:ILE:HD13	1.92	0.52
1:J:78:PHE:HB3	1:J:81:VAL:HG23	1.90	0.52
1:J:118:LEU:N	1:J:118:LEU:HD23	2.24	0.52
1:A:263:GLN:HA	1:A:266:ILE:HG12	1.92	0.52
1:B:230:ARG:HB3	1:B:279:ILE:HD13	1.92	0.52
1:G:286:GLN:HB2	1:G:288:ASN:H	1.75	0.52
1:H:112:ASN:OD1	1:H:113:ASP:N	2.43	0.52
1:H:204:LEU:HA	1:H:208:ILE:HG12	1.92	0.52
1:H:211:LEU:CD1	1:H:264:MET:HB3	2.40	0.52
1:J:306:GLY:O	1:J:310:ILE:HG13	2.10	0.52
1:A:288:ASN:CG	1:A:289:GLY:N	2.53	0.52
1:B:223:TRP:CE3	1:C:280:ILE:CG2	2.93	0.52
1:D:87:THR:HG21	1:D:90:LYS:HE2	1.91	0.52
1:F:172:ILE:CD1	1:F:189:ARG:HB3	2.40	0.52
1:F:296:ILE:HG23	1:F:297:GLN:N	2.25	0.52
1:I:301:LEU:C	1:I:304:PRO:HD2	2.30	0.52
1:J:180:VAL:HG11	1:J:184:GLN:HB2	1.92	0.52
1:J:224:LEU:O	1:J:230:ARG:HD2	2.10	0.52
1:D:172:ILE:CD1	1:D:189:ARG:HB3	2.40	0.52
1:E:172:ILE:CD1	1:E:189:ARG:HB3	2.40	0.52
1:G:164:LYS:HZ2	1:G:164:LYS:CA	2.22	0.52
1:G:246:PHE:CD2	1:H:246:PHE:HE2	2.28	0.52
1:I:40:VAL:HA	1:I:102:TYR:O	2.09	0.52
1:I:182:PRO:HB2	1:I:184:GLN:NE2	2.24	0.52
1:B:162:ILE:HG22	1:B:163:ARG:N	2.17	0.51
1:B:210:PRO:HB3	1:C:269:TYR:CD1	2.45	0.51
1:D:172:ILE:HD12	1:D:172:ILE:N	2.25	0.51
1:E:27:ASN:HB3	1:E:32:THR:HB	1.91	0.51
1:F:150:GLU:H	1:F:150:GLU:CD	2.13	0.51
1:G:286:GLN:HB3	1:G:291:GLU:CB	2.31	0.51
1:H:28:THR:HG21	1:H:253:PRO:HB2	1.92	0.51
1:H:54:LYS:HB3	1:H:55:PRO:HD2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:149:THR:HG22	1:I:150:GLU:CD	2.30	0.51
1:I:203:TYR:O	1:I:207:PHE:HB2	2.10	0.51
1:J:211:LEU:HD23	1:J:244:TYR:CE2	2.44	0.51
1:D:91:ARG:HB2	1:E:133:PHE:CE2	2.45	0.51
1:F:28:THR:HG21	1:F:253:PRO:HB2	1.93	0.51
1:E:211:LEU:HD23	1:E:244:TYR:CE2	2.45	0.51
1:E:254:ARG:O	1:E:255:LEU:HD23	2.09	0.51
1:F:112:ASN:OD1	1:F:113:ASP:N	2.44	0.51
1:G:61:THR:HG21	1:H:64:GLU:CG	2.40	0.51
1:I:87:THR:HG21	1:I:90:LYS:HE2	1.91	0.51
1:I:93:MET:SD	1:J:178:SER:CB	2.99	0.51
1:I:172:ILE:HD12	1:I:172:ILE:N	2.26	0.51
1:I:211:LEU:HD23	1:I:244:TYR:CD2	2.45	0.51
1:A:83:GLY:HA2	1:E:107:LEU:HD23	1.91	0.51
1:A:136:ASN:ND2	1:A:184:GLN:HA	2.25	0.51
1:C:94:LEU:HD23	1:C:100:VAL:HG22	1.92	0.51
1:C:262:ASP:O	1:C:266:ILE:HG12	2.10	0.51
1:D:239:LEU:O	1:D:239:LEU:HD13	2.11	0.51
1:D:306:GLY:O	1:D:310:ILE:HG13	2.10	0.51
1:E:56:LEU:HD13	1:E:57:ILE:N	2.25	0.51
1:E:211:LEU:CD1	1:E:264:MET:HB3	2.40	0.51
1:E:306:GLY:O	1:E:310:ILE:HG13	2.09	0.51
1:I:311:GLY:O	1:I:315:VAL:HG23	2.10	0.51
1:C:223:TRP:CE3	1:D:280:ILE:HG22	2.46	0.51
1:C:296:ILE:HG23	1:C:297:GLN:N	2.25	0.51
1:C:300:ARG:O	1:C:304:PRO:HG2	2.10	0.51
1:D:143:SER:HB3	1:D:167:THR:HG21	1.92	0.51
1:H:224:LEU:O	1:H:230:ARG:HD2	2.09	0.51
1:H:296:ILE:HG23	1:H:297:GLN:N	2.26	0.51
1:I:230:ARG:HB3	1:I:279:ILE:HD13	1.92	0.51
1:I:305:LEU:HD12	1:I:306:GLY:N	2.26	0.51
1:J:231:LEU:HD23	1:J:232:GLN:N	2.25	0.51
1:A:167:THR:CG2	1:A:168:HIS:H	2.19	0.51
1:A:172:ILE:CD1	1:A:189:ARG:HB3	2.41	0.51
1:B:157:ILE:HD11	1:C:115:ASP:OD2	2.11	0.51
1:H:226:SER:HB3	1:H:229:GLU:CG	2.40	0.51
1:J:27:ASN:HB3	1:J:32:THR:HB	1.93	0.51
1:A:246:PHE:CD2	1:B:246:PHE:HE2	2.29	0.51
1:B:27:ASN:HB3	1:B:32:THR:HB	1.93	0.51
1:B:305:LEU:HD12	1:B:306:GLY:N	2.24	0.51
1:C:172:ILE:CD1	1:C:189:ARG:HB3	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:180:VAL:CG2	1:D:184:GLN:HB2	2.39	0.51
1:D:294:LEU:HD12	1:D:297:GLN:NE2	2.25	0.51
1:G:78:PHE:HB3	1:G:81:VAL:CG2	2.40	0.51
1:G:91:ARG:HB2	1:H:133:PHE:HE2	1.75	0.51
1:H:81:VAL:HG11	1:H:85:PRO:HD3	1.91	0.51
1:I:147:VAL:O	1:I:149:THR:N	2.41	0.51
1:J:204:LEU:HA	1:J:208:ILE:CG1	2.41	0.51
1:J:311:GLY:O	1:J:315:VAL:HG23	2.11	0.51
1:A:150:GLU:CG	1:A:153:ASP:HB2	2.41	0.51
1:A:231:LEU:HD23	1:A:231:LEU:C	2.30	0.51
1:A:249:SER:HB3	1:E:251:ILE:HG13	1.93	0.51
1:B:263:GLN:HA	1:B:266:ILE:HG12	1.93	0.51
1:C:147:VAL:CG2	1:C:165:ALA:HB2	2.40	0.51
1:C:178:SER:O	1:C:180:VAL:N	2.44	0.51
1:C:210:PRO:O	1:C:214:ILE:HG12	2.10	0.51
1:C:248:THR:HG23	1:C:252:LEU:HD22	1.93	0.51
1:D:125:GLN:HG3	1:D:125:GLN:O	2.11	0.51
1:D:301:LEU:C	1:D:304:PRO:HD2	2.31	0.51
1:I:28:THR:HG21	1:I:253:PRO:HB2	1.92	0.51
1:I:112:ASN:OD1	1:I:113:ASP:N	2.44	0.51
1:A:239:LEU:HD23	1:E:240:THR:HA	1.92	0.51
1:D:81:VAL:HG11	1:D:85:PRO:HD3	1.93	0.51
1:D:280:ILE:HG22	1:D:280:ILE:O	2.10	0.51
1:E:239:LEU:O	1:E:239:LEU:HD13	2.11	0.51
1:E:296:ILE:HG23	1:E:297:GLN:N	2.25	0.51
1:G:28:THR:HG21	1:G:253:PRO:HB2	1.93	0.51
1:G:204:LEU:HA	1:G:208:ILE:CG1	2.40	0.51
1:H:301:LEU:C	1:H:304:PRO:HD2	2.31	0.51
1:I:306:GLY:O	1:I:310:ILE:HG13	2.11	0.51
1:J:87:THR:HG21	1:J:90:LYS:HE2	1.92	0.51
1:C:28:THR:HG21	1:C:253:PRO:HB2	1.93	0.51
1:C:91:ARG:HD3	1:D:134:SER:HB3	1.93	0.51
1:C:306:GLY:O	1:C:310:ILE:HG13	2.11	0.51
1:D:76:LEU:HB3	1:D:130:LEU:HD22	1.93	0.51
1:E:21:ASN:HB2	1:E:36:ASP:O	2.11	0.51
1:I:21:ASN:HD21	1:I:38:TYR:HE1	1.59	0.51
1:J:296:ILE:HG23	1:J:297:GLN:N	2.26	0.51
1:A:280:ILE:O	1:A:280:ILE:HG22	2.11	0.50
1:B:101:ILE:CD1	1:C:178:SER:HB3	2.41	0.50
1:B:211:LEU:HD23	1:B:244:TYR:CE2	2.45	0.50
1:C:21:ASN:HB2	1:C:36:ASP:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:78:PHE:HB3	1:F:81:VAL:CG2	2.40	0.50
1:A:13:ASP:HB3	1:A:141:ARG:HD2	1.94	0.50
1:A:112:ASN:OD1	1:A:113:ASP:N	2.44	0.50
1:A:147:VAL:C	1:A:149:THR:H	2.14	0.50
1:F:27:ASN:HB3	1:F:32:THR:HB	1.93	0.50
1:H:99:ARG:NH1	1:I:179:SER:CB	2.74	0.50
1:H:203:TYR:O	1:H:207:PHE:HB2	2.11	0.50
1:J:167:THR:O	1:J:168:HIS:HB2	2.11	0.50
1:A:23:ILE:HD11	1:A:194:ILE:HD12	1.93	0.50
1:A:296:ILE:HG23	1:A:297:GLN:N	2.25	0.50
1:B:52:GLY:O	1:B:53:ASP:HB2	2.12	0.50
1:D:14:VAL:O	1:D:141:ARG:N	2.40	0.50
1:E:112:ASN:OD1	1:E:113:ASP:N	2.43	0.50
1:E:176:HIS:N	1:E:176:HIS:CD2	2.79	0.50
1:E:224:LEU:O	1:E:230:ARG:HD2	2.11	0.50
1:G:150:GLU:HG2	1:G:154:ASN:H	1.76	0.50
1:J:13:ASP:HB3	1:J:141:ARG:HD2	1.94	0.50
1:A:167:THR:O	1:A:168:HIS:HB2	2.11	0.50
1:D:177:LEU:HD12	1:D:185:ASN:CA	2.37	0.50
1:F:306:GLY:O	1:F:310:ILE:HG13	2.11	0.50
1:G:172:ILE:N	1:G:172:ILE:HD12	2.26	0.50
1:G:280:ILE:O	1:G:280:ILE:HG22	2.11	0.50
1:H:311:GLY:O	1:H:315:VAL:HG23	2.11	0.50
1:J:150:GLU:CG	1:J:154:ASN:H	2.24	0.50
1:A:240:THR:OG1	1:B:239:LEU:HD23	2.10	0.50
1:A:301:LEU:C	1:A:304:PRO:HD2	2.31	0.50
1:A:305:LEU:HD12	1:A:306:GLY:N	2.26	0.50
1:C:296:ILE:CG2	1:C:297:GLN:N	2.75	0.50
1:D:28:THR:HG21	1:D:253:PRO:HB2	1.94	0.50
1:H:18:ILE:HB	1:H:145:ILE:HG22	1.94	0.50
1:H:294:LEU:HG	1:H:298:ARG:HH21	1.77	0.50
1:I:125:GLN:OE1	1:I:193:ARG:HD3	2.12	0.50
1:I:154:ASN:O	1:I:155:GLU:CG	2.59	0.50
1:J:173:ARG:HA	1:J:185:ASN:O	2.12	0.50
1:J:182:PRO:HB2	1:J:184:GLN:HE22	1.76	0.50
1:A:21:ASN:HD21	1:A:38:TYR:HE1	1.60	0.50
1:B:87:THR:HG21	1:B:90:LYS:HE2	1.93	0.50
1:I:220:SER:HB2	1:J:280:ILE:CD1	2.42	0.50
1:I:224:LEU:O	1:I:230:ARG:HD2	2.11	0.50
1:E:19:PHE:CE2	1:E:146:GLN:HG3	2.47	0.50
1:E:155:GLU:HB3	1:E:161:TRP:CD1	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:167:THR:O	1:E:168:HIS:HB2	2.10	0.50
1:F:280:ILE:O	1:F:280:ILE:HG22	2.12	0.50
1:H:27:ASN:HB3	1:H:32:THR:HB	1.93	0.50
1:H:210:PRO:O	1:H:214:ILE:HG12	2.12	0.50
1:H:247:TYR:HD1	1:I:246:PHE:HA	1.76	0.50
1:I:164:LYS:NZ	1:I:164:LYS:HA	2.27	0.50
1:I:239:LEU:CD1	1:J:239:LEU:HD21	2.42	0.50
1:J:305:LEU:HD12	1:J:306:GLY:N	2.27	0.50
1:A:266:ILE:HD12	1:E:205:TRP:O	2.12	0.50
1:G:157:ILE:HD11	1:H:115:ASP:CG	2.33	0.50
1:G:203:TYR:O	1:G:207:PHE:HB2	2.12	0.50
1:G:296:ILE:HG23	1:G:297:GLN:N	2.27	0.50
1:H:91:ARG:HD3	1:I:134:SER:HB3	1.92	0.50
1:I:286:GLN:HB3	1:I:291:GLU:H	1.76	0.50
1:E:150:GLU:CG	1:E:150:GLU:O	2.59	0.50
1:F:205:TRP:O	1:G:266:ILE:HD12	2.12	0.50
1:G:306:GLY:O	1:G:310:ILE:HG13	2.12	0.50
1:I:91:ARG:HB2	1:J:133:PHE:HE2	1.76	0.50
1:J:210:PRO:O	1:J:214:ILE:HG12	2.12	0.50
1:J:290:VAL:O	1:J:290:VAL:HG12	2.12	0.50
1:A:211:LEU:CD1	1:A:264:MET:HB3	2.42	0.49
1:B:28:THR:HG21	1:B:253:PRO:HB2	1.94	0.49
1:B:81:VAL:HG11	1:B:85:PRO:HD3	1.94	0.49
1:D:177:LEU:HD11	1:D:187:PHE:CE1	2.41	0.49
1:E:150:GLU:CG	1:E:153:ASP:HB3	2.40	0.49
1:F:150:GLU:CG	1:F:154:ASN:H	2.24	0.49
1:F:230:ARG:HB3	1:F:279:ILE:HD13	1.94	0.49
1:I:136:ASN:ND2	1:I:184:GLN:HA	2.26	0.49
1:I:286:GLN:HG2	1:I:289:GLY:C	2.32	0.49
1:J:292:ASP:O	1:J:294:LEU:N	2.45	0.49
1:J:296:ILE:CG2	1:J:297:GLN:N	2.75	0.49
1:B:152:ILE:HG23	1:B:155:GLU:OE1	2.12	0.49
1:C:66:TRP:HB3	1:C:71:LEU:HD12	1.93	0.49
1:C:280:ILE:HG22	1:C:280:ILE:O	2.13	0.49
1:D:28:THR:HB	1:D:255:LEU:CD2	2.42	0.49
1:D:78:PHE:HB3	1:D:81:VAL:CG2	2.43	0.49
1:H:219:TRP:C	1:H:221:VAL:H	2.14	0.49
1:J:211:LEU:CD1	1:J:264:MET:HB3	2.42	0.49
1:J:223:TRP:CD1	1:J:300:ARG:HD3	2.47	0.49
1:A:180:VAL:HG21	1:A:184:GLN:HB2	1.94	0.49
1:B:40:VAL:HA	1:B:102:TYR:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:286:GLN:HG2	1:C:289:GLY:C	2.32	0.49
1:D:57:ILE:O	1:D:57:ILE:HG22	2.11	0.49
1:D:180:VAL:HG21	1:D:184:GLN:CB	2.40	0.49
1:D:226:SER:HB3	1:D:229:GLU:CG	2.41	0.49
1:F:13:ASP:HB3	1:F:141:ARG:HD2	1.95	0.49
1:F:313:VAL:HA	1:F:316:ILE:CG1	2.43	0.49
1:H:149:THR:CG2	1:H:150:GLU:H	2.16	0.49
1:I:81:VAL:HG11	1:I:85:PRO:HD3	1.93	0.49
1:J:20:ILE:HG13	1:J:194:ILE:HD11	1.95	0.49
1:J:28:THR:HG21	1:J:253:PRO:HB2	1.94	0.49
1:B:296:ILE:HG23	1:B:297:GLN:N	2.27	0.49
1:D:67:ILE:HD11	1:D:73:VAL:HG21	1.94	0.49
1:E:204:LEU:HA	1:E:208:ILE:CG1	2.43	0.49
1:E:301:LEU:C	1:E:304:PRO:HD2	2.32	0.49
1:G:211:LEU:HD23	1:G:244:TYR:CE2	2.47	0.49
1:H:19:PHE:CE2	1:H:146:GLN:HG3	2.47	0.49
1:J:112:ASN:OD1	1:J:113:ASP:N	2.45	0.49
1:A:28:THR:HB	1:A:255:LEU:CD2	2.40	0.49
1:A:56:LEU:HD13	1:A:57:ILE:N	2.27	0.49
1:A:285:ARG:HA	1:A:285:ARG:CZ	2.42	0.49
1:B:20:ILE:HG13	1:B:194:ILE:HD11	1.95	0.49
1:B:147:VAL:O	1:B:149:THR:N	2.44	0.49
1:C:78:PHE:HB3	1:C:81:VAL:HG23	1.93	0.49
1:D:13:ASP:HB3	1:D:141:ARG:HD2	1.93	0.49
1:D:209:LEU:HB3	1:D:210:PRO:HD3	1.94	0.49
1:F:87:THR:HG21	1:F:90:LYS:CE	2.41	0.49
1:F:247:TYR:HD1	1:G:246:PHE:HA	1.78	0.49
1:G:173:ARG:HA	1:G:185:ASN:O	2.13	0.49
1:A:230:ARG:HB3	1:A:279:ILE:HD13	1.93	0.49
1:A:303:PHE:N	1:A:304:PRO:HD3	2.28	0.49
1:C:152:ILE:N	1:C:152:ILE:HD13	2.27	0.49
1:D:211:LEU:CD1	1:D:264:MET:HB3	2.42	0.49
1:E:76:LEU:HB3	1:E:130:LEU:HD22	1.95	0.49
1:E:305:LEU:HD12	1:E:306:GLY:N	2.28	0.49
1:E:311:GLY:O	1:E:315:VAL:HG23	2.12	0.49
1:F:231:LEU:HD23	1:F:231:LEU:C	2.32	0.49
1:I:72:TRP:CE2	1:I:74:PRO:HG3	2.48	0.49
1:B:148:TYR:HH	1:C:176:HIS:CE1	2.31	0.49
1:C:167:THR:CG2	1:C:168:HIS:H	2.19	0.49
1:D:203:TYR:O	1:D:207:PHE:HB2	2.12	0.49
1:E:285:ARG:HA	1:E:285:ARG:CZ	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:157:ILE:HD12	1:H:115:ASP:HA	1.94	0.49
1:H:230:ARG:HB3	1:H:279:ILE:HD13	1.93	0.49
1:I:167:THR:O	1:I:168:HIS:HB2	2.13	0.49
1:A:19:PHE:CE2	1:A:146:GLN:HG3	2.48	0.49
1:A:172:ILE:HD12	1:A:172:ILE:N	2.28	0.49
1:E:203:TYR:O	1:E:207:PHE:HB2	2.13	0.49
1:F:203:TYR:O	1:F:207:PHE:HB2	2.13	0.49
1:F:211:LEU:HD11	1:F:264:MET:HB3	1.95	0.49
1:F:296:ILE:CG2	1:F:297:GLN:N	2.75	0.49
1:F:301:LEU:C	1:F:304:PRO:HD2	2.33	0.49
1:F:313:VAL:O	1:F:316:ILE:HB	2.12	0.49
1:G:87:THR:HG21	1:G:90:LYS:CE	2.42	0.49
1:H:17:SER:O	1:H:40:VAL:HG23	2.13	0.49
1:I:259:THR:O	1:I:263:GLN:HG3	2.12	0.49
1:J:143:SER:HB3	1:J:167:THR:HG21	1.94	0.49
1:J:152:ILE:HA	1:J:155:GLU:OE1	2.12	0.49
1:A:14:VAL:O	1:A:141:ARG:N	2.43	0.49
1:E:226:SER:HB3	1:E:229:GLU:CG	2.42	0.49
1:E:296:ILE:CG2	1:E:297:GLN:N	2.76	0.49
1:H:288:ASN:OD1	1:H:291:GLU:HB2	2.12	0.49
1:I:76:LEU:HB3	1:I:130:LEU:HD22	1.95	0.49
1:J:288:ASN:CG	1:J:289:GLY:H	2.16	0.49
1:J:305:LEU:HD12	1:J:305:LEU:C	2.32	0.49
1:A:63:ILE:O	1:A:67:ILE:HD13	2.13	0.49
1:A:280:ILE:CD1	1:E:220:SER:HB2	2.42	0.49
1:A:296:ILE:CG2	1:A:297:GLN:N	2.76	0.49
1:A:311:GLY:O	1:A:315:VAL:HG23	2.13	0.49
1:B:311:GLY:O	1:B:315:VAL:HG23	2.13	0.49
1:C:303:PHE:N	1:C:304:PRO:HD3	2.28	0.49
1:I:18:ILE:HB	1:I:145:ILE:HG22	1.95	0.49
1:I:149:THR:HG22	1:I:150:GLU:H	1.78	0.49
1:A:66:TRP:HE3	1:A:71:LEU:HD12	1.78	0.48
1:A:283:HIS:HA	1:A:292:ASP:OD1	2.13	0.48
1:A:315:VAL:O	1:A:315:VAL:HG12	2.13	0.48
1:B:176:HIS:N	1:B:176:HIS:CD2	2.81	0.48
1:B:209:LEU:HB3	1:B:210:PRO:HD3	1.95	0.48
1:B:231:LEU:C	1:B:231:LEU:HD23	2.32	0.48
1:C:259:THR:O	1:C:263:GLN:HG3	2.13	0.48
1:E:13:ASP:HB3	1:E:141:ARG:HD2	1.93	0.48
1:G:185:ASN:N	1:G:185:ASN:ND2	2.61	0.48
1:I:237:LEU:HD13	1:J:235:PHE:CD2	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:303:PHE:N	1:I:304:PRO:HD3	2.28	0.48
1:J:172:ILE:CD1	1:J:189:ARG:HB3	2.42	0.48
1:A:62:GLN:HE22	1:A:65:ARG:HH11	1.60	0.48
1:A:143:SER:HB3	1:A:167:THR:HG21	1.94	0.48
1:C:21:ASN:HD21	1:C:38:TYR:HE1	1.60	0.48
1:C:167:THR:O	1:C:168:HIS:HB2	2.13	0.48
1:D:296:ILE:HG23	1:D:297:GLN:N	2.27	0.48
1:E:286:GLN:HA	1:E:291:GLU:HB3	1.95	0.48
1:F:28:THR:HB	1:F:255:LEU:CD2	2.42	0.48
1:F:311:GLY:O	1:F:315:VAL:HG23	2.14	0.48
1:J:28:THR:HB	1:J:255:LEU:CD2	2.40	0.48
1:B:56:LEU:CD1	1:B:58:VAL:HG23	2.42	0.48
1:C:72:TRP:O	1:C:72:TRP:CD1	2.65	0.48
1:D:222:PHE:HB3	1:D:300:ARG:HG2	1.95	0.48
1:E:28:THR:HB	1:E:255:LEU:CD2	2.43	0.48
1:F:65:ARG:HD2	1:G:68:ASN:ND2	2.29	0.48
1:F:263:GLN:HA	1:F:266:ILE:HG12	1.94	0.48
1:G:40:VAL:HA	1:G:102:TYR:O	2.14	0.48
1:G:65:ARG:HD2	1:H:68:ASN:HD21	1.75	0.48
1:G:177:LEU:CD1	1:G:185:ASN:HA	2.43	0.48
1:H:40:VAL:HA	1:H:102:TYR:O	2.13	0.48
1:H:180:VAL:HG22	1:H:181:GLN:N	2.28	0.48
1:H:303:PHE:N	1:H:304:PRO:HD3	2.28	0.48
1:J:23:ILE:HD11	1:J:194:ILE:HD12	1.95	0.48
1:J:40:VAL:HA	1:J:102:TYR:O	2.13	0.48
1:A:226:SER:HB3	1:A:229:GLU:CG	2.43	0.48
1:D:204:LEU:HA	1:D:208:ILE:CG1	2.42	0.48
1:D:252:LEU:HG	1:D:253:PRO:HD2	1.95	0.48
1:G:226:SER:HB3	1:G:229:GLU:CG	2.43	0.48
1:G:263:GLN:HA	1:G:266:ILE:HG12	1.96	0.48
1:B:97:ASP:OD1	1:B:99:ARG:HG2	2.14	0.48
1:B:294:LEU:HG	1:B:298:ARG:NH2	2.28	0.48
1:C:91:ARG:HB2	1:D:133:PHE:HE2	1.79	0.48
1:C:252:LEU:HG	1:C:253:PRO:HD2	1.93	0.48
1:D:286:GLN:HG2	1:D:289:GLY:C	2.34	0.48
1:D:296:ILE:CG2	1:D:297:GLN:N	2.76	0.48
1:E:40:VAL:HA	1:E:102:TYR:O	2.13	0.48
1:E:211:LEU:HD21	1:E:265:ILE:HD13	1.94	0.48
1:E:288:ASN:CG	1:E:289:GLY:H	2.16	0.48
1:F:23:ILE:HD11	1:F:194:ILE:HD12	1.94	0.48
1:H:172:ILE:CD1	1:H:189:ARG:HB3	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:296:ILE:CG2	1:H:297:GLN:N	2.76	0.48
1:I:239:LEU:O	1:I:239:LEU:HD13	2.14	0.48
1:J:167:THR:CG2	1:J:168:HIS:H	2.18	0.48
1:A:115:ASP:OD2	1:E:157:ILE:HD11	2.13	0.48
1:A:292:ASP:O	1:A:297:GLN:NE2	2.47	0.48
1:B:157:ILE:HD12	1:C:115:ASP:HA	1.95	0.48
1:B:167:THR:O	1:B:168:HIS:CB	2.61	0.48
1:B:204:LEU:HA	1:B:208:ILE:CG1	2.42	0.48
1:C:70:GLY:O	1:C:71:LEU:C	2.51	0.48
1:C:223:TRP:CD1	1:C:300:ARG:HD3	2.48	0.48
1:C:288:ASN:CG	1:C:289:GLY:N	2.67	0.48
1:D:65:ARG:HD2	1:E:68:ASN:ND2	2.29	0.48
1:D:167:THR:O	1:D:168:HIS:HB2	2.14	0.48
1:D:200:PRO:O	1:D:201:SER:C	2.52	0.48
1:D:293:ASP:CB	1:D:296:ILE:HG22	2.32	0.48
1:F:204:LEU:HA	1:F:208:ILE:CG1	2.44	0.48
1:G:66:TRP:HB3	1:G:71:LEU:HD12	1.94	0.48
1:G:76:LEU:HB3	1:G:130:LEU:HD22	1.95	0.48
1:I:20:ILE:HG13	1:I:194:ILE:HD11	1.95	0.48
1:J:66:TRP:HB3	1:J:71:LEU:HD12	1.96	0.48
1:C:56:LEU:HD13	1:C:57:ILE:H	1.76	0.48
1:D:311:GLY:O	1:D:315:VAL:HG23	2.13	0.48
1:E:21:ASN:HD21	1:E:38:TYR:HE1	1.61	0.48
1:E:181:GLN:N	1:E:182:PRO:CD	2.76	0.48
1:F:58:VAL:HB	1:F:92:LEU:HB2	1.96	0.48
1:H:147:VAL:HG23	1:H:165:ALA:HB2	1.95	0.48
1:B:292:ASP:O	1:B:297:GLN:NE2	2.47	0.48
1:C:14:VAL:O	1:C:141:ARG:N	2.44	0.48
1:C:18:ILE:HB	1:C:145:ILE:HG22	1.96	0.48
1:D:185:ASN:N	1:D:185:ASN:ND2	2.62	0.48
1:E:200:PRO:O	1:E:201:SER:C	2.52	0.48
1:F:237:LEU:HD13	1:G:235:PHE:CE2	2.49	0.48
1:I:292:ASP:O	1:I:297:GLN:NE2	2.47	0.48
1:A:203:TYR:O	1:A:207:PHE:HB2	2.14	0.48
1:B:61:THR:HG21	1:C:64:GLU:HG3	1.96	0.48
1:B:157:ILE:CD1	1:C:115:ASP:HA	2.43	0.48
1:E:147:VAL:O	1:E:149:THR:N	2.45	0.48
1:F:167:THR:O	1:F:168:HIS:HB2	2.13	0.48
1:H:21:ASN:HD21	1:H:38:TYR:HE1	1.61	0.48
1:J:301:LEU:C	1:J:304:PRO:HD2	2.34	0.48
1:A:231:LEU:HD23	1:A:232:GLN:N	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:280:ILE:HG22	1:E:223:TRP:CE3	2.49	0.48
1:B:151:ASN:HD22	1:B:151:ASN:H	1.61	0.48
1:C:143:SER:HB3	1:C:167:THR:HG21	1.96	0.48
1:C:209:LEU:HB3	1:C:210:PRO:HD3	1.96	0.48
1:D:303:PHE:N	1:D:304:PRO:HD3	2.29	0.48
1:E:20:ILE:HG13	1:E:194:ILE:HD11	1.96	0.48
1:E:180:VAL:O	1:E:180:VAL:HG13	2.13	0.48
1:F:239:LEU:HD23	1:J:240:THR:HA	1.96	0.48
1:G:303:PHE:N	1:G:304:PRO:HD3	2.29	0.48
1:I:215:ILE:HD12	1:I:268:GLY:HA2	1.96	0.48
1:I:292:ASP:O	1:I:293:ASP:C	2.52	0.48
1:J:125:GLN:HG3	1:J:125:GLN:O	2.14	0.48
1:A:173:ARG:HA	1:A:185:ASN:O	2.13	0.47
1:B:28:THR:HB	1:B:255:LEU:CD2	2.44	0.47
1:B:76:LEU:HB3	1:B:130:LEU:HD22	1.95	0.47
1:C:28:THR:HB	1:C:255:LEU:CD2	2.42	0.47
1:D:173:ARG:HA	1:D:185:ASN:O	2.13	0.47
1:E:177:LEU:HD11	1:E:185:ASN:HB3	1.96	0.47
1:F:147:VAL:CG2	1:F:165:ALA:HB2	2.44	0.47
1:F:276:ILE:O	1:F:280:ILE:HG13	2.14	0.47
1:H:72:TRP:O	1:H:72:TRP:CD1	2.66	0.47
1:I:72:TRP:O	1:I:72:TRP:CD1	2.67	0.47
1:I:286:GLN:CA	1:I:291:GLU:HB3	2.44	0.47
1:J:231:LEU:HD23	1:J:231:LEU:C	2.34	0.47
1:C:231:LEU:HD23	1:C:231:LEU:C	2.35	0.47
1:H:13:ASP:HB3	1:H:141:ARG:HD2	1.96	0.47
1:B:220:SER:HB2	1:C:280:ILE:CD1	2.44	0.47
1:C:76:LEU:HB3	1:C:130:LEU:HD22	1.95	0.47
1:C:173:ARG:HA	1:C:185:ASN:O	2.14	0.47
1:F:231:LEU:HD22	1:J:224:LEU:HD21	1.97	0.47
1:F:294:LEU:HD12	1:F:297:GLN:NE2	2.29	0.47
1:G:48:ARG:HB2	1:G:48:ARG:CZ	2.44	0.47
1:G:62:GLN:HE22	1:G:65:ARG:HH11	1.63	0.47
1:G:172:ILE:HD13	1:G:189:ARG:CB	2.44	0.47
1:G:296:ILE:CG2	1:G:297:GLN:N	2.77	0.47
1:I:283:HIS:HA	1:I:292:ASP:OD1	2.14	0.47
1:A:276:ILE:O	1:A:280:ILE:HG13	2.14	0.47
1:D:112:ASN:OD1	1:D:113:ASP:N	2.47	0.47
1:D:263:GLN:HA	1:D:266:ILE:HG12	1.95	0.47
1:D:286:GLN:HB3	1:D:291:GLU:HB3	1.96	0.47
1:F:40:VAL:HA	1:F:102:TYR:O	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:231:LEU:HD23	1:F:232:GLN:N	2.30	0.47
1:J:293:ASP:O	1:J:296:ILE:HG22	2.14	0.47
1:B:17:SER:O	1:B:40:VAL:HG23	2.14	0.47
1:B:164:LYS:HG2	1:I:163:ARG:CB	2.29	0.47
1:C:286:GLN:CB	1:C:291:GLU:HB3	2.45	0.47
1:D:15:SER:HG	1:D:142:PHE:HD1	1.60	0.47
1:G:147:VAL:CG2	1:G:165:ALA:HB2	2.43	0.47
1:G:175:ASP:HB2	1:G:176:HIS:CE1	2.50	0.47
1:G:283:HIS:O	1:G:286:GLN:HG3	2.14	0.47
1:I:28:THR:HB	1:I:255:LEU:CD2	2.45	0.47
1:I:296:ILE:HG23	1:I:297:GLN:N	2.27	0.47
1:A:176:HIS:NE2	1:E:148:TYR:OH	2.39	0.47
1:A:200:PRO:O	1:A:201:SER:C	2.53	0.47
1:B:211:LEU:CD1	1:B:264:MET:HB3	2.44	0.47
1:C:13:ASP:HB3	1:C:141:ARG:HD2	1.97	0.47
1:D:305:LEU:HA	1:D:308:LEU:HD13	1.97	0.47
1:E:303:PHE:N	1:E:304:PRO:HD3	2.30	0.47
1:F:133:PHE:HE2	1:J:91:ARG:HB2	1.78	0.47
1:G:140:LEU:CD1	1:G:190:ILE:HG13	2.27	0.47
1:G:205:TRP:O	1:H:266:ILE:HD12	2.14	0.47
1:G:220:SER:HB2	1:H:280:ILE:CD1	2.45	0.47
1:G:276:ILE:O	1:G:280:ILE:HG13	2.14	0.47
1:I:231:LEU:HD23	1:I:232:GLN:N	2.29	0.47
1:A:66:TRP:CE3	1:A:71:LEU:HD12	2.49	0.47
1:A:87:THR:HG21	1:A:90:LYS:CE	2.44	0.47
1:A:285:ARG:HD3	1:A:285:ARG:O	2.14	0.47
1:B:203:TYR:O	1:B:207:PHE:HB2	2.15	0.47
1:B:303:PHE:N	1:B:304:PRO:HD3	2.29	0.47
1:C:181:GLN:O	1:C:182:PRO:C	2.53	0.47
1:D:40:VAL:HA	1:D:102:TYR:O	2.14	0.47
1:D:147:VAL:CG2	1:D:165:ALA:HB2	2.44	0.47
1:E:150:GLU:O	1:E:150:GLU:OE2	2.33	0.47
1:F:21:ASN:HD21	1:F:38:TYR:HE1	1.62	0.47
1:F:200:PRO:O	1:F:201:SER:C	2.52	0.47
1:F:223:TRP:CE3	1:G:280:ILE:HG22	2.50	0.47
1:G:27:ASN:HB3	1:G:32:THR:HB	1.97	0.47
1:G:99:ARG:NH1	1:H:179:SER:CB	2.78	0.47
1:G:220:SER:HB2	1:H:280:ILE:HD13	1.95	0.47
1:G:239:LEU:O	1:G:239:LEU:HD13	2.14	0.47
1:I:177:LEU:CD1	1:I:185:ASN:HA	2.44	0.47
1:I:211:LEU:HD23	1:I:244:TYR:CE2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:296:ILE:CG2	1:I:297:GLN:N	2.78	0.47
1:J:18:ILE:HB	1:J:145:ILE:HG22	1.95	0.47
1:J:67:ILE:HD11	1:J:73:VAL:HG21	1.97	0.47
1:A:40:VAL:HA	1:A:102:TYR:O	2.15	0.47
1:C:180:VAL:HG21	1:C:184:GLN:CB	2.37	0.47
1:C:231:LEU:HD23	1:C:232:GLN:N	2.29	0.47
1:D:27:ASN:HB3	1:D:32:THR:HB	1.97	0.47
1:F:91:ARG:HB2	1:G:133:PHE:HE2	1.80	0.47
1:I:13:ASP:HB3	1:I:141:ARG:HD2	1.96	0.47
1:I:181:GLN:N	1:I:182:PRO:CD	2.73	0.47
1:J:76:LEU:HB3	1:J:130:LEU:HD22	1.97	0.47
1:J:150:GLU:H	1:J:150:GLU:CD	2.18	0.47
1:J:263:GLN:HA	1:J:266:ILE:HG12	1.97	0.47
1:C:174:TYR:HB2	1:C:177:LEU:CD2	2.40	0.47
1:C:301:LEU:C	1:C:304:PRO:HD2	2.35	0.47
1:F:145:ILE:H	1:F:145:ILE:CD1	2.20	0.47
1:F:211:LEU:O	1:F:211:LEU:HD13	2.15	0.47
1:G:210:PRO:HB3	1:H:269:TYR:CD1	2.50	0.47
1:H:276:ILE:O	1:H:280:ILE:HG13	2.15	0.47
1:H:282:ALA:O	1:H:292:ASP:HA	2.15	0.47
1:H:305:LEU:HA	1:H:308:LEU:HD13	1.97	0.47
1:I:162:ILE:HG22	1:I:163:ARG:N	2.19	0.47
1:A:177:LEU:HD11	1:A:185:ASN:CB	2.45	0.47
1:C:58:VAL:HB	1:C:92:LEU:HB2	1.97	0.47
1:D:66:TRP:HB3	1:D:71:LEU:HD12	1.97	0.47
1:E:185:ASN:N	1:E:185:ASN:ND2	2.63	0.47
1:F:83:GLY:CA	1:J:107:LEU:HD23	2.43	0.47
1:F:99:ARG:NH1	1:G:179:SER:CB	2.78	0.47
1:G:285:ARG:NE	1:G:285:ARG:CA	2.78	0.47
1:B:169:ILE:HD12	1:B:190:ILE:HG12	1.97	0.46
1:F:67:ILE:HD11	1:F:73:VAL:HG21	1.97	0.46
1:F:115:ASP:OD2	1:J:157:ILE:HD11	2.15	0.46
1:I:66:TRP:HB3	1:I:71:LEU:HD12	1.97	0.46
1:A:61:THR:HG21	1:B:64:GLU:HG3	1.97	0.46
1:B:23:ILE:HD11	1:B:194:ILE:HD12	1.96	0.46
1:B:78:PHE:HB3	1:B:81:VAL:CG2	2.45	0.46
1:B:301:LEU:C	1:B:304:PRO:HD2	2.35	0.46
1:E:39:ILE:HD11	1:E:78:PHE:CE1	2.49	0.46
1:E:149:THR:CG2	1:E:150:GLU:N	2.78	0.46
1:F:173:ARG:HA	1:F:185:ASN:O	2.16	0.46
1:G:288:ASN:CG	1:G:289:GLY:H	2.18	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:151:ASN:O	1:H:152:ILE:HD13	2.16	0.46
1:I:48:ARG:HB2	1:I:48:ARG:CZ	2.45	0.46
1:J:17:SER:O	1:J:40:VAL:HG23	2.15	0.46
1:J:292:ASP:O	1:J:297:GLN:NE2	2.49	0.46
1:J:292:ASP:O	1:J:293:ASP:C	2.53	0.46
1:A:145:ILE:CD1	1:A:165:ALA:HB1	2.43	0.46
1:B:292:ASP:O	1:B:293:ASP:C	2.52	0.46
1:C:40:VAL:HA	1:C:102:TYR:O	2.15	0.46
1:D:177:LEU:HB3	1:D:178:SER:H	1.47	0.46
1:E:78:PHE:HB3	1:E:81:VAL:CG2	2.45	0.46
1:H:246:PHE:CD2	1:I:246:PHE:HE2	2.34	0.46
1:H:248:THR:HG23	1:H:252:LEU:HD22	1.97	0.46
1:I:173:ARG:HA	1:I:185:ASN:O	2.15	0.46
1:I:211:LEU:CD1	1:I:264:MET:HB3	2.45	0.46
1:J:181:GLN:H	1:J:182:PRO:HD3	1.80	0.46
1:B:173:ARG:HA	1:B:185:ASN:O	2.16	0.46
1:B:257:TYR:CD2	1:B:257:TYR:N	2.82	0.46
1:C:20:ILE:HG13	1:C:194:ILE:HD11	1.97	0.46
1:D:136:ASN:ND2	1:D:184:GLN:HA	2.30	0.46
1:F:181:GLN:H	1:F:182:PRO:HD3	1.80	0.46
1:G:167:THR:O	1:G:168:HIS:CB	2.63	0.46
1:G:209:LEU:HB3	1:G:210:PRO:HD3	1.96	0.46
1:H:176:HIS:CD2	1:H:176:HIS:N	2.82	0.46
1:J:276:ILE:O	1:J:280:ILE:HG13	2.16	0.46
1:B:13:ASP:HB3	1:B:141:ARG:HD2	1.97	0.46
1:B:87:THR:HG21	1:B:90:LYS:CE	2.45	0.46
1:E:23:ILE:HD11	1:E:194:ILE:HD12	1.98	0.46
1:E:231:LEU:C	1:E:231:LEU:HD23	2.36	0.46
1:F:48:ARG:CZ	1:F:48:ARG:HB2	2.46	0.46
1:F:56:LEU:HD13	1:F:57:ILE:N	2.31	0.46
1:G:223:TRP:CD1	1:G:300:ARG:HD3	2.50	0.46
1:G:248:THR:HG23	1:G:252:LEU:HD22	1.98	0.46
1:J:180:VAL:HG22	1:J:181:GLN:N	2.31	0.46
1:J:257:TYR:CD2	1:J:257:TYR:N	2.83	0.46
1:A:209:LEU:HB3	1:A:210:PRO:HD3	1.96	0.46
1:A:239:LEU:HD21	1:E:239:LEU:CD1	2.46	0.46
1:C:157:ILE:HD13	1:C:157:ILE:HA	1.77	0.46
1:D:56:LEU:HD13	1:D:57:ILE:H	1.79	0.46
1:E:294:LEU:HA	1:E:297:GLN:HG2	1.98	0.46
1:F:174:TYR:O	1:F:177:LEU:HD11	2.16	0.46
1:F:303:PHE:N	1:F:304:PRO:HD3	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:LEU:HA	1:A:208:ILE:CG1	2.43	0.46
1:C:178:SER:O	1:C:180:VAL:HG12	2.16	0.46
1:E:117:ARG:HG2	1:E:117:ARG:HH11	1.80	0.46
1:F:14:VAL:O	1:F:141:ARG:N	2.45	0.46
1:J:48:ARG:CZ	1:J:48:ARG:HB2	2.44	0.46
1:A:246:PHE:CE2	1:E:246:PHE:CD2	3.03	0.46
1:C:148:TYR:HH	1:D:176:HIS:CE1	2.34	0.46
1:C:218:SER:CA	1:C:237:LEU:HD21	2.42	0.46
1:D:87:THR:HG21	1:D:90:LYS:CE	2.46	0.46
1:F:179:SER:CB	1:J:99:ARG:NH1	2.79	0.46
1:F:209:LEU:HB3	1:F:210:PRO:HD3	1.95	0.46
1:H:204:LEU:HA	1:H:208:ILE:CG1	2.46	0.46
1:I:172:ILE:CD1	1:I:189:ARG:HB3	2.44	0.46
1:J:203:TYR:O	1:J:207:PHE:HB2	2.16	0.46
1:J:222:PHE:HB3	1:J:300:ARG:HG2	1.97	0.46
1:A:68:ASN:HA	1:E:65:ARG:NH1	2.31	0.46
1:A:178:SER:C	1:A:180:VAL:H	2.20	0.46
1:B:200:PRO:O	1:B:201:SER:C	2.54	0.46
1:G:150:GLU:HB2	1:G:153:ASP:CB	2.45	0.46
1:I:52:GLY:O	1:I:53:ASP:CB	2.61	0.46
1:I:143:SER:HB3	1:I:167:THR:HG21	1.97	0.46
1:I:162:ILE:N	1:I:162:ILE:CD1	2.76	0.46
1:J:305:LEU:HA	1:J:308:LEU:HD13	1.97	0.46
1:A:162:ILE:N	1:A:162:ILE:CD1	2.74	0.46
1:A:281:PHE:CZ	1:A:285:ARG:HG2	2.51	0.46
1:B:18:ILE:HB	1:B:145:ILE:HG22	1.98	0.46
1:B:145:ILE:HD12	1:B:145:ILE:N	2.17	0.46
1:C:147:VAL:C	1:C:149:THR:H	2.18	0.46
1:C:285:ARG:HA	1:C:285:ARG:CZ	2.43	0.46
1:D:219:TRP:HZ2	1:D:307:PHE:CD2	2.34	0.46
1:E:143:SER:HB3	1:E:167:THR:HG21	1.98	0.46
1:F:266:ILE:HD12	1:J:205:TRP:O	2.16	0.46
1:J:145:ILE:CD1	1:J:165:ALA:HB1	2.42	0.46
1:J:177:LEU:HD11	1:J:187:PHE:CE1	2.39	0.46
1:A:92:LEU:HD23	1:A:92:LEU:HA	1.83	0.45
1:A:157:ILE:HD11	1:B:115:ASP:CG	2.37	0.45
1:D:211:LEU:HD23	1:D:244:TYR:CE2	2.51	0.45
1:E:218:SER:CA	1:E:237:LEU:HD21	2.45	0.45
1:H:185:ASN:N	1:H:185:ASN:ND2	2.64	0.45
1:I:185:ASN:N	1:I:185:ASN:ND2	2.64	0.45
1:J:226:SER:HB3	1:J:229:GLU:CG	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:ILE:HD11	1:A:73:VAL:HG21	1.98	0.45
1:A:223:TRP:CE3	1:B:280:ILE:HG22	2.50	0.45
1:B:145:ILE:N	1:B:145:ILE:CD1	2.79	0.45
1:B:293:ASP:OD2	1:B:293:ASP:N	2.43	0.45
1:B:296:ILE:CG2	1:B:297:GLN:N	2.78	0.45
1:C:18:ILE:HB	1:C:145:ILE:CG2	2.46	0.45
1:C:23:ILE:HD11	1:C:194:ILE:HD12	1.98	0.45
1:C:286:GLN:OE1	1:C:289:GLY:HA2	2.16	0.45
1:C:293:ASP:O	1:C:296:ILE:N	2.48	0.45
1:D:72:TRP:O	1:D:72:TRP:CD1	2.69	0.45
1:D:185:ASN:HD22	1:D:185:ASN:H	1.64	0.45
1:E:219:TRP:HZ2	1:E:307:PHE:CD2	2.35	0.45
1:F:50:THR:O	1:F:51:PRO:C	2.54	0.45
1:F:152:ILE:HG22	1:F:152:ILE:O	2.17	0.45
1:F:286:GLN:CB	1:F:291:GLU:HB3	2.45	0.45
1:G:237:LEU:HD13	1:H:235:PHE:CD2	2.51	0.45
1:G:305:LEU:HA	1:G:308:LEU:HD13	1.99	0.45
1:H:150:GLU:CG	1:H:154:ASN:H	2.27	0.45
1:C:48:ARG:CZ	1:C:48:ARG:HB2	2.46	0.45
1:D:231:LEU:HD23	1:D:231:LEU:C	2.36	0.45
1:F:143:SER:HB3	1:F:167:THR:HG21	1.97	0.45
1:F:315:VAL:HG12	1:F:315:VAL:O	2.16	0.45
1:G:200:PRO:O	1:G:201:SER:C	2.54	0.45
1:H:18:ILE:HB	1:H:145:ILE:CG2	2.46	0.45
1:H:239:LEU:O	1:H:239:LEU:HD13	2.16	0.45
1:H:257:TYR:CD2	1:H:257:TYR:N	2.83	0.45
1:I:209:LEU:HB3	1:I:210:PRO:HD3	1.96	0.45
1:A:292:ASP:O	1:A:294:LEU:N	2.50	0.45
1:B:286:GLN:CB	1:B:291:GLU:HB3	2.45	0.45
1:D:21:ASN:HB2	1:D:36:ASP:O	2.15	0.45
1:E:181:GLN:O	1:E:182:PRO:C	2.55	0.45
1:E:231:LEU:HD23	1:E:232:GLN:N	2.32	0.45
1:E:294:LEU:CG	1:E:298:ARG:HH21	2.25	0.45
1:G:119:PHE:O	1:G:120:PRO:C	2.54	0.45
1:I:67:ILE:HD11	1:I:73:VAL:HG21	1.99	0.45
1:I:72:TRP:CD1	1:I:72:TRP:C	2.90	0.45
1:I:147:VAL:CG2	1:I:165:ALA:HB2	2.45	0.45
1:A:91:ARG:HB2	1:B:133:PHE:HE2	1.82	0.45
1:A:147:VAL:CG2	1:A:165:ALA:HB2	2.46	0.45
1:C:87:THR:HG21	1:C:90:LYS:CE	2.47	0.45
1:D:248:THR:HG23	1:D:252:LEU:HD22	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:48:ARG:CZ	1:E:48:ARG:HB2	2.45	0.45
1:E:177:LEU:CD2	1:E:187:PHE:HE1	2.30	0.45
1:F:99:ARG:CZ	1:G:179:SER:HB2	2.46	0.45
1:F:177:LEU:CD2	1:F:185:ASN:HA	2.46	0.45
1:F:177:LEU:HD21	1:F:185:ASN:HA	1.98	0.45
1:G:18:ILE:HB	1:G:145:ILE:HG22	1.98	0.45
1:I:154:ASN:O	1:I:155:GLU:HG2	2.16	0.45
1:B:248:THR:HG23	1:B:252:LEU:HD22	1.98	0.45
1:E:293:ASP:O	1:E:296:ILE:N	2.50	0.45
1:F:150:GLU:CG	1:F:153:ASP:HB3	2.47	0.45
1:H:150:GLU:CG	1:H:150:GLU:O	2.64	0.45
1:I:149:THR:HG22	1:I:150:GLU:N	2.31	0.45
1:I:305:LEU:HA	1:I:308:LEU:HD13	1.98	0.45
1:J:18:ILE:HB	1:J:145:ILE:CG2	2.46	0.45
1:J:32:THR:HG22	1:J:33:TYR:N	2.31	0.45
1:J:87:THR:HG21	1:J:90:LYS:CE	2.47	0.45
1:A:62:GLN:HE22	1:A:65:ARG:NH1	2.14	0.45
1:D:117:ARG:HG2	1:D:117:ARG:HH11	1.81	0.45
1:D:150:GLU:CG	1:D:153:ASP:HB3	2.46	0.45
1:D:294:LEU:HG	1:D:298:ARG:HH21	1.82	0.45
1:E:32:THR:HG22	1:E:33:TYR:N	2.30	0.45
1:F:107:LEU:HD23	1:G:83:GLY:HA2	1.97	0.45
1:H:150:GLU:HG2	1:H:150:GLU:O	2.16	0.45
1:J:78:PHE:HB3	1:J:81:VAL:CG2	2.47	0.45
1:C:224:LEU:O	1:C:230:ARG:HD2	2.17	0.45
1:I:151:ASN:C	1:I:152:ILE:HG12	2.36	0.45
1:J:219:TRP:HZ2	1:J:307:PHE:CD2	2.35	0.45
1:A:224:LEU:O	1:A:230:ARG:HD2	2.17	0.45
1:B:143:SER:CB	1:B:169:ILE:HD11	2.47	0.45
1:B:150:GLU:H	1:B:150:GLU:CD	2.21	0.45
1:C:145:ILE:HD12	1:C:145:ILE:N	2.18	0.45
1:E:87:THR:HG21	1:E:90:LYS:HE2	1.98	0.45
1:E:174:TYR:HB2	1:E:177:LEU:HG	1.98	0.45
1:F:179:SER:HB3	1:J:99:ARG:NH1	2.32	0.45
1:F:249:SER:HB3	1:J:251:ILE:HG13	1.98	0.45
1:H:62:GLN:HE22	1:H:65:ARG:HH11	1.65	0.45
1:J:209:LEU:HB3	1:J:210:PRO:HD3	1.98	0.45
1:B:91:ARG:HD3	1:C:134:SER:HB3	1.95	0.45
1:C:145:ILE:CD1	1:C:165:ALA:HB1	2.45	0.45
1:C:257:TYR:CD2	1:C:257:TYR:N	2.84	0.45
1:C:286:GLN:HA	1:C:291:GLU:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:145:ILE:H	1:E:145:ILE:CD1	2.18	0.45
1:E:145:ILE:CD1	1:E:165:ALA:HB1	2.45	0.45
1:F:99:ARG:NH1	1:G:179:SER:HB2	2.32	0.45
1:F:239:LEU:CD1	1:G:239:LEU:HD21	2.47	0.45
1:G:181:GLN:N	1:G:182:PRO:CD	2.80	0.45
1:H:119:PHE:O	1:H:120:PRO:C	2.55	0.45
1:H:173:ARG:HA	1:H:185:ASN:O	2.17	0.45
1:I:178:SER:O	1:I:180:VAL:HG12	2.16	0.45
1:J:135:TYR:HB3	1:J:138:GLN:HB2	1.98	0.45
1:B:246:PHE:CD2	1:C:246:PHE:HE2	2.34	0.44
1:B:276:ILE:O	1:B:280:ILE:HG13	2.17	0.44
1:C:286:GLN:HB3	1:C:291:GLU:H	1.82	0.44
1:D:286:GLN:CA	1:D:291:GLU:HB3	2.48	0.44
1:G:294:LEU:HD12	1:G:297:GLN:NE2	2.32	0.44
1:I:57:ILE:HD13	1:J:134:SER:O	2.16	0.44
1:J:200:PRO:O	1:J:201:SER:C	2.55	0.44
1:A:219:TRP:HZ2	1:A:307:PHE:CD2	2.35	0.44
1:B:66:TRP:HB3	1:B:71:LEU:HD12	1.98	0.44
1:C:200:PRO:O	1:C:201:SER:C	2.56	0.44
1:C:205:TRP:O	1:D:266:ILE:HD12	2.16	0.44
1:E:222:PHE:HB3	1:E:300:ARG:HG2	1.98	0.44
1:F:21:ASN:HB2	1:F:36:ASP:O	2.17	0.44
1:F:219:TRP:HZ2	1:F:307:PHE:CD2	2.35	0.44
1:F:246:PHE:CD2	1:G:246:PHE:HE2	2.34	0.44
1:G:23:ILE:HD11	1:G:194:ILE:HD12	1.99	0.44
1:I:21:ASN:HB2	1:I:36:ASP:O	2.17	0.44
1:I:62:GLN:HE22	1:I:65:ARG:HH11	1.64	0.44
1:I:222:PHE:HB3	1:I:300:ARG:HG2	1.99	0.44
1:A:199:ASN:C	1:A:199:ASN:HD22	2.21	0.44
1:C:181:GLN:H	1:C:182:PRO:HD2	1.79	0.44
1:C:246:PHE:CD2	1:D:246:PHE:HE2	2.35	0.44
1:D:237:LEU:HD13	1:E:235:PHE:CE2	2.52	0.44
1:F:167:THR:CG2	1:F:168:HIS:H	2.21	0.44
1:F:305:LEU:HA	1:F:308:LEU:HD13	1.99	0.44
1:G:152:ILE:HA	1:G:155:GLU:OE1	2.18	0.44
1:I:78:PHE:HB3	1:I:81:VAL:CG2	2.46	0.44
1:I:92:LEU:HD23	1:I:92:LEU:HA	1.86	0.44
1:I:246:PHE:CD2	1:J:246:PHE:CE2	3.06	0.44
1:A:97:ASP:OD1	1:A:99:ARG:HG2	2.16	0.44
1:A:182:PRO:HB2	1:A:184:GLN:HE22	1.82	0.44
1:B:101:ILE:HD13	1:C:178:SER:HB3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:222:PHE:HB3	1:C:300:ARG:HG2	1.98	0.44
1:D:48:ARG:HB2	1:D:48:ARG:CZ	2.47	0.44
1:E:145:ILE:HD12	1:E:145:ILE:N	2.18	0.44
1:F:257:TYR:CD2	1:F:257:TYR:N	2.85	0.44
1:H:20:ILE:HG13	1:H:194:ILE:HD11	1.99	0.44
1:H:177:LEU:HD12	1:H:177:LEU:N	2.33	0.44
1:J:303:PHE:N	1:J:304:PRO:HD3	2.31	0.44
1:A:248:THR:HG23	1:A:252:LEU:HD22	2.00	0.44
1:A:305:LEU:HA	1:A:308:LEU:HD13	1.99	0.44
1:B:164:LYS:NZ	1:B:165:ALA:N	2.43	0.44
1:B:239:LEU:O	1:B:239:LEU:HD13	2.17	0.44
1:F:125:GLN:O	1:F:125:GLN:HG3	2.18	0.44
1:F:282:ALA:O	1:F:292:ASP:HA	2.18	0.44
1:G:92:LEU:HD23	1:G:92:LEU:HA	1.86	0.44
1:H:200:PRO:O	1:H:201:SER:C	2.56	0.44
1:H:239:LEU:CD1	1:I:239:LEU:HD21	2.48	0.44
1:J:157:ILE:HD13	1:J:157:ILE:HA	1.81	0.44
1:A:239:LEU:HD23	1:E:240:THR:OG1	2.17	0.44
1:B:298:ARG:O	1:B:298:ARG:HG2	2.18	0.44
1:C:97:ASP:OD1	1:C:99:ARG:HG2	2.17	0.44
1:F:66:TRP:CE3	1:F:71:LEU:HD12	2.52	0.44
1:G:140:LEU:HD13	1:G:190:ILE:CD1	2.48	0.44
1:H:174:TYR:HB2	1:H:177:LEU:HD21	2.00	0.44
1:H:181:GLN:HG3	1:H:182:PRO:CD	2.42	0.44
1:H:222:PHE:C	1:H:224:LEU:H	2.21	0.44
1:I:200:PRO:O	1:I:201:SER:C	2.56	0.44
1:B:231:LEU:HD23	1:B:232:GLN:N	2.33	0.44
1:D:61:THR:HG21	1:E:64:GLU:HG3	1.99	0.44
1:D:72:TRP:CD1	1:D:72:TRP:C	2.91	0.44
1:E:72:TRP:CD1	1:E:72:TRP:O	2.71	0.44
1:E:173:ARG:HA	1:E:185:ASN:O	2.17	0.44
1:F:72:TRP:CZ3	1:F:135:TYR:CZ	3.03	0.44
1:G:14:VAL:O	1:G:141:ARG:N	2.45	0.44
1:H:62:GLN:HE22	1:H:65:ARG:NH1	2.16	0.44
1:H:223:TRP:CD1	1:H:300:ARG:HD3	2.53	0.44
1:I:32:THR:HG22	1:I:33:TYR:N	2.33	0.44
1:J:81:VAL:HG11	1:J:85:PRO:HD3	1.98	0.44
1:A:65:ARG:NH1	1:B:68:ASN:HA	2.33	0.44
1:C:240:THR:OG1	1:D:239:LEU:HD23	2.17	0.44
1:D:54:LYS:O	1:D:55:PRO:C	2.56	0.44
1:E:259:THR:HG23	1:E:262:ASP:OD2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:185:ASN:N	1:F:185:ASN:ND2	2.64	0.44
1:G:107:LEU:HD23	1:H:83:GLY:CA	2.48	0.44
1:G:118:LEU:N	1:G:118:LEU:CD2	2.80	0.44
1:H:23:ILE:HD11	1:H:194:ILE:HD12	1.98	0.44
1:I:72:TRP:CZ3	1:I:135:TYR:CZ	3.01	0.44
1:A:17:SER:O	1:A:40:VAL:HG23	2.17	0.44
1:A:39:ILE:HD11	1:A:78:PHE:CE1	2.50	0.44
1:A:78:PHE:HB3	1:A:81:VAL:CG2	2.47	0.44
1:A:246:PHE:HZ	1:E:246:PHE:CE1	2.36	0.44
1:B:66:TRP:CE3	1:B:71:LEU:HD12	2.53	0.44
1:B:72:TRP:CD1	1:B:72:TRP:O	2.70	0.44
1:D:20:ILE:HG13	1:D:194:ILE:HD11	1.98	0.44
1:F:77:GLU:O	1:F:130:LEU:HD23	2.18	0.44
1:F:89:ASN:O	1:F:104:ALA:HA	2.18	0.44
1:G:32:THR:HG22	1:G:33:TYR:N	2.32	0.44
1:H:76:LEU:HB3	1:H:130:LEU:HD22	1.99	0.44
1:I:204:LEU:HA	1:I:208:ILE:CG1	2.48	0.44
1:C:185:ASN:N	1:C:185:ASN:ND2	2.66	0.43
1:D:145:ILE:CD1	1:D:165:ALA:HB1	2.41	0.43
1:D:231:LEU:HD23	1:D:232:GLN:N	2.32	0.43
1:E:18:ILE:HB	1:E:145:ILE:HG22	2.00	0.43
1:E:223:TRP:CD1	1:E:300:ARG:HD3	2.53	0.43
1:F:17:SER:O	1:F:40:VAL:HG23	2.18	0.43
1:F:237:LEU:HD13	1:G:235:PHE:CD2	2.53	0.43
1:G:231:LEU:HD23	1:G:231:LEU:C	2.37	0.43
1:H:48:ARG:CZ	1:H:48:ARG:HB2	2.47	0.43
1:H:143:SER:HB3	1:H:167:THR:HG21	2.01	0.43
1:H:181:GLN:N	1:H:182:PRO:CD	2.72	0.43
1:H:205:TRP:O	1:I:266:ILE:HD12	2.18	0.43
1:H:220:SER:HB2	1:I:280:ILE:CD1	2.48	0.43
1:J:177:LEU:HB3	1:J:178:SER:H	1.53	0.43
1:J:291:GLU:HG2	1:J:291:GLU:O	2.18	0.43
1:A:235:PHE:CE2	1:E:237:LEU:HD13	2.53	0.43
1:B:48:ARG:CZ	1:B:48:ARG:HB2	2.48	0.43
1:B:293:ASP:HB2	1:B:296:ILE:HG22	2.00	0.43
1:B:294:LEU:HG	1:B:298:ARG:HH21	1.84	0.43
1:C:61:THR:HG21	1:D:64:GLU:HG3	2.00	0.43
1:D:162:ILE:N	1:D:162:ILE:CD1	2.76	0.43
1:D:180:VAL:HG23	1:D:182:PRO:HD2	2.00	0.43
1:E:150:GLU:HG2	1:E:150:GLU:O	2.19	0.43
1:F:97:ASP:OD1	1:F:99:ARG:HG2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:46:LYS:O	1:H:47:PRO:C	2.56	0.43
1:I:143:SER:CB	1:I:169:ILE:HD11	2.47	0.43
1:I:150:GLU:CG	1:I:150:GLU:O	2.66	0.43
1:I:294:LEU:HD12	1:I:297:GLN:NE2	2.33	0.43
1:B:157:ILE:HD11	1:C:115:ASP:CB	2.49	0.43
1:B:185:ASN:N	1:B:185:ASN:ND2	2.63	0.43
1:B:240:THR:HA	1:C:239:LEU:HD23	2.01	0.43
1:C:17:SER:O	1:C:40:VAL:HG23	2.18	0.43
1:C:56:LEU:O	1:C:93:MET:HA	2.18	0.43
1:C:162:ILE:N	1:C:162:ILE:CD1	2.76	0.43
1:C:182:PRO:HB2	1:C:184:GLN:NE2	2.33	0.43
1:D:46:LYS:HA	1:D:47:PRO:HD2	1.89	0.43
1:D:257:TYR:CD2	1:D:257:TYR:N	2.86	0.43
1:F:81:VAL:HG11	1:F:85:PRO:HD3	1.99	0.43
1:F:211:LEU:CD1	1:F:264:MET:HB3	2.48	0.43
1:F:313:VAL:HA	1:F:316:ILE:CD1	2.48	0.43
1:H:14:VAL:O	1:H:141:ARG:N	2.47	0.43
1:I:223:TRP:CE3	1:J:280:ILE:HG22	2.52	0.43
1:A:72:TRP:O	1:A:72:TRP:CD1	2.71	0.43
1:B:70:GLY:O	1:B:71:LEU:C	2.57	0.43
1:E:16:VAL:HG12	1:E:17:SER:N	2.33	0.43
1:E:72:TRP:CZ3	1:E:135:TYR:CZ	3.02	0.43
1:E:97:ASP:OD1	1:E:99:ARG:HG2	2.18	0.43
1:E:154:ASN:O	1:E:155:GLU:HG3	2.18	0.43
1:F:205:TRP:N	1:F:205:TRP:CD1	2.87	0.43
1:G:13:ASP:HB3	1:G:141:ARG:HD2	2.00	0.43
1:H:65:ARG:HD2	1:I:68:ASN:ND2	2.33	0.43
1:B:32:THR:CG2	1:B:33:TYR:N	2.82	0.43
1:D:72:TRP:CE2	1:D:74:PRO:HG3	2.53	0.43
1:D:89:ASN:O	1:D:104:ALA:HA	2.17	0.43
1:E:172:ILE:N	1:E:172:ILE:CD1	2.81	0.43
1:F:64:GLU:CG	1:J:61:THR:HG21	2.48	0.43
1:G:62:GLN:HE22	1:G:65:ARG:NH1	2.16	0.43
1:G:224:LEU:HB2	1:G:230:ARG:HG3	1.99	0.43
1:H:91:ARG:HD2	1:I:134:SER:HB2	1.98	0.43
1:H:254:ARG:N	1:H:254:ARG:HD2	2.34	0.43
1:I:150:GLU:CD	1:I:150:GLU:H	2.20	0.43
1:I:219:TRP:HZ2	1:I:307:PHE:CD2	2.36	0.43
1:A:64:GLU:CG	1:E:61:THR:HG21	2.48	0.43
1:A:76:LEU:HB3	1:A:130:LEU:HD22	2.00	0.43
1:C:157:ILE:HD11	1:D:115:ASP:CG	2.38	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:230:ARG:HB3	1:D:279:ILE:HD13	2.00	0.43
1:E:145:ILE:CD1	1:E:145:ILE:N	2.80	0.43
1:F:119:PHE:O	1:F:120:PRO:C	2.56	0.43
1:F:154:ASN:O	1:F:155:GLU:HG3	2.18	0.43
1:F:224:LEU:O	1:F:230:ARG:HD2	2.18	0.43
1:G:28:THR:HB	1:G:255:LEU:CD2	2.45	0.43
1:G:72:TRP:CZ3	1:G:135:TYR:CZ	3.01	0.43
1:G:257:TYR:CD2	1:G:257:TYR:N	2.86	0.43
1:H:39:ILE:HD11	1:H:78:PHE:CE1	2.51	0.43
1:I:150:GLU:CG	1:I:154:ASN:HB2	2.41	0.43
1:A:143:SER:CB	1:A:169:ILE:HD11	2.49	0.43
1:A:222:PHE:HB3	1:A:300:ARG:HG2	2.00	0.43
1:B:21:ASN:HB2	1:B:36:ASP:O	2.18	0.43
1:B:72:TRP:CE2	1:B:74:PRO:HG3	2.54	0.43
1:D:161:TRP:CZ2	1:D:199:ASN:ND2	2.87	0.43
1:F:66:TRP:HE3	1:F:71:LEU:HD12	1.84	0.43
1:G:181:GLN:CG	1:G:182:PRO:HD3	2.44	0.43
1:G:211:LEU:HD21	1:G:265:ILE:HD13	2.00	0.43
1:G:278:LEU:O	1:G:281:PHE:HB3	2.18	0.43
1:H:162:ILE:N	1:H:162:ILE:CD1	2.74	0.43
1:B:32:THR:HG22	1:B:33:TYR:N	2.33	0.43
1:B:140:LEU:HD13	1:B:190:ILE:CD1	2.48	0.43
1:C:117:ARG:HG2	1:C:117:ARG:HH11	1.84	0.43
1:C:305:LEU:HA	1:C:308:LEU:HD13	2.00	0.43
1:D:205:TRP:O	1:E:266:ILE:HD12	2.19	0.43
1:D:276:ILE:O	1:D:280:ILE:HG13	2.19	0.43
1:F:180:VAL:HG21	1:F:184:GLN:HB2	2.01	0.43
1:H:91:ARG:HB2	1:I:133:PHE:HE2	1.83	0.43
1:H:145:ILE:HG21	1:H:192:VAL:CG1	2.46	0.43
1:H:145:ILE:CD1	1:H:165:ALA:HB1	2.46	0.43
1:H:222:PHE:HB3	1:H:300:ARG:HG2	2.01	0.43
1:I:119:PHE:O	1:I:120:PRO:C	2.57	0.43
1:I:211:LEU:O	1:I:211:LEU:HD13	2.19	0.43
1:I:257:TYR:CD2	1:I:257:TYR:N	2.87	0.43
1:I:285:ARG:HA	1:I:285:ARG:CZ	2.49	0.43
1:A:278:LEU:O	1:A:281:PHE:HB3	2.18	0.43
1:B:251:ILE:HG13	1:C:249:SER:HB3	2.01	0.43
1:B:294:LEU:HA	1:B:297:GLN:NE2	2.34	0.43
1:C:78:PHE:HB3	1:C:81:VAL:CG2	2.49	0.43
1:C:141:ARG:HB3	1:C:142:PHE:H	1.72	0.43
1:D:180:VAL:HG21	1:D:184:GLN:CG	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:68:ASN:HD21	1:J:65:ARG:HD2	1.81	0.43
1:F:70:GLY:O	1:F:71:LEU:C	2.56	0.43
1:G:182:PRO:O	1:G:183:ASN:HB2	2.19	0.43
1:G:222:PHE:HB3	1:G:300:ARG:HG2	2.01	0.43
1:I:56:LEU:HD22	1:I:56:LEU:HA	1.77	0.43
1:A:211:LEU:HD21	1:A:265:ILE:HD13	2.01	0.43
1:A:303:PHE:CD1	1:A:303:PHE:C	2.92	0.43
1:C:248:THR:O	1:C:252:LEU:HB2	2.19	0.43
1:D:23:ILE:HD11	1:D:194:ILE:HD12	2.01	0.43
1:D:143:SER:CB	1:D:169:ILE:HD11	2.49	0.43
1:D:286:GLN:CB	1:D:291:GLU:HB3	2.48	0.43
1:E:147:VAL:CG2	1:E:165:ALA:HB2	2.49	0.43
1:E:209:LEU:HB3	1:E:210:PRO:HD3	1.98	0.43
1:E:287:ALA:HB3	1:E:291:GLU:OE2	2.19	0.43
1:F:145:ILE:CD1	1:F:165:ALA:HB1	2.44	0.43
1:G:50:THR:O	1:G:51:PRO:C	2.57	0.43
1:G:157:ILE:HA	1:G:157:ILE:HD13	1.78	0.43
1:H:167:THR:O	1:H:168:HIS:CB	2.67	0.43
1:H:263:GLN:HA	1:H:266:ILE:HG12	2.01	0.43
1:I:14:VAL:O	1:I:141:ARG:N	2.43	0.43
1:J:89:ASN:O	1:J:104:ALA:HA	2.18	0.43
1:A:62:GLN:O	1:A:65:ARG:HB2	2.19	0.42
1:A:257:TYR:CD2	1:A:257:TYR:N	2.87	0.42
1:A:269:TYR:CD1	1:E:210:PRO:HB3	2.54	0.42
1:B:177:LEU:CD1	1:B:187:PHE:HE1	2.31	0.42
1:B:219:TRP:HZ2	1:B:307:PHE:CD2	2.37	0.42
1:D:157:ILE:HD11	1:E:115:ASP:CG	2.40	0.42
1:E:180:VAL:HG21	1:E:184:GLN:CB	2.49	0.42
1:H:21:ASN:HB2	1:H:36:ASP:O	2.19	0.42
1:A:239:LEU:CD1	1:B:239:LEU:HD21	2.48	0.42
1:D:18:ILE:HB	1:D:145:ILE:HG22	2.01	0.42
1:E:145:ILE:HG21	1:E:192:VAL:CG1	2.45	0.42
1:F:117:ARG:HG2	1:F:117:ARG:HH11	1.84	0.42
1:G:143:SER:HB3	1:G:167:THR:HG21	2.01	0.42
1:G:211:LEU:O	1:G:211:LEU:HD13	2.20	0.42
1:A:72:TRP:CD1	1:A:72:TRP:C	2.93	0.42
1:B:39:ILE:HD11	1:B:78:PHE:CE1	2.52	0.42
1:B:66:TRP:HE3	1:B:71:LEU:HD12	1.85	0.42
1:B:223:TRP:CD1	1:B:300:ARG:HD3	2.55	0.42
1:C:72:TRP:CD1	1:C:72:TRP:C	2.92	0.42
1:C:222:PHE:CE1	1:C:299:CYS:SG	3.13	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:62:GLN:O	1:E:65:ARG:HB2	2.19	0.42
1:E:248:THR:HG23	1:E:252:LEU:HD22	1.99	0.42
1:G:219:TRP:HZ2	1:G:307:PHE:CD2	2.37	0.42
1:I:32:THR:CG2	1:I:33:TYR:N	2.82	0.42
1:I:65:ARG:HD2	1:J:68:ASN:ND2	2.33	0.42
1:A:181:GLN:H	1:A:182:PRO:CD	2.32	0.42
1:B:172:ILE:HD13	1:B:189:ARG:CB	2.48	0.42
1:B:234:SER:HA	1:B:237:LEU:HB2	2.01	0.42
1:B:305:LEU:HA	1:B:308:LEU:HD13	2.02	0.42
1:C:155:GLU:HB3	1:C:161:TRP:CD1	2.54	0.42
1:G:65:ARG:NH1	1:H:68:ASN:HA	2.34	0.42
1:G:150:GLU:CG	1:G:150:GLU:O	2.67	0.42
1:H:72:TRP:CZ3	1:H:135:TYR:CZ	3.04	0.42
1:H:89:ASN:O	1:H:104:ALA:HA	2.19	0.42
1:J:32:THR:CG2	1:J:33:TYR:N	2.82	0.42
1:J:248:THR:HG23	1:J:252:LEU:HD22	2.01	0.42
1:B:14:VAL:O	1:B:141:ARG:N	2.48	0.42
1:B:119:PHE:O	1:B:120:PRO:C	2.57	0.42
1:B:247:TYR:CD1	1:C:246:PHE:HA	2.44	0.42
1:C:32:THR:CG2	1:C:33:TYR:N	2.82	0.42
1:D:65:ARG:NH1	1:E:68:ASN:HA	2.33	0.42
1:E:305:LEU:HA	1:E:308:LEU:HD13	2.00	0.42
1:F:176:HIS:CD2	1:J:146:GLN:NE2	2.87	0.42
1:G:32:THR:CG2	1:G:33:TYR:N	2.82	0.42
1:H:231:LEU:HD23	1:H:231:LEU:C	2.38	0.42
1:I:149:THR:HG22	1:I:150:GLU:OE1	2.20	0.42
1:J:147:VAL:CG2	1:J:165:ALA:HB2	2.48	0.42
1:A:48:ARG:HB2	1:A:48:ARG:CZ	2.49	0.42
1:A:125:GLN:O	1:A:125:GLN:HG3	2.19	0.42
1:A:167:THR:O	1:A:168:HIS:CB	2.67	0.42
1:B:209:LEU:C	1:B:209:LEU:HD23	2.40	0.42
1:C:32:THR:HG22	1:C:33:TYR:N	2.34	0.42
1:C:54:LYS:HB3	1:C:55:PRO:HD2	2.02	0.42
1:E:119:PHE:O	1:E:120:PRO:C	2.58	0.42
1:E:219:TRP:O	1:E:221:VAL:N	2.53	0.42
1:E:293:ASP:O	1:E:295:LEU:N	2.52	0.42
1:H:145:ILE:H	1:H:145:ILE:CD1	2.13	0.42
1:H:177:LEU:HD12	1:H:177:LEU:H	1.83	0.42
1:J:145:ILE:HG21	1:J:192:VAL:CG1	2.46	0.42
1:A:185:ASN:N	1:A:185:ASN:ND2	2.64	0.42
1:C:172:ILE:HD13	1:C:189:ARG:CB	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:46:LYS:O	1:D:47:PRO:C	2.58	0.42
1:D:181:GLN:O	1:D:182:PRO:C	2.58	0.42
1:D:220:SER:HB2	1:E:280:ILE:HD13	2.02	0.42
1:E:224:LEU:HB2	1:E:230:ARG:HG3	2.01	0.42
1:F:46:LYS:O	1:F:47:PRO:C	2.57	0.42
1:G:62:GLN:O	1:G:65:ARG:HB2	2.20	0.42
1:G:145:ILE:CD1	1:G:145:ILE:N	2.80	0.42
1:G:240:THR:HA	1:H:239:LEU:HD23	2.02	0.42
1:I:87:THR:HG21	1:I:90:LYS:CE	2.49	0.42
1:I:276:ILE:O	1:I:280:ILE:HG13	2.19	0.42
1:A:223:TRP:CD1	1:A:300:ARG:HD3	2.54	0.42
1:B:220:SER:HB2	1:C:280:ILE:HD13	2.02	0.42
1:C:199:ASN:C	1:C:199:ASN:HD22	2.23	0.42
1:D:110:PHE:CD1	1:D:110:PHE:N	2.87	0.42
1:F:172:ILE:HD13	1:F:189:ARG:CB	2.49	0.42
1:H:210:PRO:HB3	1:I:269:TYR:CD1	2.55	0.42
1:H:219:TRP:HZ2	1:H:307:PHE:CD2	2.37	0.42
1:I:145:ILE:CD1	1:I:165:ALA:HB1	2.45	0.42
1:I:149:THR:HG22	1:I:150:GLU:OE2	2.20	0.42
1:J:62:GLN:HE22	1:J:65:ARG:HH11	1.68	0.42
1:B:166:SER:HB3	1:B:193:ARG:O	2.18	0.42
1:B:313:VAL:HA	1:B:316:ILE:CD1	2.49	0.42
1:C:294:LEU:HG	1:C:298:ARG:HH21	1.85	0.42
1:D:284:HIS:CA	1:D:286:GLN:HE21	2.31	0.42
1:E:141:ARG:HB3	1:E:142:PHE:H	1.72	0.42
1:E:257:TYR:CD2	1:E:257:TYR:N	2.87	0.42
1:E:313:VAL:HA	1:E:316:ILE:CD1	2.50	0.42
1:G:72:TRP:CD1	1:G:72:TRP:O	2.73	0.42
1:G:209:LEU:O	1:G:212:GLY:N	2.53	0.42
1:H:248:THR:O	1:H:252:LEU:HB2	2.20	0.42
1:I:215:ILE:HD12	1:I:268:GLY:CA	2.49	0.42
1:J:70:GLY:O	1:J:71:LEU:C	2.57	0.42
1:J:164:LYS:HZ2	1:J:164:LYS:CA	2.33	0.42
1:B:185:ASN:HD22	1:B:185:ASN:H	1.67	0.42
1:C:27:ASN:HB3	1:C:32:THR:HB	2.02	0.42
1:C:143:SER:CB	1:C:169:ILE:HD11	2.50	0.42
1:D:119:PHE:O	1:D:120:PRO:C	2.59	0.42
1:E:46:LYS:O	1:E:47:PRO:C	2.58	0.42
1:E:81:VAL:HG11	1:E:85:PRO:HD3	2.02	0.42
1:E:135:TYR:HB3	1:E:138:GLN:HB2	2.02	0.42
1:E:167:THR:CG2	1:E:168:HIS:H	2.23	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:157:ILE:HD13	1:F:157:ILE:HA	1.87	0.42
1:G:18:ILE:HB	1:G:145:ILE:CG2	2.50	0.42
1:G:148:TYR:HH	1:H:176:HIS:CE1	2.38	0.42
1:G:226:SER:HB3	1:G:229:GLU:OE1	2.19	0.42
1:H:181:GLN:H	1:H:182:PRO:HD3	1.83	0.42
1:J:224:LEU:HB2	1:J:230:ARG:HG3	2.01	0.42
1:A:303:PHE:C	1:A:303:PHE:HD1	2.23	0.41
1:A:307:PHE:HD1	1:A:310:ILE:HD12	1.85	0.41
1:B:110:PHE:N	1:B:110:PHE:CD1	2.87	0.41
1:B:237:LEU:HD13	1:C:235:PHE:CD2	2.55	0.41
1:C:46:LYS:O	1:C:47:PRO:C	2.58	0.41
1:E:18:ILE:HB	1:E:145:ILE:CG2	2.50	0.41
1:E:182:PRO:CB	1:E:184:GLN:HE22	2.33	0.41
1:F:182:PRO:HB2	1:F:184:GLN:NE2	2.31	0.41
1:G:66:TRP:CE3	1:G:71:LEU:HD12	2.55	0.41
1:G:199:ASN:C	1:G:199:ASN:HD22	2.23	0.41
1:G:222:PHE:C	1:G:224:LEU:H	2.24	0.41
1:H:72:TRP:CD1	1:H:72:TRP:C	2.93	0.41
1:I:46:LYS:O	1:I:47:PRO:C	2.58	0.41
1:J:72:TRP:CZ3	1:J:135:TYR:CZ	3.02	0.41
1:F:75:ALA:HB3	1:J:59:GLU:OE2	2.19	0.41
1:F:209:LEU:HD23	1:F:209:LEU:C	2.41	0.41
1:H:87:THR:HG21	1:H:90:LYS:CE	2.50	0.41
1:H:182:PRO:HB2	1:H:184:GLN:NE2	2.35	0.41
1:I:302:ALA:N	1:I:304:PRO:HD2	2.35	0.41
1:A:20:ILE:HG13	1:A:194:ILE:HD11	2.01	0.41
1:A:176:HIS:CE1	1:E:148:TYR:HH	2.32	0.41
1:A:239:LEU:CD2	1:E:240:THR:HA	2.51	0.41
1:B:18:ILE:HB	1:B:145:ILE:CG2	2.49	0.41
1:B:61:THR:HG21	1:C:64:GLU:CG	2.51	0.41
1:B:72:TRP:CD1	1:B:72:TRP:C	2.94	0.41
1:C:254:ARG:N	1:C:254:ARG:HD2	2.34	0.41
1:E:181:GLN:O	1:E:182:PRO:O	2.38	0.41
1:F:72:TRP:CE2	1:F:74:PRO:HG3	2.55	0.41
1:F:226:SER:HB3	1:F:229:GLU:OE1	2.20	0.41
1:G:298:ARG:O	1:G:298:ARG:HG2	2.20	0.41
1:H:99:ARG:NH1	1:I:179:SER:HB3	2.34	0.41
1:I:248:THR:HG23	1:I:252:LEU:HD22	2.02	0.41
1:J:63:ILE:O	1:J:67:ILE:HD13	2.20	0.41
1:A:15:SER:HG	1:A:142:PHE:HD1	1.65	0.41
1:A:91:ARG:HD3	1:B:134:SER:HB3	1.99	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:SER:HB3	1:A:167:THR:CG2	2.50	0.41
1:B:62:GLN:HE22	1:B:65:ARG:HH11	1.67	0.41
1:C:62:GLN:HE22	1:C:65:ARG:HH11	1.68	0.41
1:C:303:PHE:CD1	1:C:303:PHE:C	2.94	0.41
1:F:147:VAL:O	1:F:149:THR:N	2.47	0.41
1:I:54:LYS:O	1:I:55:PRO:C	2.56	0.41
1:I:89:ASN:O	1:I:104:ALA:HA	2.21	0.41
1:I:181:GLN:HG3	1:I:182:PRO:HD3	2.03	0.41
1:J:48:ARG:CB	1:J:48:ARG:NH1	2.84	0.41
1:J:167:THR:O	1:J:168:HIS:CB	2.68	0.41
1:A:72:TRP:CE2	1:A:74:PRO:HG3	2.53	0.41
1:A:209:LEU:HD23	1:A:209:LEU:C	2.41	0.41
1:B:65:ARG:HD2	1:C:68:ASN:HD21	1.82	0.41
1:C:167:THR:O	1:C:168:HIS:CB	2.69	0.41
1:D:120:PRO:HD2	1:D:260:VAL:HG23	2.02	0.41
1:D:151:ASN:O	1:D:152:ILE:HD13	2.21	0.41
1:D:286:GLN:HG2	1:D:289:GLY:CA	2.50	0.41
1:E:150:GLU:HG3	1:E:154:ASN:H	1.85	0.41
1:E:219:TRP:C	1:E:221:VAL:N	2.72	0.41
1:F:62:GLN:HE22	1:F:65:ARG:HH11	1.69	0.41
1:F:150:GLU:HG3	1:F:154:ASN:H	1.84	0.41
1:G:117:ARG:HG2	1:G:117:ARG:HH11	1.86	0.41
1:G:151:ASN:C	1:G:152:ILE:HD13	2.40	0.41
1:G:151:ASN:O	1:G:152:ILE:HD13	2.20	0.41
1:G:185:ASN:HD22	1:G:185:ASN:H	1.65	0.41
1:G:285:ARG:O	1:G:285:ARG:HD3	2.20	0.41
1:I:125:GLN:O	1:I:125:GLN:HG3	2.19	0.41
1:I:285:ARG:C	1:I:285:ARG:HD3	2.41	0.41
1:J:164:LYS:HZ1	1:J:165:ALA:H	1.64	0.41
1:J:185:ASN:HD22	1:J:185:ASN:H	1.69	0.41
1:A:162:ILE:CG2	1:A:163:ARG:N	2.81	0.41
1:A:302:ALA:N	1:A:304:PRO:HD2	2.35	0.41
1:B:91:ARG:HD2	1:C:134:SER:HB2	2.01	0.41
1:C:119:PHE:O	1:C:120:PRO:C	2.59	0.41
1:C:145:ILE:H	1:C:145:ILE:CD1	2.19	0.41
1:C:211:LEU:HD21	1:C:265:ILE:HD13	2.02	0.41
1:D:39:ILE:HD11	1:D:78:PHE:CE1	2.56	0.41
1:D:255:LEU:HB3	1:D:256:PRO:HD2	2.03	0.41
1:D:294:LEU:N	1:D:297:GLN:HE21	2.17	0.41
1:E:125:GLN:O	1:E:125:GLN:HG3	2.19	0.41
1:E:143:SER:CB	1:E:169:ILE:HD11	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:302:ALA:N	1:E:304:PRO:HD2	2.36	0.41
1:F:39:ILE:HD11	1:F:78:PHE:CE1	2.55	0.41
1:F:140:LEU:HD12	1:F:188:SER:O	2.20	0.41
1:F:251:ILE:O	1:F:251:ILE:HG22	2.20	0.41
1:H:119:PHE:HB3	1:H:259:THR:HB	2.02	0.41
1:I:205:TRP:CD1	1:I:205:TRP:N	2.89	0.41
1:J:119:PHE:O	1:J:120:PRO:C	2.58	0.41
1:J:185:ASN:N	1:J:185:ASN:ND2	2.65	0.41
1:J:303:PHE:C	1:J:303:PHE:CD1	2.94	0.41
1:A:18:ILE:HB	1:A:145:ILE:CG2	2.51	0.41
1:A:246:PHE:CD2	1:B:246:PHE:CE2	3.09	0.41
1:B:224:LEU:HB2	1:B:230:ARG:HG3	2.03	0.41
1:G:46:LYS:O	1:G:47:PRO:C	2.59	0.41
1:I:150:GLU:O	1:I:151:ASN:C	2.59	0.41
1:I:202:TYR:HB2	1:J:256:PRO:O	2.21	0.41
1:D:125:GLN:O	1:D:125:GLN:CG	2.68	0.41
1:D:181:GLN:N	1:D:182:PRO:CD	2.83	0.41
1:F:20:ILE:HG13	1:F:194:ILE:HD11	2.01	0.41
1:F:179:SER:HB2	1:J:99:ARG:CZ	2.49	0.41
1:F:211:LEU:HD13	1:F:211:LEU:C	2.41	0.41
1:G:218:SER:CA	1:G:237:LEU:HD21	2.46	0.41
1:G:230:ARG:HB3	1:G:279:ILE:HD13	2.02	0.41
1:G:248:THR:O	1:G:252:LEU:HB2	2.20	0.41
1:H:209:LEU:HB3	1:H:210:PRO:HD3	2.01	0.41
1:J:39:ILE:HD11	1:J:78:PHE:CE1	2.54	0.41
1:A:222:PHE:CE1	1:A:299:CYS:SG	3.14	0.41
1:A:254:ARG:N	1:A:254:ARG:HD2	2.36	0.41
1:A:285:ARG:C	1:A:285:ARG:CD	2.89	0.41
1:B:46:LYS:O	1:B:47:PRO:C	2.59	0.41
1:B:91:ARG:HB2	1:C:133:PHE:HE2	1.86	0.41
1:B:211:LEU:O	1:B:211:LEU:HD13	2.20	0.41
1:B:216:ALA:C	1:B:218:SER:N	2.74	0.41
1:C:63:ILE:O	1:C:67:ILE:HD13	2.20	0.41
1:C:120:PRO:HB2	1:C:121:PHE:CE1	2.56	0.41
1:C:181:GLN:H	1:C:182:PRO:HD3	1.84	0.41
1:D:143:SER:HB3	1:D:169:ILE:HD11	2.03	0.41
1:D:150:GLU:HB2	1:D:153:ASP:HB2	1.97	0.41
1:D:215:ILE:HD12	1:D:268:GLY:CA	2.51	0.41
1:E:32:THR:CG2	1:E:33:TYR:N	2.83	0.41
1:E:72:TRP:CE2	1:E:74:PRO:HG3	2.54	0.41
1:E:87:THR:HG21	1:E:90:LYS:CE	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:164:LYS:NZ	1:E:165:ALA:N	2.57	0.41
1:E:209:LEU:C	1:E:209:LEU:HD23	2.42	0.41
1:F:120:PRO:HB2	1:F:121:PHE:CE1	2.56	0.41
1:F:246:PHE:CE2	1:J:246:PHE:CD2	3.05	0.41
1:F:286:GLN:HA	1:F:291:GLU:HB3	2.03	0.41
1:H:162:ILE:CG2	1:H:163:ARG:N	2.80	0.41
1:H:303:PHE:C	1:H:303:PHE:CD1	2.94	0.41
1:I:18:ILE:HB	1:I:145:ILE:CG2	2.50	0.41
1:I:39:ILE:HD11	1:I:78:PHE:CE1	2.56	0.41
1:I:110:PHE:CD1	1:I:110:PHE:N	2.89	0.41
1:I:259:THR:HG23	1:I:262:ASP:OD2	2.20	0.41
1:J:46:LYS:HA	1:J:47:PRO:HD2	1.92	0.41
1:J:143:SER:CB	1:J:169:ILE:HD11	2.51	0.41
1:J:209:LEU:C	1:J:209:LEU:HD23	2.41	0.41
1:D:226:SER:HB3	1:D:229:GLU:OE1	2.21	0.41
1:F:91:ARG:HD3	1:G:134:SER:HB3	2.03	0.41
1:G:17:SER:O	1:G:40:VAL:HG23	2.21	0.41
1:G:231:LEU:HD23	1:G:232:GLN:N	2.36	0.41
1:G:301:LEU:O	1:G:305:LEU:HG	2.21	0.41
1:I:62:GLN:HE22	1:I:65:ARG:NH1	2.19	0.41
1:I:146:GLN:NE2	1:J:176:HIS:CD2	2.89	0.41
1:J:119:PHE:HB3	1:J:259:THR:HB	2.03	0.41
1:A:119:PHE:HB3	1:A:259:THR:HB	2.02	0.40
1:B:143:SER:HB3	1:B:167:THR:HG21	2.02	0.40
1:B:178:SER:C	1:B:180:VAL:H	2.24	0.40
1:D:57:ILE:HD13	1:E:134:SER:O	2.22	0.40
1:D:92:LEU:HD23	1:D:92:LEU:HA	1.83	0.40
1:E:72:TRP:CD1	1:E:72:TRP:C	2.94	0.40
1:E:185:ASN:HD22	1:E:185:ASN:H	1.66	0.40
1:E:276:ILE:O	1:E:280:ILE:HG13	2.21	0.40
1:F:222:PHE:HB3	1:F:300:ARG:HG2	2.02	0.40
1:G:141:ARG:HB3	1:G:142:PHE:H	1.72	0.40
1:G:219:TRP:O	1:G:221:VAL:N	2.54	0.40
1:I:219:TRP:C	1:I:221:VAL:N	2.75	0.40
1:J:286:GLN:HG2	1:J:289:GLY:O	2.20	0.40
1:A:18:ILE:HB	1:A:145:ILE:HG22	2.03	0.40
1:A:147:VAL:O	1:A:149:THR:N	2.49	0.40
1:B:117:ARG:HH11	1:B:117:ARG:HG2	1.86	0.40
1:B:162:ILE:CG2	1:B:163:ARG:H	2.17	0.40
1:B:226:SER:HB3	1:B:229:GLU:OE1	2.21	0.40
1:B:307:PHE:HD1	1:B:310:ILE:HD12	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:237:LEU:HD12	1:E:237:LEU:HA	1.97	0.40
1:G:110:PHE:CD1	1:G:110:PHE:N	2.89	0.40
1:H:16:VAL:HG12	1:H:17:SER:N	2.36	0.40
1:H:70:GLY:O	1:H:71:LEU:C	2.60	0.40
1:H:167:THR:CG2	1:H:168:HIS:H	2.19	0.40
1:H:184:GLN:OE1	1:H:184:GLN:N	2.54	0.40
1:H:292:ASP:O	1:H:293:ASP:C	2.59	0.40
1:I:169:ILE:HD12	1:I:190:ILE:HG12	2.04	0.40
1:A:32:THR:HG22	1:A:33:TYR:N	2.35	0.40
1:A:120:PRO:HB2	1:A:121:PHE:CE1	2.57	0.40
1:B:62:GLN:O	1:B:65:ARG:HB2	2.21	0.40
1:B:219:TRP:C	1:B:221:VAL:N	2.75	0.40
1:C:220:SER:HB2	1:D:280:ILE:CD1	2.51	0.40
1:D:145:ILE:HG21	1:D:192:VAL:CG1	2.44	0.40
1:D:281:PHE:O	1:D:285:ARG:HB2	2.21	0.40
1:E:288:ASN:ND2	1:E:289:GLY:H	2.19	0.40
1:F:211:LEU:HD21	1:F:265:ILE:HD13	2.03	0.40
1:F:248:THR:O	1:F:252:LEU:HB2	2.21	0.40
1:G:72:TRP:CE2	1:G:74:PRO:HG3	2.55	0.40
1:G:187:PHE:CD1	1:G:187:PHE:N	2.89	0.40
1:I:246:PHE:CE2	1:J:246:PHE:HE2	2.39	0.40
1:J:307:PHE:HD1	1:J:310:ILE:HD12	1.86	0.40
1:A:46:LYS:O	1:A:47:PRO:C	2.59	0.40
1:A:66:TRP:HB3	1:A:71:LEU:CD1	2.51	0.40
1:A:135:TYR:HB3	1:A:138:GLN:HB2	2.04	0.40
1:A:210:PRO:HB3	1:B:269:TYR:CD1	2.55	0.40
1:B:58:VAL:HG13	1:B:62:GLN:CB	2.52	0.40
1:B:254:ARG:N	1:B:254:ARG:HD2	2.36	0.40
1:B:286:GLN:HA	1:B:291:GLU:HB3	2.03	0.40
1:B:304:PRO:O	1:B:308:LEU:HD13	2.21	0.40
1:C:66:TRP:CE3	1:C:71:LEU:HD12	2.57	0.40
1:C:89:ASN:O	1:C:104:ALA:HA	2.22	0.40
1:C:125:GLN:O	1:C:125:GLN:HG3	2.20	0.40
1:C:219:TRP:O	1:C:221:VAL:N	2.54	0.40
1:D:219:TRP:C	1:D:221:VAL:N	2.75	0.40
1:D:223:TRP:CD1	1:D:300:ARG:HD3	2.56	0.40
1:E:62:GLN:HE22	1:E:65:ARG:HH11	1.68	0.40
1:F:303:PHE:CD1	1:F:303:PHE:C	2.95	0.40
1:H:234:SER:HA	1:H:237:LEU:HB2	2.04	0.40
1:H:302:ALA:N	1:H:304:PRO:HD2	2.37	0.40
1:I:94:LEU:CD2	1:I:100:VAL:HG22	2.49	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:181:GLN:H	1:J:182:PRO:HD2	1.86	0.40
1:J:285:ARG:C	1:J:285:ARG:HD3	2.42	0.40
1:C:54:LYS:O	1:C:55:PRO:C	2.60	0.40
1:C:219:TRP:HZ2	1:C:307:PHE:CD2	2.38	0.40
1:C:298:ARG:HG2	1:C:298:ARG:O	2.22	0.40
1:D:150:GLU:HG2	1:D:150:GLU:O	2.21	0.40
1:D:211:LEU:HD21	1:D:265:ILE:HD13	2.03	0.40
1:E:14:VAL:O	1:E:141:ARG:N	2.46	0.40
1:F:52:GLY:O	1:F:53:ASP:HB2	2.20	0.40
1:F:134:SER:HB3	1:J:91:ARG:HD3	1.99	0.40
1:F:167:THR:O	1:F:168:HIS:CB	2.69	0.40
1:F:254:ARG:N	1:F:254:ARG:HD2	2.37	0.40
1:G:288:ASN:CG	1:G:289:GLY:N	2.75	0.40
1:G:304:PRO:O	1:G:308:LEU:HD13	2.21	0.40
1:H:101:ILE:CD1	1:I:178:SER:HB3	2.51	0.40
1:H:147:VAL:O	1:H:149:THR:N	2.53	0.40
1:I:149:THR:CG2	1:I:150:GLU:OE2	2.69	0.40
1:I:157:ILE:HD11	1:J:115:ASP:CG	2.41	0.40
1:I:177:LEU:HD11	1:I:185:ASN:HA	2.04	0.40
1:J:143:SER:HB3	1:J:167:THR:CG2	2.51	0.40









There are no symmetry-related clashes.

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	304/321 (95%)	234 (77%)	46 (15%)	24 (8%)		
1	B	304/321 (95%)	236 (78%)	45 (15%)	23 (8%)		
1	C	304/321 (95%)	237 (78%)	41 (14%)	26 (9%)		
1	D	304/321 (95%)	237 (78%)	45 (15%)	22 (7%)		

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	304/321 (95%)	236 (78%)	43 (14%)	25 (8%)	1	5
1	F	304/321 (95%)	236 (78%)	44 (14%)	24 (8%)	1	6
1	G	304/321 (95%)	236 (78%)	48 (16%)	20 (7%)	1	8
1	H	304/321 (95%)	238 (78%)	46 (15%)	20 (7%)	1	8
1	I	304/321 (95%)	237 (78%)	46 (15%)	21 (7%)	1	8
1	J	304/321 (95%)	237 (78%)	44 (14%)	23 (8%)	1	6
All	All	3040/3210 (95%)	2364 (78%)	448 (15%)	228 (8%)	1	7

All (228) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	53	ASP
1	A	119	PHE
1	A	141	ARG
1	A	151	ASN
1	A	168	HIS
1	A	201	SER
1	B	53	ASP
1	B	60	ASN
1	B	119	PHE
1	B	141	ARG
1	B	168	HIS
1	B	181	GLN
1	B	201	SER
1	B	294	LEU
1	C	53	ASP
1	C	119	PHE
1	C	141	ARG
1	C	151	ASN
1	C	168	HIS
1	C	201	SER
1	C	293	ASP
1	D	53	ASP
1	D	141	ARG
1	D	168	HIS
1	D	177	LEU
1	D	183	ASN
1	D	201	SER
1	E	119	PHE
1	E	141	ARG

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Mol	Chain	Res	Type
1	E	168	HIS
1	E	176	HIS
1	E	182	PRO
1	E	201	SER
1	E	293	ASP
1	F	119	PHE
1	F	141	ARG
1	F	168	HIS
1	F	183	ASN
1	F	201	SER
1	G	119	PHE
1	G	141	ARG
1	G	151	ASN
1	G	168	HIS
1	G	183	ASN
1	G	201	SER
1	H	119	PHE
1	H	141	ARG
1	H	168	HIS
1	H	201	SER
1	I	60	ASN
1	I	119	PHE
1	I	141	ARG
1	I	168	HIS
1	I	201	SER
1	J	53	ASP
1	J	119	PHE
1	J	141	ARG
1	J	168	HIS
1	J	179	SER
1	J	181	GLN
1	J	183	ASN
1	J	201	SER
1	A	85	PRO
1	A	99	ARG
1	A	165	ALA
1	A	183	ASN
1	A	288	ASN
1	B	85	PRO
1	B	99	ARG
1	B	148	TYR
1	B	165	ALA

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Mol	Chain	Res	Type
1	B	176	HIS
1	B	183	ASN
1	B	220	SER
1	B	226	SER
1	B	293	ASP
1	C	85	PRO
1	C	99	ARG
1	C	155	GLU
1	C	165	ALA
1	C	177	LEU
1	C	179	SER
1	C	294	LEU
1	D	55	PRO
1	D	60	ASN
1	D	85	PRO
1	D	99	ARG
1	D	119	PHE
1	E	53	ASP
1	E	99	ARG
1	E	220	SER
1	E	288	ASN
1	E	294	LEU
1	F	53	ASP
1	F	99	ARG
1	F	153	ASP
1	F	165	ALA
1	F	220	SER
1	G	53	ASP
1	G	99	ARG
1	G	148	TYR
1	G	155	GLU
1	G	165	ALA
1	G	220	SER
1	H	53	ASP
1	H	99	ARG
1	H	155	GLU
1	H	181	GLN
1	I	53	ASP
1	I	99	ARG
1	I	182	PRO
1	I	293	ASP
1	J	60	ASN

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Mol	Chain	Res	Type
1	A	185	ASN
1	A	220	SER
1	A	226	SER
1	A	293	ASP
1	B	79	ILE
1	B	155	GLU
1	B	185	ASN
1	C	182	PRO
1	C	185	ASN
1	C	220	SER
1	C	226	SER
1	D	148	TYR
1	D	165	ALA
1	D	220	SER
1	D	226	SER
1	E	85	PRO
1	E	153	ASP
1	E	177	LEU
1	F	47	PRO
1	F	85	PRO
1	F	179	SER
1	F	185	ASN
1	F	226	SER
1	G	85	PRO
1	G	185	ASN
1	G	226	SER
1	H	85	PRO
1	H	182	PRO
1	H	185	ASN
1	H	220	SER
1	H	226	SER
1	I	85	PRO
1	I	148	TYR
1	I	181	GLN
1	I	185	ASN
1	I	220	SER
1	I	294	LEU
1	J	85	PRO
1	J	99	ARG
1	J	165	ALA
1	J	185	ASN
1	J	220	SER

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Mol	Chain	Res	Type
1	A	47	PRO
1	A	55	PRO
1	A	79	ILE
1	A	148	TYR
1	B	47	PRO
1	C	47	PRO
1	D	47	PRO
1	D	155	GLU
1	D	185	ASN
1	E	47	PRO
1	E	55	PRO
1	E	79	ILE
1	E	148	TYR
1	E	185	ASN
1	E	226	SER
1	F	79	ILE
1	F	155	GLU
1	F	177	LEU
1	G	47	PRO
1	G	60	ASN
1	H	47	PRO
1	H	79	ILE
1	H	165	ALA
1	I	47	PRO
1	I	55	PRO
1	I	165	ALA
1	I	226	SER
1	J	59	GLU
1	J	226	SER
1	J	293	ASP
1	A	60	ASN
1	A	181	GLN
1	A	289	GLY
1	B	225	GLU
1	C	79	ILE
1	C	181	GLN
1	C	183	ASN
1	D	79	ILE
1	D	181	GLN
1	E	59	GLU
1	F	148	TYR
1	F	293	ASP

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Mol	Chain	Res	Type
1	H	55	PRO
1	H	148	TYR
1	J	47	PRO
1	J	148	TYR
1	J	155	GLU
1	E	165	ALA
1	F	181	GLN
1	G	79	ILE
1	G	181	GLN
1	H	293	ASP
1	J	289	GLY
1	A	182	PRO
1	C	152	ILE
1	E	289	GLY
1	I	79	ILE
1	J	79	ILE
1	C	55	PRO
1	F	289	GLY
1	C	289	GLY
1	C	303	PHE
1	G	303	PHE
1	A	303	PHE
1	D	162	ILE
1	D	303	PHE
1	E	303	PHE
1	F	303	PHE
1	H	303	PHE
1	I	303	PHE
1	J	303	PHE
1	B	303	PHE
1	F	162	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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	275/284 (97%)	250 (91%)	25 (9%)	9	31
1	B	275/284 (97%)	251 (91%)	24 (9%)	10	34
1	C	275/284 (97%)	252 (92%)	23 (8%)	11	35
1	D	275/284 (97%)	252 (92%)	23 (8%)	11	35
1	E	275/284 (97%)	250 (91%)	25 (9%)	9	31
1	F	275/284 (97%)	252 (92%)	23 (8%)	11	35
1	G	275/284 (97%)	251 (91%)	24 (9%)	10	34
1	H	275/284 (97%)	249 (90%)	26 (10%)	8	29
1	I	275/284 (97%)	250 (91%)	25 (9%)	9	31
1	J	275/284 (97%)	255 (93%)	20 (7%)	14	41
All	All	2750/2840 (97%)	2512 (91%)	238 (9%)	10	34

All (238) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	LEU
1	A	40	VAL
1	A	43	TRP
1	A	50	THR
1	A	71	LEU
1	A	72	TRP
1	A	78	PHE
1	A	118	LEU
1	A	138	GLN
1	A	142	PHE
1	A	145	ILE
1	A	154	ASN
1	A	157	ILE
1	A	162	ILE
1	A	171	ASP
1	A	176	HIS
1	A	177	LEU
1	A	181	GLN
1	A	184	GLN
1	A	185	ASN
1	A	199	ASN
1	A	252	LEU

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Mol	Chain	Res	Type
1	A	285	ARG
1	A	286	GLN
1	A	303	PHE
1	B	29	LEU
1	B	40	VAL
1	B	43	TRP
1	B	50	THR
1	B	71	LEU
1	B	72	TRP
1	B	78	PHE
1	B	118	LEU
1	B	138	GLN
1	B	142	PHE
1	B	145	ILE
1	B	150	GLU
1	B	151	ASN
1	B	157	ILE
1	B	162	ILE
1	B	171	ASP
1	B	176	HIS
1	B	184	GLN
1	B	185	ASN
1	B	199	ASN
1	B	285	ARG
1	B	286	GLN
1	B	293	ASP
1	B	303	PHE
1	C	29	LEU
1	C	40	VAL
1	C	43	TRP
1	C	50	THR
1	C	71	LEU
1	C	72	TRP
1	C	78	PHE
1	C	118	LEU
1	C	138	GLN
1	C	142	PHE
1	C	145	ILE
1	C	150	GLU
1	C	152	ILE
1	C	157	ILE
1	C	162	ILE

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Mol	Chain	Res	Type
1	C	171	ASP
1	C	176	HIS
1	C	184	GLN
1	C	185	ASN
1	C	199	ASN
1	C	285	ARG
1	C	286	GLN
1	C	303	PHE
1	D	29	LEU
1	D	40	VAL
1	D	43	TRP
1	D	50	THR
1	D	71	LEU
1	D	72	TRP
1	D	78	PHE
1	D	118	LEU
1	D	142	PHE
1	D	145	ILE
1	D	150	GLU
1	D	157	ILE
1	D	162	ILE
1	D	171	ASP
1	D	175	ASP
1	D	176	HIS
1	D	184	GLN
1	D	185	ASN
1	D	199	ASN
1	D	246	PHE
1	D	285	ARG
1	D	286	GLN
1	D	303	PHE
1	E	29	LEU
1	E	40	VAL
1	E	43	TRP
1	E	50	THR
1	E	71	LEU
1	E	72	TRP
1	E	78	PHE
1	E	118	LEU
1	E	124	GLN
1	E	138	GLN
1	E	142	PHE

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Mol	Chain	Res	Type
1	E	145	ILE
1	E	150	GLU
1	E	157	ILE
1	E	162	ILE
1	E	171	ASP
1	E	176	HIS
1	E	177	LEU
1	E	184	GLN
1	E	185	ASN
1	E	199	ASN
1	E	246	PHE
1	E	285	ARG
1	E	286	GLN
1	E	303	PHE
1	F	29	LEU
1	F	40	VAL
1	F	43	TRP
1	F	50	THR
1	F	71	LEU
1	F	72	TRP
1	F	78	PHE
1	F	118	LEU
1	F	138	GLN
1	F	142	PHE
1	F	145	ILE
1	F	150	GLU
1	F	162	ILE
1	F	171	ASP
1	F	175	ASP
1	F	176	HIS
1	F	177	LEU
1	F	184	GLN
1	F	185	ASN
1	F	199	ASN
1	F	285	ARG
1	F	286	GLN
1	F	303	PHE
1	G	29	LEU
1	G	40	VAL
1	G	43	TRP
1	G	50	THR
1	G	71	LEU

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Mol	Chain	Res	Type
1	G	72	TRP
1	G	78	PHE
1	G	118	LEU
1	G	138	GLN
1	G	142	PHE
1	G	145	ILE
1	G	150	GLU
1	G	152	ILE
1	G	157	ILE
1	G	162	ILE
1	G	171	ASP
1	G	176	HIS
1	G	184	GLN
1	G	185	ASN
1	G	199	ASN
1	G	252	LEU
1	G	285	ARG
1	G	286	GLN
1	G	303	PHE
1	H	29	LEU
1	H	40	VAL
1	H	43	TRP
1	H	50	THR
1	H	71	LEU
1	H	72	TRP
1	H	78	PHE
1	H	118	LEU
1	H	138	GLN
1	H	142	PHE
1	H	145	ILE
1	H	150	GLU
1	H	153	ASP
1	H	157	ILE
1	H	162	ILE
1	H	171	ASP
1	H	175	ASP
1	H	176	HIS
1	H	177	LEU
1	H	184	GLN
1	H	185	ASN
1	H	199	ASN
1	H	252	LEU

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Mol	Chain	Res	Type
1	H	285	ARG
1	H	286	GLN
1	H	303	PHE
1	I	29	LEU
1	I	40	VAL
1	I	43	TRP
1	I	50	THR
1	I	56	LEU
1	I	71	LEU
1	I	72	TRP
1	I	78	PHE
1	I	118	LEU
1	I	142	PHE
1	I	145	ILE
1	I	150	GLU
1	I	152	ILE
1	I	157	ILE
1	I	162	ILE
1	I	164	LYS
1	I	171	ASP
1	I	176	HIS
1	I	181	GLN
1	I	184	GLN
1	I	185	ASN
1	I	199	ASN
1	I	285	ARG
1	I	286	GLN
1	I	303	PHE
1	J	29	LEU
1	J	40	VAL
1	J	43	TRP
1	J	50	THR
1	J	56	LEU
1	J	71	LEU
1	J	72	TRP
1	J	78	PHE
1	J	118	LEU
1	J	142	PHE
1	J	145	ILE
1	J	150	GLU
1	J	157	ILE
1	J	162	ILE

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Mol	Chain	Res	Type
1	J	171	ASP
1	J	184	GLN
1	J	185	ASN
1	J	199	ASN
1	J	286	GLN
1	J	303	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (76) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	GLN
1	A	124	GLN
1	A	151	ASN
1	A	154	ASN
1	A	185	ASN
1	A	199	ASN
1	A	297	GLN
1	B	42	GLN
1	B	62	GLN
1	B	124	GLN
1	B	151	ASN
1	B	154	ASN
1	B	176	HIS
1	B	185	ASN
1	B	199	ASN
1	B	286	GLN
1	B	297	GLN
1	C	42	GLN
1	C	62	GLN
1	C	124	GLN
1	C	185	ASN
1	C	199	ASN
1	C	232	GLN
1	C	297	GLN
1	D	68	ASN
1	D	124	GLN
1	D	184	GLN
1	D	185	ASN
1	D	199	ASN
1	D	286	GLN
1	D	297	GLN
1	E	42	GLN

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Mol	Chain	Res	Type
1	E	62	GLN
1	E	124	GLN
1	E	154	ASN
1	E	176	HIS
1	E	185	ASN
1	E	199	ASN
1	E	297	GLN
1	F	42	GLN
1	F	62	GLN
1	F	124	GLN
1	F	176	HIS
1	F	184	GLN
1	F	185	ASN
1	F	199	ASN
1	F	297	GLN
1	G	42	GLN
1	G	62	GLN
1	G	103	ASN
1	G	124	GLN
1	G	184	GLN
1	G	185	ASN
1	G	199	ASN
1	G	297	GLN
1	H	42	GLN
1	H	62	GLN
1	H	124	GLN
1	H	185	ASN
1	H	199	ASN
1	H	297	GLN
1	I	62	GLN
1	I	124	GLN
1	I	139	GLN
1	I	184	GLN
1	I	185	ASN
1	I	199	ASN
1	I	283	HIS
1	I	297	GLN
1	J	62	GLN
1	J	124	GLN
1	J	176	HIS
1	J	184	GLN
1	J	185	ASN

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Mol	Chain	Res	Type
1	J	199	ASN
1	J	297	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	306/321 (95%)	0.04	27 (8%)	10 10	89, 125, 172, 183	0
1	B	306/321 (95%)	-0.02	14 (4%)	32 30	88, 122, 175, 190	0
1	C	306/321 (95%)	-0.10	9 (2%)	51 50	88, 123, 174, 190	0
1	D	306/321 (95%)	0.08	19 (6%)	20 20	83, 122, 175, 188	0
1	E	306/321 (95%)	-0.07	13 (4%)	36 34	91, 125, 175, 186	0
1	F	306/321 (95%)	0.06	19 (6%)	20 20	85, 127, 178, 190	0
1	G	306/321 (95%)	0.07	19 (6%)	20 20	88, 122, 174, 184	0
1	H	306/321 (95%)	0.24	24 (7%)	13 12	90, 124, 175, 195	0
1	I	306/321 (95%)	0.15	24 (7%)	13 12	87, 124, 176, 191	0
1	J	306/321 (95%)	0.00	16 (5%)	27 25	92, 127, 174, 187	0
All	All	3060/3210 (95%)	0.04	184 (6%)	21 21	83, 124, 175, 195	0

All (184) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	288	ASN	15.0
1	H	289	GLY	14.6
1	F	177	LEU	11.7
1	F	178	SER	11.3
1	H	290	VAL	11.3
1	A	152	ILE	8.6
1	H	178	SER	8.3
1	G	314	LEU	8.1
1	D	178	SER	8.1
1	H	179	SER	7.2
1	I	178	SER	7.2
1	E	178	SER	7.0
1	F	316	ILE	6.9

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Mol	Chain	Res	Type	RSRZ
1	F	176	HIS	6.9
1	I	181	GLN	6.6
1	E	179	SER	6.6
1	I	177	LEU	6.5
1	F	152	ILE	6.5
1	H	292	ASP	6.4
1	H	152	ILE	6.3
1	D	179	SER	6.3
1	D	177	LEU	6.1
1	F	151	ASN	6.0
1	G	313	VAL	6.0
1	H	314	LEU	5.9
1	I	179	SER	5.8
1	F	148	TYR	5.7
1	H	287	ALA	5.7
1	A	177	LEU	5.6
1	A	176	HIS	5.6
1	I	153	ASP	5.5
1	C	316	ILE	5.2
1	F	181	GLN	4.9
1	J	151	ASN	4.9
1	G	316	ILE	4.9
1	D	153	ASP	4.7
1	A	51	PRO	4.7
1	I	313	VAL	4.7
1	C	287	ALA	4.7
1	E	289	GLY	4.7
1	C	314	LEU	4.7
1	G	312	CYS	4.6
1	I	314	LEU	4.6
1	J	236	THR	4.5
1	E	290	VAL	4.5
1	H	184	GLN	4.4
1	C	315	VAL	4.3
1	D	181	GLN	4.3
1	D	225	GLU	4.2
1	E	148	TYR	4.2
1	H	313	VAL	4.1
1	E	181	GLN	4.1
1	G	151	ASN	4.0
1	G	152	ILE	4.0
1	A	178	SER	3.8

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Mol	Chain	Res	Type	RSRZ
1	I	315	VAL	3.8
1	H	151	ASN	3.8
1	B	296	ILE	3.8
1	C	313	VAL	3.8
1	I	184	GLN	3.8
1	A	295	LEU	3.8
1	A	298	ARG	3.8
1	A	314	LEU	3.7
1	E	177	LEU	3.7
1	H	316	ILE	3.7
1	H	310	ILE	3.6
1	D	182	PRO	3.6
1	I	152	ILE	3.5
1	A	316	ILE	3.5
1	D	152	ILE	3.5
1	H	291	GLU	3.5
1	F	175	ASP	3.4
1	B	288	ASN	3.4
1	G	156	GLU	3.4
1	A	297	GLN	3.4
1	G	290	VAL	3.4
1	J	153	ASP	3.4
1	G	178	SER	3.2
1	I	182	PRO	3.2
1	H	153	ASP	3.2
1	A	296	ILE	3.2
1	E	123	ARG	3.2
1	F	182	PRO	3.1
1	I	148	TYR	3.1
1	I	236	THR	3.1
1	F	315	VAL	3.1
1	H	148	TYR	3.1
1	G	296	ILE	3.1
1	B	240	THR	3.0
1	H	123	ARG	3.0
1	H	177	LEU	3.0
1	B	297	GLN	3.0
1	I	183	ASN	3.0
1	B	152	ILE	3.0
1	D	123	ARG	3.0
1	H	180	VAL	3.0
1	C	288	ASN	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	290	VAL	3.0
1	J	150	GLU	3.0
1	J	123	ARG	2.9
1	D	313	VAL	2.9
1	J	294	LEU	2.9
1	J	154	ASN	2.9
1	E	284	HIS	2.9
1	H	294	LEU	2.9
1	C	171	ASP	2.8
1	A	236	THR	2.8
1	A	153	ASP	2.8
1	A	294	LEU	2.8
1	D	70	GLY	2.8
1	F	174	TYR	2.8
1	F	149	THR	2.8
1	G	315	VAL	2.7
1	A	301	LEU	2.7
1	J	163	ARG	2.7
1	G	286	GLN	2.7
1	B	290	VAL	2.7
1	J	296	ILE	2.7
1	F	290	VAL	2.7
1	F	314	LEU	2.7
1	G	294	LEU	2.6
1	I	290	VAL	2.6
1	A	240	THR	2.6
1	A	175	ASP	2.6
1	I	150	GLU	2.6
1	A	313	VAL	2.6
1	F	288	ASN	2.6
1	A	184	GLN	2.6
1	B	289	GLY	2.6
1	B	316	ILE	2.5
1	G	289	GLY	2.5
1	D	288	ASN	2.5
1	A	52	GLY	2.5
1	F	49	LYS	2.4
1	H	236	THR	2.4
1	H	232	GLN	2.4
1	I	311	GLY	2.4
1	J	148	TYR	2.4
1	I	316	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	314	LEU	2.4
1	I	288	ASN	2.4
1	I	176	HIS	2.4
1	A	138	GLN	2.4
1	J	313	VAL	2.3
1	B	295	LEU	2.3
1	D	176	HIS	2.3
1	D	180	VAL	2.3
1	F	150	GLU	2.3
1	C	294	LEU	2.3
1	I	138	GLN	2.3
1	I	180	VAL	2.3
1	E	54	LYS	2.3
1	B	314	LEU	2.2
1	A	142	PHE	2.2
1	J	103	ASN	2.2
1	J	152	ILE	2.2
1	G	148	TYR	2.2
1	G	311	GLY	2.2
1	G	157	ILE	2.2
1	J	181	GLN	2.2
1	B	294	LEU	2.2
1	A	151	ASN	2.2
1	G	240	THR	2.2
1	C	236	THR	2.1
1	B	315	VAL	2.1
1	B	151	ASN	2.1
1	J	303	PHE	2.1
1	A	150	GLU	2.1
1	E	288	ASN	2.1
1	D	289	GLY	2.1
1	E	286	GLN	2.1
1	F	289	GLY	2.1
1	D	148	TYR	2.1
1	H	284	HIS	2.1
1	I	312	CYS	2.1
1	J	240	THR	2.1
1	E	51	PRO	2.1
1	G	295	LEU	2.1
1	B	287	ALA	2.0
1	A	179	SER	2.0
1	A	315	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	53	ASP	2.0
1	I	247	TYR	2.0
1	D	138	GLN	2.0

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

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

6.3 Carbohydrates [i](#)

There are no 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.